



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:28 PM EDT

PDB ID : 6OIW / pdb_00006oiw
Title : Structure of Escherichia coli dGTPase bound to dGTP-1-thiol
Authors : Barnes, C.O.; Wu, Y.; Calero, G.
Deposited on : 2019-04-09
Resolution : 3.35 Å(reported)

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

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

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:

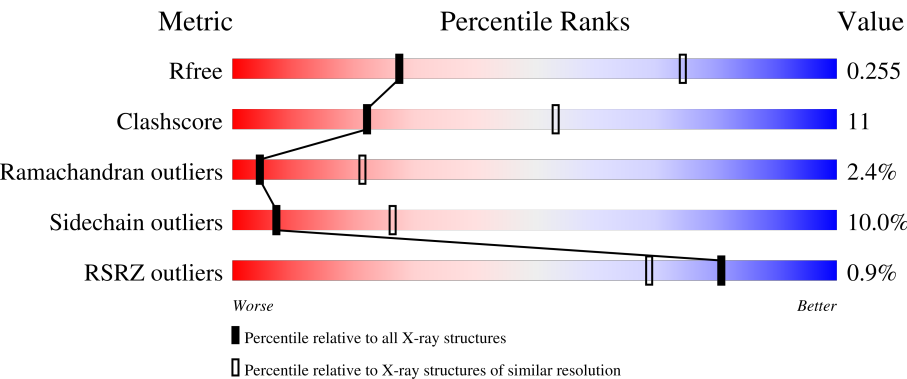
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	% 69% 25% 5% .
1	B	505	% 63% 27% 9% .
1	C	505	70% 24% 5% .
1	D	505	2% 68% 26% 5% .
1	E	505	% 70% 24% 5% .

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Mol	Chain	Length	Quality of chain
1	F	505	70% 24% 6% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25272 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Deoxyguanosinetriphosphate triphosphohydrolase.

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

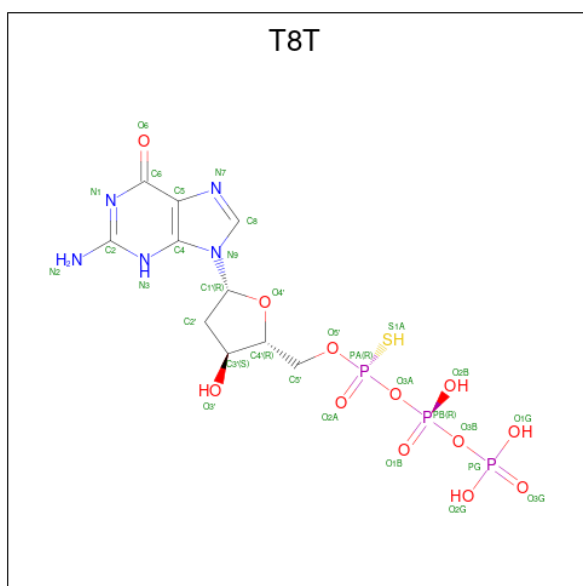
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

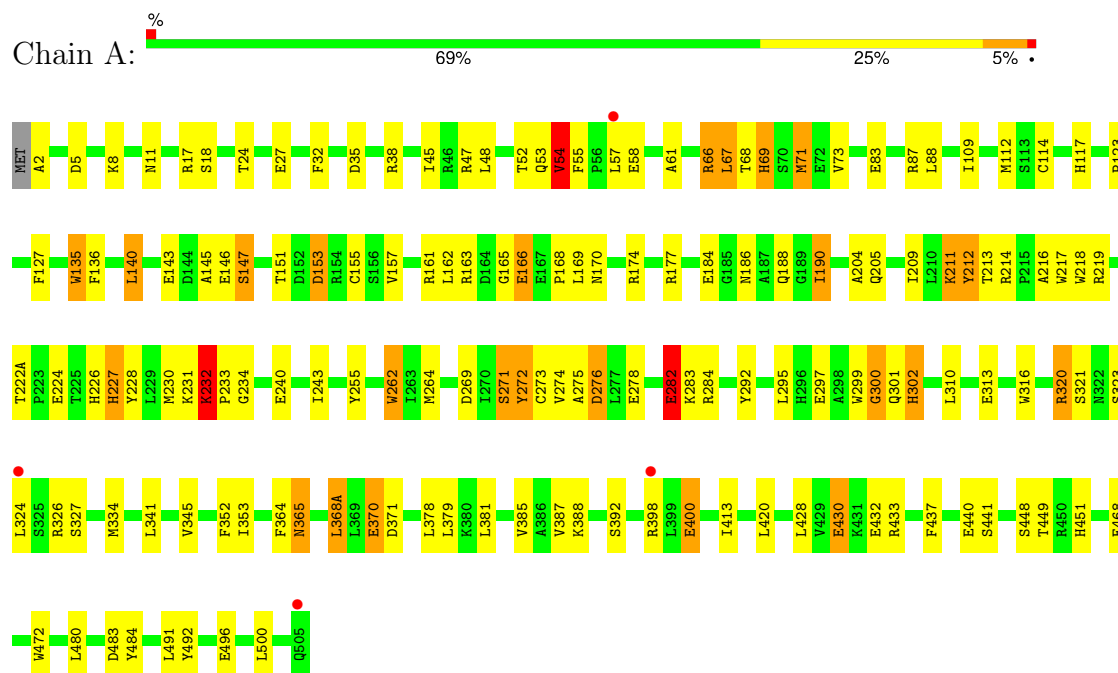
- Molecule 5 is water.

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

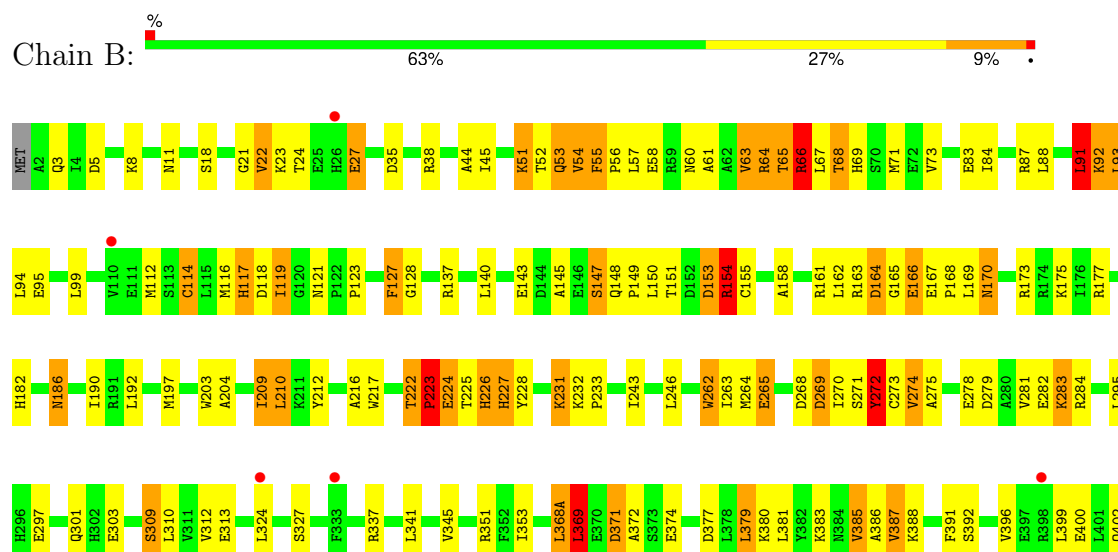
3 Residue-property plots

These plots are drawn for all protein, RNA, 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



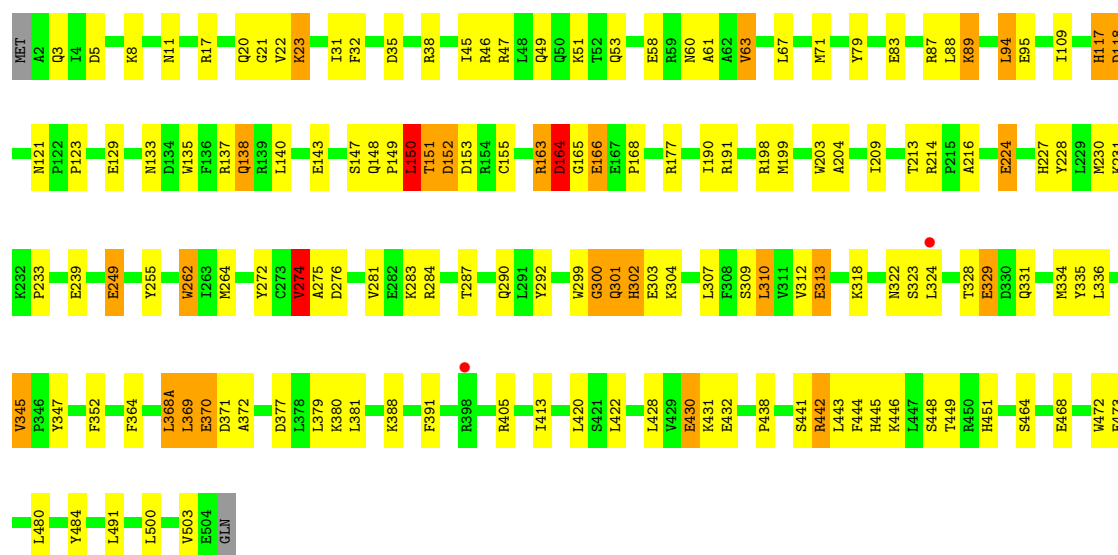
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase





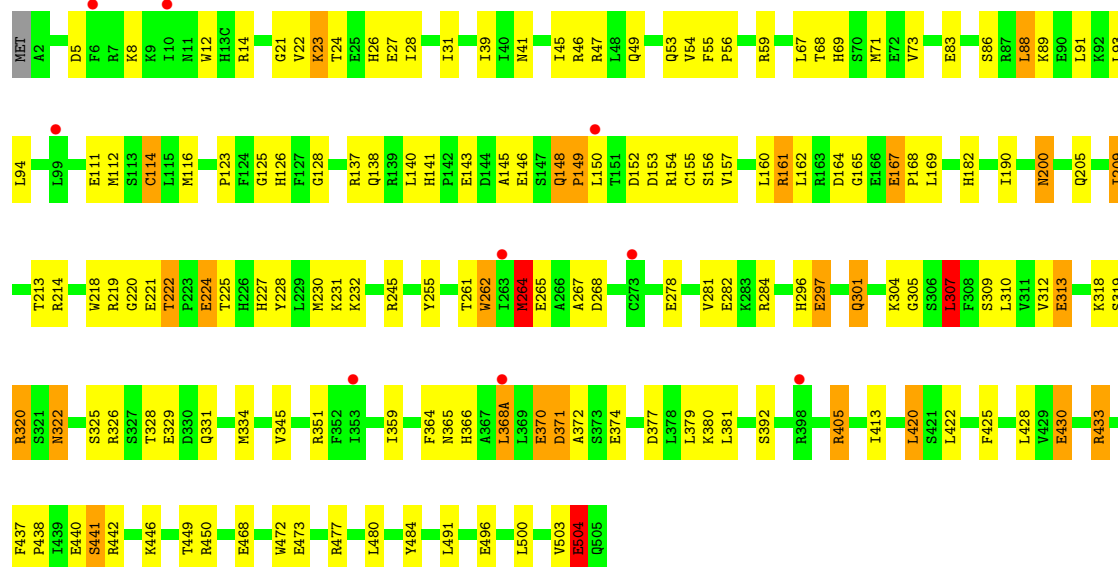
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain C: 70% 24% 5%



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

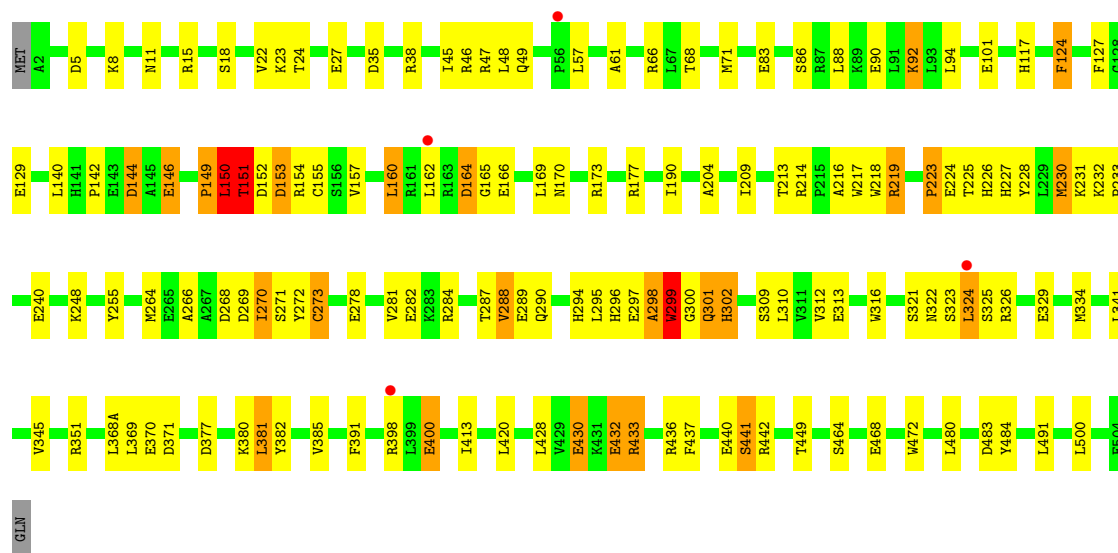
Chain D: 2% 68% 26% 5%



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

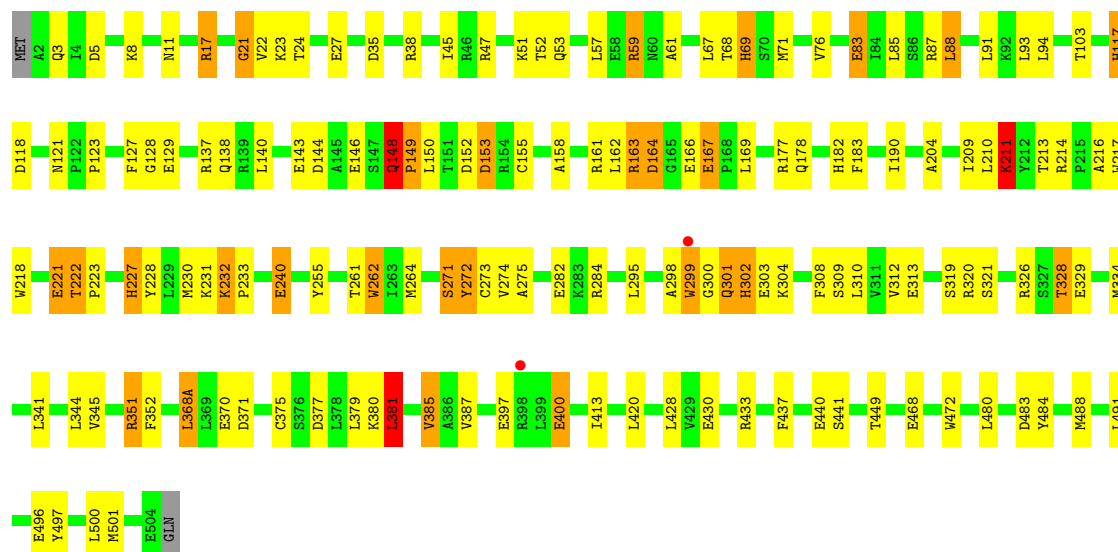
Chain E: 70% 24% 5%





• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain F: 70% 24% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	191.24Å 191.24Å 298.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 3.35 48.48 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.48-3.35) 99.7 (48.48-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.29	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.178 , 0.212 0.233 , 0.255	Depositor DCC
R_{free} test set	2451 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	112.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 122.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25272	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, T8T, 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	1.08	18/4282 (0.4%)	1.53	39/5792 (0.7%)
1	B	0.94	5/4277 (0.1%)	1.59	60/5784 (1.0%)
1	C	0.95	6/4277 (0.1%)	1.53	39/5784 (0.7%)
1	D	0.86	3/4282 (0.1%)	1.53	45/5792 (0.8%)
1	E	0.94	6/4277 (0.1%)	1.51	33/5784 (0.6%)
1	F	0.97	8/4277 (0.2%)	1.53	37/5784 (0.6%)
All	All	0.96	46/25672 (0.2%)	1.53	253/34720 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	THR	C-O	-10.97	1.09	1.24
1	A	232	LYS	C-O	-10.56	1.15	1.24
1	E	232	LYS	C-O	-10.39	1.15	1.24
1	E	230	MET	SD-CE	-9.26	1.56	1.79
1	C	275	ALA	CA-C	-8.61	1.41	1.52
1	F	232	LYS	C-O	-7.63	1.17	1.24
1	A	67	LEU	CA-C	-7.43	1.42	1.52
1	C	272	TYR	CA-C	-7.29	1.43	1.52
1	C	275	ALA	C-O	-7.18	1.15	1.24
1	A	69	HIS	C-O	-6.80	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	LEU	C-O	-6.71	1.15	1.24
1	A	272	TYR	CA-C	-6.23	1.44	1.52
1	B	386	ALA	CA-C	-6.06	1.45	1.52
1	A	112	MET	SD-CE	-5.91	1.64	1.79
1	C	276	ASP	C-O	-5.83	1.16	1.24
1	B	232	LYS	C-O	-5.82	1.18	1.24
1	A	186	ASN	CA-C	-5.80	1.45	1.52
1	E	273	CYS	C-O	-5.80	1.17	1.24
1	C	150	LEU	CA-C	5.72	1.57	1.52
1	A	282	GLU	C-O	-5.69	1.17	1.24
1	E	299	TRP	CA-C	5.58	1.60	1.52
1	F	167	GLU	CA-C	5.56	1.59	1.52
1	B	127	PHE	C-O	-5.53	1.16	1.24
1	A	275	ALA	C-O	-5.51	1.17	1.24
1	F	275	ALA	C-O	-5.50	1.17	1.24
1	A	275	ALA	CA-C	-5.47	1.45	1.52
1	D	149	PRO	CA-C	5.47	1.58	1.53
1	D	222	THR	CA-C	5.46	1.59	1.52
1	A	66	ARG	C-O	-5.38	1.17	1.24
1	F	127	PHE	C-O	-5.31	1.17	1.24
1	B	385	VAL	CA-C	-5.30	1.46	1.52
1	F	69	HIS	C-O	-5.22	1.18	1.24
1	D	268	ASP	C-O	-5.21	1.18	1.24
1	A	272	TYR	N-CA	-5.20	1.39	1.46
1	A	273	CYS	C-O	-5.19	1.18	1.24
1	B	442	ARG	C-O	-5.18	1.18	1.24
1	E	400	GLU	C-O	-5.17	1.18	1.24
1	A	68	THR	CB-OG1	-5.16	1.35	1.43
1	F	400	GLU	C-O	-5.14	1.18	1.24
1	A	400	GLU	C-O	-5.14	1.18	1.24
1	C	274	VAL	C-O	-5.12	1.18	1.24
1	F	275	ALA	CA-C	-5.11	1.46	1.52
1	A	212	TYR	C-O	-5.11	1.17	1.23
1	A	276	ASP	C-O	-5.07	1.17	1.24
1	E	270	ILE	C-O	-5.05	1.18	1.24
1	F	273	CYS	C-O	-5.02	1.18	1.24

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ILE	CA-C-N	12.84	137.88	120.54
1	B	263	ILE	C-N-CA	12.84	137.88	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ARG	N-CA-CB	-12.55	89.28	110.49
1	B	170	ASN	CA-CB-CG	9.88	122.48	112.60
1	B	153	ASP	CA-C-N	-9.70	103.01	121.54
1	B	153	ASP	C-N-CA	-9.70	103.01	121.54
1	C	199	MET	CA-C-N	-9.43	110.16	122.79
1	C	199	MET	C-N-CA	-9.43	110.16	122.79
1	E	153	ASP	CA-CB-CG	9.18	121.78	112.60
1	A	135	TRP	N-CA-C	-9.17	98.42	110.53
1	B	265	GLU	CB-CA-C	-8.99	95.86	110.79
1	E	302	HIS	N-CA-C	-8.89	101.50	114.39
1	B	92	LYS	CA-C-N	8.83	137.59	121.70
1	B	92	LYS	C-N-CA	8.83	137.59	121.70
1	E	150	LEU	CA-C-N	8.71	137.38	121.70
1	E	150	LEU	C-N-CA	8.71	137.38	121.70
1	B	263	ILE	O-C-N	-8.53	113.03	121.90
1	C	322	ASN	CA-C-N	8.40	135.39	122.29
1	C	322	ASN	C-N-CA	8.40	135.39	122.29
1	B	147	SER	O-C-N	8.27	128.51	121.65
1	E	271	SER	N-CA-C	8.16	120.26	111.36
1	F	123	PRO	CA-C-N	-7.99	111.26	123.17
1	F	123	PRO	C-N-CA	-7.99	111.26	123.17
1	C	118	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	123	PRO	CA-C-N	-7.83	111.50	123.17
1	A	123	PRO	C-N-CA	-7.83	111.50	123.17
1	F	117	HIS	N-CA-C	-7.67	98.67	110.10
1	B	123	PRO	CA-C-N	-7.63	110.28	122.95
1	B	123	PRO	C-N-CA	-7.63	110.28	122.95
1	B	275	ALA	N-CA-C	7.59	119.56	111.28
1	C	199	MET	N-CA-C	-7.51	98.33	110.20
1	A	211	LYS	N-CA-C	7.48	119.51	111.36
1	A	324	LEU	N-CA-C	-7.45	103.65	112.89
1	E	142	PRO	CA-C-N	7.41	130.21	120.28
1	E	142	PRO	C-N-CA	7.41	130.21	120.28
1	D	224	GLU	N-CA-C	-7.38	104.13	113.72
1	F	370	GLU	CA-C-N	7.34	135.56	121.54
1	F	370	GLU	C-N-CA	7.34	135.56	121.54
1	C	163	ARG	CA-C-N	7.29	134.81	121.70
1	C	163	ARG	C-N-CA	7.29	134.81	121.70
1	F	210	LEU	CA-C-N	7.27	130.61	120.29
1	F	210	LEU	C-N-CA	7.27	130.61	120.29
1	D	149	PRO	CA-C-N	7.23	134.72	121.70
1	D	149	PRO	C-N-CA	7.23	134.72	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	THR	CA-CB-OG1	-7.14	98.89	109.60
1	B	385	VAL	CB-CA-C	-7.13	102.84	111.97
1	E	149	PRO	CA-C-N	7.08	134.45	121.70
1	E	149	PRO	C-N-CA	7.08	134.45	121.70
1	B	166	GLU	CA-C-N	7.02	134.34	121.70
1	B	166	GLU	C-N-CA	7.02	134.34	121.70
1	C	123	PRO	CA-C-N	-6.99	111.35	122.95
1	C	123	PRO	C-N-CA	-6.99	111.35	122.95
1	E	124	PHE	CA-C-N	6.93	134.18	121.70
1	E	124	PHE	C-N-CA	6.93	134.18	121.70
1	B	51	LYS	N-CA-C	-6.90	95.77	107.99
1	A	135	TRP	CA-C-O	-6.88	113.88	121.87
1	B	91	LEU	CA-C-N	6.87	134.06	121.70
1	B	91	LEU	C-N-CA	6.87	134.06	121.70
1	C	323	SER	N-CA-C	-6.83	103.36	113.61
1	F	211	LYS	N-CA-C	6.83	118.80	111.36
1	B	227	HIS	CA-C-N	6.75	129.61	120.44
1	B	227	HIS	C-N-CA	6.75	129.61	120.44
1	C	307	LEU	N-CA-C	-6.74	104.08	112.90
1	F	221	GLU	N-CA-C	-6.70	104.67	112.92
1	D	504	GLU	CA-C-N	6.52	133.44	121.70
1	D	504	GLU	C-N-CA	6.52	133.44	121.70
1	D	484	TYR	CA-C-N	6.49	128.82	120.70
1	D	484	TYR	C-N-CA	6.49	128.82	120.70
1	D	297	GLU	CB-CG-CD	6.48	123.61	112.60
1	F	387	VAL	CB-CA-C	-6.47	103.41	112.14
1	D	345	VAL	N-CA-CB	6.45	115.48	110.45
1	A	483	ASP	CA-CB-CG	6.45	119.05	112.60
1	F	149	PRO	CA-C-N	6.42	133.25	121.70
1	F	149	PRO	C-N-CA	6.42	133.25	121.70
1	F	163	ARG	CA-C-N	6.40	133.22	121.70
1	F	163	ARG	C-N-CA	6.40	133.22	121.70
1	C	117	HIS	N-CA-C	-6.39	101.66	110.35
1	A	345	VAL	N-CA-CB	6.36	115.41	110.45
1	A	165	GLY	CA-C-N	6.33	133.64	121.54
1	A	165	GLY	C-N-CA	6.33	133.64	121.54
1	B	484	TYR	CA-C-N	6.28	128.55	120.70
1	B	484	TYR	C-N-CA	6.28	128.55	120.70
1	F	169	LEU	CA-C-N	6.27	128.97	120.38
1	F	169	LEU	C-N-CA	6.27	128.97	120.38
1	B	272	TYR	N-CA-C	6.26	118.18	111.36
1	C	168	PRO	CA-C-N	6.26	129.83	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	PRO	C-N-CA	6.26	129.83	120.31
1	B	327	SER	CA-C-N	6.26	128.95	120.38
1	B	327	SER	C-N-CA	6.26	128.95	120.38
1	F	302	HIS	CA-C-N	6.25	133.48	121.54
1	F	302	HIS	C-N-CA	6.25	133.48	121.54
1	C	150	LEU	CA-C-N	6.20	132.86	121.70
1	C	150	LEU	C-N-CA	6.20	132.86	121.70
1	F	21	GLY	CA-C-N	6.20	133.13	121.97
1	F	21	GLY	C-N-CA	6.20	133.13	121.97
1	D	21	GLY	N-CA-C	6.15	117.61	111.21
1	F	484	TYR	CA-C-N	6.13	128.37	120.70
1	F	484	TYR	C-N-CA	6.13	128.37	120.70
1	C	484	TYR	CA-C-N	6.12	128.34	120.70
1	C	484	TYR	C-N-CA	6.12	128.34	120.70
1	A	71	MET	CA-C-N	6.10	128.45	120.28
1	A	71	MET	C-N-CA	6.10	128.45	120.28
1	B	55	PHE	CB-CA-C	-6.10	102.90	109.85
1	E	129	GLU	N-CA-C	-6.09	104.55	111.07
1	A	484	TYR	CA-C-N	6.08	128.31	120.70
1	A	484	TYR	C-N-CA	6.08	128.31	120.70
1	E	484	TYR	CA-C-N	6.05	128.26	120.70
1	E	484	TYR	C-N-CA	6.05	128.26	120.70
1	A	274	VAL	CB-CA-C	-5.97	103.98	112.22
1	E	272	TYR	N-CA-C	5.97	117.79	111.28
1	A	271	SER	N-CA-C	5.94	120.71	112.45
1	F	326	ARG	CA-C-N	5.92	129.79	121.02
1	F	326	ARG	C-N-CA	5.92	129.79	121.02
1	A	18	SER	N-CA-C	5.90	117.33	109.83
1	B	114	CYS	N-CA-C	-5.85	105.80	113.12
1	D	128	GLY	N-CA-C	-5.85	105.41	112.49
1	D	23	LYS	N-CA-C	5.81	116.94	107.23
1	E	324	LEU	CA-C-N	5.81	131.67	122.61
1	E	324	LEU	C-N-CA	5.81	131.67	122.61
1	A	67	LEU	O-C-N	5.79	130.20	122.43
1	D	123	PRO	CA-C-N	-5.79	112.31	122.62
1	D	123	PRO	C-N-CA	-5.79	112.31	122.62
1	E	18	SER	N-CA-C	5.77	116.97	109.64
1	D	372	ALA	CA-C-N	5.74	129.26	120.82
1	D	372	ALA	C-N-CA	5.74	129.26	120.82
1	B	270	ILE	N-CA-C	5.73	116.50	110.72
1	D	89	LYS	CA-C-N	5.70	127.92	120.28
1	D	89	LYS	C-N-CA	5.70	127.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	THR	CA-C-N	5.67	131.21	122.42
1	C	151	THR	C-N-CA	5.67	131.21	122.42
1	A	127	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	68	THR	CB-CA-C	5.66	120.81	110.11
1	B	66	ARG	N-CA-C	-5.65	105.20	111.36
1	B	374	GLU	CA-C-N	5.63	127.76	120.44
1	B	374	GLU	C-N-CA	5.63	127.76	120.44
1	C	303	GLU	CA-C-N	5.62	132.28	121.54
1	C	303	GLU	C-N-CA	5.62	132.28	121.54
1	B	223	PRO	CA-C-N	5.62	132.27	121.54
1	B	223	PRO	C-N-CA	5.62	132.27	121.54
1	B	18	SER	N-CA-C	5.61	116.77	109.64
1	B	387	VAL	N-CA-CB	5.61	118.17	110.54
1	C	345	VAL	N-CA-CB	5.61	114.83	110.45
1	F	271	SER	N-CA-C	5.55	117.41	111.36
1	B	168	PRO	CA-C-N	5.55	129.99	120.72
1	B	168	PRO	C-N-CA	5.55	129.99	120.72
1	B	163	ARG	CA-C-N	5.55	131.68	121.70
1	B	163	ARG	C-N-CA	5.55	131.68	121.70
1	E	345	VAL	N-CA-CB	5.52	114.75	110.45
1	D	262	TRP	CA-C-N	5.52	127.62	120.56
1	D	262	TRP	C-N-CA	5.52	127.62	120.56
1	D	370	GLU	CA-C-N	5.49	132.02	121.54
1	D	370	GLU	C-N-CA	5.49	132.02	121.54
1	A	300	GLY	CA-C-N	5.47	131.55	121.70
1	A	300	GLY	C-N-CA	5.47	131.55	121.70
1	F	345	VAL	N-CA-CB	5.46	114.70	110.45
1	F	381	LEU	CD1-CG-CD2	5.45	122.80	110.80
1	B	21	GLY	CA-C-N	5.45	131.78	121.97
1	B	21	GLY	C-N-CA	5.45	131.78	121.97
1	B	128	GLY	N-CA-C	-5.45	105.89	112.49
1	C	276	ASP	CA-C-N	5.41	129.83	120.58
1	C	276	ASP	C-N-CA	5.41	129.83	120.58
1	D	220	GLY	CA-C-N	5.41	131.87	121.54
1	D	220	GLY	C-N-CA	5.41	131.87	121.54
1	F	52	THR	N-CA-C	5.40	118.27	110.28
1	C	300	GLY	CA-C-N	5.38	131.83	121.54
1	C	300	GLY	C-N-CA	5.38	131.83	121.54
1	C	370	GLU	CB-CG-CD	5.38	121.75	112.60
1	D	365	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	127	PHE	N-CA-C	-5.38	106.56	113.23
1	C	224	GLU	CA-C-N	5.37	130.53	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	GLU	C-N-CA	5.37	130.53	121.14
1	C	324	LEU	N-CA-C	-5.37	106.24	112.89
1	C	129	GLU	CB-CG-CD	5.36	121.71	112.60
1	D	261	THR	CA-C-N	5.36	127.72	120.38
1	D	261	THR	C-N-CA	5.36	127.72	120.38
1	D	224	GLU	CA-C-N	5.35	129.73	120.58
1	D	224	GLU	C-N-CA	5.35	129.73	120.58
1	C	165	GLY	CA-C-N	5.34	131.75	121.54
1	C	165	GLY	C-N-CA	5.34	131.75	121.54
1	E	298	ALA	CA-C-N	5.31	131.69	121.54
1	E	298	ALA	C-N-CA	5.31	131.69	121.54
1	A	2	ALA	CA-C-N	5.31	128.77	120.75
1	A	2	ALA	C-N-CA	5.31	128.77	120.75
1	E	219	ARG	CA-C-N	5.29	125.13	120.10
1	E	219	ARG	C-N-CA	5.29	125.13	120.10
1	F	272	TYR	N-CA-C	5.29	117.13	111.36
1	D	21	GLY	CA-C-N	5.28	128.68	120.34
1	D	21	GLY	C-N-CA	5.28	128.68	120.34
1	F	483	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	321	SER	CA-C-N	5.27	131.18	121.70
1	A	321	SER	C-N-CA	5.27	131.18	121.70
1	B	372	ALA	N-CA-C	-5.27	107.03	112.93
1	D	267	ALA	CA-C-N	5.26	127.28	120.44
1	D	267	ALA	C-N-CA	5.26	127.28	120.44
1	A	297	GLU	CA-C-N	5.25	127.75	120.29
1	A	297	GLU	C-N-CA	5.25	127.75	120.29
1	A	170	ASN	N-CA-C	-5.24	105.74	111.82
1	A	387	VAL	CB-CA-C	-5.24	105.06	112.14
1	D	278	GLU	CA-C-N	5.23	127.29	120.28
1	D	278	GLU	C-N-CA	5.23	127.29	120.28
1	B	226	HIS	CA-C-N	5.22	128.05	120.79
1	B	226	HIS	C-N-CA	5.22	128.05	120.79
1	D	86	SER	CA-C-N	5.22	127.28	120.28
1	D	86	SER	C-N-CA	5.22	127.28	120.28
1	D	245	ARG	CA-C-N	5.22	127.28	120.28
1	D	245	ARG	C-N-CA	5.22	127.28	120.28
1	B	95	GLU	CA-C-N	5.20	127.77	120.28
1	B	95	GLU	C-N-CA	5.20	127.77	120.28
1	D	307	LEU	N-CA-C	-5.20	105.29	111.69
1	D	264	MET	CA-C-N	5.19	127.19	120.44
1	D	264	MET	C-N-CA	5.19	127.19	120.44
1	E	301	GLN	CA-C-N	5.19	129.92	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	301	GLN	C-N-CA	5.19	129.92	121.98
1	C	302	HIS	CA-C-N	5.18	131.03	121.70
1	C	302	HIS	C-N-CA	5.18	131.03	121.70
1	B	442	ARG	CA-C-N	5.18	127.64	120.29
1	B	442	ARG	C-N-CA	5.18	127.64	120.29
1	E	124	PHE	N-CA-C	5.17	121.82	110.80
1	F	328	THR	CA-C-N	5.17	127.21	120.28
1	F	328	THR	C-N-CA	5.17	127.21	120.28
1	B	278	GLU	N-CA-C	-5.16	105.34	110.97
1	B	345	VAL	N-CA-CB	5.15	114.47	110.45
1	A	278	GLU	CA-C-N	5.15	127.18	120.28
1	A	278	GLU	C-N-CA	5.15	127.18	120.28
1	E	483	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	309	SER	CA-C-N	5.14	127.88	120.38
1	B	309	SER	C-N-CA	5.14	127.88	120.38
1	F	144	ASP	CA-CB-CG	5.14	117.74	112.60
1	E	400	GLU	CA-C-N	5.13	127.16	120.28
1	E	400	GLU	C-N-CA	5.13	127.16	120.28
1	F	169	LEU	N-CA-C	-5.10	106.16	112.38
1	C	464	SER	CA-C-N	5.09	127.10	120.28
1	C	464	SER	C-N-CA	5.09	127.10	120.28
1	A	186	ASN	N-CA-C	5.08	116.90	111.36
1	A	188	GLN	CA-C-N	5.08	125.48	119.94
1	A	188	GLN	C-N-CA	5.08	125.48	119.94
1	A	323	SER	N-CA-C	5.08	117.43	108.75
1	B	371	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	168	PRO	CA-C-N	5.06	127.57	120.28
1	D	168	PRO	C-N-CA	5.06	127.57	120.28
1	F	178	GLN	CA-C-N	5.06	127.02	120.44
1	F	178	GLN	C-N-CA	5.06	127.02	120.44
1	F	385	VAL	CB-CA-C	-5.06	105.31	112.14
1	B	441	SER	CA-C-N	5.05	127.05	120.28
1	B	441	SER	C-N-CA	5.05	127.05	120.28
1	A	54	VAL	CB-CA-C	-5.02	103.05	111.29
1	D	268	ASP	N-CA-CB	-5.02	102.73	110.01
1	A	323	SER	CA-C-N	5.01	129.90	121.14
1	A	323	SER	C-N-CA	5.01	129.90	121.14
1	E	278	GLU	CA-C-N	5.00	126.98	120.28
1	E	278	GLU	C-N-CA	5.00	126.98	120.28
1	E	464	SER	CA-C-N	5.00	126.98	120.28
1	E	464	SER	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4179	0	4129	86	0
1	B	4174	0	4129	159	0
1	C	4174	0	4132	76	0
1	D	4179	0	4129	87	0
1	E	4174	0	4132	82	0
1	F	4174	0	4132	76	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	13	7	0
4	B	31	0	13	1	0
4	C	31	0	13	4	0
4	D	31	0	13	2	0
4	E	31	0	13	3	0
4	F	31	0	13	4	0
5	A	5	0	0	1	0
5	B	4	0	0	0	0
5	C	2	0	0	0	0
5	D	5	0	0	0	0
5	E	4	0	0	0	0
5	F	3	0	0	0	0
All	All	25272	0	24861	533	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 11.

All (533) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:O	1:B:155:CYS:N	1.58	1.32
1:A:53:GLN:NE2	4:A:603:T8T:O3'	1.67	1.25
1:C:53:GLN:NE2	4:C:602:T8T:O3'	1.70	1.24
1:B:147:SER:OG	1:B:148:GLN:OE1	1.55	1.22
1:A:58:GLU:CD	1:A:283:LYS:NZ	1.98	1.22
1:F:53:GLN:NE2	4:F:603:T8T:O3'	1.74	1.19
1:C:58:GLU:CD	1:C:283:LYS:NZ	2.05	1.12
1:A:58:GLU:OE1	1:A:283:LYS:NZ	1.82	1.11
1:B:116:MET:CE	1:B:209:ILE:HG21	1.82	1.10
1:B:52:THR:HG21	1:B:57:LEU:H	1.17	1.09
1:B:147:SER:CB	1:B:148:GLN:OE1	2.01	1.08
1:B:54:VAL:HG23	1:B:55:PHE:HD1	1.13	1.08
1:A:58:GLU:CD	1:A:283:LYS:HZ1	1.55	1.08
1:B:92:LYS:H	1:B:93:LEU:HB2	1.01	1.08
1:B:55:PHE:HE2	1:B:283:LYS:HD3	1.18	1.06
1:B:55:PHE:CE2	1:B:283:LYS:HD3	1.92	1.05
1:B:400:GLU:OE1	1:C:442:ARG:NH2	1.91	1.02
1:A:232:LYS:NZ	4:A:603:T8T:O1G	1.94	0.98
1:B:92:LYS:N	1:B:93:LEU:HB2	1.78	0.98
1:B:54:VAL:HG23	1:B:55:PHE:CD1	1.98	0.98
1:A:67:LEU:HD21	1:F:71:MET:HE1	1.45	0.95
1:C:58:GLU:OE1	1:C:283:LYS:NZ	1.98	0.94
1:A:400:GLU:OE1	1:B:442:ARG:NH2	2.02	0.93
1:A:53:GLN:NE2	4:A:603:T8T:HO3'	1.52	0.93
1:C:58:GLU:CD	1:C:283:LYS:HZ2	1.69	0.93
1:B:52:THR:HG21	1:B:57:LEU:N	1.82	0.92
4:E:603:T8T:S1A	4:E:603:T8T:O3G	2.29	0.91
1:F:299:TRP:CD1	1:F:308:PHE:HB2	2.06	0.91
1:B:55:PHE:CE2	1:B:283:LYS:CD	2.52	0.91
1:A:71:MET:HE1	1:F:67:LEU:HD21	1.54	0.89
1:B:55:PHE:HE2	1:B:283:LYS:CD	1.86	0.89
1:B:153:ASP:OD2	1:B:162:LEU:N	2.07	0.87
4:C:602:T8T:O2G	4:C:602:T8T:O2B	1.85	0.87
1:A:58:GLU:CD	1:A:283:LYS:HZ3	1.72	0.87
1:B:148:GLN:OE1	1:B:148:GLN:N	2.07	0.87
1:E:299:TRP:HB3	1:E:300:GLY:CA	2.05	0.87
1:B:67:LEU:HD21	1:D:71:MET:HE1	1.55	0.86
1:A:58:GLU:OE2	1:A:283:LYS:NZ	2.04	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:SER:OG	1:B:148:GLN:CD	2.19	0.85
1:C:198:ARG:HG3	1:E:325:SER:HB3	1.55	0.85
1:E:117:HIS:NE2	1:E:268:ASP:OD1	2.09	0.85
1:F:149:PRO:HA	1:F:150:LEU:HB2	1.58	0.85
1:E:298:ALA:HB3	1:E:381:LEU:HD12	1.58	0.85
1:B:116:MET:HE2	1:B:209:ILE:HG21	1.56	0.84
1:B:212:TYR:OH	1:B:231:LYS:NZ	2.10	0.84
4:A:603:T8T:H5'	4:A:603:T8T:H8	1.60	0.83
1:E:226:HIS:CB	1:E:230:MET:HE3	2.07	0.83
1:B:147:SER:HB2	1:B:148:GLN:OE1	1.77	0.83
1:D:351:ARG:NH2	1:D:370:GLU:HB2	1.93	0.83
1:E:299:TRP:HB3	1:E:300:GLY:HA2	1.58	0.83
1:B:73:VAL:HG22	1:B:271:SER:OG	1.80	0.82
1:B:116:MET:HE3	1:B:209:ILE:HG21	1.59	0.82
1:A:55:PHE:CE2	1:A:283:LYS:HG3	2.16	0.81
1:B:52:THR:O	1:B:66:ARG:NH1	2.13	0.81
1:B:54:VAL:CG2	1:B:55:PHE:HD1	1.94	0.80
1:C:299:TRP:HE1	1:C:302:HIS:HB2	1.46	0.80
1:A:67:LEU:HG	1:A:71:MET:HE2	1.63	0.80
1:D:23:LYS:HB2	1:D:28:ILE:HD11	1.64	0.79
1:D:442:ARG:NE	1:E:400:GLU:OE1	2.15	0.79
1:B:69:HIS:O	1:B:73:VAL:HG23	1.83	0.79
1:B:222:THR:HB	1:B:223:PRO:HA	1.64	0.79
1:C:262:TRP:H	1:C:262:TRP:CD1	2.01	0.79
1:F:309:SER:HA	1:F:313:GLU:HB3	1.66	0.78
1:B:153:ASP:O	1:B:154:ARG:C	2.21	0.77
1:E:226:HIS:HB3	1:E:230:MET:HE3	1.66	0.77
1:F:262:TRP:H	1:F:262:TRP:CD1	1.99	0.77
1:A:262:TRP:H	1:A:262:TRP:CD1	1.99	0.76
1:F:211:LYS:NZ	4:F:603:T8T:O2G	2.18	0.76
1:A:53:GLN:OE1	1:A:66:ARG:NH1	2.18	0.76
1:B:153:ASP:C	1:B:155:CYS:N	2.42	0.76
4:E:603:T8T:O1G	4:E:603:T8T:O2B	2.01	0.76
1:B:197:MET:HE2	1:B:197:MET:HA	1.68	0.75
1:F:217:TRP:CH2	1:F:240:GLU:HG2	2.21	0.75
1:F:117:HIS:O	1:F:118:ASP:HB2	1.84	0.75
1:B:265:GLU:O	1:B:269:ASP:OD1	2.02	0.75
1:F:299:TRP:HD1	1:F:308:PHE:HB2	1.53	0.73
1:A:69:HIS:O	1:A:73:VAL:HG23	1.88	0.73
1:E:150:LEU:HA	1:E:151:THR:HB	1.69	0.73
1:D:364:PHE:HE1	1:D:366:HIS:HB2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:TRP:HE3	1:F:300:GLY:H	1.35	0.73
1:C:438:PRO:O	1:C:442:ARG:CD	2.37	0.73
1:B:268:ASP:O	1:B:272:TYR:CD2	2.42	0.73
1:A:292:TYR:OH	1:A:313:GLU:HG2	1.88	0.72
1:B:262:TRP:CD1	1:B:262:TRP:H	2.08	0.72
1:B:65:THR:HG21	1:D:49:GLN:OE1	1.88	0.72
1:B:92:LYS:H	1:B:93:LEU:CB	1.93	0.72
1:B:116:MET:HE2	1:B:209:ILE:CG2	2.20	0.72
1:B:400:GLU:CD	1:C:442:ARG:HH21	1.97	0.71
1:C:53:GLN:NE2	4:C:602:T8T:HO3'	1.89	0.71
1:F:437:PHE:HB3	1:F:440:GLU:HB2	1.73	0.71
1:C:67:LEU:HD21	1:E:71:MET:HE1	1.73	0.70
1:F:221:GLU:C	1:F:223:PRO:HD2	2.17	0.70
1:B:309:SER:HA	1:B:313:GLU:HB3	1.74	0.70
1:C:118:ASP:HA	1:C:121:ASN:HD22	1.56	0.70
1:E:226:HIS:HB2	1:E:230:MET:HE3	1.70	0.70
1:C:203:TRP:CD1	1:C:249:GLU:HG2	2.26	0.69
1:A:398:ARG:HH11	1:B:499:ARG:HH11	1.40	0.69
1:B:216:ALA:HA	1:B:233:PRO:HB3	1.73	0.69
1:C:428:LEU:HD11	1:C:441:SER:HA	1.75	0.69
1:A:269:ASP:OD2	5:A:701:HOH:O	2.10	0.68
1:B:71:MET:HE1	1:D:67:LEU:HD21	1.75	0.68
1:B:116:MET:CE	1:B:209:ILE:CG2	2.67	0.68
1:A:109:ILE:HA	1:A:205:GLN:HE22	1.58	0.68
1:C:224:GLU:HA	1:C:227:HIS:CD2	2.29	0.68
1:D:503:VAL:O	1:D:504:GLU:HB2	1.93	0.67
1:E:299:TRP:CB	1:E:300:GLY:HA2	2.24	0.67
1:C:443:LEU:O	1:C:446:LYS:N	2.28	0.67
1:F:217:TRP:HH2	1:F:240:GLU:HG2	1.60	0.67
1:B:150:LEU:N	1:B:150:LEU:HD12	2.10	0.67
1:E:164:ASP:H	1:E:165:GLY:HA3	1.59	0.66
1:E:309:SER:HA	1:E:313:GLU:HB3	1.76	0.66
1:B:55:PHE:CE2	1:B:283:LYS:CG	2.79	0.66
1:A:168:PRO:HD2	1:A:169:LEU:HD23	1.78	0.66
1:D:91:LEU:HB3	1:D:93:LEU:HD13	1.76	0.66
1:C:287:THR:HG23	1:C:290:GLN:H	1.61	0.65
1:D:164:ASP:N	1:D:165:GLY:HA3	2.11	0.65
1:F:309:SER:HA	1:F:313:GLU:CB	2.26	0.65
1:C:438:PRO:O	1:C:442:ARG:HD3	1.96	0.65
1:F:381:LEU:O	1:F:385:VAL:HG23	1.95	0.65
1:B:55:PHE:CD2	1:B:283:LYS:CD	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLN:HG3	1:B:54:VAL:HG13	1.80	0.64
1:B:186:ASN:HD22	1:B:186:ASN:H	1.45	0.64
1:B:145:ALA:HA	1:B:162:LEU:HD11	1.78	0.64
1:E:433:ARG:NH2	1:F:397:GLU:OE2	2.30	0.64
1:B:69:HIS:NE2	1:B:272:TYR:HB3	2.13	0.64
1:B:149:PRO:HB3	1:B:162:LEU:O	1.98	0.64
1:A:226:HIS:HA	1:A:365:ASN:HD21	1.62	0.64
1:B:118:ASP:HA	1:B:121:ASN:HD22	1.63	0.63
1:D:364:PHE:CE1	1:D:366:HIS:HB2	2.34	0.63
1:C:58:GLU:HG2	1:C:63:VAL:HG11	1.81	0.63
1:C:443:LEU:O	1:C:444:PHE:C	2.42	0.63
1:B:153:ASP:HB3	1:B:177:ARG:HH22	1.63	0.62
1:B:170:ASN:HB3	1:B:173:ARG:HH11	1.65	0.62
1:C:299:TRP:NE1	1:C:302:HIS:HB2	2.13	0.62
1:B:186:ASN:H	1:B:186:ASN:ND2	1.97	0.62
1:B:496:GLU:HG2	1:B:499:ARG:NH2	2.13	0.62
1:C:58:GLU:HG3	1:C:60:ASN:H	1.64	0.62
1:E:127:PHE:CE2	1:E:400:GLU:HG2	2.34	0.62
1:A:370:GLU:HG3	1:A:371:ASP:HB2	1.82	0.62
1:C:331:GLN:HG3	1:C:335:TYR:CE2	2.34	0.61
1:C:117:HIS:O	1:C:118:ASP:HB2	1.99	0.61
1:B:150:LEU:HD12	1:B:150:LEU:H	1.65	0.61
1:B:438:PRO:O	1:B:442:ARG:HD2	2.01	0.61
1:B:150:LEU:H	1:B:150:LEU:CD1	2.14	0.60
1:F:351:ARG:HD2	1:F:368(A):LEU:O	2.01	0.60
1:B:55:PHE:CE2	1:B:283:LYS:HG3	2.36	0.60
1:E:226:HIS:CB	1:E:230:MET:CE	2.79	0.60
1:B:127:PHE:CE2	1:B:400:GLU:HB3	2.37	0.60
1:E:287:THR:HG23	1:E:290:GLN:H	1.67	0.60
1:E:351:ARG:NH2	1:E:370:GLU:HB2	2.16	0.60
1:C:438:PRO:O	1:C:442:ARG:HD2	2.01	0.60
1:E:149:PRO:HB3	1:E:162:LEU:HB3	1.84	0.60
1:D:157:VAL:HG11	1:D:160:LEU:HD23	1.84	0.60
1:B:88:LEU:HD13	1:B:353:ILE:HG12	1.84	0.59
1:C:309:SER:HA	1:C:313:GLU:HB2	1.82	0.59
1:C:287:THR:HG22	1:C:290:GLN:HE21	1.67	0.59
1:B:368(A):LEU:O	1:B:369:LEU:HB2	2.01	0.59
1:A:428:LEU:HD11	1:A:441:SER:HA	1.84	0.59
1:B:55:PHE:CD2	1:B:283:LYS:HD2	2.38	0.59
1:A:55:PHE:CD2	1:A:283:LYS:HE2	2.38	0.59
1:A:155:CYS:HB2	1:A:177:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:CYS:HB2	1:E:177:ARG:NH1	2.18	0.59
1:B:438:PRO:HG2	1:B:439:ILE:HD12	1.83	0.58
1:D:359:ILE:HG13	1:D:364:PHE:HD2	1.67	0.58
1:E:150:LEU:CA	1:E:151:THR:HB	2.33	0.58
1:E:216:ALA:HA	1:E:233:PRO:HB3	1.86	0.58
1:F:295:LEU:HD23	1:F:385:VAL:HG21	1.84	0.58
1:F:223:PRO:HB2	1:F:227:HIS:HA	1.84	0.58
1:D:148:GLN:HE21	1:D:149:PRO:HG3	1.69	0.58
1:C:53:GLN:HE21	4:C:602:T8T:HO3'	1.40	0.57
1:B:60:ASN:O	1:B:63:VAL:HG23	2.03	0.57
1:E:226:HIS:HB3	1:E:230:MET:CE	2.33	0.57
1:C:224:GLU:HA	1:C:227:HIS:HD2	1.67	0.57
1:E:428:LEU:HD11	1:E:441:SER:HA	1.86	0.57
1:C:163:ARG:HG2	1:C:164:ASP:HB2	1.87	0.57
1:E:442:ARG:NE	1:F:400:GLU:OE1	2.37	0.57
1:C:155:CYS:HB2	1:C:177:ARG:NH1	2.20	0.57
1:F:158:ALA:HA	1:F:161:ARG:HE	1.70	0.57
1:B:387:VAL:HG13	1:B:388:LYS:HD2	1.86	0.57
1:A:224:GLU:HA	1:A:227:HIS:CD2	2.40	0.56
1:A:398:ARG:NH1	1:B:499:ARG:HH11	2.03	0.56
1:B:351:ARG:NH1	1:B:371:ASP:HB2	2.20	0.56
1:D:433:ARG:NH2	1:D:442:ARG:HH22	2.03	0.56
1:B:273:CYS:SG	1:B:379:LEU:HD22	2.46	0.56
1:D:167:GLU:HG3	1:D:169:LEU:HB2	1.87	0.56
1:A:48:LEU:HD22	1:A:66:ARG:HB3	1.87	0.55
4:B:602:T8T:S1A	4:B:602:T8T:O1G	2.64	0.55
1:F:428:LEU:HD11	1:F:441:SER:HA	1.88	0.55
1:C:216:ALA:HA	1:C:233:PRO:HB3	1.88	0.55
1:C:292:TYR:OH	1:C:313:GLU:HG2	2.06	0.55
1:B:55:PHE:HE2	1:B:283:LYS:CG	2.17	0.55
1:A:212:TYR:O	1:A:234:GLY:HA3	2.06	0.55
1:B:337:ARG:NE	1:D:41:ASN:OD1	2.40	0.55
1:B:379:LEU:O	1:B:383:LYS:HG3	2.06	0.55
1:A:295:LEU:HD23	1:A:385:VAL:HG21	1.89	0.55
1:B:491:LEU:HD21	1:D:59:ARG:NE	2.21	0.55
1:E:164:ASP:N	1:E:165:GLY:HA3	2.21	0.55
1:F:216:ALA:HA	1:F:233:PRO:HB3	1.87	0.55
1:A:352:PHE:HB2	1:A:368(A):LEU:HD21	1.89	0.55
1:B:222:THR:HB	1:B:223:PRO:CA	2.33	0.54
1:C:352:PHE:HB2	1:C:368(A):LEU:HD21	1.87	0.54
1:D:214:ARG:HH11	1:D:218:TRP:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:OD2	4:A:603:T8T:H2'A	2.07	0.54
1:B:388:LYS:O	1:B:392:SER:OG	2.12	0.54
1:B:391:PHE:N	1:B:391:PHE:CD1	2.72	0.54
1:D:442:ARG:NH2	1:E:400:GLU:OE1	2.40	0.54
1:A:492:TYR:HD1	1:F:59:ARG:HH12	1.55	0.54
1:A:282:GLU:C	1:A:284:ARG:H	2.14	0.54
1:E:287:THR:HG22	1:E:290:GLN:HE21	1.73	0.54
1:D:304:LYS:N	1:D:305:GLY:HA2	2.22	0.54
1:B:61:ALA:HB1	1:D:47:ARG:HA	1.89	0.54
1:A:153:ASP:HB3	1:A:161:ARG:HG2	1.91	0.53
1:A:299:TRP:O	1:A:301:GLN:HA	2.07	0.53
1:D:145:ALA:HA	1:D:162:LEU:HD11	1.89	0.53
1:A:67:LEU:CD2	1:F:71:MET:HE1	2.31	0.53
1:B:54:VAL:CG2	1:B:55:PHE:CD1	2.78	0.53
1:B:210:LEU:HD11	1:B:243:ILE:HD12	1.89	0.53
1:A:146:GLU:HB2	1:A:219:ARG:NH1	2.23	0.53
1:A:213:THR:HB	1:A:255:TYR:HA	1.91	0.53
1:F:155:CYS:HB2	1:F:177:ARG:NH1	2.22	0.53
4:F:603:T8T:O1B	4:F:603:T8T:H5'A	2.08	0.53
1:A:381:LEU:C	1:A:381:LEU:HD12	2.32	0.53
1:A:87:ARG:HG2	1:A:353:ILE:HD13	1.91	0.52
1:B:203:TRP:HE3	1:B:246:LEU:HD12	1.73	0.52
1:A:53:GLN:HG3	1:A:54:VAL:HG23	1.90	0.52
1:D:262:TRP:HB3	1:D:368(A):LEU:HD13	1.90	0.52
1:E:299:TRP:HB3	1:E:300:GLY:C	2.35	0.52
1:A:381:LEU:HD12	1:A:381:LEU:O	2.10	0.52
1:A:400:GLU:OE2	4:A:603:T8T:N2	2.35	0.52
1:D:155:CYS:HB3	1:D:161:ARG:HG3	1.92	0.52
1:C:213:THR:HB	1:C:255:TYR:HA	1.91	0.52
1:D:28:ILE:HA	1:D:31:ILE:HD12	1.92	0.52
1:A:135:TRP:O	1:A:136:PHE:HB2	2.10	0.52
1:B:64:ARG:NH2	1:D:46:ARG:CZ	2.72	0.52
1:C:135:TRP:O	1:C:138:GLN:HG3	2.10	0.51
1:B:405:ARG:HD2	1:C:500:LEU:O	2.10	0.51
4:A:603:T8T:H8	4:A:603:T8T:C5'	2.35	0.51
1:D:24:THR:HB	1:D:27:GLU:HB2	1.93	0.51
1:D:446:LYS:NZ	1:E:398:ARG:HH21	2.09	0.51
1:F:163:ARG:HA	1:F:164:ASP:HB2	1.93	0.51
1:B:69:HIS:HE1	1:B:117:HIS:HE1	1.59	0.51
1:D:309:SER:HA	1:D:313:GLU:HB3	1.91	0.51
1:D:392:SER:HA	1:F:433:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:GLY:O	1:F:129:GLU:C	2.51	0.51
1:F:213:THR:HB	1:F:255:TYR:HA	1.92	0.51
1:A:378:LEU:O	1:A:381:LEU:HB3	2.11	0.51
1:C:377:ASP:HA	1:C:380:LYS:HD2	1.93	0.51
1:B:351:ARG:HH12	1:B:371:ASP:HB2	1.75	0.50
1:B:377:ASP:HA	1:B:380:LYS:HD2	1.94	0.50
1:E:266:ALA:O	1:E:270:ILE:HG13	2.11	0.50
1:E:213:THR:HB	1:E:255:TYR:HA	1.93	0.50
1:E:144:ASP:HB2	1:E:153:ASP:HB2	1.93	0.50
1:B:112:MET:C	1:B:114:CYS:H	2.19	0.50
1:E:298:ALA:HB3	1:E:381:LEU:CD1	2.37	0.50
1:B:65:THR:CG2	1:D:49:GLN:OE1	2.57	0.50
1:B:273:CYS:SG	1:B:274:VAL:N	2.84	0.50
1:B:55:PHE:CD2	1:B:283:LYS:HD3	2.41	0.50
1:C:391:PHE:CD1	1:C:391:PHE:N	2.77	0.50
1:E:309:SER:HA	1:E:313:GLU:CB	2.41	0.50
1:C:413:ILE:HG21	1:C:500:LEU:HD13	1.94	0.50
1:D:428:LEU:HD11	1:D:441:SER:HA	1.93	0.50
1:B:413:ILE:HG21	1:B:500:LEU:HD13	1.94	0.50
1:B:428:LEU:HD11	1:B:441:SER:HA	1.93	0.50
1:B:503:VAL:HG21	1:C:503:VAL:HG12	1.94	0.50
1:E:299:TRP:HB3	1:E:301:GLN:N	2.27	0.50
1:D:5:ASP:HB3	1:D:8:LYS:HD2	1.94	0.49
1:D:54:VAL:HG13	1:D:55:PHE:CD2	2.47	0.49
1:D:150:LEU:HD13	1:D:164:ASP:HB3	1.93	0.49
1:B:52:THR:HG21	1:B:56:PRO:HA	1.94	0.49
1:B:92:LYS:HB3	1:B:93:LEU:HD13	1.95	0.49
1:D:116:MET:HB2	1:D:209:ILE:HG21	1.95	0.49
1:D:137:ARG:HH12	1:D:182:HIS:CE1	2.30	0.49
1:A:5:ASP:HB3	1:A:8:LYS:HD2	1.93	0.49
1:A:216:ALA:HA	1:A:233:PRO:HB3	1.94	0.49
1:C:133:ASN:O	1:C:137:ARG:HB2	2.12	0.49
1:E:5:ASP:HB3	1:E:8:LYS:HD2	1.94	0.49
1:F:68:THR:HA	1:F:71:MET:HE3	1.94	0.49
1:F:352:PHE:HB2	1:F:368(A):LEU:HD21	1.94	0.49
1:F:118:ASP:HA	1:F:121:ASN:HD22	1.77	0.49
1:D:264:MET:HG3	1:D:265:GLU:N	2.27	0.49
1:C:5:ASP:HB3	1:C:8:LYS:HD2	1.95	0.49
1:D:126:HIS:NE2	4:D:602:T8T:S1A	2.80	0.49
1:D:213:THR:HB	1:D:255:TYR:HA	1.94	0.49
1:A:226:HIS:HA	1:A:365:ASN:ND2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:THR:CB	1:B:56:PRO:HA	2.42	0.48
1:B:150:LEU:N	1:B:150:LEU:CD1	2.73	0.48
1:B:439:ILE:HD12	1:B:439:ILE:H	1.78	0.48
1:E:90:GLU:O	1:E:92:LYS:HD2	2.12	0.48
1:F:53:GLN:NE2	4:F:603:T8T:HO3'	2.01	0.48
1:B:11:ASN:H	1:B:204:ALA:HB2	1.78	0.48
1:E:150:LEU:HA	1:E:151:THR:CB	2.41	0.48
1:E:377:ASP:HA	1:E:380:LYS:HD2	1.96	0.48
1:A:145:ALA:HB1	1:A:174:ARG:HG2	1.94	0.48
1:F:87:ARG:O	1:F:91:LEU:HG	2.13	0.48
1:A:47:ARG:HA	1:F:61:ALA:HB1	1.94	0.48
1:B:148:GLN:CD	1:B:148:GLN:H	2.06	0.48
1:B:153:ASP:HB3	1:B:177:ARG:NH2	2.28	0.48
1:B:166:GLU:HA	1:B:167:GLU:HB2	1.96	0.48
1:D:359:ILE:HG13	1:D:364:PHE:CD2	2.47	0.48
1:D:405:ARG:HD2	1:F:500:LEU:O	2.14	0.48
1:D:413:ILE:HG21	1:D:500:LEU:HD13	1.95	0.48
1:B:87:ARG:O	1:B:91:LEU:HG	2.13	0.48
1:D:304:LYS:H	1:D:305:GLY:HA2	1.78	0.48
1:B:158:ALA:HA	1:B:161:ARG:NH1	2.29	0.48
1:D:377:ASP:HA	1:D:380:LYS:HD2	1.95	0.48
1:D:442:ARG:CZ	1:E:400:GLU:OE1	2.62	0.48
1:F:228:TYR:O	1:F:231:LYS:HB2	2.14	0.48
1:A:228:TYR:O	1:A:231:LYS:HB2	2.14	0.47
1:B:5:ASP:HB3	1:B:8:LYS:HD2	1.95	0.47
1:B:56:PRO:O	1:B:58:GLU:N	2.47	0.47
1:B:65:THR:HG21	1:D:49:GLN:CD	2.39	0.47
1:D:24:THR:HB	1:D:27:GLU:H	1.80	0.47
1:E:289:GLU:HG3	1:E:316:TRP:HH2	1.79	0.47
1:B:186:ASN:ND2	1:B:186:ASN:N	2.60	0.47
1:C:262:TRP:CD1	1:C:262:TRP:N	2.78	0.47
1:C:301:GLN:HB3	1:C:302:HIS:HA	1.96	0.47
1:D:307:LEU:HB2	1:D:374:GLU:HG2	1.95	0.47
1:A:24:THR:HB	1:A:27:GLU:H	1.79	0.47
1:D:433:ARG:HH21	1:D:442:ARG:HH22	1.61	0.47
1:F:148:GLN:H	1:F:149:PRO:CD	2.27	0.47
1:B:24:THR:HB	1:B:27:GLU:H	1.79	0.47
1:B:64:ARG:HH22	1:D:46:ARG:CZ	2.28	0.47
1:B:67:LEU:HG	1:B:71:MET:HE2	1.95	0.47
1:B:119:ILE:HD13	1:B:192:LEU:HD22	1.95	0.47
1:D:12:TRP:HZ2	1:D:23:LYS:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:LYS:HZ3	1:E:398:ARG:HH21	1.61	0.47
1:F:24:THR:HB	1:F:27:GLU:H	1.80	0.47
1:A:69:HIS:CE1	1:A:272:TYR:HB3	2.49	0.47
1:C:23:LYS:HD2	1:C:31:ILE:HD11	1.97	0.47
1:C:214:ARG:HG3	1:C:230:MET:HE2	1.97	0.47
1:D:503:VAL:O	1:D:504:GLU:CB	2.62	0.47
1:B:269:ASP:OD1	1:B:269:ASP:N	2.48	0.47
1:D:14:ARG:HB3	1:D:200:ASN:OD1	2.15	0.47
1:C:11:ASN:H	1:C:204:ALA:HB2	1.79	0.46
1:F:413:ILE:HG21	1:F:500:LEU:HD13	1.96	0.46
1:A:35:ASP:HA	1:A:38:ARG:HD2	1.97	0.46
1:C:287:THR:HG22	1:C:290:GLN:NE2	2.30	0.46
1:A:282:GLU:O	1:A:282:GLU:HG3	2.10	0.46
1:B:396:VAL:O	1:B:400:GLU:HG3	2.14	0.46
1:C:274:VAL:HG12	1:C:336:LEU:HD23	1.98	0.46
1:B:210:LEU:HD11	1:B:243:ILE:CD1	2.46	0.46
1:D:39:ILE:HD13	1:D:112:MET:HB3	1.97	0.46
1:E:170:ASN:HA	1:E:173:ARG:HD2	1.98	0.46
1:D:68:THR:HA	1:D:71:MET:HE3	1.96	0.46
1:F:51:LYS:HE2	1:F:488:MET:O	2.16	0.46
1:B:69:HIS:ND1	1:B:69:HIS:C	2.73	0.46
1:C:35:ASP:HA	1:C:38:ARG:HD2	1.97	0.46
1:C:61:ALA:HB1	1:E:47:ARG:HA	1.97	0.46
1:B:400:GLU:OE1	1:C:442:ARG:CZ	2.61	0.46
1:E:413:ILE:HG21	1:E:500:LEU:HD13	1.97	0.46
1:F:377:ASP:HA	1:F:380:LYS:HD2	1.96	0.46
1:D:116:MET:HE1	1:D:205:GLN:HG3	1.97	0.46
1:E:228:TYR:O	1:E:231:LYS:HB2	2.15	0.46
1:C:283:LYS:O	1:C:284:ARG:HB2	2.15	0.46
1:C:422:LEU:CD1	1:C:473:GLU:HG3	2.46	0.46
1:E:226:HIS:HB2	1:E:230:MET:CE	2.44	0.46
1:D:304:LYS:N	1:D:305:GLY:CA	2.79	0.46
1:A:413:ILE:HG21	1:A:500:LEU:HD13	1.97	0.45
1:C:228:TYR:O	1:C:231:LYS:HB2	2.16	0.45
1:F:5:ASP:HB3	1:F:8:LYS:HD2	1.97	0.45
1:F:69:HIS:CE1	1:F:272:TYR:HB3	2.51	0.45
1:B:170:ASN:HA	1:B:173:ARG:HD2	1.97	0.45
1:A:114:CYS:SG	1:A:264:MET:HB2	2.56	0.45
1:E:146:GLU:CD	1:E:219:ARG:HH11	2.24	0.45
1:F:35:ASP:HA	1:F:38:ARG:HD2	1.99	0.45
1:F:222:THR:O	1:F:223:PRO:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD13	1:B:99:LEU:HB3	1.98	0.45
1:C:347:TYR:HD2	1:C:369:LEU:HD23	1.81	0.45
1:B:112:MET:C	1:B:114:CYS:N	2.73	0.45
1:D:301:GLN:HG3	1:D:304:LYS:HD2	1.98	0.45
1:E:127:PHE:CD2	1:E:400:GLU:HG2	2.51	0.45
1:A:370:GLU:HG3	1:A:371:ASP:CB	2.47	0.45
1:B:52:THR:HB	1:B:55:PHE:O	2.17	0.45
1:B:224:GLU:C	1:B:226:HIS:H	2.25	0.45
1:D:422:LEU:CD1	1:D:473:GLU:HG3	2.47	0.45
1:E:24:THR:HB	1:E:27:GLU:H	1.82	0.45
1:E:269:ASP:O	1:E:270:ILE:C	2.59	0.45
1:E:437:PHE:O	1:E:441:SER:HB2	2.17	0.45
1:D:111:GLU:O	1:D:114:CYS:HB2	2.17	0.45
1:B:54:VAL:CG2	1:B:55:PHE:N	2.79	0.44
1:B:164:ASP:H	1:B:165:GLY:C	2.24	0.44
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.89	0.44
1:D:262:TRP:CD1	1:D:359:ILE:HG23	2.52	0.44
1:A:11:ASN:H	1:A:204:ALA:HB2	1.82	0.44
1:A:54:VAL:HB	1:A:55:PHE:CD1	2.52	0.44
1:B:402:GLN:O	1:B:403:GLY:C	2.57	0.44
1:A:145:ALA:HB3	1:A:219:ARG:NH2	2.32	0.44
1:C:150:LEU:HB2	1:C:152:ASP:N	2.32	0.44
1:C:163:ARG:HA	1:C:164:ASP:HB2	1.99	0.44
1:A:299:TRP:NE1	1:A:302:HIS:HD2	2.16	0.44
1:B:56:PRO:C	1:B:58:GLU:N	2.73	0.44
1:D:14:ARG:HD3	1:D:200:ASN:ND2	2.31	0.44
1:A:388:LYS:O	1:A:392:SER:OG	2.20	0.44
1:D:446:LYS:NZ	1:E:398:ARG:HE	2.16	0.44
1:E:282:GLU:C	1:E:284:ARG:H	2.26	0.44
1:A:316:TRP:CZ2	1:A:320:ARG:HD2	2.53	0.44
1:B:44:ALA:CB	1:B:119:ILE:HD11	2.47	0.44
1:B:68:THR:HA	1:B:71:MET:HE3	2.00	0.44
1:B:35:ASP:HA	1:B:38:ARG:HD2	1.99	0.44
1:B:69:HIS:O	1:B:69:HIS:CG	2.70	0.44
1:D:228:TYR:O	1:D:231:LYS:HB2	2.18	0.44
1:F:183:PHE:CD1	1:F:183:PHE:C	2.95	0.44
1:F:282:GLU:C	1:F:284:ARG:H	2.25	0.44
1:D:146:GLU:HG2	1:D:219:ARG:HE	1.83	0.44
1:F:214:ARG:HG3	1:F:230:MET:HE2	2.00	0.44
1:B:150:LEU:HA	1:B:151:THR:HA	1.59	0.43
1:B:222:THR:CB	1:B:223:PRO:HA	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:PHE:CE2	1:B:477:ARG:HG3	2.53	0.43
1:C:443:LEU:O	1:C:445:HIS:N	2.50	0.43
1:E:230:MET:HE2	1:E:255:TYR:HB3	1.99	0.43
1:B:53:GLN:HB2	1:B:66:ARG:HD3	1.99	0.43
1:D:12:TRP:CZ2	1:D:23:LYS:HD3	2.53	0.43
1:E:442:ARG:HG2	1:F:397:GLU:HB3	2.00	0.43
1:B:268:ASP:O	1:B:272:TYR:HD2	1.95	0.43
1:B:468:GLU:HB3	1:B:472:TRP:CD1	2.53	0.43
1:C:150:LEU:HB2	1:C:151:THR:C	2.43	0.43
1:A:190:ILE:HG21	1:A:243:ILE:HD11	1.99	0.43
1:B:64:ARG:HH22	1:D:46:ARG:NH2	2.16	0.43
1:B:84:ILE:O	1:B:88:LEU:HB2	2.18	0.43
1:D:322:ASN:CG	1:D:331:GLN:HE21	2.27	0.43
1:A:300:GLY:HA2	1:A:301:GLN:HG3	1.99	0.43
1:D:141:HIS:HB2	1:D:154:ARG:O	2.18	0.43
1:F:117:HIS:NE2	1:F:118:ASP:OD2	2.51	0.43
1:E:68:THR:HA	1:E:71:MET:HE3	2.00	0.43
1:B:262:TRP:CD1	1:B:262:TRP:N	2.83	0.43
1:A:437:PHE:HB3	1:A:440:GLU:HB2	2.01	0.43
1:C:318:LYS:HB3	1:C:335:TYR:CE2	2.54	0.43
1:E:437:PHE:HB3	1:E:440:GLU:HB2	2.01	0.43
1:D:153:ASP:HB3	1:D:161:ARG:HG2	2.00	0.43
1:D:318:LYS:C	1:D:320:ARG:H	2.27	0.43
1:E:149:PRO:HA	1:E:150:LEU:CB	2.49	0.43
1:F:301:GLN:CD	1:F:303:GLU:HB3	2.43	0.43
1:A:282:GLU:C	1:A:284:ARG:N	2.77	0.43
1:E:162:LEU:HD22	1:E:170:ASN:HB3	2.01	0.43
1:F:11:ASN:H	1:F:204:ALA:HB2	1.84	0.43
1:E:468:GLU:HB3	1:E:472:TRP:CD1	2.54	0.42
1:A:214:ARG:HE	1:A:218:TRP:HB3	1.84	0.42
1:A:232:LYS:HB2	1:A:233:PRO:CD	2.50	0.42
1:A:448:SER:HB2	1:A:451:HIS:CD2	2.54	0.42
1:B:175:LYS:HE2	1:B:217:TRP:CZ3	2.53	0.42
1:B:399:LEU:HD23	1:B:402:GLN:OE1	2.19	0.42
1:F:262:TRP:CD1	1:F:262:TRP:N	2.77	0.42
1:A:32:PHE:CE1	1:A:109:ILE:HD11	2.54	0.42
1:B:387:VAL:O	1:B:387:VAL:HG22	2.19	0.42
1:F:88:LEU:HD12	1:F:88:LEU:HA	1.90	0.42
1:C:32:PHE:CE1	1:C:109:ILE:HD11	2.55	0.42
1:E:214:ARG:HE	1:E:218:TRP:HB3	1.84	0.42
1:E:288:VAL:HG11	1:E:329:GLU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PHE:CD2	1:B:400:GLU:HB3	2.54	0.42
1:B:437:PHE:HB3	1:B:440:GLU:HB2	2.00	0.42
1:C:422:LEU:HD13	1:C:473:GLU:HG3	2.01	0.42
1:E:223:PRO:HG2	1:E:230:MET:HE1	2.01	0.42
1:C:310:LEU:H	1:C:310:LEU:HG	1.64	0.42
1:E:273:CYS:HB3	1:E:382:TYR:CB	2.50	0.42
1:C:79:TYR:CD2	1:C:345:VAL:HG21	2.55	0.42
1:C:329:GLU:CD	1:C:329:GLU:H	2.27	0.42
1:E:157:VAL:HG11	1:E:160:LEU:HD23	2.01	0.42
4:E:603:T8T:O3G	4:E:603:T8T:PA	2.77	0.42
1:A:140:LEU:HD23	1:A:157:VAL:HG21	2.02	0.41
1:A:217:TRP:HH2	1:A:240:GLU:HG3	1.85	0.41
1:A:316:TRP:CE2	1:A:320:ARG:HD2	2.56	0.41
1:B:272:TYR:CD1	1:B:272:TYR:C	2.98	0.41
1:B:295:LEU:HD23	1:B:385:VAL:HG21	2.02	0.41
1:D:437:PHE:HB3	1:D:440:GLU:HB2	2.01	0.41
1:E:35:ASP:HA	1:E:38:ARG:HD2	2.02	0.41
1:F:91:LEU:C	1:F:93:LEU:H	2.28	0.41
1:A:262:TRP:CH2	1:A:364:PHE:O	2.73	0.41
1:B:60:ASN:HB3	1:B:63:VAL:CG2	2.51	0.41
1:A:54:VAL:HB	1:A:55:PHE:HD1	1.85	0.41
1:B:279:ASP:O	1:B:282:GLU:HB3	2.19	0.41
1:B:415:ARG:N	1:B:416:PRO:HD2	2.35	0.41
1:E:391:PHE:N	1:E:391:PHE:CD1	2.87	0.41
1:F:85:LEU:HD13	1:F:103:THR:HG23	2.03	0.41
1:A:87:ARG:HG2	1:A:353:ILE:CD1	2.51	0.41
1:A:184:GLU:HG2	1:A:233:PRO:O	2.20	0.41
1:B:228:TYR:O	1:B:231:LYS:HB2	2.20	0.41
1:D:73:VAL:HG12	1:D:114:CYS:SG	2.61	0.41
1:D:371:ASP:HA	1:D:380:LYS:NZ	2.35	0.41
1:D:392:SER:HA	1:F:433:ARG:HH21	1.86	0.41
1:F:295:LEU:HD22	1:F:381:LEU:HD11	2.01	0.41
1:A:146:GLU:HB2	1:A:219:ARG:HH11	1.84	0.41
1:C:468:GLU:HB3	1:C:472:TRP:CD1	2.56	0.41
1:D:468:GLU:HB3	1:D:472:TRP:CD1	2.55	0.41
1:E:287:THR:HG22	1:E:290:GLN:NE2	2.36	0.41
1:F:76:VAL:HG21	1:F:271:SER:HB3	2.02	0.41
1:A:61:ALA:HB1	1:F:47:ARG:HA	2.01	0.41
1:B:55:PHE:HD2	1:B:283:LYS:HD2	1.81	0.41
1:C:262:TRP:CH2	1:C:364:PHE:O	2.73	0.41
1:E:296:HIS:CE1	1:E:299:TRP:HE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:SER:HB3	1:E:326:ARG:O	2.20	0.41
1:F:83:GLU:O	1:F:87:ARG:HG2	2.20	0.41
1:F:150:LEU:HD23	1:F:153:ASP:HB2	2.02	0.41
1:E:295:LEU:HD23	1:E:385:VAL:HG21	2.02	0.41
1:C:191:ARG:HD2	1:C:239:GLU:OE2	2.21	0.41
1:D:53:GLN:OE1	1:D:69:HIS:CG	2.74	0.41
1:E:294:HIS:O	1:E:297:GLU:HB2	2.20	0.41
1:A:73:VAL:HG21	1:A:117:HIS:CE1	2.56	0.41
1:A:214:ARG:HG3	1:A:230:MET:HE2	2.02	0.41
1:B:137:ARG:HH12	1:B:182:HIS:CE1	2.39	0.41
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.82	0.41
1:C:46:ARG:O	1:C:49:GLN:HG2	2.20	0.41
1:C:448:SER:HB2	1:C:451:HIS:CD2	2.56	0.41
1:E:11:ASN:H	1:E:204:ALA:HB2	1.85	0.41
1:E:127:PHE:CE2	1:E:400:GLU:CG	3.04	0.41
1:E:217:TRP:HH2	1:E:240:GLU:HG3	1.86	0.41
1:F:468:GLU:HB3	1:F:472:TRP:CD1	2.56	0.41
1:B:282:GLU:C	1:B:284:ARG:H	2.28	0.41
1:B:468:GLU:HB3	1:B:472:TRP:HD1	1.85	0.41
1:D:232:LYS:NZ	4:D:602:T8T:O1G	2.44	0.41
1:D:438:PRO:O	1:D:442:ARG:HD2	2.21	0.41
1:E:230:MET:HE2	1:E:255:TYR:CB	2.51	0.41
1:B:52:THR:CG2	1:B:57:LEU:H	2.08	0.40
1:B:448:SER:HB2	1:B:451:HIS:CD2	2.56	0.40
1:F:211:LYS:HA	1:F:261:THR:HG21	2.03	0.40
1:F:344:LEU:CD2	1:F:375:CYS:HB3	2.51	0.40
1:C:89:LYS:HE3	1:C:94:LEU:HD22	2.03	0.40
1:E:46:ARG:O	1:E:49:GLN:HG2	2.21	0.40
1:A:468:GLU:HB3	1:A:472:TRP:CD1	2.56	0.40
1:C:47:ARG:HA	1:E:61:ALA:HB1	2.02	0.40
1:D:55:PHE:HA	1:D:56:PRO:HD3	1.91	0.40
1:D:282:GLU:C	1:D:284:ARG:H	2.28	0.40
1:D:420:LEU:CD1	1:D:440:GLU:HG2	2.52	0.40
1:E:48:LEU:HD22	1:E:66:ARG:HB3	2.03	0.40
1:F:232:LYS:HB3	1:F:233:PRO:CD	2.51	0.40
1:F:298:ALA:HB3	1:F:381:LEU:CD2	2.51	0.40
1:B:279:ASP:O	1:B:282:GLU:N	2.55	0.40
1:F:17:ARG:HH12	1:F:38:ARG:HH22	1.67	0.40
1:F:137:ARG:HH12	1:F:182:HIS:CE1	2.40	0.40
1:F:148:GLN:H	1:F:149:PRO:HD3	1.85	0.40
1:F:214:ARG:HE	1:F:218:TRP:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TRP:CH2	1:C:364:PHE:HB3	2.55	0.40
1:D:425:PHE:CE2	1:D:477:ARG:HG3	2.56	0.40
1:F:497:TYR:O	1:F:501:MET:HG2	2.22	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	502/505 (99%)	463 (92%)	29 (6%)	10 (2%)	6	24
1	B	501/505 (99%)	460 (92%)	31 (6%)	10 (2%)	6	24
1	C	501/505 (99%)	457 (91%)	28 (6%)	16 (3%)	3	17
1	D	502/505 (99%)	456 (91%)	36 (7%)	10 (2%)	6	24
1	E	501/505 (99%)	455 (91%)	31 (6%)	15 (3%)	3	18
1	F	501/505 (99%)	452 (90%)	38 (8%)	11 (2%)	5	23
All	All	3008/3030 (99%)	2743 (91%)	193 (6%)	72 (2%)	4	21

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	166	GLU
1	B	22	VAL
1	B	93	LEU
1	B	154	ARG
1	B	223	PRO
1	B	369	LEU
1	B	432	GLU
1	C	304	LYS

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Mol	Chain	Res	Type
1	D	221	GLU
1	D	371	ASP
1	D	504	GLU
1	E	152	ASP
1	E	223	PRO
1	F	21	GLY
1	F	22	VAL
1	F	321	SER
1	F	371	ASP
1	B	23	LYS
1	C	21	GLY
1	C	22	VAL
1	C	164	ASP
1	C	301	GLN
1	E	22	VAL
1	E	151	THR
1	E	225	THR
1	E	299	TRP
1	E	371	ASP
1	E	432	GLU
1	F	162	LEU
1	F	164	ASP
1	F	320	ARG
1	A	162	LEU
1	A	302	HIS
1	A	327	SER
1	A	432	GLU
1	C	23	LYS
1	C	166	GLU
1	C	300	GLY
1	C	328	THR
1	C	372	ALA
1	C	432	GLU
1	D	125	GLY
1	D	322	ASN
1	E	124	PHE
1	E	321	SER
1	A	57	LEU
1	B	301	GLN
1	C	371	ASP
1	D	200	ASN
1	D	325	SER

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Mol	Chain	Res	Type
1	E	23	LYS
1	E	57	LEU
1	E	322	ASN
1	F	152	ASP
1	A	222(A)	THR
1	A	430	GLU
1	B	303	GLU
1	C	147	SER
1	C	149	PRO
1	C	430	GLU
1	D	319	SER
1	D	430	GLU
1	E	430	GLU
1	F	57	LEU
1	A	326	ARG
1	B	430	GLU
1	C	148	GLN
1	D	326	ARG
1	E	154	ARG
1	F	23	LYS
1	F	148	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/450 (100%)	412 (92%)	36 (8%)	11	36
1	B	448/450 (100%)	397 (89%)	51 (11%)	5	20
1	C	448/450 (100%)	402 (90%)	46 (10%)	7	25
1	D	448/450 (100%)	400 (89%)	48 (11%)	6	23
1	E	448/450 (100%)	404 (90%)	44 (10%)	7	27
1	F	448/450 (100%)	403 (90%)	45 (10%)	7	26
All	All	2688/2700 (100%)	2418 (90%)	270 (10%)	7	26

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	45	ILE
1	A	52	THR
1	A	54	VAL
1	A	83	GLU
1	A	88	LEU
1	A	140	LEU
1	A	143	GLU
1	A	147	SER
1	A	151	THR
1	A	153	ASP
1	A	163	ARG
1	A	166	GLU
1	A	190	ILE
1	A	209	ILE
1	A	211	LYS
1	A	227	HIS
1	A	232	LYS
1	A	262	TRP
1	A	271	SER
1	A	282	GLU
1	A	310	LEU
1	A	320	ARG
1	A	334	MET
1	A	341	LEU
1	A	365	ASN
1	A	368(A)	LEU
1	A	370	GLU
1	A	379	LEU
1	A	420	LEU
1	A	430	GLU
1	A	433	ARG
1	A	449	THR
1	A	480	LEU
1	A	491	LEU
1	A	496	GLU
1	B	3	GLN
1	B	22	VAL
1	B	27	GLU
1	B	45	ILE
1	B	51	LYS
1	B	53	GLN

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Mol	Chain	Res	Type
1	B	54	VAL
1	B	63	VAL
1	B	65	THR
1	B	66	ARG
1	B	83	GLU
1	B	91	LEU
1	B	117	HIS
1	B	119	ILE
1	B	140	LEU
1	B	143	GLU
1	B	164	ASP
1	B	169	LEU
1	B	186	ASN
1	B	190	ILE
1	B	209	ILE
1	B	210	LEU
1	B	222	THR
1	B	224	GLU
1	B	225	THR
1	B	227	HIS
1	B	231	LYS
1	B	262	TRP
1	B	264	MET
1	B	269	ASP
1	B	272	TYR
1	B	274	VAL
1	B	281	VAL
1	B	283	LYS
1	B	297	GLU
1	B	310	LEU
1	B	312	VAL
1	B	324	LEU
1	B	341	LEU
1	B	368(A)	LEU
1	B	369	LEU
1	B	379	LEU
1	B	381	LEU
1	B	405	ARG
1	B	420	LEU
1	B	430	GLU
1	B	432	GLU
1	B	435	LYS

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Mol	Chain	Res	Type
1	B	449	THR
1	B	491	LEU
1	B	504	GLU
1	C	3	GLN
1	C	17	ARG
1	C	20	GLN
1	C	45	ILE
1	C	51	LYS
1	C	63	VAL
1	C	71	MET
1	C	83	GLU
1	C	87	ARG
1	C	88	LEU
1	C	89	LYS
1	C	94	LEU
1	C	95	GLU
1	C	138	GLN
1	C	140	LEU
1	C	143	GLU
1	C	150	LEU
1	C	152	ASP
1	C	153	ASP
1	C	164	ASP
1	C	166	GLU
1	C	190	ILE
1	C	209	ILE
1	C	249	GLU
1	C	262	TRP
1	C	264	MET
1	C	274	VAL
1	C	281	VAL
1	C	310	LEU
1	C	312	VAL
1	C	313	GLU
1	C	329	GLU
1	C	334	MET
1	C	368(A)	LEU
1	C	369	LEU
1	C	370	GLU
1	C	379	LEU
1	C	381	LEU
1	C	388	LYS

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Mol	Chain	Res	Type
1	C	405	ARG
1	C	420	LEU
1	C	430	GLU
1	C	431	LYS
1	C	449	THR
1	C	480	LEU
1	C	491	LEU
1	D	22	VAL
1	D	26	HIS
1	D	45	ILE
1	D	83	GLU
1	D	88	LEU
1	D	94	LEU
1	D	114	CYS
1	D	138	GLN
1	D	140	LEU
1	D	143	GLU
1	D	148	GLN
1	D	152	ASP
1	D	156	SER
1	D	161	ARG
1	D	167	GLU
1	D	190	ILE
1	D	209	ILE
1	D	222	THR
1	D	224	GLU
1	D	225	THR
1	D	227	HIS
1	D	230	MET
1	D	264	MET
1	D	281	VAL
1	D	296	HIS
1	D	297	GLU
1	D	301	GLN
1	D	307	LEU
1	D	310	LEU
1	D	312	VAL
1	D	313	GLU
1	D	320	ARG
1	D	328	THR
1	D	329	GLU
1	D	334	MET

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Mol	Chain	Res	Type
1	D	368(A)	LEU
1	D	379	LEU
1	D	381	LEU
1	D	405	ARG
1	D	420	LEU
1	D	430	GLU
1	D	433	ARG
1	D	441	SER
1	D	449	THR
1	D	450	ARG
1	D	480	LEU
1	D	491	LEU
1	D	496	GLU
1	E	15	ARG
1	E	45	ILE
1	E	83	GLU
1	E	86	SER
1	E	88	LEU
1	E	92	LYS
1	E	94	LEU
1	E	101	GLU
1	E	140	LEU
1	E	144	ASP
1	E	146	GLU
1	E	150	LEU
1	E	151	THR
1	E	160	LEU
1	E	164	ASP
1	E	166	GLU
1	E	169	LEU
1	E	190	ILE
1	E	209	ILE
1	E	224	GLU
1	E	227	HIS
1	E	248	LYS
1	E	264	MET
1	E	281	VAL
1	E	288	VAL
1	E	299	TRP
1	E	302	HIS
1	E	310	LEU
1	E	312	VAL

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Mol	Chain	Res	Type
1	E	324	LEU
1	E	334	MET
1	E	341	LEU
1	E	368(A)	LEU
1	E	369	LEU
1	E	381	LEU
1	E	420	LEU
1	E	430	GLU
1	E	432	GLU
1	E	433	ARG
1	E	436	ARG
1	E	441	SER
1	E	449	THR
1	E	480	LEU
1	E	491	LEU
1	F	3	GLN
1	F	17	ARG
1	F	45	ILE
1	F	59	ARG
1	F	83	GLU
1	F	88	LEU
1	F	94	LEU
1	F	138	GLN
1	F	140	LEU
1	F	143	GLU
1	F	146	GLU
1	F	148	GLN
1	F	153	ASP
1	F	166	GLU
1	F	167	GLU
1	F	190	ILE
1	F	209	ILE
1	F	211	LYS
1	F	222	THR
1	F	227	HIS
1	F	240	GLU
1	F	262	TRP
1	F	264	MET
1	F	274	VAL
1	F	299	TRP
1	F	301	GLN
1	F	302	HIS

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Mol	Chain	Res	Type
1	F	304	LYS
1	F	310	LEU
1	F	312	VAL
1	F	319	SER
1	F	328	THR
1	F	329	GLU
1	F	334	MET
1	F	341	LEU
1	F	351	ARG
1	F	368(A)	LEU
1	F	379	LEU
1	F	381	LEU
1	F	420	LEU
1	F	430	GLU
1	F	449	THR
1	F	480	LEU
1	F	491	LEU
1	F	496	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	26	HIS
1	A	49	GLN
1	A	60	ASN
1	A	205	GLN
1	A	290	GLN
1	A	296	HIS
1	A	301	GLN
1	A	302	HIS
1	A	314	ASN
1	A	331	GLN
1	A	505	GLN
1	B	20	GLN
1	B	49	GLN
1	B	53	GLN
1	B	60	ASN
1	B	69	HIS
1	B	121	ASN
1	B	178	GLN
1	B	186	ASN

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Mol	Chain	Res	Type
1	B	188	GLN
1	B	290	GLN
1	B	301	GLN
1	B	331	GLN
1	B	445	HIS
1	B	451	HIS
1	C	26	HIS
1	C	49	GLN
1	C	53	GLN
1	C	60	ASN
1	C	121	ASN
1	C	141	HIS
1	C	290	GLN
1	C	322	ASN
1	C	339	ASN
1	C	451	HIS
1	D	3	GLN
1	D	60	ASN
1	D	138	GLN
1	D	148	GLN
1	D	182	HIS
1	D	188	GLN
1	D	331	GLN
1	D	339	ASN
1	D	350	GLN
1	D	445	HIS
1	D	451	HIS
1	D	505	GLN
1	E	53	GLN
1	E	60	ASN
1	E	290	GLN
1	E	296	HIS
1	E	331	GLN
1	E	339	ASN
1	F	26	HIS
1	F	49	GLN
1	F	53	GLN
1	F	60	ASN
1	F	69	HIS
1	F	121	ASN
1	F	148	GLN
1	F	170	ASN

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Mol	Chain	Res	Type
1	F	290	GLN
1	F	339	ASN
1	F	445	HIS
1	F	451	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	T8T	A	603	2	29,33,33	1.64	4 (13%)	36,52,52	0.75	0
4	T8T	C	602	-	29,33,33	1.24	2 (6%)	36,52,52	1.01	1 (2%)
4	T8T	B	602	-	29,33,33	1.15	4 (13%)	36,52,52	0.64	0
4	T8T	E	603	-	29,33,33	1.10	4 (13%)	36,52,52	1.06	1 (2%)
4	T8T	F	603	-	29,33,33	1.01	2 (6%)	36,52,52	0.62	0
4	T8T	D	602	-	29,33,33	0.93	2 (6%)	36,52,52	0.69	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	T8T	A	603	2	-	6/19/34/34	0/3/3/3
4	T8T	C	602	-	-	7/19/34/34	0/3/3/3
4	T8T	B	602	-	-	4/19/34/34	0/3/3/3
4	T8T	E	603	-	-	1/19/34/34	0/3/3/3
4	T8T	F	603	-	-	2/19/34/34	0/3/3/3
4	T8T	D	602	-	-	6/19/34/34	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	T8T	PG-O3G	-6.39	1.30	1.50
4	C	602	T8T	PG-O3G	-4.19	1.37	1.50
4	B	602	T8T	PG-O3G	-3.65	1.39	1.50
4	A	603	T8T	PG-O2G	-3.38	1.42	1.54
4	C	602	T8T	PG-O2G	-3.25	1.42	1.54
4	A	603	T8T	PA-O2A	-3.02	1.40	1.46
4	E	603	T8T	PG-O1G	-2.76	1.44	1.54
4	B	602	T8T	PG-O2G	-2.74	1.44	1.54
4	F	603	T8T	PG-O3G	-2.65	1.42	1.50
4	A	603	T8T	PG-O1G	-2.58	1.45	1.54
4	E	603	T8T	PG-O2G	-2.57	1.45	1.54
4	F	603	T8T	PG-O2G	-2.41	1.45	1.54
4	B	602	T8T	PA-O2A	-2.35	1.41	1.46
4	D	602	T8T	PA-O2A	-2.15	1.41	1.46
4	E	603	T8T	PA-O2A	-2.10	1.42	1.46
4	B	602	T8T	PG-O1G	-2.08	1.47	1.54
4	D	602	T8T	PG-O2G	-2.03	1.47	1.54
4	E	603	T8T	PG-O3G	-2.01	1.44	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	T8T	O2B-PB-O3B	-4.08	96.25	107.27
4	C	602	T8T	O2B-PB-O3B	-2.24	101.23	107.27
4	D	602	T8T	O2B-PB-O3A	2.14	113.05	107.27

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

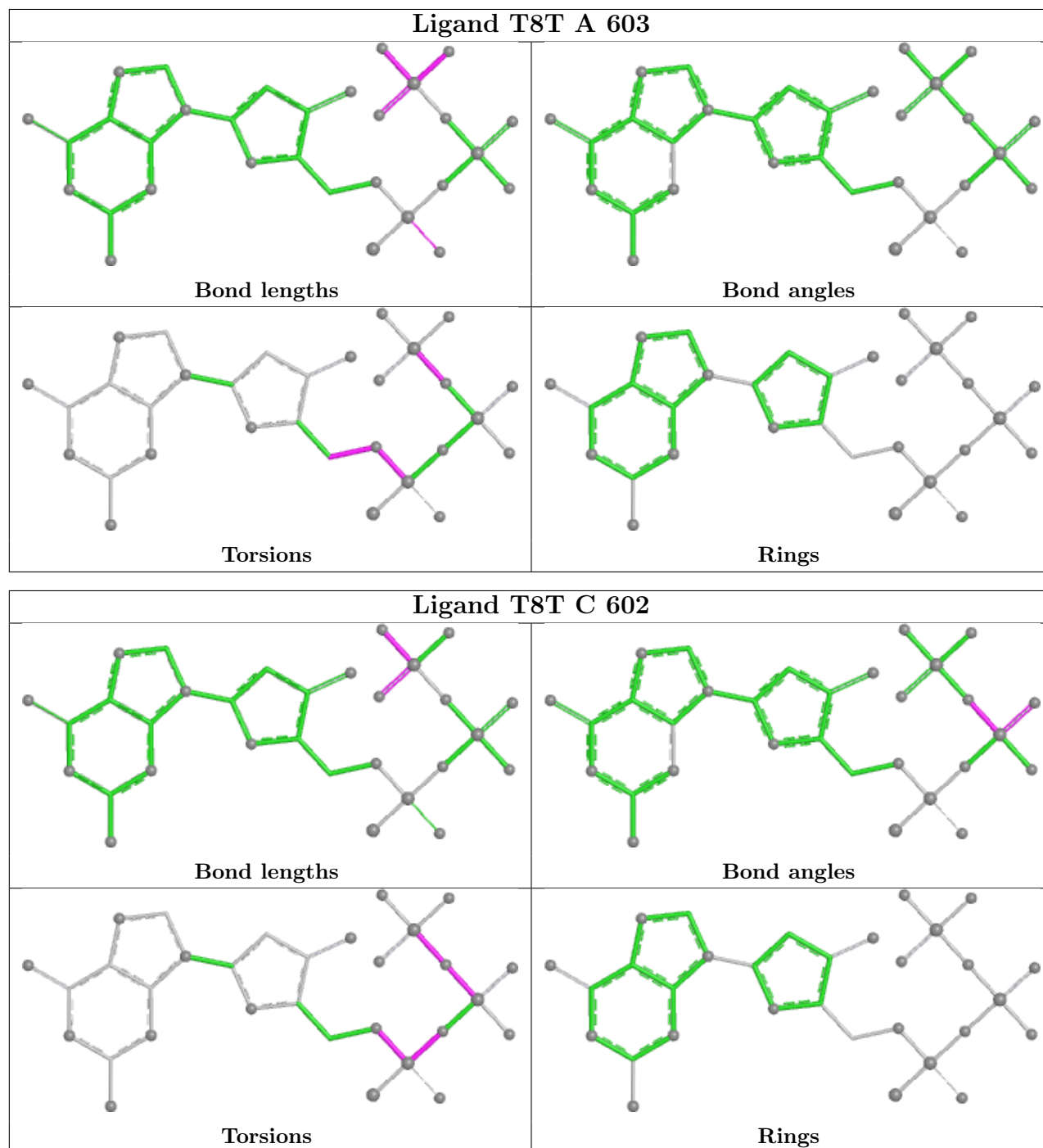
There are no ring outliers.

6 monomers are involved in 21 short contacts:

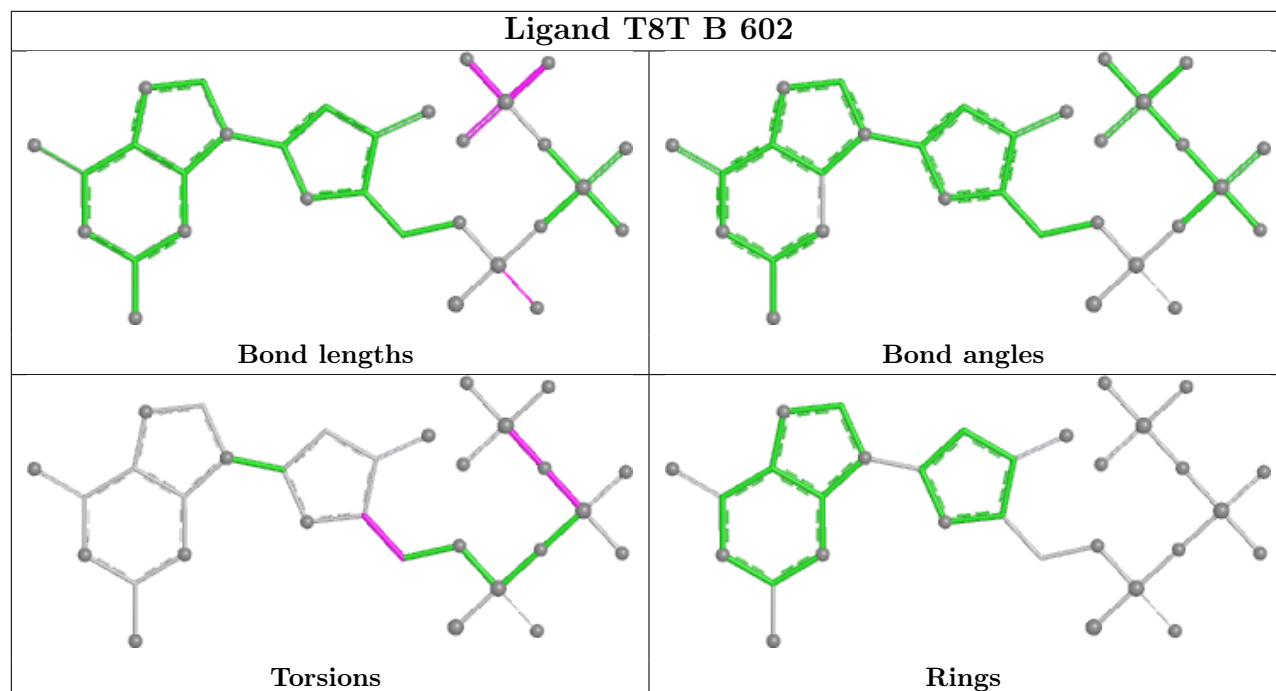
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	T8T	7	0
4	C	602	T8T	4	0
4	B	602	T8T	1	0
4	E	603	T8T	3	0
4	F	603	T8T	4	0
4	D	602	T8T	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

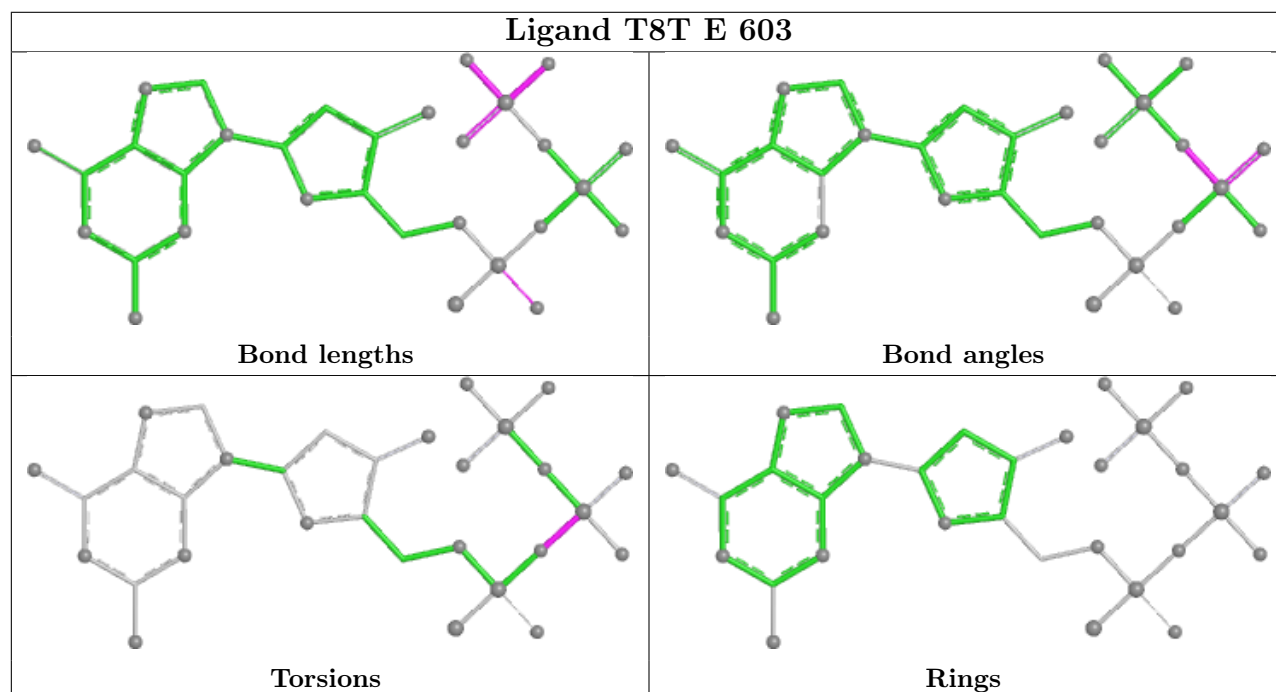
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

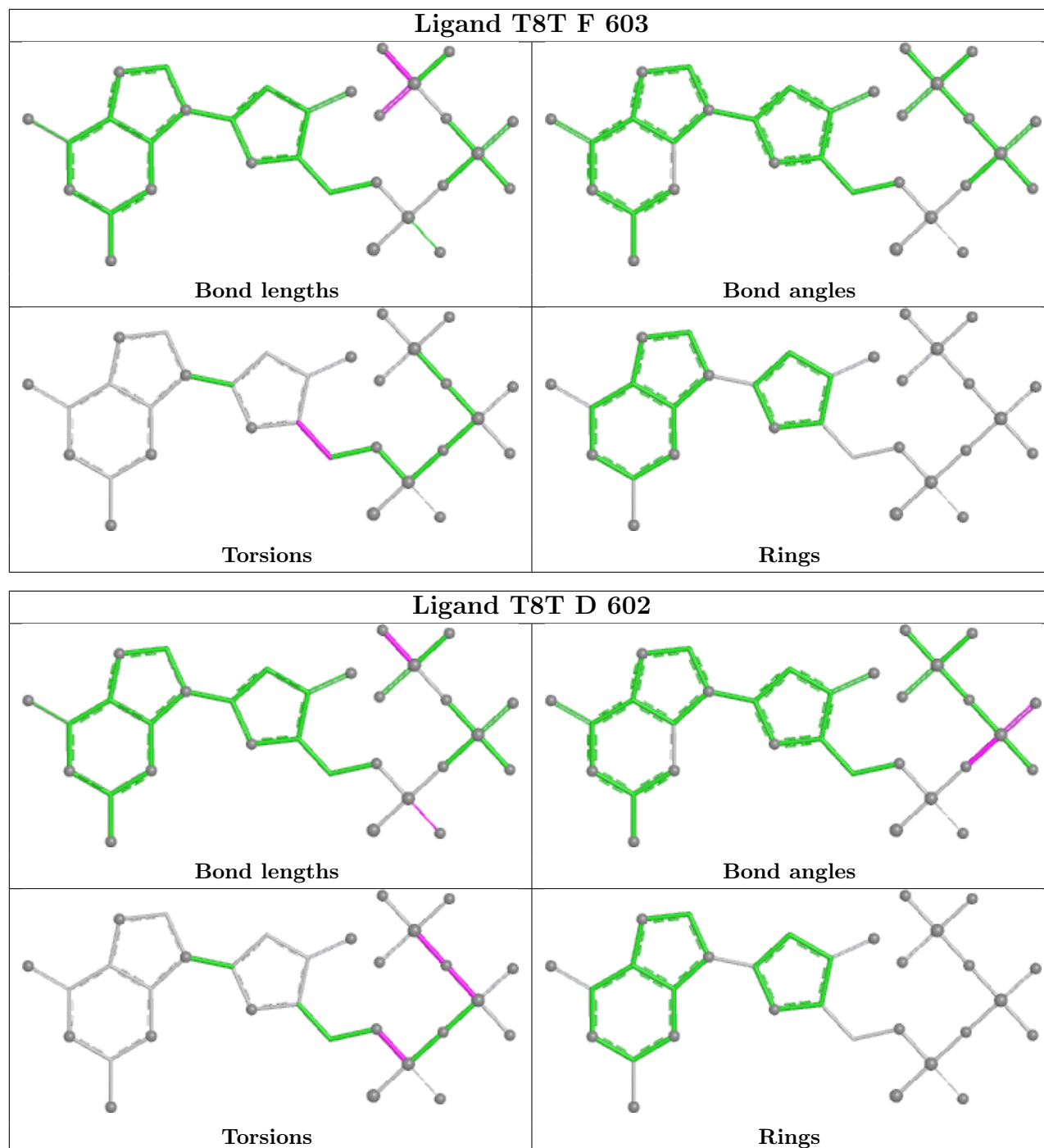


Ligand T8T B 602



Ligand T8T E 603





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	504/505 (99%)	-0.18	4 (0%) 82 71	59, 108, 166, 205	0
1	B	503/505 (99%)	0.12	5 (0%) 79 66	59, 153, 210, 235	0
1	C	503/505 (99%)	-0.18	2 (0%) 88 81	58, 109, 169, 209	0
1	D	504/505 (99%)	0.22	9 (1%) 67 51	62, 162, 212, 233	0
1	E	503/505 (99%)	-0.07	4 (0%) 82 71	62, 125, 188, 221	0
1	F	503/505 (99%)	-0.11	2 (0%) 88 81	61, 121, 181, 211	0
All	All	3020/3030 (99%)	-0.03	26 (0%) 81 69	58, 128, 199, 235	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	398	ARG	4.2
1	A	324	LEU	4.0
1	A	398	ARG	3.5
1	E	324	LEU	3.2
1	E	398	ARG	3.1
1	C	398	ARG	2.9
1	D	99	LEU	2.6
1	D	150	LEU	2.5
1	B	398	ARG	2.5
1	A	57	LEU	2.5
1	B	324	LEU	2.5
1	B	333	PHE	2.4
1	E	56	PRO	2.4
1	D	10	ILE	2.4
1	D	353	ILE	2.3
1	A	505	GLN	2.2
1	D	6	PHE	2.2
1	D	368(A)	LEU	2.1
1	F	299	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	398	ARG	2.1
1	D	263	ILE	2.1
1	C	324	LEU	2.1
1	E	162	LEU	2.1
1	D	273	CYS	2.1
1	B	26	HIS	2.0
1	B	110	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

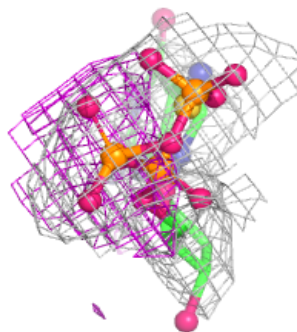
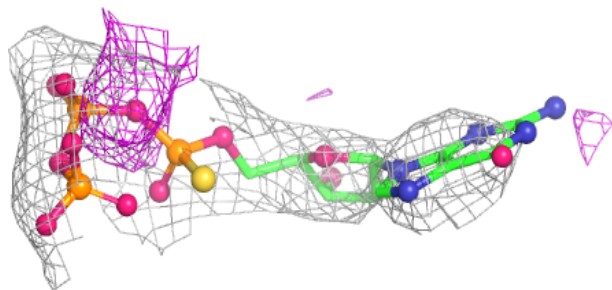
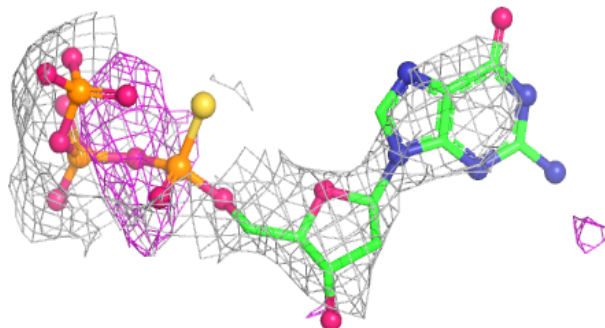
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	F	601	1/1	0.72	0.24	120,120,120,120	0
4	T8T	E	603	31/31	0.81	0.12	212,224,248,249	0
4	T8T	A	603	31/31	0.83	0.10	135,149,210,216	0
2	MG	E	601	1/1	0.83	0.09	95,95,95,95	0
4	T8T	F	603	31/31	0.85	0.10	153,170,217,218	0
4	T8T	C	602	31/31	0.86	0.09	170,187,224,224	0
4	T8T	D	602	31/31	0.86	0.09	148,177,226,228	0
4	T8T	B	602	31/31	0.89	0.09	150,180,229,232	0
3	MN	B	601	1/1	0.91	0.12	194,194,194,194	0
3	MN	E	602	1/1	0.91	0.11	174,174,174,174	0
3	MN	F	602	1/1	0.92	0.10	168,168,168,168	0
3	MN	A	602	1/1	0.94	0.06	119,119,119,119	0
3	MN	C	601	1/1	0.95	0.06	128,128,128,128	0
3	MN	D	601	1/1	0.96	0.06	183,183,183,183	0
2	MG	A	601	1/1	0.98	0.10	108,108,108,108	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.

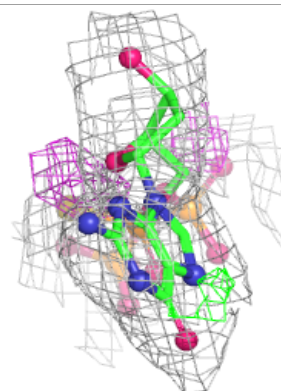
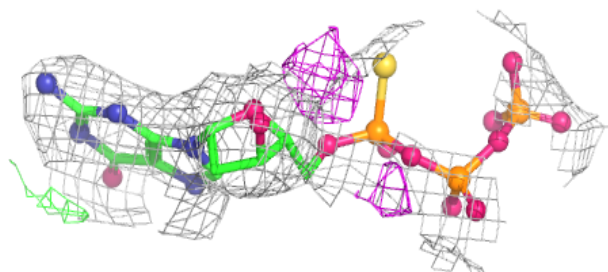
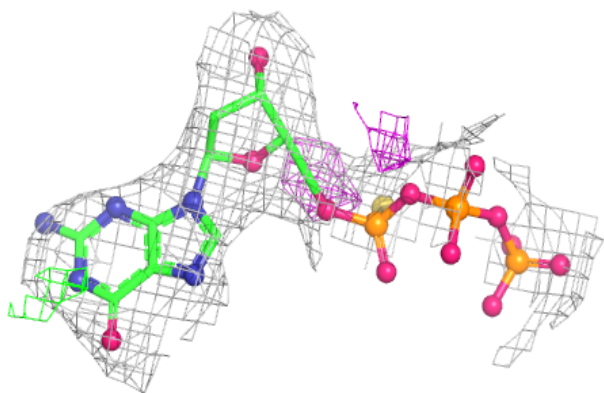
Electron density around T8T E 603:

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

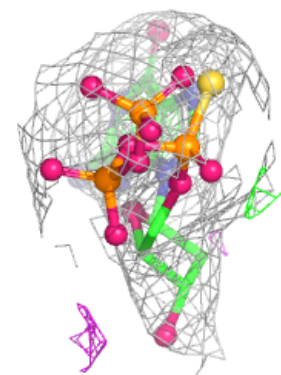
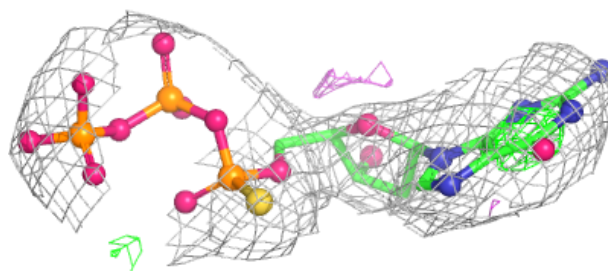
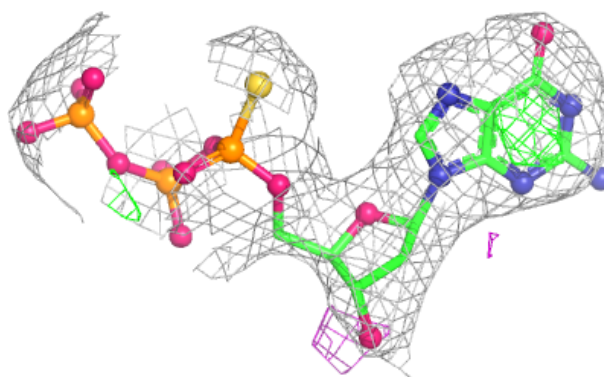


Electron density around T8T A 603:

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

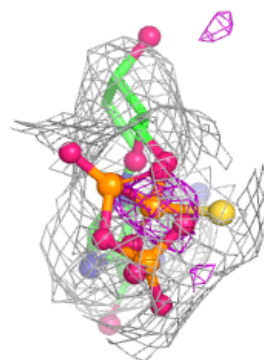
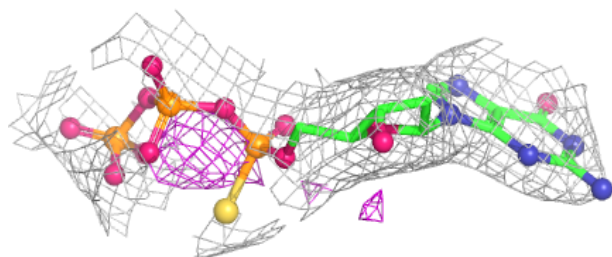
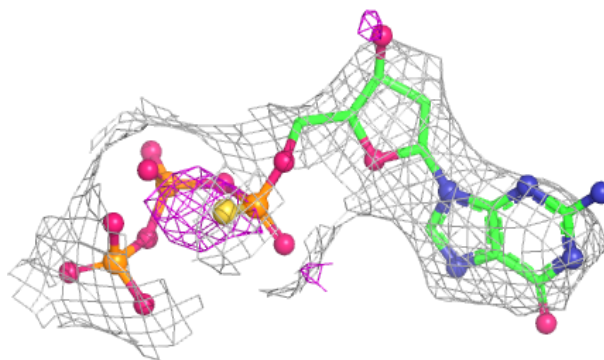
**Electron density around T8T F 603:**

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

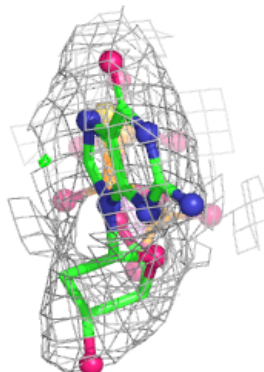
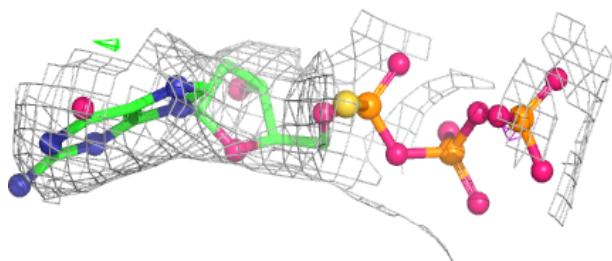


Electron density around T8T C 602:

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

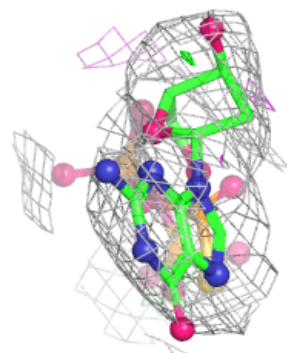
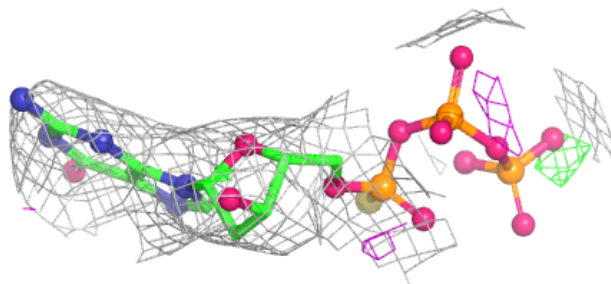
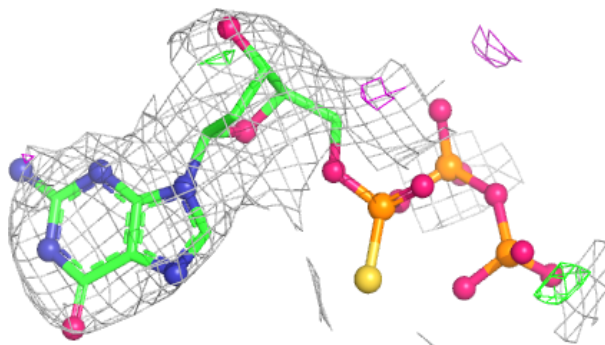
**Electron density around T8T D 602:**

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



Electron density around T8T B 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.