



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:34 AM UTC

PDB ID : 6FJF / pdb_00006fjf
Title : Tubulin-FcMaytansine complex
Authors : Menchon, G.; Protá, A.E.; Lucena Angell, D.; Bucher, P.; Mueller, R.; Paterson, I.; Diaz, J.F.; Altmann, K.-H.; Steinmetz, M.O.
Deposited on : 2018-01-22
Resolution : 2.40 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

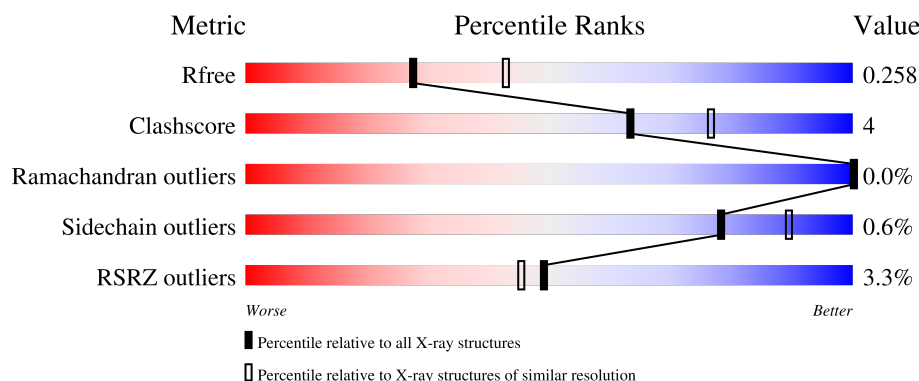
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	3% 83% 14% .
1	C	451	% 91% 6% .
2	B	445	3% 84% 10% 5%
2	D	445	2% 84% 10% 5%
3	E	143	4% 82% . 14%

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Mol	Chain	Length	Quality of chain
4	F	384	8% 75% 15% • 10%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18138 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	440	Total	C	N	O	S	0	1	0
			3450	2182	587	659	22			
1	C	440	Total	C	N	O	S	0	4	0
			3454	2185	585	660	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	2	0
			3348	2104	572	646	26			
2	D	422	Total	C	N	O	S	0	0	0
			3314	2083	563	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	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	345	Total	C	N	O	S	0	1	0
			2828	1814	481	518	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 (CCD ID: 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 (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		
6	D	1	Total	Mg	0	0
			1	1		

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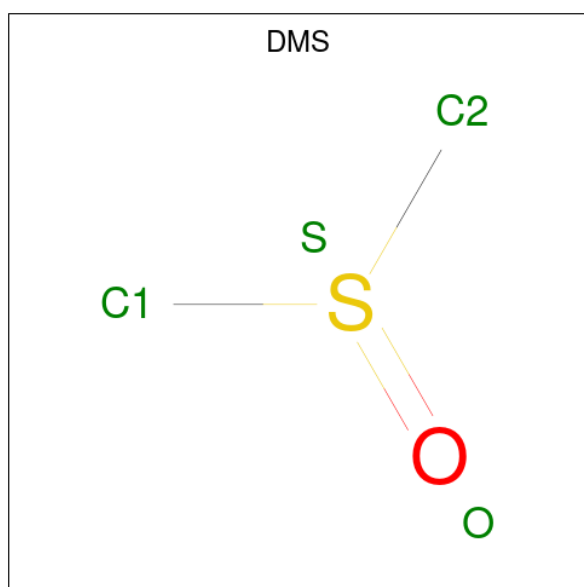
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

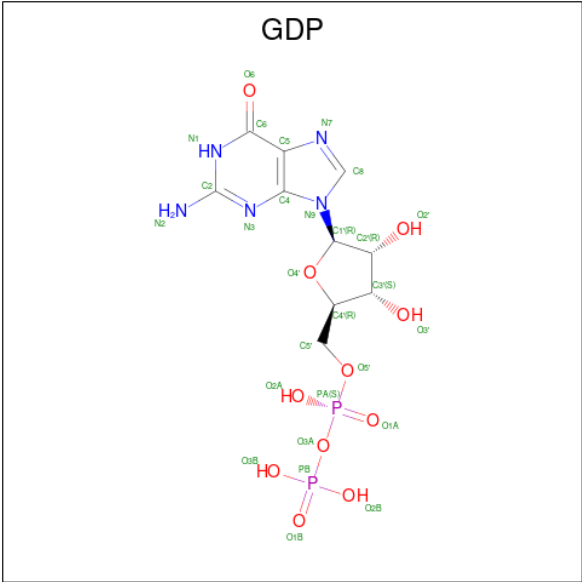
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



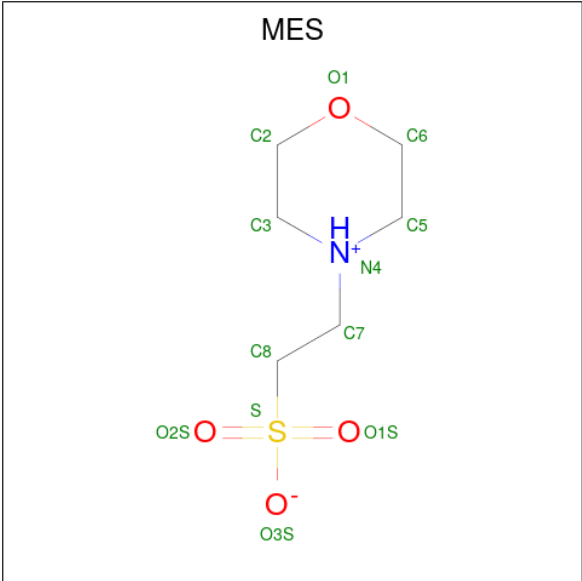
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	S	0	0
			4	2	1	1		
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



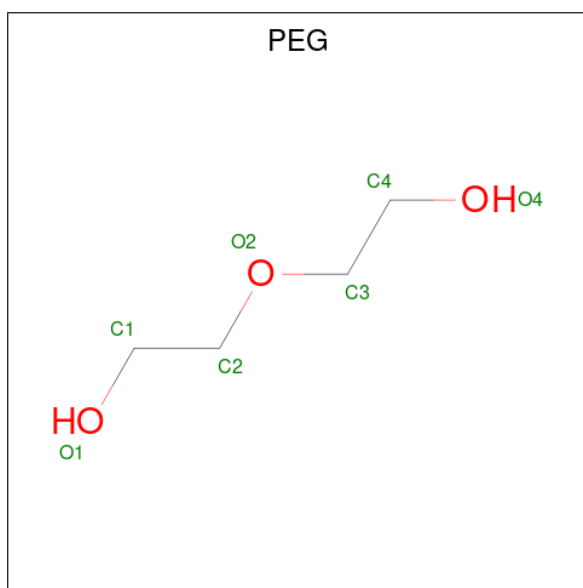
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



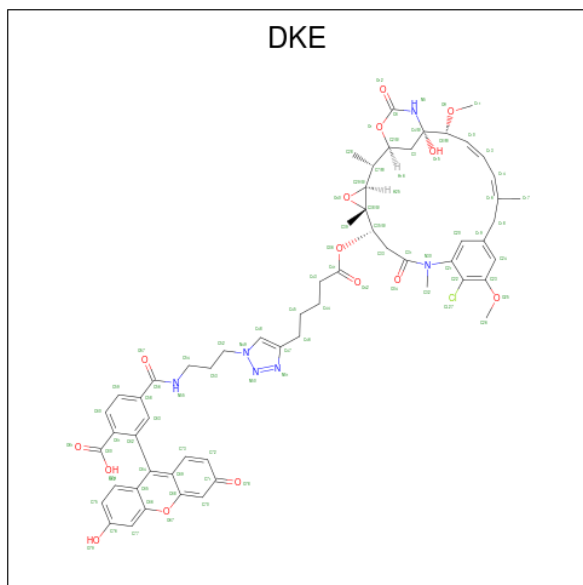
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			7	4	3		

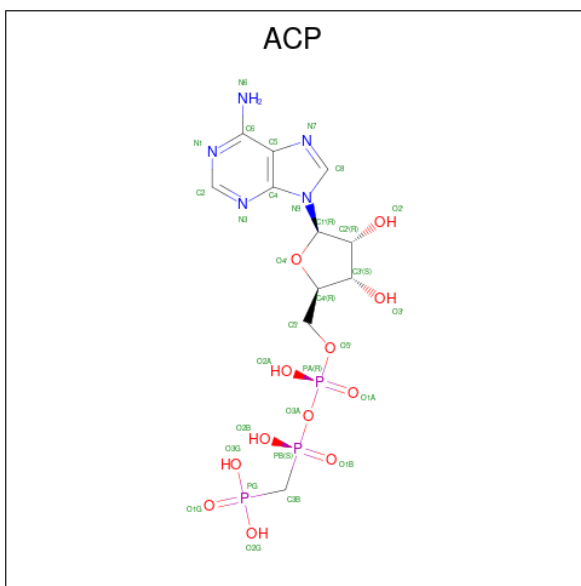
- Molecule 12 is FcMaytansine (CCD ID: DKE) (formula: $C_{59}H_{64}ClN_6O_{15}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	Cl	N	O	0	0
			81	59	1	6	15		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD

ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).

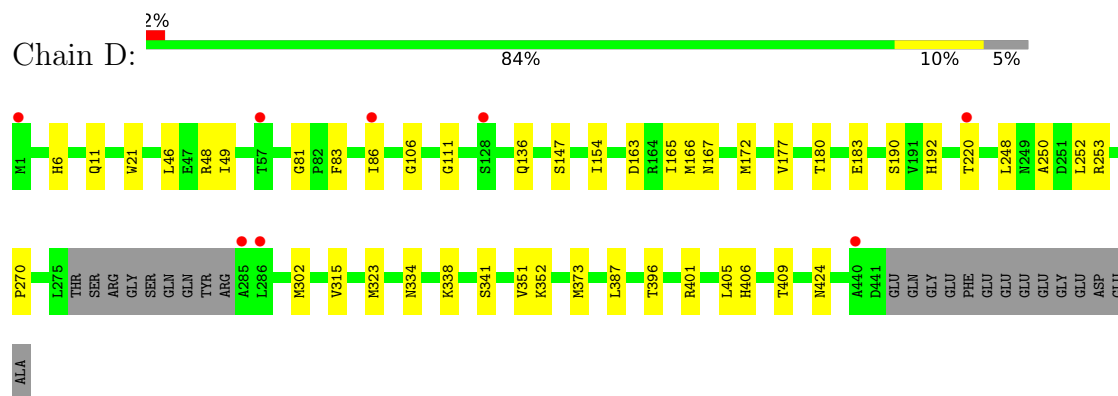


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

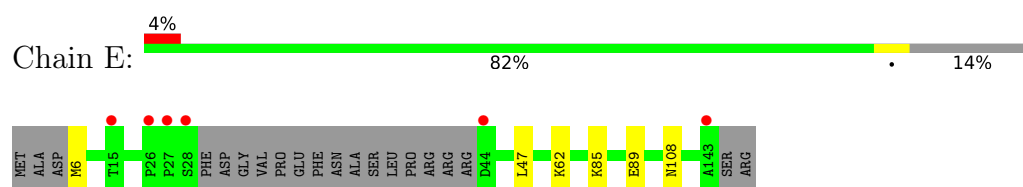
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	75	Total O 75 75	0	0
14	B	67	Total O 67 67	0	0
14	C	181	Total O 181 181	0	0
14	D	72	Total O 72 72	0	0
14	E	15	Total O 15 15	0	0
14	F	42	Total O 42 42	0	0

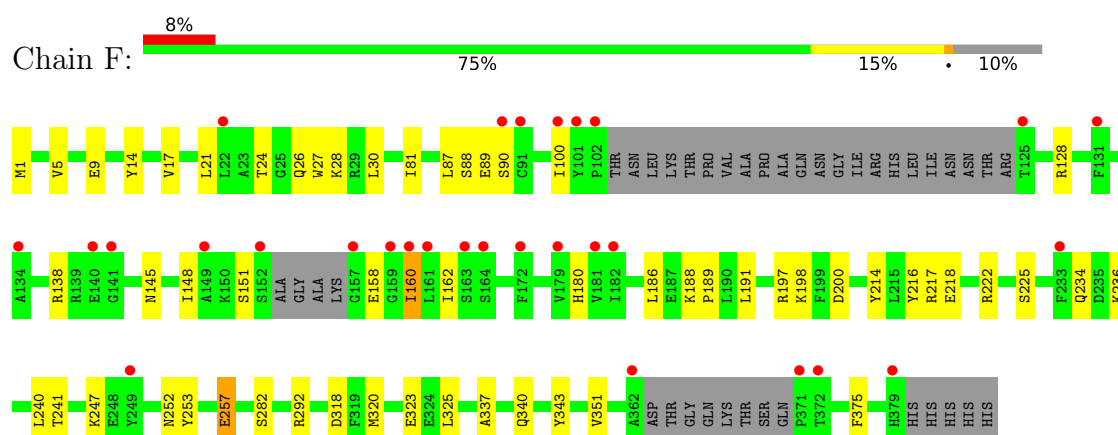
- Molecule 2: Tubulin beta-2B chain



- 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	104.37Å 156.74Å 180.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 2.40 49.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.55-2.40) 100.0 (49.55-2.40)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, R_{free}	0.201 , 0.258 0.202 , 0.258	Depositor DCC
R_{free} test set	5732 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18138	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMS, CA, DKE, PEG, ACP, GDP, GTP, MES

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	0.12	0/3530	0.30	0/4789
1	C	0.12	0/3541	0.31	0/4808
2	B	0.12	0/3425	0.31	0/4638
2	D	0.11	0/3387	0.28	0/4588
3	E	0.11	0/1022	0.25	0/1356
4	F	0.11	0/2895	0.32	0/3909
All	All	0.12	0/17800	0.30	0/24088

There are no bond length outliers.

There are no bond angle outliers.

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	3450	0	3358	41	0
1	C	3454	0	3366	15	0
2	B	3348	0	3226	27	0
2	D	3314	0	3194	24	0
3	E	1014	0	1029	5	0
4	F	2828	0	2799	32	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	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
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	4	0	6	0	0
8	B	4	0	6	0	0
8	C	12	0	18	1	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	12	0	12	1	0
11	C	7	0	10	1	0
12	D	81	0	0	1	0
13	F	31	0	14	0	0
14	A	75	0	0	2	0
14	B	67	0	0	1	0
14	C	181	0	0	1	0
14	D	72	0	0	2	0
14	E	15	0	0	1	0
14	F	42	0	0	0	0
All	All	18138	0	17086	139	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 4.

All (139) 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)
2:D:147:SER:HG	2:D:190:SER:HG	1.35	0.72
1:A:36:MET:HE3	1:A:39:ASP:HB2	1.73	0.71
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.77	0.66
4:F:88:SER:O	4:F:90:SER:N	2.27	0.65
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.80	0.64
4:F:24:THR:HG23	4:F:26:GLN:H	1.63	0.63
2:D:406:HIS:HA	2:D:409:THR:HG22	1.82	0.61
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.83	0.61
1:A:215:ARG:NH2	1:A:299:ALA:O	2.34	0.60
1:A:297:GLU:OE1	1:A:339:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:14:TYR:HA	4:F:17:VAL:HG12	1.84	0.59
2:D:172:MET:HG2	2:D:387:LEU:HD11	1.85	0.59
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.84	0.59
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.85	0.59
1:A:293:ASN:OD1	1:A:339:ARG:NH1	2.37	0.58
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.86	0.57
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.87	0.56
2:B:311:ARG:NH2	2:B:345:GLU:OE1	2.39	0.56
2:B:276:THR:HG21	2:B:371:LEU:HD11	1.88	0.55
2:D:401:ARG:NH2	12:D:503:DKE:O79	2.39	0.55
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.89	0.55
2:B:223:THR:HG23	2:B:226:ASP:H	1.72	0.55
1:A:166:LYS:NZ	14:A:605:HOH:O	2.40	0.54
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.91	0.53
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.40	0.52
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.90	0.52
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.90	0.52
1:A:449:GLU:HG3	4:F:337:ALA:HB2	1.92	0.51
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.91	0.51
1:A:261:PRO:HG2	1:A:313:MET:HE2	1.92	0.51
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.45	0.51
1:A:329:ASN:HB3	3:E:6:MET:HE1	1.93	0.50
2:D:180:THR:HG22	2:D:183:GLU:HG3	1.92	0.50
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.47	0.50
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.94	0.50
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.94	0.49
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.95	0.49
2:B:147:SER:HG	2:B:190:SER:HG	1.60	0.49
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.95	0.49
2:B:90:ASP:OD1	2:B:90:ASP:N	2.41	0.48
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.52	0.48
2:B:282:GLN:N	14:B:609:HOH:O	2.45	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.31	0.48
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.48
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.47	0.48
2:D:323:MET:HE2	2:D:373:MET:HG2	1.95	0.48
3:E:62:LYS:HZ2	3:E:62:LYS:HB2	1.78	0.48
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.47	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.49	0.47
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.95	0.47
4:F:222:ARG:NH2	4:F:318:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:HB2	1:A:193:THR:HB	1.97	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.14	0.47
4:F:247:LYS:NZ	4:F:253:TYR:OH	2.27	0.47
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.46
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.97	0.46
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.15	0.46
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.46
2:D:192:HIS:CE1	2:D:424:ASN:HD22	2.32	0.46
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.97	0.46
1:C:253:THR:HB	11:C:507:PEG:H11	1.98	0.46
1:A:164:LYS:NZ	14:A:607:HOH:O	2.49	0.46
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.46
4:F:158:GLU:HB2	4:F:160:ILE:HG23	1.98	0.46
1:C:327:ASP:OD2	14:C:601:HOH:O	2.20	0.46
2:B:253[A]:ARG:NH1	10:B:503:MES:O2S	2.39	0.46
1:A:409:VAL:HA	1:A:413:MET:O	2.17	0.45
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.97	0.45
1:A:223:THR:HG22	1:A:226:ASN:OD1	2.17	0.45
1:C:296:PHE:HZ	1:C:351:PHE:HE2	1.64	0.45
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.45
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.99	0.45
1:A:209:ILE:HD12	1:A:227:LEU:HB3	1.99	0.45
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.99	0.45
3:E:108:ASN:ND2	14:E:201:HOH:O	2.36	0.45
2:B:230:LEU:O	2:B:234:THR:HG23	2.16	0.45
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.97	0.45
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.51	0.45
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.51	0.45
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.98	0.44
2:D:83:PHE:O	2:D:86:ILE:HG12	2.17	0.44
4:F:21:LEU:O	4:F:27:TRP:HB2	2.17	0.44
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.98	0.44
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.32	0.44
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.99	0.44
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.99	0.44
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.98	0.44
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.99	0.44
1:A:100:ALA:HA	2:B:254:LYS:HG3	2.00	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.52	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ARG:HH12	2:D:250:ALA:HB1	1.82	0.43
2:D:106:GLY:O	2:D:111:GLY:HA3	2.18	0.43
1:C:288:VAL:N	8:C:504:DMS:O	2.36	0.43
4:F:236:LYS:HB3	4:F:240:LEU:HD22	1.99	0.43
2:B:291:LEU:HD11	2:B:373:MET:HB3	2.00	0.43
4:F:5:VAL:HG12	4:F:30:LEU:HB2	2.00	0.43
2:D:46:LEU:HA	2:D:49:ILE:HB	2.01	0.43
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.54	0.43
4:F:151:SER:HB3	4:F:180:HIS:CG	2.54	0.43
1:A:209:ILE:HD13	1:A:231:ILE:HD11	2.01	0.43
2:B:158:ARG:NH1	2:B:196:GLU:O	2.51	0.43
2:D:11:GLN:NE2	14:D:607:HOH:O	2.51	0.42
4:F:234:GLN:O	4:F:236:LYS:NZ	2.33	0.42
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.55	0.42
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.42
4:F:188:LYS:HG2	4:F:323:GLU:CD	2.45	0.42
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.37	0.42
2:D:81:GLY:O	14:D:601:HOH:O	2.21	0.42
4:F:160:ILE:HB	4:F:236:LYS:HD3	2.02	0.42
1:A:3:GLU:O	1:A:133:GLN:HG2	2.19	0.42
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.41
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.41
4:F:17:VAL:HG23	4:F:351:VAL:HG22	2.02	0.41
4:F:148:ILE:HG13	4:F:162:ILE:HG12	2.02	0.41
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.86	0.41
4:F:1:MET:SD	4:F:28:LYS:HG3	2.61	0.41
1:A:88:HIS:ND1	1:A:90:GLU:OE1	2.53	0.41
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.02	0.41
4:F:160:ILE:O	4:F:160:ILE:HG13	2.21	0.41
2:B:216:THR:HG21	2:B:275:LEU:HD12	2.02	0.41
2:D:163:ASP:O	2:D:253:ARG:NH2	2.51	0.41
3:E:85:LYS:NZ	3:E:89:GLU:OE2	2.53	0.41
2:B:136:GLN:HA	2:B:167:ASN:O	2.21	0.41
2:D:83:PHE:HD2	2:D:86:ILE:HD13	1.85	0.41
1:A:174:ALA:O	1:A:178:SER:HB3	2.21	0.41
1:C:166:LYS:HE2	1:C:197:HIS:O	2.21	0.41
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.02	0.41
2:D:334:ASN:ND2	2:D:338:LYS:HE2	2.36	0.41
4:F:189:PRO:HG2	4:F:191:LEU:HD21	2.03	0.40
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:THR:O	2:B:243:ARG:HG3	2.21	0.40
4:F:138:ARG:HB3	4:F:145:ASN:ND2	2.36	0.40
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.57	0.40
1:A:105[B]:ARG:NE	1:A:411:GLU:OE2	2.54	0.40
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.92	0.40
4:F:225:SER:OG	4:F:252:ASN:O	2.39	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	437/451 (97%)	425 (97%)	12 (3%)	0	100	100
1	C	442/451 (98%)	434 (98%)	8 (2%)	0	100	100
2	B	421/445 (95%)	414 (98%)	7 (2%)	0	100	100
2	D	418/445 (94%)	408 (98%)	10 (2%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	338/384 (88%)	324 (96%)	13 (4%)	1 (0%)	36	50
All	All	2175/2319 (94%)	2123 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	160	ILE

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	372/379 (98%)	372 (100%)	0	100	100
1	C	375/379 (99%)	372 (99%)	3 (1%)	73	86
2	B	368/383 (96%)	367 (100%)	1 (0%)	86	93
2	D	364/383 (95%)	360 (99%)	4 (1%)	65	82
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	311/342 (91%)	307 (99%)	4 (1%)	61	80
All	All	1900/1993 (95%)	1888 (99%)	12 (1%)	78	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	282	GLN
1	C	71	GLU
1	C	218	ASP
1	C	381	THR
2	D	177	VAL
2	D	220	THR
2	D	341	SER
2	D	396	THR
4	F	9	GLU
4	F	89	GLU
4	F	257	GLU
4	F	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	101	ASN
1	A	216	ASN
1	A	309	HIS
2	B	282	GLN
2	B	336	GLN
2	B	436	GLN
1	C	283	HIS
1	C	356	ASN

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Mol	Chain	Res	Type
1	C	380	ASN
2	D	85	GLN
2	D	334	ASN
3	E	108	ASN
3	E	136	ASN
4	F	45	ASN
4	F	196	HIS
4	F	333	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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
8	DMS	C	506	-	3,3,3	0.67	0	3,3,3	0.47	0
5	GTP	C	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.50	10 (20%)
10	MES	B	503	-	12,12,12	2.30	1 (8%)	15,16,16	1.94	4 (26%)
9	GDP	B	501	6	29,30,30	1.21	4 (13%)	45,47,47	1.68	6 (13%)
9	GDP	D	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.70	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	DMS	C	504	-	3,3,3	0.67	0	3,3,3	0.61	0
13	ACP	F	401	6	31,33,33	1.55	7 (22%)	47,52,52	1.96	11 (23%)
11	PEG	C	507	-	6,6,6	0.42	0	5,5,5	0.49	0
5	GTP	A	501	6	33,34,34	1.03	4 (12%)	50,54,54	1.53	9 (18%)
8	DMS	C	505	-	3,3,3	0.66	0	3,3,3	0.51	0
8	DMS	B	504	-	3,3,3	0.67	0	3,3,3	0.53	0
12	DKE	D	503	-	87,89,89	1.27	9 (10%)	113,131,131	1.46	14 (12%)
8	DMS	A	504	-	3,3,3	0.68	0	3,3,3	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
9	GDP	D	501	6	-	4/16/32/32	0/3/3/3
13	ACP	F	401	6	-	9/19/38/38	0/3/3/3
11	PEG	C	507	-	-	3/4/4/4	-
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
12	DKE	D	503	-	-	16/74/123/123	0/7/9/9
10	MES	B	503	-	-	4/6/14/14	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.70	1.66	1.77
12	D	503	DKE	O40-C29	-4.71	1.39	1.45
12	D	503	DKE	O81-C80	4.58	1.35	1.22
12	D	503	DKE	C31-N30	3.50	1.42	1.35
13	F	401	ACP	C5-N7	-3.36	1.33	1.39
13	F	401	ACP	C5-C4	3.14	1.44	1.39
9	D	501	GDP	C5-C4	3.09	1.47	1.38
9	B	501	GDP	C5-C4	3.04	1.47	1.38
13	F	401	ACP	C4-N9	-2.87	1.31	1.37
12	D	503	DKE	C48-N49	2.84	1.39	1.34
13	F	401	ACP	PG-O3G	2.76	1.61	1.55
13	F	401	ACP	C8-N9	-2.71	1.32	1.37
9	B	501	GDP	C6-N1	-2.45	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	PA-O3A	2.43	1.62	1.59
9	D	501	GDP	C6-N1	-2.34	1.34	1.38
5	A	501	GTP	PB-O3B	2.31	1.62	1.59
12	D	503	DKE	C56-N55	2.31	1.38	1.33
13	F	401	ACP	PG-O2G	2.30	1.60	1.55
12	D	503	DKE	C73-C69	2.29	1.45	1.40
5	A	501	GTP	PA-O3A	2.29	1.62	1.59
12	D	503	DKE	O82-C80	-2.15	1.24	1.30
12	D	503	DKE	C6-N5	2.15	1.39	1.34
5	A	501	GTP	PB-O3A	2.12	1.61	1.59
5	A	501	GTP	C2-N3	2.12	1.38	1.33
5	C	501	GTP	C2-N3	2.11	1.38	1.33
12	D	503	DKE	O1-C2	-2.03	1.43	1.46
9	B	501	GDP	C5-N7	-2.01	1.35	1.39
13	F	401	ACP	PG-O1G	-2.01	1.46	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	401	ACP	C5-C4-N3	-5.84	118.67	126.72
9	D	501	GDP	C5-C4-N3	-5.75	119.24	128.39
9	B	501	GDP	C5-C4-N3	-5.63	119.43	128.39
13	F	401	ACP	N3-C4-N9	5.11	135.86	127.17
9	D	501	GDP	C2-N3-C4	4.94	120.81	112.30
9	B	501	GDP	C2-N3-C4	4.92	120.78	112.30
10	B	503	MES	C5-N4-C3	4.92	119.43	108.84
5	C	501	GTP	C5-C4-N3	-4.59	121.09	128.39
5	A	501	GTP	C2-N3-C4	4.52	120.09	112.30
5	A	501	GTP	C5-C4-N3	-4.51	121.22	128.39
5	C	501	GTP	C2-N3-C4	4.39	119.87	112.30
12	D	503	DKE	O40-C38-C29	-4.38	56.61	59.38
12	D	503	DKE	O40-C29-C7	4.31	122.58	117.41
12	D	503	DKE	O82-C80-C61	4.31	127.54	115.28
9	B	501	GDP	N9-C4-N3	4.18	134.30	125.95
9	D	501	GDP	N9-C4-N3	4.15	134.24	125.95
12	D	503	DKE	O36-C35-C38	3.95	114.39	105.48
13	F	401	ACP	C4-N9-C8	3.90	109.84	105.74
13	F	401	ACP	C2-N3-C4	3.88	121.31	111.83
13	F	401	ACP	N3-C2-N1	-3.80	122.83	128.58
12	D	503	DKE	O36-C35-C33	3.63	112.10	105.09
13	F	401	ACP	PB-O3A-PA	-3.62	120.55	132.37
9	D	501	GDP	C6-C5-N7	3.57	136.78	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C6-C5-N7	3.53	136.72	130.29
12	D	503	DKE	C38-O40-C29	3.41	62.74	60.81
12	D	503	DKE	O82-C80-O81	-3.34	116.18	123.35
12	D	503	DKE	C2-C7-C29	3.28	119.61	111.19
5	C	501	GTP	N9-C4-N3	2.94	131.84	125.95
13	F	401	ACP	C4-C5-N7	-2.85	107.33	110.58
5	A	501	GTP	N9-C4-N3	2.82	131.58	125.95
13	F	401	ACP	N9-C8-N7	-2.79	109.98	113.94
5	A	501	GTP	C2-N1-C6	-2.78	120.06	125.11
5	C	501	GTP	C2-N1-C6	-2.73	120.16	125.11
5	A	501	GTP	N9-C8-N7	-2.70	108.39	113.40
5	C	501	GTP	N9-C8-N7	-2.66	108.46	113.40
12	D	503	DKE	C52-N49-N50	2.66	126.11	120.78
9	D	501	GDP	C4-C5-N7	-2.63	106.50	110.67
12	D	503	DKE	C61-C62-C64	2.63	127.11	123.42
13	F	401	ACP	O2G-PG-C3B	2.62	112.76	106.40
5	A	501	GTP	C5-C6-N1	2.57	119.79	113.25
13	F	401	ACP	C5-N7-C8	2.50	107.39	103.45
5	C	501	GTP	C5-C6-N1	2.49	119.60	113.25
5	C	501	GTP	C8-N7-C5	2.49	108.70	104.26
5	A	501	GTP	C8-N7-C5	2.45	108.63	104.26
9	B	501	GDP	C4-C5-N7	-2.43	106.81	110.67
12	D	503	DKE	O81-C80-C61	-2.38	116.28	121.97
12	D	503	DKE	C52-N49-C48	-2.38	124.39	128.83
12	D	503	DKE	O25-C23-C22	2.32	117.99	115.44
5	A	501	GTP	O2A-PA-O3A	2.31	113.50	107.27
10	B	503	MES	O1S-S-C8	2.29	110.18	106.73
5	C	501	GTP	O2B-PB-O3A	2.20	113.23	107.27
12	D	503	DKE	C46-C47-C48	-2.20	126.01	130.26
5	C	501	GTP	O6-C6-C5	-2.14	120.88	126.53
5	A	501	GTP	O6-C6-C5	-2.14	120.89	126.53
9	B	501	GDP	O6-C6-C5	-2.08	121.03	126.53
5	C	501	GTP	O2A-PA-O3A	2.08	112.90	107.27
10	B	503	MES	C7-N4-C5	2.05	116.71	111.24
9	D	501	GDP	O6-C6-C5	-2.04	121.14	126.53
13	F	401	ACP	C3'-C2'-C1'	2.03	105.31	101.46
10	B	503	MES	C7-N4-C3	2.01	116.61	111.24

There are no chirality outliers.

All (54) 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	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
12	D	503	DKE	C4-C8-O9-C11
12	D	503	DKE	C22-C23-O25-C26
12	D	503	DKE	C44-C45-C46-C47
12	D	503	DKE	C58-C56-N55-C54
12	D	503	DKE	O57-C56-N55-C54
12	D	503	DKE	C62-C64-C65-C74
12	D	503	DKE	C69-C64-C65-C74
13	F	401	ACP	PB-C3B-PG-O1G
13	F	401	ACP	PB-C3B-PG-O2G
13	F	401	ACP	PB-C3B-PG-O3G
13	F	401	ACP	PG-C3B-PB-O1B
13	F	401	ACP	PG-C3B-PB-O3A
13	F	401	ACP	C5'-O5'-PA-O1A
13	F	401	ACP	C5'-O5'-PA-O3A
12	D	503	DKE	C24-C23-O25-C26
12	D	503	DKE	C41-C43-C44-C45
12	D	503	DKE	C10-C8-O9-C11
12	D	503	DKE	N49-C52-C53-C54
12	D	503	DKE	C43-C44-C45-C46
10	B	503	MES	C7-C8-S-O3S
12	D	503	DKE	C45-C46-C47-N51
10	B	503	MES	C8-C7-N4-C5
12	D	503	DKE	C45-C46-C47-C48
5	C	501	GTP	PB-O3B-PG-O3G
11	C	507	PEG	C1-C2-O2-C3
11	C	507	PEG	O2-C3-C4-O4
12	D	503	DKE	C3-C2-C7-C28
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O2A
13	F	401	ACP	PG-C3B-PB-O2B

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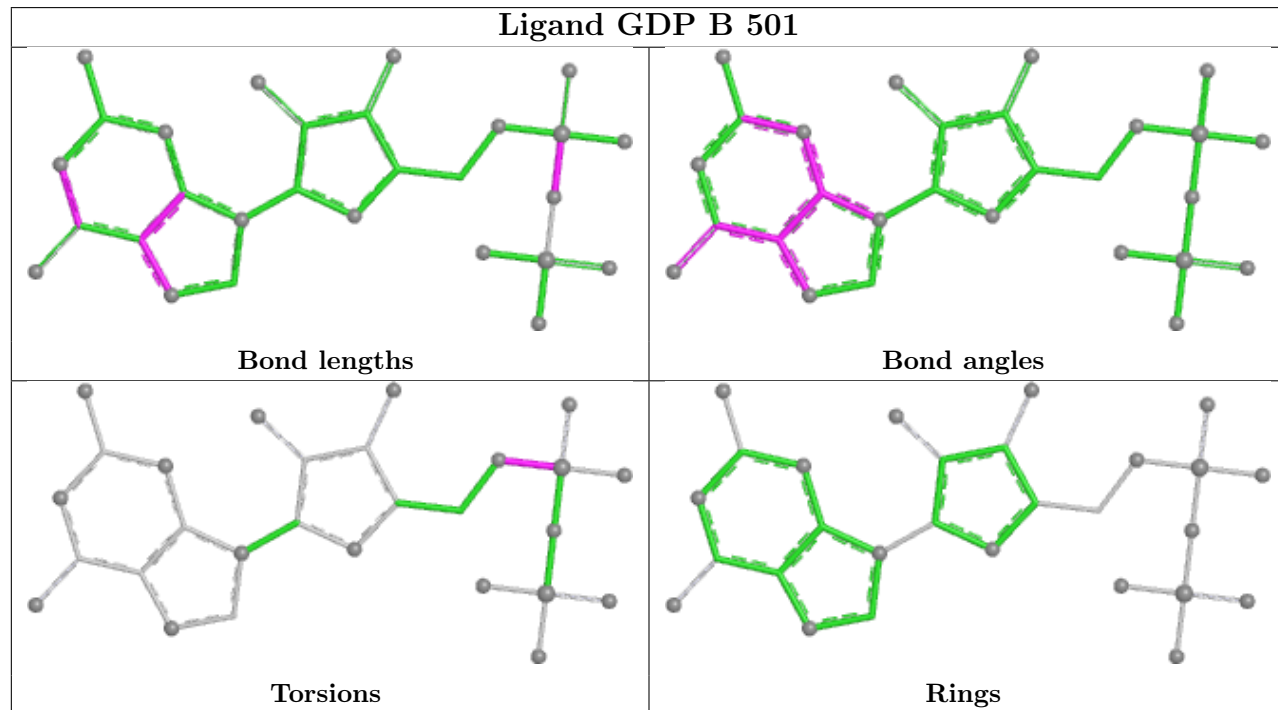
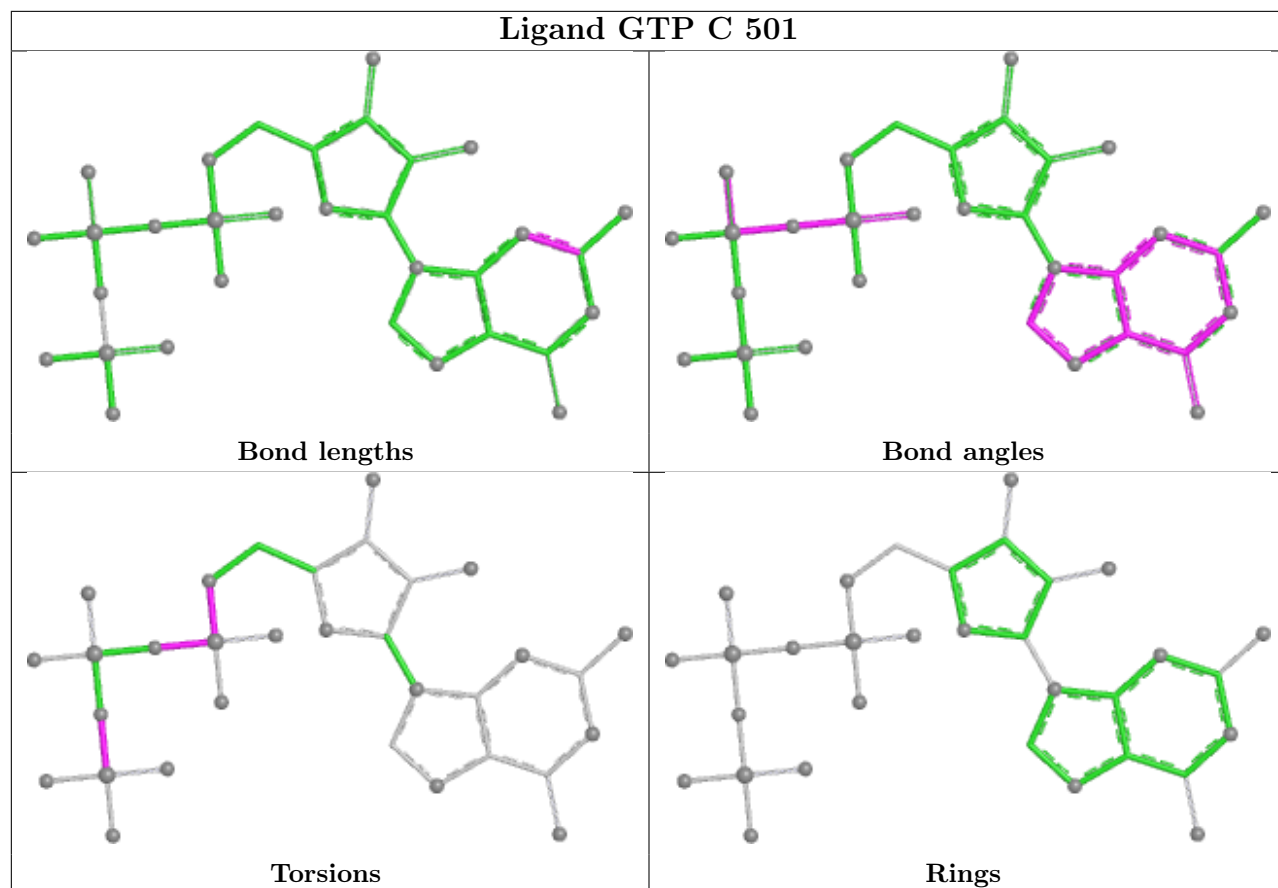
Mol	Chain	Res	Type	Atoms
13	F	401	ACP	C5'-O5'-PA-O2A
11	C	507	PEG	C4-C3-O2-C2
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
9	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3A-PA-O1A
12	D	503	DKE	O36-C41-C43-C44

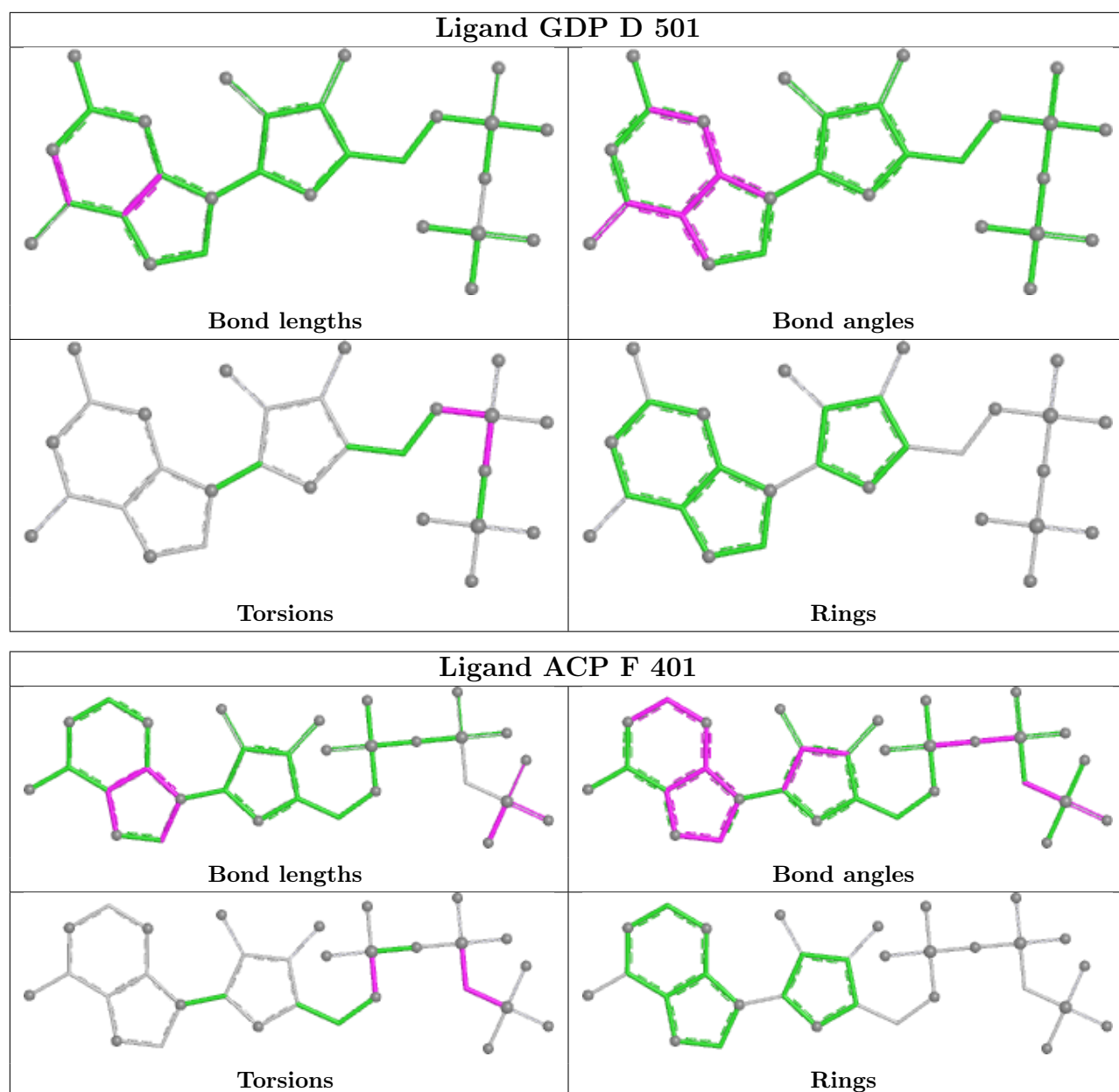
There are no ring outliers.

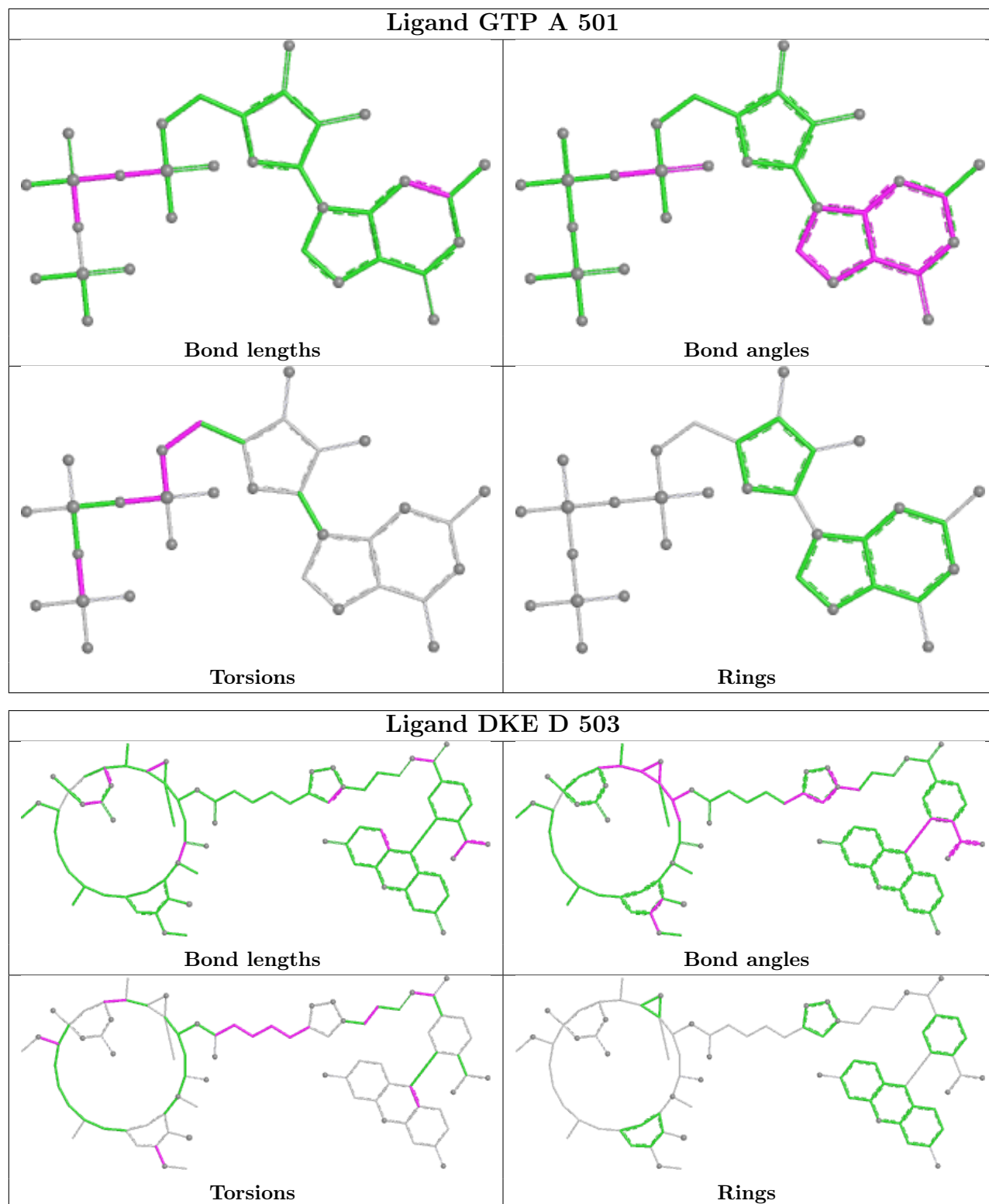
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
10	B	503	MES	1	0
8	C	504	DMS	1	0
11	C	507	PEG	1	0
12	D	503	DKE	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	440/451 (97%)	0.03	13 (2%)	52	48	26, 55, 94, 123	1 (0%)
1	C	440/451 (97%)	-0.29	4 (0%)	81	78	22, 43, 72, 105	4 (0%)
2	B	423/445 (95%)	0.03	13 (3%)	51	47	24, 52, 88, 140	4 (0%)
2	D	422/445 (94%)	0.14	8 (1%)	66	62	36, 60, 94, 131	6 (1%)
3	E	123/143 (86%)	0.43	6 (4%)	35	31	45, 68, 105, 129	0
4	F	345/384 (89%)	0.63	29 (8%)	17	14	31, 81, 145, 181	1 (0%)
All	All	2193/2319 (94%)	0.10	73 (3%)	49	45	22, 57, 109, 181	16 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	160	ILE	5.0
4	F	371	PRO	4.4
2	B	438	ALA	4.3
2	D	285	ALA	4.2
4	F	157	GLY	4.2
1	C	440	VAL	3.8
2	B	57	THR	3.6
2	D	1	MET	3.6
4	F	181	VAL	3.6
4	F	152	SER	3.5
4	F	125	THR	3.5
4	F	159	GLY	3.4
4	F	362	ALA	3.4
1	A	179	THR	3.3
3	E	143	ALA	3.3
1	C	340	SER	3.2
2	D	57	THR	3.0
4	F	141	GLY	3.0
4	F	102	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	325	MET	2.9
1	A	282	TYR	2.9
4	F	161	LEU	2.9
2	D	220	THR	2.8
1	A	437	VAL	2.8
1	C	357	TYR	2.8
4	F	22	LEU	2.7
2	B	2	ARG	2.7
2	B	284	ARG	2.7
2	D	286	LEU	2.7
4	F	249	TYR	2.6
4	F	91	CYS	2.6
4	F	131	PHE	2.5
3	E	26	PRO	2.5
3	E	44	ASP	2.5
1	A	96	LYS	2.5
4	F	179	VAL	2.4
2	D	86	ILE	2.4
2	B	248	LEU	2.4
2	B	85	GLN	2.4
2	B	282	GLN	2.4
4	F	101	TYR	2.3
4	F	149	ALA	2.3
1	A	346	TRP	2.3
1	A	85	GLN	2.3
4	F	90	SER	2.3
1	A	88	HIS	2.2
4	F	163	SER	2.2
1	A	46	ASP	2.2
4	F	134	ALA	2.2
2	B	247	GLN	2.2
4	F	233	PHE	2.2
3	E	15	THR	2.2
4	F	140	GLU	2.2
2	B	272	PHE	2.2
1	A	438	ASP	2.1
4	F	164	SER	2.1
1	C	1	MET	2.1
4	F	379	HIS	2.1
3	E	27	PRO	2.1
4	F	172	PHE	2.1
1	A	285	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	56	ALA	2.1
4	F	372	THR	2.1
2	B	285	ALA	2.1
4	F	182	ILE	2.1
1	A	262	TYR	2.1
4	F	100	ILE	2.0
2	D	128	SER	2.0
1	A	283	HIS	2.0
2	D	440	ALA	2.0
1	A	164	LYS	2.0
2	B	277	SER	2.0
3	E	28	SER	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.

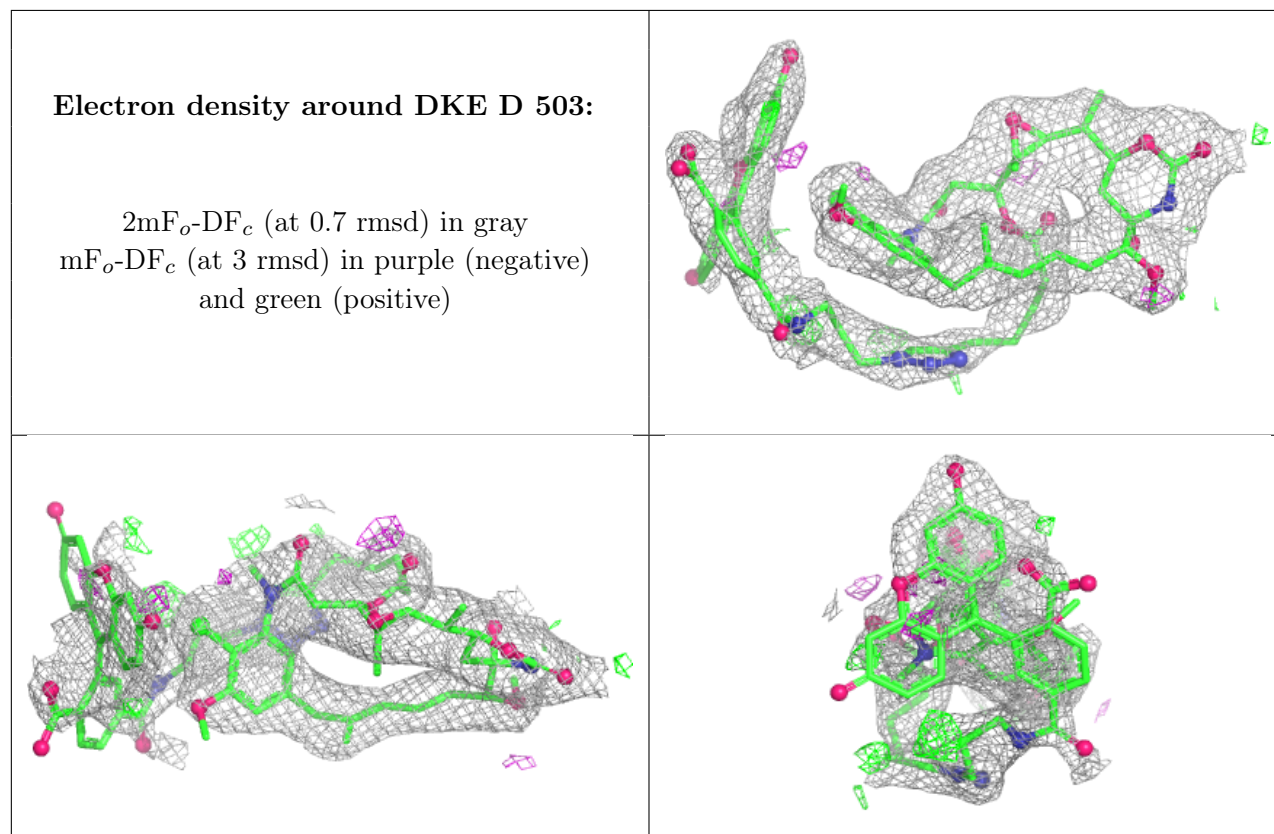
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	DMS	B	504	4/4	0.78	0.22	102,108,113,117	0
8	DMS	A	504	4/4	0.81	0.21	83,89,91,92	0
12	DKE	D	503	81/81	0.82	0.16	49,93,134,137	0
8	DMS	C	504	4/4	0.85	0.20	66,83,89,92	0
13	ACP	F	401	31/31	0.86	0.12	83,89,121,129	0
6	MG	F	402	1/1	0.87	0.12	97,97,97,97	0
11	PEG	C	507	7/7	0.87	0.22	76,78,81,81	0
8	DMS	C	505	4/4	0.89	0.25	86,95,96,97	0
10	MES	B	503	12/12	0.90	0.16	68,84,99,107	0
8	DMS	C	506	4/4	0.93	0.17	70,81,83,84	0
9	GDP	D	501	28/28	0.93	0.09	42,55,70,82	0

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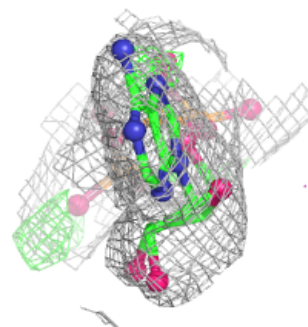
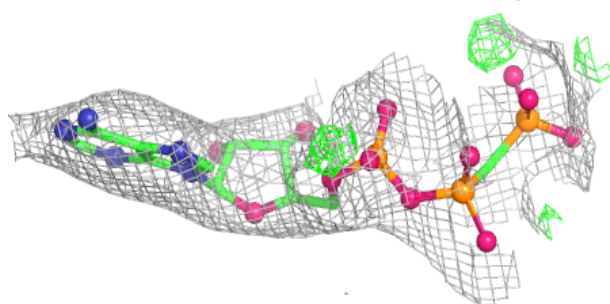
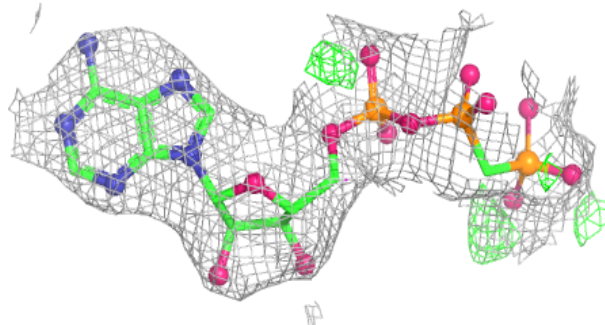
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	502	1/1	0.95	0.08	52,52,52,52	0
7	CA	A	503	1/1	0.95	0.07	96,96,96,96	0
7	CA	C	503	1/1	0.97	0.04	65,65,65,65	0
5	GTP	C	501	32/32	0.98	0.05	24,33,41,47	0
6	MG	B	502	1/1	0.98	0.07	34,34,34,34	0
9	GDP	B	501	28/28	0.98	0.06	27,36,44,45	0
5	GTP	A	501	32/32	0.98	0.05	31,38,46,49	0
6	MG	A	502	1/1	0.99	0.03	39,39,39,39	0
6	MG	C	502	1/1	1.00	0.01	30,30,30,30	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.



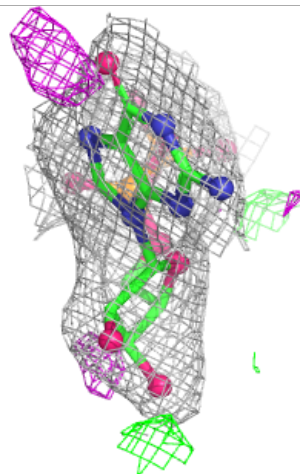
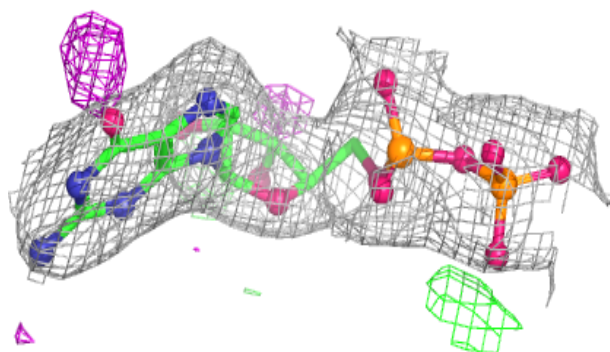
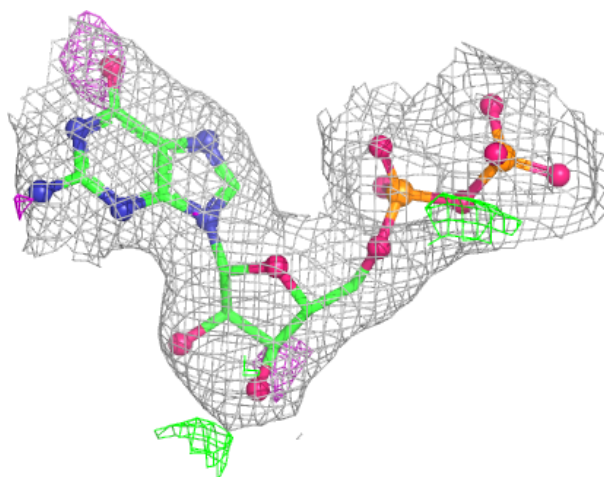
Electron density around ACP F 401:

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



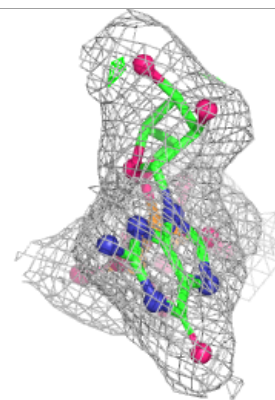
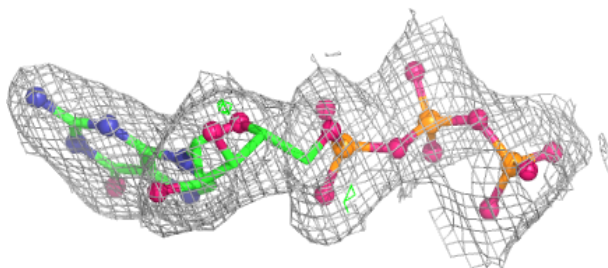
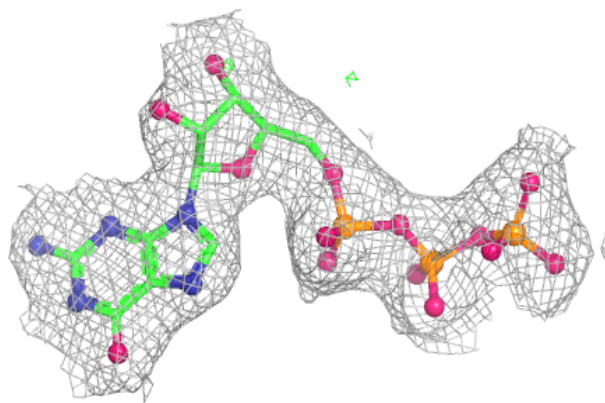
Electron density around GDP D 501:

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



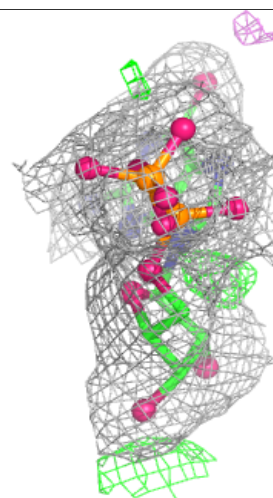
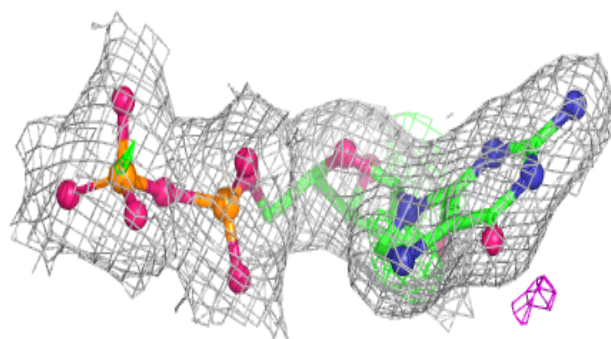
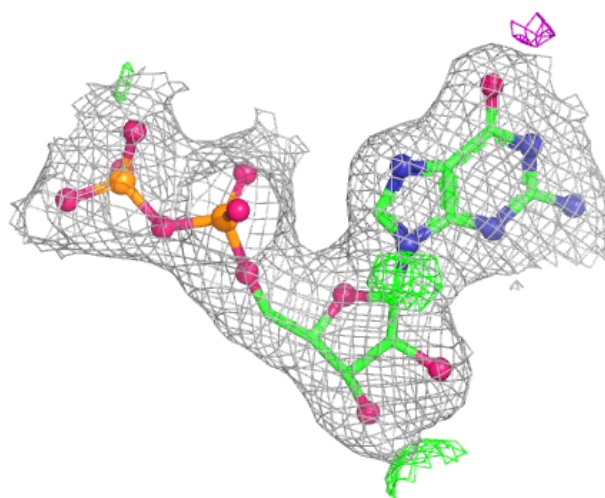
Electron density around GTP C 501:

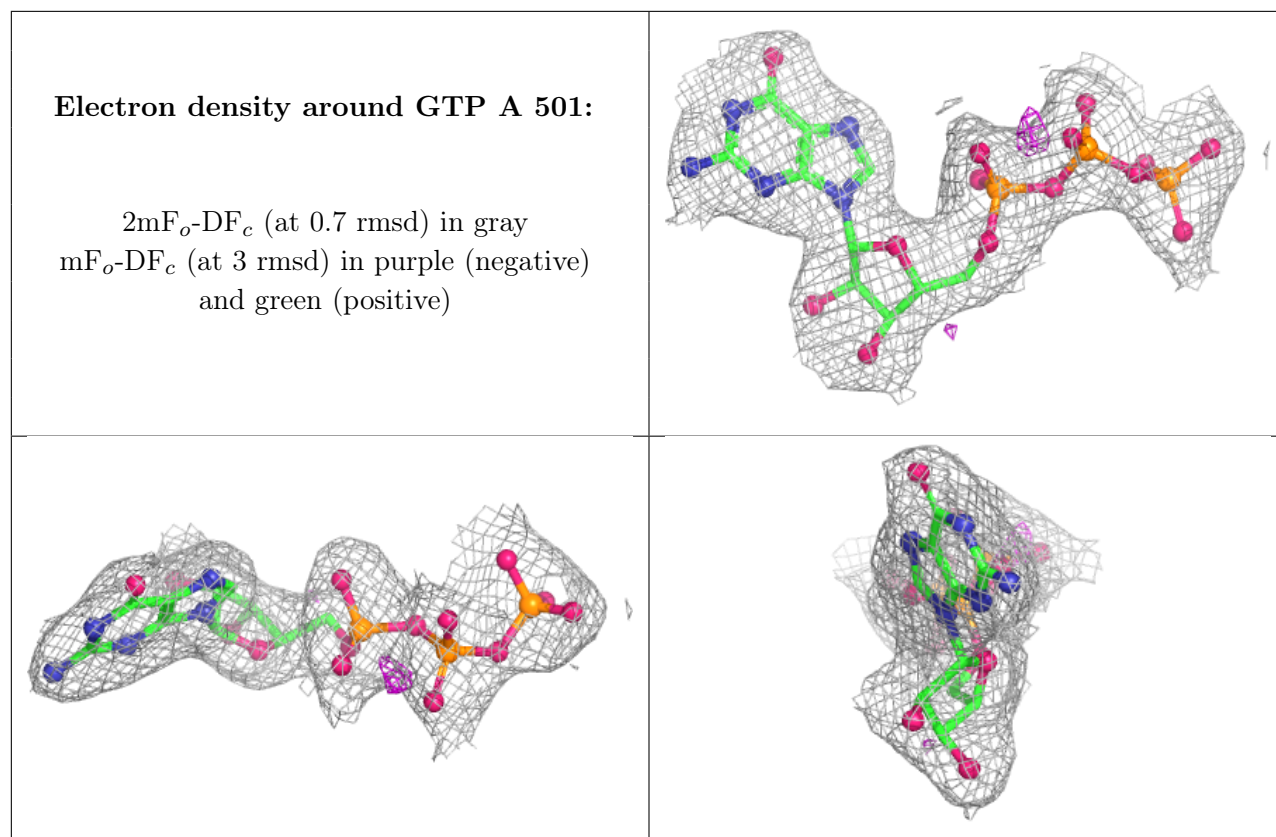
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.