



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 05:38 PM EDT

PDB ID : 3G6W
Title : Asymmetric GTP bound structure of UPRTase from *Sulfolobus solfataricus* containing PRPP-mg²⁺ in half of the active sites and R5P and PPi in the other half
Authors : Kadziola, A.; Christoffersen, S.
Deposited on : 2009-02-09
Resolution : 2.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

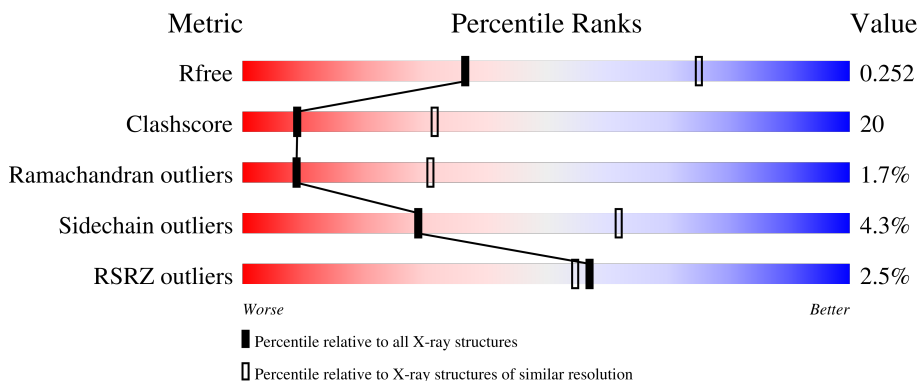
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	216	 6% 57% 39% .
1	B	216	 2% 58% 35% . 5%
1	C	216	 % 63% 31% . .
1	D	216	 56% 38% 5%

2 Entry composition [i](#)

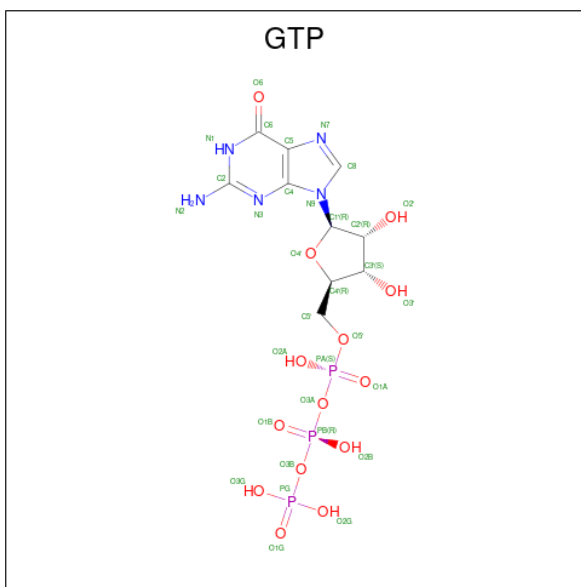
There are 7 unique types of molecules in this entry. The entry contains 6923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uracil phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	Total	C	N	O	S	0	0	0
			1695	1102	279	311	3			
1	B	206	Total	C	N	O	S	0	0	0
			1628	1060	269	296	3			
1	C	207	Total	C	N	O	S	0	0	0
			1635	1065	270	297	3			
1	D	215	Total	C	N	O	S	0	0	0
			1695	1102	279	311	3			

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
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		

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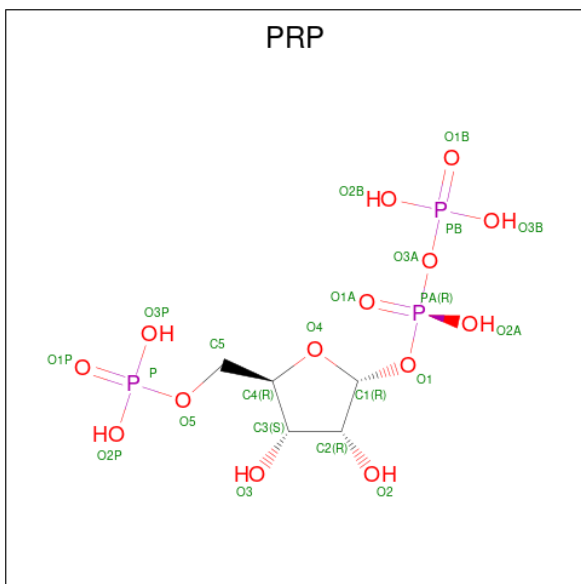
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

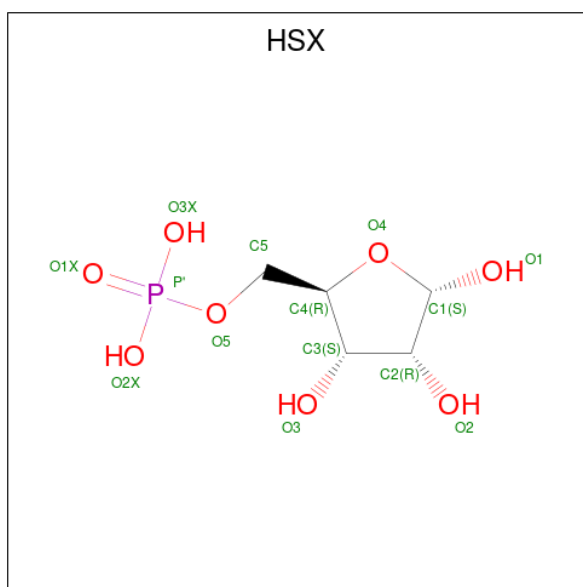
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (three-letter code: PRP) (formula: C₅H₁₃O₁₄P₃).



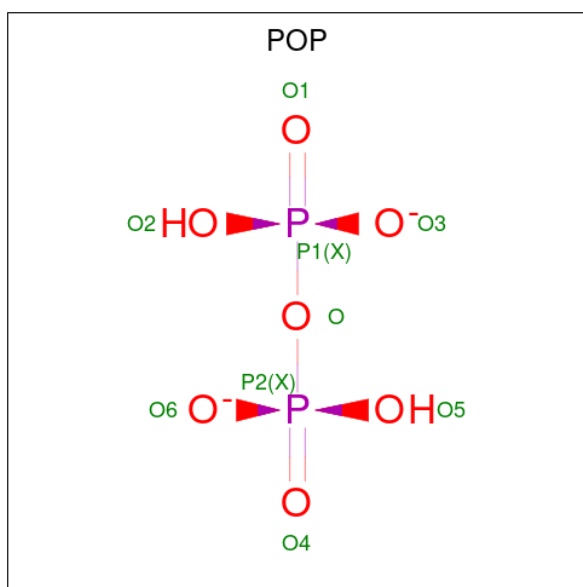
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	A	1	Total	C	O	P	0	0
			22	5	14	3		
4	D	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 5 is 5-O-phosphono-alpha-D-ribofuranose (three-letter code: HSX) (formula: C₅H₁₁O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			14	5	8	1		
5	C	1	Total	C	O	P	0	0
			14	5	8	1		
5	D	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			9	7	2		

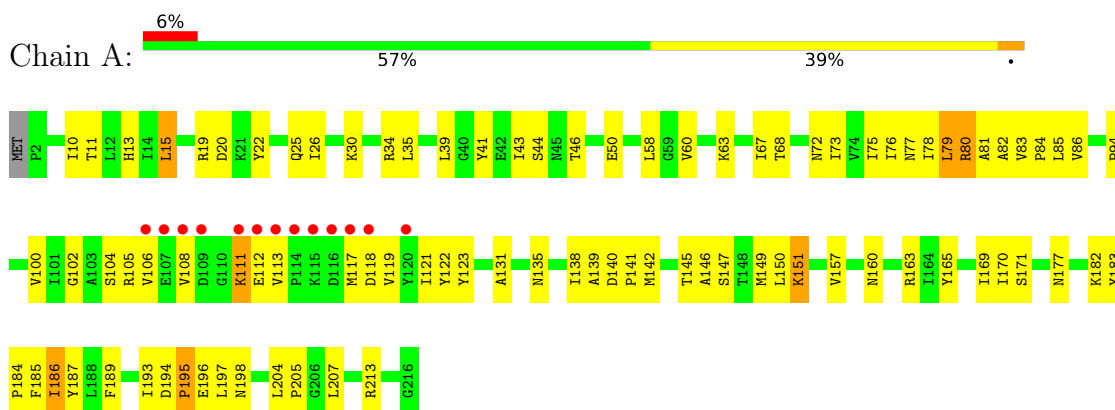
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total	O	0	0
			13	13		
7	B	5	Total	O	0	0
			5	5		
7	C	8	Total	O	0	0
			8	8		
7	D	8	Total	O	0	0
			8	8		

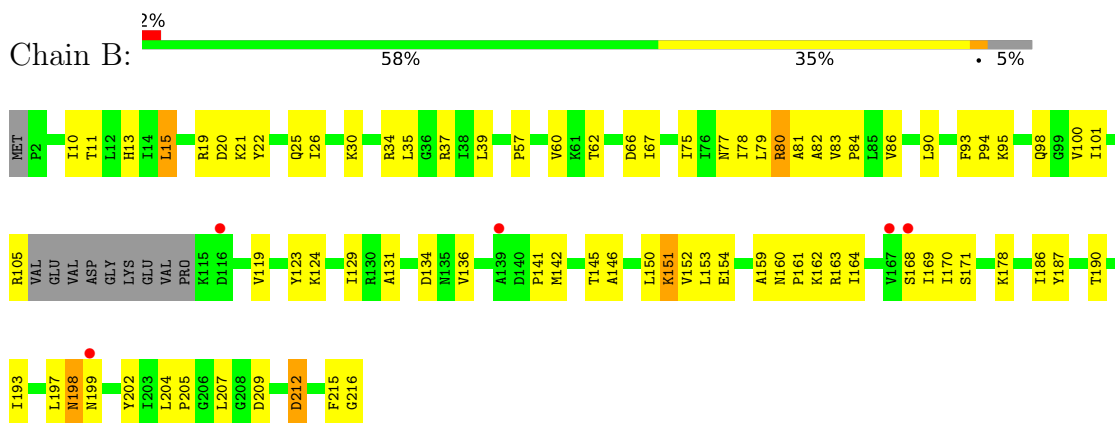
3 Residue-property plots

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.

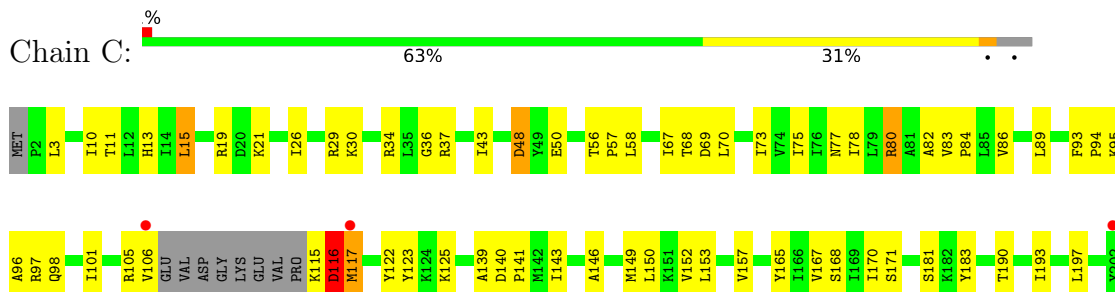
• Molecule 1: Uracil phosphoribosyltransferase



• Molecule 1: Uracil phosphoribosyltransferase



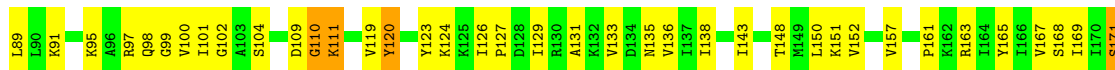
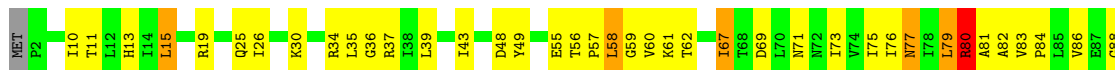
• Molecule 1: Uracil phosphoribosyltransferase





- Molecule 1: Uracil phosphoribosyltransferase

Chain D: 56% 38% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.04Å 98.76Å 73.53Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 24.52 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.90) 98.7 (24.52-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.89Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.274 0.197 , 0.252	Depositor DCC
R_{free} test set	984 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtrriage
Anisotropy	0.380	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.040 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.10% 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: GTP, POP, MG, HSX, PRP

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	0.39	0/1724	0.67	0/2338
1	B	0.42	0/1655	0.68	0/2242
1	C	0.39	0/1662	0.69	0/2252
1	D	0.42	0/1724	0.71	1/2338 (0.0%)
All	All	0.40	0/6765	0.69	1/9170 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	LEU	N-CA-C	5.69	126.36	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1695	0	1789	82	0
1	B	1628	0	1722	68	0
1	C	1635	0	1731	58	0
1	D	1695	0	1789	102	0
2	A	32	0	12	3	0
2	B	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	64	0	24	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	22	0	8	0	0
4	D	22	0	8	2	0
5	B	14	0	0	0	0
5	C	14	0	0	0	0
5	D	14	0	0	1	0
6	B	9	0	0	0	0
6	C	9	0	0	0	0
7	A	13	0	0	3	0
7	B	5	0	0	0	0
7	C	8	0	0	2	0
7	D	8	0	0	1	0
All	All	6923	0	7095	283	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 20.

All (283) 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:163:ARG:HD3	1:B:187:TYR:CE2	2.10	0.87
1:C:67:ILE:H	1:D:13:HIS:HD2	1.19	0.85
1:B:101:ILE:HD13	1:B:152:VAL:HG22	1.63	0.80
1:A:13:HIS:CD2	1:B:67:ILE:H	2.00	0.79
1:C:67:ILE:H	1:D:13:HIS:CD2	2.01	0.78
1:C:106:VAL:HG22	1:C:117:MET:SD	2.24	0.78
1:A:67:ILE:H	1:B:13:HIS:HD2	1.29	0.78
1:D:79:LEU:HB2	1:D:102:GLY:HA2	1.67	0.77
1:D:76:ILE:HD11	1:D:138:ILE:HG23	1.67	0.77
1:A:13:HIS:HD2	1:B:67:ILE:H	1.32	0.76
1:D:49:TYR:HB3	1:D:67:ILE:HG23	1.68	0.74
1:A:67:ILE:H	1:B:13:HIS:CD2	2.04	0.74
1:A:111:LYS:HG3	1:A:112:GLU:H	1.51	0.74
1:B:79:LEU:O	1:B:80:ARG:HB2	1.86	0.73
1:A:113:VAL:HG11	1:A:197:LEU:HB2	1.70	0.73
1:D:80:ARG:HB2	4:D:303:PRP:O3B	1.88	0.72
1:A:177:ASN:HB2	7:A:228:HOH:O	1.90	0.71
1:A:105:ARG:HD2	1:A:117:MET:HE3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ALA:HB3	7:D:220:HOH:O	1.90	0.69
1:D:35:LEU:HD13	1:D:169:ILE:HD12	1.74	0.69
1:D:76:ILE:HG12	1:D:138:ILE:HA	1.74	0.69
1:C:205:PRO:HG3	1:D:62:THR:HB	1.73	0.69
1:B:209:ASP:OD2	1:B:212:ASP:HB2	1.94	0.68
1:D:101:ILE:HG13	1:D:126:ILE:HD11	1.75	0.67
1:D:77:ASN:ND2	1:D:82:ALA:HB3	2.10	0.67
1:A:35:LEU:HD13	1:A:169:ILE:HD12	1.76	0.66
1:D:73:ILE:HD13	1:D:135:ASN:HB2	1.77	0.66
1:D:143:ILE:HB	1:D:171:SER:HB3	1.77	0.66
1:A:151:LYS:NZ	1:A:151:LYS:HA	2.10	0.65
1:D:76:ILE:CD1	1:D:152:VAL:HG11	2.26	0.65
1:C:115:LYS:O	1:C:115:LYS:HD3	1.95	0.65
1:B:20:ASP:OD1	1:B:22:TYR:HB2	1.97	0.65
1:B:81:ALA:HB1	1:B:141:PRO:HG3	1.78	0.65
1:A:58:LEU:HD22	1:B:204:LEU:HD21	1.78	0.65
1:D:129:ILE:HD13	1:D:136:VAL:HG21	1.79	0.65
1:D:60:VAL:HG12	1:D:61:LYS:N	2.10	0.64
1:C:153:LEU:O	1:C:157:VAL:HG23	1.98	0.64
1:A:63:LYS:HG2	7:A:222:HOH:O	1.98	0.64
1:D:104:SER:HB3	1:D:120:TYR:HD2	1.62	0.64
1:D:76:ILE:CD1	1:D:138:ILE:HG12	2.28	0.64
1:C:13:HIS:CD2	1:D:67:ILE:HG13	2.32	0.64
1:A:63:LYS:HE2	7:A:222:HOH:O	1.99	0.63
1:B:83:VAL:HB	1:B:84:PRO:HD3	1.80	0.62
1:D:77:ASN:C	1:D:77:ASN:HD22	2.02	0.62
1:A:105:ARG:HD2	1:A:117:MET:CE	2.29	0.62
1:B:145:THR:O	1:B:146:ALA:HB3	2.00	0.61
1:A:151:LYS:HA	1:A:151:LYS:HZ2	1.65	0.61
1:C:122:TYR:HB2	7:C:223:HOH:O	2.00	0.61
1:A:163:ARG:HD3	1:A:187:TYR:CE2	2.35	0.61
1:D:39:LEU:HD23	1:D:167:VAL:HG12	1.82	0.61
1:D:80:ARG:CB	4:D:303:PRP:O3B	2.49	0.61
1:A:106:VAL:HG23	1:A:118:ASP:O	2.00	0.60
1:D:60:VAL:HG12	1:D:61:LYS:H	1.66	0.60
1:C:13:HIS:HD2	1:D:67:ILE:H	1.50	0.60
1:B:100:VAL:HG23	1:B:123:TYR:HE2	1.67	0.60
1:D:110:GLY:HA2	1:D:199:ASN:HB2	1.84	0.59
1:D:76:ILE:HG13	1:D:76:ILE:O	2.01	0.59
1:D:209:ASP:OD2	1:D:212:ASP:HB2	2.03	0.59
1:B:142:MET:CE	1:B:207:LEU:HG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:MET:HB2	7:C:222:HOH:O	2.03	0.58
1:D:163:ARG:CD	1:D:187:TYR:CE2	2.86	0.58
1:A:150:LEU:HD22	1:A:182:LYS:HD3	1.85	0.58
1:C:146:ALA:O	1:C:150:LEU:HG	2.04	0.58
1:B:82:ALA:O	1:B:86:VAL:HG23	2.03	0.58
1:A:131:ALA:HA	1:A:160:ASN:O	2.04	0.58
1:B:197:LEU:HA	1:B:202:TYR:O	2.03	0.58
1:D:39:LEU:HD23	1:D:167:VAL:CG1	2.34	0.57
1:D:71:ASN:OD1	1:D:95:LYS:HD2	2.04	0.57
1:D:109:ASP:O	1:D:111:LYS:HG3	2.04	0.57
1:A:163:ARG:HD2	1:A:165:TYR:CE1	2.40	0.57
1:B:81:ALA:O	1:B:84:PRO:HD2	2.04	0.57
1:C:36:GLY:O	1:C:89:LEU:HD23	2.05	0.57
1:C:19:ARG:HD3	1:D:62:THR:HG21	1.87	0.57
1:C:78:ILE:CD1	1:C:152:VAL:HG21	2.35	0.57
1:D:57:PRO:C	1:D:59:GLY:H	2.08	0.56
1:B:100:VAL:CG2	1:B:123:TYR:HE2	2.18	0.56
1:D:104:SER:HB3	1:D:120:TYR:CD2	2.40	0.56
1:A:77:ASN:HD21	1:A:83:VAL:HA	1.71	0.56
1:B:15:LEU:HD21	1:B:170:ILE:HD11	1.87	0.56
1:D:75:ILE:HG21	1:D:86:VAL:HG13	1.87	0.56
1:D:77:ASN:ND2	1:D:77:ASN:C	2.59	0.56
1:C:75:ILE:HG21	1:C:86:VAL:HG13	1.88	0.56
1:A:58:LEU:HD22	1:B:204:LEU:CD2	2.36	0.55
1:D:76:ILE:HD11	1:D:138:ILE:CG2	2.36	0.55
1:A:111:LYS:HG3	1:A:112:GLU:N	2.20	0.55
1:D:83:VAL:HB	1:D:84:PRO:HD3	1.87	0.55
1:D:163:ARG:HD2	1:D:187:TYR:CE2	2.41	0.55
1:D:79:LEU:O	1:D:80:ARG:HB2	2.06	0.55
1:C:205:PRO:HB2	1:D:56:THR:HG21	1.88	0.54
1:B:95:LYS:HG3	1:D:26:ILE:HD11	1.88	0.54
1:C:157:VAL:HG21	1:C:183:TYR:CE2	2.43	0.54
1:D:25:GLN:OE1	1:D:216:GLY:HA3	2.06	0.54
1:B:207:LEU:C	1:B:207:LEU:HD12	2.28	0.54
1:A:111:LYS:HE3	1:A:112:GLU:HG3	1.88	0.54
1:A:79:LEU:O	1:A:80:ARG:HB2	2.07	0.54
1:A:102:GLY:HA3	1:A:122:TYR:CE1	2.43	0.54
1:A:79:LEU:HB2	1:A:102:GLY:HA2	1.90	0.54
1:A:83:VAL:HB	1:A:84:PRO:HD3	1.90	0.53
1:A:121:ILE:HG22	1:A:123:TYR:O	2.09	0.53
1:B:198:ASN:HD21	1:B:202:TYR:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ASP:HB2	5:D:306:HSX:C3	2.38	0.53
1:C:82:ALA:O	1:C:86:VAL:HG23	2.08	0.53
1:C:171:SER:O	1:C:193:ILE:HA	2.09	0.53
1:B:215:PHE:HD1	1:D:98:GLN:HB3	1.74	0.52
1:C:83:VAL:HB	1:C:84:PRO:HD3	1.91	0.52
1:B:77:ASN:HD21	1:B:83:VAL:HA	1.74	0.52
1:D:101:ILE:HG12	1:D:124:LYS:HG3	1.91	0.52
1:A:50:GLU:OE2	1:A:68:THR:HG21	2.10	0.52
1:A:15:LEU:HD22	1:A:19:ARG:HG3	1.91	0.52
1:C:15:LEU:HD21	1:C:170:ILE:HD11	1.92	0.52
1:D:77:ASN:HB2	1:D:86:VAL:HG21	1.91	0.52
2:A:301:GTP:H4'	1:B:94:PRO:HG3	1.91	0.52
1:B:25:GLN:OE1	1:B:216:GLY:HA3	2.09	0.52
1:B:78:ILE:HA	1:B:101:ILE:HG22	1.93	0.51
1:D:58:LEU:C	1:D:60:VAL:H	2.14	0.51
1:D:76:ILE:HG12	1:D:138:ILE:HG12	1.92	0.51
1:A:35:LEU:CD1	1:A:169:ILE:HD12	2.40	0.51
1:A:39:LEU:O	1:A:43:ILE:HG13	2.10	0.51
1:A:204:LEU:HA	1:A:205:PRO:C	2.31	0.51
1:C:209:ASP:HB3	1:C:212:ASP:HB2	1.92	0.51
1:A:157:VAL:HG21	1:A:183:TYR:CE2	2.45	0.51
1:A:111:LYS:HB2	1:A:111:LYS:NZ	2.26	0.51
1:B:131:ALA:HA	1:B:160:ASN:O	2.11	0.51
1:D:25:GLN:HG3	1:D:213:ARG:O	2.11	0.51
1:A:26:ILE:HD11	1:C:95:LYS:HG2	1.94	0.50
1:B:35:LEU:O	1:B:39:LEU:HB2	2.11	0.50
1:D:76:ILE:HD12	1:D:152:VAL:HG11	1.93	0.50
1:D:110:GLY:O	1:D:111:LYS:HG3	2.10	0.50
2:A:301:GTP:H2'	2:D:217:GTP:O6	2.11	0.50
1:A:75:ILE:HG21	1:A:86:VAL:HG13	1.92	0.50
1:C:67:ILE:O	1:C:67:ILE:HG22	2.12	0.50
1:D:99:GLY:HA2	1:D:127:PRO:HD3	1.93	0.50
1:C:73:ILE:HB	1:C:96:ALA:HB2	1.92	0.50
1:A:171:SER:O	1:A:193:ILE:HA	2.11	0.50
1:B:171:SER:O	1:B:193:ILE:HA	2.11	0.50
1:A:19:ARG:HD3	1:B:62:THR:HG21	1.94	0.49
1:D:163:ARG:HG2	1:D:165:TYR:CE1	2.47	0.49
1:B:75:ILE:HG21	1:B:86:VAL:HG13	1.94	0.49
1:B:35:LEU:HD13	1:B:169:ILE:HD12	1.93	0.49
1:D:195:PRO:HG2	1:D:196:GLU:H	1.78	0.49
1:D:77:ASN:HD22	1:D:82:ALA:HB3	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ASN:HB3	1:D:204:LEU:HD11	1.95	0.49
1:B:129:ILE:HB	1:B:159:ALA:HB1	1.94	0.48
1:A:77:ASN:ND2	1:A:86:VAL:HG21	2.29	0.48
1:B:10:ILE:HG23	1:B:11:THR:N	2.28	0.48
1:D:10:ILE:HG23	1:D:11:THR:N	2.28	0.48
1:C:15:LEU:HD22	1:C:19:ARG:HG3	1.95	0.48
1:C:26:ILE:O	1:C:30:LYS:HB2	2.13	0.48
1:C:197:LEU:HD23	1:C:197:LEU:N	2.28	0.48
1:C:21:LYS:HB3	1:D:55:GLU:O	2.13	0.48
1:A:85:LEU:HD23	1:A:139:ALA:HB1	1.96	0.48
2:A:301:GTP:O6	2:D:217:GTP:H2'	2.13	0.48
1:B:134:ASP:O	1:B:162:LYS:HB3	2.13	0.48
1:A:102:GLY:HA3	1:A:123:TYR:HB3	1.95	0.48
1:C:101:ILE:HG23	1:C:101:ILE:O	2.14	0.48
1:D:58:LEU:O	1:D:60:VAL:HG23	2.14	0.48
1:D:79:LEU:HD23	1:D:79:LEU:HA	1.45	0.48
1:A:82:ALA:O	1:A:86:VAL:HG23	2.13	0.47
1:A:145:THR:O	1:A:146:ALA:HB3	2.14	0.47
1:B:142:MET:HE2	1:B:207:LEU:HG	1.95	0.47
1:A:122:TYR:CD1	1:A:122:TYR:C	2.88	0.47
1:A:184:PRO:HG2	1:A:185:PHE:CD1	2.49	0.47
1:A:207:LEU:O	1:A:213:ARG:NH1	2.48	0.47
1:B:80:ARG:HG3	1:D:123:TYR:OH	2.14	0.47
1:C:10:ILE:HG23	1:C:11:THR:N	2.29	0.47
1:D:80:ARG:HH11	1:D:80:ARG:HB3	1.78	0.47
1:D:150:LEU:HD11	1:D:178:LYS:HG2	1.97	0.47
1:A:108:VAL:HG23	1:A:108:VAL:O	2.15	0.47
1:B:90:LEU:HD11	1:B:98:GLN:HE22	1.78	0.47
1:A:20:ASP:OD1	1:A:22:TYR:HB2	2.15	0.47
1:A:10:ILE:HG23	1:A:11:THR:N	2.30	0.47
1:B:168:SER:O	1:B:190:THR:HA	2.14	0.47
1:D:15:LEU:HD22	1:D:19:ARG:HG3	1.97	0.47
1:D:30:LYS:O	1:D:34:ARG:HG3	2.15	0.46
1:A:170:ILE:HD12	1:A:207:LEU:HG	1.96	0.46
1:A:195:PRO:HG2	1:A:196:GLU:H	1.79	0.46
1:D:83:VAL:CB	1:D:84:PRO:HD3	2.46	0.46
1:A:194:ASP:HB3	1:A:204:LEU:O	2.15	0.46
1:A:122:TYR:CD1	1:C:123:TYR:HB2	2.51	0.46
1:B:100:VAL:HG23	1:B:123:TYR:CE2	2.50	0.46
1:A:213:ARG:NH1	1:B:57:PRO:HG2	2.30	0.46
1:B:15:LEU:HD22	1:B:19:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:HG3	1:B:105:ARG:HH11	1.80	0.46
1:B:145:THR:O	1:B:146:ALA:CB	2.62	0.46
1:A:30:LYS:O	1:A:34:ARG:HG3	2.16	0.46
1:C:168:SER:O	1:C:190:THR:HA	2.14	0.46
1:C:116:ASP:O	1:C:117:MET:C	2.54	0.45
1:D:157:VAL:HG21	1:D:183:TYR:CE2	2.52	0.45
1:D:171:SER:O	1:D:193:ILE:HA	2.16	0.45
1:C:56:THR:HG22	1:D:19:ARG:HB3	1.99	0.45
1:B:93:PHE:N	1:B:94:PRO:HD3	2.30	0.45
1:C:68:THR:C	1:C:70:LEU:N	2.70	0.45
1:A:78:ILE:HD12	1:A:140:ASP:HB2	1.98	0.45
1:A:138:ILE:HG21	1:A:149:MET:SD	2.56	0.45
1:D:73:ILE:CD1	1:D:135:ASN:HB2	2.45	0.45
1:B:142:MET:HE1	1:B:207:LEU:HG	1.98	0.45
1:D:43:ILE:HG23	1:D:165:TYR:CE2	2.51	0.45
1:A:13:HIS:HD2	1:B:67:ILE:N	2.06	0.45
1:A:41:TYR:O	1:A:44:SER:HB2	2.16	0.45
1:A:79:LEU:HD13	1:A:100:VAL:HG13	1.98	0.45
1:A:163:ARG:HD2	1:A:165:TYR:CZ	2.52	0.45
1:A:25:GLN:HE22	1:C:97:ARG:HG3	1.82	0.44
1:C:48:ASP:HB2	1:C:69:ASP:OD2	2.17	0.44
1:B:105:ARG:HA	1:B:119:VAL:HG12	1.99	0.44
1:B:204:LEU:HA	1:B:205:PRO:C	2.37	0.44
1:C:30:LYS:O	1:C:34:ARG:HG3	2.17	0.44
1:A:198:ASN:HB3	1:A:204:LEU:HD11	1.99	0.44
1:C:29:ARG:HG3	1:C:29:ARG:HH11	1.82	0.44
1:C:43:ILE:HD11	1:C:167:VAL:HG22	1.99	0.44
1:A:67:ILE:N	1:B:13:HIS:HD2	2.07	0.44
1:B:30:LYS:O	1:B:34:ARG:HG3	2.18	0.44
1:C:106:VAL:HA	1:C:117:MET:CG	2.47	0.44
1:D:60:VAL:CG1	1:D:61:LYS:N	2.78	0.44
1:A:81:ALA:O	1:A:84:PRO:HD2	2.17	0.44
1:A:117:MET:HE2	1:A:145:THR:HG21	1.99	0.44
1:C:143:ILE:HB	1:C:171:SER:CB	2.48	0.44
1:D:76:ILE:CG1	1:D:138:ILE:HG12	2.48	0.44
1:D:110:GLY:C	1:D:111:LYS:HG3	2.38	0.44
1:A:183:TYR:CB	1:A:186:ILE:HD12	2.48	0.44
1:D:77:ASN:CB	1:D:86:VAL:HG21	2.48	0.44
1:A:79:LEU:HD13	1:A:100:VAL:CG1	2.48	0.43
1:B:150:LEU:HD11	1:B:178:LYS:HG3	1.99	0.43
1:D:168:SER:O	1:D:190:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:VAL:HA	1:C:117:MET:SD	2.58	0.43
1:A:72:ASN:O	1:A:73:ILE:HD13	2.17	0.43
1:B:119:VAL:O	1:B:151:LYS:HG3	2.18	0.43
1:B:124:LYS:O	1:B:124:LYS:HG2	2.18	0.43
1:C:43:ILE:HG23	1:C:165:TYR:CE2	2.53	0.43
1:D:88:GLY:HA2	1:D:91:LYS:HG2	2.00	0.43
1:D:131:ALA:C	1:D:133:VAL:H	2.21	0.43
1:A:119:VAL:HG21	1:A:147:SER:HB3	2.00	0.43
1:C:123:TYR:OH	1:C:125:LYS:HB2	2.18	0.43
1:D:60:VAL:CG1	1:D:61:LYS:H	2.31	0.43
1:C:77:ASN:O	1:C:101:ILE:HG22	2.18	0.43
1:C:93:PHE:N	1:C:94:PRO:HD3	2.33	0.43
1:A:76:ILE:HB	1:A:138:ILE:HA	2.01	0.43
1:B:215:PHE:CD1	1:D:98:GLN:HB3	2.53	0.43
1:A:46:THR:HG21	1:A:189:PHE:HZ	1.83	0.43
1:C:116:ASP:O	1:C:117:MET:O	2.36	0.43
1:D:76:ILE:CD1	1:D:138:ILE:HG23	2.44	0.43
1:D:148:THR:O	1:D:151:LYS:HB3	2.18	0.43
1:D:204:LEU:HA	1:D:205:PRO:C	2.38	0.43
1:B:26:ILE:O	1:B:30:LYS:HB2	2.19	0.43
1:A:13:HIS:CD2	1:B:66:ASP:HA	2.54	0.43
1:B:80:ARG:CG	1:D:123:TYR:OH	2.67	0.43
1:C:58:LEU:HD22	1:C:58:LEU:N	2.34	0.43
1:B:150:LEU:HA	1:B:153:LEU:HD12	2.01	0.42
1:C:67:ILE:N	1:D:13:HIS:HD2	2.00	0.42
1:B:129:ILE:HG21	1:B:161:PRO:HB3	2.00	0.42
1:D:76:ILE:CG1	1:D:138:ILE:HA	2.46	0.42
1:B:164:ILE:HB	1:B:186:ILE:HG12	2.01	0.42
1:D:163:ARG:HD3	1:D:187:TYR:CE2	2.54	0.42
1:C:68:THR:C	1:C:70:LEU:H	2.22	0.42
1:C:139:ALA:O	1:C:140:ASP:HB2	2.18	0.42
1:D:71:ASN:OD1	1:D:95:LYS:CD	2.67	0.42
1:D:207:LEU:C	1:D:207:LEU:HD12	2.39	0.42
1:A:94:PRO:HG3	2:B:301:GTP:O2'	2.20	0.42
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.74	0.42
1:D:35:LEU:O	1:D:39:LEU:HB2	2.19	0.42
1:D:79:LEU:HG	1:D:100:VAL:CG1	2.50	0.42
1:B:90:LEU:HD11	1:B:98:GLN:NE2	2.34	0.42
1:C:67:ILE:CG2	1:C:70:LEU:HG	2.50	0.42
1:D:36:GLY:O	1:D:89:LEU:HD23	2.19	0.42
1:A:104:SER:HB2	1:A:122:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ASP:O	1:D:110:GLY:C	2.58	0.42
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.59	0.42
1:A:142:MET:HA	1:A:170:ILE:O	2.19	0.42
1:C:3:LEU:HD21	1:C:193:ILE:HD11	2.01	0.42
1:C:67:ILE:HG22	1:C:70:LEU:HG	2.02	0.42
1:D:79:LEU:HD22	1:D:80:ARG:H	1.83	0.42
1:A:184:PRO:HG2	1:A:185:PHE:CE1	2.54	0.41
1:D:76:ILE:HD11	1:D:152:VAL:HG11	2.02	0.41
1:C:86:VAL:HG11	1:C:98:GLN:HE21	1.85	0.41
1:D:119:VAL:HG21	1:D:148:THR:HA	2.01	0.41
1:D:80:ARG:O	1:D:81:ALA:C	2.58	0.41
1:B:151:LYS:HD3	1:B:154:GLU:OE2	2.20	0.41
1:B:129:ILE:HD13	1:B:136:VAL:HG21	2.02	0.41
1:D:57:PRO:C	1:D:59:GLY:N	2.73	0.41
1:D:129:ILE:HG21	1:D:161:PRO:HB3	2.03	0.41
1:A:73:ILE:HD13	1:A:135:ASN:HB2	2.03	0.41
1:A:30:LYS:HA	1:A:30:LYS:HD2	1.89	0.40
1:C:140:ASP:HA	1:C:141:PRO:HD2	1.86	0.40
1:D:143:ILE:HB	1:D:171:SER:CB	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/216 (99%)	183 (86%)	28 (13%)	2 (1%)	17	48
1	B	202/216 (94%)	180 (89%)	20 (10%)	2 (1%)	15	45
1	C	203/216 (94%)	176 (87%)	22 (11%)	5 (2%)	5	21
1	D	213/216 (99%)	185 (87%)	23 (11%)	5 (2%)	6	23
All	All	831/864 (96%)	724 (87%)	93 (11%)	14 (2%)	9	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	ARG
1	C	80	ARG
1	C	105	ARG
1	C	116	ASP
1	C	117	MET
1	D	80	ARG
1	A	80	ARG
1	B	198	ASN
1	D	58	LEU
1	D	110	GLY
1	D	111	LYS
1	A	195	PRO
1	C	57	PRO
1	D	195	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/189 (100%)	181 (96%)	7 (4%)	34	68
1	B	180/189 (95%)	173 (96%)	7 (4%)	32	66
1	C	181/189 (96%)	174 (96%)	7 (4%)	32	66
1	D	188/189 (100%)	177 (94%)	11 (6%)	19	49
All	All	737/756 (98%)	705 (96%)	32 (4%)	29	62

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	60	VAL
1	A	79	LEU
1	A	111	LYS
1	A	141	PRO
1	A	151	LYS

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Mol	Chain	Res	Type
1	A	186	ILE
1	B	15	LEU
1	B	21	LYS
1	B	37	ARG
1	B	60	VAL
1	B	151	LYS
1	B	199	ASN
1	B	212	ASP
1	C	15	LEU
1	C	37	ARG
1	C	48	ASP
1	C	50	GLU
1	C	80	ARG
1	C	116	ASP
1	C	181	SER
1	D	15	LEU
1	D	37	ARG
1	D	48	ASP
1	D	67	ILE
1	D	69	ASP
1	D	77	ASN
1	D	80	ARG
1	D	97	ARG
1	D	120	TYR
1	D	171	SER
1	D	199	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	25	GLN
1	A	77	ASN
1	A	160	ASN
1	B	13	HIS
1	B	17	GLN
1	B	77	ASN
1	B	98	GLN
1	C	13	HIS
1	C	98	GLN
1	C	177	ASN
1	D	13	HIS

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Mol	Chain	Res	Type
1	D	17	GLN
1	D	77	ASN
1	D	135	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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
6	POP	C	307	-	6,8,8	1.04	0	13,13,13	1.06	1 (7%)
5	HSX	D	306	-	14,14,14	0.96	1 (7%)	20,21,21	1.43	3 (15%)
4	PRP	A	303	3	19,22,22	0.97	1 (5%)	33,35,35	1.03	2 (6%)
5	HSX	C	306	-	14,14,14	0.73	0	20,21,21	1.35	4 (20%)
6	POP	B	307	-	6,8,8	1.23	1 (16%)	13,13,13	1.07	0
2	GTP	A	301	3	26,34,34	1.43	3 (11%)	32,54,54	1.17	3 (9%)
2	GTP	B	301	3	26,34,34	1.52	4 (15%)	32,54,54	1.11	2 (6%)
4	PRP	D	303	3	19,22,22	1.14	2 (10%)	33,35,35	1.12	3 (9%)
2	GTP	D	301	3	26,34,34	1.51	3 (11%)	32,54,54	1.17	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GTP	D	217	3	26,34,34	1.49	3 (11%)	32,54,54	1.08	2 (6%)
5	HSX	B	306	-	14,14,14	0.81	0	20,21,21	1.34	2 (10%)

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
6	POP	C	307	-	-	2/6/6/6	-
5	HSX	D	306	-	-	1/6/22/22	0/1/1/1
4	PRP	A	303	3	-	2/16/33/33	0/1/1/1
5	HSX	C	306	-	-	2/6/22/22	0/1/1/1
6	POP	B	307	-	-	0/6/6/6	-
2	GTP	A	301	3	-	2/18/38/38	0/3/3/3
2	GTP	B	301	3	-	3/18/38/38	0/3/3/3
4	PRP	D	303	3	-	11/16/33/33	0/1/1/1
2	GTP	D	301	3	-	3/18/38/38	0/3/3/3
2	GTP	D	217	3	-	8/18/38/38	0/3/3/3
5	HSX	B	306	-	-	2/6/22/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	GTP	C6-N1	4.66	1.44	1.37
2	D	217	GTP	C6-N1	4.26	1.44	1.37
2	B	301	GTP	C6-N1	4.04	1.43	1.37
2	D	217	GTP	C8-N7	-3.44	1.29	1.35
2	A	301	GTP	C6-N1	3.40	1.42	1.37
2	B	301	GTP	C8-N7	-3.26	1.29	1.35
2	D	301	GTP	C2'-C1'	-3.07	1.49	1.53
2	D	301	GTP	C8-N7	-3.03	1.29	1.35
2	A	301	GTP	C8-N7	-3.00	1.29	1.35
2	A	301	GTP	O4'-C1'	2.83	1.45	1.41
2	B	301	GTP	C2'-C1'	-2.82	1.49	1.53
2	D	217	GTP	C2'-C1'	-2.70	1.49	1.53
4	A	303	PRP	O4-C4	2.60	1.50	1.45
2	B	301	GTP	O4'-C1'	2.51	1.44	1.41
4	D	303	PRP	O4-C4	2.51	1.50	1.45
4	D	303	PRP	PA-O1	2.28	1.66	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	306	HSX	O4-C1	-2.26	1.40	1.43
6	B	307	POP	P1-O2	-2.05	1.46	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	GTP	C3'-C2'-C1'	4.51	107.78	100.98
2	B	301	GTP	C3'-C2'-C1'	4.24	107.37	100.98
2	A	301	GTP	C3'-C2'-C1'	4.14	107.21	100.98
2	D	217	GTP	C3'-C2'-C1'	3.92	106.87	100.98
5	B	306	HSX	O1-C1-O4	-3.16	107.08	111.13
5	D	306	HSX	O4-C4-C3	3.13	111.30	105.11
5	D	306	HSX	O1-C1-O4	-3.07	107.21	111.13
5	C	306	HSX	O1-C1-O4	-2.95	107.36	111.13
5	B	306	HSX	O4-C4-C3	2.61	110.28	105.11
2	D	301	GTP	O6-C6-C5	2.54	129.34	124.37
4	D	303	PRP	P-O5-C5	2.51	125.22	118.30
2	A	301	GTP	O6-C6-N1	-2.51	117.69	120.65
5	D	306	HSX	O4-C1-C2	2.47	107.50	104.46
2	D	217	GTP	O6-C6-C5	2.47	129.19	124.37
5	C	306	HSX	O4-C4-C3	2.44	109.94	105.11
2	A	301	GTP	O6-C6-C5	2.43	129.12	124.37
4	A	303	PRP	P-O5-C5	2.42	124.97	118.30
4	D	303	PRP	O3P-P-O5	-2.27	100.68	106.73
5	C	306	HSX	O5-C5-C4	2.27	116.79	108.99
2	B	301	GTP	O6-C6-C5	2.25	128.78	124.37
6	C	307	POP	O2-P1-O	2.20	112.02	104.64
4	A	303	PRP	O3P-P-O5	-2.12	101.10	106.73
5	C	306	HSX	P'-O5-C5	-2.08	112.57	118.30
4	D	303	PRP	O4-C1-O1	2.06	113.27	109.18

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GTP	PB-O3B-PG-O2G
2	D	217	GTP	C5'-O5'-PA-O3A
4	D	303	PRP	C1-O1-PA-O2A
4	D	303	PRP	C5-O5-P-O2P
4	D	303	PRP	C5-O5-P-O3P
5	B	306	HSX	O4-C4-C5-O5
4	D	303	PRP	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
5	B	306	HSX	C3-C4-C5-O5
5	C	306	HSX	O4-C4-C5-O5
5	C	306	HSX	C3-C4-C5-O5
4	D	303	PRP	C1-O1-PA-O3A
2	D	301	GTP	C3'-C4'-C5'-O5'
2	D	301	GTP	O4'-C4'-C5'-O5'
4	A	303	PRP	C5-O5-P-O1P
4	D	303	PRP	C5-O5-P-O1P
4	D	303	PRP	O4-C4-C5-O5
4	D	303	PRP	PB-O3A-PA-O1
6	C	307	POP	P2-O-P1-O3
2	A	301	GTP	PG-O3B-PB-O1B
2	A	301	GTP	PA-O3A-PB-O1B
2	D	301	GTP	PB-O3A-PA-O1A
4	D	303	PRP	C1-O1-PA-O1A
2	D	217	GTP	C5'-O5'-PA-O1A
2	D	217	GTP	O4'-C4'-C5'-O5'
4	D	303	PRP	C4-C5-O5-P
2	B	301	GTP	PB-O3A-PA-O1A
2	D	217	GTP	PA-O3A-PB-O1B
2	D	217	GTP	C3'-C4'-C5'-O5'
5	D	306	HSX	O4-C4-C5-O5
6	C	307	POP	P2-O-P1-O1
4	A	303	PRP	C3-C4-C5-O5
2	B	301	GTP	PB-O3B-PG-O3G
2	D	217	GTP	PG-O3B-PB-O2B
2	D	217	GTP	PB-O3A-PA-O2A
2	D	217	GTP	C5'-O5'-PA-O2A
4	D	303	PRP	C2-C1-O1-PA

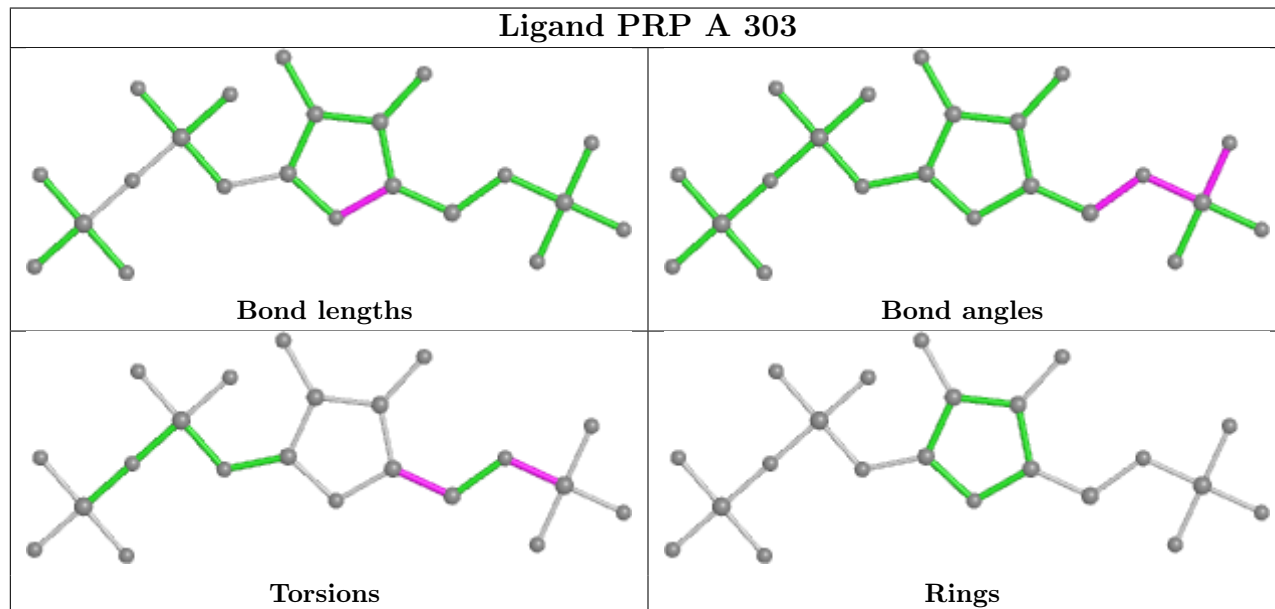
There are no ring outliers.

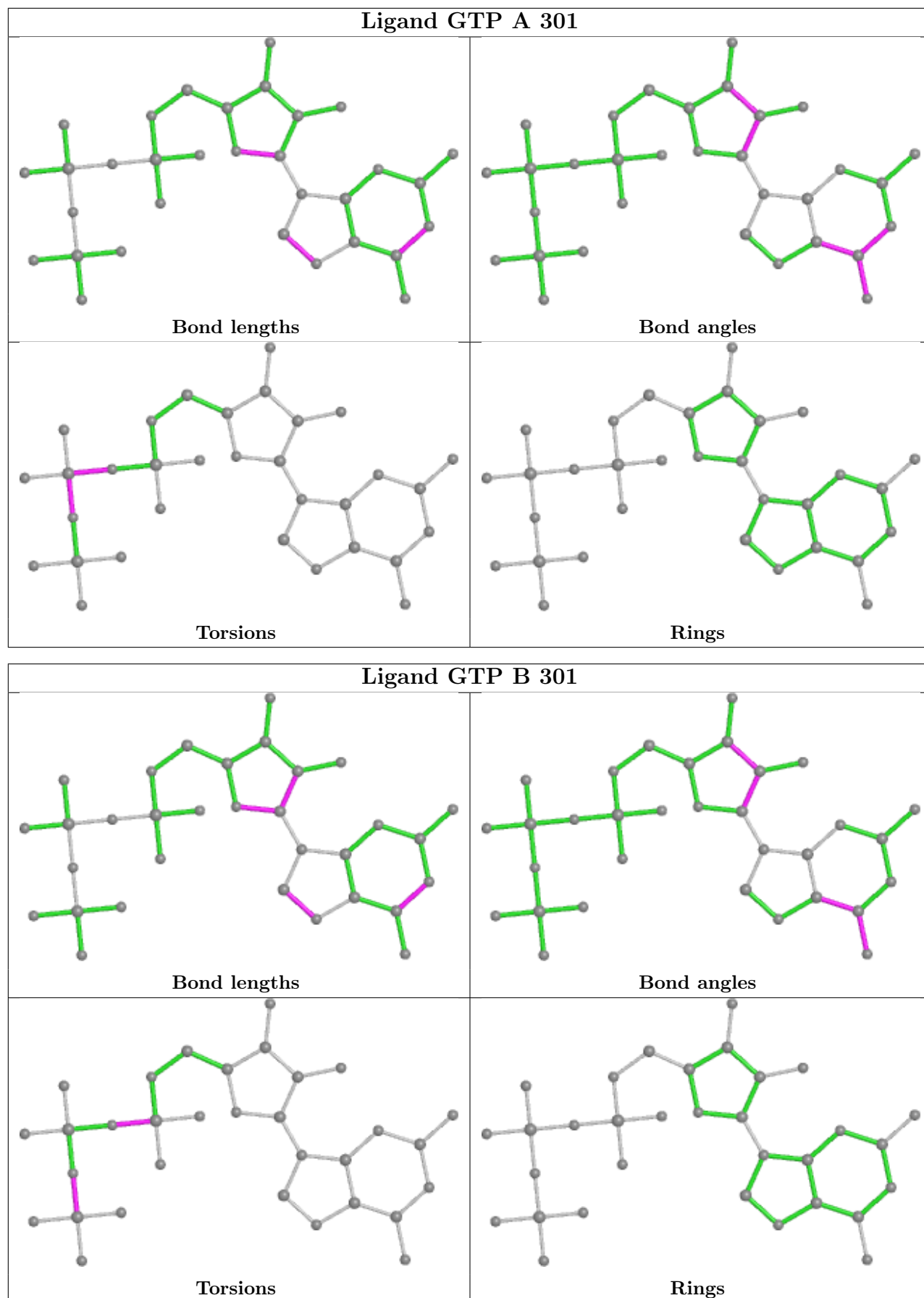
5 monomers are involved in 7 short contacts:

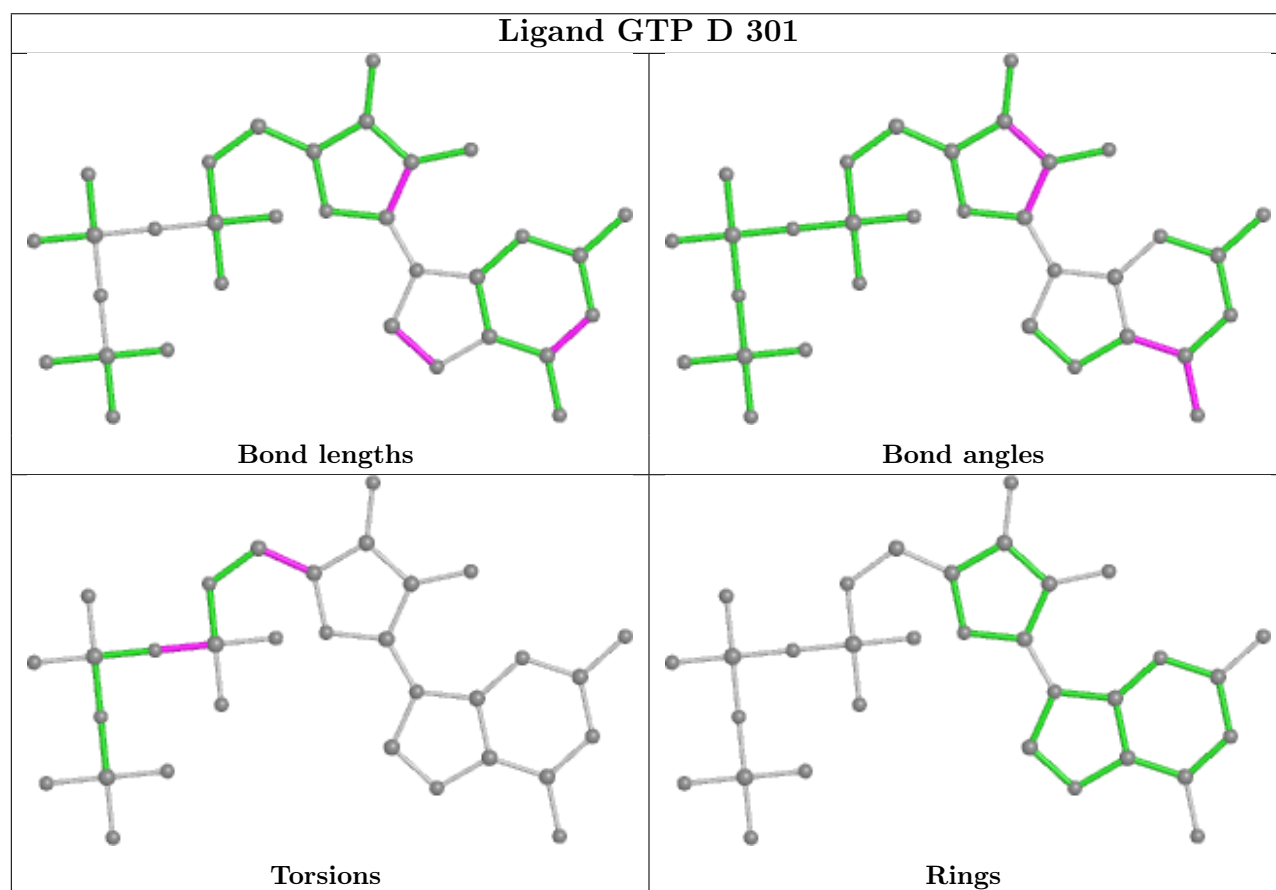
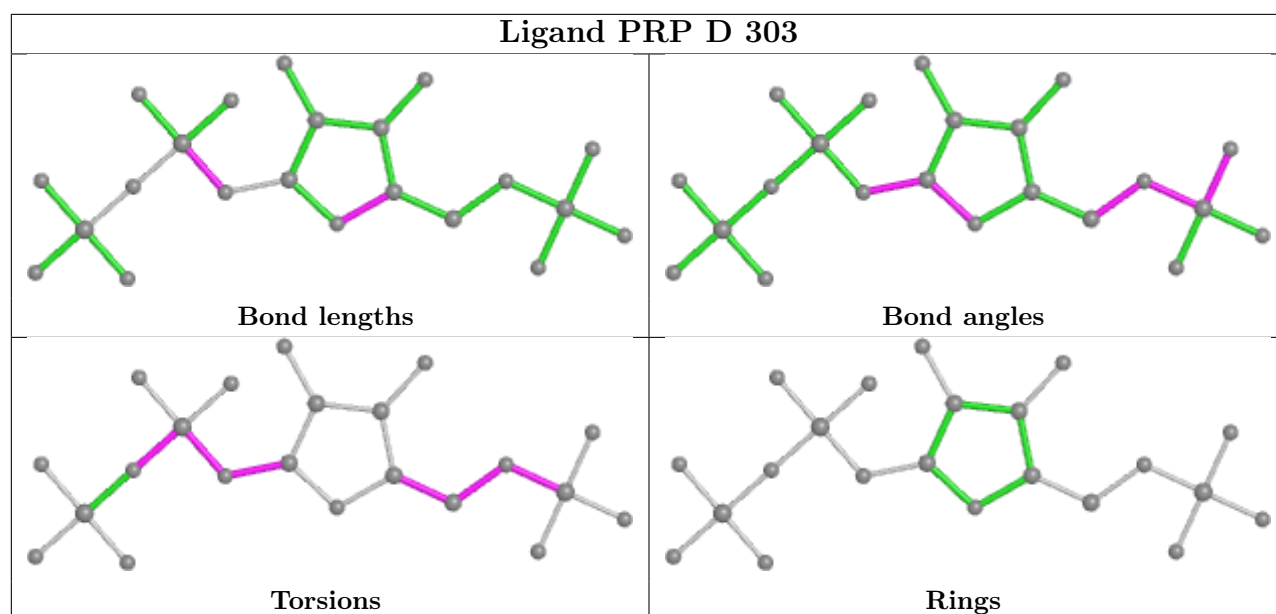
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	306	HSX	1	0
2	A	301	GTP	3	0
2	B	301	GTP	1	0
4	D	303	PRP	2	0
2	D	217	GTP	2	0

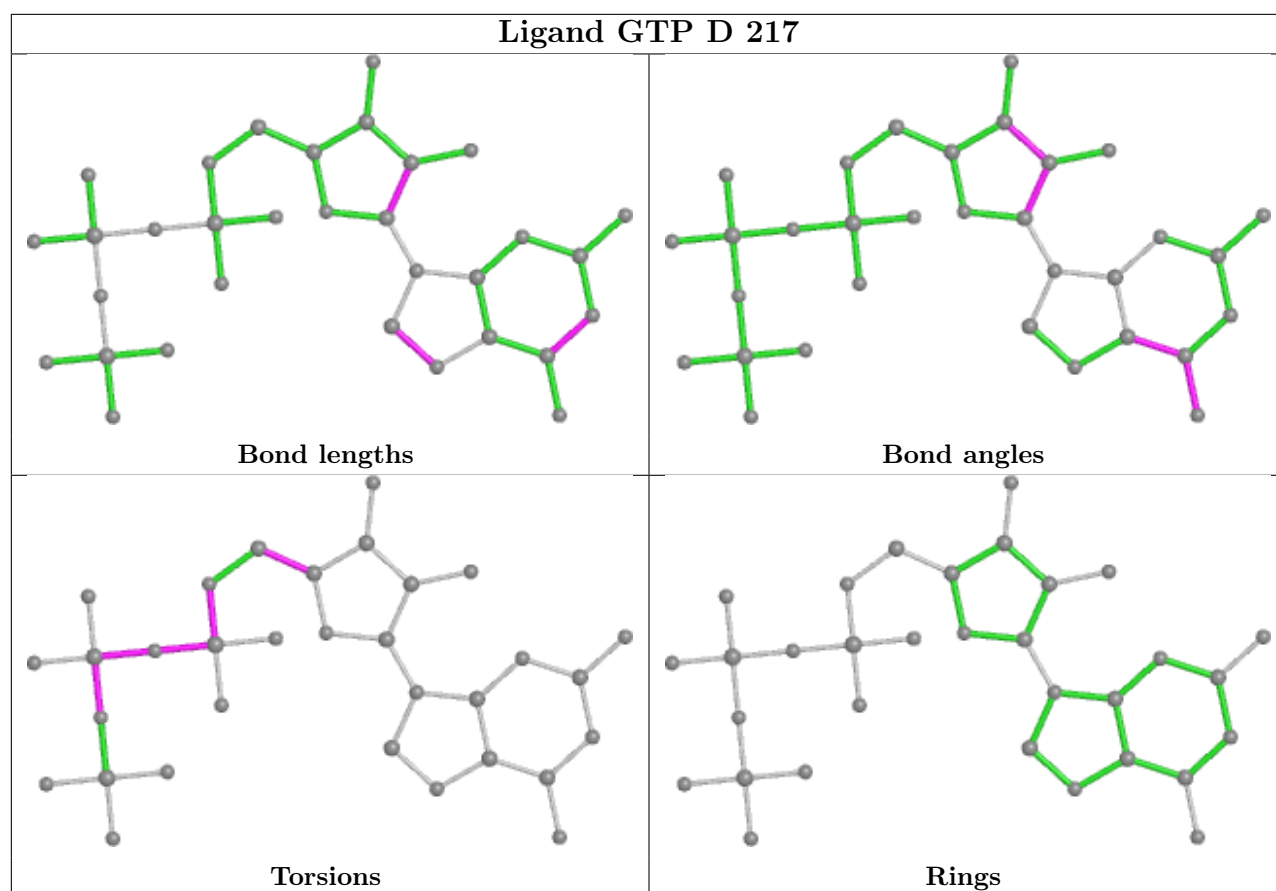
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.









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	215/216 (99%)	-0.23	13 (6%) 21 18	22, 39, 105, 124	0
1	B	206/216 (95%)	-0.32	5 (2%) 59 56	23, 38, 60, 88	0
1	C	207/216 (95%)	-0.33	3 (1%) 75 75	20, 39, 71, 103	0
1	D	215/216 (99%)	-0.48	0 100 100	18, 35, 65, 80	0
All	All	843/864 (97%)	-0.34	21 (2%) 57 55	18, 38, 70, 124	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	LYS	5.3
1	A	120	TYR	4.8
1	C	117	MET	3.6
1	A	113	VAL	3.3
1	A	107	GLU	3.1
1	A	117	MET	3.1
1	A	108	VAL	3.1
1	A	106	VAL	3.0
1	B	116	ASP	3.0
1	A	114	PRO	3.0
1	A	112	GLU	2.9
1	A	109	ASP	2.8
1	C	202	TYR	2.7
1	A	115	LYS	2.6
1	A	116	ASP	2.6
1	B	168	SER	2.4
1	C	106	VAL	2.4
1	A	118	ASP	2.1
1	B	199	ASN	2.1
1	B	139	ALA	2.1
1	B	167	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

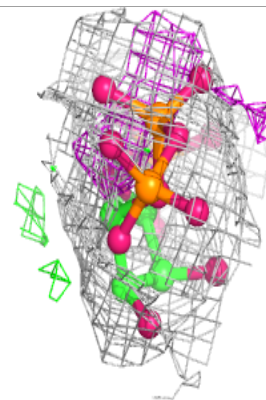
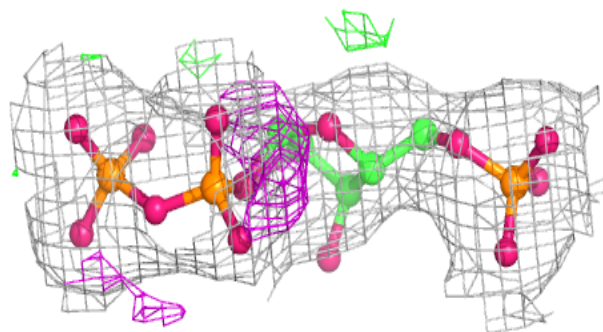
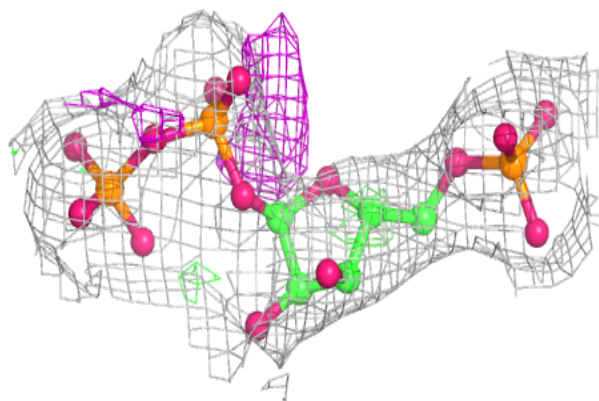
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	POP	C	307	9/9	0.67	0.35	93,93,94,94	9
5	HSX	D	306	14/14	0.83	0.26	97,99,109,109	0
6	POP	B	307	9/9	0.85	0.23	94,94,97,97	9
3	MG	A	305	1/1	0.85	0.12	65,65,65,65	0
3	MG	A	302	1/1	0.90	0.15	92,92,92,92	0
4	PRP	D	303	22/22	0.91	0.18	40,59,66,67	0
4	PRP	A	303	22/22	0.91	0.17	44,66,71,72	0
5	HSX	C	306	14/14	0.94	0.19	56,66,69,70	0
5	HSX	B	306	14/14	0.94	0.17	48,54,58,59	0
3	MG	B	302	1/1	0.95	0.06	35,35,35,35	0
2	GTP	D	301	32/32	0.95	0.14	32,39,42,45	0
3	MG	D	304	1/1	0.97	0.06	80,80,80,80	0
2	GTP	B	301	32/32	0.97	0.10	35,39,42,42	0
2	GTP	A	301	32/32	0.97	0.12	24,30,35,37	0
2	GTP	D	217	32/32	0.97	0.12	21,25,29,30	0

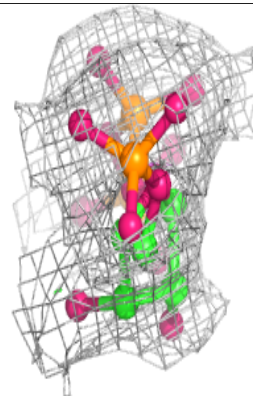
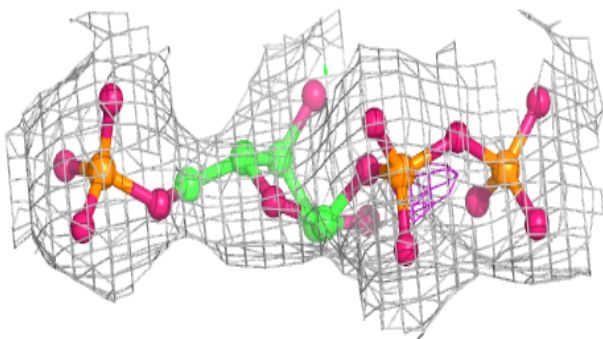
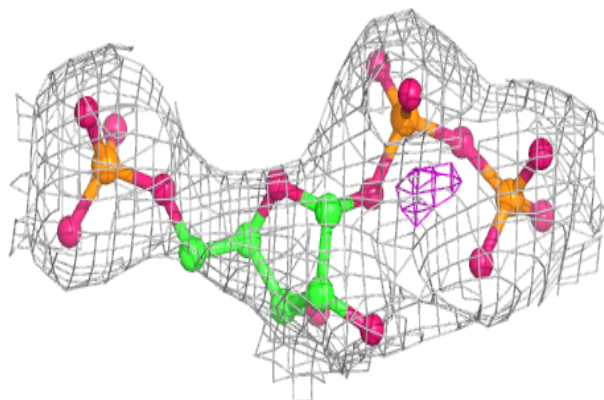
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

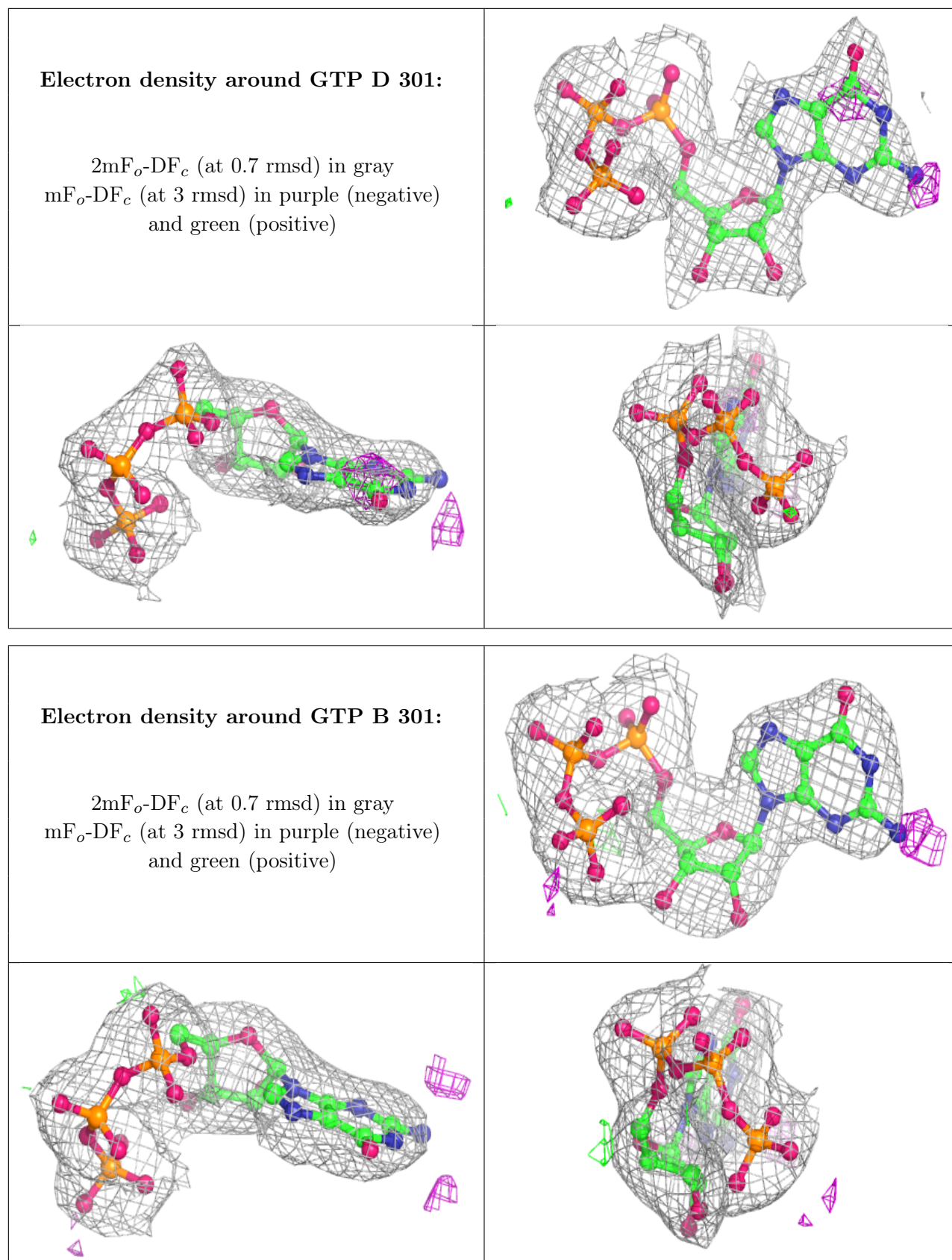
Electron density around PRP D 303:

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

**Electron density around PRP A 303:**

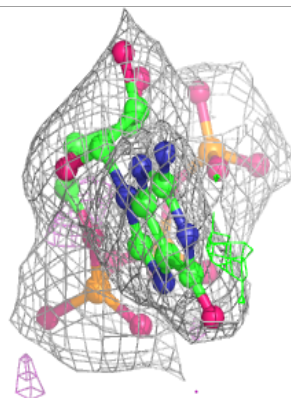
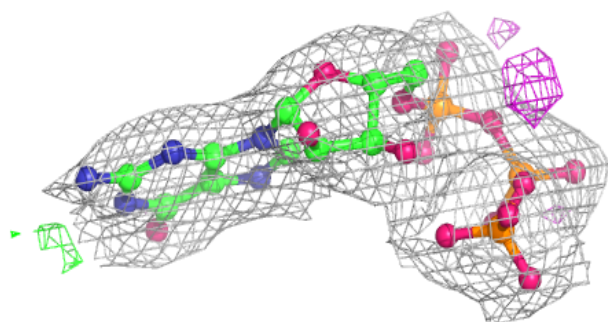
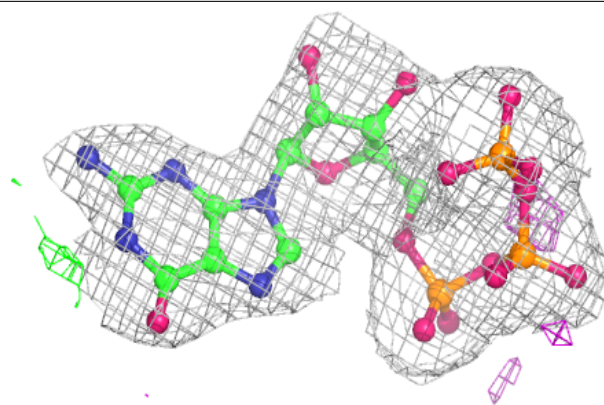
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



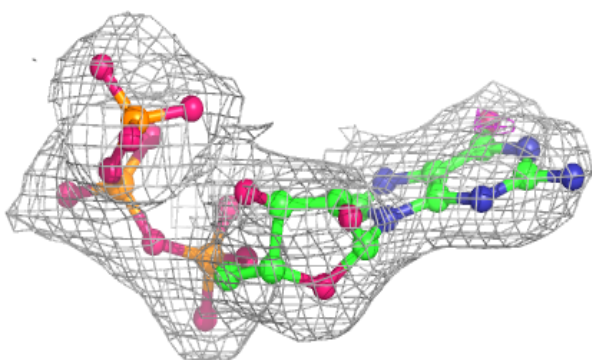
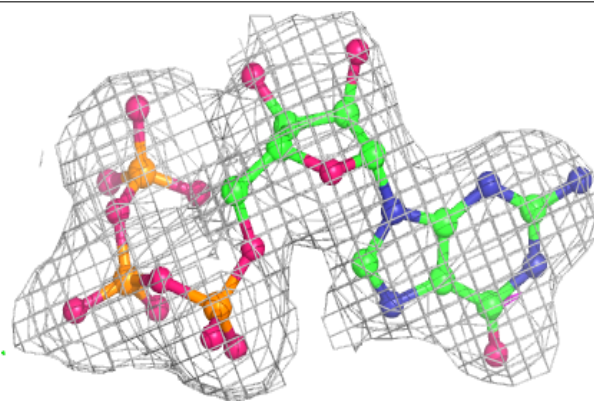


Electron density around GTP A 301:

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

**Electron density around GTP D 217:**

$2mF_o-DF_c$ (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.