



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:10 PM JST

PDB ID : 7DBA
Title : RYX in complex with tubulin
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2020-10-19
Resolution : 2.46 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 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 : 2.23.2
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) : 2.23.2

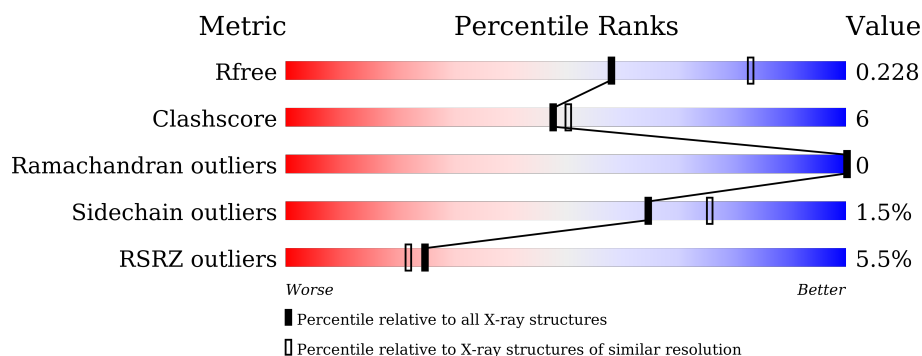
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	451	<div> <div>2%</div> <div>82% 15% .</div> </div>
1	C	451	<div> <div>87% 10% .</div> </div>
2	B	445	<div> <div>4%</div> <div>81% 13% . 5%</div> </div>
2	D	445	<div> <div>4%</div> <div>78% 16% 6%</div> </div>
3	E	143	<div> <div>8%</div> <div>73% 13% 14%</div> </div>
4	F	384	<div> <div>16%</div> <div>71% 20% . 8%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18135 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3427	2170	580	653	24			
1	C	440	Total	C	N	O	S	0	11	0
			3479	2203	586	664	26			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	5	0
			3369	2119	576	648	26			
2	D	420	Total	C	N	O	S	0	4	0
			3301	2076	557	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	3	0
			1031	637	186	202	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	5	0
			2913	1871	502	525	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

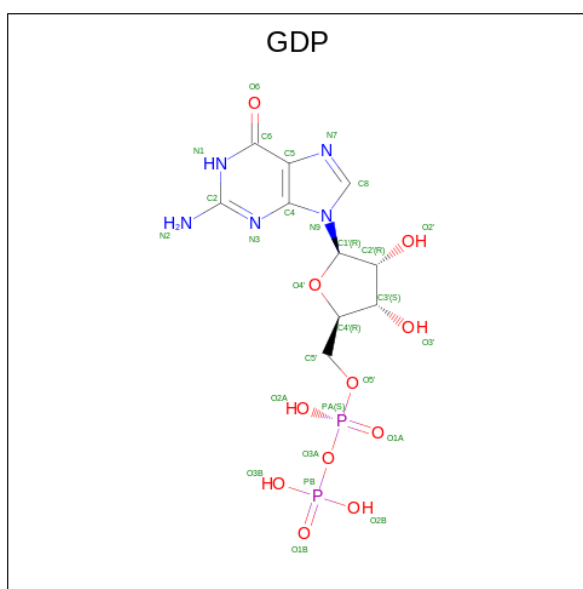
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

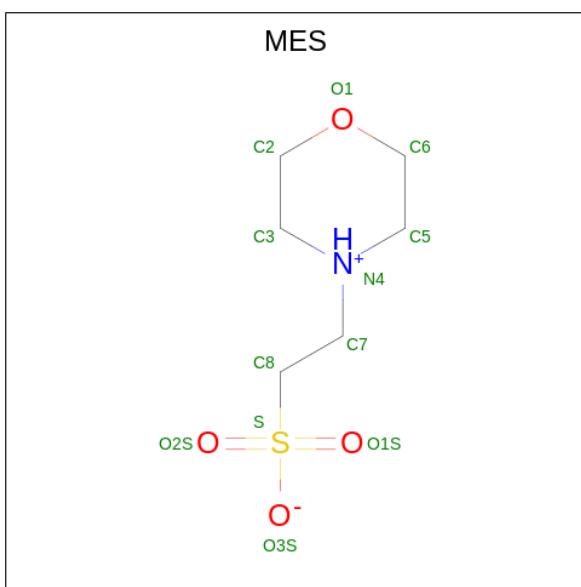
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

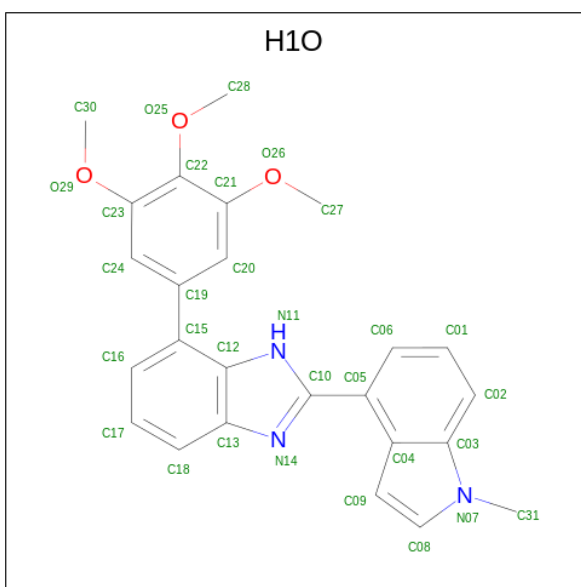
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-(1-methylindol-4-yl)-7-(3,4,5-trimethoxyphenyl)-1 {H}-benzimidazole (three-letter code: H1O) (formula: C₂₅H₂₃N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			31	25	3	3		

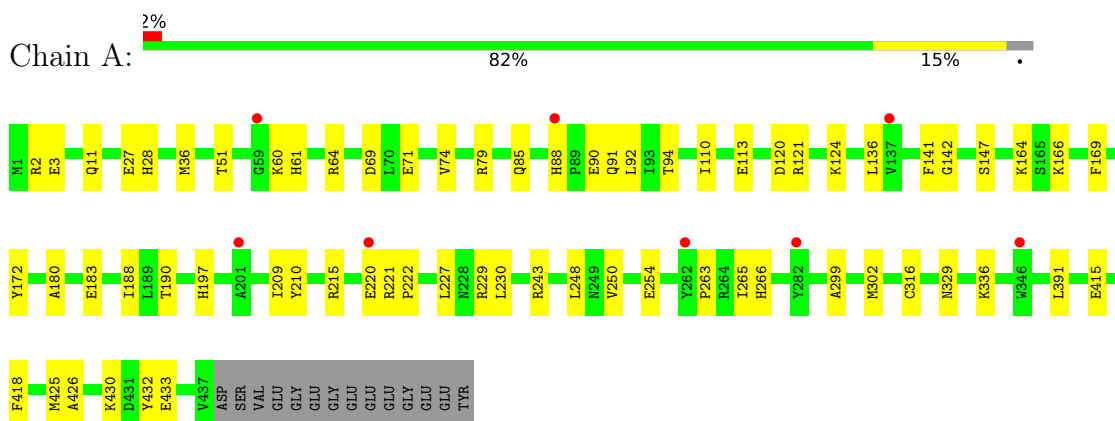
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	89	Total 89	O 89	0	0
12	B	83	Total 83	O 83	0	0
12	C	174	Total 174	O 174	0	0
12	D	41	Total 41	O 41	0	0
12	E	18	Total 18	O 18	0	0
12	F	28	Total 28	O 28	0	0

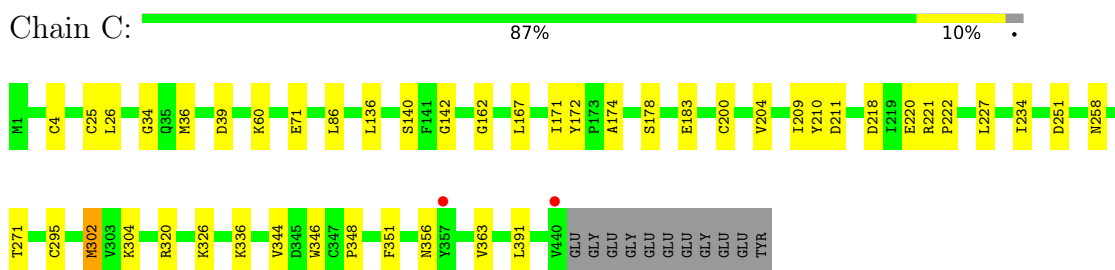
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

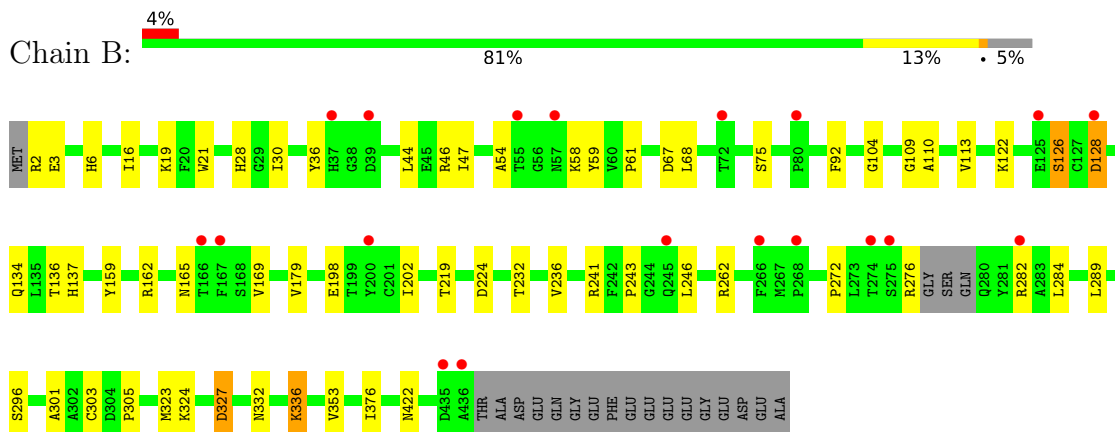
• Molecule 1: Tubulin alpha-1B chain




• Molecule 1: Tubulin alpha-1B chain

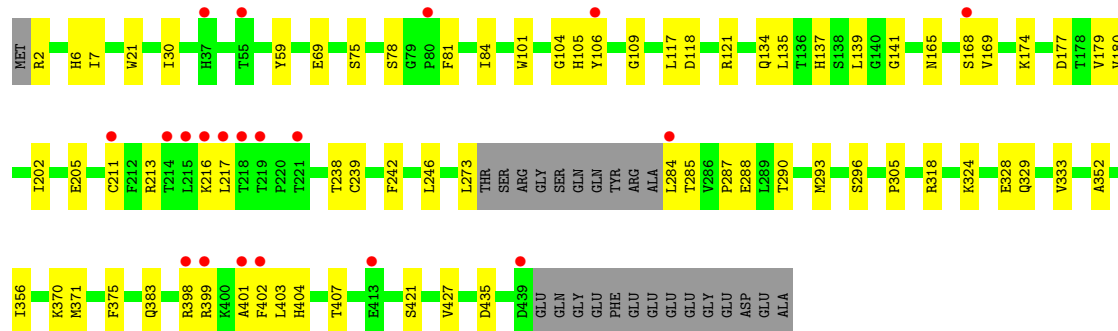


• Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.45Å 158.88Å 181.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.30 – 2.46 31.30 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.1 (31.30-2.46) 99.1 (31.30-2.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.188 , 0.228 0.189 , 0.228	Depositor DCC
R_{free} test set	1997 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18135	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: MES, H1O, GTP, CA, GDP, MG, CL

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	0.29	0/3517	0.48	0/4776
1	C	0.31	0/3587	0.50	0/4870
2	B	0.32	0/3455	0.49	1/4678 (0.0%)
2	D	0.31	0/3383	0.49	0/4586
3	E	0.34	0/1049	0.45	0/1392
4	F	0.32	0/2996	0.55	2/4048 (0.0%)
All	All	0.31	0/17987	0.50	3/24350 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	282	ARG	NE-CZ-NH1	-5.85	117.37	120.30
4	F	159	GLY	N-CA-C	5.60	127.09	113.10
4	F	225	SER	C-N-CA	5.31	134.98	121.70

There are no chirality outliers.

There are no planarity outliers.

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	3427	0	3340	44	0
1	C	3479	0	3405	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3369	0	3257	41	0
2	D	3301	0	3172	44	0
3	E	1031	0	1051	14	0
4	F	2913	0	2889	53	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	24	0	24	0	0
11	B	31	0	0	1	0
12	A	89	0	0	1	0
12	B	83	0	0	2	0
12	C	174	0	0	1	0
12	D	41	0	0	2	0
12	E	18	0	0	3	0
12	F	28	0	0	0	0
All	All	18135	0	17186	212	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 (212) 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:234:ILE:HG21	1:C:302[B]:MET:SD	2.19	0.83
2:D:399:ARG:HD2	2:D:401:ALA:HB2	1.66	0.77
2:D:105:HIS:HD2	2:D:106:TYR:CE2	2.03	0.76
4:F:86:GLU:O	4:F:87:LEU:HD23	1.86	0.75
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.25	0.69
4:F:277:THR:HG21	4:F:282:SER:HB3	1.74	0.69
1:C:336:LYS:NZ	12:C:601:HOH:O	2.25	0.69
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.25	0.69
2:D:239[B]:CYS:SG	12:D:636:HOH:O	2.51	0.69
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.26	0.67
1:A:60:LYS:NZ	1:A:85:GLN:O	2.27	0.66
4:F:137:ARG:NH1	4:F:137:ARG:HB2	2.11	0.66
2:D:404:HIS:HA	2:D:407:THR:HG22	1.79	0.64
2:D:238[B]:THR:HG21	2:D:318:ARG:HD2	1.78	0.64
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.80	0.63
2:D:324:LYS:O	2:D:328:GLU:HG3	1.99	0.62
3:E:109:LYS:NZ	12:E:202:HOH:O	2.31	0.62
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.80	0.62
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.81	0.62
2:B:165:ASN:OD1	2:B:198:GLU:HG3	1.99	0.61
4:F:135:TYR:OH	4:F:165:GLU:HA	2.00	0.61
4:F:128:ARG:HD3	4:F:170:LEU:HD23	1.82	0.61
2:B:122:LYS:HG3	12:B:632:HOH:O	2.00	0.61
3:E:80:ARG:NH2	12:E:203:HOH:O	2.33	0.61
1:A:209:ILE:HD11	1:A:302:MET:SD	2.41	0.60
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.41	0.60
4:F:286:GLN:O	4:F:290:ILE:HG13	2.02	0.60
2:D:101:TRP:CZ3	2:D:106:TYR:HE2	2.20	0.60
2:B:332:ASN:O	2:B:336:LYS:HB2	2.03	0.59
4:F:251:LYS:HB2	4:F:252:ASN:ND2	2.17	0.59
4:F:31:ARG:NE	4:F:32:LYS:H	2.00	0.59
4:F:161:LEU:HA	4:F:236:LYS:NZ	2.18	0.59
4:F:166:ALA:O	4:F:169:LEU:N	2.36	0.59
2:D:134:GLN:HA	2:D:165:ASN:O	2.03	0.59
4:F:160:ILE:HD12	4:F:240:LEU:HD13	1.86	0.58
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.22	0.58
3:E:124:GLN:OE1	3:E:124:GLN:HA	2.03	0.57
1:C:204:VAL:HG22	1:C:302[B]:MET:HE3	1.87	0.57
2:D:370:LYS:HE3	2:D:370:LYS:HA	1.87	0.57
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.87	0.56
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.87	0.56
2:D:105:HIS:HD2	2:D:106:TYR:CZ	2.22	0.56
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.88	0.56
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.21	0.56
2:D:211:CYS:HB3	2:D:217:LEU:HD12	1.88	0.56
4:F:141:GLY:O	4:F:142:ARG:HB2	2.06	0.55
2:B:126:SER:OG	2:B:126:SER:O	2.25	0.55
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.88	0.55
3:E:47:LEU:HD11	3:E:51:GLN:NE2	2.22	0.55
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.08	0.55
1:A:426:ALA:O	1:A:430:LYS:HG2	2.07	0.54
1:C:36:MET:SD	1:C:39:ASP:HB2	2.48	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.43	0.54
2:B:134:GLN:HA	2:B:165:ASN:O	2.07	0.54
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.72	0.54
2:D:329:GLN:O	2:D:333:VAL:HG23	2.08	0.54
1:C:220:GLU:OE2	2:D:324:LYS:NZ	2.41	0.54
4:F:14:TYR:HA	4:F:17:VAL:HB	1.90	0.53
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.26	0.53
4:F:237:THR:O	4:F:246:GLN:NE2	2.41	0.53
2:D:30:ILE:HD13	2:D:59:TYR:HB2	1.90	0.53
3:E:80:ARG:NE	12:E:207:HOH:O	2.41	0.53
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.44	0.53
1:A:141:PHE:O	1:A:147:SER:HB3	2.09	0.52
2:D:105:HIS:CD2	2:D:106:TYR:CE2	2.92	0.52
2:D:404:HIS:HA	2:D:407:THR:CG2	2.40	0.52
2:D:117:LEU:HB3	2:D:121:ARG:NH2	2.24	0.52
4:F:166:ALA:HA	4:F:169:LEU:HD12	1.90	0.52
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.44	0.52
2:D:213:ARG:O	2:D:216:LYS:HE3	2.10	0.52
4:F:99:VAL:O	4:F:100:ILE:HG13	2.09	0.52
2:B:284:LEU:HD23	2:B:289:LEU:HD23	1.91	0.52
2:B:30:ILE:HD13	2:B:59:TYR:HB2	1.90	0.52
4:F:161:LEU:HA	4:F:236:LYS:HZ1	1.75	0.51
2:D:293:MET:HE2	2:D:375:PHE:HB2	1.93	0.51
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.46	0.51
4:F:277:THR:HG22	4:F:278:THR:H	1.76	0.51
4:F:170:LEU:H	4:F:170:LEU:HD12	1.76	0.51
3:E:28:SER:O	3:E:28:SER:OG	2.28	0.51
2:D:118:ASP:OD1	2:D:121:ARG:NH1	2.41	0.51
1:C:140:SER:HA	1:C:171:ILE:HB	1.93	0.50
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.76	0.50
1:A:90:GLU:O	1:A:121:ARG:HD2	2.11	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.45	0.50
2:B:246:LEU:HG	11:B:505:H1O:C16	2.42	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.46	0.50
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.46	0.50
2:D:285:THR:HB	2:D:287:PRO:HD2	1.94	0.50
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.11	0.50
2:B:67:ASP:O	2:B:92:PHE:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:31:ARG:HE	4:F:32:LYS:H	1.59	0.49
1:A:28:HIS:HB3	1:A:36:MET:HE3	1.94	0.49
2:D:296:SER:HB2	2:D:305:PRO:HD2	1.94	0.49
2:B:44:LEU:HA	2:B:47:ILE:HB	1.94	0.49
3:E:72:LEU:O	3:E:76:ARG:HG2	2.12	0.49
2:D:401:ALA:HB1	2:D:402:PHE:CD1	2.48	0.49
4:F:318:ASP:O	4:F:330:ILE:HG12	2.13	0.49
2:B:128:ASP:OD2	2:B:128:ASP:N	2.46	0.48
4:F:15:ALA:O	4:F:19:ARG:HG3	2.13	0.48
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.13	0.48
1:A:263:PRO:O	1:A:266:HIS:HD2	1.96	0.48
2:B:28:HIS:NE2	2:B:241:ARG:HB3	2.29	0.48
2:B:54:ALA:HB3	2:B:58:LYS:HB2	1.96	0.48
1:A:69:ASP:O	1:A:94:THR:HA	2.14	0.47
2:D:246:LEU:HD23	2:D:352:ALA:HB2	1.97	0.47
1:A:229:ARG:NH1	12:A:601:HOH:O	2.21	0.47
2:D:383:GLN:HB2	2:D:427:VAL:HG13	1.95	0.47
4:F:246:GLN:O	4:F:250:SER:HB3	2.14	0.47
2:B:272:PRO:HB3	2:B:284:LEU:HD22	1.97	0.47
2:B:36:TYR:CE2	2:B:44:LEU:HD11	2.50	0.47
1:C:336:LYS:HE2	1:C:351:PHE:CE1	2.49	0.47
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.97	0.47
4:F:128:ARG:HH11	4:F:170:LEU:HD23	1.80	0.47
4:F:125:THR:OG1	4:F:126:ASP:N	2.48	0.47
1:A:110:ILE:O	1:A:113:GLU:HG2	2.14	0.46
2:D:179:VAL:HG13	2:D:180:VAL:HG13	1.97	0.46
4:F:129:GLU:HG2	4:F:130:VAL:N	2.30	0.46
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.50	0.46
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.96	0.46
1:A:221:ARG:NH1	2:B:327:ASP:OD2	2.48	0.46
2:D:399:ARG:CD	2:D:401:ALA:HB2	2.39	0.46
2:B:16[A]:ILE:HD11	2:B:136:THR:HB	1.97	0.46
2:B:301:ALA:O	2:B:303:CYS:N	2.46	0.46
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.16	0.46
2:D:81:PHE:O	2:D:84:ILE:HG22	2.15	0.46
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.98	0.46
3:E:126:LYS:HE3	3:E:126:LYS:HB3	1.62	0.46
1:A:220:GLU:HG2	2:B:324:LYS:HE2	1.98	0.45
2:B:104:GLY:O	2:B:109:GLY:HA3	2.16	0.45
2:B:262:ARG:HH12	2:B:422[A]:ASN:HD21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.98	0.45
2:B:296:SER:HB2	2:B:305:PRO:HD2	1.99	0.45
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.49	0.45
2:B:232:THR:O	2:B:236:VAL:HG13	2.17	0.45
1:A:166:LYS:HB2	1:A:166:LYS:HE2	1.84	0.45
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.52	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.52	0.45
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.75	0.44
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.17	0.44
4:F:101:TYR:N	4:F:126:ASP:OD2	2.49	0.44
1:A:79:ARG:HG2	1:A:92:LEU:CD1	2.48	0.44
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.44
2:B:46:ARG:NH2	2:B:243:PRO:HA	2.33	0.44
4:F:162:ILE:HD12	4:F:236:LYS:HZ3	1.82	0.44
2:B:159:TYR:HB3	2:B:162[B]:ARG:HG2	1.99	0.44
2:D:104:GLY:O	2:D:109:GLY:HA3	2.17	0.44
2:D:242:PHE:CZ	2:D:356:ILE:HD11	2.52	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.18	0.44
2:D:284:LEU:HD12	2:D:288:GLU:HG3	1.99	0.44
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.49	0.44
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.52	0.44
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.00	0.44
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.98	0.44
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.99	0.43
1:A:329:ASN:OD1	3:E:22:VAL:HG21	2.18	0.43
2:B:2:ARG:HB3	2:B:3:GLU:H	1.60	0.43
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.17	0.43
4:F:99:VAL:O	4:F:127:GLU:HB2	2.18	0.43
2:D:169:VAL:HA	2:D:202:ILE:O	2.18	0.43
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.54	0.43
2:D:75:SER:HA	2:D:78:SER:HB2	2.00	0.43
4:F:137:ARG:HB2	4:F:137:ARG:HH11	1.79	0.43
2:D:174:LYS:NZ	2:D:205:GLU:OE2	2.50	0.42
4:F:95:PRO:HB2	4:F:183:GLN:HG3	2.01	0.42
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.01	0.42
1:C:34:GLY:HA3	1:C:60:LYS:HG3	2.01	0.42
2:D:435:ASP:OD2	12:D:601:HOH:O	2.22	0.42
4:F:251:LYS:HB2	4:F:252:ASN:HD22	1.83	0.42
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:150:LYS:HG2	4:F:160:ILE:HG12	2.00	0.42
2:B:323:MET:HG2	2:B:353:VAL:HG21	2.02	0.42
1:C:26:LEU:HD12	1:C:363:VAL:HG12	2.01	0.42
3:E:80:ARG:O	3:E:84:GLN:HG3	2.20	0.42
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.42
1:C:174:ALA:O	1:C:178:SER:HB3	2.20	0.42
2:D:273:LEU:HD23	2:D:273:LEU:HA	1.89	0.42
2:B:110:ALA:O	2:B:113:VAL:HG12	2.20	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.20	0.42
2:D:403:LEU:O	2:D:403:LEU:HD23	2.19	0.42
1:A:221:ARG:HD3	2:B:324:LYS:HA	2.02	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
1:A:433:GLU:OE1	4:F:46:ARG:NH2	2.53	0.41
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.54	0.41
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.93	0.41
1:C:25:CYS:SG	1:C:86:LEU:HD21	2.60	0.41
2:D:401:ALA:HB1	2:D:402:PHE:HD1	1.85	0.41
2:D:7:ILE:O	2:D:135:LEU:HD12	2.20	0.41
4:F:106:LYS:HA	4:F:106:LYS:HD3	1.87	0.41
1:A:136:LEU:HD23	1:A:169:PHE:HE1	1.85	0.41
1:A:2:ARG:O	1:A:51:THR:HG23	2.21	0.41
2:B:219:THR:HG21	1:C:326:LYS:HA	2.02	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.19	0.41
4:F:318:ASP:HB3	4:F:330:ILE:HD11	2.02	0.41
1:A:248:LEU:HD21	1:A:316[B]:CYS:SG	2.61	0.41
4:F:191:LEU:HD12	4:F:197:ARG:C	2.41	0.41
1:A:88:HIS:O	1:A:91:GLN:HG3	2.21	0.41
2:B:219:THR:O	12:B:601:HOH:O	2.22	0.41
2:D:371:MET:HE3	2:D:371:MET:HB3	1.96	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.20	0.40
1:C:220:GLU:H	1:C:220:GLU:HG2	1.66	0.40
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.03	0.40
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.02	0.40
4:F:138:ARG:HA	4:F:143:GLU:OE1	2.21	0.40
1:A:415:GLU:O	1:A:418:PHE:HB2	2.21	0.40
2:B:236:VAL:HB	2:B:376:ILE:HD11	2.04	0.40
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
1	C	448/451 (99%)	437 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	D	419/445 (94%)	406 (97%)	13 (3%)	0	100	100
3	E	122/143 (85%)	122 (100%)	0	0	100	100
4	F	349/384 (91%)	333 (95%)	16 (5%)	0	100	100
All	All	2202/2319 (95%)	2135 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	371/379 (98%)	367 (99%)	4 (1%)	73	82
1	C	381/379 (100%)	375 (98%)	6 (2%)	62	74
2	B	371/383 (97%)	365 (98%)	6 (2%)	62	74
2	D	364/383 (95%)	358 (98%)	6 (2%)	62	74
3	E	113/127 (89%)	111 (98%)	2 (2%)	59	71
4	F	321/342 (94%)	313 (98%)	8 (2%)	47	60
All	All	1921/1993 (96%)	1889 (98%)	32 (2%)	65	73

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	120[A]	ASP
1	A	120[B]	ASP
1	A	164	LYS
2	B	75	SER
2	B	126	SER
2	B	128	ASP
2	B	137	HIS
2	B	327	ASP
2	B	336	LYS
1	C	71	GLU
1	C	218	ASP
1	C	221	ARG
1	C	251	ASP
1	C	302[A]	MET
1	C	302[B]	MET
2	D	2	ARG
2	D	69	GLU
2	D	137	HIS
2	D	177	ASP
2	D	398	ARG
2	D	421	SER
3	E	52	LYS
3	E	100	LYS
4	F	138	ARG
4	F	143	GLU
4	F	164	SER
4	F	211	TYR
4	F	222	ARG
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	269	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	285	GLN
2	B	291	GLN
2	D	48	ASN
2	D	57	ASN

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Mol	Chain	Res	Type
2	D	105	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\# Z > 2$
9	GDP	D	501	6	24,30,30	1.21	2 (8%)	31,47,47	1.81	6 (19%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.67	6 (18%)
9	GDP	B	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.95	9 (29%)
10	MES	B	504	-	12,12,12	4.48	7 (58%)	14,16,16	2.27	4 (28%)
11	H1O	B	505	-	31,35,35	1.27	6 (19%)	38,51,51	1.34	8 (21%)
10	MES	B	503	-	12,12,12	4.83	7 (58%)	14,16,16	2.77	6 (42%)
5	GTP	A	501	6	26,34,34	1.03	1 (3%)	33,54,54	1.72	6 (18%)

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
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
11	H1O	B	505	-	-	3/14/14/14	0/5/5/5
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C7-N4	-8.46	1.28	1.47
10	B	503	MES	O1S-S	8.23	1.69	1.45
10	B	503	MES	C7-N4	-7.77	1.29	1.47
10	B	503	MES	O2S-S	7.63	1.67	1.45
10	B	504	MES	O1S-S	7.27	1.66	1.45
10	B	504	MES	O2S-S	7.02	1.65	1.45
10	B	503	MES	O3S-S	6.02	1.68	1.47
10	B	503	MES	C8-S	5.99	1.86	1.77
10	B	504	MES	O3S-S	5.21	1.66	1.47
10	B	504	MES	C8-S	4.46	1.83	1.77
9	D	501	GDP	C6-C5	4.25	1.48	1.41
9	B	501	GDP	C6-C5	4.09	1.48	1.41
5	A	501	GTP	C6-N1	3.23	1.38	1.33
5	C	501	GTP	C6-N1	3.23	1.38	1.33
10	B	504	MES	C5-N4	-2.97	1.38	1.46
11	B	505	H1O	C08-N07	-2.91	1.32	1.37
10	B	503	MES	C3-N4	-2.89	1.38	1.46
10	B	503	MES	C5-N4	-2.67	1.39	1.46
10	B	504	MES	C3-N4	-2.63	1.39	1.46
9	D	501	GDP	C5-C4	2.44	1.47	1.40
11	B	505	H1O	C10-N14	-2.43	1.32	1.35
11	B	505	H1O	C10-N11	-2.36	1.32	1.35
9	B	501	GDP	C5-C4	2.30	1.47	1.40
11	B	505	H1O	C15-C19	2.10	1.53	1.49
11	B	505	H1O	O29-C23	2.07	1.40	1.37
11	B	505	H1O	O26-C21	2.06	1.40	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	C6-C5-N4	5.79	118.88	110.10
5	A	501	GTP	N3-C2-N1	-5.33	120.12	127.22
5	C	501	GTP	N3-C2-N1	-5.23	120.25	127.22
10	B	504	MES	C2-C3-N4	4.92	117.57	110.10
10	B	504	MES	C5-N4-C3	4.68	119.37	108.83
9	D	501	GDP	C2-N3-C4	4.66	120.68	115.36
10	B	503	MES	C2-C3-N4	4.65	117.16	110.10
9	B	501	GDP	C2-N3-C4	4.55	120.55	115.36
9	B	501	GDP	C6-N1-C2	4.31	122.78	115.93
9	B	501	GDP	C6-C5-C4	-4.21	116.78	120.80
9	B	501	GDP	C5-C6-N1	-4.18	117.72	123.43
10	B	503	MES	C5-N4-C3	4.14	118.15	108.83
9	D	501	GDP	C5-C6-N1	-4.03	117.92	123.43
9	D	501	GDP	C6-N1-C2	4.00	122.29	115.93
5	A	501	GTP	C2-N3-C4	3.92	119.84	115.36
5	C	501	GTP	C2-N3-C4	3.87	119.77	115.36
10	B	503	MES	O3S-S-C8	3.66	111.69	105.77
9	D	501	GDP	C6-C5-C4	-3.64	117.32	120.80
9	B	501	GDP	N3-C2-N1	-3.46	122.61	127.22
5	C	501	GTP	C5-C6-N1	-3.22	119.03	123.43
5	A	501	GTP	PA-O3A-PB	-3.21	121.81	132.83
9	D	501	GDP	N3-C2-N1	-3.17	122.99	127.22
10	B	503	MES	O1S-S-C8	3.05	110.59	106.92
5	A	501	GTP	C5-C6-N1	-2.98	119.36	123.43
11	B	505	H1O	C10-C05-C04	-2.97	119.98	123.46
9	B	501	GDP	C4-C5-N7	-2.93	106.34	109.40
9	D	501	GDP	C4-C5-N7	-2.88	106.40	109.40
5	C	501	GTP	C6-N1-C2	2.84	120.44	115.93
11	B	505	H1O	O26-C21-C22	2.76	120.02	115.16
11	B	505	H1O	O29-C23-C22	2.74	119.98	115.16
5	A	501	GTP	C6-N1-C2	2.71	120.23	115.93
10	B	504	MES	C6-C5-N4	2.60	114.04	110.10
10	B	503	MES	C7-N4-C5	2.49	117.60	111.23
11	B	505	H1O	C30-O29-C23	-2.42	113.88	117.53
10	B	504	MES	O2S-S-C8	2.41	109.81	106.92
11	B	505	H1O	O26-C21-C20	-2.40	119.99	124.12
11	B	505	H1O	C27-O26-C21	-2.39	113.93	117.53
11	B	505	H1O	O29-C23-C24	-2.37	120.04	124.12
9	B	501	GDP	PA-O3A-PB	-2.29	124.97	132.83
5	C	501	GTP	PA-O3A-PB	-2.27	125.03	132.83
5	A	501	GTP	PB-O3B-PG	-2.26	125.08	132.83
5	C	501	GTP	PB-O3B-PG	-2.15	125.44	132.83
9	B	501	GDP	C1'-N9-C4	-2.12	122.92	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	O2B-PB-O3A	2.09	111.66	104.64
11	B	505	H1O	C10-N14-C13	2.00	107.75	103.78

There are no chirality outliers.

All (29) torsion outliers are listed below:

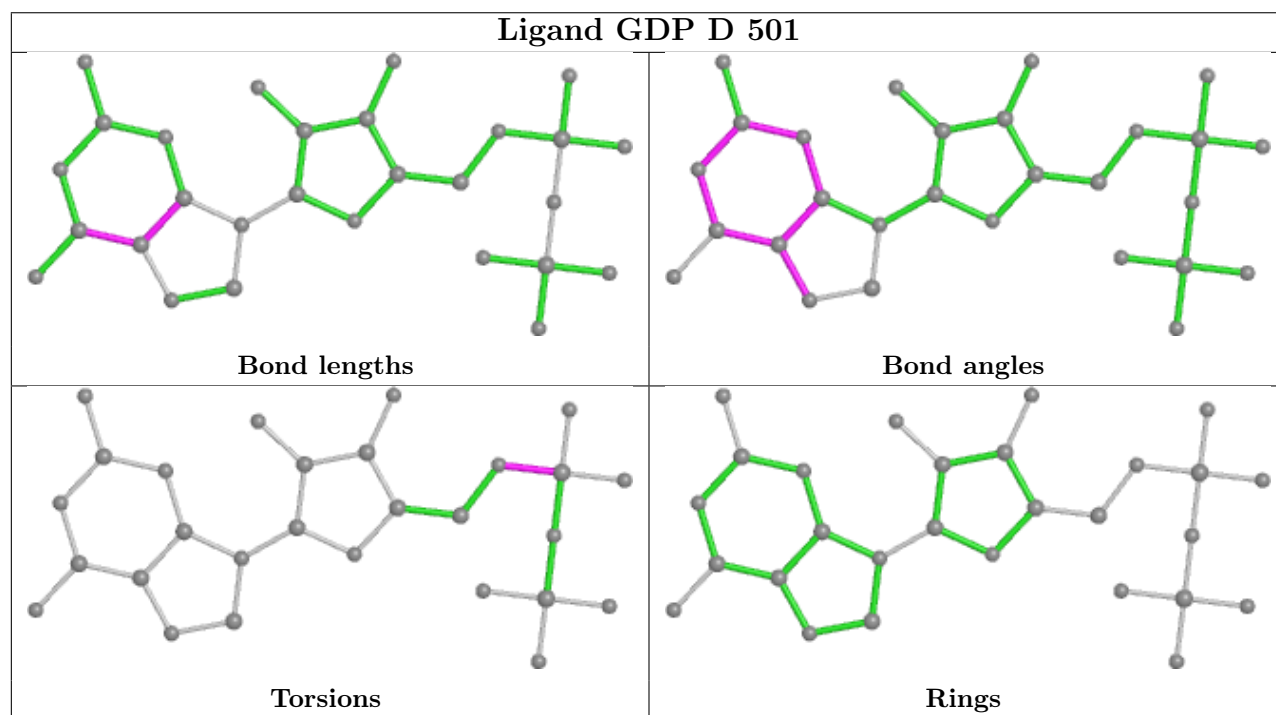
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
5	C	501	GTP	PB-O3B-PG-O1G
11	B	505	H1O	C22-C21-O26-C27
5	A	501	GTP	PB-O3B-PG-O1G
11	B	505	H1O	C20-C21-O26-C27
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	B	505	H1O	C16-C15-C19-C20
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A
10	B	504	MES	C8-C7-N4-C5

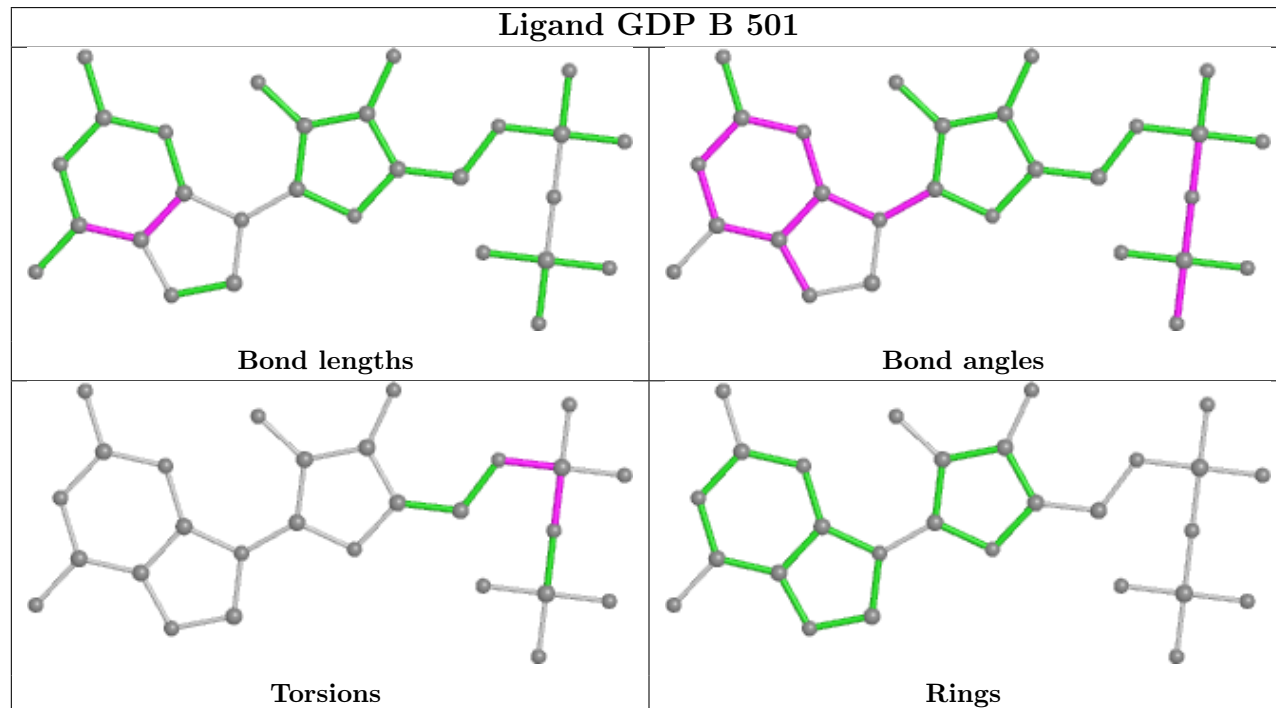
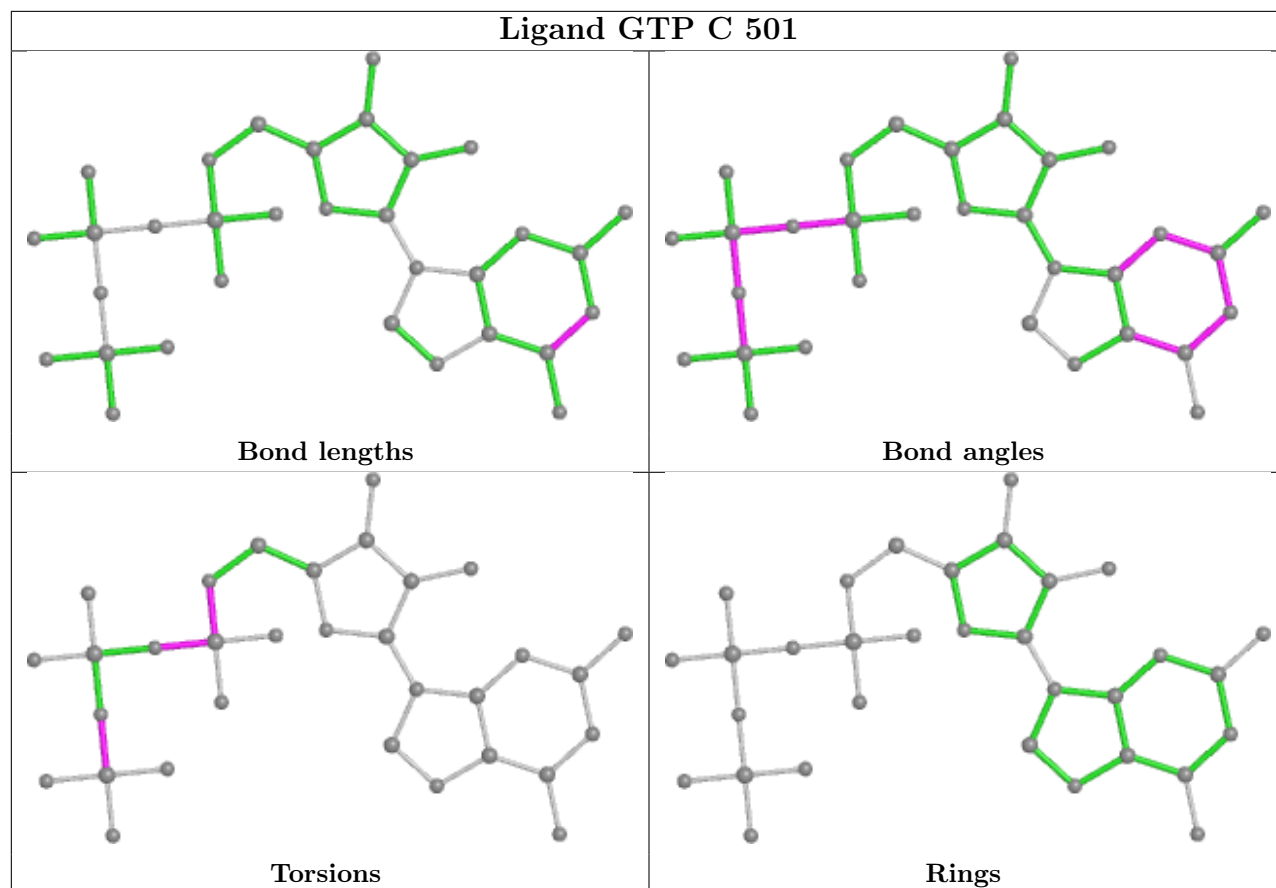
There are no ring outliers.

2 monomers are involved in 2 short contacts:

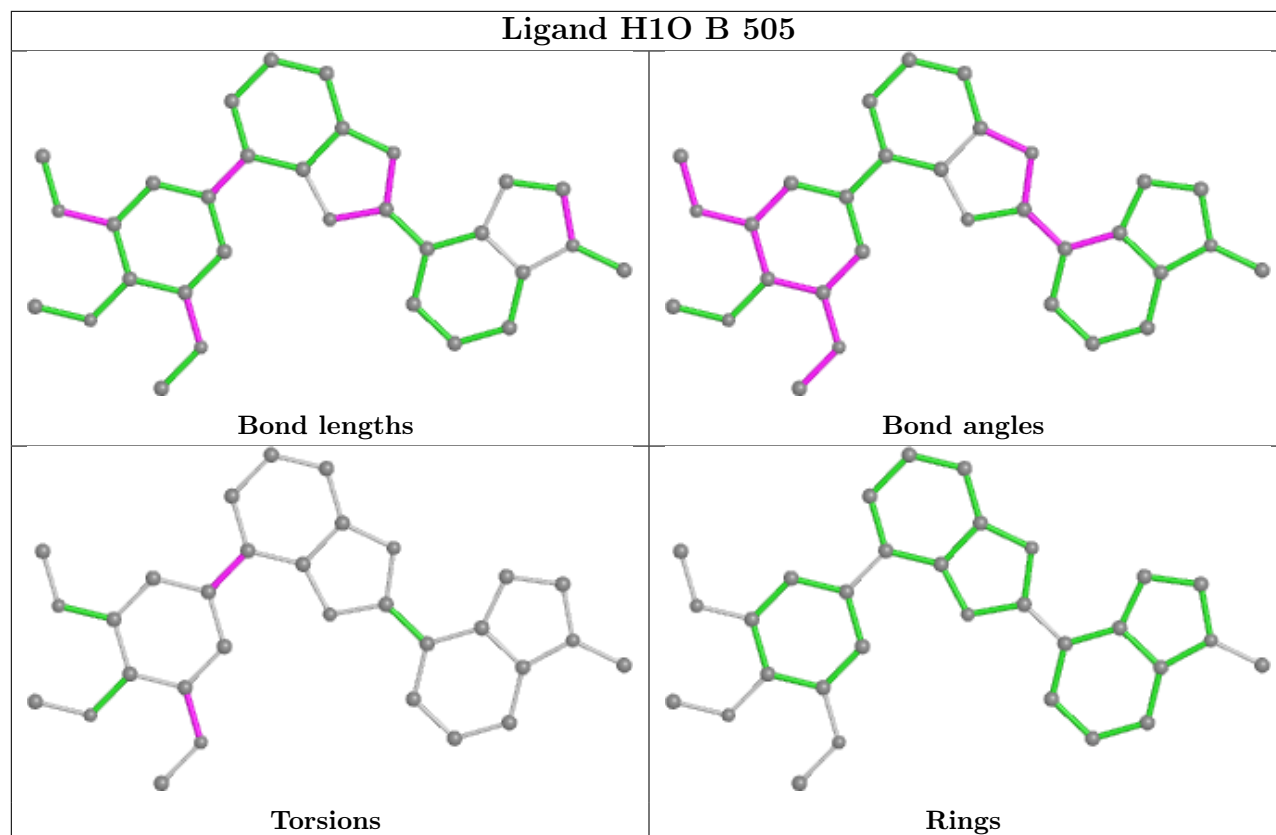
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
11	B	505	H1O	1	0

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.

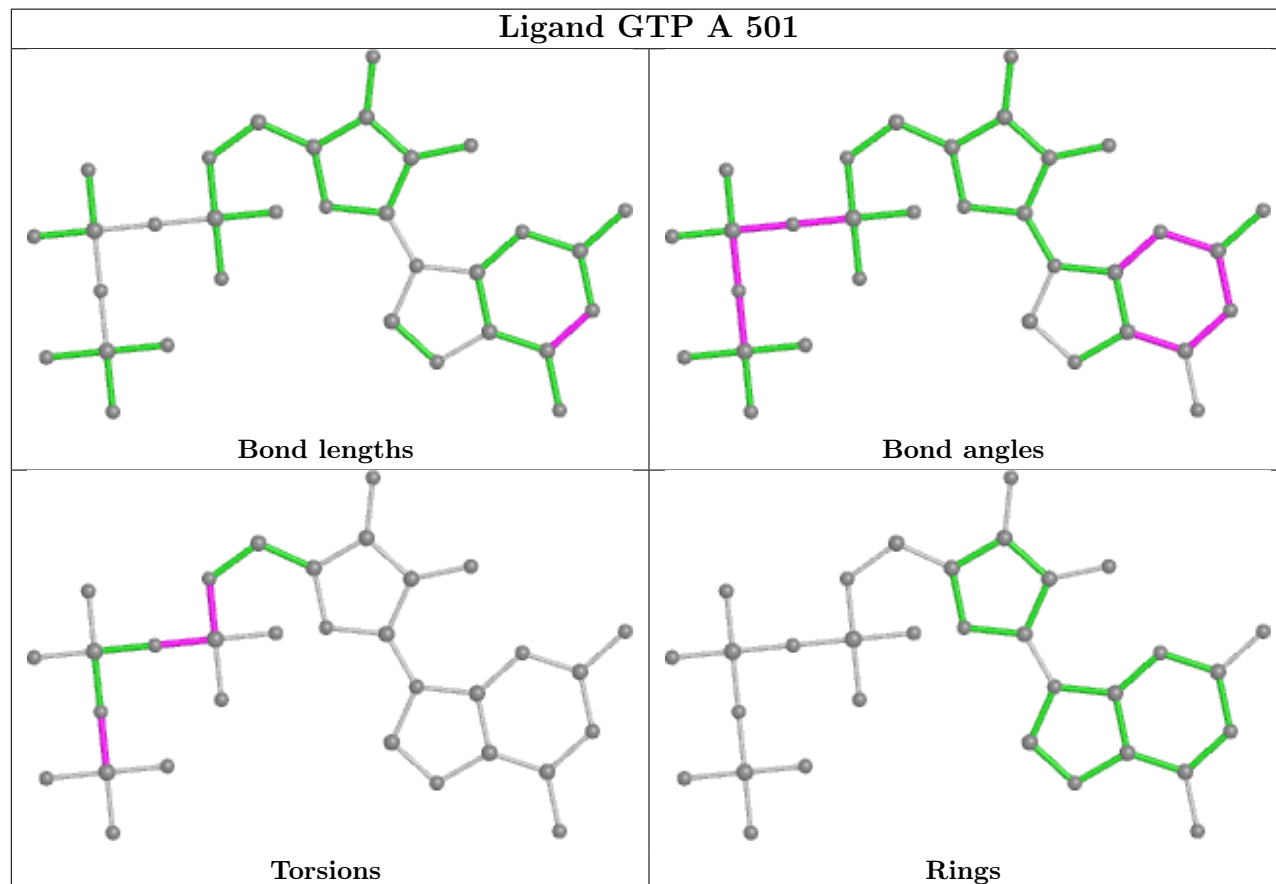




Ligand H1O B 505



Ligand GTP A 501



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	437/451 (96%)	0.01	8 (1%) 68 65	30, 45, 71, 88	0
1	C	440/451 (97%)	-0.26	2 (0%) 91 92	22, 35, 58, 94	0
2	B	424/445 (95%)	0.11	19 (4%) 33 30	23, 44, 74, 117	2 (0%)
2	D	420/445 (94%)	0.20	20 (4%) 30 28	30, 54, 84, 126	3 (0%)
3	E	123/143 (86%)	0.45	11 (8%) 9 6	32, 57, 92, 125	0
4	F	352/384 (91%)	0.73	61 (17%) 1 1	35, 69, 141, 163	0
All	All	2196/2319 (94%)	0.15	121 (5%) 25 22	22, 48, 96, 163	5 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	8.3
4	F	104	ASN	6.2
4	F	177	GLY	5.6
4	F	102	PRO	5.3
4	F	106	LYS	5.3
4	F	244	CYS	5.3
4	F	143	GLU	5.1
4	F	248	GLU	5.1
4	F	142	ARG	5.0
2	D	55	THR	4.9
4	F	101	TYR	4.7
4	F	255[A]	ARG	4.6
4	F	103	THR	4.5
4	F	125	THR	4.4
4	F	178	GLN	4.3
4	F	152	SER	4.2
2	B	245	GLN	4.2
2	D	219	THR	4.1
4	F	362	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	139	ARG	4.0
4	F	245	ILE	4.0
4	F	176	GLN	4.0
2	D	398	ARG	4.0
4	F	251	LYS	3.9
3	E	139	LEU	3.8
4	F	25	GLY	3.8
4	F	169	LEU	3.7
4	F	372	THR	3.7
3	E	143	ALA	3.6
4	F	10	ASN	3.6
2	B	436	ALA	3.6
1	A	262	TYR	3.5
4	F	137	ARG	3.5
2	B	274	THR	3.4
3	E	48	GLU	3.4
2	D	216	LYS	3.4
4	F	175	GLU	3.3
4	F	173	ILE	3.3
4	F	174	ASP	3.3
2	D	215	LEU	3.3
4	F	232	ASN	3.3
4	F	140	GLU	3.2
4	F	45	ASN	3.2
4	F	138	ARG	3.2
2	D	218	THR	3.2
4	F	234	GLN	3.2
3	E	140	LYS	3.2
4	F	141	GLY	3.2
2	D	214	THR	3.2
4	F	231	ALA	3.2
2	D	399	ARG	3.2
4	F	132	LEU	3.2
2	B	275	SER	3.1
2	B	57	ASN	3.1
2	D	217	LEU	3.1
4	F	158	GLU	3.1
4	F	233	PHE	3.1
3	E	141	GLU	3.0
2	B	282	ARG	3.0
3	E	142	GLU	3.0
4	F	89	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	243	HIS	3.0
4	F	159	GLY	2.9
4	F	133	ALA	2.9
1	A	346	TRP	2.9
4	F	161	LEU	2.9
4	F	253	TYR	2.9
4	F	247	LYS	2.9
2	D	221	THR	2.8
2	D	284	LEU	2.7
4	F	252	ASN	2.7
2	D	439	ASP	2.7
4	F	381	HIS	2.7
4	F	24	THR	2.7
4	F	136	ASN	2.7
2	B	80	PRO	2.7
2	B	435	ASP	2.6
2	D	106	TYR	2.6
4	F	225	SER	2.6
4	F	379	HIS	2.6
2	B	55	THR	2.6
4	F	165	GLU	2.6
2	B	72	THR	2.6
3	E	44	ASP	2.6
1	C	440	VAL	2.5
2	B	268	PRO	2.5
2	D	37	HIS	2.5
4	F	151	SER	2.5
4	F	249	TYR	2.5
2	B	200	TYR	2.5
2	B	167	PHE	2.5
4	F	134	ALA	2.5
1	A	282	TYR	2.4
2	D	401	ALA	2.4
2	B	128	ASP	2.4
3	E	46	SER	2.4
2	D	211	CYS	2.4
4	F	135	TYR	2.3
4	F	167	SER	2.3
3	E	138	GLU	2.3
1	A	59	GLY	2.3
4	F	196	HIS	2.3
1	A	137	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	28	SER	2.3
4	F	256	TYR	2.3
1	C	357	TYR	2.3
2	D	168	SER	2.3
2	B	166	THR	2.3
1	A	201	ALA	2.2
4	F	361	LEU	2.2
2	B	39	ASP	2.2
1	A	220	GLU	2.2
2	B	37	HIS	2.2
2	D	413	GLU	2.2
2	D	80	PRO	2.2
2	B	125	GLU	2.1
2	D	402	PHE	2.1
1	A	88	HIS	2.1
2	B	266	PHE	2.1
4	F	145	ASN	2.0
3	E	45	PRO	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	MG	D	502	1/1	0.89	0.11	57,57,57,57	0
8	CL	A	504	1/1	0.90	0.09	79,79,79,79	0
11	H1O	B	505	31/31	0.90	0.15	30,48,55,58	0
6	MG	C	502	1/1	0.91	0.14	31,31,31,31	0
10	MES	B	504	12/12	0.94	0.24	65,73,82,92	0

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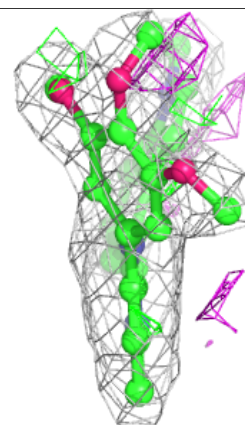
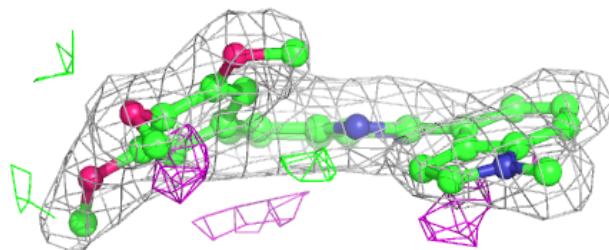
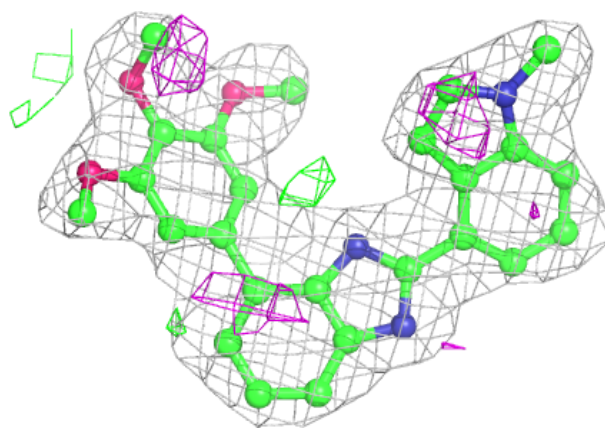
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	A	503	1/1	0.95	0.06	66,66,66,66	0
10	MES	B	503	12/12	0.96	0.14	38,54,60,61	0
7	CA	C	503	1/1	0.96	0.04	49,49,49,49	0
9	GDP	D	501	28/28	0.96	0.12	43,50,68,80	0
6	MG	A	502	1/1	0.97	0.09	32,32,32,32	0
5	GTP	C	501	32/32	0.98	0.14	22,29,34,40	0
5	GTP	A	501	32/32	0.98	0.11	24,37,42,48	0
6	MG	B	502	1/1	0.98	0.13	23,23,23,23	0
9	GDP	B	501	28/28	0.99	0.13	20,31,40,41	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.

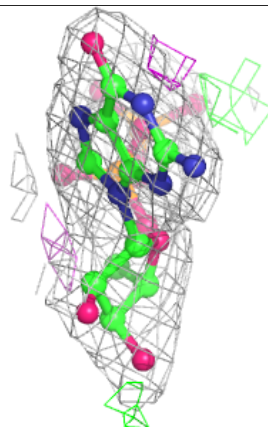
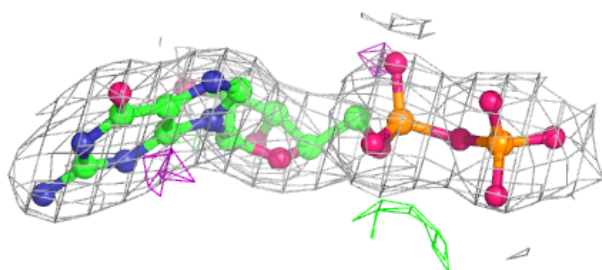
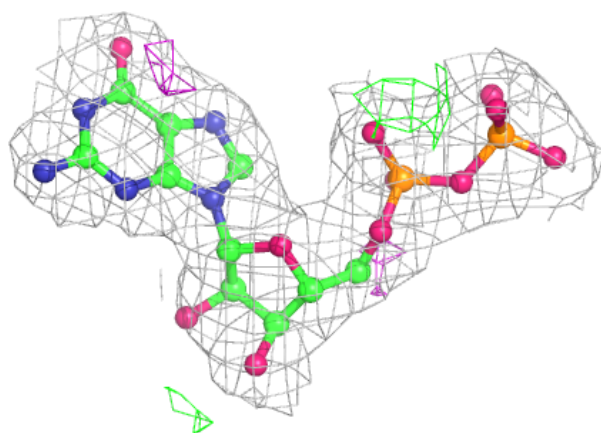
Electron density around H1O B 505:

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

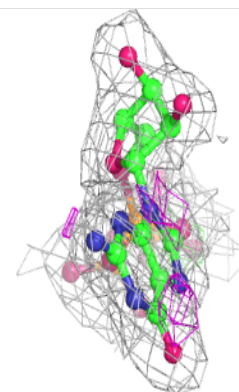
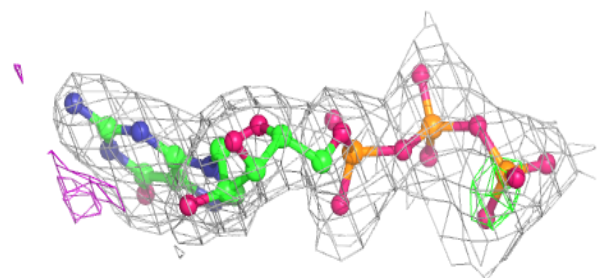
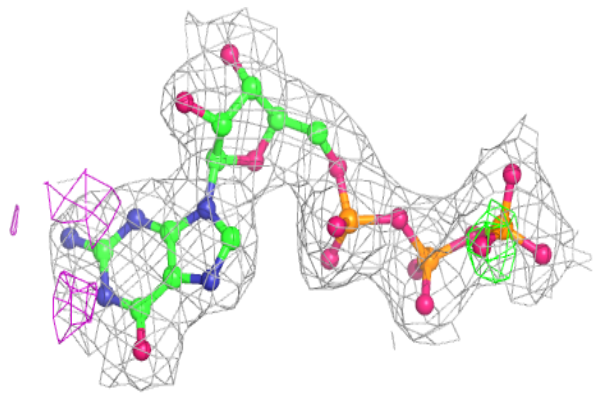


Electron density around GDP D 501:

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

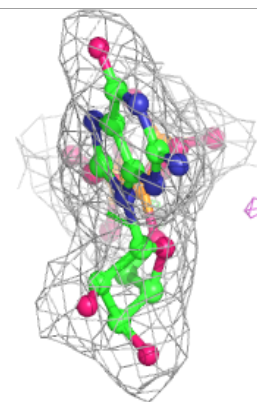
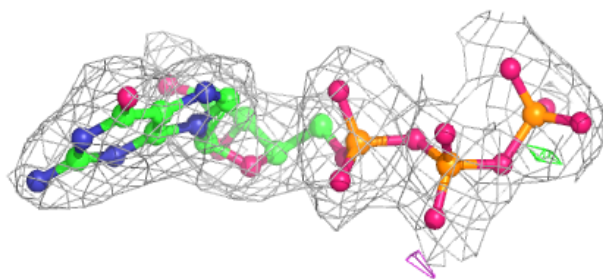
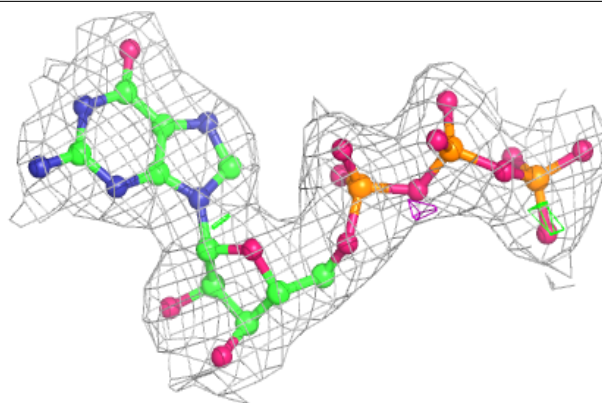
**Electron density around GTP C 501:**

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

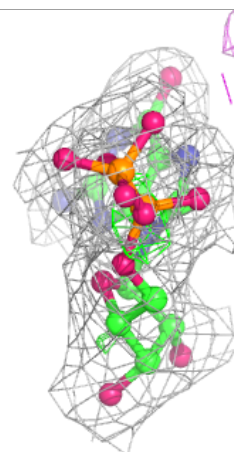
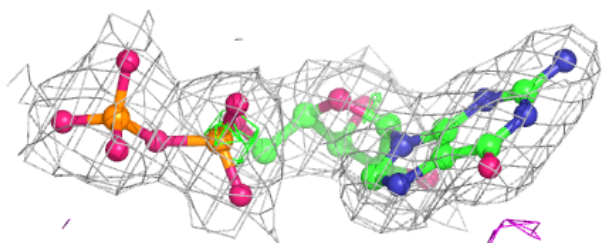
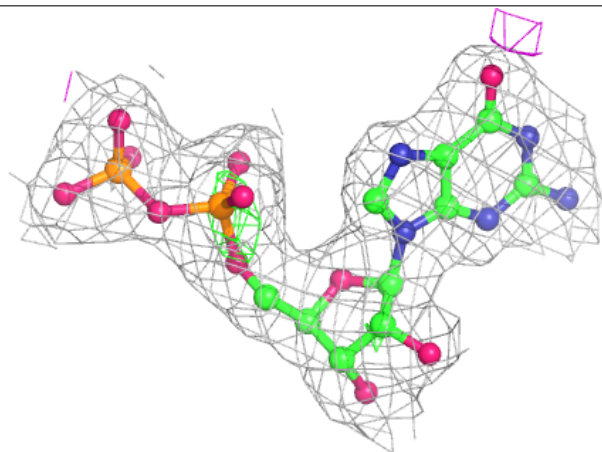


Electron density around GTP A 501:

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

**Electron density around GDP B 501:**

$2mF_o-DF_c$ (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.