



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:38 PM UTC

PDB ID : 6OIY / pdb_00006oiy
Title : Structure of Escherichia coli bound to dGTP
Authors : Barnes, C.O.; Wu, Y.; Calero, G.
Deposited on : 2019-04-09
Resolution : 3.29 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:

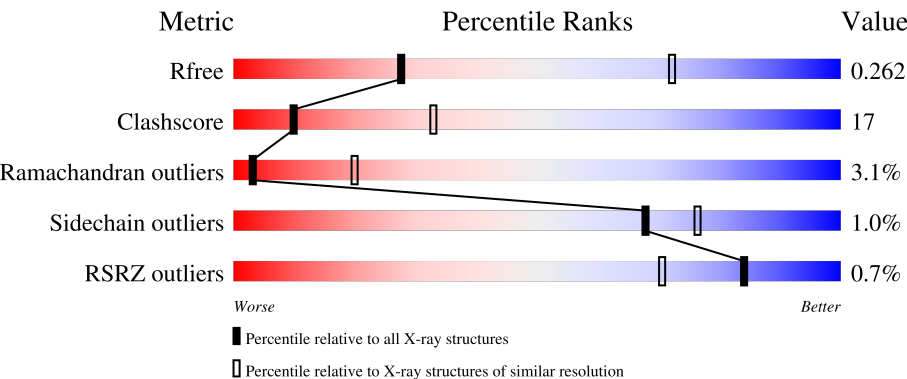
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	505	% 63%32%..
1	B	505	% 50%45%..
1	C	505	% 72%25%.
1	D	505	% 67%28%...
1	E	505	% 70%26%...

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Mol	Chain	Length	Quality of chain
1	F	505	 74% 22% . .

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	601	-	-	X	-

2 Entry composition [i](#)

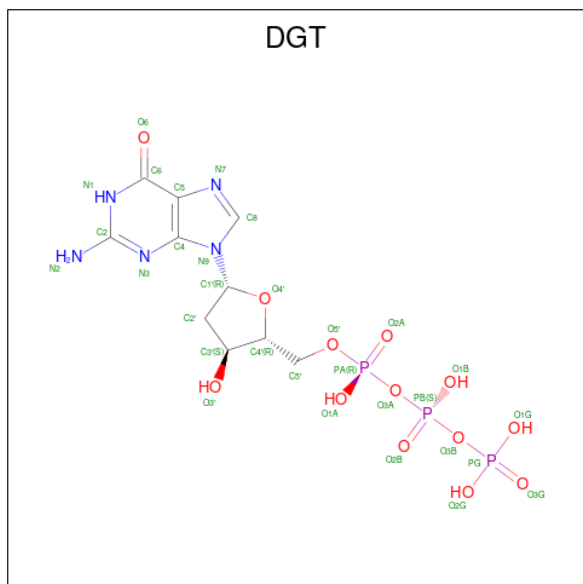
There are 4 unique types of molecules in this entry. The entry contains 24717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	503	Total	C	N	O	S	0	0	0
			4115	2627	737	735	16			
1	B	503	Total	C	N	O	S	0	0	0
			4112	2624	737	735	16			
1	C	503	Total	C	N	O	S	0	0	0
			4112	2624	737	735	16			
1	D	492	Total	C	N	O	S	0	0	0
			4058	2592	726	724	16			
1	E	492	Total	C	N	O	S	0	0	0
			4058	2592	726	724	16			
1	F	492	Total	C	N	O	S	0	0	0
			4058	2592	726	724	16			

- 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	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

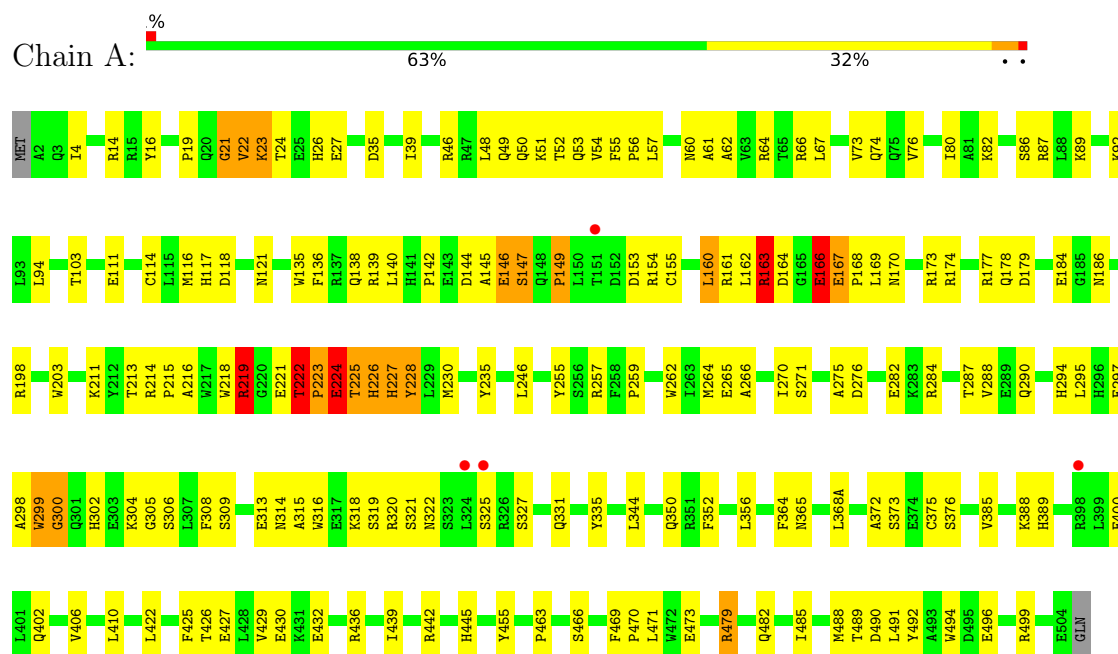
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		
4	C	3	Total	O	0	0
			3	3		
4	D	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		
4	F	2	Total	O	0	0
			2	2		

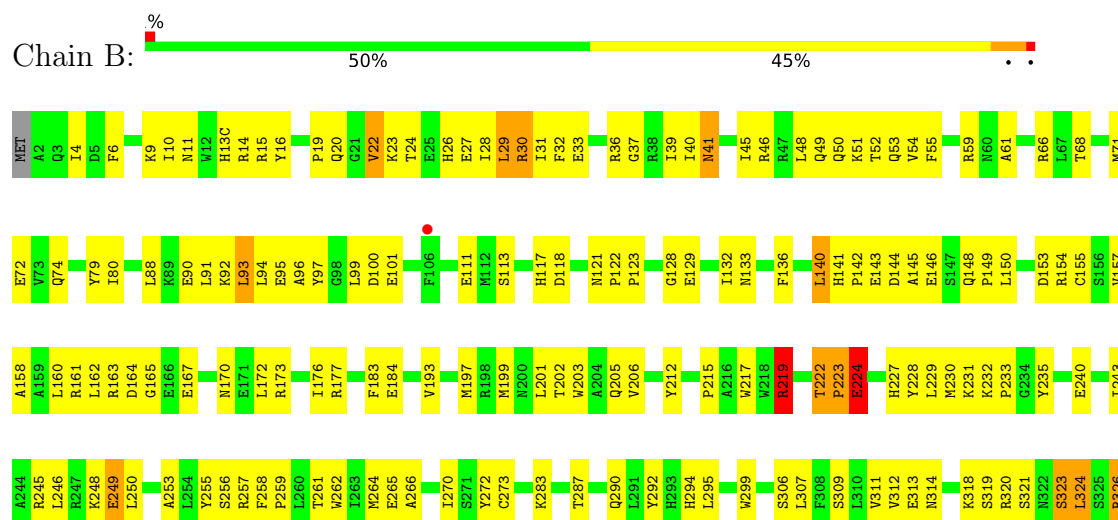
3 Residue-property plots

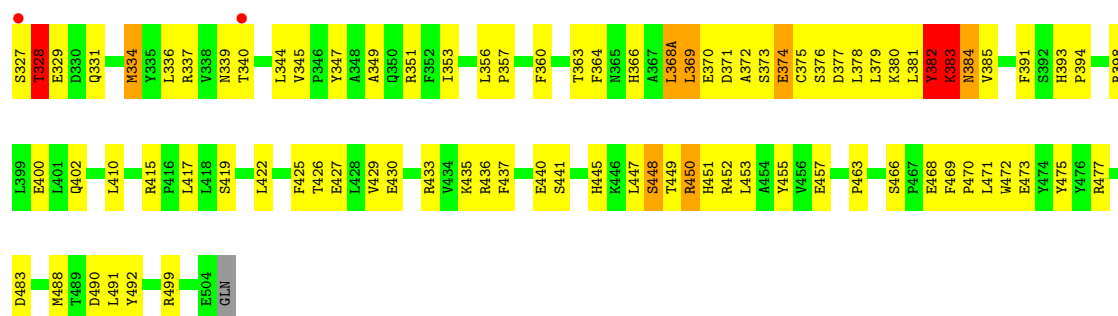
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

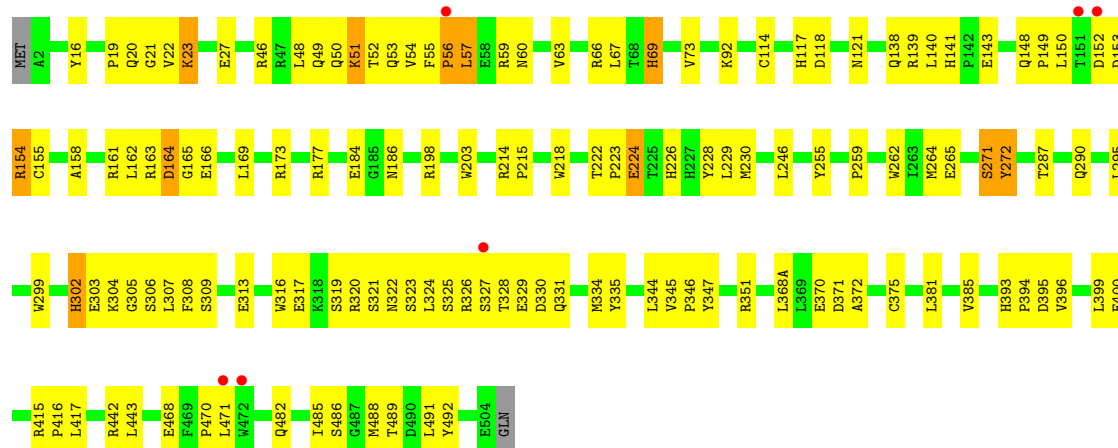
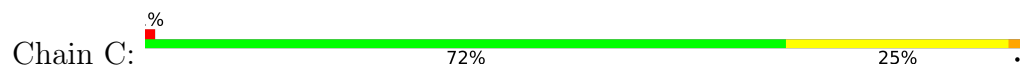


• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

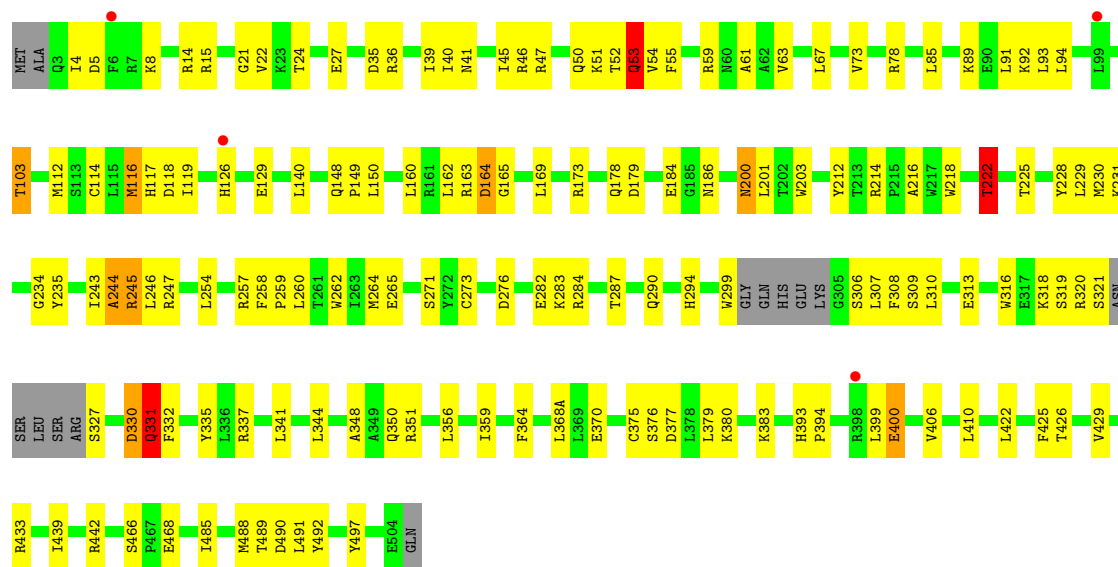




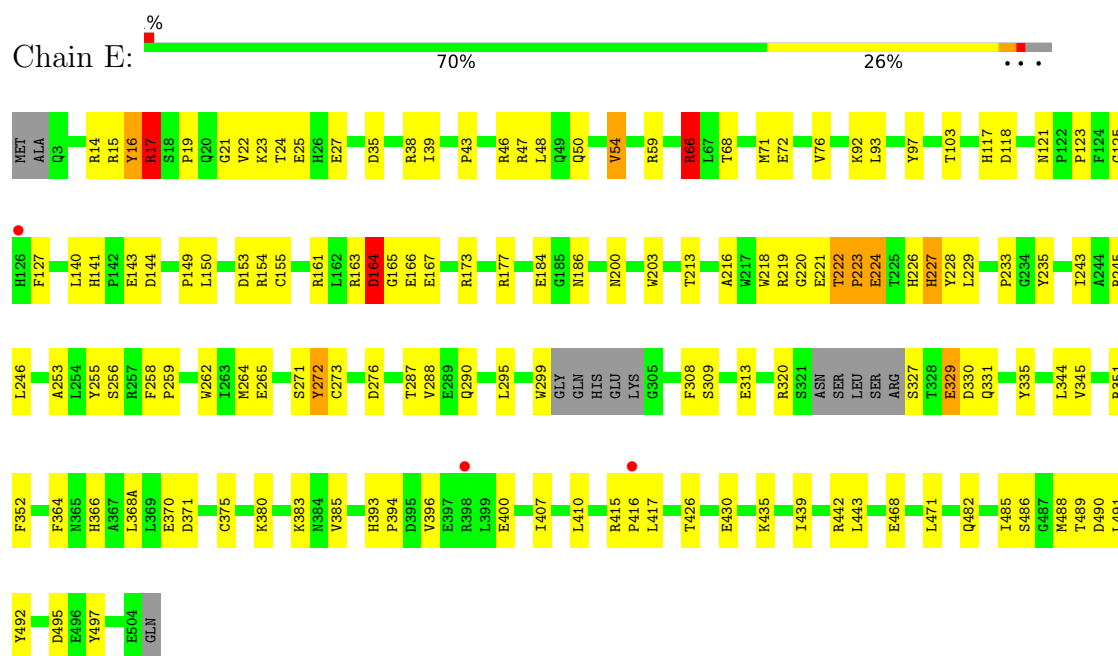
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



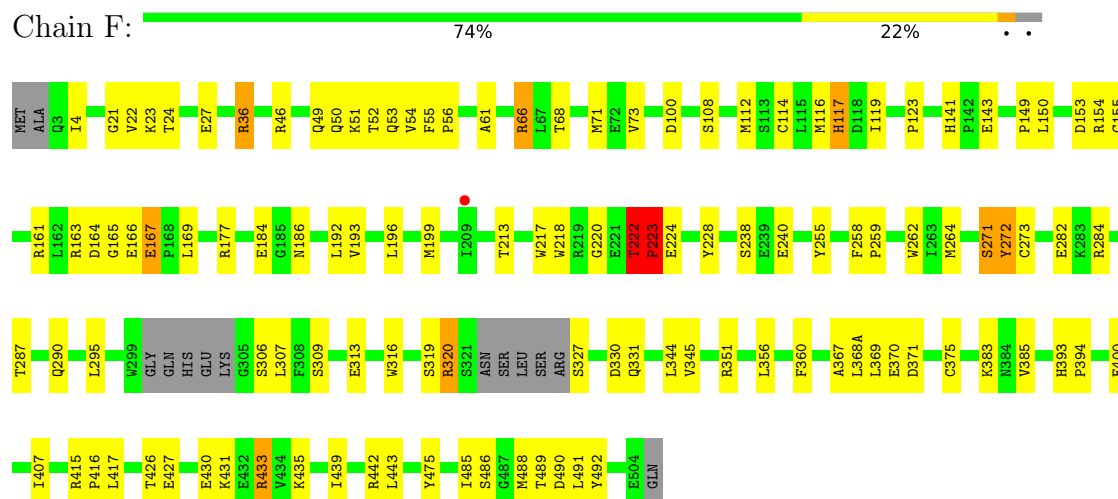
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	192.18Å 192.18Å 299.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.87 – 3.29 46.87 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.87-3.29) 99.8 (46.87-3.29)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.241 0.251 , 0.262	Depositor DCC
R_{free} test set	2552 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	151.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 142.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24717	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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: MN, DGT

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	0.76	7/4216 (0.2%)	0.86	8/5705 (0.1%)
1	B	0.59	3/4213 (0.1%)	0.92	17/5699 (0.3%)
1	C	0.68	4/4213 (0.1%)	0.81	12/5699 (0.2%)
1	D	0.54	4/4157 (0.1%)	0.82	21/5618 (0.4%)
1	E	0.61	2/4157 (0.0%)	0.79	7/5618 (0.1%)
1	F	0.67	6/4157 (0.1%)	0.75	6/5618 (0.1%)
All	All	0.65	26/25113 (0.1%)	0.83	71/33957 (0.2%)

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	A	0	3
1	B	0	2
1	C	0	1
1	D	0	2
1	E	0	4
1	F	0	1
All	All	0	13

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	MET	CG-SD	-14.24	1.45	1.80
1	F	345	VAL	CA-CB	-12.36	1.47	1.54
1	A	160	LEU	CG-CD1	11.73	1.91	1.52
1	F	112	MET	C-O	-10.43	1.11	1.24
1	C	69	HIS	C-O	-10.23	1.12	1.24
1	E	66	ARG	C-O	-8.17	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ARG	CD-NE	-7.67	1.35	1.46
1	F	36	ARG	C-O	-7.51	1.15	1.24
1	A	479	ARG	NE-CZ	-7.45	1.24	1.33
1	F	66	ARG	C-O	-7.35	1.14	1.24
1	A	479	ARG	CZ-NH2	-7.27	1.24	1.33
1	F	272	TYR	C-O	-6.04	1.16	1.24
1	A	160	LEU	CA-CB	-6.00	1.43	1.53
1	B	41	ASN	C-N	-5.79	1.21	1.33
1	D	331	GLN	CA-C	-5.62	1.45	1.52
1	C	272	TYR	C-O	-5.51	1.17	1.24
1	F	117	HIS	CG-ND1	-5.49	1.32	1.38
1	D	331	GLN	CD-OE1	5.43	1.33	1.23
1	B	227	HIS	CA-C	5.40	1.60	1.52
1	E	345	VAL	CA-CB	5.33	1.57	1.53
1	A	297	GLU	CA-C	-5.33	1.43	1.52
1	D	332	PHE	CB-CG	5.21	1.62	1.50
1	C	345	VAL	CA-CB	5.20	1.57	1.54
1	C	69	HIS	CE1-NE2	-5.11	1.27	1.32
1	D	41	ASN	C-N	-5.08	1.23	1.33
1	A	149	PRO	C-O	-5.04	1.17	1.24

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	ARG	CB-CG-CD	12.66	140.42	111.30
1	B	383	LYS	CD-CE-NZ	-11.29	75.78	111.90
1	D	245	ARG	N-CA-CB	10.52	125.58	110.12
1	E	17	ARG	CA-CB-CG	9.87	133.85	114.10
1	E	17	ARG	CG-CD-NE	9.78	133.50	112.00
1	D	245	ARG	CB-CG-CD	9.77	133.76	111.30
1	A	228	TYR	N-CA-C	9.62	123.13	111.40
1	E	17	ARG	N-CA-CB	9.09	125.85	110.49
1	D	245	ARG	CB-CA-C	-9.03	95.81	110.79
1	B	334	MET	CA-CB-CG	8.60	131.31	114.10
1	D	245	ARG	CD-NE-CZ	7.88	135.43	124.40
1	D	331	GLN	N-CA-CB	7.69	123.49	110.49
1	D	164	ASP	N-CA-C	7.63	120.48	111.71
1	E	164	ASP	N-CA-C	7.43	120.44	111.82
1	E	17	ARG	N-CA-C	-7.42	94.99	110.80
1	B	334	MET	CB-CG-SD	-7.12	91.35	112.70
1	D	245	ARG	CA-CB-CG	-6.94	100.22	114.10
1	A	149	PRO	N-CA-CB	6.93	110.53	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	TYR	N-CA-CB	-6.93	99.88	110.13
1	D	331	GLN	CA-CB-CG	6.74	127.57	114.10
1	B	328	THR	N-CA-C	6.73	125.13	110.80
1	B	227	HIS	CA-C-O	6.63	127.07	119.18
1	B	384	ASN	N-CA-CB	6.60	120.23	110.33
1	C	69	HIS	CB-CA-C	-6.54	100.62	110.88
1	D	245	ARG	CG-CD-NE	6.43	126.14	112.00
1	B	227	HIS	N-CA-CB	-6.41	100.40	110.46
1	B	140	LEU	CA-CB-CG	6.16	137.87	116.30
1	D	244	ALA	CA-C-N	-6.09	112.12	120.28
1	D	244	ALA	C-N-CA	-6.09	112.12	120.28
1	D	331	GLN	CG-CD-NE2	6.04	125.46	116.40
1	A	226	HIS	N-CA-C	-5.97	102.77	111.30
1	B	224	GLU	N-CA-C	-5.91	107.88	114.62
1	B	383	LYS	CA-CB-CG	5.90	125.90	114.10
1	C	271	SER	CA-C-N	-5.77	111.94	121.92
1	C	271	SER	C-N-CA	-5.77	111.94	121.92
1	D	331	GLN	CB-CG-CD	-5.76	102.81	112.60
1	B	29	LEU	CA-C-N	5.75	128.25	120.38
1	B	29	LEU	C-N-CA	5.75	128.25	120.38
1	B	30	ARG	N-CA-CB	-5.73	101.47	110.06
1	F	433	ARG	N-CA-CB	5.71	119.57	110.65
1	C	69	HIS	CA-C-O	-5.64	114.90	120.82
1	D	53	GLN	CA-C-N	5.64	132.12	121.97
1	D	53	GLN	C-N-CA	5.64	132.12	121.97
1	A	226	HIS	CB-CA-C	5.63	121.09	111.46
1	C	302	HIS	CA-C-N	5.60	131.79	121.70
1	C	302	HIS	C-N-CA	5.60	131.79	121.70
1	D	331	GLN	CG-CD-OE1	-5.55	109.69	120.80
1	E	17	ARG	CD-NE-CZ	-5.53	116.65	124.40
1	D	399	LEU	N-CA-C	-5.49	105.45	111.82
1	B	30	ARG	CG-CD-NE	5.47	124.04	112.00
1	D	332	PHE	N-CA-CB	5.46	118.22	110.13
1	F	271	SER	CA-C-N	-5.32	112.29	121.66
1	F	271	SER	C-N-CA	-5.32	112.29	121.66
1	F	222	THR	CA-C-N	5.31	126.47	119.84
1	F	222	THR	C-N-CA	5.31	126.47	119.84
1	A	224	GLU	CA-C-N	-5.26	111.49	121.54
1	A	224	GLU	C-N-CA	-5.26	111.49	121.54
1	D	400	GLU	N-CA-C	-5.24	105.48	111.14
1	F	66	ARG	N-CA-C	-5.17	106.48	112.89
1	A	227	HIS	N-CA-C	5.16	117.30	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	MET	CA-C-N	-5.16	111.69	121.54
1	D	116	MET	C-N-CA	-5.16	111.69	121.54
1	B	329	GLU	CA-CB-CG	5.10	124.31	114.10
1	B	383	LYS	CB-CG-CD	5.09	123.00	111.30
1	C	272	TYR	N-CA-C	-5.07	107.26	113.50
1	C	57	LEU	CA-C-N	-5.05	115.98	123.05
1	C	57	LEU	C-N-CA	-5.05	115.98	123.05
1	C	272	TYR	CA-C-N	-5.05	113.77	120.79
1	C	272	TYR	C-N-CA	-5.05	113.77	120.79
1	C	302	HIS	N-CA-C	5.02	121.50	110.80
1	B	140	LEU	CB-CA-C	-5.01	104.29	111.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	222	THR	Peptide
1	B	219	ARG	Sidechain
1	B	382	TYR	Peptide
1	C	325	SER	Peptide
1	D	222	THR	Peptide
1	D	330	ASP	Peptide
1	E	16	TYR	Peptide
1	E	164	ASP	Peptide
1	E	17	ARG	Peptide
1	E	66	ARG	Sidechain
1	F	66	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	4115	0	4033	173	0
1	B	4112	0	4027	248	0
1	C	4112	0	4031	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4058	0	4003	130	0
1	E	4058	0	4000	113	0
1	F	4058	0	4002	92	0
2	A	31	0	12	5	0
2	B	31	0	12	11	0
2	C	31	0	12	3	0
2	D	31	0	12	6	0
2	E	31	0	12	2	0
2	F	31	0	12	4	0
3	A	1	0	0	0	0
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	2	0	0	0	0
4	B	3	0	0	1	0
4	C	3	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
All	All	24717	0	24168	854	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (854) 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:A:160:LEU:CD1	1:A:160:LEU:CG	1.91	1.47
1:E:127:PHE:CE2	1:E:400:GLU:OE1	1.70	1.43
1:F:218:TRP:NE1	1:F:220:GLY:O	1.62	1.29
2:F:601:DGT:C4'	2:F:601:DGT:O4'	1.67	1.28
2:C:601:DGT:C4'	2:C:601:DGT:O4'	1.66	1.27
1:E:218:TRP:NE1	1:E:220:GLY:O	1.76	1.18
1:A:142:PRO:O	1:A:219:ARG:NH2	1.78	1.16
1:F:222:THR:OG1	1:F:223:PRO:HD2	1.44	1.13
1:A:223:PRO:O	1:A:227:HIS:HA	1.53	1.09
1:E:222:THR:H	1:E:223:PRO:HD3	1.15	1.08
1:A:146:GLU:HG2	1:A:219:ARG:NH1	1.68	1.07
1:C:66:ARG:NH2	4:C:701:HOH:O	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:602:DGT:H8	2:D:602:DGT:H5'A	1.08	1.06
1:A:146:GLU:HG2	1:A:219:ARG:HH12	1.19	1.03
1:E:222:THR:H	1:E:223:PRO:CD	1.71	1.02
1:E:228:TYR:OH	1:E:265:GLU:OE2	1.76	1.02
1:A:163:ARG:HE	1:A:163:ARG:HA	1.26	0.99
1:F:222:THR:OG1	1:F:223:PRO:CD	2.13	0.97
2:D:602:DGT:H5'A	2:D:602:DGT:C8	1.95	0.96
1:A:219:ARG:HH11	1:A:219:ARG:HB3	1.31	0.94
1:F:36:ARG:HD2	1:F:108:SER:OG	1.69	0.91
1:B:351:ARG:NH1	1:B:371:ASP:OD1	2.02	0.91
1:B:118:ASP:HA	1:B:121:ASN:HD22	1.36	0.89
1:D:169:LEU:HD11	1:D:468:GLU:HB3	1.53	0.89
1:F:327:SER:HB3	1:F:330:ASP:HB2	1.54	0.89
1:C:302:HIS:O	1:C:308:PHE:HB3	1.74	0.88
1:D:218:TRP:HZ2	1:D:222:THR:OG1	1.56	0.88
2:D:602:DGT:H8	2:D:602:DGT:C5'	2.03	0.86
1:B:92:LYS:N	1:B:93:LEU:HB2	1.90	0.86
1:E:222:THR:N	1:E:223:PRO:CD	2.37	0.86
1:D:114:CYS:O	1:D:117:HIS:CE1	2.29	0.86
1:E:127:PHE:HE2	1:E:400:GLU:OE1	1.26	0.85
1:C:324:LEU:HA	1:C:328:THR:HA	1.55	0.85
1:E:163:ARG:HD2	1:E:173:ARG:HH12	1.41	0.84
1:D:114:CYS:O	1:D:117:HIS:ND1	2.10	0.84
1:C:51:LYS:NZ	1:C:121:ASN:O	2.11	0.83
1:B:415:ARG:NH1	1:B:419:SER:OG	2.11	0.83
1:A:223:PRO:O	1:A:227:HIS:CA	2.27	0.83
1:D:273:CYS:HB3	1:D:383:LYS:NZ	1.94	0.82
1:E:327:SER:HB3	1:E:330:ASP:HB2	1.60	0.82
1:C:489:THR:HG22	1:C:491:LEU:H	1.42	0.82
1:B:51:LYS:HB3	1:B:66:ARG:HG3	1.60	0.82
1:E:16:TYR:O	1:E:200:ASN:ND2	2.12	0.82
1:B:222:THR:HB	1:B:223:PRO:CD	2.11	0.80
1:C:321:SER:O	1:C:323:SER:N	2.15	0.79
1:B:435:LYS:H	1:B:435:LYS:HD3	1.46	0.79
1:E:489:THR:HG22	1:E:491:LEU:H	1.45	0.79
1:E:442:ARG:NE	1:F:400:GLU:OE1	2.15	0.79
1:D:89:LYS:HA	1:D:94:LEU:HD11	1.65	0.79
1:F:218:TRP:CD1	1:F:220:GLY:O	2.36	0.79
1:A:50:GLN:HE21	1:F:61:ALA:HB2	1.48	0.79
1:A:299:TRP:HD1	1:A:308:PHE:HD2	1.30	0.78
1:B:79:TYR:HD1	1:B:345:VAL:HG11	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:396:VAL:O	1:E:400:GLU:HG3	1.83	0.78
1:B:54:VAL:CG2	2:B:601:DGT:H2'	2.14	0.78
1:A:14:ARG:NH2	1:A:35:ASP:OD1	2.17	0.77
1:B:93:LEU:O	1:B:95:GLU:N	2.16	0.77
1:A:219:ARG:HH11	1:A:219:ARG:CB	1.98	0.77
1:F:489:THR:HG22	1:F:491:LEU:H	1.50	0.77
1:A:224:GLU:OE2	1:A:225:THR:N	2.17	0.77
1:A:298:ALA:O	1:A:300:GLY:N	2.18	0.77
2:B:601:DGT:H8	2:B:601:DGT:H5'A	1.67	0.77
1:D:53:GLN:HG3	1:D:53:GLN:O	1.85	0.77
1:D:489:THR:HG22	1:D:491:LEU:H	1.50	0.76
1:B:224:GLU:N	1:B:224:GLU:OE1	2.18	0.76
1:E:218:TRP:HE1	1:E:220:GLY:C	1.92	0.76
1:D:400:GLU:OE1	1:F:442:ARG:NE	2.17	0.76
1:C:327:SER:HB2	1:C:330:ASP:HB2	1.67	0.75
1:B:380:LYS:O	1:B:384:ASN:ND2	2.20	0.75
1:B:54:VAL:HG22	2:B:601:DGT:H1'	1.68	0.74
1:A:257:ARG:NH2	1:A:265:GLU:OE1	2.21	0.74
1:B:299:TRP:HH2	1:B:377:ASP:HB3	1.53	0.74
1:B:382:TYR:O	1:B:385:VAL:N	2.21	0.73
1:C:226:HIS:HB3	1:C:229:LEU:HB2	1.70	0.73
1:E:218:TRP:CE2	1:E:220:GLY:O	2.41	0.73
1:A:262:TRP:H	1:A:262:TRP:CD1	2.06	0.72
1:B:141:HIS:O	1:B:177:ARG:NH1	2.22	0.72
1:B:449:THR:O	1:B:452:ARG:N	2.20	0.72
1:B:203:TRP:HE3	1:B:246:LEU:HD12	1.53	0.72
1:A:22:VAL:O	1:A:23:LYS:HB2	1.90	0.72
1:D:218:TRP:HZ2	1:D:222:THR:HG1	1.35	0.72
1:A:479:ARG:NH2	1:A:482:GLN:OE1	2.22	0.72
1:C:309:SER:HA	1:C:313:GLU:HB2	1.72	0.72
1:B:257:ARG:NH2	1:B:265:GLU:OE1	2.21	0.72
1:B:92:LYS:H	1:B:93:LEU:HB2	1.51	0.72
1:A:163:ARG:H	1:A:173:ARG:NH1	1.87	0.71
1:A:21:GLY:O	1:A:22:VAL:HG12	1.89	0.71
1:A:24:THR:HB	1:A:27:GLU:H	1.54	0.71
1:A:299:TRP:HD1	1:A:308:PHE:CD2	2.08	0.71
1:E:309:SER:HA	1:E:313:GLU:HB2	1.72	0.71
1:B:164:ASP:H	1:B:165:GLY:C	1.99	0.71
1:A:163:ARG:HA	1:A:163:ARG:NE	2.04	0.71
1:B:340:THR:O	1:B:344:LEU:HB2	1.90	0.71
1:C:491:LEU:HD21	1:E:59:ARG:HE	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:HIS:O	1:B:30:ARG:HG3	1.91	0.71
1:B:309:SER:HA	1:B:313:GLU:HB2	1.73	0.71
1:C:262:TRP:H	1:C:262:TRP:CD1	2.09	0.70
1:D:327:SER:HB3	1:D:330:ASP:HB2	1.73	0.70
1:D:228:TYR:OH	1:D:265:GLU:OE1	2.10	0.70
1:B:262:TRP:CD1	1:B:262:TRP:H	2.09	0.70
1:B:129:GLU:O	1:B:133:ASN:ND2	2.23	0.69
1:C:153:ASP:O	1:C:155:CYS:N	2.22	0.69
1:D:327:SER:O	1:D:331:GLN:HB2	1.92	0.69
1:F:155:CYS:HB3	1:F:161:ARG:HG3	1.73	0.69
1:F:309:SER:HA	1:F:313:GLU:HB2	1.75	0.69
1:B:80:ILE:HG12	1:B:345:VAL:HG13	1.74	0.69
1:B:257:ARG:HH21	1:B:261:THR:HG22	1.56	0.69
1:F:262:TRP:H	1:F:262:TRP:CD1	2.09	0.69
1:A:46:ARG:O	1:A:49:GLN:HG2	1.93	0.68
1:C:488:MET:HG2	1:C:492:TYR:HD2	1.58	0.68
1:E:287:THR:H	1:E:290:GLN:HB2	1.58	0.68
1:A:167:GLU:HB2	1:A:168:PRO:HD2	1.73	0.68
1:E:262:TRP:H	1:E:262:TRP:CD1	2.10	0.68
1:D:50:GLN:HB3	1:D:489:THR:CG2	2.24	0.67
1:F:50:GLN:HB3	1:F:489:THR:CG2	2.24	0.67
1:B:54:VAL:HG22	2:B:601:DGT:H2'	1.76	0.67
1:A:146:GLU:CG	1:A:219:ARG:HH12	2.00	0.67
1:A:489:THR:HG22	1:A:491:LEU:H	1.60	0.67
1:A:160:LEU:CD1	1:A:160:LEU:HG	2.19	0.67
1:D:488:MET:HG2	1:D:492:TYR:HD2	1.60	0.67
1:B:463:PRO:HB2	1:B:466:SER:HB2	1.77	0.67
1:D:309:SER:HA	1:D:313:GLU:HB2	1.77	0.67
1:A:203:TRP:HE3	1:A:246:LEU:HD12	1.60	0.66
1:A:87:ARG:NE	1:A:350:GLN:OE1	2.28	0.66
1:C:396:VAL:O	1:C:400:GLU:HG3	1.95	0.66
1:A:463:PRO:HB2	1:A:466:SER:HB2	1.78	0.66
1:D:50:GLN:OE1	1:D:489:THR:HG21	1.95	0.66
1:A:219:ARG:NH1	1:A:219:ARG:HB3	2.07	0.66
1:B:52:THR:HB	1:B:490:ASP:OD2	1.96	0.66
1:A:145:ALA:HB1	1:A:174:ARG:HG3	1.76	0.66
1:A:388:LYS:HD2	1:B:433:ARG:HH12	1.59	0.66
1:D:299:TRP:CD1	1:D:308:PHE:CD2	2.85	0.65
1:C:306:SER:OG	1:C:307:LEU:N	2.27	0.65
1:D:299:TRP:CD1	1:D:308:PHE:HD2	2.14	0.65
1:D:299:TRP:NE1	1:D:308:PHE:HB2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HD22	1:B:170:ASN:HB3	1.78	0.65
1:B:235:TYR:CG	1:B:243:ILE:HD12	2.31	0.65
1:B:299:TRP:CH2	1:B:377:ASP:HB3	2.32	0.65
1:B:79:TYR:CD1	1:B:345:VAL:HG11	2.30	0.65
1:E:50:GLN:HB3	1:E:489:THR:CG2	2.26	0.65
2:F:601:DGT:H5'A	2:F:601:DGT:H8	1.79	0.65
1:E:127:PHE:CD2	1:E:400:GLU:OE1	2.45	0.65
1:F:164:ASP:H	1:F:166:GLU:N	1.95	0.65
1:C:48:LEU:HD23	1:C:51:LYS:HD2	1.78	0.64
1:E:218:TRP:NE1	1:E:220:GLY:C	2.50	0.64
1:A:67:LEU:HD21	1:F:71:MET:HE1	1.79	0.64
1:C:153:ASP:CG	1:C:161:ARG:HG2	2.23	0.64
1:F:222:THR:CB	1:F:223:PRO:CD	2.75	0.64
1:C:299:TRP:HB2	1:C:381:LEU:HD13	1.80	0.64
1:C:230:MET:HE3	1:C:255:TYR:CD1	2.33	0.64
1:A:50:GLN:HB3	1:A:489:THR:CG2	2.28	0.63
1:A:167:GLU:HB2	1:A:169:LEU:HD23	1.81	0.63
1:F:435:LYS:H	1:F:435:LYS:HD3	1.62	0.63
1:A:223:PRO:HB3	1:A:230:MET:HB2	1.80	0.63
1:B:158:ALA:HA	1:B:161:ARG:NH1	2.13	0.63
1:C:319:SER:O	1:C:324:LEU:N	2.30	0.63
1:D:63:VAL:HG21	1:D:283:LYS:HE2	1.79	0.63
1:A:402:GLN:NE2	1:B:499:ARG:O	2.30	0.63
1:C:302:HIS:HA	1:C:305:GLY:H	1.64	0.63
1:A:496:GLU:OE2	1:A:499:ARG:NH2	2.31	0.63
1:B:425:PHE:CE2	1:B:477:ARG:HG3	2.33	0.63
1:D:229:LEU:HD21	1:D:262:TRP:CH2	2.34	0.63
1:D:319:SER:HA	1:D:331:GLN:OE1	1.98	0.63
1:B:90:GLU:HB3	1:B:91:LEU:HD23	1.81	0.63
1:D:117:HIS:O	1:D:119:ILE:N	2.31	0.63
1:B:157:VAL:HG12	1:B:158:ALA:H	1.63	0.63
1:B:373:SER:C	1:B:375:CYS:H	2.08	0.62
1:B:51:LYS:NZ	1:B:488:MET:O	2.30	0.62
1:B:455:TYR:OH	1:B:473:GLU:OE2	2.16	0.62
1:C:153:ASP:OD1	1:C:177:ARG:NH2	2.33	0.62
1:F:488:MET:HG2	1:F:492:TYR:HD2	1.64	0.62
1:A:52:THR:HG21	1:A:56:PRO:HA	1.81	0.62
1:C:54:VAL:HG13	1:C:55:PHE:CD2	2.34	0.62
1:A:442:ARG:NE	1:C:400:GLU:OE1	2.30	0.62
1:B:222:THR:CB	1:B:223:PRO:CD	2.74	0.62
1:B:323:SER:O	1:B:331:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:HB2	1:A:168:PRO:CD	2.28	0.62
1:B:197:MET:HE3	1:B:197:MET:HA	1.82	0.62
1:B:379:LEU:O	1:B:383:LYS:HG3	2.00	0.62
1:F:193:VAL:HG12	1:F:199:MET:HE3	1.82	0.62
1:B:92:LYS:HG2	1:B:93:LEU:HA	1.81	0.62
1:B:203:TRP:CE3	1:B:246:LEU:HD12	2.35	0.62
1:C:169:LEU:HD23	1:C:173:ARG:HH21	1.65	0.62
1:F:164:ASP:H	1:F:166:GLU:H	1.48	0.62
1:B:172:LEU:O	1:B:176:ILE:HG13	1.99	0.62
1:C:164:ASP:H	1:C:165:GLY:C	2.08	0.61
1:A:318:LYS:HB2	1:A:335:TYR:CE2	2.36	0.61
1:B:54:VAL:HG22	2:B:601:DGT:C1'	2.31	0.61
1:B:229:LEU:HD22	1:B:257:ARG:HD3	1.82	0.61
1:B:441:SER:O	1:B:445:HIS:ND1	2.33	0.61
1:C:228:TYR:OH	1:C:265:GLU:OE2	2.19	0.61
1:C:46:ARG:O	1:C:49:GLN:HG2	2.00	0.61
1:D:377:ASP:HA	1:D:380:LYS:HE3	1.82	0.61
1:E:226:HIS:HD2	1:E:255:TYR:O	1.84	0.61
1:D:276:ASP:OD2	2:D:602:DGT:H2'	2.01	0.60
1:F:114:CYS:O	1:F:117:HIS:ND1	2.32	0.60
1:E:218:TRP:HE1	1:E:221:GLU:CA	2.14	0.60
1:B:400:GLU:OE1	1:C:442:ARG:NE	2.33	0.60
1:E:488:MET:HG2	1:E:492:TYR:HD2	1.65	0.60
1:A:316:TRP:CZ2	1:A:320:ARG:HD2	2.36	0.60
1:C:329:GLU:CD	1:C:329:GLU:H	2.07	0.60
1:A:178:GLN:CD	1:A:219:ARG:HG2	2.26	0.60
1:B:222:THR:HB	1:B:223:PRO:HD3	1.83	0.60
1:B:349:ALA:O	1:B:353:ILE:HD12	2.01	0.60
1:C:351:ARG:NH2	1:C:370:GLU:HB3	2.17	0.60
1:F:351:ARG:NH2	1:F:370:GLU:HB2	2.17	0.60
1:B:222:THR:HB	1:B:223:PRO:HD2	1.82	0.60
1:F:50:GLN:HB3	1:F:489:THR:HG23	1.84	0.60
1:F:164:ASP:H	1:F:166:GLU:HG3	1.67	0.60
1:C:153:ASP:C	1:C:155:CYS:H	2.09	0.60
1:D:89:LYS:CA	1:D:94:LEU:HD11	2.32	0.60
1:B:11:ASN:HD21	1:B:13(C):HIS:HB2	1.66	0.59
1:A:223:PRO:HB3	1:A:226:HIS:O	2.01	0.59
1:B:145:ALA:HB2	1:B:177:ARG:NH2	2.16	0.59
1:D:24:THR:HB	1:D:27:GLU:H	1.67	0.59
1:D:50:GLN:HB3	1:D:489:THR:HG23	1.82	0.59
1:A:228:TYR:OH	1:A:265:GLU:OE2	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:HB3	1:B:161:ARG:HD3	1.83	0.59
1:A:173:ARG:HE	1:A:471:LEU:HD21	1.68	0.59
1:B:23:LYS:HA	1:B:27:GLU:OE1	2.02	0.59
1:E:54:VAL:HG21	1:E:276:ASP:CG	2.28	0.59
1:E:50:GLN:HB3	1:E:489:THR:HG23	1.85	0.59
1:B:202:THR:O	1:B:205:GLN:N	2.36	0.59
1:D:162:LEU:HD23	1:D:173:ARG:HD2	1.84	0.59
1:A:316:TRP:CH2	1:A:320:ARG:HD2	2.38	0.59
1:B:328:THR:HA	1:B:331:GLN:OE1	2.03	0.58
1:B:425:PHE:HE2	1:B:477:ARG:HG3	1.68	0.58
1:D:164:ASP:N	1:D:165:GLY:HA3	2.17	0.58
1:B:435:LYS:H	1:B:435:LYS:CD	2.10	0.58
1:E:371:ASP:HB3	1:E:380:LYS:HZ1	1.68	0.58
1:A:53:GLN:OE1	1:A:66:ARG:NH1	2.36	0.58
1:C:52:THR:O	1:C:66:ARG:NE	2.36	0.58
1:C:117:HIS:O	1:C:118:ASP:HB2	2.04	0.58
1:A:167:GLU:HG3	1:A:169:LEU:CD2	2.33	0.58
1:B:6:PHE:HD2	1:B:99:LEU:HD21	1.69	0.58
1:C:59:ARG:NH1	1:E:495:ASP:OD2	2.36	0.58
1:C:50:GLN:HB3	1:C:489:THR:HG23	1.84	0.58
1:C:56:PRO:O	1:C:399:LEU:HD13	2.03	0.58
1:F:68:THR:HA	1:F:71:MET:HE3	1.85	0.58
1:B:368(A):LEU:O	1:B:369:LEU:HG	2.03	0.58
1:A:218:TRP:CZ2	1:A:222:THR:HG22	2.38	0.58
1:B:371:ASP:C	1:B:373:SER:H	2.10	0.58
1:C:53:GLN:NE2	2:C:601:DGT:O3'	2.37	0.58
1:B:232:LYS:NZ	2:B:601:DGT:O2G	2.37	0.57
1:F:316:TRP:CE2	1:F:320:ARG:HD2	2.38	0.57
1:A:163:ARG:HB2	1:A:173:ARG:HH12	1.69	0.57
1:D:117:HIS:C	1:D:119:ILE:H	2.12	0.57
1:A:50:GLN:HB3	1:A:489:THR:HG21	1.87	0.57
1:B:140:LEU:O	1:B:142:PRO:HD3	2.05	0.57
1:B:46:ARG:O	1:B:49:GLN:HG2	2.05	0.57
1:B:292:TYR:HE2	1:B:312:VAL:HG22	1.68	0.57
1:E:327:SER:HB3	1:E:330:ASP:CB	2.32	0.57
1:F:164:ASP:N	1:F:166:GLU:HG3	2.20	0.57
1:A:144:ASP:OD1	1:A:154:ARG:NH1	2.37	0.57
1:B:309:SER:HA	1:B:313:GLU:CB	2.34	0.57
2:C:601:DGT:H5'A	2:C:601:DGT:H8	1.87	0.57
1:F:287:THR:H	1:F:290:GLN:HB2	1.69	0.57
1:A:60:ASN:C	1:A:62:ALA:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TRP:CD1	1:A:308:PHE:HB2	2.40	0.56
1:C:153:ASP:OD2	1:C:162:LEU:N	2.37	0.56
1:D:287:THR:H	1:D:290:GLN:HB2	1.69	0.56
1:D:318:LYS:HB3	1:D:335:TYR:CE2	2.40	0.56
1:C:287:THR:H	1:C:290:GLN:HB2	1.69	0.56
1:D:306:SER:O	1:D:310:LEU:HG	2.05	0.56
1:F:344:LEU:CD2	1:F:375:CYS:HB3	2.35	0.56
1:A:16:TYR:OH	1:A:198:ARG:NH1	2.38	0.56
1:B:118:ASP:HA	1:B:121:ASN:ND2	2.12	0.56
1:E:68:THR:HA	1:E:71:MET:HE3	1.87	0.56
1:A:295:LEU:HD23	1:A:385:VAL:HG21	1.87	0.56
1:A:60:ASN:O	1:A:62:ALA:N	2.39	0.56
1:B:59:ARG:HE	1:D:491:LEU:HD21	1.71	0.56
1:C:302:HIS:C	1:C:308:PHE:HB3	2.29	0.56
1:E:262:TRP:CH2	1:E:364:PHE:O	2.59	0.56
1:D:485:ILE:O	1:D:488:MET:HB2	2.06	0.56
1:E:166:GLU:O	1:E:167:GLU:HG3	2.06	0.56
1:B:290:GLN:O	1:B:294:HIS:ND1	2.37	0.56
1:B:488:MET:HG2	1:B:492:TYR:HD2	1.71	0.56
1:E:164:ASP:N	1:E:165:GLY:HA3	2.21	0.56
1:F:272:TYR:C	1:F:272:TYR:CD1	2.84	0.56
1:B:217:TRP:CH2	1:B:240:GLU:HG3	2.41	0.56
1:B:257:ARG:HH22	1:B:265:GLU:CD	2.11	0.55
1:F:153:ASP:HB3	1:F:161:ARG:HG2	1.87	0.55
2:D:602:DGT:O2A	2:D:602:DGT:H4'	2.06	0.55
1:E:435:LYS:H	1:E:435:LYS:HD2	1.70	0.55
1:B:163:ARG:HG3	1:B:164:ASP:HB2	1.88	0.55
1:D:327:SER:O	1:D:330:ASP:N	2.30	0.55
1:A:262:TRP:HB3	1:A:368(A):LEU:HD13	1.88	0.55
1:B:259:PRO:O	1:B:262:TRP:HD1	1.90	0.55
1:C:203:TRP:HE3	1:C:246:LEU:HD12	1.70	0.55
1:B:54:VAL:HG22	2:B:601:DGT:C2'	2.36	0.55
1:B:176:ILE:HG23	1:B:475:TYR:CD1	2.42	0.55
1:E:426:THR:O	1:E:430:GLU:HG3	2.07	0.55
1:A:218:TRP:HZ2	1:A:222:THR:HG22	1.71	0.55
1:A:319:SER:HA	1:A:331:GLN:HG2	1.89	0.55
1:E:253:ALA:N	1:E:256:SER:OG	2.39	0.55
1:F:50:GLN:HB3	1:F:489:THR:HG21	1.89	0.55
1:A:282:GLU:C	1:A:284:ARG:H	2.13	0.55
1:A:288:VAL:HG12	1:A:316:TRP:HZ3	1.70	0.55
1:D:422:LEU:O	1:D:426:THR:OG1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:MET:HG2	1:A:492:TYR:HD2	1.72	0.54
1:B:54:VAL:HG12	1:B:55:PHE:CD1	2.42	0.54
1:C:259:PRO:O	1:C:262:TRP:HD1	1.89	0.54
1:E:228:TYR:OH	1:E:265:GLU:CD	2.49	0.54
1:A:352:PHE:HB2	1:A:368(A):LEU:HD21	1.88	0.54
1:B:74:GLN:HG2	1:B:111:GLU:HG3	1.88	0.54
1:D:348:ALA:HB1	1:D:368(A):LEU:HD23	1.90	0.54
1:E:141:HIS:O	1:E:177:ARG:NH1	2.40	0.54
1:D:39:ILE:HG12	1:D:116:MET:SD	2.48	0.54
1:D:258:PHE:CE2	1:D:260:LEU:HB2	2.42	0.54
1:E:163:ARG:HD2	1:E:173:ARG:NH1	2.16	0.54
1:C:331:GLN:HA	1:C:334:MET:HB3	1.88	0.54
1:A:162:LEU:HD22	1:A:170:ASN:HB3	1.89	0.54
1:B:235:TYR:CD2	1:B:243:ILE:HD12	2.43	0.54
1:B:427:GLU:CD	1:B:436:ARG:HH22	2.16	0.54
1:D:203:TRP:HE3	1:D:246:LEU:HD12	1.73	0.54
1:D:273:CYS:HB3	1:D:383:LYS:HZ1	1.72	0.54
1:F:427:GLU:HG2	1:F:431:LYS:HE2	1.89	0.54
1:A:321:SER:HB3	1:A:322:ASN:HA	1.90	0.54
1:B:11:ASN:CG	1:B:13(C):HIS:H	2.14	0.54
1:B:314:ASN:OD1	1:B:318:LYS:HD2	2.07	0.54
1:E:203:TRP:HE3	1:E:246:LEU:HD12	1.73	0.54
1:B:88:LEU:HD13	1:B:353:ILE:HG12	1.89	0.53
1:D:245:ARG:O	1:D:245:ARG:HG2	2.07	0.53
1:A:51:LYS:HA	1:A:490:ASP:OD1	2.08	0.53
1:E:144:ASP:OD1	1:E:154:ARG:NH1	2.39	0.53
1:A:299:TRP:CD1	1:A:308:PHE:CD2	2.95	0.53
1:B:136:PHE:O	1:B:140:LEU:HD12	2.09	0.53
1:D:5:ASP:HB3	1:D:8:LYS:HD2	1.89	0.53
1:A:73:VAL:HG22	1:A:271:SER:OG	2.07	0.53
1:D:54:VAL:HG13	1:D:55:PHE:CD2	2.43	0.53
1:F:141:HIS:O	1:F:177:ARG:NH1	2.41	0.53
1:F:485:ILE:O	1:F:488:MET:HB2	2.07	0.53
1:B:33:GLU:OE2	1:D:78:ARG:NE	2.35	0.53
1:C:485:ILE:O	1:C:488:MET:HB2	2.09	0.53
1:E:262:TRP:HH2	1:E:364:PHE:O	1.91	0.53
1:F:426:THR:O	1:F:430:GLU:HG3	2.08	0.53
1:A:82:LYS:O	1:A:86:SER:OG	2.21	0.53
1:C:141:HIS:O	1:C:177:ARG:NH1	2.41	0.53
1:C:114:CYS:O	1:C:117:HIS:ND1	2.40	0.53
1:A:400:GLU:OE2	2:A:601:DGT:N2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LEU:HD22	1:B:257:ARG:CD	2.38	0.53
1:B:326:ARG:O	1:B:327:SER:OG	2.26	0.53
1:C:59:ARG:CZ	1:E:491:LEU:HD21	2.39	0.53
1:C:73:VAL:HG22	1:C:271:SER:OG	2.09	0.53
1:C:158:ALA:O	1:C:163:ARG:NH1	2.31	0.53
1:C:344:LEU:CD2	1:C:375:CYS:HB3	2.39	0.53
1:A:373:SER:HB2	1:A:376:SER:H	1.74	0.53
1:B:9:LYS:HE2	1:B:250:LEU:O	2.09	0.53
1:B:53:GLN:O	1:B:55:PHE:N	2.38	0.53
1:B:117:HIS:HB2	4:B:702:HOH:O	2.09	0.53
1:B:319:SER:O	1:B:321:SER:N	2.39	0.53
1:C:23:LYS:HA	1:C:27:GLU:OE1	2.09	0.53
1:C:163:ARG:HA	1:C:164:ASP:HB2	1.90	0.53
2:A:601:DGT:H5'A	2:A:601:DGT:H8	1.90	0.52
1:B:26:HIS:HA	1:B:29:LEU:HD23	1.91	0.52
1:D:218:TRP:CZ2	1:D:222:THR:OG1	2.48	0.52
1:B:307:LEU:HD23	1:B:374:GLU:O	2.09	0.52
1:E:50:GLN:HB3	1:E:489:THR:HG21	1.90	0.52
1:A:138:GLN:HG3	1:A:139:ARG:N	2.23	0.52
1:D:50:GLN:HB3	1:D:489:THR:HG21	1.90	0.52
1:F:282:GLU:C	1:F:284:ARG:H	2.18	0.52
1:A:219:ARG:NH1	1:A:219:ARG:CG	2.73	0.52
1:A:259:PRO:O	1:A:262:TRP:HD1	1.92	0.52
1:A:314:ASN:OD1	1:A:318:LYS:HE3	2.09	0.52
1:B:356:LEU:O	1:B:360:PHE:HB3	2.09	0.52
1:D:4:ILE:HD13	1:D:356:LEU:HG	1.92	0.52
1:A:427:GLU:OE1	1:A:436:ARG:NH2	2.41	0.52
1:D:91:LEU:CB	1:D:93:LEU:HD13	2.40	0.52
1:B:157:VAL:HG12	1:B:158:ALA:N	2.25	0.52
1:E:163:ARG:HH11	1:E:173:ARG:HH12	1.57	0.52
1:A:114:CYS:O	1:A:117:HIS:ND1	2.38	0.52
1:A:294:HIS:CD2	1:A:389:HIS:CE1	2.98	0.52
1:B:93:LEU:HD23	1:B:96:ALA:HB3	1.92	0.52
1:B:167:GLU:OE2	1:B:173:ARG:NH1	2.42	0.52
1:A:153:ASP:HB3	1:A:161:ARG:HG2	1.91	0.51
1:A:214:ARG:HE	1:A:218:TRP:HB3	1.75	0.51
1:A:50:GLN:HB3	1:A:489:THR:HG23	1.92	0.51
1:A:309:SER:HA	1:A:313:GLU:HB2	1.92	0.51
1:B:334:MET:HB3	1:B:337:ARG:NH1	2.25	0.51
1:F:54:VAL:HG13	1:F:55:PHE:CD2	2.46	0.51
1:B:93:LEU:HD11	1:B:97:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLN:HB3	1:C:489:THR:CG2	2.40	0.51
1:D:290:GLN:O	1:D:294:HIS:ND1	2.43	0.51
1:B:253:ALA:O	1:B:256:SER:OG	2.25	0.51
1:B:364:PHE:CZ	1:B:366:HIS:HB2	2.46	0.51
1:B:371:ASP:O	1:B:373:SER:N	2.44	0.51
1:E:272:TYR:CD1	1:E:272:TYR:C	2.88	0.51
1:F:262:TRP:HB3	1:F:368(A):LEU:HD13	1.92	0.51
1:B:164:ASP:HB3	1:B:165:GLY:HA3	1.91	0.51
1:C:489:THR:HG22	1:C:491:LEU:N	2.19	0.51
1:A:227:HIS:HB3	1:A:365:ASN:HD21	1.75	0.51
1:B:228:TYR:HD2	1:B:229:LEU:HD23	1.75	0.51
1:D:184:GLU:HG3	1:D:186:ASN:H	1.75	0.51
1:F:488:MET:HE2	1:F:492:TYR:CE2	2.46	0.51
1:B:491:LEU:HD21	1:D:59:ARG:NE	2.26	0.51
1:D:179:ASP:OD2	1:D:216:ALA:HB3	2.11	0.51
1:B:4:ILE:HD11	1:B:357:PRO:HA	1.92	0.50
1:B:36:ARG:O	1:B:40:ILE:HD12	2.11	0.50
1:C:287:THR:HB	1:C:290:GLN:H	1.75	0.50
1:C:319:SER:HA	1:C:323:SER:CB	2.41	0.50
1:F:415:ARG:N	1:F:416:PRO:HD2	2.26	0.50
1:F:24:THR:HB	1:F:27:GLU:H	1.75	0.50
1:E:226:HIS:CD2	1:E:255:TYR:O	2.64	0.50
1:A:262:TRP:CD1	1:A:262:TRP:N	2.78	0.50
1:B:257:ARG:NH2	1:B:261:THR:HG22	2.24	0.50
1:B:266:ALA:O	1:B:270:ILE:HG13	2.11	0.50
1:E:410:LEU:HD11	1:E:497:TYR:HB2	1.92	0.50
1:B:373:SER:C	1:B:375:CYS:N	2.70	0.50
1:C:306:SER:O	1:C:309:SER:OG	2.28	0.50
1:D:410:LEU:HD11	1:D:497:TYR:HB2	1.93	0.50
1:B:201:LEU:HB2	1:B:206:VAL:CG2	2.41	0.50
1:B:249:GLU:C	1:B:250:LEU:HD23	2.36	0.50
1:E:117:HIS:O	1:E:118:ASP:HB2	2.11	0.50
1:B:15:ARG:HG3	1:B:16:TYR:CE1	2.47	0.50
1:B:155:CYS:HB3	1:B:161:ARG:HG2	1.93	0.50
1:B:248:LYS:O	1:B:250:LEU:N	2.45	0.50
1:B:160:LEU:HA	1:B:173:ARG:HG2	1.94	0.50
1:D:406:VAL:O	1:D:410:LEU:HD13	2.12	0.50
1:F:51:LYS:HE2	1:F:488:MET:O	2.11	0.50
1:F:272:TYR:CD1	1:F:273:CYS:N	2.80	0.50
1:A:4:ILE:HD13	1:A:356:LEU:HG	1.92	0.49
1:A:22:VAL:HG22	1:A:23:LYS:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ALA:O	1:A:147:SER:N	2.44	0.49
1:A:167:GLU:OE1	1:A:167:GLU:N	2.38	0.49
1:B:376:SER:O	1:B:380:LYS:HG3	2.12	0.49
1:F:213:THR:HB	1:F:255:TYR:HA	1.94	0.49
1:B:117:HIS:O	1:B:118:ASP:HB2	2.13	0.49
1:D:258:PHE:HE2	1:D:260:LEU:HB2	1.78	0.49
1:D:379:LEU:O	1:D:383:LYS:HG3	2.11	0.49
1:A:344:LEU:CD2	1:A:375:CYS:HB3	2.43	0.49
1:B:113:SER:HB3	1:B:205:GLN:NE2	2.27	0.49
1:C:491:LEU:HD21	1:E:59:ARG:HH21	1.77	0.49
1:D:235:TYR:CG	1:D:243:ILE:HG13	2.48	0.49
1:A:117:HIS:O	1:A:118:ASP:HB2	2.11	0.49
1:B:54:VAL:CG2	2:B:601:DGT:C2'	2.90	0.49
2:E:601:DGT:H8	2:E:601:DGT:H5'A	1.95	0.49
1:F:167:GLU:HB3	1:F:169:LEU:H	1.77	0.49
1:A:89:LYS:HG3	1:A:94:LEU:HD22	1.93	0.49
1:A:178:GLN:HG2	1:A:219:ARG:HG3	1.93	0.49
1:B:250:LEU:HD13	1:B:258:PHE:CE1	2.48	0.49
1:C:69:HIS:CE1	1:C:272:TYR:HB3	2.47	0.49
1:D:15:ARG:HD2	1:D:245:ARG:NH2	2.27	0.49
1:B:28:ILE:O	1:B:31:ILE:HG22	2.13	0.49
1:C:327:SER:HB2	1:C:330:ASP:CB	2.41	0.49
1:D:117:HIS:C	1:D:119:ILE:N	2.70	0.49
1:E:35:ASP:O	1:E:39:ILE:HD12	2.13	0.49
2:F:601:DGT:H5'A	2:F:601:DGT:C8	2.42	0.49
1:A:167:GLU:N	1:A:167:GLU:CD	2.71	0.49
1:A:214:ARG:HG3	1:A:230:MET:HE3	1.94	0.49
1:B:158:ALA:HA	1:B:161:ARG:HH12	1.78	0.49
1:E:66:ARG:HH22	1:E:125:GLY:HA2	1.78	0.49
1:F:258:PHE:CD1	1:F:259:PRO:HD2	2.48	0.49
1:C:67:LEU:HD21	1:E:71:MET:HE1	1.95	0.48
1:C:302:HIS:H	1:C:303:GLU:CB	2.26	0.48
1:A:422:LEU:O	1:A:426:THR:OG1	2.22	0.48
1:B:11:ASN:OD1	1:B:13(C):HIS:N	2.43	0.48
1:B:93:LEU:CD2	1:B:96:ALA:HB3	2.43	0.48
1:C:417:LEU:HD11	1:C:443:LEU:HB3	1.95	0.48
1:E:140:LEU:HD12	1:E:140:LEU:O	2.13	0.48
1:A:14:ARG:HG3	1:A:19:PRO:HD3	1.95	0.48
1:B:167:GLU:HB3	1:B:170:ASN:OD1	2.13	0.48
1:E:235:TYR:CG	1:E:243:ILE:HG13	2.49	0.48
1:A:52:THR:HG22	1:A:490:ASP:OD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:H	1:B:290:GLN:HB2	1.78	0.48
1:C:303:GLU:N	1:C:308:PHE:HB3	2.28	0.48
1:A:142:PRO:HB3	1:A:177:ARG:O	2.13	0.48
1:A:163:ARG:CB	1:A:173:ARG:HH12	2.26	0.48
1:B:48:LEU:C	1:B:50:GLN:H	2.21	0.48
1:B:422:LEU:O	1:B:426:THR:OG1	2.30	0.48
1:C:482:GLN:O	1:C:486:SER:OG	2.24	0.48
1:D:299:TRP:HD1	1:D:308:PHE:CD2	2.31	0.48
1:E:273:CYS:SG	1:E:383:LYS:HE2	2.53	0.48
1:A:455:TYR:OH	1:A:473:GLU:OE2	2.25	0.48
1:B:142:PRO:HD2	1:B:143:GLU:OE1	2.14	0.48
1:B:347:TYR:C	1:B:347:TYR:CD1	2.88	0.48
1:C:316:TRP:O	1:C:319:SER:OG	2.30	0.48
1:F:164:ASP:N	1:F:166:GLU:H	2.11	0.48
1:A:170:ASN:HA	1:A:173:ARG:HG3	1.95	0.48
1:C:415:ARG:N	1:C:416:PRO:HD2	2.28	0.48
1:D:163:ARG:C	1:D:165:GLY:HA3	2.39	0.48
1:E:23:LYS:HA	1:E:27:GLU:OE1	2.13	0.48
1:B:449:THR:O	1:B:451:HIS:N	2.47	0.48
1:D:91:LEU:HB2	1:D:93:LEU:HD13	1.96	0.48
1:E:222:THR:N	1:E:223:PRO:HD2	2.25	0.48
1:A:140:LEU:HD12	1:A:177:ARG:HA	1.95	0.48
1:A:439:ILE:HD12	1:A:439:ILE:H	1.78	0.48
1:B:373:SER:O	1:B:375:CYS:N	2.47	0.48
1:D:344:LEU:HD21	1:D:375:CYS:HB3	1.96	0.48
1:E:17:ARG:HH11	1:E:17:ARG:HD2	1.46	0.48
1:F:164:ASP:N	1:F:165:GLY:HA2	2.28	0.48
1:A:299:TRP:HE3	1:A:299:TRP:O	1.97	0.47
1:A:469:PHE:HB3	1:A:470:PRO:HD3	1.96	0.47
1:B:319:SER:HA	1:B:331:GLN:OE1	2.14	0.47
1:C:313:GLU:O	1:C:317:GLU:HG2	2.14	0.47
1:F:4:ILE:HD13	1:F:356:LEU:HG	1.96	0.47
1:A:135:TRP:O	1:A:138:GLN:HG2	2.13	0.47
1:A:218:TRP:CZ2	1:A:222:THR:CG2	2.97	0.47
1:A:490:ASP:OD1	1:A:490:ASP:N	2.45	0.47
1:F:393:HIS:CG	1:F:394:PRO:HD2	2.49	0.47
1:A:163:ARG:N	1:A:173:ARG:NH1	2.61	0.47
1:A:318:LYS:HB2	1:A:335:TYR:HE2	1.78	0.47
1:B:123:PRO:HG3	1:B:488:MET:O	2.14	0.47
1:D:160:LEU:O	1:D:173:ARG:HG2	2.14	0.47
1:F:417:LEU:HD11	1:F:443:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:H	1:A:173:ARG:HH11	1.61	0.47
1:B:39:ILE:O	1:B:45:ILE:HD12	2.15	0.47
1:F:163:ARG:HG2	1:F:164:ASP:HB2	1.95	0.47
1:F:439:ILE:HD12	1:F:439:ILE:H	1.79	0.47
1:A:54:VAL:HG13	1:A:55:PHE:CD2	2.49	0.47
1:B:176:ILE:HG23	1:B:475:TYR:HD1	1.79	0.47
1:B:292:TYR:CE2	1:B:312:VAL:HG22	2.47	0.47
1:D:351:ARG:NH2	1:D:370:GLU:HG2	2.30	0.47
1:A:24:THR:HG22	1:A:26:HIS:H	1.80	0.47
1:A:178:GLN:CG	1:A:219:ARG:HG3	2.45	0.47
1:A:320:ARG:O	1:A:321:SER:HB2	2.13	0.47
1:B:9:LYS:HD2	1:B:259:PRO:HG2	1.96	0.47
1:B:93:LEU:O	1:B:95:GLU:HG2	2.14	0.47
1:B:398:ARG:HG2	1:B:402:GLN:HE21	1.80	0.47
1:B:417:LEU:O	1:B:477:ARG:NH1	2.47	0.47
1:C:164:ASP:H	1:C:165:GLY:CA	2.27	0.47
1:E:155:CYS:HB3	1:E:161:ARG:HG3	1.97	0.47
1:F:184:GLU:HG3	1:F:186:ASN:H	1.80	0.47
1:C:302:HIS:CB	1:C:306:SER:HB3	2.44	0.47
1:E:439:ILE:HD12	1:E:439:ILE:H	1.80	0.47
1:F:295:LEU:HD23	1:F:385:VAL:HG21	1.96	0.47
1:A:162:LEU:CD2	1:A:170:ASN:HB3	2.45	0.47
1:B:4:ILE:HD13	1:B:360:PHE:CD1	2.50	0.47
1:B:230:MET:HE3	1:B:255:TYR:CG	2.49	0.47
1:B:410:LEU:HA	1:B:410:LEU:HD12	1.71	0.47
1:C:153:ASP:HB3	1:C:161:ARG:HG2	1.96	0.47
1:B:351:ARG:HE	1:B:351:ARG:HB3	1.49	0.47
1:C:393:HIS:CG	1:C:394:PRO:HD2	2.50	0.47
1:D:350:GLN:OE1	1:D:350:GLN:N	2.48	0.47
1:E:351:ARG:HH21	1:E:370:GLU:HB3	1.79	0.47
1:B:68:THR:HG21	1:D:46:ARG:HG2	1.95	0.46
1:B:164:ASP:N	1:B:165:GLY:O	2.48	0.46
1:B:212:TYR:OH	1:B:231:LYS:HE2	2.15	0.46
1:B:264:MET:HB3	1:B:264:MET:HE2	1.74	0.46
1:D:376:SER:O	1:D:380:LYS:HG2	2.14	0.46
1:D:410:LEU:CD1	1:D:497:TYR:HB2	2.45	0.46
1:B:39:ILE:HG23	1:B:45:ILE:CD1	2.44	0.46
1:B:184:GLU:HG2	1:B:233:PRO:O	2.14	0.46
1:C:320:ARG:HA	1:C:320:ARG:NE	2.29	0.46
1:E:184:GLU:HG3	1:E:186:ASN:H	1.80	0.46
1:A:117:HIS:HB3	1:A:264:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:HIS:CG	1:B:394:PRO:HD2	2.50	0.46
1:C:138:GLN:HG3	1:C:139:ARG:N	2.29	0.46
1:E:364:PHE:CZ	1:E:366:HIS:HB2	2.50	0.46
1:E:488:MET:HE2	1:E:492:TYR:CE2	2.50	0.46
1:B:14:ARG:NH2	1:B:201:LEU:HA	2.30	0.46
1:B:272:TYR:O	1:B:273:CYS:C	2.59	0.46
1:E:224:GLU:HA	1:E:227:HIS:CD2	2.50	0.46
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.59	0.46
1:B:26:HIS:CE1	1:B:30:ARG:HD2	2.51	0.46
1:B:203:TRP:CH2	1:B:245:ARG:HG2	2.50	0.46
1:B:270:ILE:HD11	1:B:369:LEU:HD11	1.97	0.46
1:B:427:GLU:OE2	1:B:436:ARG:NH2	2.37	0.46
1:D:307:LEU:HD12	1:D:310:LEU:HB2	1.97	0.46
1:E:344:LEU:CD2	1:E:375:CYS:HB3	2.45	0.46
1:D:258:PHE:CD1	1:D:259:PRO:HD2	2.51	0.46
1:F:46:ARG:O	1:F:49:GLN:HG2	2.16	0.46
1:F:433:ARG:NH1	1:F:442:ARG:HH22	2.13	0.46
1:A:167:GLU:CD	1:A:167:GLU:H	2.19	0.46
1:B:162:LEU:CD2	1:B:170:ASN:HB3	2.45	0.46
1:E:216:ALA:HA	1:E:233:PRO:HB3	1.98	0.46
1:E:415:ARG:N	1:E:416:PRO:HD2	2.30	0.46
1:A:262:TRP:HH2	1:A:364:PHE:O	1.99	0.46
1:A:287:THR:H	1:A:290:GLN:HB2	1.81	0.46
1:C:16:TYR:OH	1:C:198:ARG:NH1	2.48	0.46
1:D:257:ARG:NH2	1:D:265:GLU:OE2	2.46	0.46
1:E:76:VAL:HG21	1:E:271:SER:HB3	1.98	0.46
1:B:19:PRO:O	1:B:20:GLN:NE2	2.49	0.46
1:C:143:GLU:HG3	1:C:154:ARG:NH1	2.31	0.46
1:A:211:LYS:HE2	2:A:601:DGT:O3G	2.15	0.45
1:B:453:LEU:O	1:B:457:GLU:HB2	2.16	0.45
1:C:309:SER:HA	1:C:313:GLU:CB	2.44	0.45
1:D:212:TYR:O	1:D:234:GLY:HA3	2.16	0.45
1:F:117:HIS:HB3	1:F:264:MET:HE3	1.97	0.45
1:F:351:ARG:CZ	1:F:370:GLU:HB2	2.45	0.45
1:A:22:VAL:O	1:A:23:LYS:CB	2.63	0.45
1:B:224:GLU:N	1:B:224:GLU:CD	2.73	0.45
1:B:364:PHE:CE2	1:B:366:HIS:HB2	2.51	0.45
1:C:53:GLN:O	1:C:54:VAL:HG12	2.17	0.45
1:D:140:LEU:O	1:D:140:LEU:HD12	2.17	0.45
1:A:76:VAL:O	1:A:80:ILE:HG13	2.15	0.45
1:A:485:ILE:O	1:A:488:MET:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASN:HD21	1:B:13(C):HIS:CB	2.28	0.45
1:C:117:HIS:HB3	1:C:264:MET:HE3	1.99	0.45
1:E:288:VAL:HG11	1:E:329:GLU:HA	1.99	0.45
1:A:179:ASP:OD1	1:A:216:ALA:HB3	2.17	0.45
1:E:15:ARG:HE	1:E:245:ARG:NH2	2.14	0.45
1:E:435:LYS:H	1:E:435:LYS:CD	2.28	0.45
1:F:238:SER:HB3	1:F:475:TYR:HE2	1.81	0.45
1:F:259:PRO:O	1:F:262:TRP:HD1	1.99	0.45
1:A:145:ALA:HB1	1:A:174:ARG:CG	2.44	0.45
1:B:37:GLY:O	1:B:41:ASN:HB2	2.16	0.45
1:B:437:PHE:HB3	1:B:440:GLU:HB2	1.98	0.45
1:C:53:GLN:O	1:C:55:PHE:N	2.45	0.45
1:C:470:PRO:HG2	1:C:471:LEU:HD12	1.97	0.45
1:D:73:VAL:HG22	1:D:271:SER:OG	2.17	0.45
1:D:299:TRP:NE1	1:D:308:PHE:HD2	2.14	0.45
1:F:192:LEU:HA	1:F:196:LEU:HD12	1.99	0.45
1:F:273:CYS:SG	1:F:383:LYS:HG3	2.57	0.45
1:B:61:ALA:HB3	1:D:47:ARG:HA	1.99	0.45
1:B:122:PRO:HG3	1:B:183:PHE:HE1	1.82	0.45
1:B:292:TYR:O	1:B:295:LEU:N	2.42	0.45
1:B:347:TYR:HE2	1:B:375:CYS:HB2	1.81	0.45
1:D:262:TRP:HH2	1:D:364:PHE:O	2.00	0.45
1:B:26:HIS:O	1:B:29:LEU:HG	2.17	0.45
1:B:163:ARG:HG3	1:B:164:ASP:CB	2.47	0.45
1:B:371:ASP:C	1:B:373:SER:N	2.74	0.45
1:E:24:THR:HG22	1:E:25:GLU:N	2.31	0.45
1:B:11:ASN:O	1:B:32:PHE:HZ	2.00	0.45
1:B:306:SER:O	1:B:309:SER:OG	2.35	0.45
1:B:382:TYR:O	1:B:383:LYS:C	2.59	0.45
1:C:50:GLN:O	1:C:489:THR:HG23	2.17	0.45
1:C:54:VAL:O	1:C:56:PRO:HD3	2.17	0.45
1:C:215:PRO:O	1:C:218:TRP:HB2	2.17	0.45
1:C:491:LEU:CD2	1:E:59:ARG:HE	2.28	0.45
1:A:213:THR:HB	1:A:255:TYR:HA	1.98	0.45
1:A:410:LEU:HD12	1:A:410:LEU:HA	1.63	0.45
1:C:52:THR:O	1:C:52:THR:HG23	2.16	0.45
1:D:53:GLN:O	1:D:54:VAL:HG12	2.17	0.45
1:D:309:SER:HA	1:D:313:GLU:CB	2.44	0.45
1:E:468:GLU:HA	1:E:471:LEU:HD13	1.98	0.45
1:F:433:ARG:HH11	1:F:442:ARG:NH2	2.15	0.45
1:A:23:LYS:HG3	1:A:27:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LYS:HA	1:D:490:ASP:OD1	2.17	0.44
1:E:417:LEU:HD11	1:E:443:LEU:HB3	1.99	0.44
1:F:489:THR:HG22	1:F:490:ASP:N	2.32	0.44
1:A:425:PHE:O	1:A:429:VAL:HG23	2.17	0.44
1:B:451:HIS:CD2	1:B:483:ASP:HB3	2.51	0.44
1:D:425:PHE:O	1:D:429:VAL:HG23	2.17	0.44
1:E:123:PRO:HB2	1:E:407:ILE:HD11	1.98	0.44
1:E:295:LEU:HD23	1:E:385:VAL:HG21	1.99	0.44
1:A:406:VAL:HG21	1:A:494:TRP:HD1	1.83	0.44
1:E:229:LEU:HD21	1:E:262:TRP:CH2	2.52	0.44
1:E:471:LEU:HD12	1:E:471:LEU:H	1.82	0.44
1:F:488:MET:HE2	1:F:492:TYR:CD2	2.53	0.44
1:A:161:ARG:O	1:A:162:LEU:C	2.60	0.44
1:B:54:VAL:CG2	2:B:601:DGT:H1'	2.43	0.44
1:B:164:ASP:N	1:B:165:GLY:C	2.73	0.44
1:D:351:ARG:NE	1:D:370:GLU:HG3	2.32	0.44
1:E:243:ILE:HD13	1:E:243:ILE:HA	1.81	0.44
1:A:426:THR:O	1:A:430:GLU:HG3	2.17	0.44
1:C:262:TRP:HB3	1:C:368(A):LEU:HD13	1.99	0.44
1:D:244:ALA:O	1:D:245:ARG:C	2.58	0.44
1:D:344:LEU:CD2	1:D:375:CYS:HB3	2.48	0.44
1:D:370:GLU:O	1:D:376:SER:HB3	2.18	0.44
1:E:213:THR:HB	1:E:255:TYR:HA	1.99	0.44
1:A:315:ALA:HB1	1:A:335:TYR:HB2	2.00	0.44
1:B:50:GLN:HB2	1:D:61:ALA:HB2	2.00	0.44
1:B:391:PHE:CZ	2:B:601:DGT:H2'A	2.53	0.44
1:B:435:LYS:HE2	1:B:436:ARG:NH1	2.32	0.44
1:D:14:ARG:HD3	1:D:200:ASN:CG	2.42	0.44
1:D:282:GLU:C	1:D:284:ARG:H	2.26	0.44
1:F:344:LEU:HD21	1:F:375:CYS:HB3	1.98	0.44
1:A:167:GLU:CB	1:A:169:LEU:HD23	2.47	0.44
1:B:72:GLU:HG2	1:D:40:ILE:HG22	1.98	0.44
1:B:215:PRO:HB3	1:B:235:TYR:CZ	2.53	0.44
1:C:59:ARG:NH1	1:E:491:LEU:HD21	2.33	0.44
1:B:128:GLY:O	1:B:132:ILE:HG13	2.18	0.44
1:B:449:THR:O	1:B:450:ARG:C	2.59	0.44
1:D:247:ARG:HD3	1:D:254:LEU:HA	2.00	0.44
1:D:262:TRP:CH2	1:D:364:PHE:O	2.70	0.44
1:D:439:ILE:HD12	1:D:439:ILE:H	1.83	0.44
1:E:143:GLU:HG3	1:E:154:ARG:NH1	2.32	0.44
1:A:167:GLU:HG3	1:A:169:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:HG3	1:A:169:LEU:HD23	2.00	0.43
1:D:316:TRP:CE2	1:D:320:ARG:HD2	2.52	0.43
1:E:38:ARG:HH12	1:E:200:ASN:HB3	1.83	0.43
1:C:395:ASP:O	1:C:399:LEU:HD12	2.19	0.43
1:D:114:CYS:HA	1:D:264:MET:HG3	2.01	0.43
1:E:155:CYS:HB2	1:E:177:ARG:NH1	2.33	0.43
1:F:4:ILE:HG23	1:F:360:PHE:CD2	2.53	0.43
1:B:488:MET:HE2	1:B:492:TYR:CE2	2.53	0.43
1:A:344:LEU:HD23	1:A:375:CYS:HB3	2.00	0.43
1:B:88:LEU:HA	1:B:88:LEU:HD12	1.87	0.43
1:B:158:ALA:C	1:B:160:LEU:H	2.26	0.43
1:D:489:THR:HG22	1:D:490:ASP:N	2.32	0.43
1:F:272:TYR:C	1:F:272:TYR:HD1	2.24	0.43
1:A:167:GLU:CB	1:A:168:PRO:CD	2.94	0.43
1:B:262:TRP:HB3	1:B:368(A):LEU:HD13	2.00	0.43
1:D:85:LEU:O	1:D:89:LYS:HB2	2.18	0.43
1:F:143:GLU:HG3	1:F:154:ARG:NH1	2.33	0.43
1:A:39:ILE:HG12	1:A:116:MET:HE2	2.01	0.43
1:C:19:PRO:C	1:C:20:GLN:HG2	2.43	0.43
1:C:184:GLU:HG3	1:C:186:ASN:H	1.83	0.43
1:C:259:PRO:O	1:C:262:TRP:CD1	2.70	0.43
1:C:326:ARG:O	1:C:327:SER:C	2.62	0.43
1:D:393:HIS:CG	1:D:394:PRO:HD2	2.53	0.43
1:A:178:GLN:CD	1:A:219:ARG:CG	2.92	0.43
1:B:71:MET:HE1	1:D:67:LEU:HD21	2.00	0.43
1:B:366:HIS:HA	1:B:370:GLU:OE1	2.19	0.43
1:C:164:ASP:N	1:C:165:GLY:CA	2.82	0.43
1:F:433:ARG:HH11	1:F:442:ARG:HH22	1.66	0.43
1:D:214:ARG:HG3	1:D:230:MET:HE2	2.01	0.43
1:A:219:ARG:HH11	1:A:219:ARG:CG	2.29	0.43
1:B:228:TYR:CD2	1:B:229:LEU:HD23	2.52	0.43
1:B:311:VAL:HG13	1:B:339:ASN:CB	2.49	0.43
1:B:323:SER:C	1:B:331:GLN:NE2	2.77	0.43
1:C:335:TYR:OH	1:E:17:ARG:NH2	2.51	0.43
1:E:331:GLN:HG3	1:E:335:TYR:CE2	2.53	0.43
1:E:442:ARG:CZ	1:F:400:GLU:OE1	2.67	0.43
1:F:53:GLN:NE2	2:F:601:DGT:O3'	2.51	0.43
1:F:489:THR:HB	1:F:492:TYR:H	1.83	0.43
1:A:35:ASP:O	1:A:39:ILE:HD12	2.19	0.43
1:A:215:PRO:HG3	1:A:235:TYR:OH	2.19	0.43
1:E:396:VAL:CG1	2:E:601:DGT:HN2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG13	1:A:23:LYS:N	2.33	0.42
1:A:64:ARG:NE	1:A:275:ALA:HB1	2.33	0.42
1:A:319:SER:OG	1:A:320:ARG:N	2.52	0.42
1:C:161:ARG:HB3	1:C:163:ARG:HH11	1.84	0.42
1:D:212:TYR:HE2	1:D:231:LYS:HB3	1.83	0.42
1:E:259:PRO:O	1:E:262:TRP:HD1	2.02	0.42
1:A:118:ASP:HA	1:A:121:ASN:OD1	2.18	0.42
1:A:166:GLU:HA	1:A:166:GLU:OE1	2.19	0.42
1:B:22:VAL:HB	1:B:23:LYS:H	1.61	0.42
1:C:163:ARG:HG3	1:C:164:ASP:HB2	2.00	0.42
1:B:55:PHE:CE2	1:B:283:LYS:HG3	2.54	0.42
1:B:153:ASP:C	1:B:155:CYS:H	2.26	0.42
1:B:347:TYR:CE2	1:B:375:CYS:HB2	2.55	0.42
1:B:378:LEU:O	1:B:381:LEU:HB3	2.19	0.42
1:D:35:ASP:O	1:D:39:ILE:HD12	2.20	0.42
1:B:447:LEU:O	1:B:448:SER:C	2.62	0.42
1:C:302:HIS:HA	1:C:305:GLY:N	2.32	0.42
1:D:85:LEU:HD13	1:D:103:THR:HG23	2.01	0.42
1:D:229:LEU:HD21	1:D:262:TRP:HH2	1.82	0.42
1:A:400:GLU:OE2	2:A:601:DGT:N1	2.52	0.42
1:B:11:ASN:O	1:B:32:PHE:CZ	2.73	0.42
1:D:488:MET:HG2	1:D:492:TYR:CD2	2.48	0.42
1:E:352:PHE:HB2	1:E:368(A):LEU:HD21	2.01	0.42
1:A:266:ALA:O	1:A:270:ILE:HG13	2.20	0.42
1:D:273:CYS:HB3	1:D:383:LYS:HZ3	1.81	0.42
1:E:393:HIS:CG	1:E:394:PRO:HD2	2.54	0.42
1:F:52:THR:OG1	1:F:56:PRO:HA	2.20	0.42
1:F:117:HIS:C	1:F:119:ILE:H	2.27	0.42
1:B:144:ASP:OD2	1:B:154:ARG:HB2	2.20	0.42
1:B:222:THR:CB	1:B:223:PRO:HD2	2.48	0.42
1:E:93:LEU:HD22	1:E:97:TYR:CZ	2.55	0.42
1:A:184:GLU:HG3	1:A:186:ASN:H	1.85	0.42
1:B:6:PHE:HB3	1:B:10:ILE:HD12	2.01	0.42
1:B:61:ALA:HB2	1:D:50:GLN:HB2	2.02	0.42
1:B:113:SER:HB3	1:B:205:GLN:HE21	1.85	0.42
1:B:382:TYR:O	1:B:384:ASN:N	2.53	0.42
1:B:445:HIS:HD1	1:B:445:HIS:N	2.17	0.42
1:C:51:LYS:HB3	1:C:52:THR:H	1.58	0.42
1:D:92:LYS:O	1:D:92:LYS:HG3	2.20	0.42
1:D:126:HIS:HA	1:D:129:GLU:OE1	2.19	0.42
1:E:46:ARG:O	1:E:48:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:HD2	1:A:140:LEU:HD21	1.85	0.42
1:C:140:LEU:HD13	1:C:177:ARG:HA	2.02	0.42
1:C:153:ASP:CB	1:C:161:ARG:HG2	2.49	0.42
1:D:466:SER:OG	1:D:468:GLU:HG2	2.20	0.42
1:F:123:PRO:HD3	1:F:486:SER:HA	2.01	0.42
1:A:155:CYS:HB3	1:A:161:ARG:HG3	2.02	0.42
1:A:218:TRP:HZ2	1:A:222:THR:CG2	2.32	0.42
1:B:157:VAL:HB	1:B:160:LEU:HB2	2.02	0.42
1:D:52:THR:OG1	1:D:55:PHE:O	2.36	0.42
1:E:258:PHE:CD1	1:E:259:PRO:HD2	2.55	0.42
1:E:489:THR:HG22	1:E:490:ASP:N	2.34	0.42
1:B:91:LEU:HA	1:B:92:LYS:HA	1.81	0.41
1:C:161:ARG:O	1:C:173:ARG:NH1	2.52	0.41
1:C:163:ARG:H	1:C:173:ARG:NH1	2.18	0.41
1:D:53:GLN:HE21	1:D:53:GLN:HB2	1.34	0.41
1:D:259:PRO:O	1:D:262:TRP:HD1	2.03	0.41
1:E:24:THR:HB	1:E:27:GLU:H	1.85	0.41
1:E:482:GLN:O	1:E:486:SER:OG	2.29	0.41
1:F:23:LYS:HA	1:F:27:GLU:OE1	2.20	0.41
1:B:92:LYS:CA	1:B:93:LEU:HB2	2.50	0.41
1:C:163:ARG:HB2	1:C:173:ARG:HH12	1.85	0.41
1:C:346:PRO:O	1:C:347:TYR:C	2.63	0.41
1:D:287:THR:HB	1:D:290:GLN:H	1.85	0.41
1:E:72:GLU:O	1:E:76:VAL:HG23	2.20	0.41
1:A:64:ARG:HG3	1:A:64:ARG:HH11	1.84	0.41
1:A:276:ASP:OD2	2:A:601:DGT:H2'	2.21	0.41
1:C:56:PRO:HA	1:C:57:LEU:HA	1.82	0.41
1:D:53:GLN:NE2	2:D:602:DGT:O3'	2.50	0.41
1:E:14:ARG:HG3	1:E:19:PRO:HD3	2.02	0.41
1:E:163:ARG:HB2	1:E:167:GLU:OE2	2.20	0.41
1:E:371:ASP:HB3	1:E:380:LYS:NZ	2.33	0.41
1:F:217:TRP:HH2	1:F:240:GLU:OE1	2.03	0.41
1:F:319:SER:HA	1:F:331:GLN:HG2	2.02	0.41
1:A:432:GLU:O	1:A:445:HIS:HE1	2.04	0.41
1:B:54:VAL:HG21	2:B:601:DGT:H2'	1.96	0.41
1:B:59:ARG:NE	1:D:491:LEU:HD21	2.36	0.41
1:B:299:TRP:CE3	1:B:299:TRP:HA	2.56	0.41
1:B:324:LEU:HA	1:B:331:GLN:CD	2.45	0.41
1:B:425:PHE:O	1:B:429:VAL:HG23	2.20	0.41
1:C:60:ASN:O	1:C:63:VAL:HG12	2.20	0.41
1:D:262:TRP:CD1	1:D:359:ILE:HG23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LYS:O	1:B:11:ASN:N	2.53	0.41
1:B:146:GLU:OE1	1:B:219:ARG:HG2	2.21	0.41
1:B:163:ARG:HB3	1:B:167:GLU:OE2	2.20	0.41
1:D:73:VAL:HG12	1:D:114:CYS:SG	2.60	0.41
1:D:433:ARG:NH2	1:D:442:ARG:NH2	2.68	0.41
1:E:344:LEU:HD23	1:E:375:CYS:HB3	2.01	0.41
1:E:485:ILE:O	1:E:488:MET:HB2	2.20	0.41
1:F:116:MET:C	1:F:117:HIS:O	2.61	0.41
1:A:203:TRP:CE3	1:A:246:LEU:HD12	2.49	0.41
1:B:54:VAL:HG12	1:B:55:PHE:HD1	1.85	0.41
1:B:379:LEU:C	1:B:383:LYS:HG3	2.45	0.41
1:B:451:HIS:HD2	1:B:483:ASP:HB3	1.85	0.41
1:D:229:LEU:HD22	1:D:257:ARG:HD3	2.02	0.41
1:E:153:ASP:HB3	1:E:161:ARG:HG2	2.01	0.41
1:F:54:VAL:O	1:F:56:PRO:HD3	2.21	0.41
1:B:11:ASN:HD21	1:B:13(C):HIS:CG	2.38	0.41
1:B:230:MET:HE3	1:B:255:TYR:CD1	2.56	0.41
1:C:214:ARG:HE	1:C:218:TRP:HB3	1.86	0.41
1:E:43:PRO:O	1:E:47:ARG:HG3	2.20	0.41
1:E:117:HIS:HB3	1:E:264:MET:HE3	2.03	0.41
1:A:48:LEU:C	1:A:50:GLN:H	2.29	0.41
1:B:469:PHE:HB3	1:B:470:PRO:HD3	2.03	0.41
1:F:100:ASP:OD1	1:F:100:ASP:N	2.53	0.41
1:F:228:TYR:OH	1:F:367:ALA:HB2	2.21	0.41
1:A:162:LEU:HD22	1:A:170:ASN:CG	2.46	0.41
1:A:224:GLU:O	1:A:227:HIS:N	2.48	0.41
1:A:262:TRP:CH2	1:A:364:PHE:O	2.74	0.41
1:B:36:ARG:HE	1:B:36:ARG:HB3	1.77	0.41
1:B:48:LEU:C	1:B:50:GLN:N	2.79	0.41
1:B:100:ASP:OD1	1:B:101:GLU:N	2.54	0.41
1:B:193:VAL:HG12	1:B:199:MET:HE3	2.02	0.41
1:B:426:THR:O	1:B:430:GLU:HG3	2.21	0.41
1:C:53:GLN:NE2	1:C:66:ARG:NH1	2.68	0.41
1:C:468:GLU:HA	1:C:471:LEU:HD13	2.02	0.41
1:D:320:ARG:O	1:D:321:SER:C	2.63	0.41
1:E:118:ASP:HA	1:E:121:ASN:OD1	2.21	0.41
1:F:123:PRO:HB2	1:F:407:ILE:HD11	2.02	0.41
1:B:24:THR:HB	1:B:27:GLU:HG3	2.03	0.41
1:B:39:ILE:HD11	1:B:201:LEU:CD1	2.51	0.41
1:B:351:ARG:HH11	1:B:351:ARG:HD3	1.70	0.41
1:B:471:LEU:HD12	1:B:471:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ARG:CZ	1:D:112:MET:HE3	2.50	0.41
1:D:51:LYS:HE2	1:D:488:MET:O	2.21	0.41
1:D:212:TYR:CE2	1:D:231:LYS:HB3	2.56	0.41
1:B:468:GLU:HB3	1:B:472:TRP:CD1	2.56	0.40
1:C:295:LEU:HD23	1:C:385:VAL:HG21	2.02	0.40
1:E:226:HIS:ND1	1:E:226:HIS:N	2.68	0.40
1:F:272:TYR:HD1	1:F:273:CYS:N	2.20	0.40
1:F:368(A):LEU:C	1:F:369:LEU:HD12	2.46	0.40
1:F:431:LYS:HB2	1:F:431:LYS:HE3	1.93	0.40
1:B:273:CYS:HB2	1:B:382:TYR:HB2	2.04	0.40
1:D:178:GLN:HE21	1:D:178:GLN:HA	1.86	0.40
1:E:299:TRP:CD1	1:E:308:PHE:HB2	2.56	0.40
1:F:73:VAL:HG22	1:F:271:SER:OG	2.21	0.40
1:A:74:GLN:HG3	1:A:111:GLU:O	2.21	0.40
1:B:336:LEU:HD12	1:B:336:LEU:O	2.21	0.40
1:B:422:LEU:HD23	1:B:426:THR:OG1	2.22	0.40
1:D:337:ARG:HG2	1:D:341:LEU:HD13	2.04	0.40
1:A:259:PRO:O	1:A:262:TRP:CD1	2.73	0.40
1:A:299:TRP:NE1	1:A:308:PHE:HB2	2.37	0.40
1:A:304:LYS:O	1:A:305:GLY:C	2.64	0.40
1:C:49:GLN:HG2	1:C:49:GLN:H	1.66	0.40
1:F:306:SER:OG	1:F:307:LEU:N	2.51	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	501/505 (99%)	448 (89%)	33 (7%)	20 (4%)	2	15
1	B	501/505 (99%)	423 (84%)	55 (11%)	23 (5%)	2	13
1	C	501/505 (99%)	444 (89%)	38 (8%)	19 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	486/505 (96%)	442 (91%)	33 (7%)	11 (2%)	5	25
1	E	486/505 (96%)	446 (92%)	31 (6%)	9 (2%)	6	28
1	F	486/505 (96%)	442 (91%)	35 (7%)	9 (2%)	6	28
All	All	2961/3030 (98%)	2645 (89%)	225 (8%)	91 (3%)	3	20

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	23	LYS
1	A	57	LEU
1	A	61	ALA
1	A	92	LYS
1	A	221	GLU
1	A	225	THR
1	A	299	TRP
1	B	94	LEU
1	B	149	PRO
1	B	150	LEU
1	B	323	SER
1	B	326	ARG
1	B	369	LEU
1	B	383	LYS
1	B	450	ARG
1	C	51	LYS
1	C	149	PRO
1	C	152	ASP
1	C	154	ARG
1	C	304	LYS
1	C	322	ASN
1	D	149	PRO
1	D	150	LEU
1	D	201	LEU
1	D	222	THR
1	D	331	GLN
1	E	17	ARG
1	E	149	PRO
1	E	150	LEU
1	F	149	PRO
1	F	150	LEU
1	F	222	THR

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Mol	Chain	Res	Type
1	F	223	PRO
1	A	21	GLY
1	A	146	GLU
1	A	166	GLU
1	A	223	PRO
1	A	325	SER
1	B	22	VAL
1	B	93	LEU
1	B	223	PRO
1	B	372	ALA
1	B	374	GLU
1	C	22	VAL
1	C	92	LYS
1	C	164	ASP
1	C	166	GLU
1	C	223	PRO
1	C	372	ALA
1	D	22	VAL
1	E	22	VAL
1	E	222	THR
1	F	21	GLY
1	F	22	VAL
1	F	167	GLU
1	F	320	ARG
1	F	371	ASP
1	A	147	SER
1	A	302	HIS
1	B	148	GLN
1	B	320	ARG
1	B	324	LEU
1	B	382	TYR
1	B	448	SER
1	C	150	LEU
1	C	224	GLU
1	D	200	ASN
1	A	300	GLY
1	A	372	ALA
1	B	222	THR
1	B	249	GLU
1	B	328	THR
1	B	363	THR
1	C	23	LYS

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Mol	Chain	Res	Type
1	D	118	ASP
1	E	92	LYS
1	A	306	SER
1	A	327	SER
1	B	368(A)	LEU
1	C	56	PRO
1	C	148	GLN
1	C	371	ASP
1	E	223	PRO
1	E	320	ARG
1	D	225	THR
1	E	21	GLY
1	A	149	PRO
1	D	148	GLN
1	D	21	GLY
1	C	21	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/450 (96%)	423 (98%)	8 (2%)	50	68
1	B	431/450 (96%)	428 (99%)	3 (1%)	76	80
1	C	431/450 (96%)	429 (100%)	2 (0%)	81	83
1	D	431/450 (96%)	428 (99%)	3 (1%)	76	80
1	E	431/450 (96%)	423 (98%)	8 (2%)	50	68
1	F	431/450 (96%)	429 (100%)	2 (0%)	81	83
All	All	2586/2700 (96%)	2560 (99%)	26 (1%)	68	76

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	THR
1	A	163	ARG

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Mol	Chain	Res	Type
1	A	164	ASP
1	A	166	GLU
1	A	167	GLU
1	A	219	ARG
1	A	222	THR
1	A	224	GLU
1	B	219	ARG
1	B	224	GLU
1	B	328	THR
1	C	222	THR
1	C	224	GLU
1	D	45	ILE
1	D	53	GLN
1	D	103	THR
1	E	54	VAL
1	E	66	ARG
1	E	103	THR
1	E	219	ARG
1	E	224	GLU
1	E	227	HIS
1	E	272	TYR
1	E	329	GLU
1	F	223	PRO
1	F	224	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	138	GLN
1	A	178	GLN
1	A	194	HIS
1	A	294	HIS
1	A	389	HIS
1	B	11	ASN
1	B	20	GLN
1	B	49	GLN
1	B	74	GLN
1	B	75	GLN
1	B	121	ASN
1	B	186	ASN
1	B	384	ASN

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Mol	Chain	Res	Type
1	B	402	GLN
1	C	53	GLN
1	C	69	HIS
1	C	138	GLN
1	C	178	GLN
1	C	182	HIS
1	C	194	HIS
1	C	402	GLN
1	D	41	ASN
1	D	53	GLN
1	D	186	ASN
1	E	20	GLN
1	E	49	GLN
1	E	194	HIS
1	E	226	HIS
1	F	53	GLN
1	F	186	ASN
1	F	194	HIS
1	F	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 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	$\# Z > 2$
2	DGT	A	601	3	32,33,33	1.75	8 (25%)	48,52,52	2.74	17 (35%)
2	DGT	D	602	-	32,33,33	2.02	9 (28%)	48,52,52	2.54	15 (31%)
2	DGT	F	601	3	32,33,33	3.62	16 (50%)	48,52,52	2.11	9 (18%)
2	DGT	B	601	-	32,33,33	1.86	10 (31%)	48,52,52	2.32	16 (33%)
2	DGT	E	601	-	32,33,33	1.72	8 (25%)	48,52,52	1.95	14 (29%)
2	DGT	C	601	-	32,33,33	3.63	16 (50%)	48,52,52	2.19	11 (22%)

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	A	601	3	-	9/22/34/34	0/3/3/3
2	DGT	D	602	-	-	6/22/34/34	0/3/3/3
2	DGT	F	601	3	-	3/22/34/34	0/3/3/3
2	DGT	B	601	-	-	5/22/34/34	0/3/3/3
2	DGT	E	601	-	-	1/22/34/34	0/3/3/3
2	DGT	C	601	-	-	1/22/34/34	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	DGT	O4'-C4'	9.91	1.67	1.45
2	C	601	DGT	O4'-C4'	9.67	1.66	1.45
2	C	601	DGT	C3'-C4'	-7.25	1.33	1.53
2	F	601	DGT	C3'-C4'	-7.24	1.34	1.53
2	C	601	DGT	C4-N3	6.60	1.49	1.34
2	F	601	DGT	C4-N3	6.28	1.48	1.34
2	C	601	DGT	PA-O3A	5.80	1.65	1.59
2	D	602	DGT	C6-N1	-5.71	1.28	1.38
2	F	601	DGT	PA-O3A	5.63	1.65	1.59
2	F	601	DGT	PB-O3A	5.61	1.65	1.59
2	C	601	DGT	PB-O3A	5.55	1.65	1.59
2	C	601	DGT	C2-N3	5.49	1.46	1.33
2	F	601	DGT	PB-O3B	5.23	1.65	1.59
2	F	601	DGT	C2-N3	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	DGT	C6-N1	-5.17	1.29	1.38
2	C	601	DGT	PB-O3B	5.15	1.65	1.59
2	F	601	DGT	O4'-C1'	-5.07	1.31	1.42
2	C	601	DGT	C2-N2	5.01	1.45	1.34
2	C	601	DGT	O4'-C1'	-4.91	1.31	1.42
2	B	601	DGT	PB-O3A	4.72	1.64	1.59
2	F	601	DGT	C2-N2	4.71	1.45	1.34
2	D	602	DGT	C5-N7	-4.61	1.29	1.39
2	A	601	DGT	C6-N1	-4.08	1.31	1.38
2	A	601	DGT	C2-N1	-3.91	1.28	1.37
2	B	601	DGT	C6-N1	-3.64	1.32	1.38
2	B	601	DGT	C4-N9	-3.46	1.29	1.38
2	D	602	DGT	C2-N1	-3.40	1.29	1.37
2	E	601	DGT	PB-O3A	3.28	1.63	1.59
2	A	601	DGT	C5-N7	-3.26	1.32	1.39
2	D	602	DGT	C8-N9	-3.22	1.30	1.37
2	D	602	DGT	PB-O3B	3.09	1.62	1.59
2	E	601	DGT	C2-N1	-2.94	1.30	1.37
2	A	601	DGT	C4-N9	-2.89	1.30	1.38
2	C	601	DGT	C2-N1	2.89	1.44	1.37
2	F	601	DGT	C2'-C1'	2.88	1.60	1.52
2	E	601	DGT	C4-N9	-2.83	1.30	1.38
2	C	601	DGT	C5-N7	-2.82	1.33	1.39
2	F	601	DGT	C2-N1	2.80	1.44	1.37
2	F	601	DGT	C5-N7	-2.78	1.33	1.39
2	E	601	DGT	C5-C4	2.76	1.46	1.38
2	C	601	DGT	C2'-C1'	2.67	1.59	1.52
2	E	601	DGT	C5-N7	-2.62	1.33	1.39
2	C	601	DGT	C6-N1	2.60	1.43	1.38
2	F	601	DGT	C6-N1	2.59	1.43	1.38
2	A	601	DGT	O4'-C4'	-2.57	1.39	1.45
2	D	602	DGT	PB-O3A	2.53	1.62	1.59
2	C	601	DGT	C5-C6	2.48	1.53	1.44
2	B	601	DGT	O4'-C4'	-2.43	1.39	1.45
2	B	601	DGT	C2-N1	-2.39	1.31	1.37
2	B	601	DGT	C3'-C4'	-2.38	1.46	1.53
2	D	602	DGT	C4-N9	-2.37	1.32	1.38
2	F	601	DGT	C5-C6	2.36	1.53	1.44
2	A	601	DGT	C8-N9	-2.35	1.32	1.37
2	F	601	DGT	C4-N9	-2.34	1.32	1.38
2	C	601	DGT	O6-C6	-2.34	1.19	1.23
2	E	601	DGT	PG-O1G	-2.31	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	DGT	C5-N7	-2.30	1.34	1.39
2	B	601	DGT	O3'-C3'	-2.27	1.38	1.43
2	B	601	DGT	C5-C4	2.25	1.44	1.38
2	A	601	DGT	PB-O3A	-2.22	1.57	1.59
2	D	602	DGT	O4'-C4'	-2.21	1.40	1.45
2	F	601	DGT	O6-C6	-2.20	1.19	1.23
2	D	602	DGT	PA-O1A	-2.17	1.45	1.55
2	A	601	DGT	PB-O1B	-2.12	1.45	1.55
2	E	601	DGT	O4'-C4'	-2.07	1.40	1.45
2	B	601	DGT	C8-N9	-2.07	1.32	1.37
2	C	601	DGT	C4-N9	-2.01	1.33	1.38

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	DGT	C5-C4-N3	-9.00	114.07	128.39
2	F	601	DGT	C1'-N9-C8	7.45	144.62	127.91
2	C	601	DGT	C1'-N9-C8	7.36	144.41	127.91
2	F	601	DGT	C1'-N9-C4	-7.30	105.80	125.50
2	A	601	DGT	C5-C4-N3	-6.95	117.34	128.39
2	C	601	DGT	C1'-N9-C4	-6.93	106.81	125.50
2	A	601	DGT	C2-N3-C4	6.81	124.03	112.30
2	D	602	DGT	C2-N3-C4	6.68	123.81	112.30
2	A	601	DGT	O1B-PB-O3A	-6.68	89.23	107.27
2	B	601	DGT	O1A-PA-O3A	6.24	124.14	107.27
2	D	602	DGT	N9-C4-N3	5.73	137.41	125.95
2	E	601	DGT	C5-C4-N3	-5.70	119.32	128.39
2	B	601	DGT	C5-C4-N3	-5.54	119.57	128.39
2	A	601	DGT	O3A-PA-O2A	-5.46	94.28	110.70
2	B	601	DGT	C2-N3-C4	5.29	121.41	112.30
2	A	601	DGT	N9-C4-N3	5.16	136.26	125.95
2	A	601	DGT	O4'-C1'-N9	-4.97	99.04	107.86
2	C	601	DGT	C5-C4-N3	-4.90	120.58	128.39
2	B	601	DGT	C6-C5-N7	4.79	139.02	130.29
2	C	601	DGT	C2-N3-C4	4.49	120.03	112.30
2	E	601	DGT	O4'-C1'-N9	-4.33	100.17	107.86
2	A	601	DGT	C2'-C1'-N9	4.28	124.53	113.81
2	F	601	DGT	C5-C4-N3	-4.25	121.63	128.39
2	D	602	DGT	O4'-C4'-C3'	-4.11	96.28	105.65
2	B	601	DGT	O2G-PG-O1G	4.07	123.06	107.80
2	E	601	DGT	N9-C4-N3	4.07	134.09	125.95
2	F	601	DGT	C2-N3-C4	3.96	119.11	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	DGT	C6-C5-N7	3.84	137.27	130.29
2	D	602	DGT	O4'-C1'-C2'	-3.65	99.43	106.25
2	A	601	DGT	O2G-PG-O1G	3.63	121.40	107.80
2	B	601	DGT	N9-C4-N3	3.52	132.99	125.95
2	D	602	DGT	O5'-C5'-C4'	3.49	120.88	108.99
2	A	601	DGT	O1B-PB-O2B	3.47	128.56	112.44
2	D	602	DGT	C4'-O4'-C1'	3.43	117.67	109.51
2	E	601	DGT	C6-C5-N7	3.43	136.53	130.29
2	E	601	DGT	C2'-C1'-N9	3.42	122.36	113.81
2	A	601	DGT	C4'-O4'-C1'	3.41	117.62	109.51
2	F	601	DGT	N9-C8-N7	-3.33	107.22	113.40
2	A	601	DGT	C6-C5-C4	-3.30	113.86	118.83
2	A	601	DGT	C5-C6-N1	3.25	121.53	113.25
2	D	602	DGT	C4-C5-N7	-3.23	105.55	110.67
2	C	601	DGT	N9-C8-N7	-3.22	107.43	113.40
2	B	601	DGT	C4-C5-N7	-3.12	105.73	110.67
2	E	601	DGT	C2-N3-C4	3.05	117.56	112.30
2	B	601	DGT	O1G-PG-O3G	-2.98	99.21	110.83
2	D	602	DGT	C2-N1-C6	-2.95	119.76	125.11
2	B	601	DGT	C4'-O4'-C1'	2.93	116.48	109.51
2	E	601	DGT	O2G-PG-O1G	2.91	118.72	107.80
2	C	601	DGT	N9-C4-N3	2.91	131.77	125.95
2	D	602	DGT	C6-C5-N7	2.90	135.57	130.29
2	E	601	DGT	C4-C5-N7	-2.84	106.16	110.67
2	B	601	DGT	O3'-C3'-C4'	-2.83	99.36	110.07
2	F	601	DGT	N9-C4-N3	2.79	131.54	125.95
2	C	601	DGT	C2-N1-C6	-2.73	120.17	125.11
2	E	601	DGT	O1A-PA-O3A	2.69	114.55	107.27
2	F	601	DGT	C2-N1-C6	-2.64	120.33	125.11
2	A	601	DGT	O6-C6-C5	-2.57	119.76	126.53
2	E	601	DGT	O2G-PG-O3B	-2.56	96.04	104.64
2	E	601	DGT	N2-C2-N1	-2.56	111.37	116.76
2	B	601	DGT	O4'-C4'-C3'	-2.53	99.88	105.65
2	F	601	DGT	O6-C6-C5	-2.51	119.90	126.53
2	D	602	DGT	C5-C6-N1	2.51	119.64	113.25
2	B	601	DGT	C2'-C3'-C4'	2.49	107.85	102.80
2	C	601	DGT	C5-C6-N1	2.48	119.56	113.25
2	B	601	DGT	O2G-PG-O3G	2.46	120.41	110.83
2	C	601	DGT	O6-C6-C5	-2.45	120.08	126.53
2	B	601	DGT	C6-C5-C4	-2.38	115.25	118.83
2	F	601	DGT	C5-C6-N1	2.30	119.12	113.25
2	D	602	DGT	C1'-N9-C4	2.30	131.71	125.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	DGT	C8-N7-C5	2.28	108.33	104.26
2	D	602	DGT	C2'-C1'-N9	2.26	119.46	113.81
2	B	601	DGT	N2-C2-N3	-2.21	115.35	119.67
2	A	601	DGT	C2-N1-C6	-2.21	121.10	125.11
2	E	601	DGT	N1-C2-N3	2.20	127.34	123.32
2	D	602	DGT	C1'-N9-C8	-2.20	122.99	127.91
2	C	601	DGT	O4'-C1'-N9	2.19	111.76	107.86
2	A	601	DGT	C2'-C3'-C4'	2.19	107.24	102.80
2	B	601	DGT	N2-C2-N1	2.13	121.27	116.76
2	E	601	DGT	O3B-PB-O2B	-2.12	104.33	110.70
2	D	602	DGT	O1G-PG-O3G	2.04	118.79	110.83
2	A	601	DGT	O5'-C5'-C4'	2.02	115.86	108.99
2	E	601	DGT	C4'-O4'-C1'	2.00	114.27	109.51

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	DGT	PB-O3B-PG-O1G
2	A	601	DGT	C5'-O5'-PA-O3A
2	A	601	DGT	C5'-O5'-PA-O1A
2	A	601	DGT	C4'-C5'-O5'-PA
2	B	601	DGT	C5'-O5'-PA-O3A
2	B	601	DGT	C5'-O5'-PA-O1A
2	B	601	DGT	C5'-O5'-PA-O2A
2	B	601	DGT	C4'-C5'-O5'-PA
2	D	602	DGT	C4'-C5'-O5'-PA
2	D	602	DGT	O4'-C4'-C5'-O5'
2	E	601	DGT	C4'-C5'-O5'-PA
2	A	601	DGT	PB-O3A-PA-O5'
2	D	602	DGT	PA-O3A-PB-O3B
2	C	601	DGT	C4'-C5'-O5'-PA
2	A	601	DGT	C5'-O5'-PA-O2A
2	F	601	DGT	C4'-C5'-O5'-PA
2	A	601	DGT	PB-O3B-PG-O3G
2	A	601	DGT	PB-O3A-PA-O2A
2	D	602	DGT	C3'-C4'-C5'-O5'
2	A	601	DGT	PG-O3B-PB-O1B
2	B	601	DGT	PB-O3A-PA-O2A
2	D	602	DGT	PA-O3A-PB-O2B
2	F	601	DGT	PG-O3B-PB-O2B
2	D	602	DGT	PB-O3A-PA-O2A

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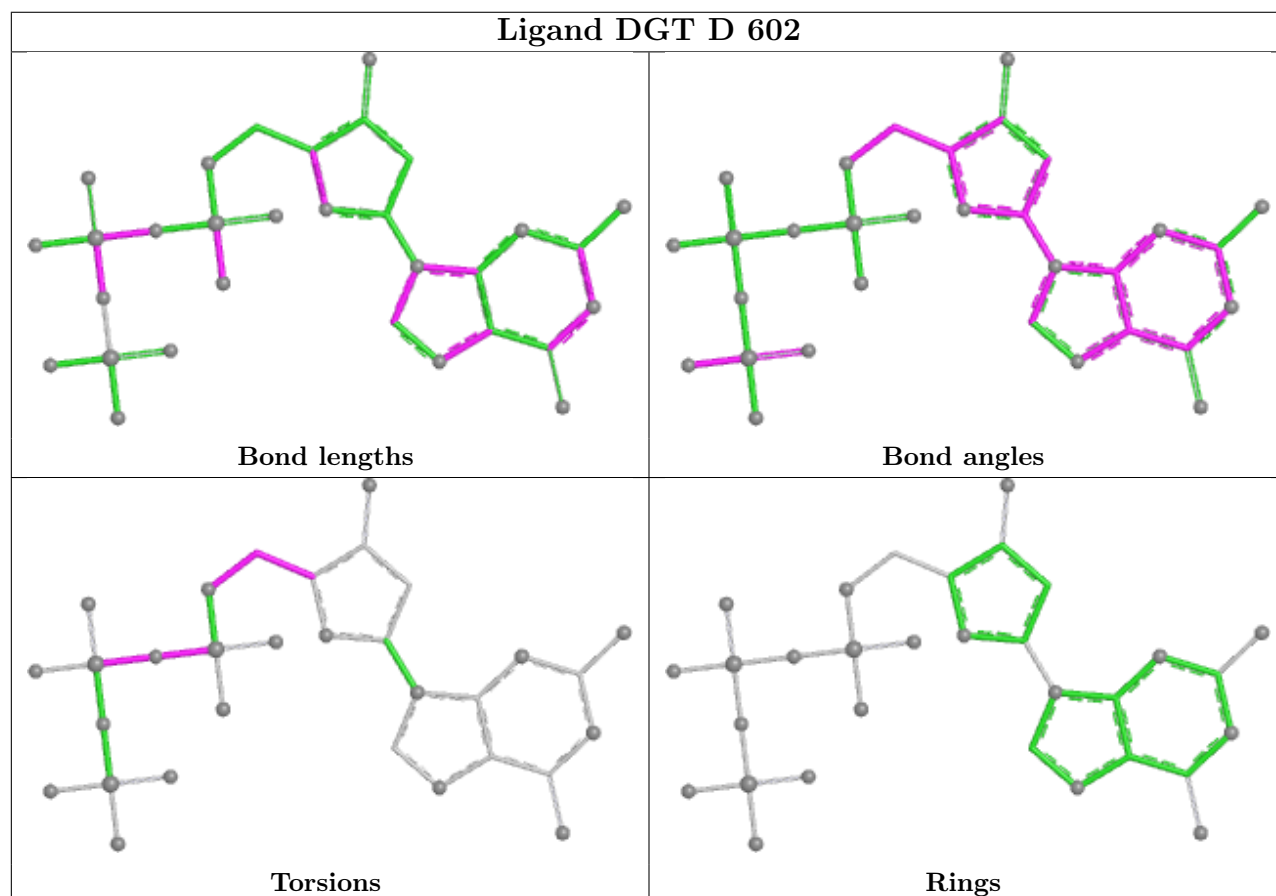
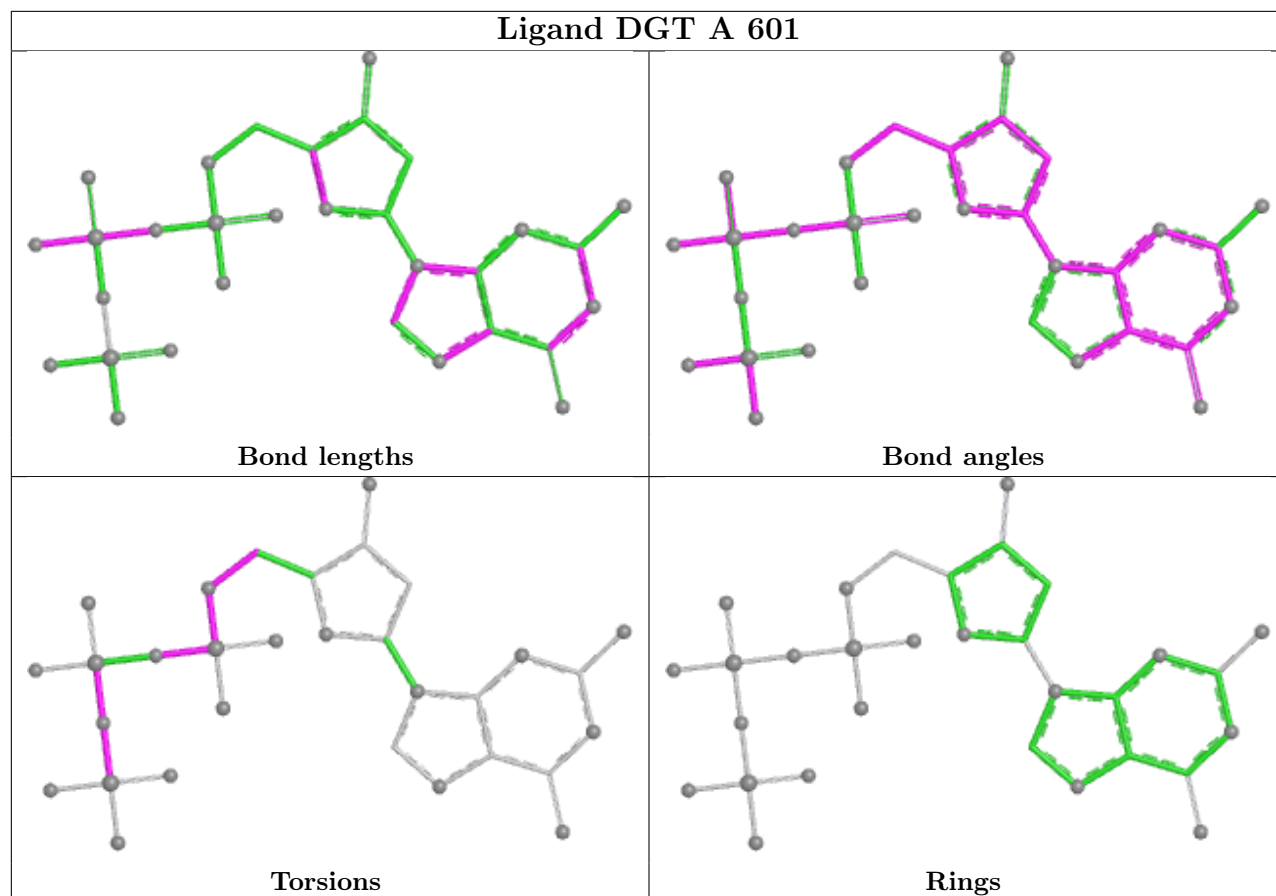
Mol	Chain	Res	Type	Atoms
2	F	601	DGT	PG-O3B-PB-O1B

There are no ring outliers.

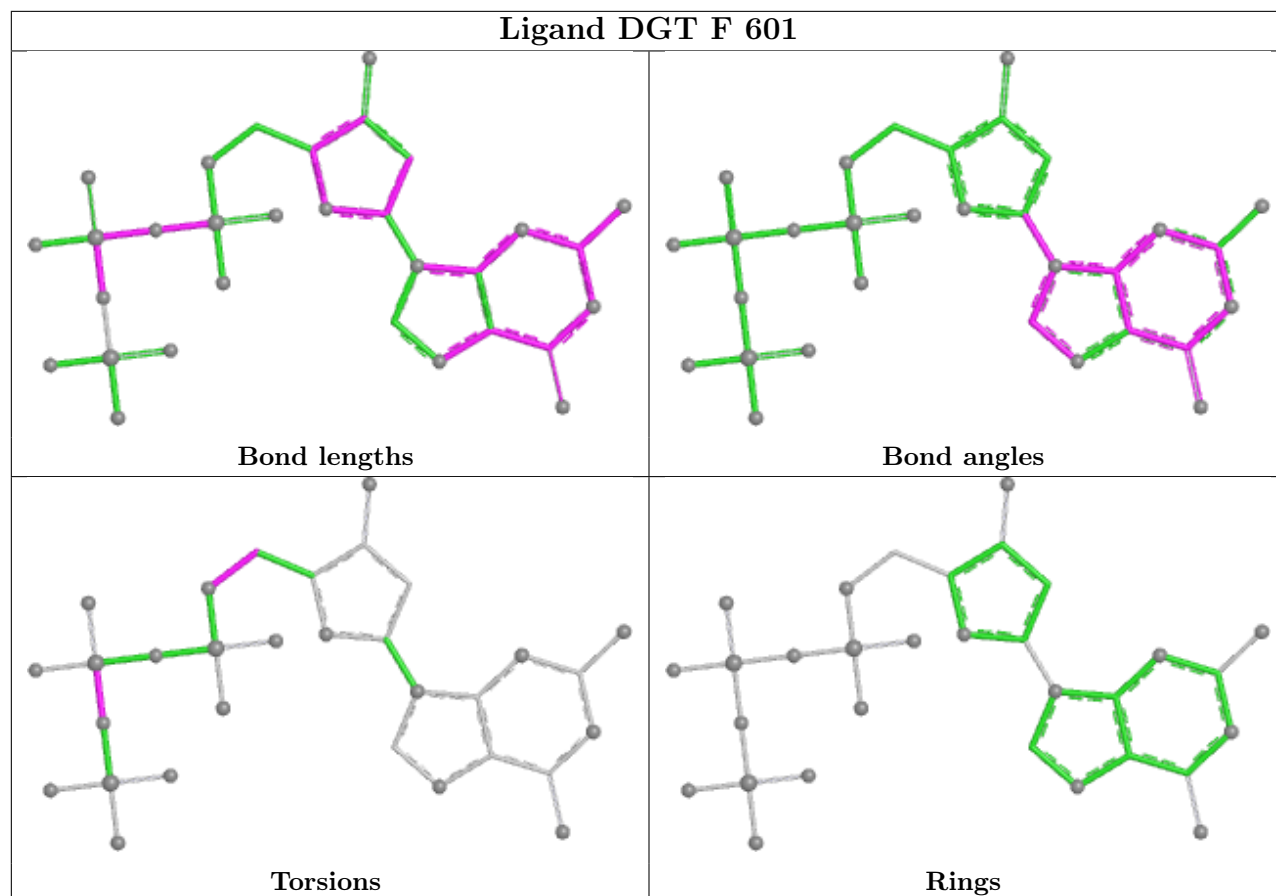
6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	DGT	5	0
2	D	602	DGT	6	0
2	F	601	DGT	4	0
2	B	601	DGT	11	0
2	E	601	DGT	2	0
2	C	601	DGT	3	0

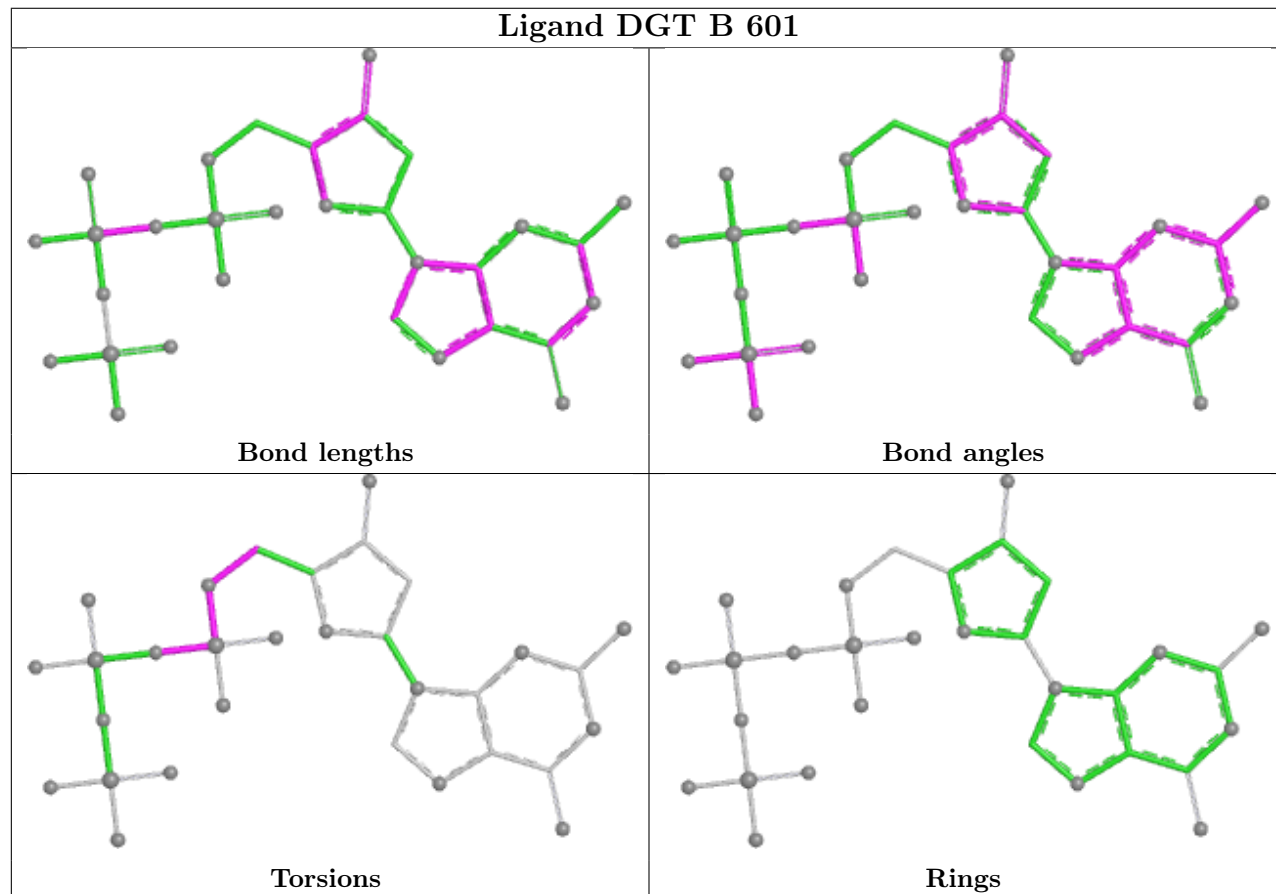
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

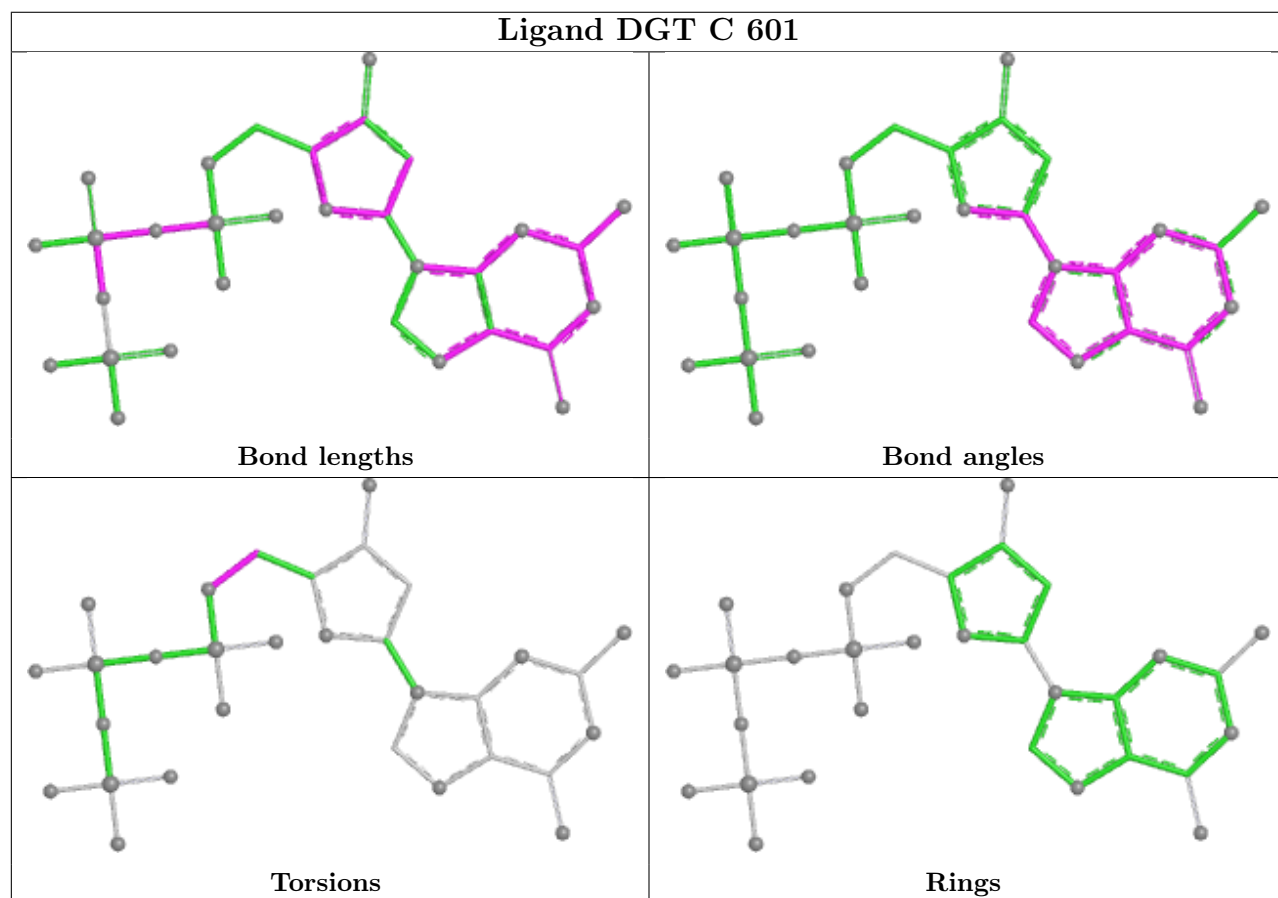
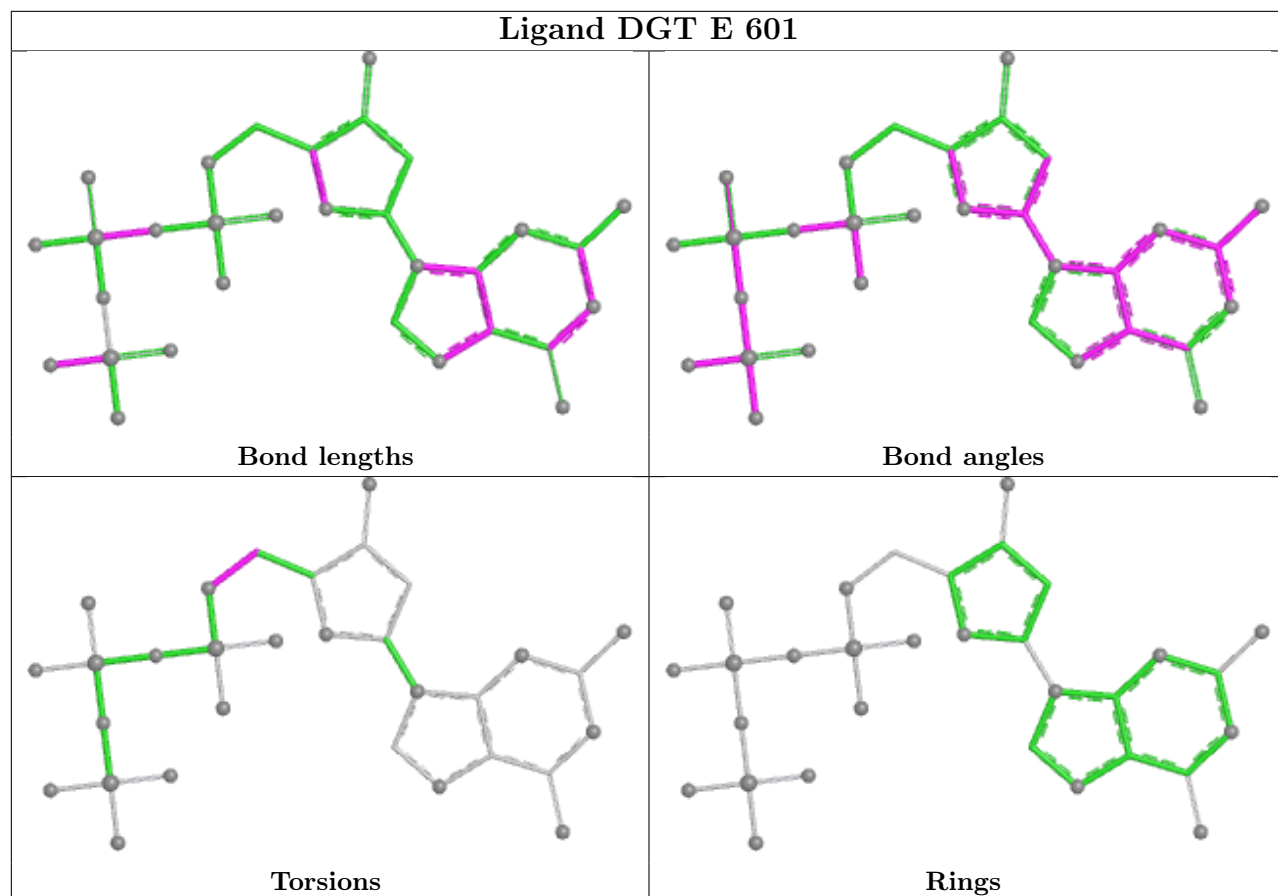


Ligand DGT F 601



Ligand DGT B 601





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	503/505 (99%)	-0.56	4 (0%)	82 68	65, 133, 200, 294	0
1	B	503/505 (99%)	-0.51	3 (0%)	85 73	71, 177, 234, 334	0
1	C	503/505 (99%)	-0.34	6 (1%)	76 58	70, 138, 202, 364	0
1	D	492/505 (97%)	-0.53	4 (0%)	82 68	77, 184, 235, 272	0
1	E	492/505 (97%)	-0.53	3 (0%)	85 73	78, 152, 203, 277	0
1	F	492/505 (97%)	-0.53	1 (0%)	91 86	76, 151, 201, 253	0
All	All	2985/3030 (98%)	-0.50	21 (0%)	84 70	65, 156, 220, 364	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	PHE	2.8
1	D	398	ARG	2.6
1	E	126	HIS	2.6
1	A	325	SER	2.5
1	B	327	SER	2.5
1	F	209	ILE	2.5
1	E	398	ARG	2.4
1	A	324	LEU	2.4
1	C	151	THR	2.3
1	D	126	HIS	2.3
1	D	6	PHE	2.3
1	C	152	ASP	2.3
1	E	416	PRO	2.2
1	C	472	TRP	2.2
1	C	56	PRO	2.2
1	A	398	ARG	2.2
1	B	340	THR	2.2
1	C	327	SER	2.2
1	D	99	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	151	THR	2.1
1	C	471	LEU	2.1

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](#)

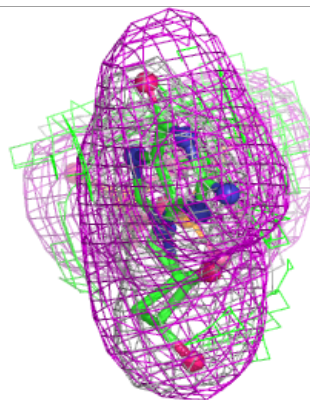
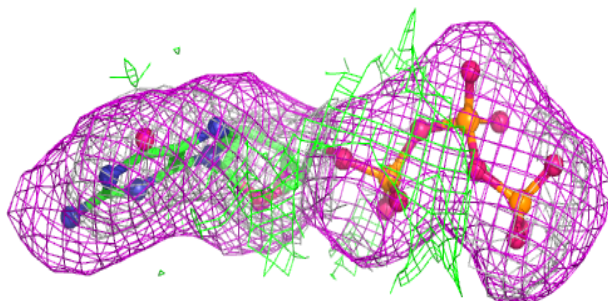
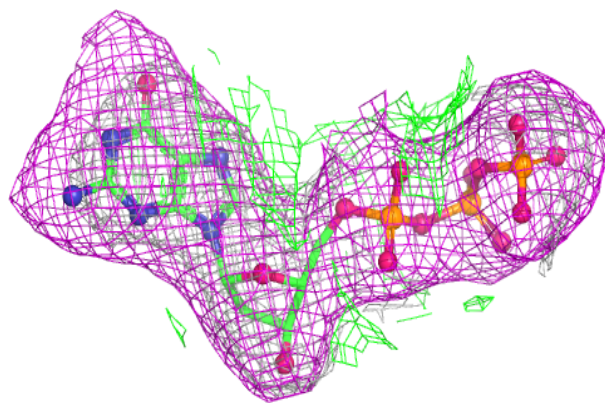
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	602	31/31	0.77	0.14	20,20,20,20	0
3	MN	F	602	1/1	0.78	0.10	206,206,206,206	0
2	DGT	A	601	31/31	0.80	0.09	166,201,225,228	0
3	MN	D	601	1/1	0.81	0.13	194,194,194,194	0
2	DGT	E	601	31/31	0.83	0.09	198,225,241,245	0
3	MN	A	602	1/1	0.86	0.08	138,138,138,138	0
2	DGT	F	601	31/31	0.88	0.06	153,181,241,248	0
2	DGT	B	601	31/31	0.89	0.07	150,200,232,240	0
2	DGT	C	601	31/31	0.89	0.07	178,210,227,237	0
3	MN	B	602	1/1	0.93	0.05	230,230,230,230	0
3	MN	C	602	1/1	0.93	0.06	147,147,147,147	0
3	MN	E	602	1/1	0.94	0.05	175,175,175,175	0

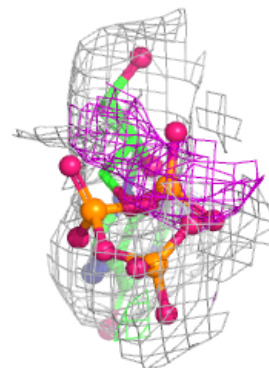
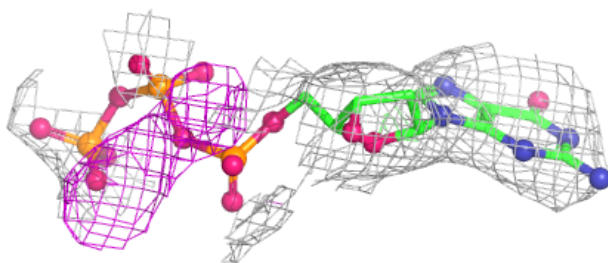
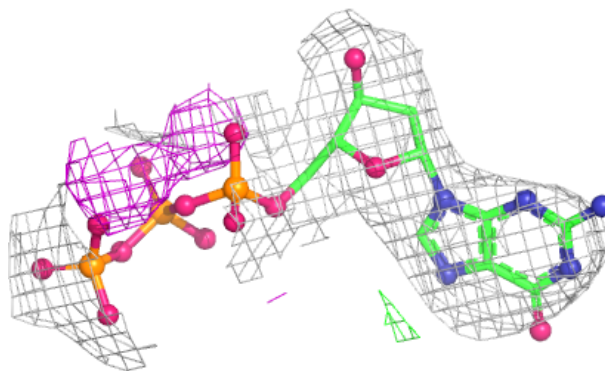
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT D 602:

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

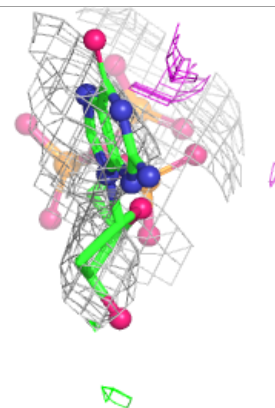
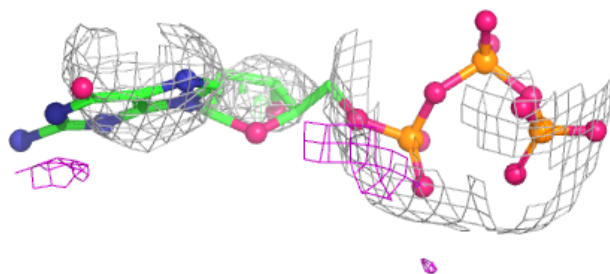
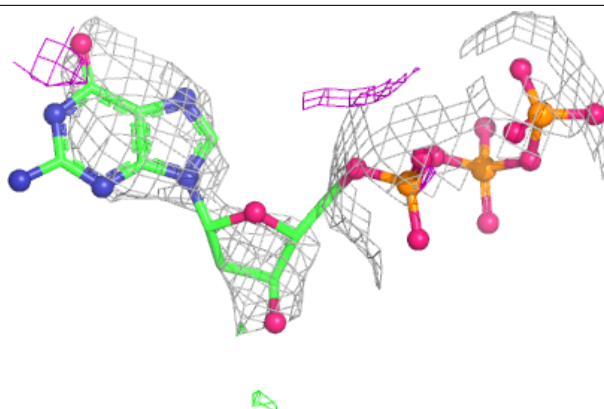
**Electron density around DGT A 601:**

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

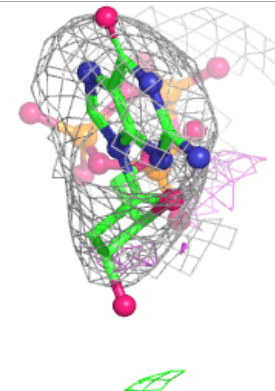
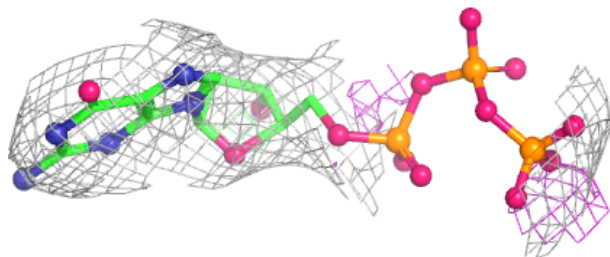
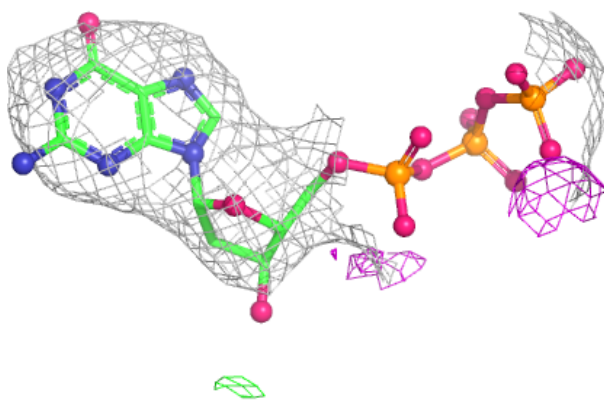


Electron density around DGT E 601:

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

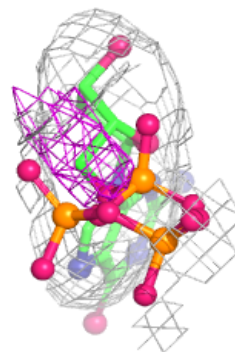
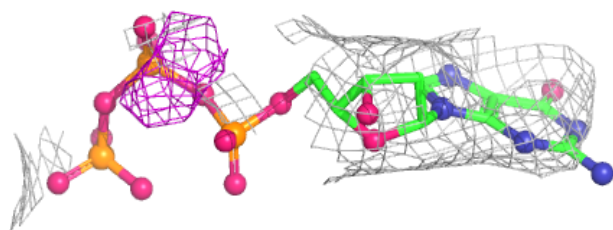
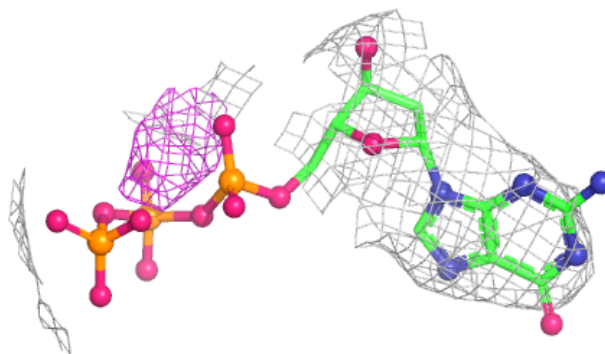
**Electron density around DGT F 601:**

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

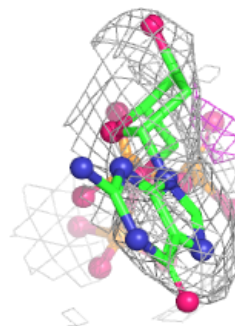
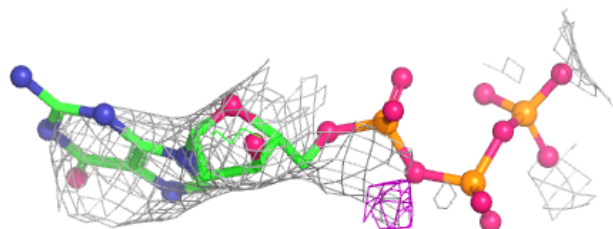
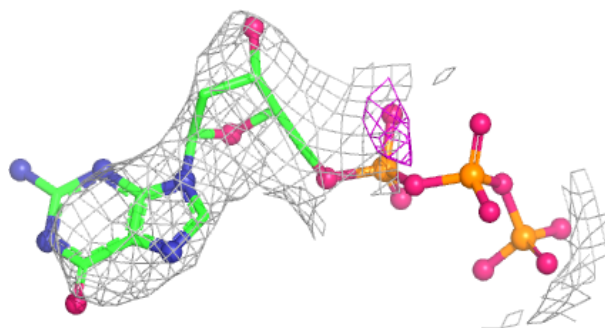


Electron density around DGT B 601:

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

**Electron density around DGT C 601:**

$2mF_o-DF_c$ (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.