



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:54 AM UTC

PDB ID : 5HCI / pdb_00005hci
Title : GPN-loop GTPase Npa3 in complex with GDP
Authors : Niesser, J.; Wagner, F.R.; Kostrewa, D.; Muehlbacher, W.; Cramer, P.
Deposited on : 2016-01-04
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

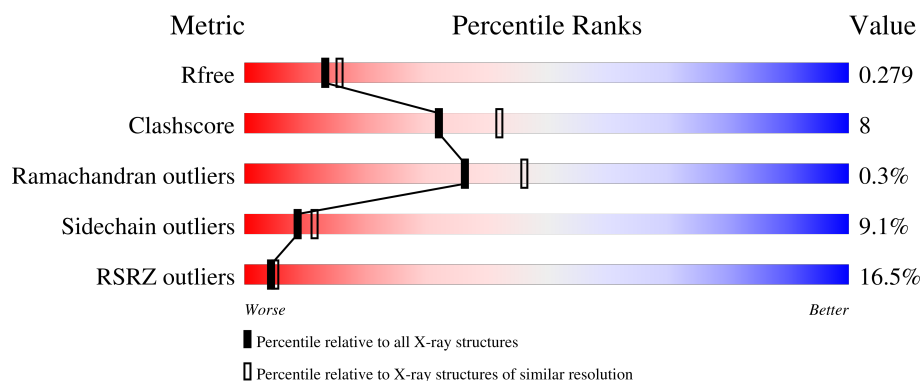
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	261	7% 79% 18% • •
1	B	261	23% 74% 20% 6% •
1	C	261	22% 71% 20% • 6%
1	D	261	14% 82% 14% • •
1	E	261	11% 79% 16% • •

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Mol	Chain	Length	Quality of chain
1	F	261	19% 80% 14% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12383 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 GPN-loop GTPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2032	1300	324	391	17			
1	B	258	Total	C	N	O	S	0	0	0
			2042	1306	327	392	17			
1	C	246	Total	C	N	O	S	0	0	0
			1937	1238	309	374	16			
1	D	258	Total	C	N	O	S	0	0	0
			2042	1306	327	392	17			
1	E	259	Total	C	N	O	S	0	0	0
			2052	1312	330	393	17			
1	F	249	Total	C	N	O	S	0	0	0
			1959	1252	314	377	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P47122
A	?	-	ASN	deletion	UNP P47122
A	?	-	GLY	deletion	UNP P47122
A	?	-	ASP	deletion	UNP P47122
A	?	-	ASN	deletion	UNP P47122
A	?	-	GLY	deletion	UNP P47122
A	?	-	LEU	deletion	UNP P47122
A	?	-	GLY	deletion	UNP P47122
A	?	-	SER	deletion	UNP P47122
A	265	LYS	-	expression tag	UNP P47122
A	266	HIS	-	expression tag	UNP P47122
A	267	HIS	-	expression tag	UNP P47122
A	268	HIS	-	expression tag	UNP P47122
A	269	HIS	-	expression tag	UNP P47122
A	270	HIS	-	expression tag	UNP P47122
A	271	HIS	-	expression tag	UNP P47122
B	?	-	LEU	deletion	UNP P47122

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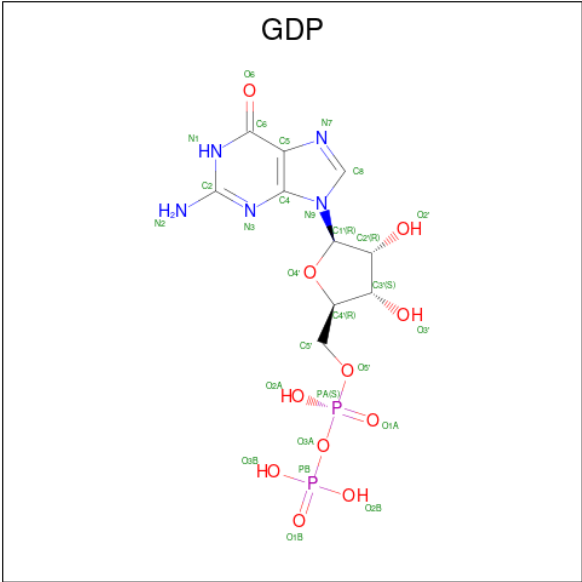
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P47122
B	?	-	GLY	deletion	UNP P47122
B	?	-	ASP	deletion	UNP P47122
B	?	-	ASN	deletion	UNP P47122
B	?	-	GLY	deletion	UNP P47122
B	?	-	LEU	deletion	UNP P47122
B	?	-	GLY	deletion	UNP P47122
B	?	-	SER	deletion	UNP P47122
B	265	LYS	-	expression tag	UNP P47122
B	266	HIS	-	expression tag	UNP P47122
B	267	HIS	-	expression tag	UNP P47122
B	268	HIS	-	expression tag	UNP P47122
B	269	HIS	-	expression tag	UNP P47122
B	270	HIS	-	expression tag	UNP P47122
B	271	HIS	-	expression tag	UNP P47122
C	?	-	LEU	deletion	UNP P47122
C	?	-	ASN	deletion	UNP P47122
C	?	-	GLY	deletion	UNP P47122
C	?	-	ASP	deletion	UNP P47122
C	?	-	ASN	deletion	UNP P47122
C	?	-	GLY	deletion	UNP P47122
C	?	-	LEU	deletion	UNP P47122
C	?	-	GLY	deletion	UNP P47122
C	?	-	SER	deletion	UNP P47122
C	265	LYS	-	expression tag	UNP P47122
C	266	HIS	-	expression tag	UNP P47122
C	267	HIS	-	expression tag	UNP P47122
C	268	HIS	-	expression tag	UNP P47122
C	269	HIS	-	expression tag	UNP P47122
C	270	HIS	-	expression tag	UNP P47122
C	271	HIS	-	expression tag	UNP P47122
D	?	-	LEU	deletion	UNP P47122
D	?	-	ASN	deletion	UNP P47122
D	?	-	GLY	deletion	UNP P47122
D	?	-	ASP	deletion	UNP P47122
D	?	-	ASN	deletion	UNP P47122
D	?	-	GLY	deletion	UNP P47122
D	?	-	LEU	deletion	UNP P47122
D	?	-	GLY	deletion	UNP P47122
D	?	-	SER	deletion	UNP P47122
D	265	LYS	-	expression tag	UNP P47122
D	266	HIS	-	expression tag	UNP P47122

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Chain	Residue	Modelled	Actual	Comment	Reference
D	267	HIS	-	expression tag	UNP P47122
D	268	HIS	-	expression tag	UNP P47122
D	269	HIS	-	expression tag	UNP P47122
D	270	HIS	-	expression tag	UNP P47122
D	271	HIS	-	expression tag	UNP P47122
E	?	-	LEU	deletion	UNP P47122
E	?	-	ASN	deletion	UNP P47122
E	?	-	GLY	deletion	UNP P47122
E	?	-	ASP	deletion	UNP P47122
E	?	-	ASN	deletion	UNP P47122
E	?	-	GLY	deletion	UNP P47122
E	?	-	LEU	deletion	UNP P47122
E	?	-	GLY	deletion	UNP P47122
E	?	-	SER	deletion	UNP P47122
E	265	LYS	-	expression tag	UNP P47122
E	266	HIS	-	expression tag	UNP P47122
E	267	HIS	-	expression tag	UNP P47122
E	268	HIS	-	expression tag	UNP P47122
E	269	HIS	-	expression tag	UNP P47122
E	270	HIS	-	expression tag	UNP P47122
E	271	HIS	-	expression tag	UNP P47122
F	?	-	LEU	deletion	UNP P47122
F	?	-	ASN	deletion	UNP P47122
F	?	-	GLY	deletion	UNP P47122
F	?	-	ASP	deletion	UNP P47122
F	?	-	ASN	deletion	UNP P47122
F	?	-	GLY	deletion	UNP P47122
F	?	-	LEU	deletion	UNP P47122
F	?	-	GLY	deletion	UNP P47122
F	?	-	SER	deletion	UNP P47122
F	265	LYS	-	expression tag	UNP P47122
F	266	HIS	-	expression tag	UNP P47122
F	267	HIS	-	expression tag	UNP P47122
F	268	HIS	-	expression tag	UNP P47122
F	269	HIS	-	expression tag	UNP P47122
F	270	HIS	-	expression tag	UNP P47122
F	271	HIS	-	expression tag	UNP P47122

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

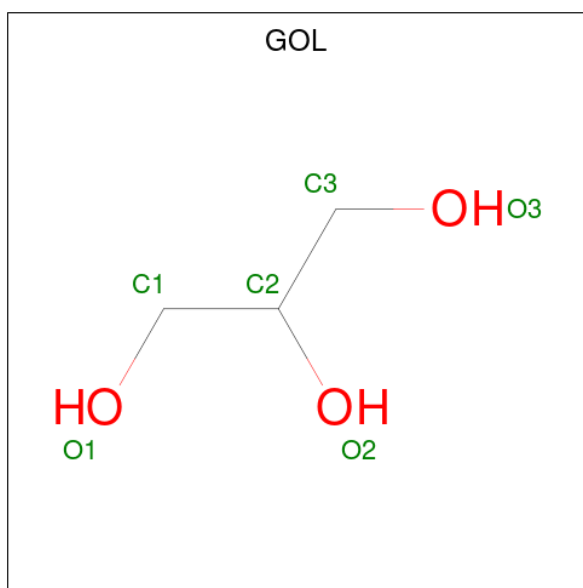


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

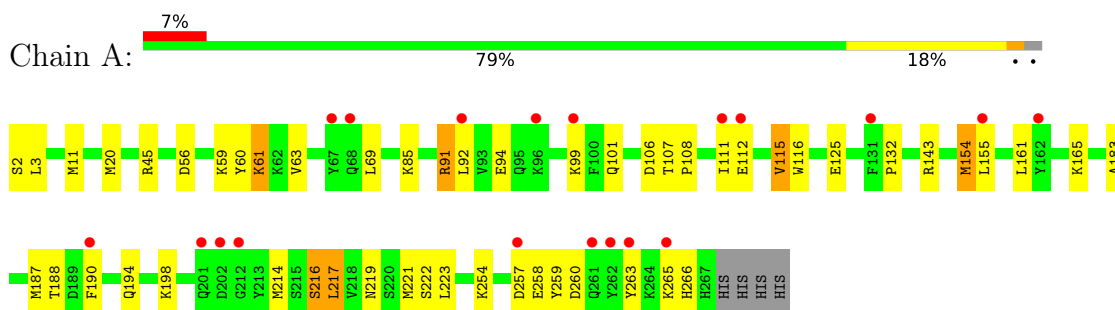
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	30	Total	O	0	0
			30	30		
5	C	16	Total	O	0	0
			16	16		
5	D	16	Total	O	0	0
			16	16		
5	E	21	Total	O	0	0
			21	21		
5	F	5	Total	O	0	0
			5	5		

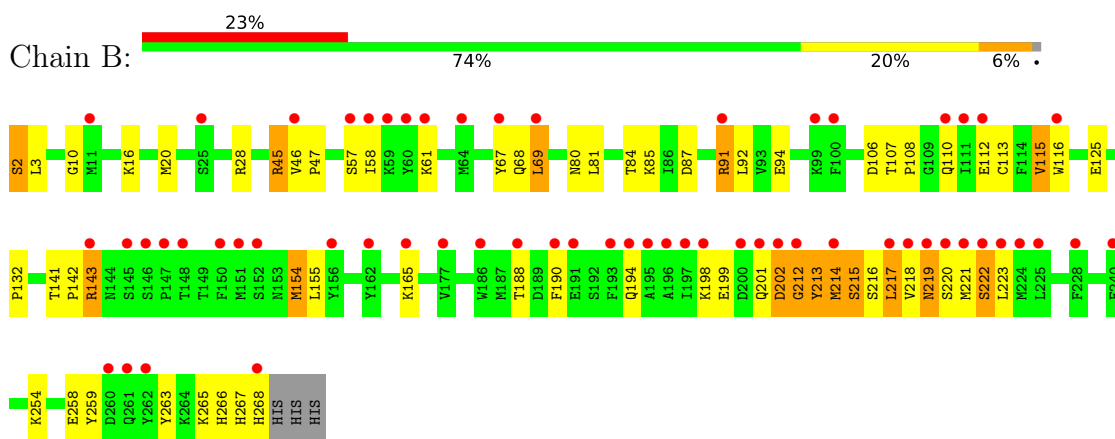
3 Residue-property plots [i](#)

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.

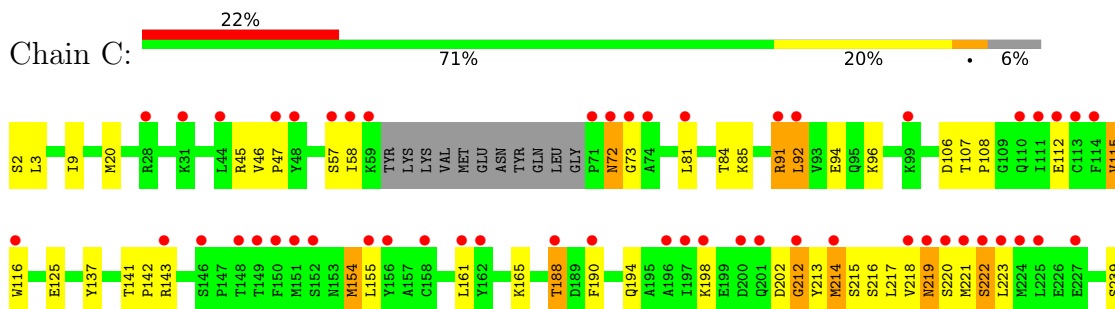
• Molecule 1: GPN-loop GTPase 1

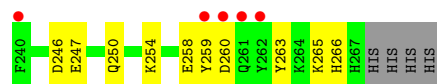


• Molecule 1: GPN-loop GTPase 1

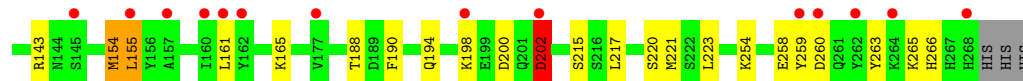
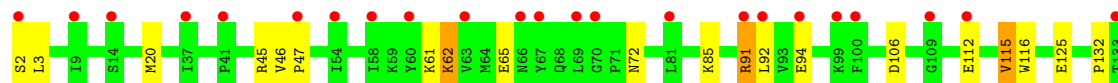
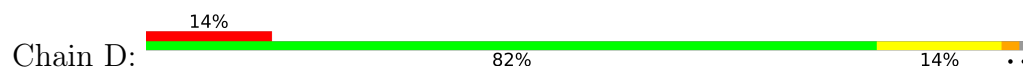


• Molecule 1: GPN-loop GTPase 1

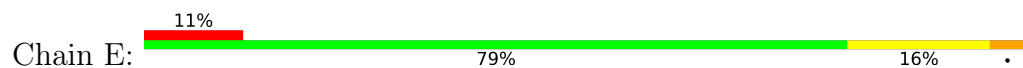




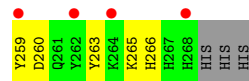
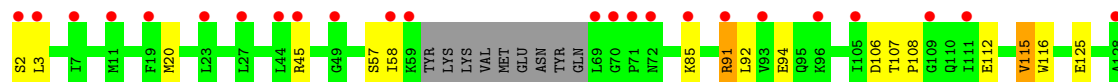
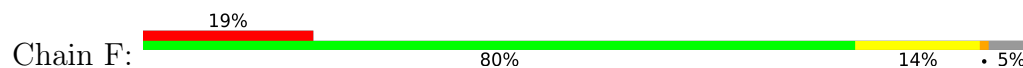
• Molecule 1: GPN-loop GTPase 1



• Molecule 1: GPN-loop GTPase 1



• Molecule 1: GPN-loop GTPase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.99Å 119.18Å 347.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.25 – 2.30 45.25 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.25-2.30) 99.7 (45.25-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.276 0.246 , 0.279	Depositor DCC
R_{free} test set	1988 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12383	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.72	0/2075	0.92	1/2806 (0.0%)
1	B	0.75	2/2086 (0.1%)	1.01	8/2821 (0.3%)
1	C	0.78	3/1977 (0.2%)	0.95	3/2673 (0.1%)
1	D	0.51	0/2086	0.82	0/2821
1	E	0.74	2/2097 (0.1%)	0.93	3/2836 (0.1%)
1	F	0.48	0/2000	0.81	0/2705
All	All	0.67	7/12321 (0.1%)	0.91	15/16662 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	ASN	C-O	7.31	1.32	1.24
1	C	219	ASN	C-O	6.88	1.31	1.24
1	E	220	SER	C-O	6.63	1.31	1.24
1	B	220	SER	C-O	5.59	1.30	1.24
1	E	224	MET	CA-C	5.26	1.59	1.52
1	C	220	SER	C-O	5.26	1.30	1.24
1	C	73	GLY	N-CA	-5.11	1.38	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ARG	NE-CZ-NH2	12.15	130.14	119.20
1	B	45	ARG	NE-CZ-NH1	-11.25	110.25	121.50
1	B	45	ARG	CD-NE-CZ	9.29	137.40	124.40
1	B	222	SER	CA-C-N	-6.03	112.60	120.44
1	B	222	SER	C-N-CA	-6.03	112.60	120.44
1	C	222	SER	CA-C-N	-5.87	112.81	120.44
1	C	222	SER	C-N-CA	-5.87	112.81	120.44
1	E	220	SER	CA-C-O	5.87	126.77	120.55
1	B	267	HIS	N-CA-C	5.74	117.72	107.80
1	C	220	SER	CA-C-O	5.50	126.39	120.55
1	B	220	SER	CA-C-O	5.46	126.34	120.55
1	E	223	LEU	CA-C-N	-5.16	113.36	120.28
1	E	223	LEU	C-N-CA	-5.16	113.36	120.28
1	B	218	VAL	N-CA-C	5.12	115.89	110.72
1	A	60	TYR	N-CA-C	5.03	116.76	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	72	ASN	Peptide
1	D	202	ASP	Peptide
1	F	202	ASP	Peptide

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	2032	0	2009	26	1
1	B	2042	0	2016	61	0
1	C	1937	0	1914	55	0
1	D	2042	0	2016	23	0
1	E	2052	0	2023	31	1
1	F	1959	0	1933	24	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	1	0
2	D	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	12	0	0
2	F	28	0	12	1	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	6	0	8	1	0
4	C	6	0	8	0	0
4	E	12	0	16	1	0
5	A	33	0	0	2	0
5	B	30	0	0	2	0
5	C	16	0	0	0	0
5	D	16	0	0	1	0
5	E	21	0	0	3	0
5	F	5	0	0	0	0
All	All	12383	0	12015	193	1

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 8.

All (193) 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:91:ARG:HG3	1:D:202:ASP:HB3	1.23	1.13
1:C:202:ASP:O	1:C:213:TYR:N	1.85	1.07
1:C:91:ARG:HG3	1:F:202:ASP:HB3	1.48	0.94
1:B:143:ARG:NH2	5:B:401:HOH:O	2.01	0.92
1:C:91:ARG:CG	1:F:202:ASP:HB3	2.08	0.82
1:C:214:MET:HB3	1:C:217:LEU:HD13	1.62	0.80
1:B:28:ARG:HE	1:C:250:GLN:CD	1.91	0.79
1:C:91:ARG:HG3	1:F:202:ASP:CB	2.12	0.79
1:B:28:ARG:HH22	1:C:247:GLU:N	1.86	0.73
1:B:45:ARG:NH2	1:C:188:THR:OG1	2.24	0.71
1:F:190:PHE:HD2	1:F:194:GLN:HE21	1.38	0.71
1:B:28:ARG:HE	1:C:250:GLN:NE2	1.87	0.71
1:B:28:ARG:HH22	1:C:246:ASP:C	2.00	0.70
1:B:154:MET:HE3	1:B:154:MET:HA	1.73	0.70
1:B:190:PHE:HD2	1:B:194:GLN:HE21	1.39	0.70
1:C:190:PHE:HD2	1:C:194:GLN:HE21	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLU:OE2	5:B:402:HOH:O	2.10	0.69
1:A:56:ASP:OD2	5:A:401:HOH:O	2.10	0.69
1:E:263:TYR:OH	5:E:401:HOH:O	2.10	0.69
1:B:212:GLY:O	1:B:215:SER:N	2.27	0.67
1:D:91:ARG:HH11	1:D:91:ARG:HG3	1.60	0.67
1:E:190:PHE:HD2	1:E:194:GLN:HE21	1.43	0.66
1:F:91:ARG:HG3	1:F:91:ARG:HH11	1.61	0.65
1:B:45:ARG:HB3	1:C:188:THR:CG2	2.26	0.65
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.62	0.65
1:B:91:ARG:HG3	1:D:202:ASP:CB	2.15	0.65
1:D:190:PHE:HD2	1:D:194:GLN:HE21	1.45	0.64
1:B:28:ARG:NH2	1:C:246:ASP:C	2.56	0.64
1:C:217:LEU:HB3	1:C:221:MET:SD	2.38	0.64
1:C:214:MET:SD	1:C:214:MET:N	2.71	0.63
1:A:190:PHE:HD2	1:A:194:GLN:HE21	1.46	0.62
1:A:99:LYS:HG3	1:B:2:SER:OG	1.99	0.62
1:B:217:LEU:O	1:B:221:MET:HG3	1.99	0.62
1:B:202:ASP:O	1:B:212:GLY:C	2.42	0.61
1:E:91:ARG:HG3	1:E:91:ARG:HH11	1.66	0.61
1:A:59:LYS:HD2	1:A:61:LYS:HZ2	1.64	0.61
1:A:154:MET:HE3	1:A:154:MET:HA	1.83	0.61
1:B:45:ARG:HD2	1:C:188:THR:HG21	1.82	0.61
1:E:154:MET:HE3	1:E:154:MET:HA	1.82	0.60
1:D:154:MET:HE3	1:D:154:MET:HA	1.83	0.60
1:B:115:VAL:HG22	1:B:116:TRP:CE3	2.36	0.60
1:C:154:MET:HE3	1:C:154:MET:HA	1.84	0.59
1:B:201:GLN:HG2	1:B:213:TYR:H	1.68	0.59
1:B:212:GLY:HA3	1:B:215:SER:HB3	1.84	0.59
1:C:214:MET:O	1:C:217:LEU:HB2	2.02	0.59
1:A:115:VAL:HG22	1:A:116:TRP:CE3	2.37	0.59
1:E:115:VAL:HG22	1:E:116:TRP:CE3	2.36	0.59
1:E:257:ASP:HB3	4:E:303:GOL:H31	1.84	0.58
1:B:28:ARG:NH2	1:C:247:GLU:N	2.52	0.58
1:F:115:VAL:HG22	1:F:116:TRP:CE3	2.39	0.58
1:B:201:GLN:HG2	1:B:213:TYR:HB3	1.86	0.56
1:C:212:GLY:HA2	1:C:215:SER:HB3	1.86	0.56
1:B:45:ARG:HB3	1:C:188:THR:HG21	1.86	0.56
1:D:115:VAL:HG22	1:D:116:TRP:CE3	2.41	0.56
1:C:91:ARG:HG3	1:C:91:ARG:HH11	1.70	0.56
1:F:154:MET:HE3	1:F:154:MET:HA	1.87	0.55
1:A:91:ARG:HH11	1:A:91:ARG:CG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HG3	1:F:202:ASP:CG	2.30	0.55
1:F:165:LYS:HE3	1:F:266:HIS:HD2	1.72	0.54
1:E:91:ARG:HH11	1:E:91:ARG:CG	2.20	0.54
1:F:91:ARG:HH11	1:F:91:ARG:CG	2.19	0.54
1:D:91:ARG:HH11	1:D:91:ARG:CG	2.20	0.54
1:D:165:LYS:HE3	1:D:266:HIS:HD2	1.72	0.54
1:E:165:LYS:HE3	1:E:266:HIS:HD2	1.73	0.53
1:C:115:VAL:HG22	1:C:116:TRP:CE3	2.42	0.53
1:A:20:MET:HE2	1:A:106:ASP:HB2	1.91	0.53
1:A:165:LYS:HE3	1:A:266:HIS:HD2	1.73	0.52
1:F:214:MET:O	1:F:218:VAL:HG23	2.10	0.52
1:B:80:ASN:HB3	1:E:177:VAL:O	2.10	0.51
1:E:254:LYS:NZ	1:E:258:GLU:OE2	2.34	0.51
1:B:165:LYS:HE3	1:B:266:HIS:HD2	1.76	0.51
1:B:212:GLY:O	1:B:214:MET:N	2.44	0.51
1:C:165:LYS:HE3	1:C:266:HIS:HD2	1.75	0.51
1:B:91:ARG:CG	1:B:91:ARG:HH11	2.24	0.50
1:A:216:SER:O	1:A:219:ASN:HB2	2.11	0.50
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.77	0.50
1:D:265:LYS:HG3	1:D:266:HIS:ND1	2.26	0.50
1:F:265:LYS:HG3	1:F:266:HIS:ND1	2.27	0.50
1:C:91:ARG:CG	1:C:91:ARG:HH11	2.24	0.50
1:B:28:ARG:NE	1:C:250:GLN:NE2	2.56	0.49
1:C:265:LYS:HG3	1:C:266:HIS:ND1	2.28	0.49
1:B:87:ASP:CG	1:E:143:ARG:HH22	2.21	0.49
1:C:20:MET:HE2	1:C:106:ASP:HB2	1.95	0.48
1:D:155:LEU:HD23	1:E:155:LEU:HD23	1.94	0.48
1:B:28:ARG:NH2	1:C:246:ASP:HB3	2.29	0.48
1:D:165:LYS:HE2	1:D:266:HIS:HB3	1.96	0.48
1:C:215:SER:O	1:C:218:VAL:N	2.46	0.48
1:E:161:LEU:HD21	5:E:401:HOH:O	2.13	0.47
1:E:202:ASP:OD1	1:E:202:ASP:N	2.47	0.47
1:A:265:LYS:HG3	1:A:266:HIS:ND1	2.29	0.47
1:B:110:GLN:HB2	1:B:113:CYS:SG	2.54	0.47
1:E:40:ASP:OD2	5:E:402:HOH:O	2.20	0.47
1:E:165:LYS:HE2	1:E:266:HIS:HB3	1.96	0.47
1:F:202:ASP:OD1	1:F:202:ASP:N	2.47	0.47
1:B:201:GLN:HE21	1:B:213:TYR:HB3	1.80	0.47
1:E:175:THR:HA	1:E:178:CYS:O	2.15	0.47
1:F:254:LYS:NZ	1:F:258:GLU:OE2	2.38	0.47
1:E:265:LYS:HG3	1:E:266:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:HE2	1:B:106:ASP:HB2	1.96	0.47
1:B:265:LYS:HG3	1:B:266:HIS:ND1	2.29	0.47
1:D:254:LYS:NZ	1:D:258:GLU:OE2	2.37	0.47
1:F:165:LYS:HE2	1:F:266:HIS:HB3	1.97	0.47
1:B:45:ARG:HB3	1:C:188:THR:HG23	1.95	0.46
1:C:222:SER:OG	1:C:223:LEU:N	2.48	0.46
1:D:220:SER:HB2	1:E:156:TYR:CE2	2.50	0.46
1:F:20:MET:HE2	1:F:106:ASP:HB2	1.97	0.46
1:A:85:LYS:N	1:A:85:LYS:HD2	2.30	0.46
1:C:91:ARG:HG2	1:F:202:ASP:HB3	1.92	0.46
1:B:222:SER:OG	1:B:223:LEU:N	2.47	0.46
1:C:141:THR:HB	1:C:142:PRO:HD3	1.96	0.46
1:B:254:LYS:NZ	1:B:258:GLU:OE2	2.38	0.46
1:F:223:LEU:HD23	1:F:223:LEU:HA	1.79	0.46
1:D:259:TYR:HA	1:D:263:TYR:HB2	1.97	0.46
1:A:101:GLN:CD	4:A:303:GOL:H32	2.41	0.46
1:B:141:THR:HB	1:B:142:PRO:HD3	1.97	0.46
1:E:151:MET:O	1:E:155:LEU:HD22	2.15	0.46
1:C:212:GLY:HA2	1:C:215:SER:CB	2.46	0.46
1:C:259:TYR:HA	1:C:263:TYR:HB2	1.97	0.46
1:A:165:LYS:HE2	1:A:266:HIS:HB3	1.98	0.45
1:B:201:GLN:HE21	1:B:213:TYR:CB	2.29	0.45
1:D:20:MET:HE2	1:D:106:ASP:HB2	1.98	0.45
1:B:202:ASP:O	1:B:213:TYR:N	2.49	0.45
1:B:259:TYR:HA	1:B:263:TYR:HB2	1.97	0.45
1:C:85:LYS:N	1:C:85:LYS:HD2	2.31	0.45
1:D:62:LYS:HE3	1:D:62:LYS:HB2	1.78	0.45
1:E:46:VAL:HA	1:E:47:PRO:HD3	1.80	0.45
1:E:259:TYR:HA	1:E:263:TYR:HB2	1.98	0.45
1:B:81:LEU:O	1:B:84:THR:HB	2.15	0.45
1:B:165:LYS:HE2	1:B:266:HIS:HB3	1.98	0.45
1:C:165:LYS:HE2	1:C:266:HIS:HB3	1.98	0.45
1:F:259:TYR:HA	1:F:263:TYR:HB2	1.98	0.44
1:A:259:TYR:HA	1:A:263:TYR:HB2	1.99	0.44
1:C:219:ASN:O	1:C:222:SER:HB3	2.17	0.44
1:D:106:ASP:OD1	5:D:402:HOH:O	2.21	0.44
1:F:85:LYS:N	1:F:85:LYS:HD2	2.33	0.44
1:C:84:THR:HG22	1:C:85:LYS:HD2	2.00	0.44
1:E:85:LYS:N	1:E:85:LYS:HD2	2.33	0.44
1:A:20:MET:HE3	1:A:20:MET:HB3	1.92	0.44
1:C:46:VAL:HA	1:C:47:PRO:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LYS:HD2	1:D:85:LYS:N	2.33	0.44
1:B:84:THR:HG22	1:B:85:LYS:HD2	1.99	0.43
1:B:213:TYR:C	1:B:214:MET:HG2	2.43	0.43
1:E:268:HIS:CD2	1:E:269:HIS:HB3	2.53	0.43
1:A:254:LYS:NZ	1:A:258:GLU:OE2	2.38	0.43
1:C:107:THR:HB	1:C:108:PRO:HD2	2.00	0.43
1:F:57:SER:OG	1:F:58:ILE:HD12	2.18	0.43
1:C:9:ILE:O	1:C:137:TYR:HA	2.18	0.43
1:F:239:SER:N	2:F:301:GDP:O6	2.51	0.43
1:B:28:ARG:NH2	1:C:247:GLU:HA	2.33	0.43
1:B:107:THR:HB	1:B:108:PRO:HD2	1.99	0.43
1:C:217:LEU:O	1:C:218:VAL:C	2.60	0.43
1:D:46:VAL:HA	1:D:47:PRO:HD3	1.82	0.43
1:C:81:LEU:O	1:C:84:THR:HB	2.19	0.43
1:C:217:LEU:O	1:C:221:MET:HG3	2.18	0.43
1:E:148:THR:HG22	1:E:214:MET:HE3	2.00	0.43
1:B:91:ARG:NH2	1:D:200:ASP:O	2.52	0.42
1:A:219:ASN:O	1:A:222:SER:HB3	2.19	0.42
1:B:57:SER:OG	1:B:58:ILE:HD12	2.19	0.42
1:C:202:ASP:OD1	1:C:202:ASP:N	2.50	0.42
1:A:107:THR:HB	1:A:108:PRO:HD2	2.02	0.42
1:A:183:ALA:O	1:A:187:MET:HG3	2.19	0.42
1:E:20:MET:HE2	1:E:106:ASP:HB2	2.02	0.42
1:B:69:LEU:HD13	1:B:69:LEU:HA	1.86	0.42
1:B:132:PRO:HA	1:B:259:TYR:CE1	2.55	0.42
1:B:219:ASN:O	1:B:222:SER:HB3	2.19	0.42
1:C:239:SER:N	2:C:301:GDP:O6	2.52	0.42
1:C:254:LYS:NZ	1:C:258:GLU:OE2	2.39	0.42
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.88	0.42
1:A:111:ILE:HA	5:A:417:HOH:O	2.20	0.41
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.90	0.41
1:B:85:LYS:HD2	1:B:85:LYS:N	2.35	0.41
1:C:190:PHE:CZ	1:C:222:SER:HA	2.55	0.41
1:F:132:PRO:HA	1:F:259:TYR:CE1	2.55	0.41
1:E:107:THR:HB	1:E:108:PRO:HD2	2.01	0.41
1:C:57:SER:OG	1:C:58:ILE:HD12	2.21	0.41
1:C:92:LEU:O	1:C:96:LYS:HG2	2.20	0.41
1:E:259:TYR:O	1:E:260:ASP:C	2.62	0.41
1:A:223:LEU:HD23	1:A:223:LEU:HA	1.79	0.41
1:B:10:GLY:N	1:B:16:LYS:HD3	2.35	0.41
1:B:67:TYR:HB3	1:B:69:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:TYR:CD1	1:E:259:TYR:C	2.99	0.41
1:A:132:PRO:HA	1:A:259:TYR:CE1	2.56	0.41
1:B:46:VAL:HA	1:B:47:PRO:HD3	1.81	0.41
1:D:223:LEU:HD23	1:D:223:LEU:HA	1.81	0.41
1:E:9:ILE:O	1:E:137:TYR:HA	2.21	0.41
1:F:107:THR:HB	1:F:108:PRO:HD2	2.03	0.41
1:A:11:MET:HE2	1:A:11:MET:HB2	1.88	0.40
1:A:217:LEU:HD12	1:A:221:MET:SD	2.61	0.40
1:B:20:MET:HE3	1:B:20:MET:HB3	2.00	0.40
1:B:190:PHE:CZ	1:B:222:SER:HA	2.57	0.40
1:D:217:LEU:O	1:D:221:MET:HG3	2.21	0.40
1:B:202:ASP:OD1	1:B:202:ASP:N	2.48	0.40
1:D:132:PRO:HA	1:D:259:TYR:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:O	1:E:91:ARG:NH2[5_455]	2.13	0.07

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	255/261 (98%)	251 (98%)	4 (2%)	0	100	100
1	B	256/261 (98%)	250 (98%)	4 (2%)	2 (1%)	16	20
1	C	242/261 (93%)	236 (98%)	5 (2%)	1 (0%)	30	38
1	D	256/261 (98%)	252 (98%)	4 (2%)	0	100	100
1	E	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	30	38
1	F	245/261 (94%)	241 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1511/1566 (96%)	1482 (98%)	25 (2%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	212	GLY
1	C	212	GLY
1	B	213	TYR
1	E	212	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/235 (98%)	209 (90%)	22 (10%)	8	10
1	B	232/235 (99%)	210 (90%)	22 (10%)	8	10
1	C	221/235 (94%)	202 (91%)	19 (9%)	10	13
1	D	232/235 (99%)	210 (90%)	22 (10%)	8	10
1	E	233/235 (99%)	211 (91%)	22 (9%)	8	11
1	F	223/235 (95%)	205 (92%)	18 (8%)	11	14
All	All	1372/1410 (97%)	1247 (91%)	125 (9%)	9	11

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	LEU
1	A	45	ARG
1	A	61	LYS
1	A	63	VAL
1	A	69	LEU
1	A	91	ARG
1	A	92	LEU

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Mol	Chain	Res	Type
1	A	94	GLU
1	A	112	GLU
1	A	115	VAL
1	A	125	GLU
1	A	143	ARG
1	A	154	MET
1	A	155	LEU
1	A	161	LEU
1	A	188	THR
1	A	198	LYS
1	A	214	MET
1	A	216	SER
1	A	217	LEU
1	A	260	ASP
1	B	2	SER
1	B	3	LEU
1	B	61	LYS
1	B	68	GLN
1	B	69	LEU
1	B	91	ARG
1	B	92	LEU
1	B	94	GLU
1	B	112	GLU
1	B	115	VAL
1	B	125	GLU
1	B	143	ARG
1	B	154	MET
1	B	155	LEU
1	B	188	THR
1	B	198	LYS
1	B	202	ASP
1	B	214	MET
1	B	215	SER
1	B	216	SER
1	B	217	LEU
1	B	268	HIS
1	C	2	SER
1	C	3	LEU
1	C	45	ARG
1	C	72	ASN
1	C	91	ARG
1	C	92	LEU

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Mol	Chain	Res	Type
1	C	94	GLU
1	C	112	GLU
1	C	115	VAL
1	C	125	GLU
1	C	143	ARG
1	C	154	MET
1	C	155	LEU
1	C	161	LEU
1	C	188	THR
1	C	198	LYS
1	C	214	MET
1	C	216	SER
1	C	260	ASP
1	D	2	SER
1	D	3	LEU
1	D	45	ARG
1	D	61	LYS
1	D	62	LYS
1	D	65	GLU
1	D	72	ASN
1	D	91	ARG
1	D	92	LEU
1	D	94	GLU
1	D	112	GLU
1	D	115	VAL
1	D	125	GLU
1	D	143	ARG
1	D	154	MET
1	D	155	LEU
1	D	161	LEU
1	D	188	THR
1	D	198	LYS
1	D	202	ASP
1	D	215	SER
1	D	260	ASP
1	E	2	SER
1	E	3	LEU
1	E	45	ARG
1	E	62	LYS
1	E	65	GLU
1	E	69	LEU
1	E	91	ARG

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Mol	Chain	Res	Type
1	E	92	LEU
1	E	94	GLU
1	E	112	GLU
1	E	115	VAL
1	E	125	GLU
1	E	143	ARG
1	E	154	MET
1	E	155	LEU
1	E	161	LEU
1	E	188	THR
1	E	198	LYS
1	E	214	MET
1	E	260	ASP
1	E	268	HIS
1	E	269	HIS
1	F	2	SER
1	F	3	LEU
1	F	45	ARG
1	F	91	ARG
1	F	92	LEU
1	F	94	GLU
1	F	112	GLU
1	F	115	VAL
1	F	125	GLU
1	F	143	ARG
1	F	154	MET
1	F	155	LEU
1	F	161	LEU
1	F	188	THR
1	F	198	LYS
1	F	202	ASP
1	F	217	LEU
1	F	260	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	26	HIS
1	A	101	GLN
1	A	102	ASN
1	A	194	GLN

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Mol	Chain	Res	Type
1	B	101	GLN
1	B	102	ASN
1	B	194	GLN
1	B	201	GLN
1	B	250	GLN
1	C	24	ASN
1	C	26	HIS
1	C	101	GLN
1	C	102	ASN
1	C	194	GLN
1	C	250	GLN
1	D	26	HIS
1	D	101	GLN
1	D	102	ASN
1	D	194	GLN
1	E	24	ASN
1	E	26	HIS
1	E	101	GLN
1	E	102	ASN
1	E	194	GLN
1	E	261	GLN
1	F	24	ASN
1	F	26	HIS
1	F	101	GLN
1	F	102	ASN
1	F	194	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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	GDP	D	301	3	29,30,30	1.15	2 (6%)	45,47,47	1.85	7 (15%)
4	GOL	A	303	-	5,5,5	0.37	0	5,5,5	0.66	0
2	GDP	B	301	3	29,30,30	1.35	5 (17%)	45,47,47	1.63	6 (13%)
4	GOL	E	303	-	5,5,5	0.36	0	5,5,5	0.23	0
2	GDP	F	301	3	29,30,30	1.22	3 (10%)	45,47,47	1.61	6 (13%)
2	GDP	C	301	-	29,30,30	1.17	3 (10%)	45,47,47	1.93	6 (13%)
2	GDP	A	301	3	29,30,30	1.20	4 (13%)	45,47,47	1.86	11 (24%)
4	GOL	E	304	-	5,5,5	0.38	0	5,5,5	0.55	0
2	GDP	E	301	3	29,30,30	1.18	2 (6%)	45,47,47	2.21	11 (24%)
4	GOL	C	303	-	5,5,5	0.37	0	5,5,5	0.31	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	GDP	D	301	3	-	4/16/32/32	0/3/3/3
4	GOL	A	303	-	-	2/4/4/4	-
2	GDP	B	301	3	-	0/16/32/32	0/3/3/3
4	GOL	E	303	-	-	2/4/4/4	-
2	GDP	F	301	3	-	5/16/32/32	0/3/3/3
2	GDP	C	301	-	-	3/16/32/32	0/3/3/3
2	GDP	A	301	3	-	0/16/32/32	0/3/3/3
4	GOL	E	304	-	-	1/4/4/4	-
2	GDP	E	301	3	-	1/16/32/32	0/3/3/3
4	GOL	C	303	-	-	3/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GDP	PA-O3A	3.69	1.63	1.59
2	A	301	GDP	C6-N1	-3.54	1.32	1.38
2	D	301	GDP	C5-C4	3.39	1.48	1.38
2	F	301	GDP	C5-C4	3.24	1.47	1.38
2	B	301	GDP	C5-C4	3.19	1.47	1.38
2	A	301	GDP	C5-C4	3.05	1.47	1.38
2	C	301	GDP	C5-C4	3.00	1.47	1.38
2	E	301	GDP	C5-C4	2.86	1.46	1.38
2	D	301	GDP	C6-N1	-2.67	1.33	1.38
2	E	301	GDP	C6-N1	-2.59	1.34	1.38
2	F	301	GDP	PA-O3A	2.57	1.62	1.59
2	A	301	GDP	C5-N7	-2.33	1.34	1.39
2	F	301	GDP	C6-N1	-2.28	1.34	1.38
2	B	301	GDP	C6-N1	-2.22	1.34	1.38
2	C	301	GDP	C5-N7	-2.14	1.34	1.39
2	C	301	GDP	C6-N1	-2.14	1.34	1.38
2	A	301	GDP	C4-N9	-2.13	1.32	1.38
2	B	301	GDP	C5-N7	-2.01	1.35	1.39
2	B	301	GDP	C4-N9	-2.00	1.33	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	GDP	C5-C4-N3	-6.84	117.50	128.39
2	E	301	GDP	C5-C4-N3	-6.80	117.57	128.39
2	E	301	GDP	C2-N3-C4	6.58	123.64	112.30
2	D	301	GDP	C5-C4-N3	-6.35	118.28	128.39
2	C	301	GDP	C2-N3-C4	6.01	122.65	112.30
2	A	301	GDP	C5-C4-N3	-5.67	119.36	128.39
2	F	301	GDP	C5-C4-N3	-5.40	119.80	128.39
2	B	301	GDP	C5-C4-N3	-5.29	119.97	128.39
2	D	301	GDP	C2-N3-C4	5.05	121.00	112.30
2	E	301	GDP	N9-C4-N3	4.81	135.57	125.95
2	C	301	GDP	N9-C4-N3	4.79	135.53	125.95
2	F	301	GDP	C2-N3-C4	4.77	120.51	112.30
2	A	301	GDP	C2-N3-C4	4.63	120.27	112.30
2	E	301	GDP	C5'-C4'-C3'	-4.47	99.11	115.21
2	A	301	GDP	N9-C4-N3	4.38	134.72	125.95
2	D	301	GDP	N9-C4-N3	4.35	134.65	125.95
2	E	301	GDP	C6-C5-N7	4.22	137.96	130.29
2	F	301	GDP	N9-C4-N3	4.10	134.14	125.95
2	B	301	GDP	C2-N3-C4	4.06	119.29	112.30
2	D	301	GDP	C6-C5-N7	3.75	137.12	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	GDP	C6-C5-N7	3.48	136.62	130.29
2	B	301	GDP	N9-C4-N3	3.39	132.73	125.95
2	F	301	GDP	C6-C5-N7	3.23	136.18	130.29
2	D	301	GDP	O4'-C1'-N9	3.14	115.48	108.36
2	E	301	GDP	C4-C5-N7	-3.12	105.73	110.67
2	D	301	GDP	C4-C5-N7	-3.11	105.74	110.67
2	A	301	GDP	C2'-C1'-N9	-3.09	104.65	113.25
2	A	301	GDP	C6-C5-N7	3.04	135.82	130.29
2	B	301	GDP	C6-C5-N7	3.01	135.77	130.29
2	C	301	GDP	C4-C5-N7	-2.94	106.01	110.67
2	A	301	GDP	C4-C5-N7	-2.88	106.11	110.67
2	A	301	GDP	O2A-PA-O3A	2.67	114.49	107.27
2	B	301	GDP	C4-C5-N7	-2.61	106.53	110.67
2	E	301	GDP	C8-N7-C5	2.42	108.58	104.26
2	A	301	GDP	O3B-PB-O3A	2.34	112.49	104.64
2	E	301	GDP	C5-C6-N1	2.30	119.11	113.25
2	A	301	GDP	C8-N7-C5	2.26	108.29	104.26
2	D	301	GDP	C8-N7-C5	2.24	108.25	104.26
2	E	301	GDP	O2A-PA-O3A	2.22	113.28	107.27
2	A	301	GDP	O4'-C1'-N9	2.22	113.38	108.36
2	B	301	GDP	C2'-C3'-C4'	2.19	106.84	102.61
2	C	301	GDP	C8-N7-C5	2.18	108.14	104.26
2	E	301	GDP	O4'-C4'-C3'	2.18	109.48	105.15
2	F	301	GDP	O6-C6-C5	-2.15	120.85	126.53
2	F	301	GDP	C4-C5-N7	-2.13	107.30	110.67
2	E	301	GDP	O6-C6-C5	-2.06	121.09	126.53
2	A	301	GDP	O2B-PB-O3A	2.02	111.42	104.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	GDP	C5'-O5'-PA-O3A
2	F	301	GDP	C5'-O5'-PA-O1A
4	A	303	GOL	O1-C1-C2-C3
4	C	303	GOL	O1-C1-C2-C3
4	E	303	GOL	C1-C2-C3-O3
4	C	303	GOL	O1-C1-C2-O2
2	F	301	GDP	C3'-C4'-C5'-O5'
4	E	304	GOL	C1-C2-C3-O3
4	A	303	GOL	O1-C1-C2-O2
4	E	303	GOL	O2-C2-C3-O3

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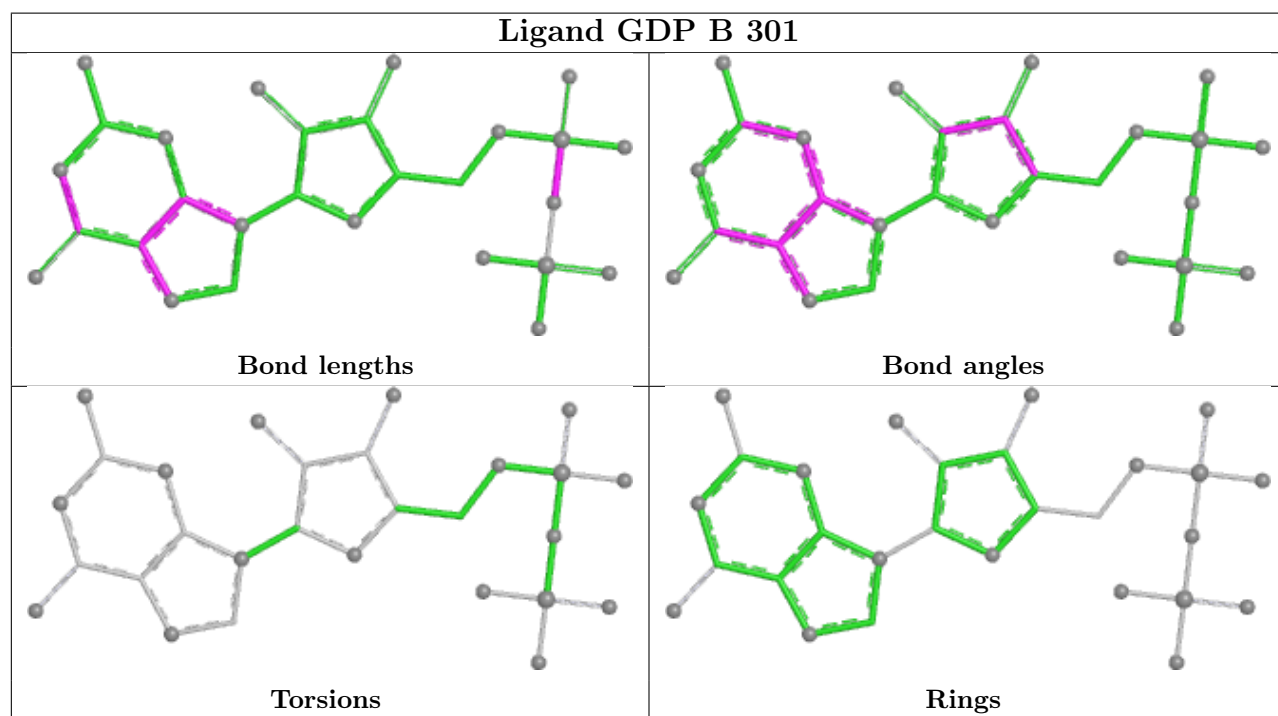
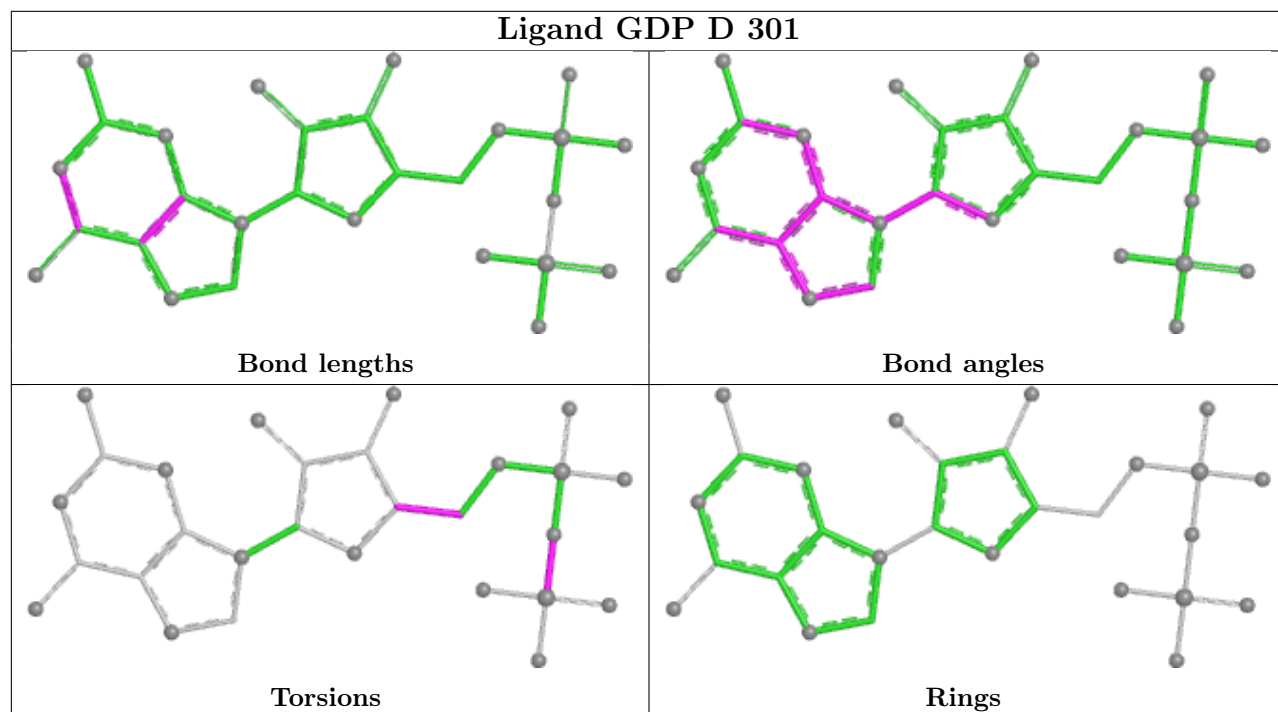
Mol	Chain	Res	Type	Atoms
2	F	301	GDP	O4'-C4'-C5'-O5'
2	D	301	GDP	O4'-C4'-C5'-O5'
2	F	301	GDP	C5'-O5'-PA-O2A
2	C	301	GDP	PA-O3A-PB-O1B
2	D	301	GDP	PA-O3A-PB-O1B
2	E	301	GDP	PA-O3A-PB-O1B
2	C	301	GDP	PA-O3A-PB-O2B
2	C	301	GDP	PA-O3A-PB-O3B
2	D	301	GDP	PA-O3A-PB-O2B
2	D	301	GDP	PA-O3A-PB-O3B
4	C	303	GOL	C1-C2-C3-O3

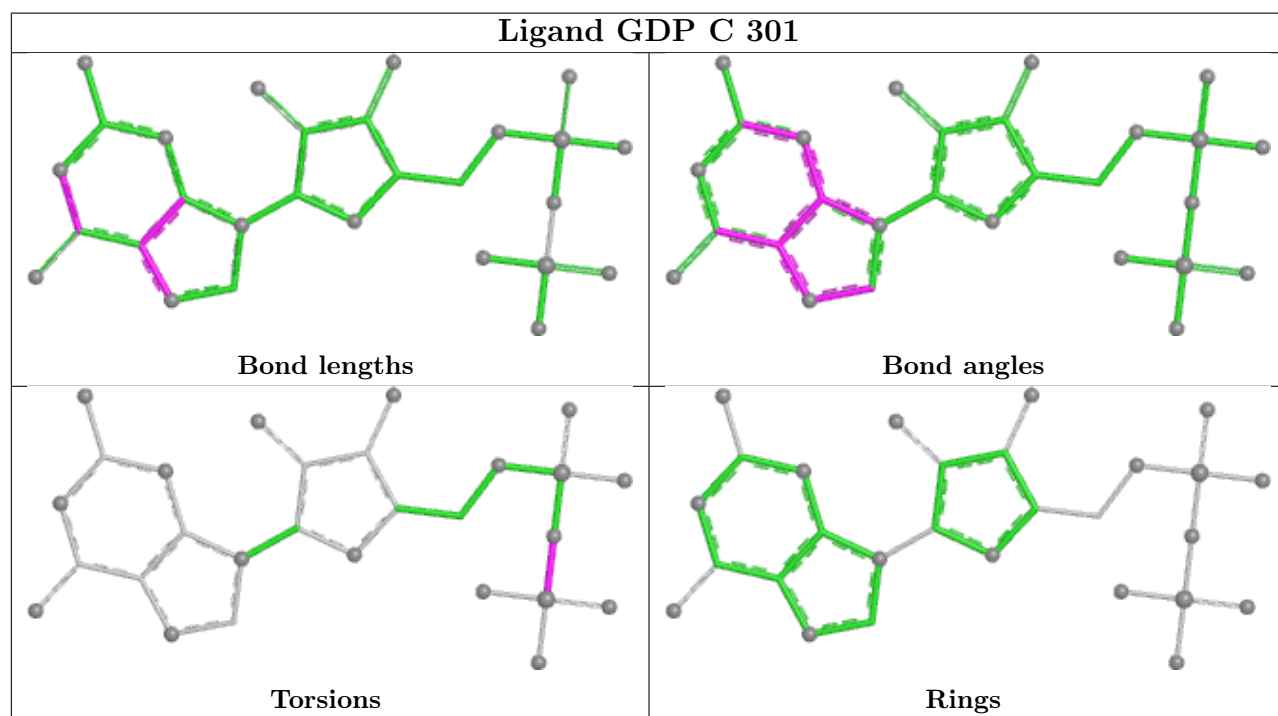
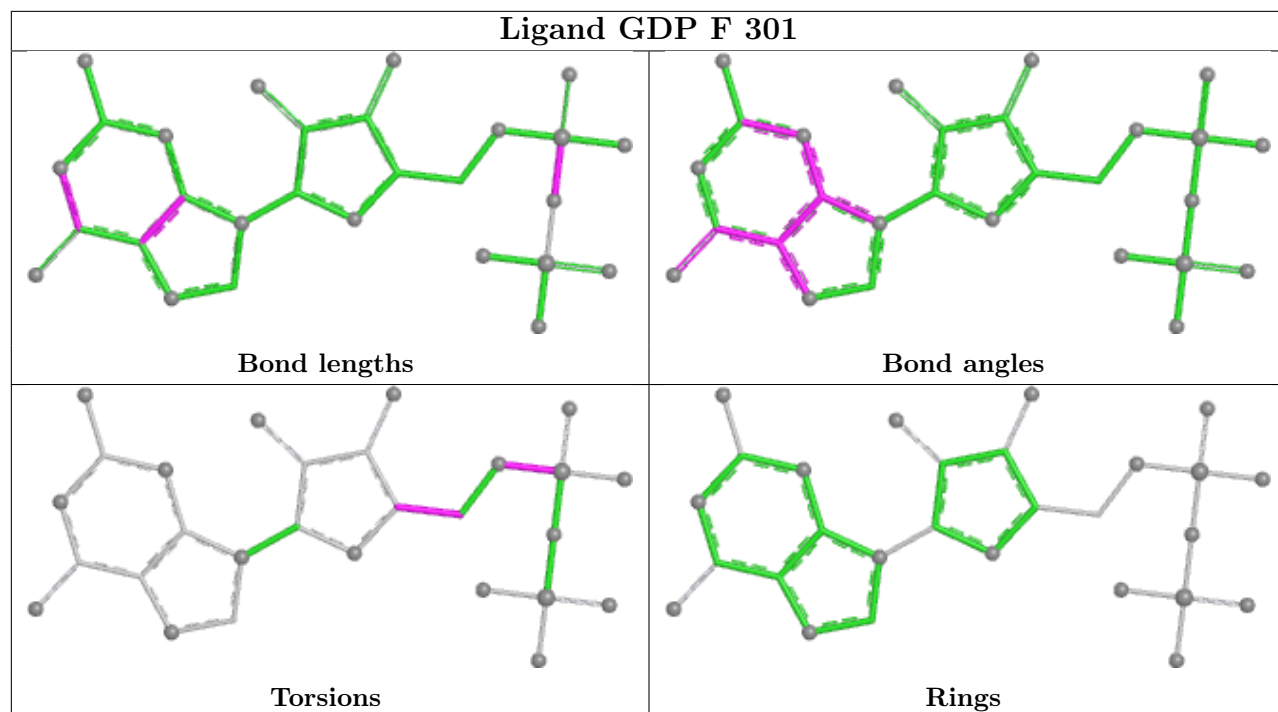
There are no ring outliers.

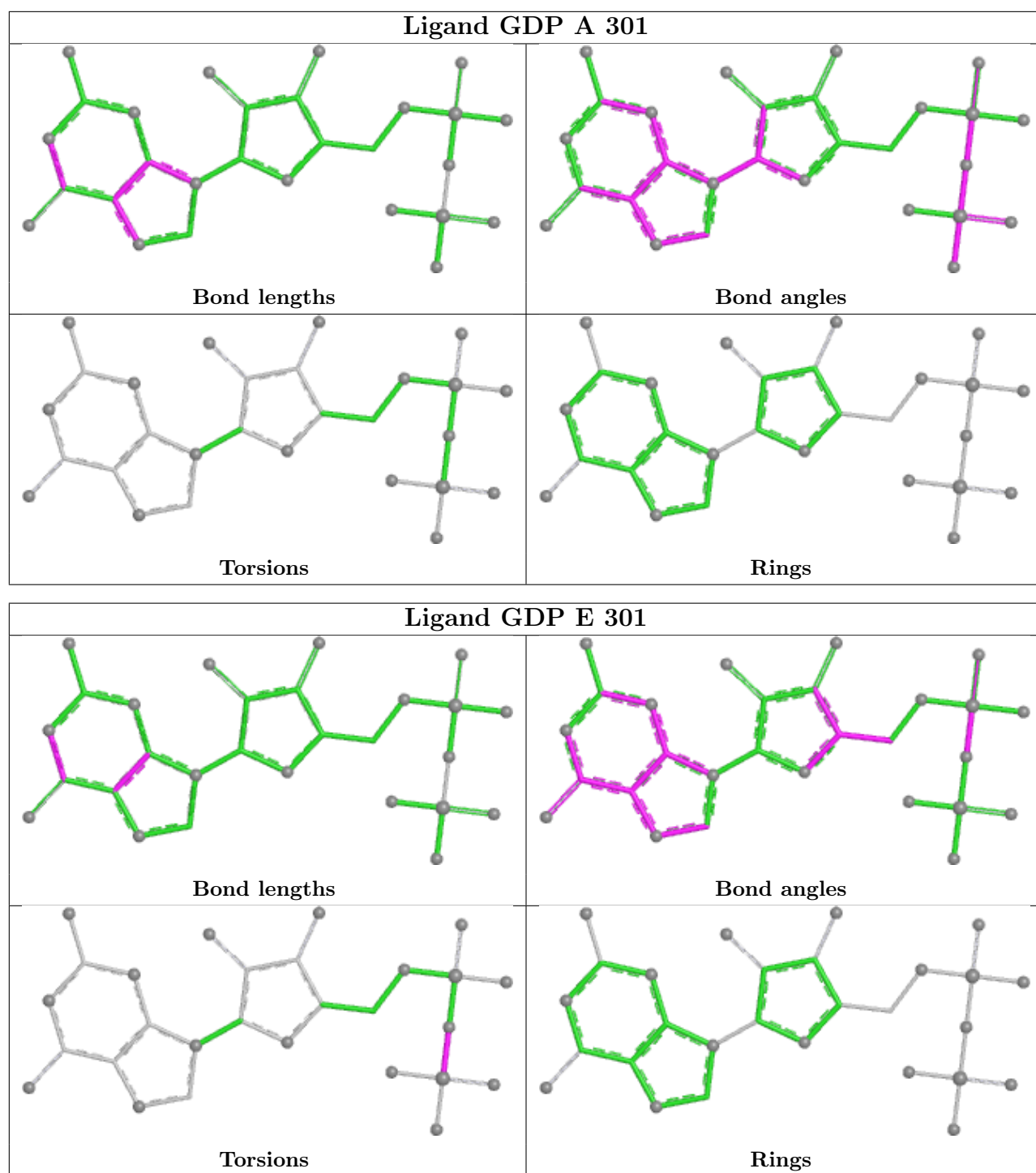
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	GOL	1	0
4	E	303	GOL	1	0
2	F	301	GDP	1	0
2	C	301	GDP	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	257/261 (98%)	0.65	19 (7%)	20 22	42, 60, 106, 198	0
1	B	258/261 (98%)	1.21	60 (23%)	2 2	44, 69, 146, 237	0
1	C	246/261 (94%)	1.18	57 (23%)	2 2	48, 72, 158, 280	0
1	D	258/261 (98%)	1.06	37 (14%)	6 7	56, 83, 135, 186	0
1	E	259/261 (99%)	0.74	30 (11%)	9 10	44, 63, 127, 211	0
1	F	249/261 (95%)	1.41	49 (19%)	3 3	55, 104, 146, 195	0
All	All	1527/1566 (97%)	1.04	252 (16%)	4 5	42, 74, 141, 280	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	220	SER	7.0
1	B	197	ILE	7.0
1	B	220	SER	6.0
1	F	234	VAL	6.0
1	B	218	VAL	5.8
1	B	223	LEU	5.5
1	C	197	ILE	5.4
1	F	93	VAL	5.2
1	F	202	ASP	5.2
1	C	218	VAL	5.0
1	B	240	PHE	5.0
1	B	162	TYR	4.9
1	F	58	ILE	4.9
1	C	58	ILE	4.7
1	C	47	PRO	4.7
1	F	71	PRO	4.7
1	C	261	GLN	4.6
1	C	73	GLY	4.6
1	B	147	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	219	ASN	4.5
1	B	196	ALA	4.4
1	F	59	LYS	4.4
1	F	19	PHE	4.4
1	B	195	ALA	4.4
1	A	257	ASP	4.4
1	B	262	TYR	4.3
1	F	105	ILE	4.2
1	B	58	ILE	4.1
1	B	202	ASP	4.1
1	B	212	GLY	4.0
1	F	69	LEU	3.9
1	B	190	PHE	3.9
1	B	221	MET	3.8
1	C	71	PRO	3.8
1	C	155	LEU	3.8
1	E	261	GLN	3.8
1	B	57	SER	3.8
1	B	201	GLN	3.7
1	C	162	TYR	3.7
1	E	269	HIS	3.7
1	E	162	TYR	3.7
1	A	99	LYS	3.7
1	F	248	PHE	3.6
1	B	116	TRP	3.6
1	B	260	ASP	3.6
1	E	66	ASN	3.6
1	F	44	LEU	3.6
1	F	262	TYR	3.6
1	F	7	ILE	3.6
1	C	262	TYR	3.5
1	B	148	THR	3.5
1	B	145	SER	3.5
1	C	151	MET	3.5
1	C	223	LEU	3.5
1	B	198	LYS	3.5
1	D	145	SER	3.5
1	C	212	GLY	3.5
1	D	112	GLU	3.5
1	D	202	ASP	3.5
1	B	224	MET	3.4
1	C	116	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	61	LYS	3.4
1	E	63	VAL	3.4
1	C	44	LEU	3.4
1	E	262	TYR	3.3
1	B	222	SER	3.3
1	C	201	GLN	3.3
1	C	190	PHE	3.3
1	E	91	ARG	3.2
1	B	152	SER	3.2
1	E	202	ASP	3.2
1	B	268	HIS	3.2
1	F	111	ILE	3.2
1	D	198	LYS	3.2
1	D	63	VAL	3.2
1	E	44	LEU	3.2
1	C	224	MET	3.2
1	C	240	PHE	3.1
1	C	200	ASP	3.1
1	D	177	VAL	3.1
1	D	69	LEU	3.1
1	F	162	TYR	3.1
1	F	259	TYR	3.1
1	B	150	PHE	3.1
1	C	221	MET	3.1
1	D	67	TYR	3.0
1	E	67	TYR	3.0
1	B	25	SER	3.0
1	C	222	SER	3.0
1	D	58	ILE	3.0
1	C	158	CYS	3.0
1	B	69	LEU	3.0
1	C	156	TYR	3.0
1	C	152	SER	3.0
1	A	261	GLN	3.0
1	A	67	TYR	3.0
1	A	162	TYR	3.0
1	B	143	ARG	3.0
1	E	57	SER	3.0
1	B	200	ASP	3.0
1	D	81	LEU	2.9
1	B	261	GLN	2.9
1	C	259	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	151	MET	2.9
1	E	257	ASP	2.9
1	E	260	ASP	2.9
1	A	202	ASP	2.9
1	B	91	ARG	2.9
1	C	196	ALA	2.9
1	D	60	TYR	2.9
1	C	143	ARG	2.9
1	F	27	LEU	2.9
1	F	134	VAL	2.9
1	F	268	HIS	2.8
1	E	92	LEU	2.8
1	C	214	MET	2.8
1	C	31	LYS	2.8
1	E	60	TYR	2.8
1	D	100	PHE	2.8
1	E	42	ALA	2.8
1	A	190	PHE	2.8
1	C	99	LYS	2.8
1	F	233	ASP	2.8
1	B	156	TYR	2.8
1	D	162	TYR	2.8
1	F	232	LEU	2.8
1	C	148	THR	2.7
1	F	180	ALA	2.7
1	B	111	ILE	2.7
1	C	111	ILE	2.7
1	B	165	LYS	2.7
1	C	81	LEU	2.7
1	C	48	TYR	2.7
1	D	133	THR	2.7
1	F	2	SER	2.7
1	A	201	GLN	2.7
1	C	112	GLU	2.6
1	C	219	ASN	2.6
1	C	260	ASP	2.6
1	E	201	GLN	2.6
1	F	201	GLN	2.6
1	D	92	LEU	2.6
1	B	11	MET	2.6
1	B	100	PHE	2.6
1	E	71	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	259	TYR	2.6
1	F	198	LYS	2.6
1	A	68	GLN	2.5
1	D	91	ARG	2.5
1	F	228	PHE	2.5
1	B	59	LYS	2.5
1	D	262	TYR	2.5
1	B	193	PHE	2.5
1	F	131	PHE	2.5
1	C	225	LEU	2.5
1	B	228	PHE	2.5
1	D	14	SER	2.5
1	D	260	ASP	2.5
1	B	188	THR	2.4
1	F	133	THR	2.4
1	F	145	SER	2.4
1	B	67	TYR	2.4
1	A	212	GLY	2.4
1	D	47	PRO	2.4
1	E	212	GLY	2.4
1	F	45	ARG	2.4
1	F	70	GLY	2.4
1	C	57	SER	2.4
1	F	3	LEU	2.4
1	D	259	TYR	2.4
1	D	109	GLY	2.4
1	D	157	ALA	2.4
1	A	96	LYS	2.4
1	A	131	PHE	2.4
1	D	70	GLY	2.4
1	D	9	ILE	2.4
1	B	225	LEU	2.4
1	C	28	ARG	2.4
1	B	191	GLU	2.4
1	C	72	ASN	2.3
1	A	265	LYS	2.3
1	D	2	SER	2.3
1	C	161	LEU	2.3
1	C	188	THR	2.3
1	F	135	ILE	2.3
1	D	161	LEU	2.3
1	B	99	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	188	THR	2.3
1	F	91	ARG	2.3
1	C	227	GLU	2.3
1	A	111	ILE	2.3
1	F	139	VAL	2.3
1	F	72	ASN	2.3
1	B	194	GLN	2.2
1	E	258	GLU	2.2
1	C	198	LYS	2.2
1	D	160	ILE	2.2
1	A	155	LEU	2.2
1	A	262	TYR	2.2
1	A	263	TYR	2.2
1	F	23	LEU	2.2
1	F	264	LYS	2.2
1	B	217	LEU	2.2
1	F	235	VAL	2.2
1	D	41	PRO	2.2
1	F	109	GLY	2.2
1	C	149	THR	2.2
1	B	60	TYR	2.1
1	E	45	ARG	2.1
1	B	214	MET	2.1
1	B	46	VAL	2.1
1	D	66	ASN	2.1
1	C	150	PHE	2.1
1	B	110	GLN	2.1
1	F	49	GLY	2.1
1	B	61	LYS	2.1
1	C	59	LYS	2.1
1	C	92	LEU	2.1
1	D	99	LYS	2.1
1	D	155	LEU	2.1
1	A	112	GLU	2.1
1	B	177	VAL	2.1
1	C	114	PHE	2.1
1	B	146	SER	2.1
1	C	146	SER	2.1
1	B	64	MET	2.1
1	D	264	LYS	2.1
1	F	11	MET	2.1
1	F	169	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	268	HIS	2.1
1	E	49	GLY	2.1
1	C	74	ALA	2.1
1	F	179	LYS	2.1
1	B	112	GLU	2.1
1	C	110	GLN	2.1
1	E	268	HIS	2.1
1	E	82	PHE	2.1
1	B	186	TRP	2.1
1	F	85	LYS	2.0
1	C	113	CYS	2.0
1	E	95	GLN	2.0
1	D	37	ILE	2.0
1	D	54	ILE	2.0
1	F	137	TYR	2.0
1	E	43	VAL	2.0
1	E	198	LYS	2.0
1	F	96	LYS	2.0
1	D	94	GLU	2.0
1	E	112	GLU	2.0
1	F	128	ALA	2.0
1	A	92	LEU	2.0
1	C	91	ARG	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.

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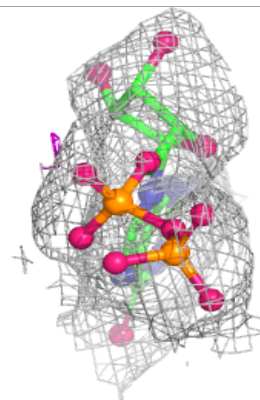
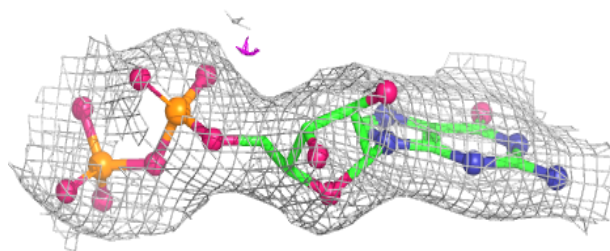
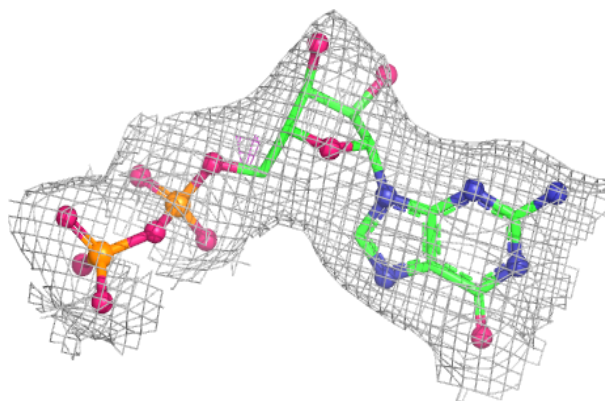
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	303	6/6	0.69	0.19	104,119,129,129	0
4	GOL	C	303	6/6	0.79	0.18	90,102,119,125	0
4	GOL	E	303	6/6	0.82	0.16	91,102,106,108	0
4	GOL	E	304	6/6	0.89	0.16	69,98,110,124	0
2	GDP	F	301	28/28	0.94	0.08	71,93,103,114	0
3	MG	F	302	1/1	0.94	0.12	85,85,85,85	0
3	MG	D	302	1/1	0.95	0.06	65,65,65,65	0
2	GDP	D	301	28/28	0.95	0.08	55,68,91,136	0
2	GDP	E	301	28/28	0.96	0.08	54,61,86,110	0
2	GDP	C	301	28/28	0.96	0.07	45,66,77,84	0
3	MG	C	302	1/1	0.96	0.07	63,63,63,63	0
3	MG	E	302	1/1	0.97	0.08	61,61,61,61	0
2	GDP	B	301	28/28	0.97	0.07	51,53,63,65	0
2	GDP	A	301	28/28	0.98	0.07	57,59,77,79	0
3	MG	A	302	1/1	0.99	0.07	55,55,55,55	0
3	MG	B	302	1/1	0.99	0.03	52,52,52,52	0

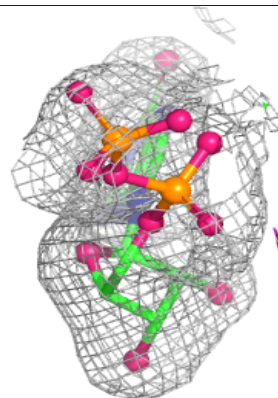
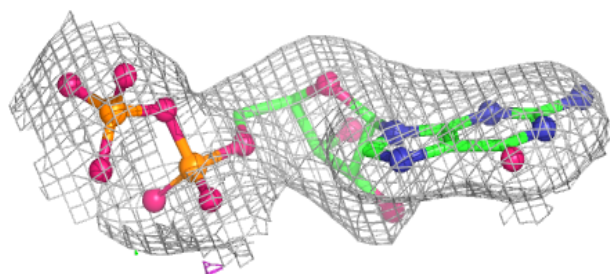
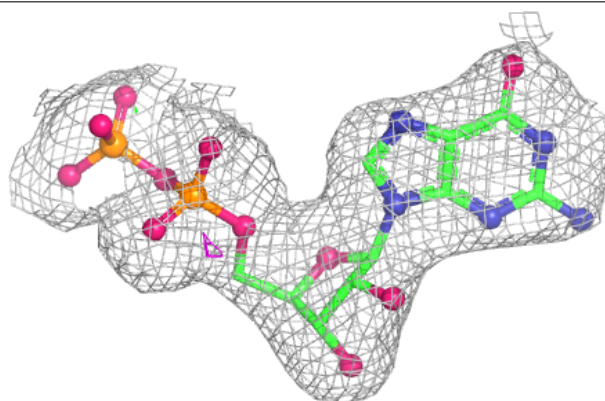
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP F 301:

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

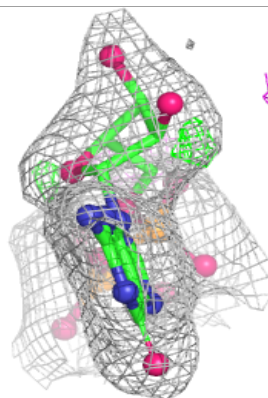
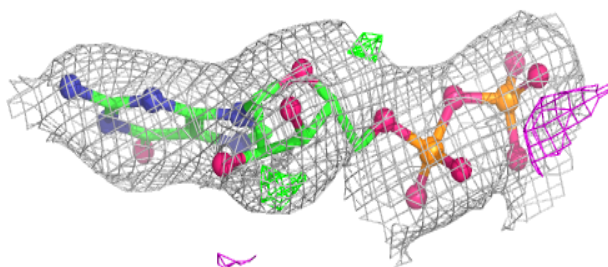
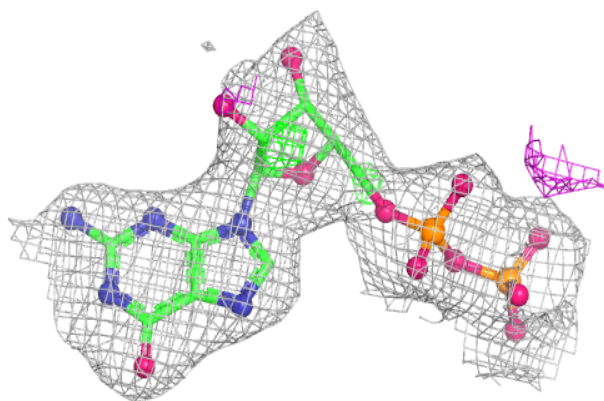
**Electron density around GDP D 301:**

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

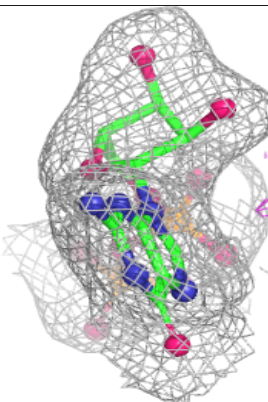
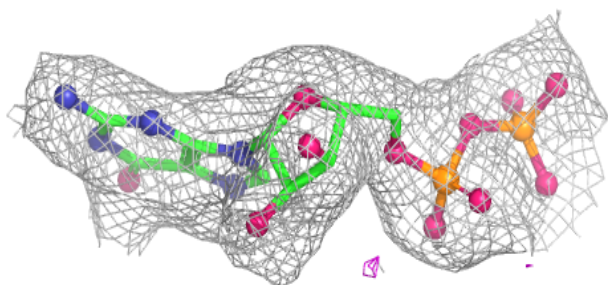
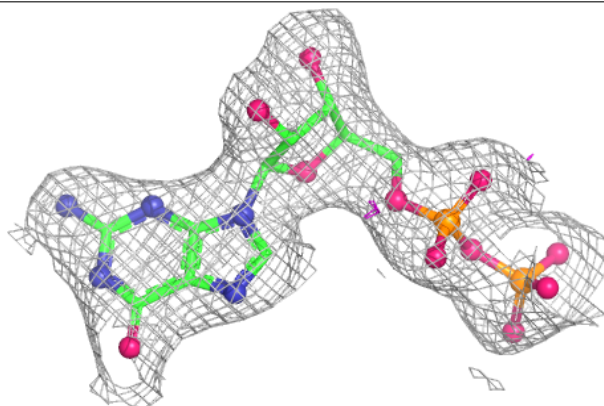


Electron density around GDP E 301:

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

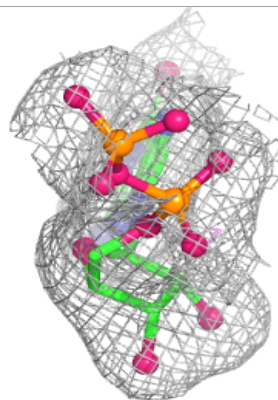
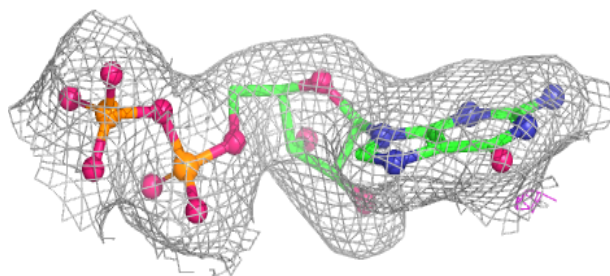
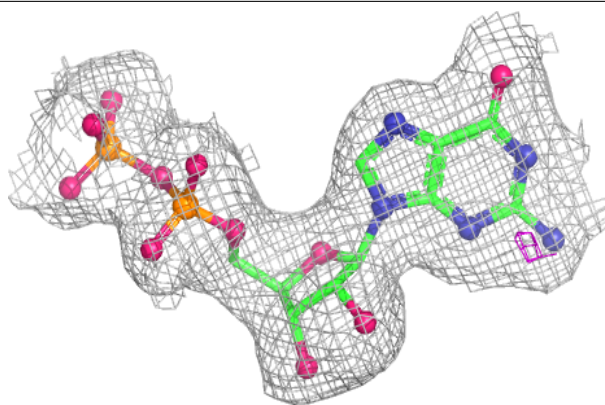
**Electron density around GDP C 301:**

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

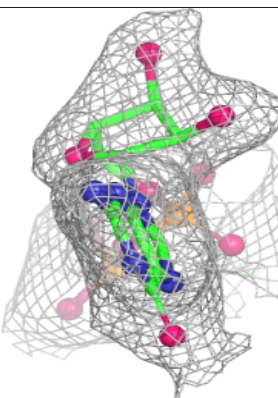
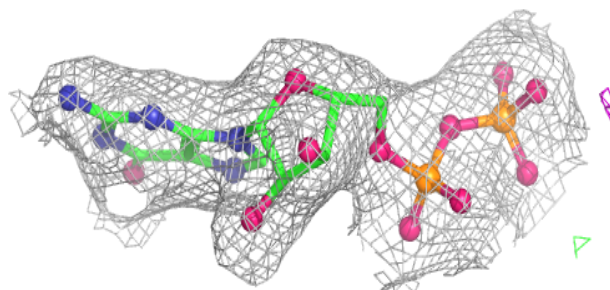
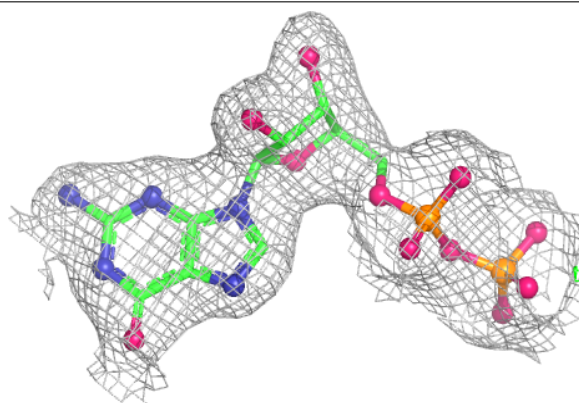


Electron density around GDP B 301:

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

**Electron density around GDP A 301:**

$2mF_o-DF_c$ (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.