



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:47 PM EDT

PDB ID : 6PC4 / pdb_00006pc4
Title : Tubulin-RB3_SLD-TTL in complex with compound ABI-274
Authors : Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on : 2019-06-15
Resolution : 2.60 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

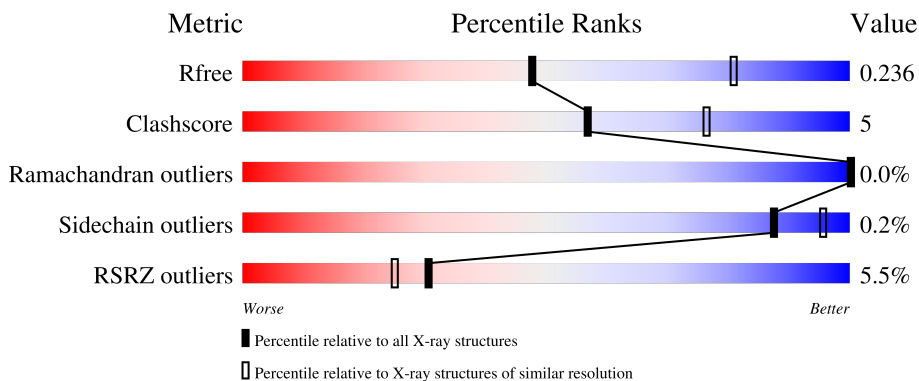
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	450	 89% 8%
1	C	450	 91% 7%
2	B	445	 87% 9%
2	D	445	 81% 13% 5%
3	E	143	 73% 12% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '17%', a large green segment labeled '74%', a yellow segment labeled '12%', and a grey segment on the right labeled '14%'.</p>

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 17742 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
			Total	C	N	O	S			
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	0	0
			997	614	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

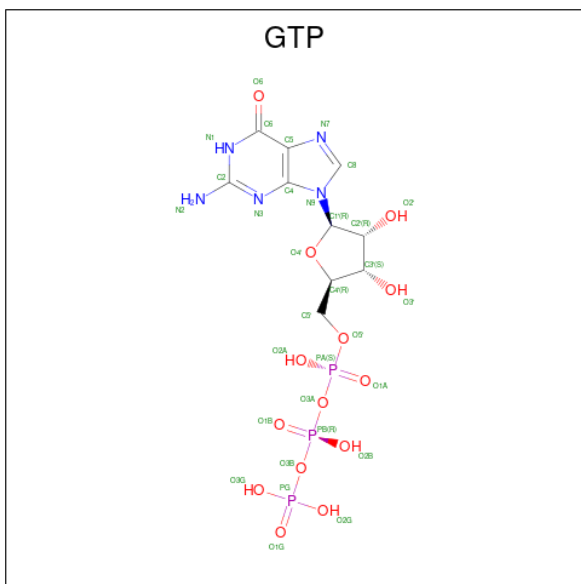
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	332	Total	C	N	O	S	0	0	0
			2617	1686	446	471	14			

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 (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
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 (CCD ID: MG) (formula: Mg).

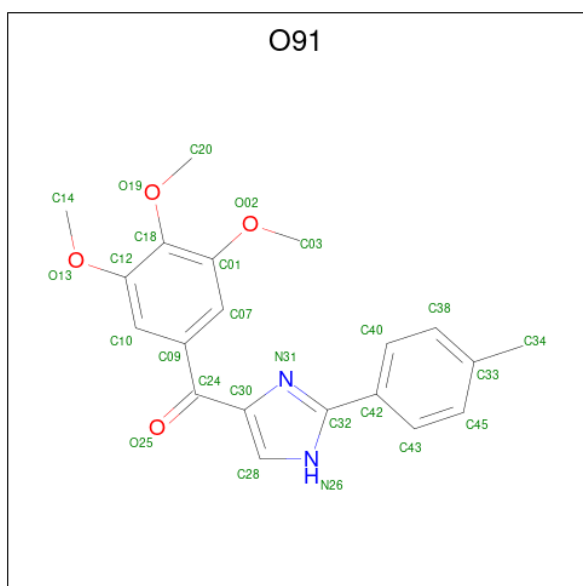
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).



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

- Molecule 10 is [2-(4-methylphenyl)-1H-imidazol-4-yl](3,4,5-trimethoxyphenyl)methanone (CCD ID: O91) (formula: C₂₀H₂₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	26	20	2	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	D	1	26	20	2	4	0	0

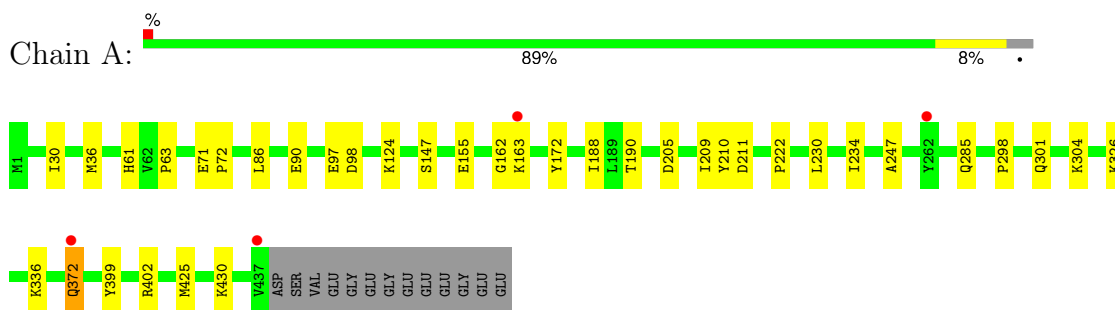
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	96	96	96	0	0
11	B	76	76	76	0	0
11	C	124	124	124	0	0
11	D	41	41	41	0	0
11	E	21	21	21	0	0
11	F	46	46	46	0	0

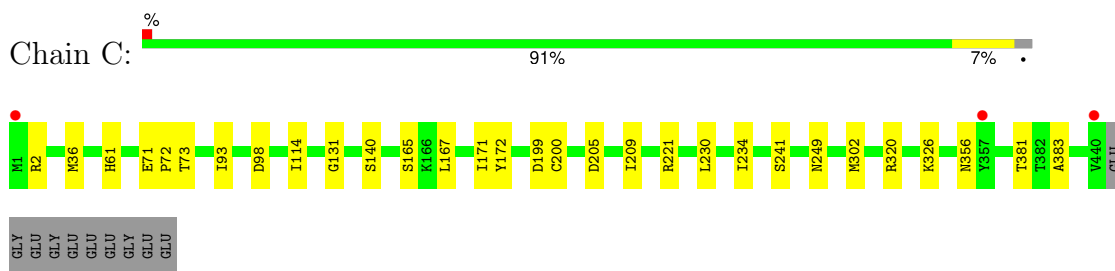
3 Residue-property plots [i](#)

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.

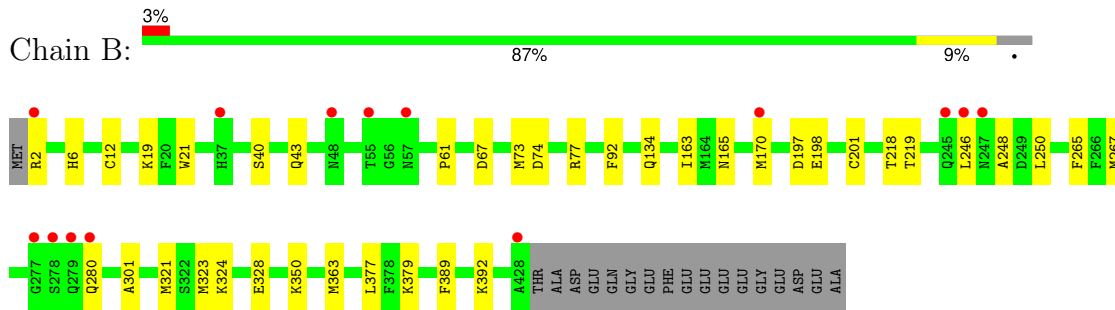
- Molecule 1: Tubulin alpha-1B chain



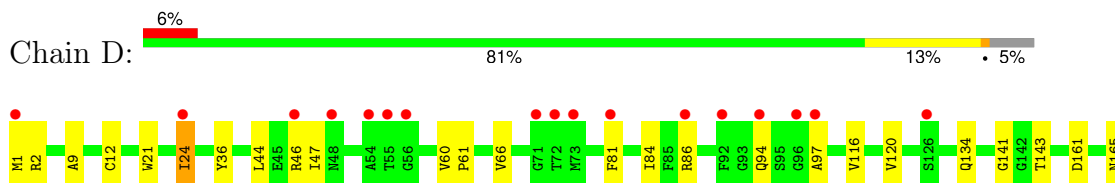
- Molecule 1: Tubulin alpha-1B chain

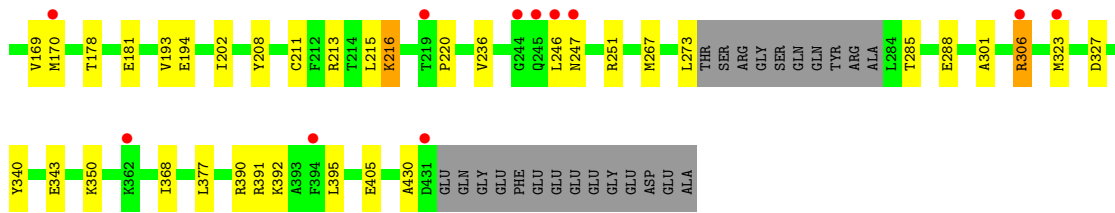


- Molecule 2: Tubulin beta-2B chain

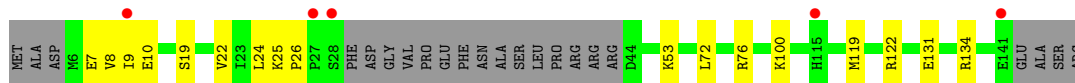


- Molecule 2: Tubulin beta-2B chain

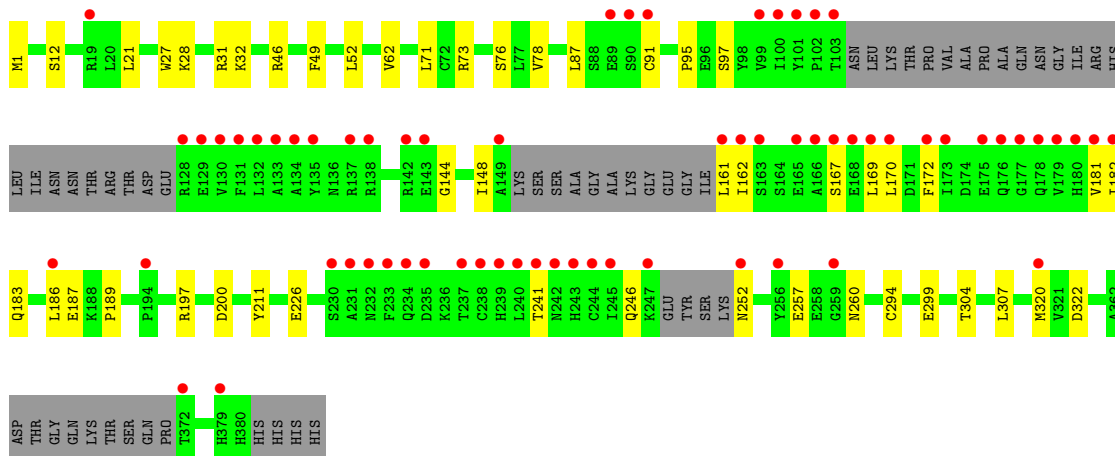
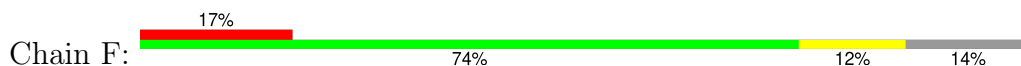




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.14Å 157.53Å 181.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.74 – 2.60 41.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.74-2.60) 98.7 (41.74-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.61Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.234 0.191 , 0.236	Depositor DCC
R_{free} test set	4594 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17742	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: MES, O91, CA, GTP, MG, 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	0.17	0/3494	0.42	3/4743 (0.1%)
1	C	0.15	0/3515	0.38	0/4772
2	B	0.13	0/3436	0.35	0/4654
2	D	0.27	1/3382 (0.0%)	0.51	7/4581 (0.2%)
3	E	0.14	0/1005	0.28	0/1333
4	F	0.13	0/2677	0.35	0/3629
All	All	0.18	1/17509 (0.0%)	0.40	10/23712 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	60	VAL	CA-C	5.61	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	24	ILE	CB-CA-C	-8.12	101.02	112.22
2	D	24	ILE	N-CA-CB	7.88	122.41	110.58
1	A	372	GLN	CA-CB-CG	7.32	128.75	114.10
2	D	24	ILE	CA-CB-CG1	6.25	121.03	110.40
2	D	306	ARG	CD-NE-CZ	5.83	132.56	124.40
2	D	86	ARG	CG-CD-NE	5.34	123.74	112.00
2	D	94	GLN	CB-CG-CD	-5.24	103.70	112.60
1	A	30	ILE	CA-C-N	5.14	135.56	120.97
1	A	30	ILE	C-N-CA	5.14	135.56	120.97
2	D	216	LYS	CG-CD-CE	-5.05	99.68	111.30

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	3416	0	3331	30	0
1	C	3437	0	3348	18	0
2	B	3361	0	3238	25	0
2	D	3309	0	3189	47	0
3	E	997	0	1009	13	0
4	F	2617	0	2516	30	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	24	0	24	1	0
10	B	26	0	0	1	0
10	D	26	0	0	3	0
11	A	96	0	0	1	0
11	B	76	0	0	1	0
11	C	124	0	0	0	0
11	D	41	0	0	3	0
11	E	21	0	0	1	0
11	F	46	0	0	1	0
All	All	17742	0	16703	158	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 5.

All (158) 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:A:285:GLN:HG3	1:A:372:GLN:NE2	1.40	1.32
1:A:285:GLN:CG	1:A:372:GLN:HE22	1.48	1.23
1:A:285:GLN:CG	1:A:372:GLN:NE2	2.11	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:HG3	1:A:372:GLN:HE22	0.83	0.97
1:C:221:ARG:NH2	2:D:323:MET:HE1	1.83	0.91
1:A:90:GLU:OE2	1:A:124:LYS:NZ	2.03	0.91
1:A:285:GLN:CB	1:A:372:GLN:HE22	1.93	0.81
4:F:52:LEU:HD13	4:F:62:VAL:HG21	1.63	0.79
2:D:1:MET:HG3	2:D:2:ARG:HG2	1.65	0.79
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.66	0.77
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.68	0.76
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.18	0.74
4:F:97:SER:OG	4:F:183:GLN:NE2	2.22	0.73
1:A:163:LYS:H	1:A:163:LYS:HD2	1.55	0.71
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.74	0.70
2:D:306:ARG:HD3	2:D:340:TYR:CZ	2.27	0.69
2:D:246:LEU:HD22	2:D:350:LYS:HZ1	1.56	0.69
1:C:381:THR:HG22	1:C:383:ALA:H	1.60	0.66
2:B:324:LYS:O	2:B:328:GLU:HG3	1.96	0.65
4:F:161:LEU:HD23	4:F:172:PHE:HZ	1.62	0.65
2:D:392:LYS:NZ	11:D:601:HOH:O	2.30	0.64
3:E:119:MET:HA	3:E:122:ARG:HE	1.63	0.62
2:D:21:TRP:CZ3	2:D:24:ILE:HD11	2.34	0.62
2:D:236:VAL:HG22	2:D:368:ILE:HD11	1.82	0.61
2:D:246:LEU:HD22	2:D:350:LYS:NZ	2.15	0.60
1:A:285:GLN:CB	1:A:372:GLN:NE2	2.60	0.60
4:F:167:SER:HA	4:F:170:LEU:HB2	1.84	0.59
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.84	0.59
2:D:97:ALA:HB2	2:D:143:THR:OG1	2.03	0.58
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.85	0.58
2:D:134:GLN:HA	2:D:165:ASN:O	2.04	0.58
3:E:25:LYS:HD3	3:E:26:PRO:O	2.04	0.58
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.87	0.57
2:B:321:MET:HB3	2:B:363:MET:HE1	1.87	0.56
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.85	0.56
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.24	0.56
2:D:46:ARG:NH2	11:D:603:HOH:O	2.38	0.56
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.38	0.56
2:B:134:GLN:HA	2:B:165:ASN:O	2.05	0.56
2:D:306:ARG:HD3	2:D:340:TYR:CE2	2.41	0.56
1:C:2:ARG:HA	1:C:131:GLY:O	2.06	0.55
2:D:246:LEU:HD12	2:D:247:ASN:H	1.70	0.55
4:F:95:PRO:HB2	4:F:183:GLN:NE2	2.22	0.55
2:B:280:GLN:NE2	2:B:280:GLN:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:O	1:C:234:ILE:HD12	2.07	0.54
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.88	0.54
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.73	0.54
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.42	0.54
2:D:36:TYR:CD1	2:D:44:LEU:HD21	2.43	0.53
2:D:2:ARG:NH2	11:D:604:HOH:O	2.42	0.53
2:D:161:ASP:O	2:D:251:ARG:NH2	2.42	0.52
2:D:246:LEU:HD21	10:D:502:O91:C30	2.39	0.52
2:D:178:THR:O	2:D:181:GLU:HG3	2.08	0.52
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.90	0.52
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.91	0.52
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.18	0.51
4:F:226:GLU:OE1	4:F:252:ASN:HA	2.10	0.51
2:D:193:VAL:HG13	2:D:194:GLU:HG2	1.93	0.51
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.92	0.51
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.93	0.50
4:F:161:LEU:HD23	4:F:172:PHE:CZ	2.46	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.50
1:A:285:GLN:CD	1:A:372:GLN:NE2	2.70	0.50
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.94	0.49
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.47	0.49
4:F:169:LEU:HA	4:F:172:PHE:HB3	1.93	0.49
2:D:208:TYR:CE1	2:D:220:PRO:HD2	2.48	0.49
2:B:389:PHE:O	2:B:392:LYS:NZ	2.38	0.49
2:D:141:GLY:HA3	8:D:501:GDP:O3A	2.13	0.49
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.52	0.49
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.95	0.48
3:E:100:LYS:NZ	11:E:201:HOH:O	2.45	0.48
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.48	0.48
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.48
2:D:323:MET:HE2	2:D:327:ASP:OD2	2.14	0.48
4:F:87:LEU:O	4:F:91:CYS:HB2	2.14	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.47
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.50	0.47
4:F:189:PRO:HA	4:F:322:ASP:HA	1.96	0.47
2:B:248:ALA:HB1	10:B:505:O91:C10	2.45	0.47
2:D:211:CYS:HB2	2:D:220:PRO:HG3	1.97	0.47
4:F:31:ARG:NE	4:F:31:ARG:HA	2.30	0.47
2:D:390:ARG:HG3	2:D:391:ARG:HG3	1.96	0.46
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.96	0.46
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.46
1:A:247:ALA:HB3	3:E:19:SER:OG	2.15	0.46
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.16	0.46
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.96	0.46
2:B:219:THR:HG21	1:C:326:LYS:HA	1.98	0.46
4:F:46:ARG:NH2	11:F:403:HOH:O	2.49	0.46
1:A:155:GLU:OE1	3:E:53:LYS:NZ	2.46	0.45
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.98	0.45
1:C:241:SER:HA	1:C:249:ASN:OD1	2.16	0.45
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.97	0.45
1:A:326:LYS:NZ	11:A:605:HOH:O	2.47	0.45
2:B:74:ASP:OD1	2:B:77:ARG:NH2	2.49	0.45
2:B:363:MET:HE2	2:B:363:MET:HB3	1.67	0.45
2:B:379:LYS:HB2	2:B:379:LYS:HE3	1.78	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.52	0.45
9:B:504:MES:H51	9:B:504:MES:H81	1.59	0.45
2:D:323:MET:HE2	2:D:327:ASP:CG	2.42	0.45
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.49	0.45
4:F:31:ARG:HD3	4:F:32:LYS:N	2.32	0.45
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.52	0.45
2:B:73:MET:N	11:B:604:HOH:O	2.48	0.45
1:A:285:GLN:HG3	1:A:372:GLN:HE21	1.61	0.44
1:A:163:LYS:H	1:A:163:LYS:CD	2.22	0.44
4:F:21:LEU:O	4:F:27:TRP:HB2	2.18	0.44
4:F:73:ARG:HB3	4:F:76:SER:OG	2.17	0.44
3:E:9:ILE:HG22	3:E:10:GLU:HB2	1.99	0.44
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.52	0.44
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.00	0.44
2:D:61:PRO:HD3	2:D:84:ILE:HG13	1.99	0.44
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.34	0.44
2:B:323:MET:HE2	2:B:323:MET:HB3	1.77	0.44
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.99	0.44
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.00	0.44
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.52	0.44
2:D:285:THR:HG23	2:D:288:GLU:H	1.82	0.44
2:B:246:LEU:HD21	2:B:350:LYS:HE2	2.00	0.43
1:A:97:GLU:OE1	2:B:2:ARG:NH2	2.51	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.00	0.43
3:E:8:VAL:C	3:E:9:ILE:HD12	2.43	0.43
2:D:323:MET:CE	2:D:327:ASP:OD2	2.66	0.43
2:D:395:LEU:HD21	2:D:405:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:186:LEU:HD13	4:F:320:MET:SD	2.58	0.43
1:C:209:ILE:HD11	1:C:302:MET:SD	2.58	0.43
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.24	0.43
3:E:7:GLU:O	3:E:22:VAL:HA	2.19	0.43
4:F:182:ILE:HD12	4:F:182:ILE:HA	1.88	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.43
2:D:44:LEU:HA	2:D:47:ILE:HB	2.00	0.43
2:B:67:ASP:O	2:B:92:PHE:HA	2.19	0.43
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.99	0.43
1:A:298:PRO:HA	1:A:301:GLN:CD	2.44	0.42
1:A:430:LYS:HE2	1:A:430:LYS:HB3	1.79	0.42
2:D:246:LEU:HD21	10:D:502:O91:C24	2.49	0.42
3:E:7:GLU:CD	3:E:9:ILE:HD11	2.44	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.42
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.42
2:D:213:ARG:O	2:D:216:LYS:HE3	2.20	0.42
2:D:116:VAL:O	2:D:120:VAL:HG23	2.19	0.42
3:E:25:LYS:CE	3:E:26:PRO:O	2.67	0.42
2:B:40:SER:HB3	2:B:43:GLN:HE21	1.85	0.42
2:D:9:ALA:HA	2:D:66:VAL:O	2.20	0.42
1:A:399:TYR:O	1:A:402:ARG:NH1	2.46	0.41
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.53	0.41
1:A:230:LEU:O	1:A:234:ILE:HD12	2.20	0.41
2:D:273:LEU:HD23	2:D:273:LEU:HA	1.88	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
2:B:197:ASP:C	2:B:198:GLU:HG3	2.45	0.41
2:D:350:LYS:HD3	10:D:502:O91:C40	2.51	0.41
2:D:211:CYS:CB	2:D:220:PRO:HG3	2.51	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.22	0.40
1:C:320:ARG:HA	1:C:356:ASN:O	2.20	0.40
2:D:170:MET:HE2	2:D:377:LEU:HD21	2.04	0.40
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.03	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	435/450 (97%)	426 (98%)	8 (2%)	1 (0%)	43	66
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	D	417/445 (94%)	405 (97%)	12 (3%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	322/384 (84%)	305 (95%)	17 (5%)	0	100	100
All	All	2154/2317 (93%)	2092 (97%)	61 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY

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	368/378 (97%)	368 (100%)	0	100	100
1	C	371/378 (98%)	371 (100%)	0	100	100
2	B	369/383 (96%)	367 (100%)	2 (0%)	81	92
2	D	364/383 (95%)	364 (100%)	0	100	100
3	E	108/127 (85%)	108 (100%)	0	100	100
4	F	272/342 (80%)	271 (100%)	1 (0%)	84	93
All	All	1852/1991 (93%)	1849 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	19	LYS
2	B	218	THR
4	F	12	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	216	ASN
1	A	309	HIS
1	A	372	GLN
1	A	393	HIS
2	B	15	GLN
2	B	43	GLN
2	B	99	ASN
2	B	280	GLN
2	B	347	ASN
2	B	424	GLN
1	C	15	GLN
1	C	85	GLN
1	C	107	HIS
1	C	256	GLN
1	C	285	GLN
1	C	372	GLN
2	D	11	GLN
2	D	247	ASN
2	D	329	GLN
2	D	335	ASN
2	D	347	ASN
2	D	375	GLN
2	D	423	GLN
3	E	12	ASN
3	E	90	ASN
3	E	108	ASN
3	E	136	ASN
4	F	183	GLN
4	F	196	HIS
4	F	229	ASN
4	F	269	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	MES	B	503	-	12,12,12	2.25	1 (8%)	15,16,16	1.77	4 (26%)
8	GDP	D	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
10	O91	B	505	-	28,28,28	1.38	8 (28%)	33,39,39	1.33	4 (12%)
9	MES	B	504	-	12,12,12	2.33	1 (8%)	15,16,16	1.89	3 (20%)
8	GDP	B	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.69	6 (13%)
5	GTP	A	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.54	8 (16%)
5	GTP	C	501	6	33,34,34	1.03	4 (12%)	50,54,54	1.53	8 (16%)
10	O91	D	502	-	28,28,28	1.38	7 (25%)	33,39,39	1.47	7 (21%)

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	MES	B	503	-	-	4/6/14/14	0/1/1/1
8	GDP	D	501	-	-	6/16/32/32	0/3/3/3
10	O91	B	505	-	-	2/18/18/18	0/3/3/3
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
10	O91	D	502	-	-	6/18/18/18	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.77	1.66	1.77
9	B	503	MES	C8-S	-7.53	1.67	1.77
10	D	502	O91	C30-N31	-3.24	1.31	1.38
10	B	505	O91	C30-N31	-3.16	1.31	1.38
8	D	501	GDP	C5-C4	3.15	1.47	1.38
8	B	501	GDP	C5-C4	3.07	1.47	1.38
10	B	505	O91	C42-C32	2.98	1.52	1.47
10	D	502	O91	C42-C32	2.78	1.52	1.47
10	D	502	O91	C30-C24	2.67	1.53	1.49
5	C	501	GTP	PA-O3A	2.64	1.62	1.59
10	B	505	O91	C30-C24	2.61	1.53	1.49
8	D	501	GDP	C6-N1	-2.38	1.34	1.38
8	B	501	GDP	C6-N1	-2.38	1.34	1.38
5	A	501	GTP	PA-O3A	2.36	1.62	1.59
10	D	502	O91	O13-C12	2.22	1.40	1.37
10	B	505	O91	O13-C12	2.19	1.40	1.37
5	A	501	GTP	C2-N3	2.19	1.38	1.33
10	D	502	O91	C28-N26	-2.15	1.31	1.36
10	D	502	O91	O25-C24	-2.12	1.18	1.23
10	B	505	O91	O25-C24	-2.10	1.18	1.23
5	C	501	GTP	PB-O3A	2.07	1.61	1.59
5	C	501	GTP	C2-N3	2.07	1.38	1.33
5	A	501	GTP	PB-O3A	2.05	1.61	1.59
10	D	502	O91	C09-C24	2.04	1.53	1.49
5	C	501	GTP	PB-O3B	2.04	1.61	1.59
10	B	505	O91	C09-C24	2.03	1.53	1.49
10	B	505	O91	C28-N26	-2.02	1.32	1.36
8	D	501	GDP	C5-N7	-2.01	1.35	1.39
10	B	505	O91	O02-C01	2.00	1.40	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-6.06	118.75	128.39
8	B	501	GDP	C5-C4-N3	-5.84	119.09	128.39
8	D	501	GDP	C2-N3-C4	5.04	120.97	112.30
8	B	501	GDP	C2-N3-C4	4.92	120.77	112.30
5	A	501	GTP	C5-C4-N3	-4.90	120.60	128.39
5	C	501	GTP	C5-C4-N3	-4.54	121.17	128.39
5	A	501	GTP	C2-N3-C4	4.52	120.09	112.30
5	C	501	GTP	C2-N3-C4	4.50	120.06	112.30
8	D	501	GDP	N9-C4-N3	4.44	134.83	125.95
8	B	501	GDP	N9-C4-N3	4.32	134.60	125.95
9	B	504	MES	C5-N4-C3	4.09	117.65	108.84
9	B	503	MES	C5-N4-C3	3.81	117.04	108.84
8	B	501	GDP	C6-C5-N7	3.39	136.47	130.29
8	D	501	GDP	C6-C5-N7	3.39	136.45	130.29
10	D	502	O91	O13-C12-C18	3.18	120.59	115.14
9	B	504	MES	C6-C5-N4	-3.07	105.45	110.12
5	A	501	GTP	N9-C4-N3	3.02	131.99	125.95
10	D	502	O91	O02-C01-C18	3.01	120.30	115.14
5	C	501	GTP	N9-C8-N7	-2.89	108.03	113.40
5	A	501	GTP	C2-N1-C6	-2.85	119.94	125.11
5	C	501	GTP	N9-C4-N3	2.75	131.45	125.95
10	B	505	O91	O02-C01-C18	2.70	119.77	115.14
5	A	501	GTP	N9-C8-N7	-2.69	108.42	113.40
10	B	505	O91	O13-C12-C18	2.67	119.71	115.14
5	C	501	GTP	C2-N1-C6	-2.66	120.28	125.11
8	D	501	GDP	C4-C5-N7	-2.66	106.45	110.67
10	B	505	O91	C42-C32-N26	2.65	126.85	124.29
5	C	501	GTP	C8-N7-C5	2.63	108.95	104.26
8	B	501	GDP	C4-C5-N7	-2.60	106.54	110.67
9	B	503	MES	C7-N4-C5	2.57	118.08	111.24
5	A	501	GTP	C8-N7-C5	2.53	108.77	104.26
9	B	503	MES	C6-C5-N4	-2.51	106.31	110.12
10	D	502	O91	O13-C12-C10	-2.51	119.76	124.08
5	A	501	GTP	C5-C6-N1	2.44	119.46	113.25
5	C	501	GTP	C5-C6-N1	2.39	119.33	113.25
5	A	501	GTP	O6-C6-C5	-2.28	120.52	126.53
10	D	502	O91	C14-O13-C12	-2.27	114.18	117.51
5	C	501	GTP	O6-C6-C5	-2.25	120.60	126.53
10	D	502	O91	C03-O02-C01	-2.24	114.23	117.51
9	B	503	MES	O3S-S-C8	2.22	110.34	106.00
10	D	502	O91	O02-C01-C07	-2.20	120.28	124.08
10	D	502	O91	C42-C32-N26	2.18	126.39	124.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	O6-C6-C5	-2.16	120.84	126.53
8	D	501	GDP	O6-C6-C5	-2.06	121.10	126.53
10	B	505	O91	O13-C12-C10	-2.05	120.55	124.08
9	B	504	MES	C7-N4-C5	2.05	116.69	111.24

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
10	B	505	O91	C09-C24-C30-C28
10	B	505	O91	O25-C24-C30-C28
10	D	502	O91	C09-C24-C30-C28
10	D	502	O91	O25-C24-C30-C28
10	D	502	O91	C18-C12-O13-C14
10	D	502	O91	C10-C12-O13-C14
10	D	502	O91	C18-C01-O02-C03
10	D	502	O91	C07-C01-O02-C03
9	B	503	MES	C7-C8-S-O1S
8	D	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
8	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A

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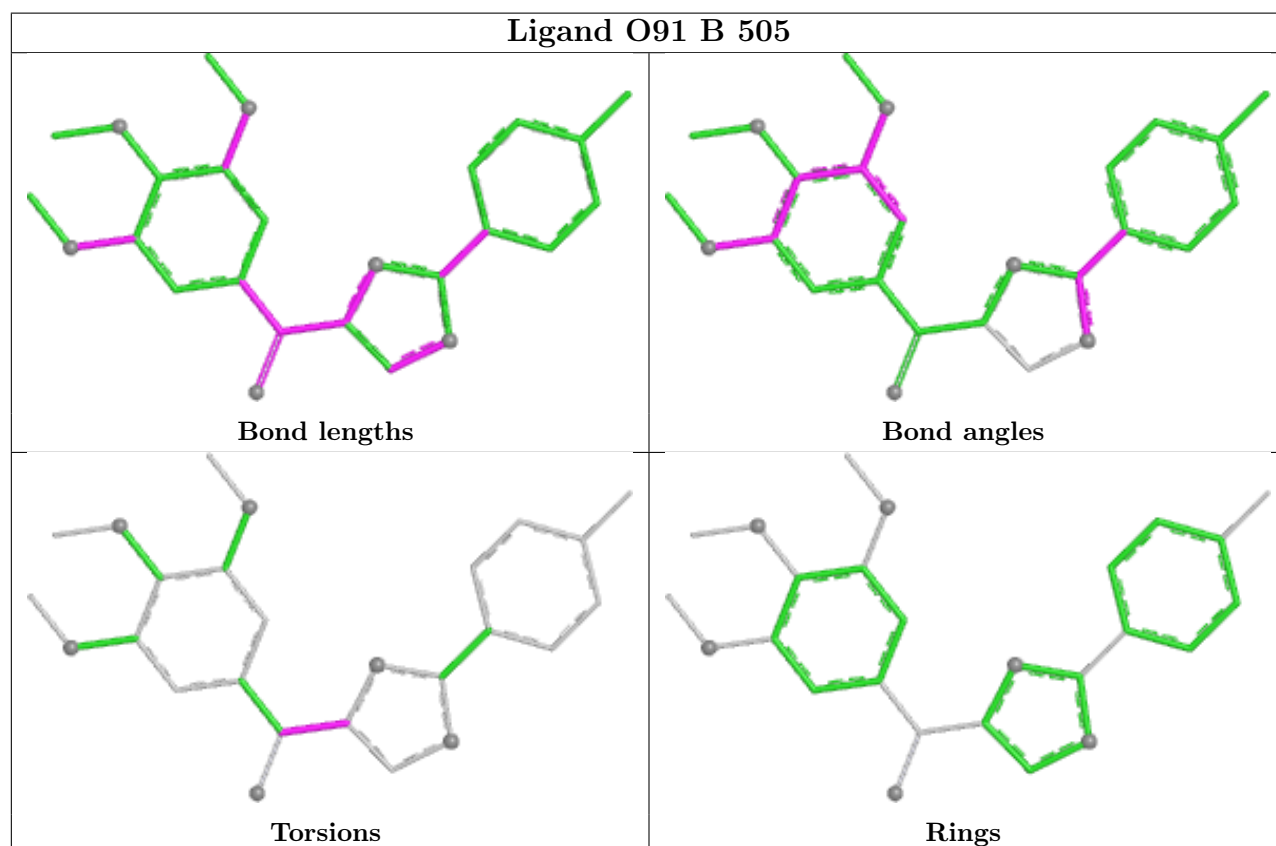
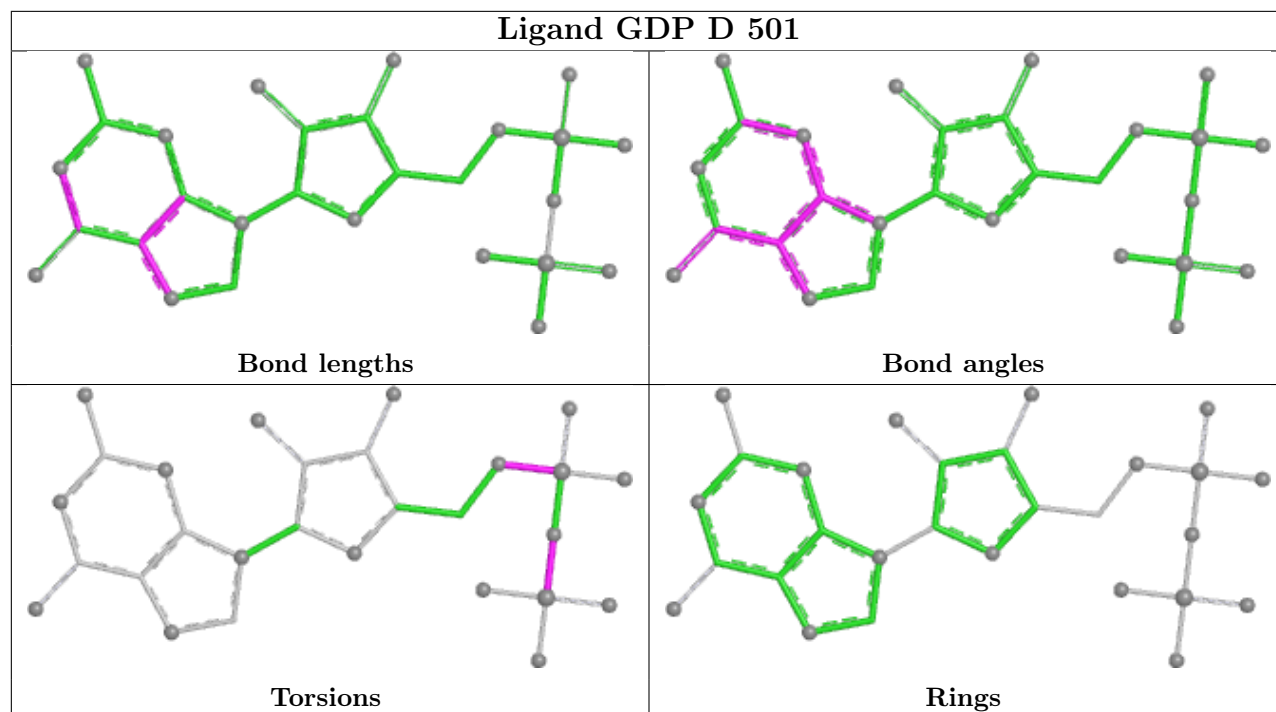
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C4'-C5'-O5'-PA

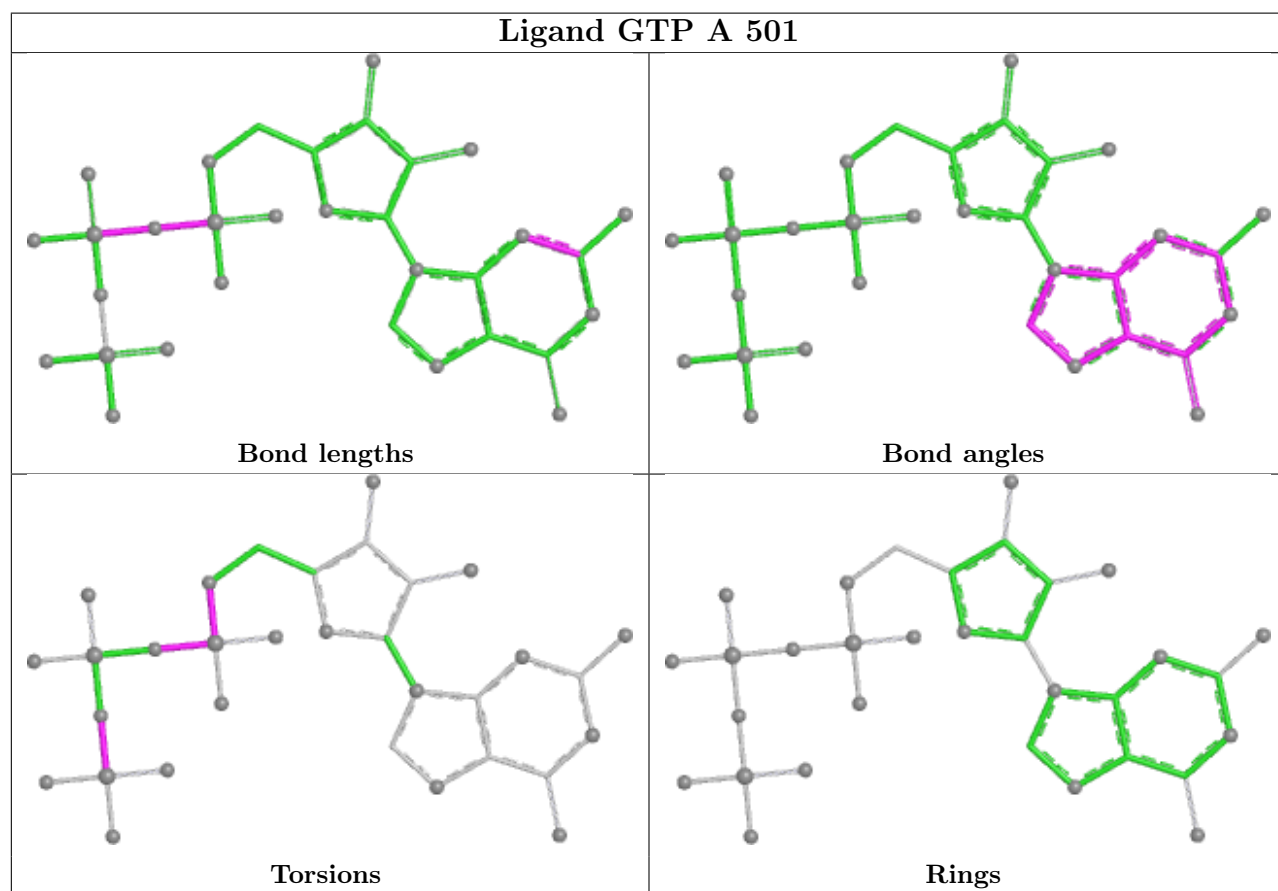
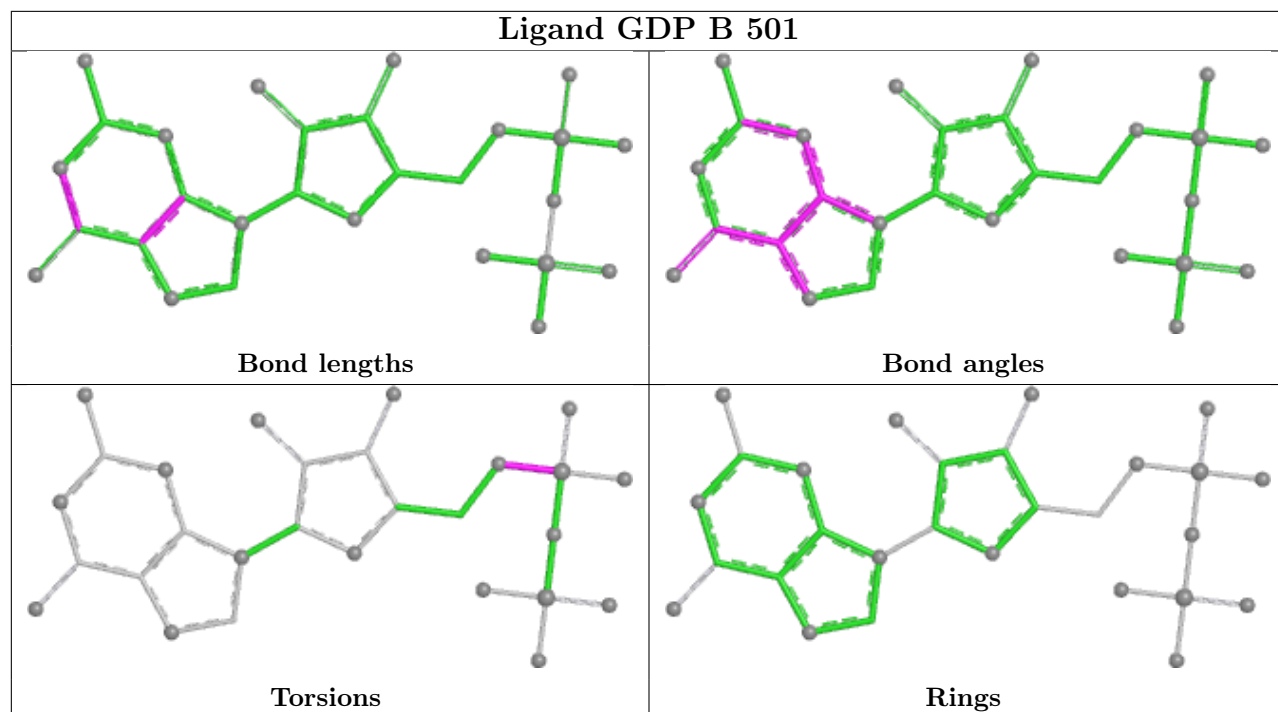
There are no ring outliers.

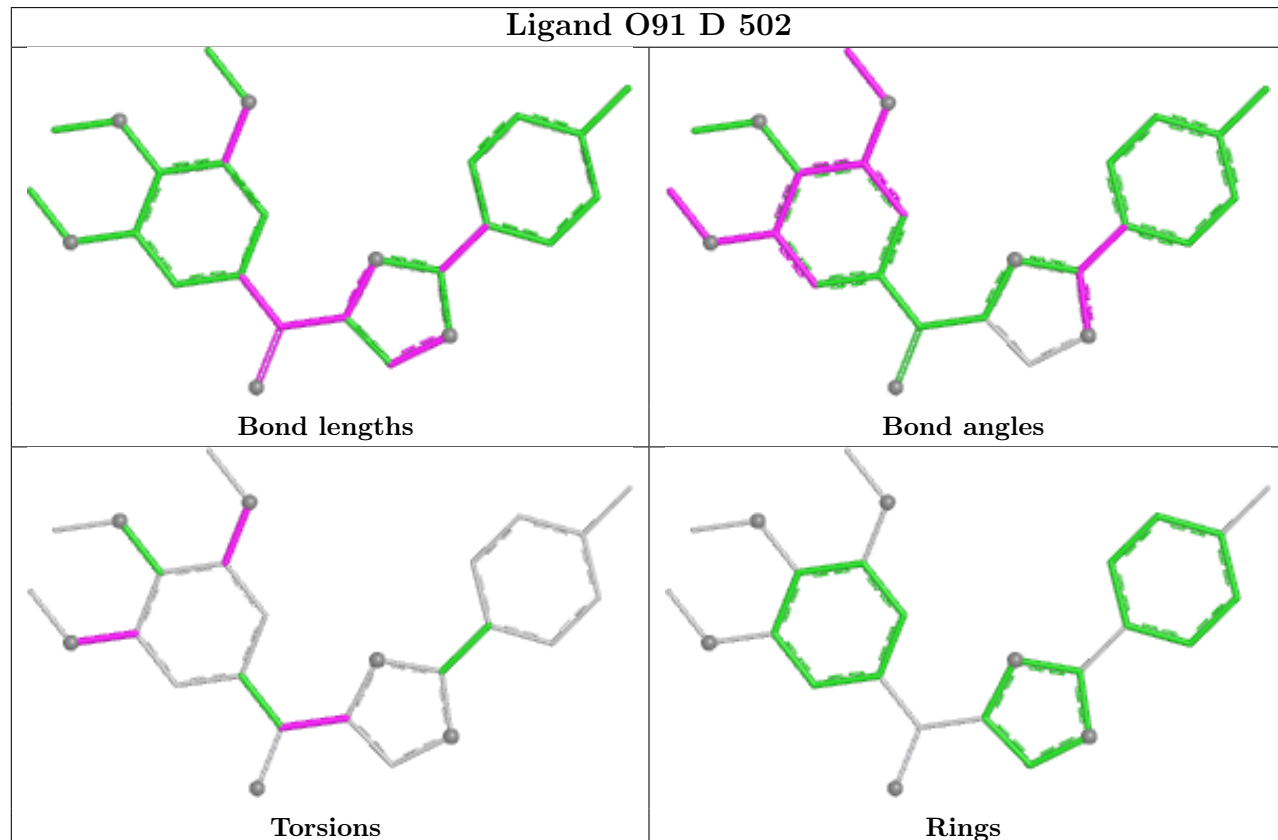
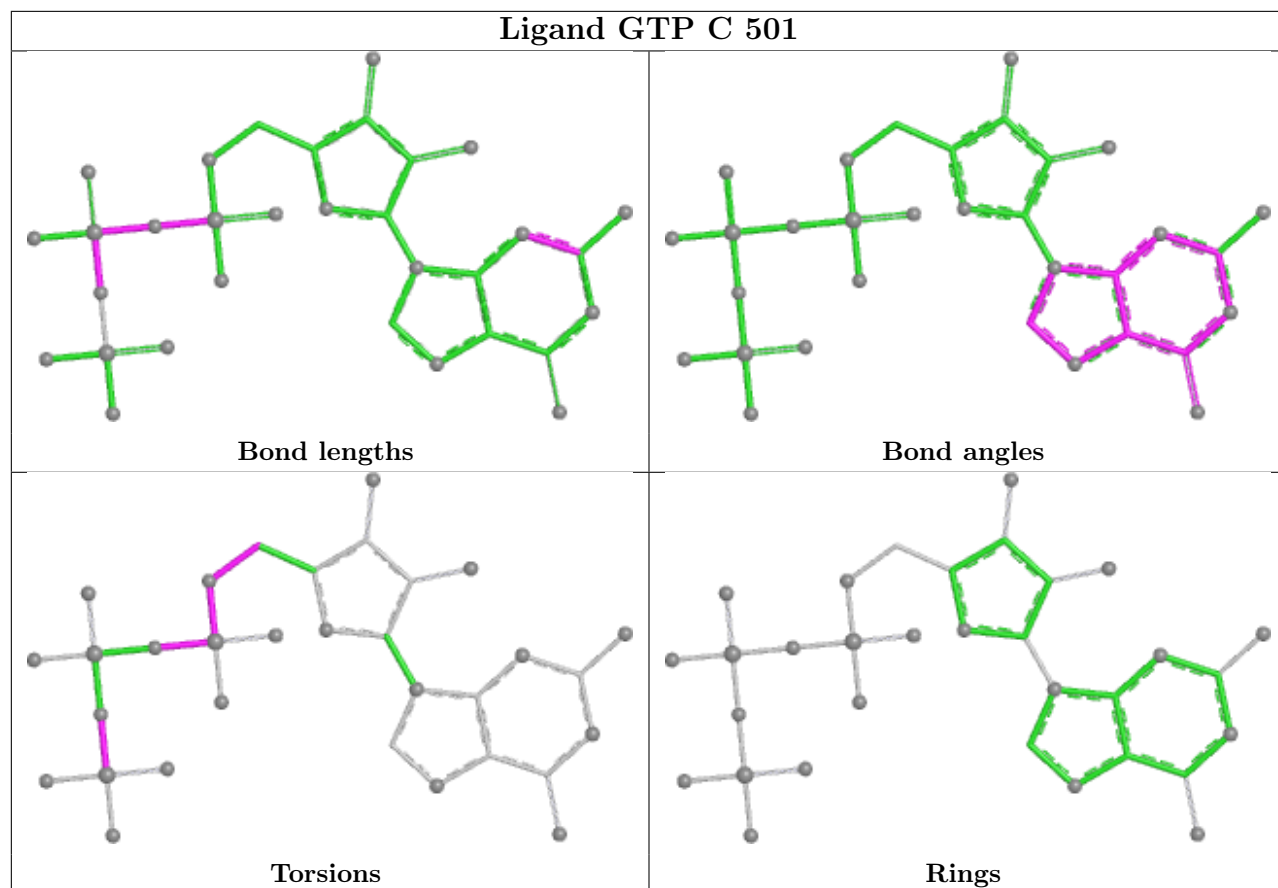
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
10	B	505	O91	1	0
9	B	504	MES	1	0
8	B	501	GDP	1	0
10	D	502	O91	3	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	437/450 (97%)	-0.30	4 (0%) 81 78	25, 41, 70, 85	0
1	C	440/450 (97%)	-0.43	3 (0%) 84 82	21, 32, 60, 91	0
2	B	427/445 (95%)	-0.20	14 (3%) 49 43	21, 39, 75, 128	0
2	D	421/445 (94%)	0.37	28 (6%) 24 19	28, 58, 100, 136	0
3	E	121/143 (84%)	0.29	5 (4%) 41 36	30, 57, 90, 125	0
4	F	332/384 (86%)	0.86	65 (19%) 3 2	30, 66, 138, 161	0
All	All	2178/2317 (94%)	0.03	119 (5%) 30 25	21, 47, 102, 161	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	7.3
4	F	103	THR	5.9
4	F	243	HIS	5.5
2	D	1	MET	5.2
4	F	235	ASP	5.1
4	F	100	ILE	4.7
4	F	90	SER	4.7
4	F	178	GLN	4.7
4	F	130	VAL	4.6
1	A	437	VAL	4.6
4	F	149	ALA	4.4
4	F	240	LEU	4.3
4	F	89	GLU	4.3
2	B	428	ALA	4.2
4	F	233	PHE	4.1
4	F	182	ILE	4.0
2	B	48	ASN	4.0
2	D	55	THR	4.0
4	F	131	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	245	GLN	3.8
4	F	166	ALA	3.8
4	F	234	GLN	3.7
4	F	172	PHE	3.7
4	F	247	LYS	3.6
4	F	180	HIS	3.6
2	D	219	THR	3.6
4	F	142	ARG	3.5
2	D	247	ASN	3.5
4	F	165	GLU	3.4
4	F	143	GLU	3.4
4	F	232	ASN	3.4
1	C	440	VAL	3.3
4	F	99	VAL	3.3
4	F	132	LEU	3.3
4	F	245	ILE	3.3
2	D	246	LEU	3.2
2	B	277	GLY	3.2
3	E	141	GLU	3.2
4	F	252	ASN	3.2
2	D	245	GLN	3.2
4	F	176	GLN	3.2
4	F	179	VAL	3.1
4	F	128	ARG	3.1
4	F	135	TYR	3.1
4	F	129	GLU	3.1
4	F	170	LEU	2.9
2	D	94	GLN	2.9
4	F	238	CYS	2.9
4	F	239	HIS	2.9
1	C	1	MET	2.9
2	B	37	HIS	2.9
4	F	101	TYR	2.8
2	D	170	MET	2.8
2	B	247	ASN	2.8
4	F	133	ALA	2.8
4	F	181	VAL	2.8
4	F	244	CYS	2.8
4	F	372	THR	2.8
1	A	262	TYR	2.8
2	D	244	GLY	2.8
2	D	81	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	102	PRO	2.7
1	A	163	LYS	2.7
4	F	173	ILE	2.7
2	D	394	PHE	2.7
4	F	138	ARG	2.7
4	F	175	GLU	2.7
2	B	280	GLN	2.6
4	F	177	GLY	2.6
2	B	55	THR	2.6
2	D	72	THR	2.6
3	E	28	SER	2.6
2	D	86	ARG	2.6
2	D	306	ARG	2.6
1	C	357	TYR	2.5
2	D	96	GLY	2.5
2	B	279	GLN	2.5
4	F	91	CYS	2.5
4	F	137	ARG	2.5
3	E	27	PRO	2.5
2	D	73	MET	2.5
2	D	323	MET	2.5
2	D	126	SER	2.5
4	F	163	SER	2.5
2	D	431	ASP	2.5
4	F	168	GLU	2.5
4	F	167	SER	2.4
4	F	134	ALA	2.4
2	B	57	ASN	2.4
4	F	162	ILE	2.4
4	F	256	TYR	2.4
2	B	246	LEU	2.4
4	F	320	MET	2.4
2	D	54	ALA	2.4
2	D	362	LYS	2.3
4	F	194	PRO	2.3
4	F	259	GLY	2.3
2	B	278	SER	2.3
2	D	46	ARG	2.3
4	F	186	LEU	2.3
2	D	24	ILE	2.3
2	D	71	GLY	2.2
4	F	379	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	241	THR	2.2
4	F	242	ASN	2.2
2	D	97	ALA	2.2
2	D	48	ASN	2.2
4	F	231	ALA	2.1
2	D	56	GLY	2.1
2	D	92	PHE	2.1
4	F	230	SER	2.1
4	F	169	LEU	2.1
3	E	9	ILE	2.1
2	B	2	ARG	2.1
2	B	170	MET	2.1
4	F	237	THR	2.0
1	A	372	GLN	2.0
3	E	115	HIS	2.0
4	F	19	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.

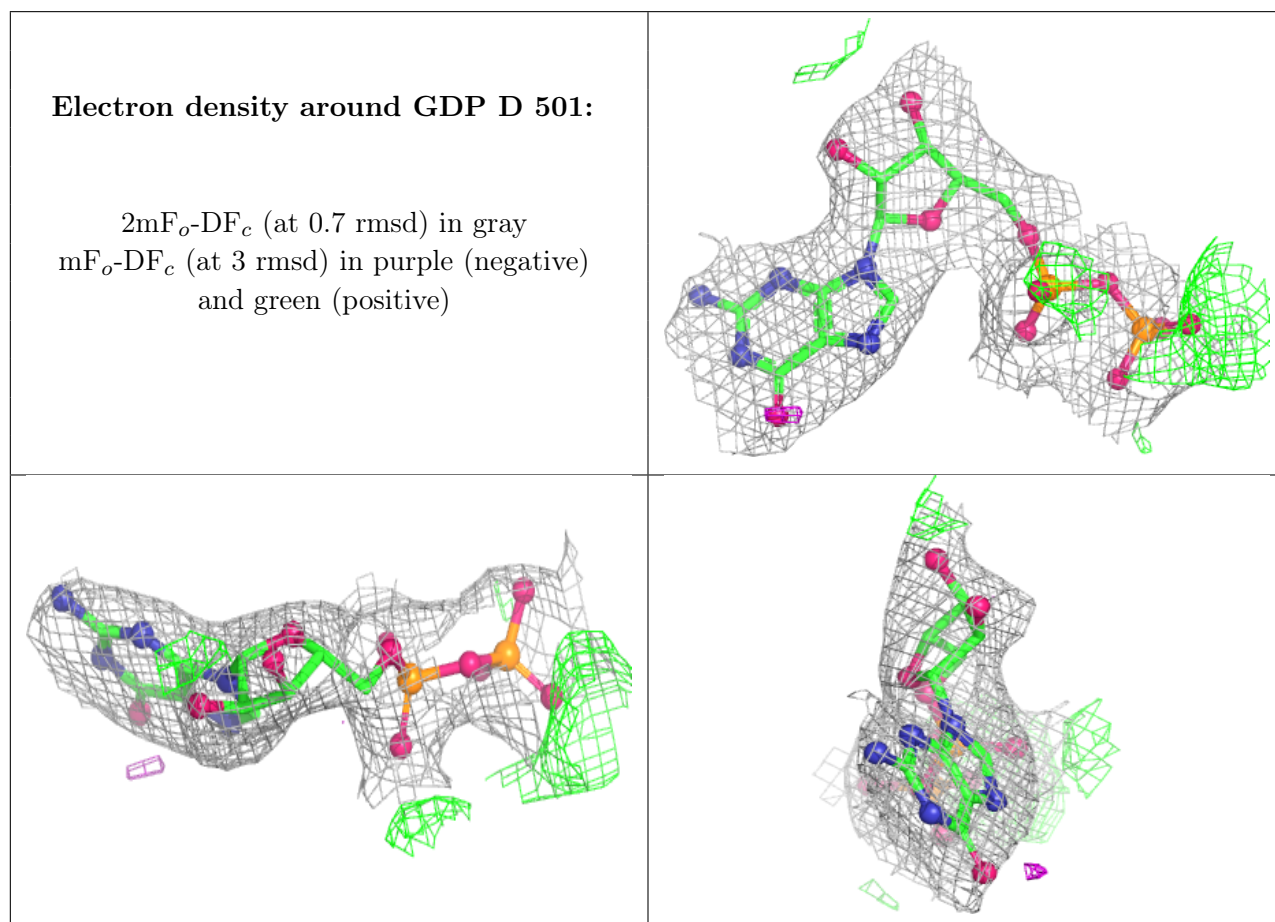
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GDP	D	501	28/28	0.90	0.10	48,55,65,66	0
10	O91	D	502	26/26	0.91	0.12	44,52,60,65	0
9	MES	B	504	12/12	0.94	0.10	57,62,70,73	0
10	O91	B	505	26/26	0.96	0.08	33,38,44,47	0
9	MES	B	503	12/12	0.97	0.07	32,46,61,64	0
8	GDP	B	501	28/28	0.98	0.05	18,25,33,35	0
5	GTP	C	501	32/32	0.98	0.05	23,28,31,34	0

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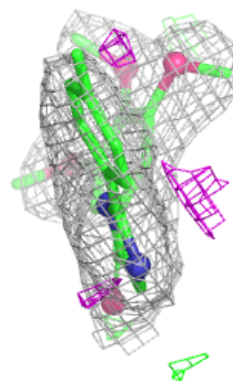
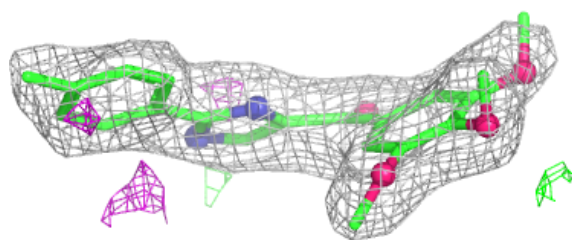
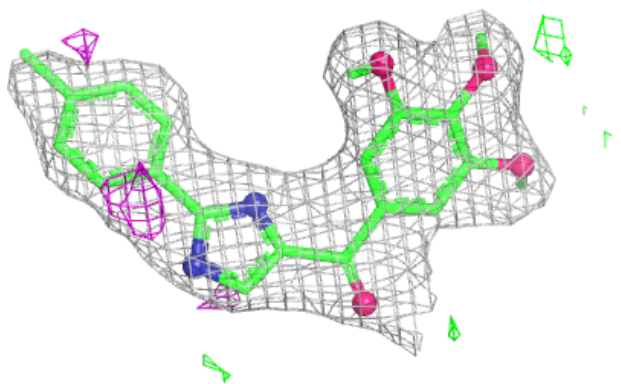
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	A	503	1/1	0.99	0.04	60,60,60,60	0
7	CA	C	503	1/1	0.99	0.02	45,45,45,45	0
5	GTP	A	501	32/32	0.99	0.05	22,28,34,39	0
6	MG	B	502	1/1	0.99	0.11	35,35,35,35	0
6	MG	A	502	1/1	1.00	0.02	24,24,24,24	0
6	MG	C	502	1/1	1.00	0.01	26,26,26,26	0

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.

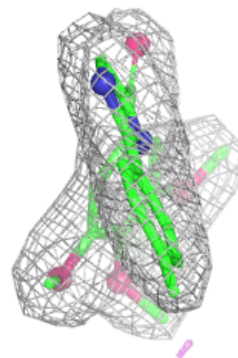
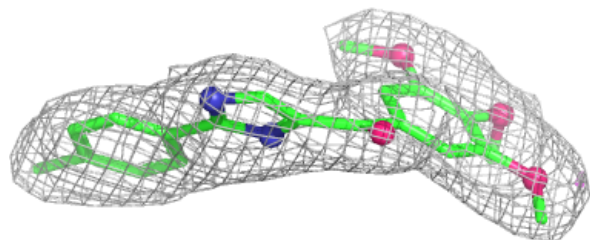
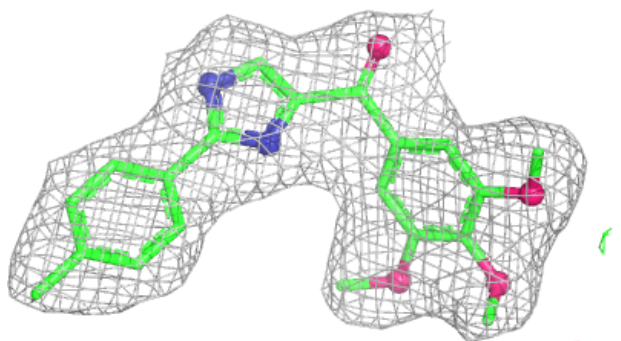


Electron density around O91 D 502:

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

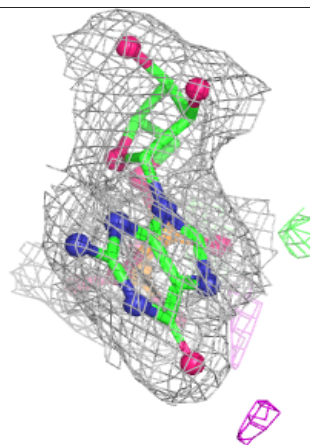
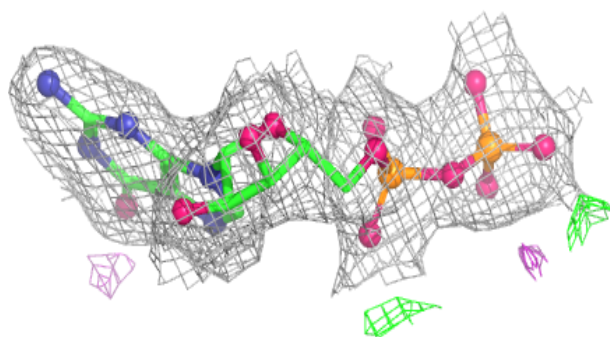
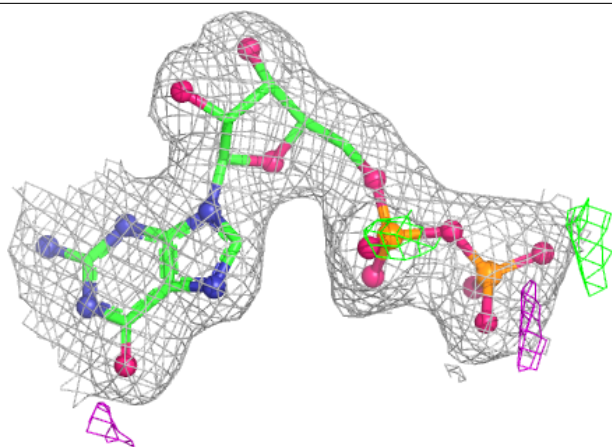
**Electron density around O91 B 505:**

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

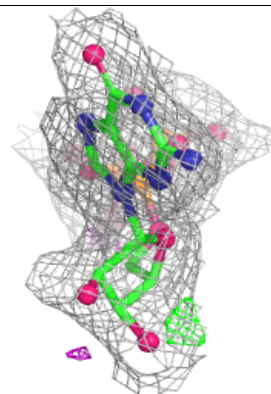
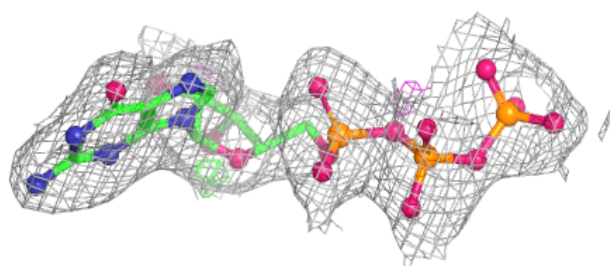
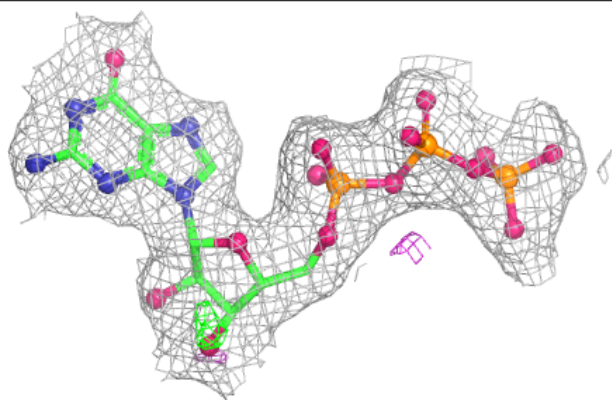


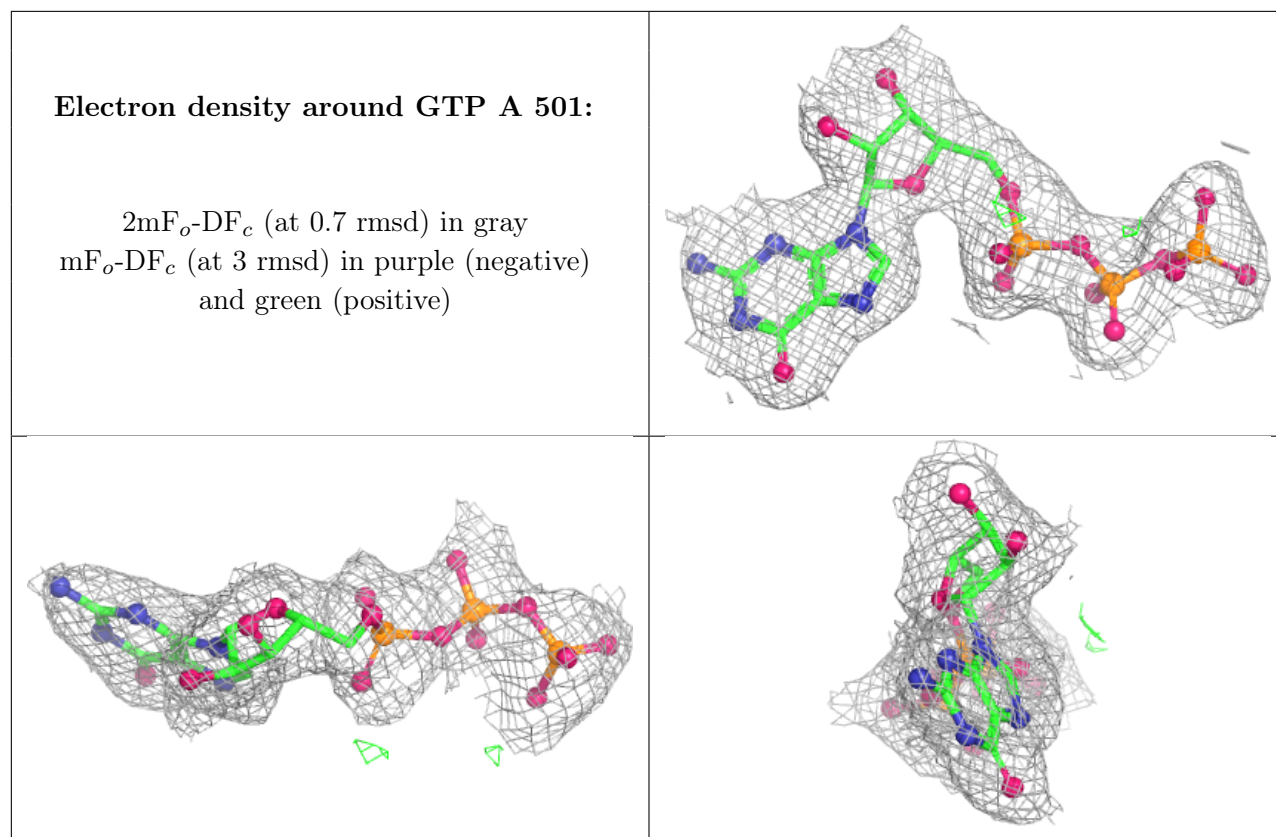
Electron density around GDP B 501:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.