



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:05 AM UTC

PDB ID : 6OIX / pdb_00006oix
Title : Structure of Escherichia coli dGTPase bound to GTP
Authors : Barnes, C.O.; Wu, Y.; Calero, G.
Deposited on : 2019-04-09
Resolution : 3.15 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:

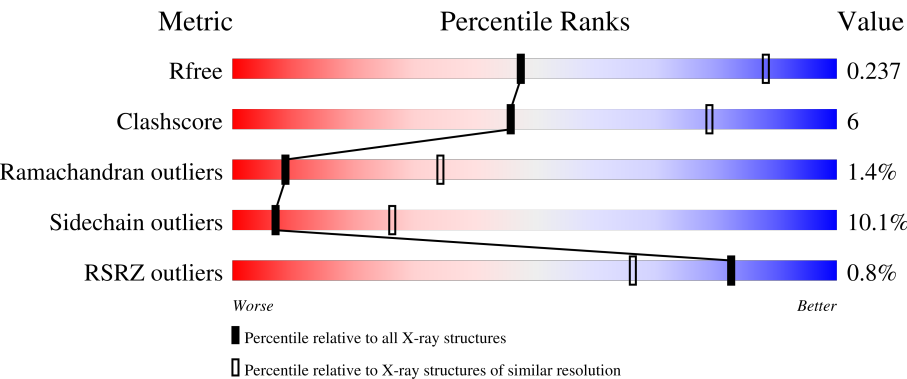
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	% 71%19%• 6%
1	B	505	72%17%• 7%
1	C	505	% 70%20%• • 5%
1	D	505	% 72%19%• 7%
1	E	505	% 73%18%• 5%

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Mol	Chain	Length	Quality of chain
1	F	505	72% 18% • 6%

2 Entry composition [i](#)

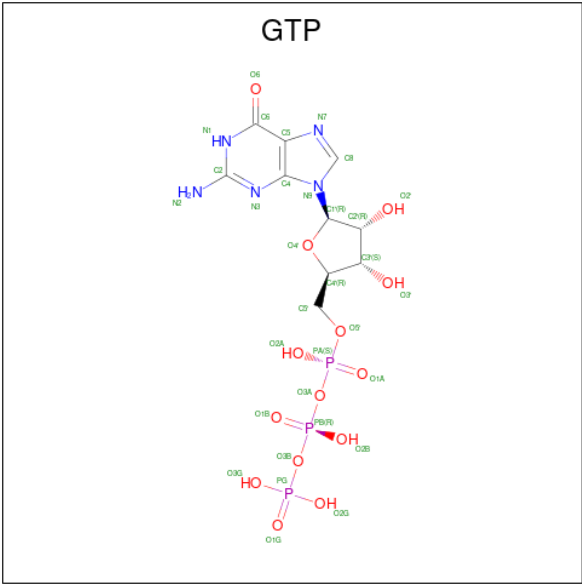
There are 4 unique types of molecules in this entry. The entry contains 24160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	477	Total	C	N	O	S	0	0	0
			3980	2549	708	708	15			
1	B	471	Total	C	N	O	S	0	0	0
			3921	2515	694	697	15			
1	C	478	Total	C	N	O	S	0	0	0
			3982	2552	708	706	16			
1	D	472	Total	C	N	O	S	0	0	0
			3927	2514	699	698	16			
1	E	478	Total	C	N	O	S	0	0	0
			3982	2549	708	709	16			
1	F	475	Total	C	N	O	S	0	0	0
			3954	2536	702	700	16			

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	F	1	Total	C	N	O	P	0	0
			32	10	5	14	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		

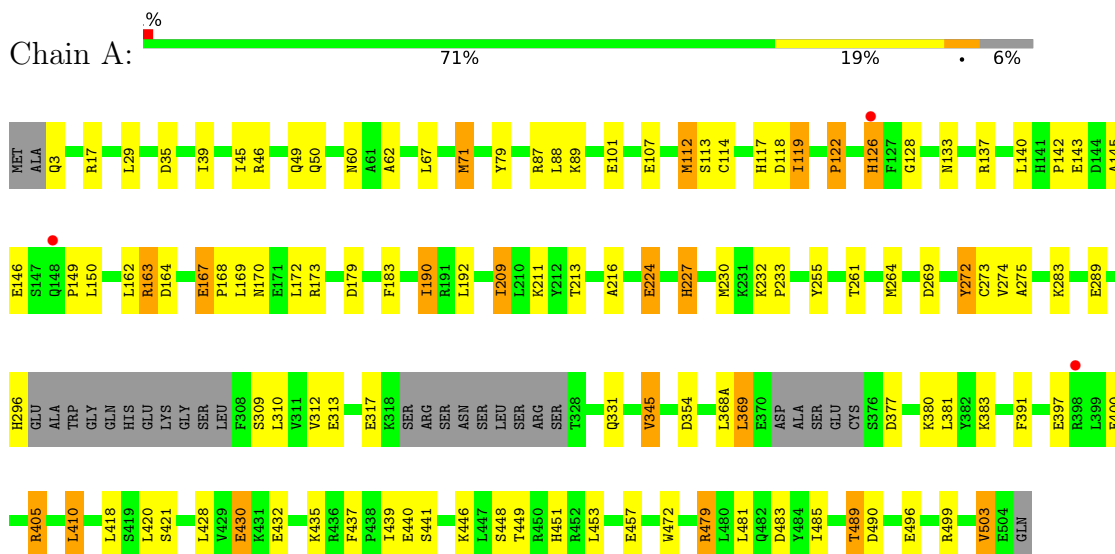
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	22	Total	O	0	0
			22	22		
4	C	38	Total	O	0	0
			38	38		
4	D	21	Total	O	0	0
			21	21		
4	E	49	Total	O	0	0
			49	49		
4	F	46	Total	O	0	0
			46	46		

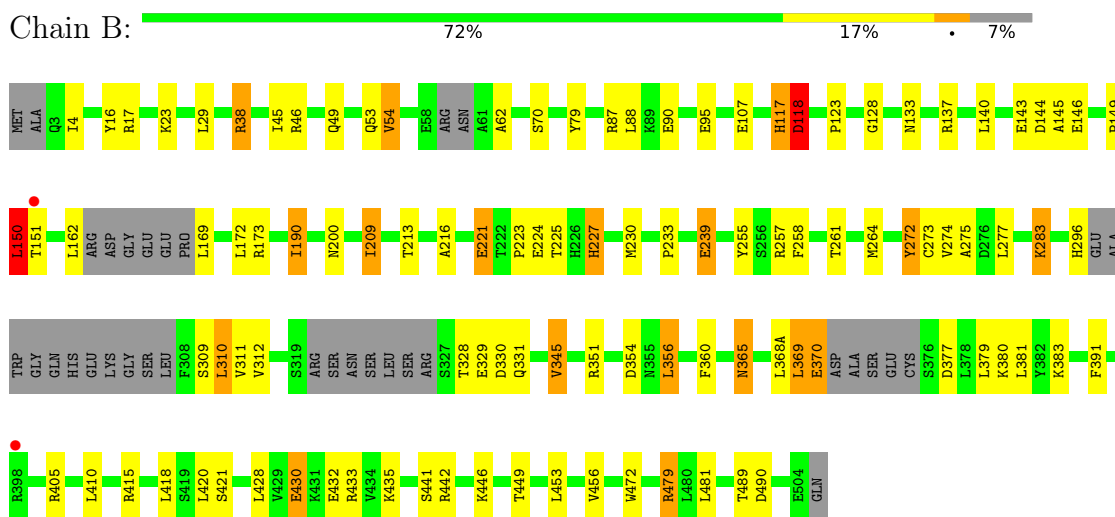
3 Residue-property plots

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

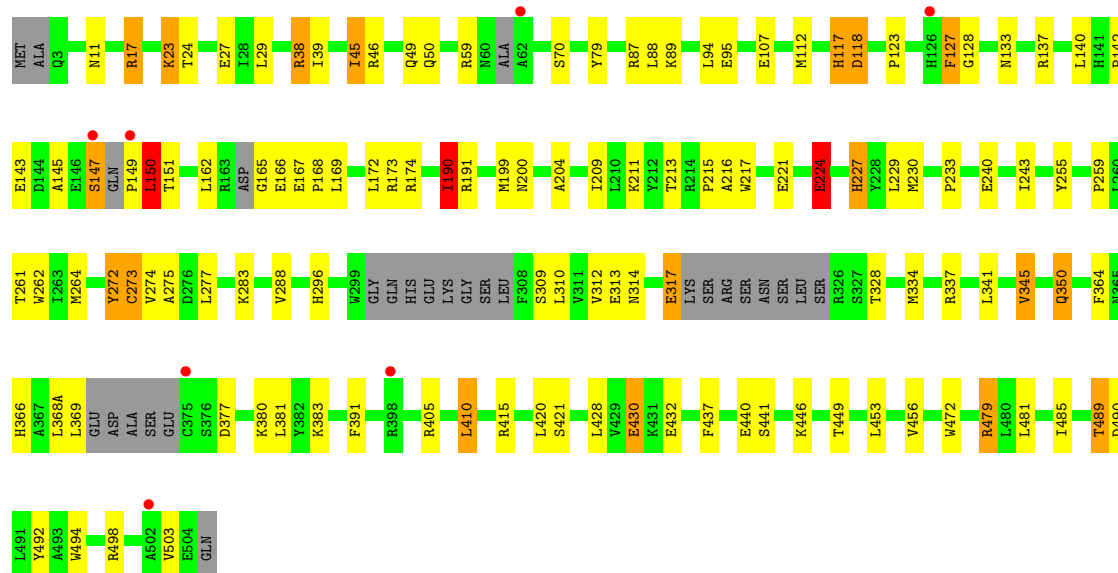


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

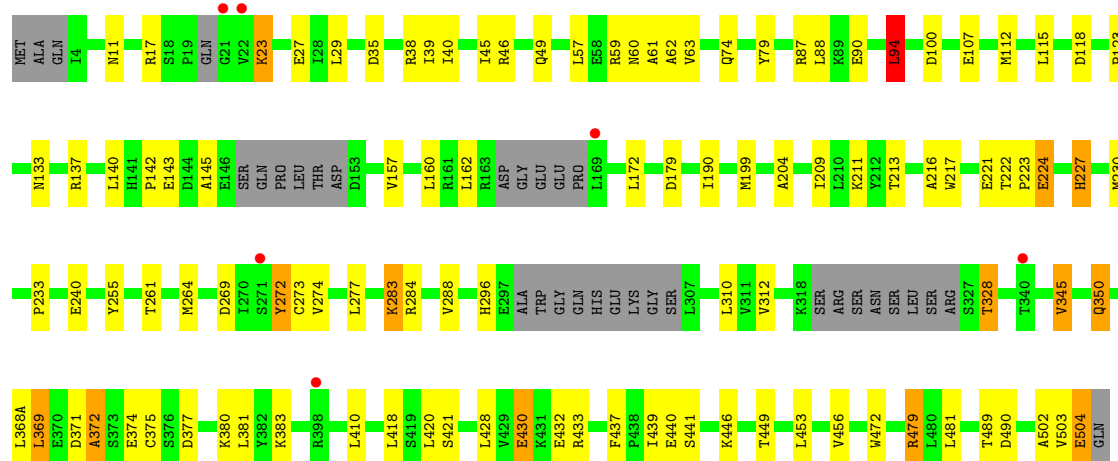


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

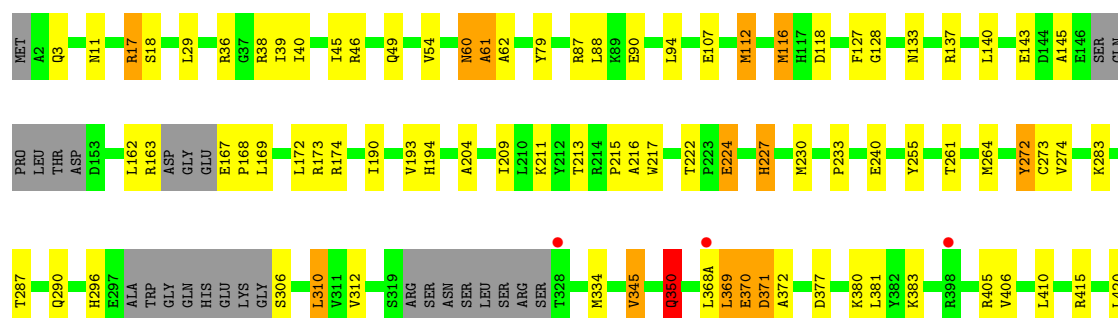
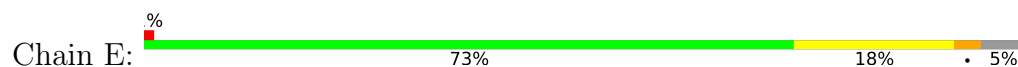


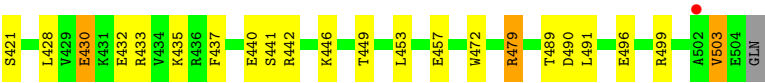


• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

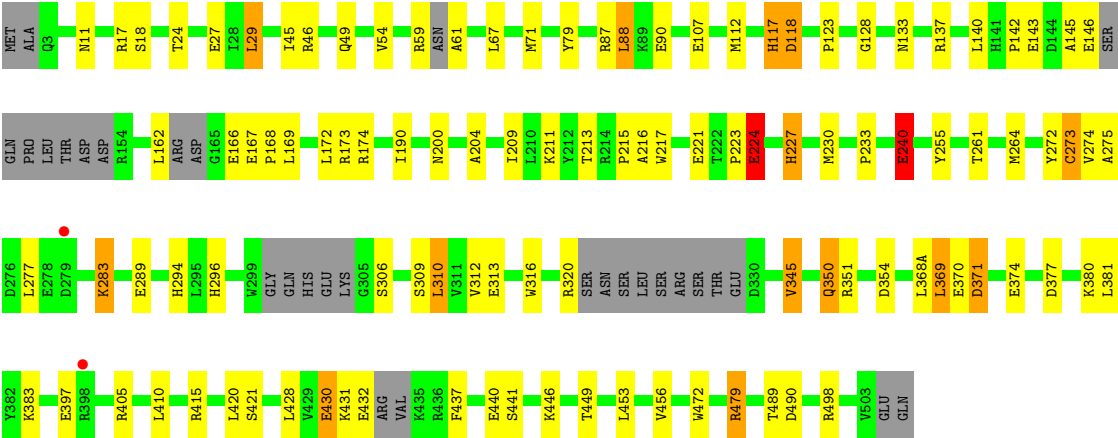


• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase





● 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	191.59Å 191.59Å 292.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.75 – 3.15 31.75 – 3.15	Depositor EDS
% Data completeness (in resolution range)	91.6 (31.75-3.15) 91.5 (31.75-3.15)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.190 , 0.208 0.218 , 0.237	Depositor DCC
R_{free} test set	2647 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 101.2	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	0.94	EDS
Total number of atoms	24160	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, GTP

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	0.92	4/4077 (0.1%)	1.44	24/5511 (0.4%)
1	B	0.83	0/4015	1.47	30/5426 (0.6%)
1	C	0.91	1/4078 (0.0%)	1.51	39/5508 (0.7%)
1	D	0.81	1/4018 (0.0%)	1.49	32/5424 (0.6%)
1	E	0.92	4/4077 (0.1%)	1.49	21/5508 (0.4%)
1	F	0.86	2/4049 (0.0%)	1.48	32/5467 (0.6%)
All	All	0.87	12/24314 (0.0%)	1.48	178/32844 (0.5%)

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	E	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	112	MET	SD-CE	-15.56	1.40	1.79
1	E	116	MET	SD-CE	-10.13	1.54	1.79
1	A	71	MET	SD-CE	-8.97	1.57	1.79
1	E	345	VAL	CA-CB	6.77	1.57	1.54
1	D	199	MET	SD-CE	-6.36	1.63	1.79
1	A	122	PRO	C-O	-6.28	1.17	1.24
1	A	503	VAL	CA-C	5.77	1.60	1.53
1	C	273	CYS	CA-C	-5.27	1.47	1.52
1	A	112	MET	SD-CE	-5.26	1.66	1.79
1	F	112	MET	SD-CE	-5.17	1.66	1.79
1	F	345	VAL	CA-CB	5.08	1.56	1.54
1	E	3	GLN	C-N	5.03	1.39	1.33

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	ASN	CA-CB-CG	-11.80	100.80	112.60
1	E	60	ASN	CA-C-N	10.81	142.19	121.54
1	E	60	ASN	C-N-CA	10.81	142.19	121.54
1	C	123	PRO	CA-C-N	-10.52	107.50	123.17
1	C	123	PRO	C-N-CA	-10.52	107.50	123.17
1	F	123	PRO	CA-C-N	-10.44	107.62	123.17
1	F	123	PRO	C-N-CA	-10.44	107.62	123.17
1	D	123	PRO	CA-C-N	-10.16	108.04	123.17
1	D	123	PRO	C-N-CA	-10.16	108.04	123.17
1	C	117	HIS	N-CA-C	-9.63	95.52	109.96
1	F	117	HIS	N-CA-C	-9.63	95.52	109.96
1	B	123	PRO	CA-C-N	-8.91	108.16	122.95
1	B	123	PRO	C-N-CA	-8.91	108.16	122.95
1	C	199	MET	N-CA-C	-8.59	96.11	109.25
1	B	117	HIS	N-CA-C	-8.32	97.48	109.96
1	C	350	GLN	CB-CG-CD	-8.04	98.94	112.60
1	A	168	PRO	CA-C-N	7.59	131.21	120.28
1	A	168	PRO	C-N-CA	7.59	131.21	120.28
1	A	163	ARG	CA-C-N	7.58	136.02	121.54
1	A	163	ARG	C-N-CA	7.58	136.02	121.54
1	C	168	PRO	CA-C-N	7.53	131.12	120.28
1	C	168	PRO	C-N-CA	7.53	131.12	120.28
1	F	240	GLU	CB-CG-CD	7.43	125.24	112.60
1	D	59	ARG	CA-C-N	7.37	135.61	121.54
1	D	59	ARG	C-N-CA	7.37	135.61	121.54
1	E	168	PRO	CA-C-N	7.34	130.85	120.28
1	E	168	PRO	C-N-CA	7.34	130.85	120.28
1	F	345	VAL	N-CA-CB	7.32	115.42	110.52
1	F	168	PRO	CA-C-N	7.10	130.50	120.28
1	F	168	PRO	C-N-CA	7.10	130.50	120.28
1	A	167	GLU	N-CA-C	7.06	120.76	108.82
1	C	345	VAL	N-CA-CB	7.04	115.24	110.52
1	C	199	MET	CA-C-N	-6.98	112.36	122.06
1	C	199	MET	C-N-CA	-6.98	112.36	122.06
1	E	345	VAL	N-CA-CB	6.86	115.11	110.52
1	E	118	ASP	CA-CB-CG	6.84	119.44	112.60
1	D	118	ASP	CA-CB-CG	6.82	119.42	112.60
1	C	224	GLU	CA-C-N	6.63	129.16	120.28
1	C	224	GLU	C-N-CA	6.63	129.16	120.28
1	B	345	VAL	N-CA-CB	6.62	114.96	110.52
1	F	224	GLU	CA-C-N	6.61	129.14	120.28
1	F	224	GLU	C-N-CA	6.61	129.14	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	224	GLU	CA-C-N	6.60	129.12	120.28
1	D	224	GLU	C-N-CA	6.60	129.12	120.28
1	D	62	ALA	N-CA-C	-6.58	105.23	113.20
1	A	224	GLU	CA-C-N	6.53	129.03	120.28
1	A	224	GLU	C-N-CA	6.53	129.03	120.28
1	B	118	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	165	GLY	CA-C-N	6.51	133.98	121.54
1	C	165	GLY	C-N-CA	6.51	133.98	121.54
1	F	118	ASP	CA-CB-CG	6.47	119.07	112.60
1	C	200	ASN	CA-CB-CG	6.38	118.98	112.60
1	C	118	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	62	ALA	CA-C-N	6.08	129.94	120.34
1	A	62	ALA	C-N-CA	6.08	129.94	120.34
1	D	345	VAL	N-CA-CB	6.06	114.58	110.52
1	A	345	VAL	N-CA-CB	6.03	114.56	110.52
1	C	230	MET	CA-C-N	6.03	128.67	120.54
1	C	230	MET	C-N-CA	6.03	128.67	120.54
1	E	230	MET	CA-C-N	6.01	128.65	120.54
1	E	230	MET	C-N-CA	6.01	128.65	120.54
1	D	62	ALA	CA-C-N	6.00	129.83	120.34
1	D	62	ALA	C-N-CA	6.00	129.83	120.34
1	B	53	GLN	N-CA-C	-6.00	98.74	108.52
1	C	317	GLU	CB-CG-CD	5.98	122.76	112.60
1	A	62	ALA	N-CA-C	-5.96	105.98	113.20
1	D	94	LEU	CD1-CG-CD2	-5.95	97.71	110.80
1	F	230	MET	CA-C-N	5.86	128.44	120.54
1	F	230	MET	C-N-CA	5.86	128.44	120.54
1	D	230	MET	CA-C-N	5.84	128.42	120.54
1	D	230	MET	C-N-CA	5.84	128.42	120.54
1	C	150	LEU	CA-C-N	5.82	132.17	121.70
1	C	150	LEU	C-N-CA	5.82	132.17	121.70
1	B	239	GLU	CB-CG-CD	5.82	122.49	112.60
1	D	372	ALA	CA-C-N	5.79	129.06	120.90
1	D	372	ALA	C-N-CA	5.79	129.06	120.90
1	A	230	MET	CA-C-N	5.75	128.31	120.54
1	A	230	MET	C-N-CA	5.75	128.31	120.54
1	B	62	ALA	CA-C-N	5.71	128.28	120.35
1	B	62	ALA	C-N-CA	5.71	128.28	120.35
1	A	101	GLU	CB-CG-CD	5.66	122.22	112.60
1	C	277	LEU	CA-C-N	5.64	127.83	120.28
1	C	277	LEU	C-N-CA	5.64	127.83	120.28
1	E	224	GLU	CA-C-N	5.62	127.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	224	GLU	C-N-CA	5.62	127.81	120.28
1	D	283	LYS	CA-C-N	5.60	130.08	122.19
1	D	283	LYS	C-N-CA	5.60	130.08	122.19
1	B	354	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	230	MET	CA-C-N	5.48	127.94	120.54
1	B	230	MET	C-N-CA	5.48	127.94	120.54
1	E	227	HIS	CA-CB-CG	5.47	119.28	113.80
1	B	309	SER	CA-C-N	5.45	127.58	120.28
1	B	309	SER	C-N-CA	5.45	127.58	120.28
1	F	142	PRO	CA-C-N	5.43	127.56	120.28
1	F	142	PRO	C-N-CA	5.43	127.56	120.28
1	A	275	ALA	CA-C-N	5.42	128.55	120.31
1	A	275	ALA	C-N-CA	5.42	128.55	120.31
1	D	142	PRO	CA-C-N	5.40	127.51	120.28
1	D	142	PRO	C-N-CA	5.40	127.51	120.28
1	C	288	VAL	CA-C-N	5.40	127.45	120.44
1	C	288	VAL	C-N-CA	5.40	127.45	120.44
1	B	277	LEU	CA-C-N	5.39	127.50	120.28
1	B	277	LEU	C-N-CA	5.39	127.50	120.28
1	D	374	GLU	CA-C-N	5.39	127.77	120.44
1	D	374	GLU	C-N-CA	5.39	127.77	120.44
1	B	150	LEU	CA-C-N	5.37	127.42	120.44
1	B	150	LEU	C-N-CA	5.37	127.42	120.44
1	D	38	ARG	CA-C-N	5.33	127.28	120.56
1	D	38	ARG	C-N-CA	5.33	127.28	120.56
1	B	456	VAL	CA-C-N	5.33	127.74	120.54
1	B	456	VAL	C-N-CA	5.33	127.74	120.54
1	C	70	SER	CA-C-N	5.31	127.39	120.28
1	C	70	SER	C-N-CA	5.31	127.39	120.28
1	E	18	SER	N-CA-C	5.31	116.51	109.93
1	F	283	LYS	CA-C-N	5.30	130.10	122.35
1	F	283	LYS	C-N-CA	5.30	130.10	122.35
1	C	275	ALA	CA-C-N	5.30	128.36	120.31
1	C	275	ALA	C-N-CA	5.30	128.36	120.31
1	E	62	ALA	CA-C-N	5.30	128.48	120.75
1	E	62	ALA	C-N-CA	5.30	128.48	120.75
1	F	128	GLY	N-CA-C	-5.29	105.99	112.77
1	F	18	SER	N-CA-C	5.29	116.49	109.93
1	B	275	ALA	CA-C-N	5.29	128.35	120.31
1	B	275	ALA	C-N-CA	5.29	128.35	120.31
1	A	354	ASP	CA-CB-CG	5.28	117.88	112.60
1	F	277	LEU	CA-C-N	5.27	127.34	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	277	LEU	C-N-CA	5.27	127.34	120.28
1	C	456	VAL	CA-C-N	5.26	127.64	120.54
1	C	456	VAL	C-N-CA	5.26	127.64	120.54
1	F	354	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	269	ASP	CA-CB-CG	5.21	117.81	112.60
1	F	275	ALA	CA-C-N	5.21	128.23	120.31
1	F	275	ALA	C-N-CA	5.21	128.23	120.31
1	F	224	GLU	CB-CG-CD	5.20	121.44	112.60
1	F	374	GLU	CA-C-N	5.20	127.52	120.44
1	F	374	GLU	C-N-CA	5.20	127.52	120.44
1	D	277	LEU	CA-C-N	5.17	127.20	120.28
1	D	277	LEU	C-N-CA	5.17	127.20	120.28
1	B	128	GLY	N-CA-C	-5.15	106.17	112.77
1	B	283	LYS	CA-C-N	5.14	129.86	122.35
1	B	283	LYS	C-N-CA	5.14	129.86	122.35
1	D	288	VAL	CA-C-N	5.13	127.12	120.44
1	D	288	VAL	C-N-CA	5.13	127.12	120.44
1	F	456	VAL	CA-C-N	5.13	127.46	120.54
1	F	456	VAL	C-N-CA	5.13	127.46	120.54
1	E	350	GLN	CB-CG-CD	5.12	121.31	112.60
1	C	127	PHE	CA-CB-CG	-5.11	108.69	113.80
1	F	313	GLU	CA-C-N	5.11	127.44	120.54
1	F	313	GLU	C-N-CA	5.11	127.44	120.54
1	F	223	PRO	CA-C-N	5.10	127.37	120.38
1	F	223	PRO	C-N-CA	5.10	127.37	120.38
1	E	372	ALA	CA-C-N	5.09	128.07	120.90
1	E	372	ALA	C-N-CA	5.09	128.07	120.90
1	D	456	VAL	CA-C-N	5.07	127.39	120.54
1	D	456	VAL	C-N-CA	5.07	127.39	120.54
1	C	190	ILE	CB-CG1-CD1	5.07	124.45	113.80
1	C	142	PRO	CA-C-N	5.07	127.07	120.28
1	C	142	PRO	C-N-CA	5.07	127.07	120.28
1	E	128	GLY	CA-C-N	5.07	127.34	120.65
1	E	128	GLY	C-N-CA	5.07	127.34	120.65
1	A	35	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	70	SER	CA-C-N	5.04	127.04	120.28
1	B	70	SER	C-N-CA	5.04	127.04	120.28
1	A	142	PRO	CA-C-N	5.04	127.03	120.28
1	A	142	PRO	C-N-CA	5.04	127.03	120.28
1	B	38	ARG	CA-C-N	5.03	126.90	120.56
1	B	38	ARG	C-N-CA	5.03	126.90	120.56
1	E	370	GLU	CA-C-N	5.02	131.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	370	GLU	C-N-CA	5.02	131.13	121.54
1	A	489	THR	N-CA-C	-5.02	103.78	110.55
1	C	38	ARG	CA-C-N	5.01	126.87	120.56
1	C	38	ARG	C-N-CA	5.01	126.87	120.56
1	D	269	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	128	GLY	CA-C-N	5.01	127.26	120.65
1	A	128	GLY	C-N-CA	5.01	127.26	120.65
1	D	35	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	128	GLY	CA-C-N	5.00	127.25	120.65
1	C	128	GLY	C-N-CA	5.00	127.25	120.65

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	60	ASN	Peptide

5.2 Too-close contacts [i](#)

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	3980	0	3954	59	0
1	B	3921	0	3893	46	0
1	C	3982	0	3944	55	0
1	D	3927	0	3906	39	0
1	E	3982	0	3955	50	0
1	F	3954	0	3924	42	0
2	A	32	0	12	4	0
2	B	32	0	12	2	0
2	C	32	0	12	1	0
2	D	32	0	12	0	0
2	E	32	0	12	0	0
2	F	32	0	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	40	0	0	2	0
4	B	22	0	0	1	0
4	C	38	0	0	0	0
4	D	21	0	0	0	0
4	E	49	0	0	1	0
4	F	46	0	0	2	0
All	All	24160	0	23648	278	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 6.

All (278) 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:C:150:LEU:HB3	1:C:151:THR:HA	1.16	1.13
1:B:17:ARG:HH22	1:B:38:ARG:HH22	1.05	1.02
1:E:272:TYR:HD2	1:E:273:CYS:HG	1.04	0.96
1:C:150:LEU:HB3	1:C:151:THR:CA	1.92	0.96
1:C:17:ARG:HH22	1:C:38:ARG:HH22	1.10	0.96
1:A:400:GLU:OE2	1:B:442:ARG:NE	2.00	0.94
1:B:4:ILE:HD13	1:B:356:LEU:HD12	1.55	0.88
1:A:126:HIS:CD2	1:A:126:HIS:H	1.92	0.85
1:C:262:TRP:HZ3	1:C:366:HIS:O	1.57	0.85
1:E:36:ARG:HA	1:E:112:MET:HE2	1.57	0.84
1:A:122:PRO:HG3	1:A:183:PHE:CE1	2.12	0.83
2:A:601:GTP:O2G	4:A:701:HOH:O	1.97	0.82
1:C:262:TRP:HH2	1:C:364:PHE:O	1.65	0.79
1:B:310:LEU:HD12	1:B:311:VAL:HG23	1.64	0.77
1:F:79:TYR:HD2	1:F:345:VAL:HG11	1.50	0.77
1:C:17:ARG:NH2	1:C:38:ARG:HH22	1.81	0.77
1:B:17:ARG:NH2	1:B:38:ARG:HH22	1.82	0.77
1:E:79:TYR:HD2	1:E:345:VAL:HG11	1.51	0.76
1:C:79:TYR:HD2	1:C:345:VAL:HG11	1.51	0.75
1:C:50:GLN:HG3	1:E:61:ALA:HB1	1.68	0.75
1:F:351:ARG:HH12	1:F:370:GLU:HG3	1.52	0.75
1:A:119:ILE:HG23	1:A:192:LEU:HD23	1.69	0.74
1:B:351:ARG:HH12	1:B:370:GLU:HG3	1.52	0.74
1:B:272:TYR:HD2	1:B:273:CYS:HG	1.37	0.72
1:B:144:ASP:HB3	1:B:150:LEU:HD21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:TYR:HD2	1:B:345:VAL:HG11	1.53	0.72
1:A:71:MET:HE2	1:F:71:MET:SD	2.30	0.72
1:D:272:TYR:HD2	1:D:273:CYS:HG	1.37	0.72
1:B:227:HIS:HB2	4:B:704:HOH:O	1.92	0.70
1:C:262:TRP:CZ3	1:C:366:HIS:O	2.45	0.67
1:B:150:LEU:H	1:B:150:LEU:HD22	1.59	0.67
1:D:79:TYR:HD2	1:D:345:VAL:HG11	1.58	0.66
1:F:289:GLU:HG3	1:F:316:TRP:HH2	1.60	0.66
1:A:122:PRO:HG3	1:A:183:PHE:HE1	1.60	0.65
1:C:262:TRP:CH2	1:C:364:PHE:O	2.48	0.64
1:C:479:ARG:HG3	1:C:479:ARG:HH11	1.63	0.63
1:C:79:TYR:CD2	1:C:345:VAL:HG11	2.33	0.62
1:C:224:GLU:HA	1:C:227:HIS:ND1	2.15	0.62
1:D:79:TYR:CD2	1:D:345:VAL:HG11	2.35	0.62
1:F:79:TYR:CD2	1:F:345:VAL:HG11	2.34	0.62
1:A:79:TYR:CD2	1:A:345:VAL:HG11	2.35	0.61
1:A:272:TYR:HD2	1:A:273:CYS:HG	1.49	0.61
1:D:224:GLU:HA	1:D:227:HIS:HD2	1.66	0.61
1:C:272:TYR:HD2	1:C:273:CYS:HG	1.48	0.60
1:D:479:ARG:HG3	1:D:479:ARG:HH11	1.66	0.60
1:A:79:TYR:HD2	1:A:345:VAL:HG11	1.65	0.60
1:C:494:TRP:CD1	1:C:498:ARG:HD3	2.36	0.60
1:B:272:TYR:HD2	1:B:273:CYS:SG	2.24	0.60
1:F:273:CYS:SG	1:F:383:LYS:HD2	2.43	0.59
1:E:39:ILE:HB	1:E:112:MET:CE	2.33	0.59
1:B:479:ARG:HH11	1:B:479:ARG:HG3	1.68	0.59
1:A:272:TYR:HD2	1:A:273:CYS:SG	2.25	0.59
1:B:79:TYR:CD2	1:B:345:VAL:HG11	2.35	0.58
1:F:224:GLU:HA	1:F:227:HIS:HD2	1.68	0.58
1:E:79:TYR:CD2	1:E:345:VAL:HG11	2.36	0.58
1:E:479:ARG:HG3	1:E:479:ARG:HH11	1.67	0.58
1:E:287:THR:HG23	1:E:290:GLN:H	1.69	0.57
1:A:122:PRO:HG3	1:A:183:PHE:CZ	2.40	0.57
1:C:272:TYR:HD2	1:C:273:CYS:SG	2.27	0.57
1:F:479:ARG:HG3	1:F:479:ARG:HH11	1.68	0.57
1:B:145:ALA:HA	1:B:162:LEU:HD11	1.85	0.57
1:F:294:HIS:HD2	4:F:736:HOH:O	1.86	0.57
1:F:217:TRP:CH2	1:F:240:GLU:HG2	2.40	0.57
1:B:257:ARG:HG2	1:B:261:THR:OG1	2.05	0.56
1:C:145:ALA:HA	1:C:162:LEU:HD11	1.86	0.56
1:A:391:PHE:CD1	2:A:601:GTP:C5	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:O	1:D:49:GLN:HG2	2.06	0.56
1:E:145:ALA:HA	1:E:162:LEU:HD11	1.88	0.56
1:A:46:ARG:O	1:A:49:GLN:HG2	2.06	0.55
1:D:94:LEU:HD23	1:D:100:ASP:HA	1.88	0.55
1:D:224:GLU:HA	1:D:227:HIS:CD2	2.40	0.55
1:E:40:ILE:HG13	1:E:112:MET:HE1	1.87	0.55
1:A:224:GLU:HA	1:A:227:HIS:ND1	2.22	0.55
1:C:217:TRP:HH2	1:C:240:GLU:HG3	1.71	0.55
1:F:46:ARG:O	1:F:49:GLN:HG2	2.06	0.55
1:A:479:ARG:HG2	1:A:479:ARG:HH11	1.71	0.55
1:C:313:GLU:O	1:C:317:GLU:OE1	2.24	0.55
1:E:46:ARG:O	1:E:49:GLN:HG2	2.07	0.55
1:A:119:ILE:HG23	1:A:192:LEU:CD2	2.38	0.54
1:B:4:ILE:CD1	1:B:356:LEU:HD12	2.35	0.54
1:A:122:PRO:CG	1:A:183:PHE:CE1	2.87	0.54
1:C:410:LEU:HD12	1:C:485:ILE:HD12	1.89	0.54
1:D:272:TYR:HD2	1:D:273:CYS:SG	2.30	0.54
1:B:54:VAL:HG11	1:B:391:PHE:HE1	1.73	0.54
1:A:122:PRO:CG	1:A:183:PHE:HE1	2.20	0.54
1:B:46:ARG:O	1:B:49:GLN:HG2	2.07	0.54
1:A:145:ALA:HA	1:A:162:LEU:HD11	1.89	0.54
1:A:397:GLU:HB3	1:B:442:ARG:HG2	1.89	0.54
1:D:145:ALA:HA	1:D:162:LEU:HD11	1.88	0.54
1:A:410:LEU:HD12	1:A:485:ILE:HD12	1.90	0.54
1:C:217:TRP:CH2	1:C:240:GLU:HG3	2.43	0.54
1:F:216:ALA:HA	1:F:233:PRO:HB3	1.89	0.53
1:A:216:ALA:HA	1:A:233:PRO:HB3	1.90	0.53
1:F:145:ALA:HA	1:F:162:LEU:HD11	1.90	0.53
1:B:356:LEU:HD13	1:B:360:PHE:HB2	1.90	0.53
1:C:46:ARG:O	1:C:49:GLN:HG2	2.09	0.53
1:E:216:ALA:HA	1:E:233:PRO:HB3	1.91	0.53
1:D:350:GLN:HA	1:D:350:GLN:NE2	2.24	0.53
1:C:216:ALA:HA	1:C:233:PRO:HB3	1.91	0.52
1:B:216:ALA:HA	1:B:233:PRO:HB3	1.90	0.52
1:F:224:GLU:HA	1:F:227:HIS:CD2	2.45	0.52
1:A:172:LEU:HD11	1:A:472:TRP:CZ2	2.45	0.52
1:E:39:ILE:HB	1:E:112:MET:HE3	1.92	0.52
1:C:147:SER:C	1:C:149:PRO:HG2	2.35	0.52
1:C:479:ARG:HG3	1:C:479:ARG:NH1	2.23	0.52
1:F:306:SER:C	1:F:310:LEU:HD12	2.35	0.52
1:E:217:TRP:HH2	1:E:240:GLU:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:HIS:CD2	1:A:126:HIS:N	2.72	0.51
1:F:172:LEU:HD11	1:F:472:TRP:CZ2	2.45	0.51
1:C:259:PRO:O	1:C:262:TRP:HD1	1.93	0.51
1:E:172:LEU:HD11	1:E:472:TRP:CZ2	2.46	0.51
1:C:229:LEU:HD21	1:C:262:TRP:CH2	2.46	0.51
1:C:337:ARG:O	1:C:341:LEU:HD23	2.11	0.50
1:D:222:THR:OG1	1:D:223:PRO:HA	2.12	0.50
1:A:126:HIS:NE2	4:A:703:HOH:O	2.35	0.50
1:D:216:ALA:HA	1:D:233:PRO:HB3	1.93	0.50
1:A:71:MET:HE1	1:F:67:LEU:HD21	1.93	0.50
1:A:400:GLU:OE2	1:B:442:ARG:CZ	2.59	0.50
1:A:448:SER:HB2	1:A:451:HIS:ND1	2.27	0.50
2:A:601:GTP:H5'	2:A:601:GTP:C8	2.47	0.50
1:D:479:ARG:HG3	1:D:479:ARG:NH1	2.27	0.50
1:C:172:LEU:HD11	1:C:472:TRP:CZ2	2.47	0.49
1:D:172:LEU:HD11	1:D:472:TRP:CZ2	2.46	0.49
1:C:494:TRP:HD1	1:C:498:ARG:HD3	1.78	0.49
1:E:479:ARG:HG3	1:E:479:ARG:NH1	2.26	0.49
1:F:17:ARG:NH2	1:F:200:ASN:HD22	2.09	0.49
1:A:50:GLN:HG3	1:F:61:ALA:HB1	1.94	0.49
1:D:94:LEU:CD2	1:D:100:ASP:HA	2.41	0.49
1:A:418:LEU:HD11	1:A:481:LEU:HD23	1.95	0.49
1:D:179:ASP:OD1	1:D:216:ALA:HB3	2.12	0.49
1:D:369:LEU:N	1:D:369:LEU:HD22	2.27	0.49
1:F:59:ARG:C	1:F:61:ALA:HB2	2.38	0.49
1:B:377:ASP:HA	1:B:380:LYS:HD2	1.94	0.49
1:E:350:GLN:HA	1:E:350:GLN:NE2	2.28	0.48
1:F:350:GLN:HA	1:F:350:GLN:NE2	2.28	0.48
1:E:377:ASP:HA	1:E:380:LYS:HD2	1.95	0.48
1:A:313:GLU:O	1:A:317:GLU:OE1	2.32	0.48
1:A:369:LEU:N	1:A:369:LEU:HD22	2.28	0.48
1:A:211:LYS:HA	1:A:261:THR:HG21	1.96	0.48
1:B:133:ASN:O	1:B:137:ARG:HB2	2.14	0.48
1:E:371:ASP:HA	1:E:380:LYS:NZ	2.29	0.48
1:E:217:TRP:CH2	1:E:240:GLU:HG3	2.48	0.48
1:A:133:ASN:O	1:A:137:ARG:HB2	2.13	0.48
1:F:371:ASP:HA	1:F:380:LYS:NZ	2.29	0.48
1:A:67:LEU:HG	1:A:71:MET:HE3	1.96	0.47
1:A:114:CYS:O	1:A:117:HIS:ND1	2.36	0.47
1:F:29:LEU:HD12	4:F:730:HOH:O	2.14	0.47
1:F:479:ARG:HG3	1:F:479:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ARG:HH22	1:C:38:ARG:NH2	1.93	0.47
1:E:17:ARG:HH22	1:E:38:ARG:HH22	1.61	0.47
1:A:113:SER:O	1:A:264:MET:HE2	2.15	0.47
1:B:117:HIS:O	1:B:118:ASP:HB2	2.14	0.47
1:B:479:ARG:HG3	1:B:479:ARG:NH1	2.29	0.47
1:C:59:ARG:HH11	1:E:491:LEU:HD23	1.79	0.47
1:C:428:LEU:HD11	1:C:441:SER:HA	1.97	0.47
1:A:232:LYS:HD2	2:A:601:GTP:O1G	2.14	0.47
1:A:377:ASP:HA	1:A:380:LYS:HD2	1.95	0.47
1:A:391:PHE:N	1:A:391:PHE:CD2	2.80	0.47
1:B:54:VAL:HG11	1:B:391:PHE:CE1	2.49	0.47
1:D:377:ASP:HA	1:D:380:LYS:HD2	1.95	0.47
1:B:172:LEU:HD11	1:B:472:TRP:CZ2	2.50	0.46
1:C:377:ASP:HA	1:C:380:LYS:HD2	1.97	0.46
1:F:377:ASP:HA	1:F:380:LYS:HD2	1.96	0.46
1:E:116:MET:HE1	1:E:193:VAL:HG11	1.97	0.46
1:A:479:ARG:HG2	1:A:479:ARG:NH1	2.31	0.46
1:C:117:HIS:O	1:C:118:ASP:HB2	2.16	0.46
1:E:496:GLU:HG2	1:E:499:ARG:HH21	1.81	0.46
1:F:169:LEU:HD23	1:F:173:ARG:NH1	2.30	0.46
1:B:405:ARG:HG3	1:B:405:ARG:HH11	1.81	0.46
1:E:211:LYS:HA	1:E:261:THR:HG21	1.97	0.46
1:A:369:LEU:HD22	1:A:369:LEU:H	1.81	0.45
1:B:16:TYR:H	1:B:200:ASN:ND2	2.14	0.45
1:D:418:LEU:HD11	1:D:481:LEU:HD23	1.98	0.45
1:B:221:GLU:O	1:B:223:PRO:HD3	2.15	0.45
1:E:369:LEU:N	1:E:369:LEU:HD22	2.32	0.45
1:A:169:LEU:HD23	1:A:173:ARG:NH1	2.30	0.45
1:F:213:THR:HB	1:F:255:TYR:HA	1.98	0.45
1:C:273:CYS:SG	1:C:383:LYS:HA	2.56	0.45
1:C:211:LYS:HA	1:C:261:THR:HG21	1.99	0.45
1:D:504:GLU:OE2	1:D:504:GLU:HA	2.16	0.45
1:E:169:LEU:HD23	1:E:173:ARG:NH1	2.31	0.45
1:E:405:ARG:HH11	1:E:405:ARG:HG3	1.82	0.45
1:A:163:ARG:HB2	1:A:167:GLU:OE1	2.16	0.45
1:B:428:LEU:HD11	1:B:441:SER:HA	1.99	0.45
1:D:133:ASN:O	1:D:137:ARG:HB2	2.17	0.45
1:F:133:ASN:O	1:F:137:ARG:HB2	2.17	0.45
1:D:369:LEU:HD22	1:D:369:LEU:H	1.81	0.45
1:D:428:LEU:HD11	1:D:441:SER:HA	1.98	0.45
1:E:369:LEU:HD22	1:E:369:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:LEU:HD22	1:F:369:LEU:N	2.32	0.45
1:C:11:ASN:H	1:C:204:ALA:HB2	1.81	0.44
1:E:133:ASN:O	1:E:137:ARG:HB2	2.17	0.44
1:E:428:LEU:HD11	1:E:441:SER:HA	1.99	0.44
1:E:503:VAL:HG12	1:F:498:ARG:HG2	1.99	0.44
1:A:410:LEU:HA	1:A:410:LEU:HD22	1.84	0.44
1:A:451:HIS:CD2	1:A:483:ASP:HB3	2.52	0.44
1:D:211:LYS:HA	1:D:261:THR:HG21	1.99	0.44
1:D:437:PHE:HB3	1:D:440:GLU:HB2	1.99	0.44
1:F:428:LEU:HD11	1:F:441:SER:HA	1.99	0.44
1:C:133:ASN:O	1:C:137:ARG:HB2	2.18	0.44
1:E:306:SER:C	1:E:310:LEU:HD12	2.42	0.44
1:B:418:LEU:HD11	1:B:481:LEU:HD23	1.99	0.44
1:A:437:PHE:HB3	1:A:440:GLU:HB2	2.00	0.44
1:B:356:LEU:HD13	1:B:356:LEU:O	2.18	0.44
1:A:428:LEU:HD11	1:A:441:SER:HA	2.00	0.44
1:F:369:LEU:HD22	1:F:369:LEU:H	1.83	0.44
1:A:179:ASP:OD1	1:A:216:ALA:HB3	2.18	0.43
1:C:391:PHE:HB3	2:C:601:GTP:C6	2.53	0.43
1:B:329:GLU:HG3	1:B:330:ASP:H	1.84	0.43
1:E:273:CYS:SG	1:E:383:LYS:HA	2.58	0.43
1:A:213:THR:HB	1:A:255:TYR:HA	2.00	0.43
1:B:169:LEU:HD23	1:B:173:ARG:NH1	2.33	0.43
1:B:391:PHE:HB3	2:B:601:GTP:O6	2.18	0.43
1:D:11:ASN:H	1:D:204:ALA:HB2	1.84	0.43
1:D:439:ILE:HD13	1:E:127:PHE:HE2	1.81	0.43
1:E:39:ILE:CG2	1:E:112:MET:HE3	2.48	0.43
1:B:258:PHE:HB3	1:B:261:THR:HG23	2.01	0.43
1:C:23:LYS:HA	1:C:27:GLU:OE1	2.19	0.43
1:F:211:LYS:HA	1:F:261:THR:HG21	2.00	0.43
1:B:369:LEU:HD13	1:B:379:LEU:HD11	2.00	0.43
1:D:213:THR:HB	1:D:255:TYR:HA	2.00	0.43
1:D:74:GLN:OE1	1:D:115:LEU:HD13	2.19	0.42
1:C:489:THR:HG23	1:C:492:TYR:HB3	2.01	0.42
1:C:213:THR:HB	1:C:255:TYR:HA	2.00	0.42
1:E:116:MET:CE	1:E:193:VAL:HG11	2.49	0.42
1:E:437:PHE:HB3	1:E:440:GLU:HB2	2.00	0.42
1:E:11:ASN:H	1:E:204:ALA:HB2	1.83	0.42
1:A:273:CYS:SG	1:A:383:LYS:HA	2.60	0.42
1:C:437:PHE:HB3	1:C:440:GLU:HB2	2.01	0.42
1:C:489:THR:HG23	1:C:492:TYR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:HD12	1:D:57:LEU:H	1.83	0.42
1:F:11:ASN:H	1:F:204:ALA:HB2	1.84	0.42
1:D:350:GLN:HA	1:D:350:GLN:HE21	1.83	0.42
1:B:272:TYR:CE1	2:B:601:GTP:H5''	2.55	0.42
1:B:273:CYS:SG	1:B:383:LYS:HA	2.60	0.42
1:E:442:ARG:HG2	1:F:397:GLU:HB3	2.01	0.42
1:A:405:ARG:HE	1:A:405:ARG:HB2	1.56	0.42
1:D:273:CYS:SG	1:D:383:LYS:HA	2.59	0.42
1:F:437:PHE:HB3	1:F:440:GLU:HB2	2.02	0.42
1:F:24:THR:HB	1:F:27:GLU:H	1.85	0.41
1:F:117:HIS:O	1:F:118:ASP:HB2	2.19	0.41
1:C:190:ILE:HG21	1:C:243:ILE:HD11	2.02	0.41
1:C:481:LEU:C	1:C:481:LEU:HD23	2.46	0.41
1:D:39:ILE:HD13	1:D:112:MET:HB3	2.00	0.41
1:D:61:ALA:HB1	1:D:63:VAL:HG12	2.01	0.41
1:A:400:GLU:OE2	1:B:442:ARG:NH2	2.53	0.41
1:F:306:SER:O	1:F:310:LEU:HD12	2.20	0.41
1:C:24:THR:HB	1:C:27:GLU:H	1.84	0.41
1:E:163:ARG:HB2	1:E:167:GLU:OE1	2.20	0.41
1:A:39:ILE:HD13	1:A:112:MET:HB3	2.02	0.41
1:C:39:ILE:HD13	1:C:112:MET:HB3	2.01	0.41
1:E:39:ILE:CB	1:E:112:MET:HE3	2.50	0.41
1:C:39:ILE:O	1:C:45:ILE:HG12	2.20	0.41
1:C:215:PRO:HB3	1:C:217:TRP:CH2	2.55	0.41
1:D:23:LYS:HA	1:D:27:GLU:OE1	2.19	0.41
1:E:213:THR:HB	1:E:255:TYR:HA	2.02	0.41
1:A:496:GLU:HG2	1:A:499:ARG:HH21	1.85	0.41
1:B:213:THR:HB	1:B:255:TYR:HA	2.02	0.41
1:F:145:ALA:HB1	1:F:174:ARG:HG2	2.01	0.41
1:A:170:ASN:HA	1:A:173:ARG:HD2	2.03	0.41
1:B:190:ILE:HG13	1:B:209:ILE:HD12	2.03	0.41
1:C:169:LEU:HD23	1:C:173:ARG:NH1	2.36	0.41
1:A:397:GLU:OE1	1:B:442:ARG:HG2	2.21	0.41
1:D:217:TRP:HH2	1:D:240:GLU:HG2	1.86	0.41
1:F:215:PRO:HB3	1:F:217:TRP:CH2	2.55	0.41
1:A:439:ILE:HD13	1:C:127:PHE:HE2	1.86	0.40
1:D:502:ALA:HB1	1:E:406:VAL:HG23	2.03	0.40
1:E:194:HIS:HD2	4:E:728:HOH:O	2.04	0.40
1:E:479:ARG:HH11	1:E:479:ARG:CG	2.34	0.40
1:F:88:LEU:HD12	1:F:88:LEU:HA	1.96	0.40
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:VAL:HG11	1:D:160:LEU:HD23	2.03	0.40
1:E:39:ILE:HD13	1:E:112:MET:HB3	2.03	0.40
1:A:190:ILE:HG13	1:A:209:ILE:HD12	2.03	0.40
1:E:94:LEU:HD12	1:E:94:LEU:HA	1.86	0.40
1:C:145:ALA:HB1	1:C:174:ARG:HG2	2.03	0.40
1:E:145:ALA:HB1	1:E:174:ARG:HG2	2.03	0.40
1:E:215:PRO:HB3	1:E:217:TRP:CH2	2.57	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	469/505 (93%)	445 (95%)	19 (4%)	5 (1%)	11	39
1	B	459/505 (91%)	430 (94%)	20 (4%)	9 (2%)	6	27
1	C	464/505 (92%)	437 (94%)	20 (4%)	7 (2%)	8	33
1	D	460/505 (91%)	429 (93%)	24 (5%)	7 (2%)	8	33
1	E	468/505 (93%)	442 (94%)	19 (4%)	7 (2%)	8	33
1	F	461/505 (91%)	438 (95%)	18 (4%)	5 (1%)	11	39
All	All	2781/3030 (92%)	2621 (94%)	120 (4%)	40 (1%)	9	34

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	GLU
1	D	60	ASN
1	E	61	ALA
1	E	222	THR
1	E	371	ASP

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Mol	Chain	Res	Type
1	F	167	GLU
1	A	164	ASP
1	B	54	VAL
1	C	328	THR
1	E	54	VAL
1	F	54	VAL
1	F	371	ASP
1	A	432	GLU
1	B	225	THR
1	B	328	THR
1	B	432	GLU
1	C	150	LEU
1	C	432	GLU
1	D	328	THR
1	D	432	GLU
1	E	432	GLU
1	A	430	GLU
1	B	118	ASP
1	B	430	GLU
1	C	23	LYS
1	C	430	GLU
1	D	272	TYR
1	D	372	ALA
1	D	430	GLU
1	E	430	GLU
1	F	272	TYR
1	F	430	GLU
1	A	272	TYR
1	B	23	LYS
1	B	272	TYR
1	C	272	TYR
1	E	272	TYR
1	A	149	PRO
1	B	149	PRO
1	D	23	LYS

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	427/450 (95%)	383 (90%)	44 (10%)	7	25
1	B	421/450 (94%)	377 (90%)	44 (10%)	6	24
1	C	426/450 (95%)	382 (90%)	44 (10%)	7	25
1	D	421/450 (94%)	379 (90%)	42 (10%)	7	27
1	E	427/450 (95%)	387 (91%)	40 (9%)	8	29
1	F	422/450 (94%)	379 (90%)	43 (10%)	7	26
All	All	2544/2700 (94%)	2287 (90%)	257 (10%)	7	26

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	17	ARG
1	A	29	LEU
1	A	45	ILE
1	A	60	ASN
1	A	87	ARG
1	A	88	LEU
1	A	89	LYS
1	A	107	GLU
1	A	118	ASP
1	A	119	ILE
1	A	126	HIS
1	A	140	LEU
1	A	143	GLU
1	A	146	GLU
1	A	150	LEU
1	A	190	ILE
1	A	209	ILE
1	A	227	HIS
1	A	274	VAL
1	A	283	LYS
1	A	289	GLU
1	A	296	HIS
1	A	309	SER
1	A	310	LEU
1	A	312	VAL
1	A	331	GLN
1	A	368(A)	LEU

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Mol	Chain	Res	Type
1	A	369	LEU
1	A	381	LEU
1	A	405	ARG
1	A	410	LEU
1	A	420	LEU
1	A	421	SER
1	A	430	GLU
1	A	435	LYS
1	A	446	LYS
1	A	449	THR
1	A	453	LEU
1	A	457	GLU
1	A	479	ARG
1	A	489	THR
1	A	490	ASP
1	A	503	VAL
1	B	29	LEU
1	B	45	ILE
1	B	87	ARG
1	B	88	LEU
1	B	90	GLU
1	B	95	GLU
1	B	107	GLU
1	B	140	LEU
1	B	143	GLU
1	B	146	GLU
1	B	150	LEU
1	B	151	THR
1	B	190	ILE
1	B	209	ILE
1	B	221	GLU
1	B	224	GLU
1	B	227	HIS
1	B	239	GLU
1	B	264	MET
1	B	274	VAL
1	B	283	LYS
1	B	296	HIS
1	B	310	LEU
1	B	312	VAL
1	B	331	GLN
1	B	356	LEU

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Mol	Chain	Res	Type
1	B	365	ASN
1	B	368(A)	LEU
1	B	369	LEU
1	B	370	GLU
1	B	381	LEU
1	B	410	LEU
1	B	415	ARG
1	B	420	LEU
1	B	421	SER
1	B	430	GLU
1	B	433	ARG
1	B	435	LYS
1	B	446	LYS
1	B	449	THR
1	B	453	LEU
1	B	479	ARG
1	B	489	THR
1	B	490	ASP
1	C	17	ARG
1	C	29	LEU
1	C	45	ILE
1	C	87	ARG
1	C	88	LEU
1	C	89	LYS
1	C	95	GLU
1	C	107	GLU
1	C	140	LEU
1	C	143	GLU
1	C	147	SER
1	C	167	GLU
1	C	190	ILE
1	C	191	ARG
1	C	209	ILE
1	C	221	GLU
1	C	224	GLU
1	C	227	HIS
1	C	264	MET
1	C	274	VAL
1	C	283	LYS
1	C	296	HIS
1	C	309	SER
1	C	310	LEU

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Mol	Chain	Res	Type
1	C	312	VAL
1	C	314	ASN
1	C	334	MET
1	C	350	GLN
1	C	368(A)	LEU
1	C	369	LEU
1	C	381	LEU
1	C	405	ARG
1	C	410	LEU
1	C	415	ARG
1	C	420	LEU
1	C	421	SER
1	C	430	GLU
1	C	446	LYS
1	C	449	THR
1	C	453	LEU
1	C	479	ARG
1	C	489	THR
1	C	490	ASP
1	C	503	VAL
1	D	17	ARG
1	D	29	LEU
1	D	40	ILE
1	D	45	ILE
1	D	87	ARG
1	D	88	LEU
1	D	90	GLU
1	D	94	LEU
1	D	107	GLU
1	D	140	LEU
1	D	143	GLU
1	D	190	ILE
1	D	209	ILE
1	D	221	GLU
1	D	227	HIS
1	D	264	MET
1	D	274	VAL
1	D	283	LYS
1	D	284	ARG
1	D	296	HIS
1	D	310	LEU
1	D	312	VAL

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Mol	Chain	Res	Type
1	D	328	THR
1	D	350	GLN
1	D	368(A)	LEU
1	D	369	LEU
1	D	371	ASP
1	D	375	CYS
1	D	381	LEU
1	D	410	LEU
1	D	420	LEU
1	D	421	SER
1	D	430	GLU
1	D	433	ARG
1	D	446	LYS
1	D	449	THR
1	D	453	LEU
1	D	479	ARG
1	D	489	THR
1	D	490	ASP
1	D	503	VAL
1	D	504	GLU
1	E	17	ARG
1	E	29	LEU
1	E	45	ILE
1	E	87	ARG
1	E	88	LEU
1	E	90	GLU
1	E	107	GLU
1	E	140	LEU
1	E	143	GLU
1	E	190	ILE
1	E	209	ILE
1	E	224	GLU
1	E	227	HIS
1	E	264	MET
1	E	274	VAL
1	E	283	LYS
1	E	296	HIS
1	E	310	LEU
1	E	312	VAL
1	E	334	MET
1	E	350	GLN
1	E	368(A)	LEU

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Mol	Chain	Res	Type
1	E	369	LEU
1	E	370	GLU
1	E	381	LEU
1	E	410	LEU
1	E	415	ARG
1	E	420	LEU
1	E	421	SER
1	E	430	GLU
1	E	433	ARG
1	E	435	LYS
1	E	446	LYS
1	E	449	THR
1	E	453	LEU
1	E	457	GLU
1	E	479	ARG
1	E	489	THR
1	E	490	ASP
1	E	503	VAL
1	F	29	LEU
1	F	45	ILE
1	F	87	ARG
1	F	88	LEU
1	F	90	GLU
1	F	107	GLU
1	F	140	LEU
1	F	143	GLU
1	F	146	GLU
1	F	166	GLU
1	F	190	ILE
1	F	209	ILE
1	F	221	GLU
1	F	224	GLU
1	F	227	HIS
1	F	240	GLU
1	F	264	MET
1	F	273	CYS
1	F	274	VAL
1	F	283	LYS
1	F	296	HIS
1	F	309	SER
1	F	310	LEU
1	F	312	VAL

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Mol	Chain	Res	Type
1	F	320	ARG
1	F	350	GLN
1	F	368(A)	LEU
1	F	369	LEU
1	F	381	LEU
1	F	405	ARG
1	F	410	LEU
1	F	415	ARG
1	F	420	LEU
1	F	421	SER
1	F	430	GLU
1	F	431	LYS
1	F	432	GLU
1	F	446	LYS
1	F	449	THR
1	F	453	LEU
1	F	479	ARG
1	F	489	THR
1	F	490	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	GLN
1	A	41	ASN
1	A	69	HIS
1	A	121	ASN
1	A	126	HIS
1	A	138	GLN
1	A	188	GLN
1	A	226	HIS
1	B	3	GLN
1	B	50	GLN
1	B	69	HIS
1	B	188	GLN
1	B	200	ASN
1	B	226	HIS
1	B	251	ASN
1	B	339	ASN
1	B	350	GLN
1	B	482	GLN

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Mol	Chain	Res	Type
1	C	20	GLN
1	C	69	HIS
1	C	188	GLN
1	C	226	HIS
1	C	251	ASN
1	C	294	HIS
1	C	350	GLN
1	C	366	HIS
1	C	389	HIS
1	C	482	GLN
1	D	50	GLN
1	D	60	ASN
1	D	69	HIS
1	D	121	ASN
1	D	188	GLN
1	D	226	HIS
1	D	227	HIS
1	D	482	GLN
1	E	41	ASN
1	E	69	HIS
1	E	188	GLN
1	E	226	HIS
1	E	294	HIS
1	E	389	HIS
1	F	50	GLN
1	F	69	HIS
1	F	188	GLN
1	F	200	ASN
1	F	226	HIS
1	F	227	HIS
1	F	251	ASN
1	F	482	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	GTP	D	601	-	33,34,34	0.43	0	50,54,54	0.52	0
2	GTP	C	601	-	33,34,34	0.57	0	50,54,54	0.68	0
2	GTP	A	601	-	33,34,34	1.31	5 (15%)	50,54,54	1.83	8 (16%)
2	GTP	E	601	-	33,34,34	0.44	0	50,54,54	0.51	0
2	GTP	B	601	-	33,34,34	0.45	0	50,54,54	0.54	0
2	GTP	F	601	-	33,34,34	0.44	0	50,54,54	0.50	0

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	GTP	D	601	-	-	9/22/38/38	0/3/3/3
2	GTP	C	601	-	-	2/22/38/38	0/3/3/3
2	GTP	A	601	-	-	2/22/38/38	0/3/3/3
2	GTP	E	601	-	-	5/22/38/38	0/3/3/3
2	GTP	B	601	-	-	1/22/38/38	0/3/3/3
2	GTP	F	601	-	-	5/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GTP	C6-N1	-2.99	1.33	1.38
2	A	601	GTP	C5-N7	-2.64	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GTP	C4-N9	-2.41	1.31	1.38
2	A	601	GTP	C5-C4	2.32	1.45	1.38
2	A	601	GTP	C2-N1	-2.09	1.32	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GTP	C5-C4-N3	-5.95	118.93	128.39
2	A	601	GTP	C2-N3-C4	4.98	120.88	112.30
2	A	601	GTP	C6-C5-N7	3.94	137.46	130.29
2	A	601	GTP	N9-C4-N3	3.89	133.73	125.95
2	A	601	GTP	C4-C5-N7	-3.04	105.86	110.67
2	A	601	GTP	O4'-C1'-N9	-2.60	102.46	108.36
2	A	601	GTP	O3G-PG-O2G	2.24	116.21	107.80
2	A	601	GTP	C3'-C2'-C1'	2.06	105.36	101.46

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GTP	PB-O3B-PG-O2G
2	C	601	GTP	PB-O3B-PG-O3G
2	D	601	GTP	PB-O3B-PG-O2G
2	D	601	GTP	C5'-O5'-PA-O1A
2	E	601	GTP	C5'-O5'-PA-O2A
2	D	601	GTP	O4'-C4'-C5'-O5'
2	D	601	GTP	C3'-C4'-C5'-O5'
2	D	601	GTP	C5'-O5'-PA-O3A
2	E	601	GTP	C5'-O5'-PA-O3A
2	F	601	GTP	C5'-O5'-PA-O3A
2	F	601	GTP	C5'-O5'-PA-O1A
2	F	601	GTP	C5'-O5'-PA-O2A
2	E	601	GTP	PB-O3A-PA-O2A
2	F	601	GTP	PA-O3A-PB-O2B
2	C	601	GTP	O4'-C4'-C5'-O5'
2	D	601	GTP	PB-O3B-PG-O3G
2	A	601	GTP	PB-O3A-PA-O1A
2	A	601	GTP	PB-O3A-PA-O2A
2	E	601	GTP	PB-O3A-PA-O1A
2	D	601	GTP	PB-O3B-PG-O1G
2	D	601	GTP	PG-O3B-PB-O2B
2	D	601	GTP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	E	601	GTP	PA-O3A-PB-O2B
2	F	601	GTP	PA-O3A-PB-O1B

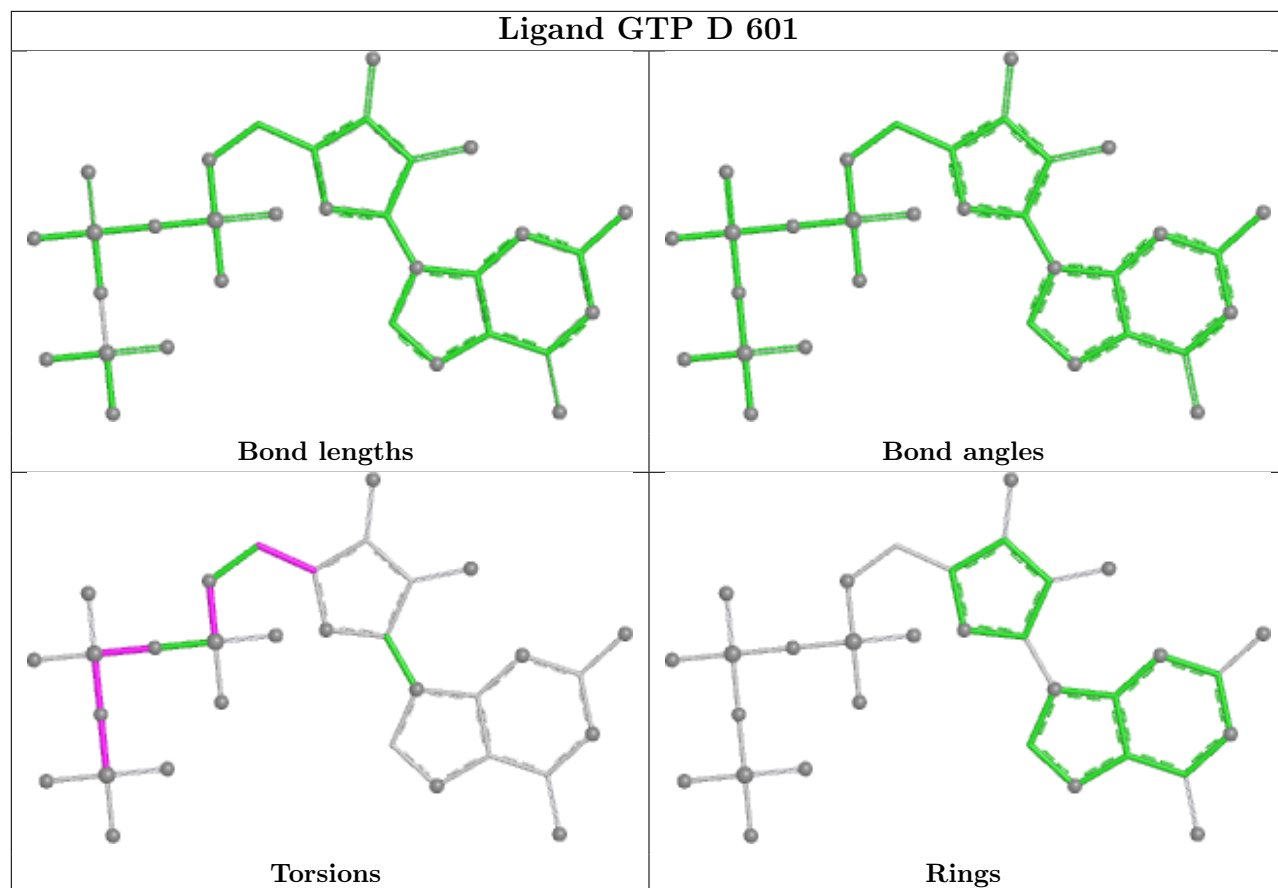
There are no ring outliers.

3 monomers are involved in 7 short contacts:

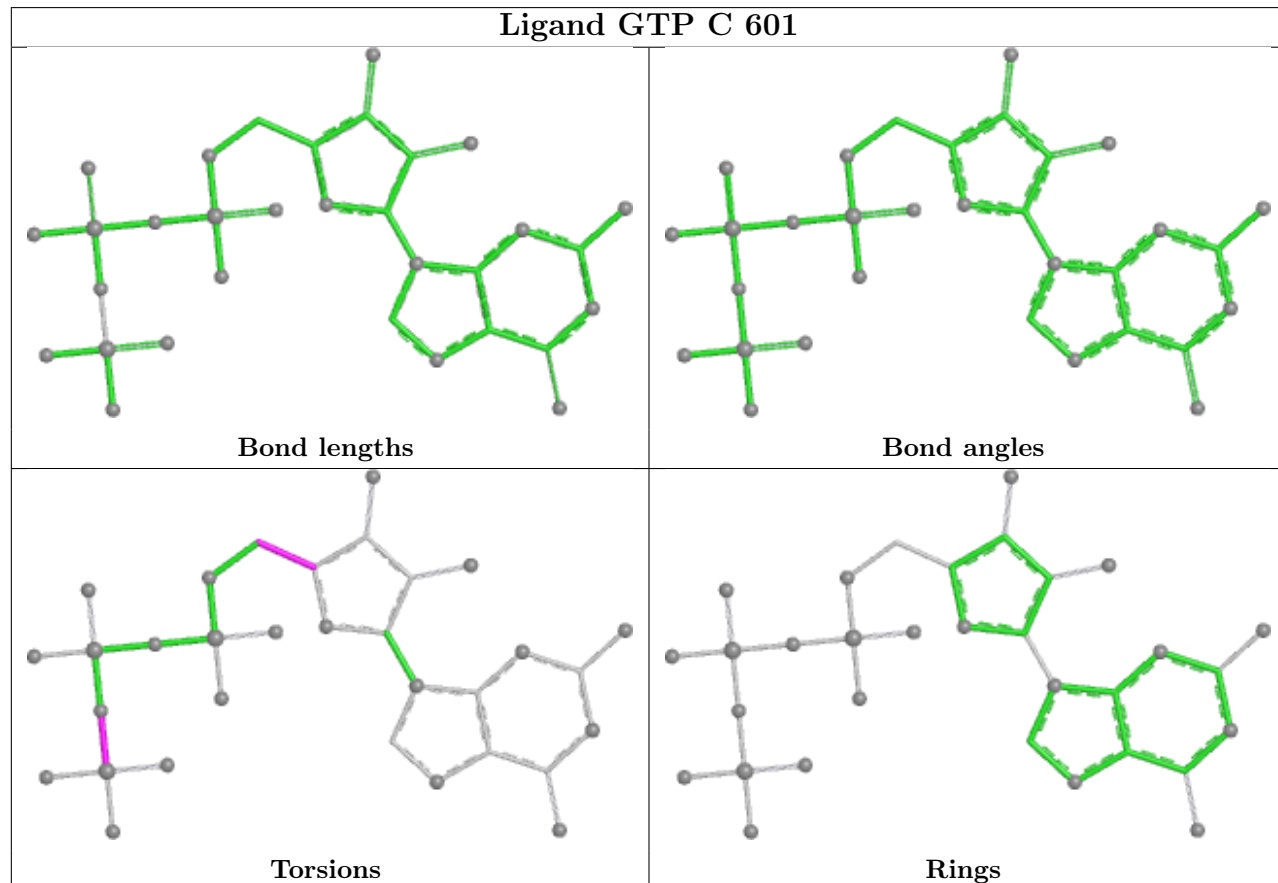
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	GTP	1	0
2	A	601	GTP	4	0
2	B	601	GTP	2	0

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.

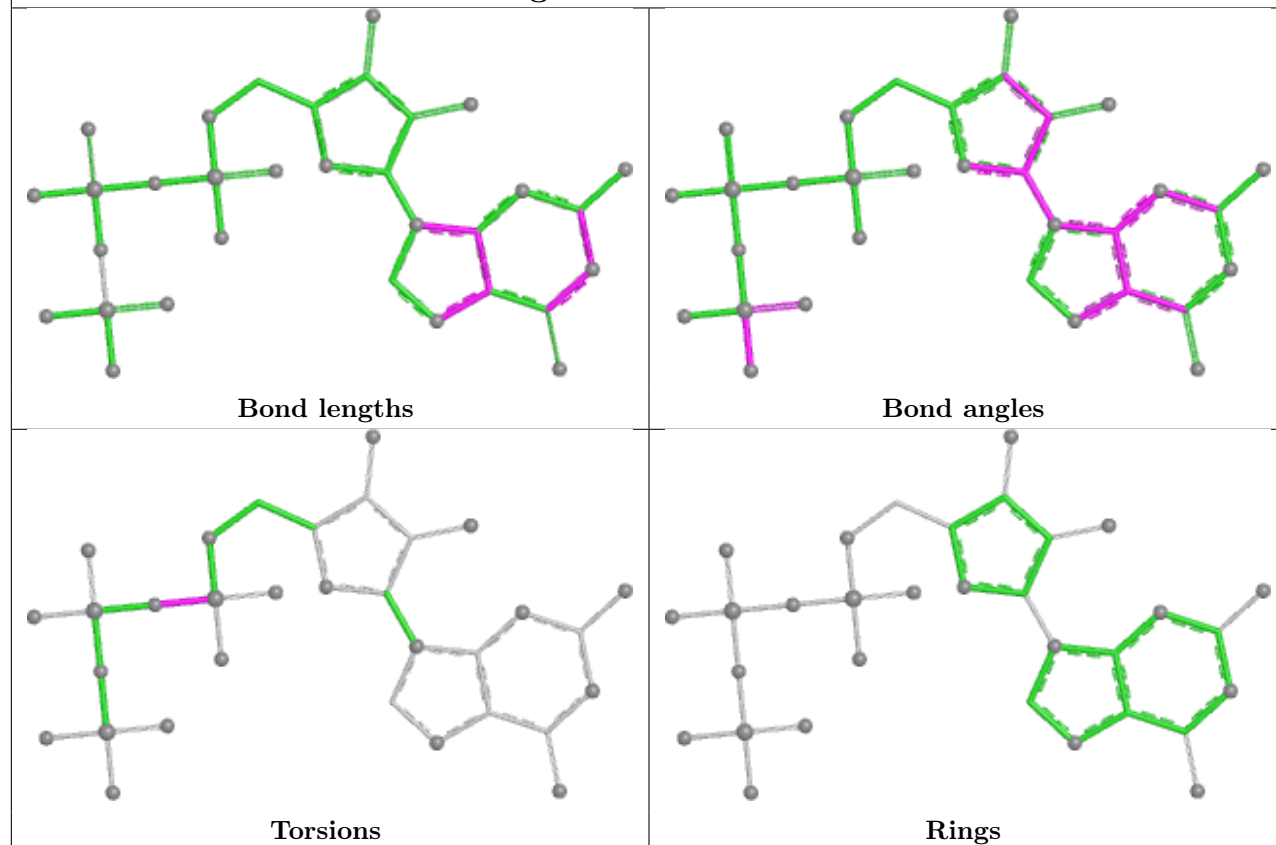
Ligand GTP D 601



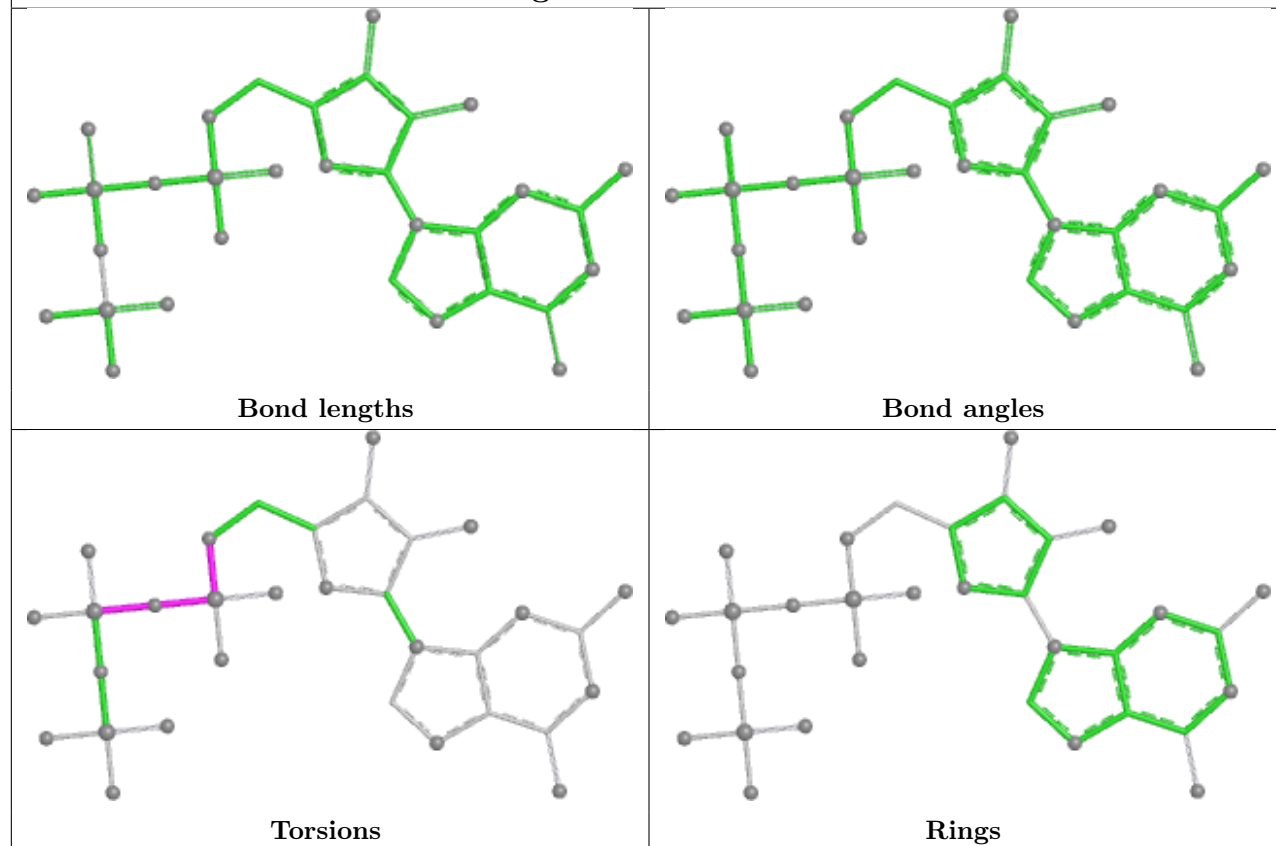
Ligand GTP C 601



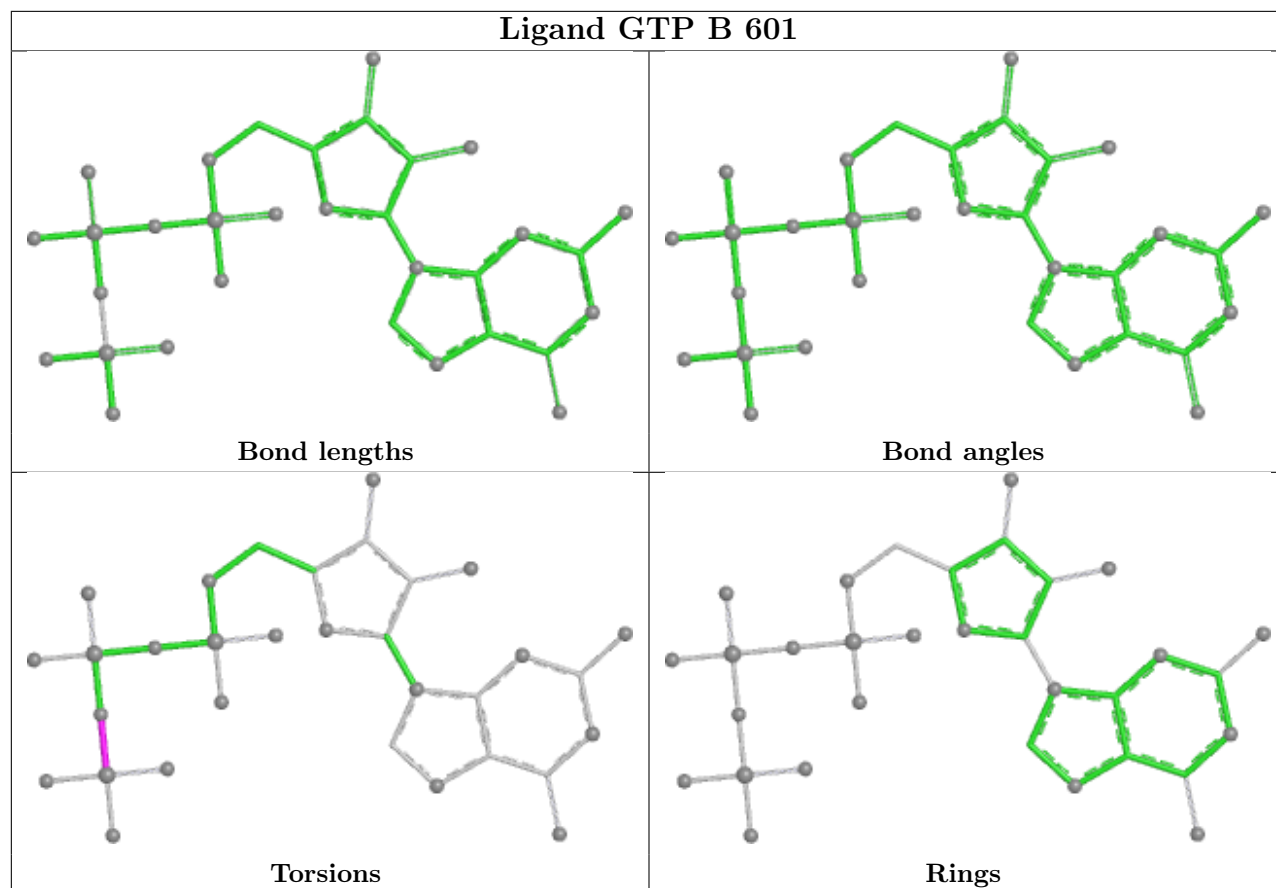
Ligand GTP A 601



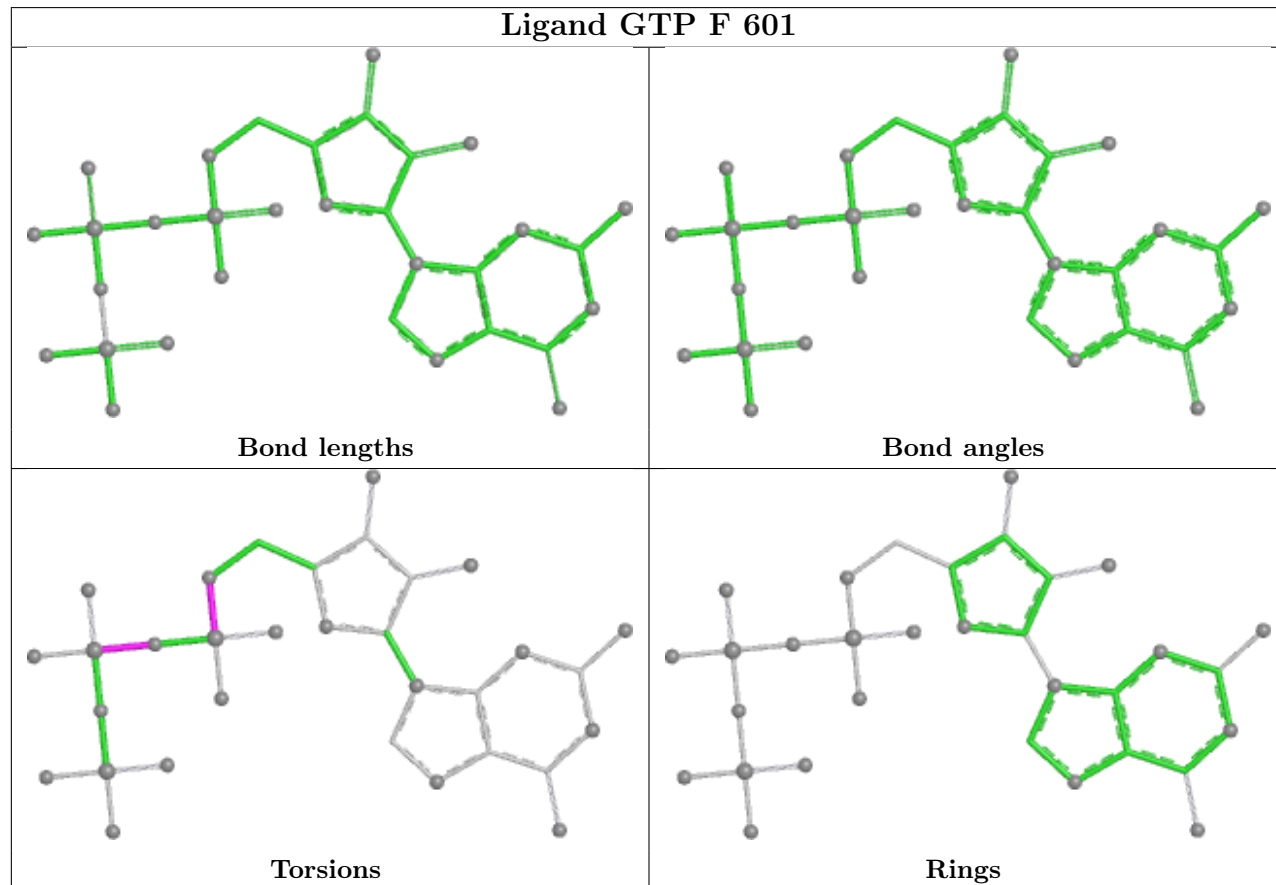
Ligand GTP E 601



Ligand GTP B 601



Ligand GTP F 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	477/505 (94%)	-0.24	3 (0%)	85 72	43, 99, 160, 189	1 (0%)
1	B	471/505 (93%)	-0.06	2 (0%)	88 78	56, 145, 198, 211	2 (0%)
1	C	478/505 (94%)	-0.26	7 (1%)	72 52	51, 101, 161, 186	2 (0%)
1	D	472/505 (93%)	-0.08	6 (1%)	75 55	58, 146, 185, 200	0
1	E	478/505 (94%)	-0.26	4 (0%)	82 66	57, 108, 162, 190	0
1	F	475/505 (94%)	-0.25	2 (0%)	88 78	52, 111, 160, 194	2 (0%)
All	All	2851/3030 (94%)	-0.19	24 (0%)	82 66	43, 118, 177, 211	7 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	HIS	5.3
1	C	149	PRO	3.6
1	C	375	CYS	3.2
1	D	21	GLY	3.0
1	C	62	ALA	2.8
1	E	398	ARG	2.8
1	D	398	ARG	2.7
1	E	502	ALA	2.6
1	F	398	ARG	2.6
1	D	169	LEU	2.6
1	C	398	ARG	2.5
1	E	368(A)	LEU	2.4
1	F	279	ASP	2.4
1	A	148	GLN	2.3
1	D	340	THR	2.3
1	B	398	ARG	2.3
1	B	151	THR	2.2
1	C	147	SER	2.2
1	D	271	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	398	ARG	2.2
1	D	22	VAL	2.1
1	E	328	THR	2.1
1	C	502	ALA	2.1
1	C	126	HIS	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](#)

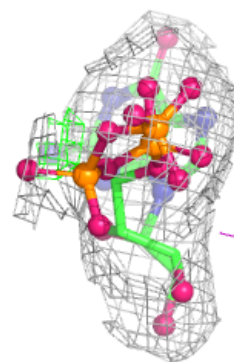
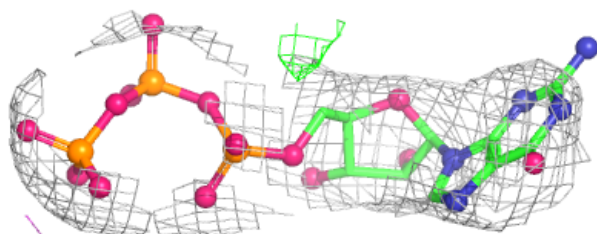
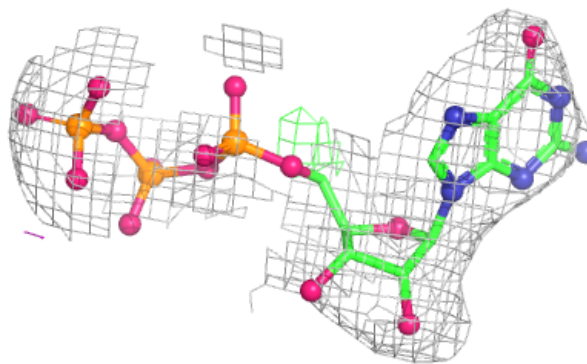
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MN	E	602	1/1	0.83	0.13	212,212,212,212	0
3	MN	B	602	1/1	0.85	0.09	174,174,174,174	0
3	MN	C	602	1/1	0.85	0.10	189,189,189,189	0
2	GTP	D	601	32/32	0.85	0.08	153,164,208,208	0
3	MN	D	602	1/1	0.87	0.09	179,179,179,179	0
3	MN	A	602	1/1	0.88	0.08	170,170,170,170	0
2	GTP	B	601	32/32	0.89	0.08	174,179,230,231	0
2	GTP	E	601	32/32	0.90	0.08	108,122,166,168	32
2	GTP	C	601	32/32	0.90	0.09	95,113,159,162	0
2	GTP	A	601	32/32	0.90	0.09	106,131,164,165	0
2	GTP	F	601	32/32	0.91	0.07	111,127,169,170	0
3	MN	F	602	1/1	0.94	0.05	167,167,167,167	0

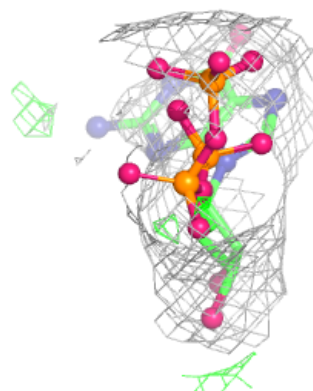
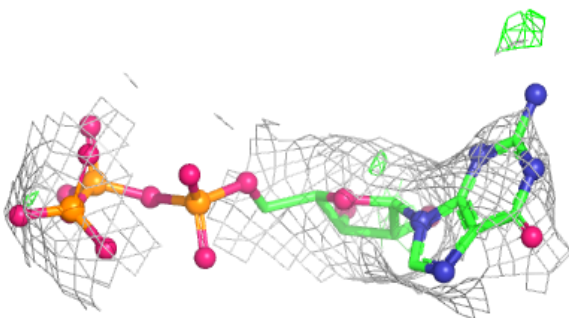
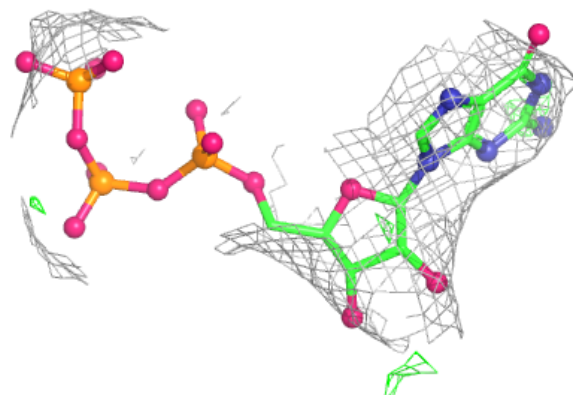
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP D 601:

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

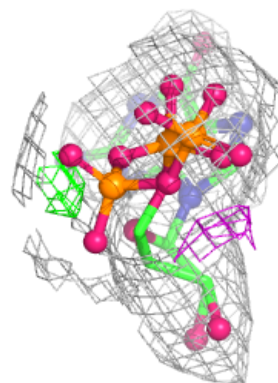
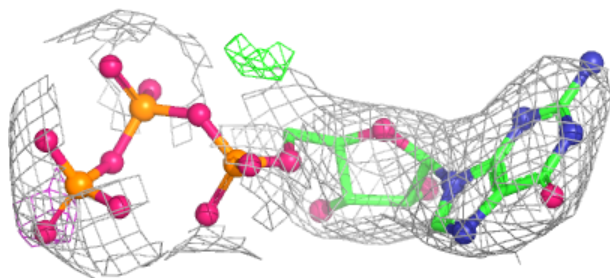
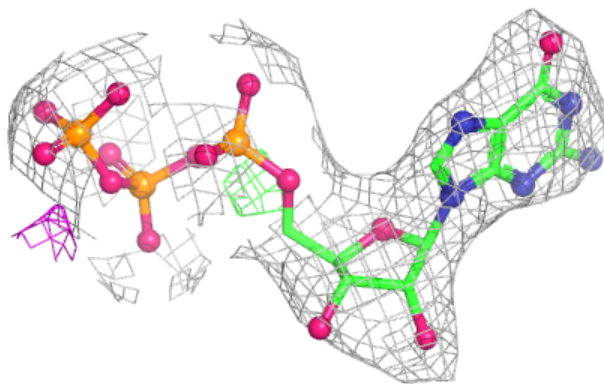
**Electron density around GTP B 601:**

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

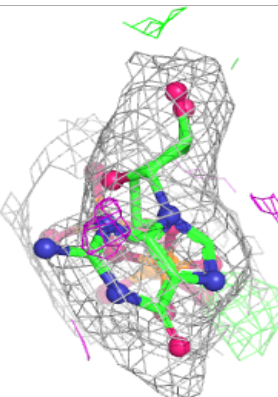
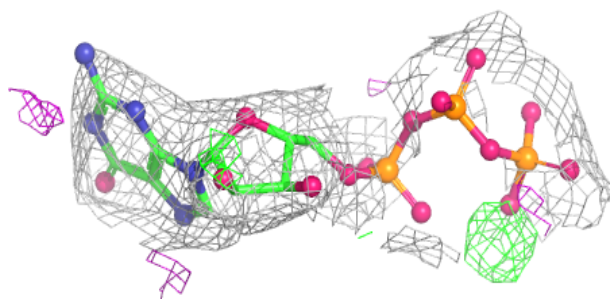
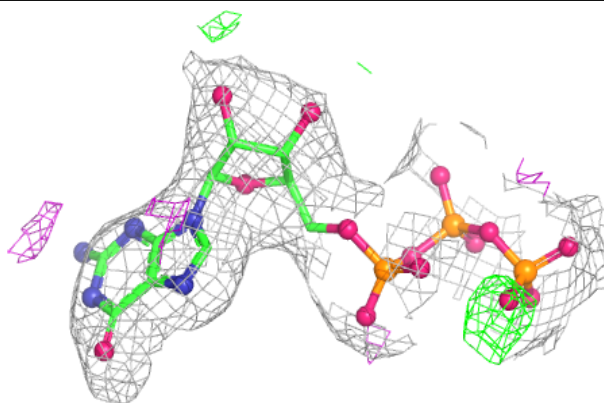


Electron density around GTP E 601:

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

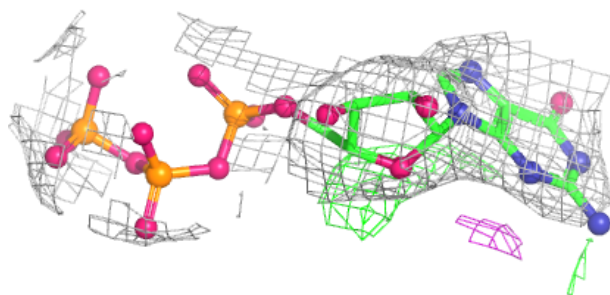
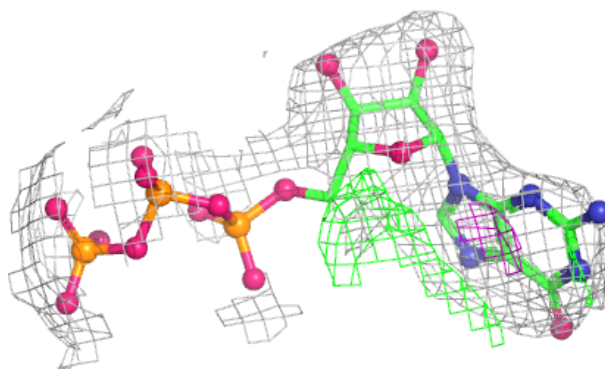
**Electron density around GTP C 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

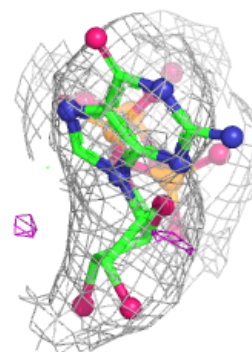
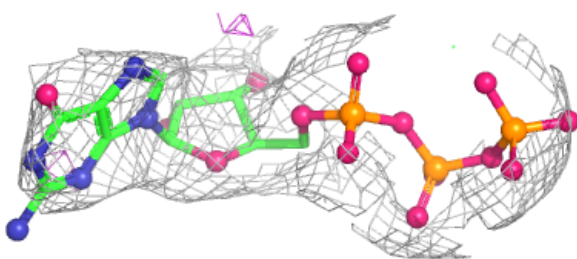
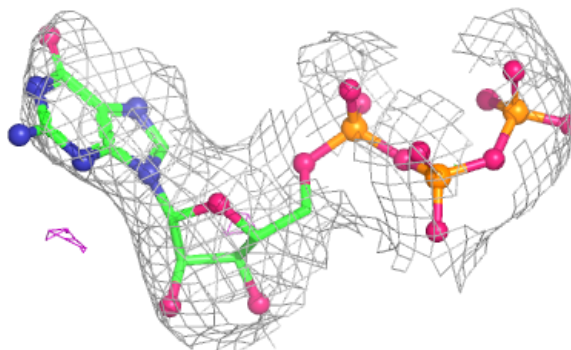


Electron density around GTP A 601:

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

**Electron density around GTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.