



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:27 PM UTC

PDB ID : 8BDE / pdb_00008bde
Title : Tubulin-baccatin III complex
Authors : Prota, A.E.; Lucena-Agell, D.; Ma, Y.; Estevez-Gallego, J.; Li, S.; Bargsten, K.; Altmann, K.H.; Gaillard, N.; Kamimura, S.; Muehlethaler, T.; Gago, F.; Oliva, M.A.; Steinmetz, M.O.; Fang, W.S.; Diaz, J.F.
Deposited on : 2022-10-19
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

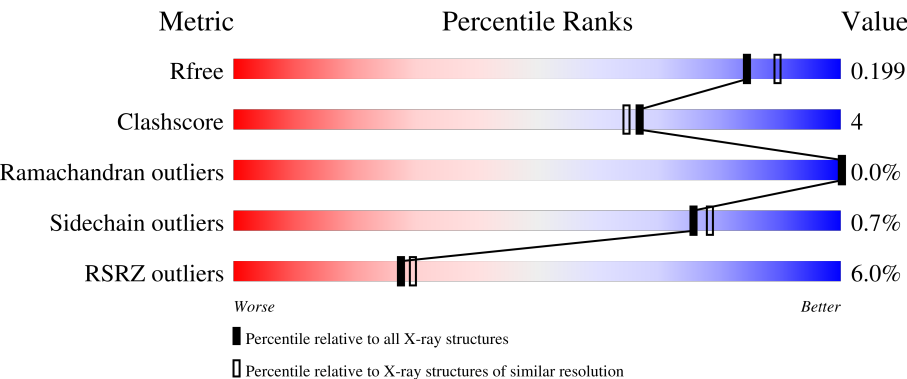
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	3% 88% 8% .
1	C	451	2% 91% 6% .
2	B	445	7% 85% 10% .
2	D	445	5% 84% 11% 5%

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Mol	Chain	Length	Quality of chain
3	E	143	6% 76% 8% 15%
4	F	384	12% 77% 10% 13%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18429 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	434	Total	C	N	O	S	0	6	0
			3412	2165	576	647	24			
1	C	440	Total	C	N	O	S	0	10	0
			3484	2208	586	665	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	5	0
			3385	2125	582	651	27			
2	D	424	Total	C	N	O	S	0	2	0
			3340	2098	568	646	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	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 beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2737	1760	466	497	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: $C_{10}H_{16}N_5O_{14}P_3$).



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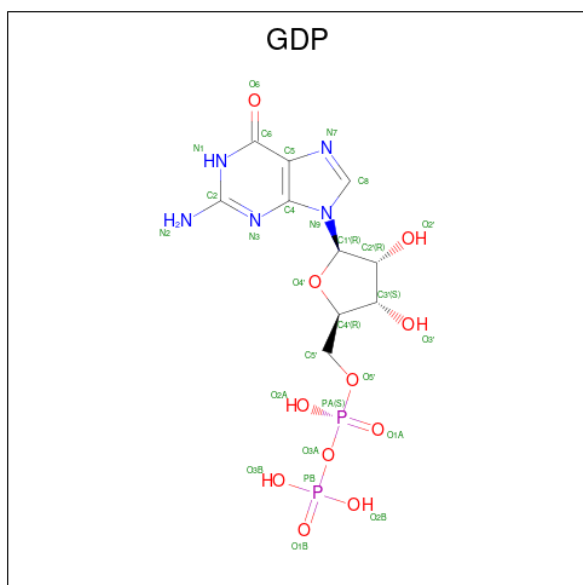
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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



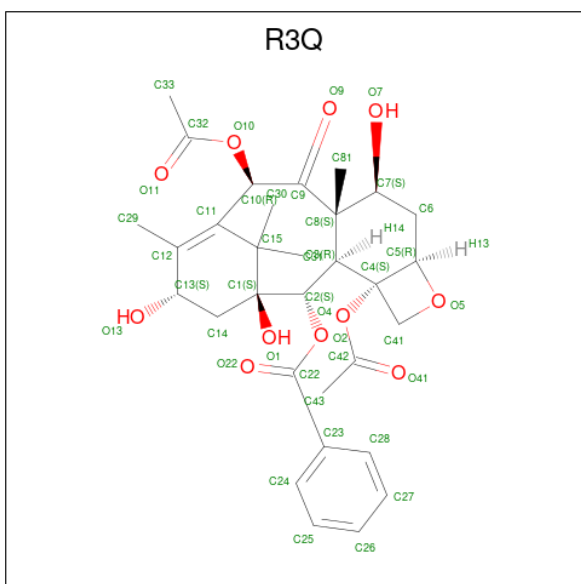
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



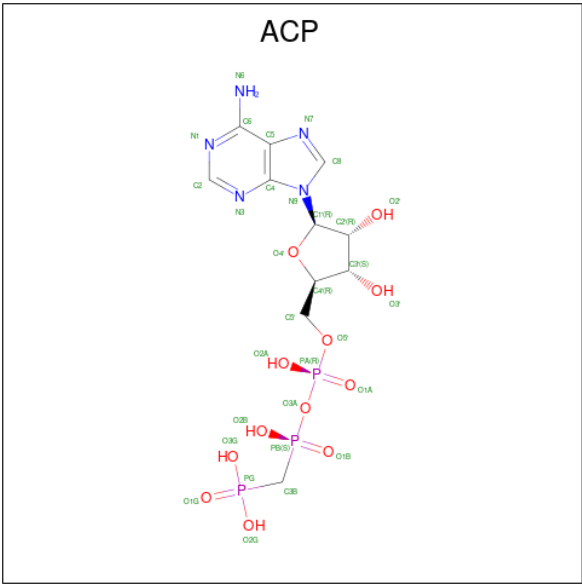
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is [(1 {S},2 {S},3 {R},4 {S},7 {R},9 {S},10 {S},12 {R},15 {S})-4,12-diacetyloxy-10,14,16,16-tetramethyl-1,9,15-tris(oxidanyl)-11-oxidanylidene-6-oxatetracyclo[11.3.1.0^{3,10}.0^{4,7}]heptadec-13-en-2-yl] benzoate (CCD ID: R3Q) (formula: C₃₁H₃₈O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			42	31	11		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

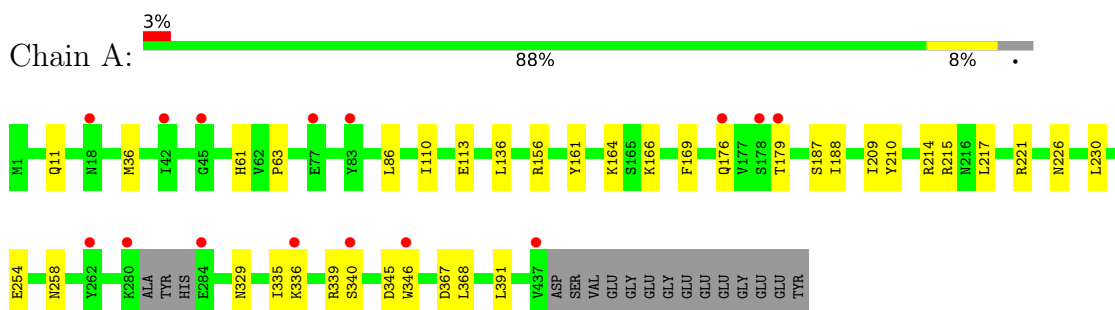
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	181	Total	O	0	0
			181	181		
12	B	153	Total	O	0	0
			153	153		
12	C	300	Total	O	0	0
			300	300		
12	D	121	Total	O	0	0
			121	121		
12	E	47	Total	O	0	0
			47	47		
12	F	57	Total	O	0	0
			57	57		

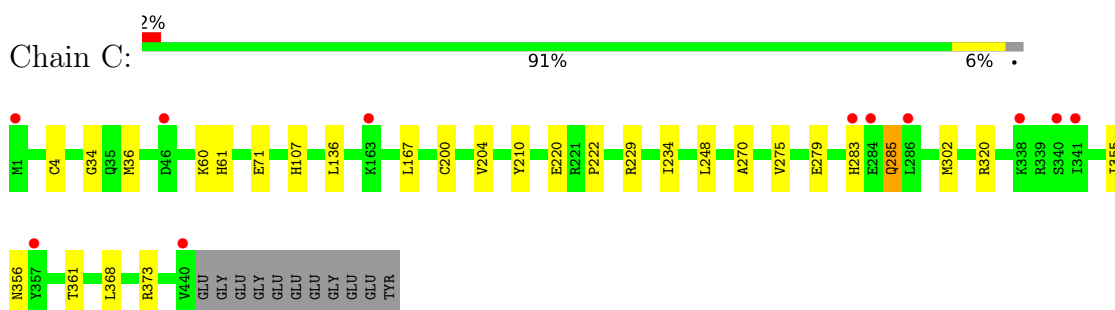
3 Residue-property plots [i](#)

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.

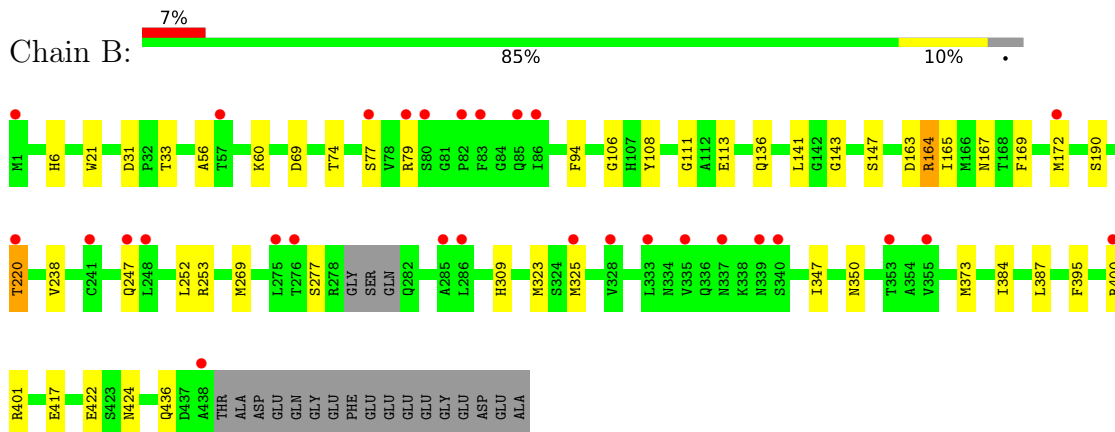
- Molecule 1: Tubulin alpha-1B chain



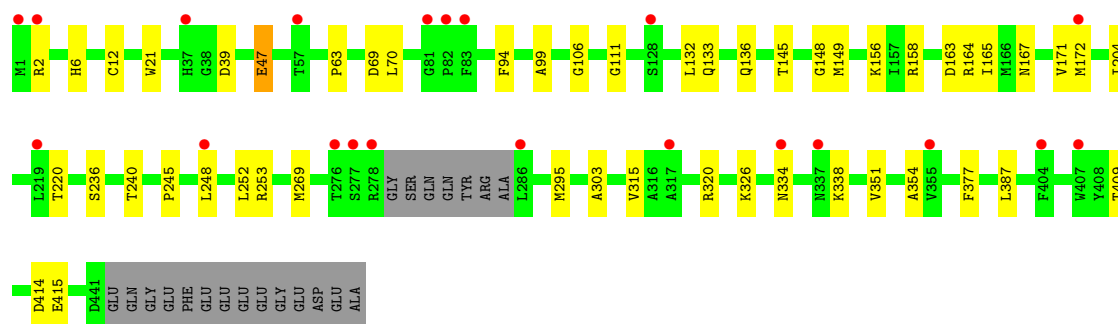
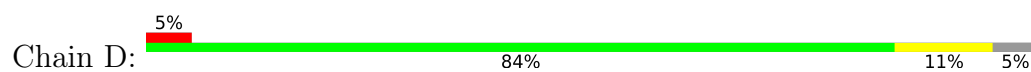
- Molecule 1: Tubulin alpha-1B chain



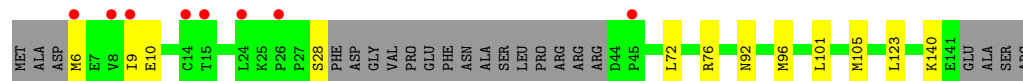
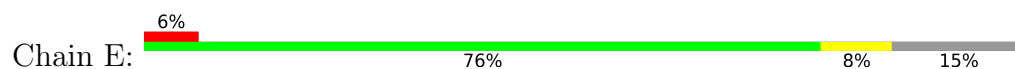
- Molecule 2: Tubulin beta-2B chain



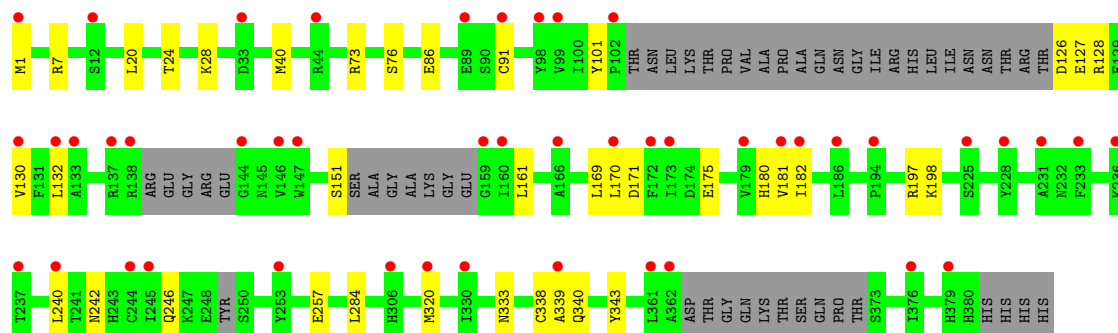
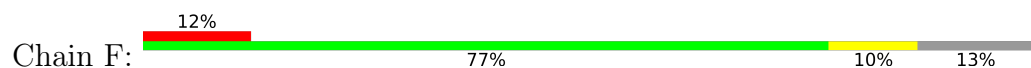
- Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.10Å 157.15Å 179.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 1.90 49.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.20-1.90) 99.9 (49.20-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.192 , 0.218 0.196 , 0.199	Depositor DCC
R_{free} test set	11325 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18429	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: GTP, R3Q, CA, MES, MG, GDP, ACP

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	0/3505	0.37	0/4757
1	C	0.18	0/3586	0.40	0/4871
2	B	0.42	0/3465	0.50	0/4690
2	D	0.14	0/3419	0.33	0/4631
3	E	0.13	0/1008	0.29	0/1337
4	F	0.12	0/2798	0.33	0/3777
All	All	0.23	0/17781	0.39	0/24063

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	163	ASP	Mainchain
2	B	164[A]	ARG	Mainchain
2	B	164[B]	ARG	Mainchain
2	B	253[A]	ARG	Mainchain
2	B	253[B]	ARG	Mainchain

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	3412	0	3354	24	0
1	C	3484	0	3413	18	1
2	B	3385	0	3273	27	1
2	D	3340	0	3226	35	0
3	E	1000	0	1018	12	0
4	F	2737	0	2709	21	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
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	12	0	13	0	0
10	D	42	0	0	0	0
11	F	31	0	14	2	0
12	A	181	0	0	5	0
12	B	153	0	0	3	0
12	C	300	0	0	3	0
12	D	121	0	0	7	0
12	E	47	0	0	0	0
12	F	57	0	0	0	0
All	All	18429	0	17068	127	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (127) 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:B:79:ARG:NH1	12:B:601:HOH:O	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ARG:NH1	12:D:601:HOH:O	2.11	0.84
1:C:270:ALA:HB3	1:C:302[B]:MET:HE2	1.64	0.81
2:D:149:MET:N	12:D:602:HOH:O	2.12	0.79
2:B:220:THR:O	12:B:602:HOH:O	2.07	0.71
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.72	0.71
12:C:808:HOH:O	3:E:105:MET:SD	2.48	0.70
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.77	0.65
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.77	0.65
2:D:145:THR:O	12:D:602:HOH:O	2.13	0.65
1:A:156:ARG:NH2	12:A:601:HOH:O	2.17	0.65
2:D:148:GLY:N	12:D:602:HOH:O	2.29	0.64
1:A:156:ARG:NE	12:A:601:HOH:O	2.22	0.64
1:C:279:GLU:O	12:C:601:HOH:O	2.15	0.64
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.30	0.64
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.81	0.62
2:D:240[A]:THR:HG21	2:D:320:ARG:HD2	1.82	0.61
1:C:220:GLU:HB3	2:D:326:LYS:HD3	1.83	0.61
1:C:107:HIS:HE1	3:E:105:MET:HE1	1.66	0.60
3:E:101:LEU:HD12	3:E:105:MET:HE3	1.83	0.60
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.83	0.59
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.84	0.59
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.42	0.59
1:C:107:HIS:CE1	3:E:105:MET:HE1	2.37	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.84	0.58
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.22	0.57
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.22	0.57
2:D:409:THR:O	3:E:140:LYS:NZ	2.33	0.57
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.47	0.56
2:B:164[B]:ARG:HA	2:B:164[B]:ARG:HE	1.67	0.56
2:D:164:ARG:NH1	12:D:609:HOH:O	2.39	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.08	0.54
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.90	0.54
1:A:11:GLN:OE1	2:B:247:GLN:NE2	2.37	0.53
3:E:9:ILE:HG13	3:E:10:GLU:HG2	1.89	0.52
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.91	0.52
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.91	0.52
4:F:127:GLU:HB2	4:F:130:VAL:HG12	1.92	0.52
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.93	0.51
4:F:161:LEU:HD23	4:F:169:LEU:HD23	1.92	0.51
1:A:329:ASN:HB3	3:E:6:MET:HE1	1.93	0.51
4:F:242:ASN:ND2	11:F:402:ACP:H3B1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:198:LYS:HG2	4:F:320:MET:HE1	1.93	0.50
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.93	0.50
2:B:424:ASN:HB3	12:B:615:HOH:O	2.12	0.50
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.45	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.12	0.49
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.24	0.49
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.94	0.49
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.77	0.49
1:A:179:THR:HG21	2:B:247:GLN:HG3	1.95	0.49
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.48	0.49
2:D:236:SER:O	2:D:240[A]:THR:HG23	2.13	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.48
2:D:136:GLN:HA	2:D:167:ASN:O	2.13	0.48
4:F:338:CYS:SG	4:F:339:ALA:N	2.86	0.48
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.95	0.48
2:D:2:ARG:NH1	12:D:607:HOH:O	2.36	0.47
4:F:101:TYR:N	4:F:126:ASP:OD2	2.43	0.47
2:D:145:THR:C	12:D:602:HOH:O	2.57	0.47
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.50	0.47
4:F:128:ARG:HD3	4:F:170:LEU:HD13	1.97	0.47
4:F:86:GLU:OE1	4:F:86:GLU:N	2.43	0.47
2:D:132:LEU:O	2:D:164:ARG:NH1	2.49	0.46
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.98	0.46
1:A:136[B]:LEU:HD23	1:A:169:PHE:HE2	1.81	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.45
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.32	0.45
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.96	0.45
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.45
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.99	0.44
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.44
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.57	0.44
2:D:163:ASP:O	2:D:253:ARG:NH2	2.51	0.44
2:D:106:GLY:O	2:D:111:GLY:HA3	2.18	0.44
4:F:171:ASP:O	4:F:175:GLU:HG3	2.18	0.44
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.00	0.44
1:A:346:TRP:CD1	1:A:346:TRP:H	2.35	0.43
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.00	0.43
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.53	0.43
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.99	0.43
1:A:166:LYS:NZ	12:A:620:HOH:O	2.51	0.43
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.43
4:F:7:ARG:CD	4:F:40:MET:HE3	2.47	0.43
2:B:74:THR:O	2:B:77:SER:HB3	2.19	0.43
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.80	0.43
2:D:334:ASN:OD1	2:D:338:LYS:HD2	2.19	0.43
1:A:36:MET:HB3	1:A:61:HIS:NE2	2.34	0.43
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.84	0.42
2:D:414:ASP:OD1	2:D:415:GLU:N	2.52	0.42
4:F:73:ARG:HB2	4:F:76:SER:OG	2.19	0.42
1:A:345:ASP:HB3	3:E:28:SER:HB2	2.00	0.42
2:B:269:MET:HG2	2:B:384:ILE:HD13	2.01	0.42
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.00	0.42
1:A:110:ILE:O	1:A:113:GLU:HG2	2.19	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.20	0.42
1:A:156:ARG:CZ	12:A:601:HOH:O	2.54	0.42
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.35	0.42
2:D:39:ASP:N	2:D:39:ASP:OD1	2.53	0.42
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.52	0.42
1:C:285:GLN:HG3	1:C:373:ARG:HH12	1.85	0.42
2:D:2:ARG:HB3	2:D:133:GLN:HG3	2.02	0.42
2:D:69:ASP:O	2:D:94:PHE:HA	2.20	0.42
3:E:101:LEU:CD1	3:E:105:MET:HE3	2.48	0.42
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.42
2:D:334:ASN:HD21	2:D:338:LYS:NZ	2.17	0.41
4:F:333:ASN:ND2	11:F:402:ACP:O3G	2.48	0.41
1:C:204:VAL:HG22	1:C:302[B]:MET:SD	2.61	0.41
2:B:141:LEU:HD12	2:B:172:MET:SD	2.60	0.41
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.02	0.41
1:C:34:GLY:HA3	1:C:60:LYS:HG3	2.01	0.41
1:A:63:PRO:HD3	1:A:86:LEU:HG	2.02	0.41
2:B:309:HIS:O	2:B:436:GLN:NE2	2.54	0.41
2:D:156:LYS:HA	2:D:156:LYS:HD2	1.83	0.41
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.36	0.41
1:A:176:GLN:HG2	12:A:742:HOH:O	2.21	0.41
1:A:221:ARG:HG3	2:B:325:MET:HB3	2.02	0.41
2:B:323:MET:HE2	2:B:373:MET:HG2	2.03	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
3:E:92:ASN:O	3:E:96:MET:HG2	2.21	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.21	0.41
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.56	0.41
1:C:229:ARG:NH2	12:C:618:HOH:O	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ALA:O	1:C:302[A]:MET:HG2	2.21	0.40
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.02	0.40
4:F:240:LEU:O	4:F:246:GLN:NE2	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLU:OE2	1:C:283:HIS:NE2[4_555]	2.13	0.07

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	436/451 (97%)	431 (99%)	5 (1%)	0	100	100
1	C	448/451 (99%)	438 (98%)	10 (2%)	0	100	100
2	B	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
2	D	422/445 (95%)	417 (99%)	5 (1%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	322/384 (84%)	308 (96%)	13 (4%)	1 (0%)	36	29
All	All	2171/2319 (94%)	2132 (98%)	38 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	91	CYS

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	372/379 (98%)	369 (99%)	3 (1%)	73	75
1	C	381/379 (100%)	377 (99%)	4 (1%)	68	70
2	B	373/383 (97%)	371 (100%)	2 (0%)	81	84
2	D	369/383 (96%)	367 (100%)	2 (0%)	81	84
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	301/342 (88%)	298 (99%)	3 (1%)	68	70
All	All	1905/1993 (96%)	1891 (99%)	14 (1%)	76	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ILE
1	A	215	ARG
1	A	340	SER
2	B	220	THR
2	B	277	SER
1	C	71	GLU
1	C	285	GLN
1	C	361[A]	THR
1	C	361[B]	THR
2	D	47	GLU
2	D	220	THR
4	F	181	VAL
4	F	182	ILE
4	F	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	393	HIS
2	B	192	HIS

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Mol	Chain	Res	Type
2	B	424	ASN
1	C	107	HIS
1	C	285	GLN
1	C	356	ASN
2	D	167	ASN
2	D	331	GLN
2	D	334	ASN
3	E	115	HIS
3	E	124	GLN
3	E	136	ASN
4	F	379	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 oligosaccharides 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
8	GDP	B	501	6	29,30,30	1.09	2 (6%)	45,47,47	1.73	7 (15%)
8	GDP	D	501	6	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MES	B	503	-	12,12,12	0.70	0	15,16,16	0.40	0
10	R3Q	D	503	-	46,46,46	0.89	1 (2%)	74,75,75	1.28	10 (13%)
5	GTP	A	501	6	33,34,34	0.94	2 (6%)	50,54,54	1.47	8 (16%)
5	GTP	C	501	6	33,34,34	0.93	2 (6%)	50,54,54	1.50	8 (16%)
11	ACP	F	402	6	31,33,33	1.72	8 (25%)	47,52,52	1.77	9 (19%)

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
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
8	GDP	D	501	6	-	5/16/32/32	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	R3Q	D	503	-	-	6/17/103/103	0/5/5/5
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
11	ACP	F	402	6	-	6/19/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	C5-C4	4.83	1.47	1.39
11	F	402	ACP	PB-O3A	3.25	1.62	1.58
8	D	501	GDP	C5-C4	3.01	1.47	1.38
11	F	402	ACP	PG-O2G	2.92	1.61	1.55
11	F	402	ACP	PG-O3G	2.86	1.61	1.55
8	B	501	GDP	C5-C4	2.80	1.46	1.38
11	F	402	ACP	C5-C6	2.73	1.48	1.41
11	F	402	ACP	PA-O3A	2.58	1.62	1.59
11	F	402	ACP	C8-N7	2.33	1.36	1.31
5	C	501	GTP	PA-O3A	2.27	1.61	1.59
11	F	402	ACP	C5-N7	-2.25	1.35	1.39
10	D	503	R3Q	O5-C5	-2.24	1.42	1.46
8	D	501	GDP	C6-N1	-2.16	1.34	1.38
5	A	501	GTP	PB-O3B	2.12	1.61	1.59
8	B	501	GDP	C6-N1	-2.10	1.34	1.38
5	C	501	GTP	C2-N3	2.07	1.38	1.33
5	A	501	GTP	C2-N3	2.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	PA-O3A	2.07	1.61	1.59

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C5-C4-N3	-5.90	118.59	126.72
8	D	501	GDP	C5-C4-N3	-5.70	119.32	128.39
8	B	501	GDP	C5-C4-N3	-5.60	119.48	128.39
8	D	501	GDP	C2-N3-C4	4.97	120.85	112.30
8	B	501	GDP	C2-N3-C4	4.78	120.54	112.30
11	F	402	ACP	N3-C4-N9	4.69	135.15	127.17
5	C	501	GTP	C5-C4-N3	-4.61	121.05	128.39
8	B	501	GDP	N9-C4-N3	4.52	135.00	125.95
5	C	501	GTP	C2-N3-C4	4.45	119.96	112.30
5	A	501	GTP	C5-C4-N3	-4.40	121.38	128.39
5	A	501	GTP	C2-N3-C4	4.30	119.70	112.30
8	D	501	GDP	N9-C4-N3	4.22	134.40	125.95
11	F	402	ACP	C2-N3-C4	3.67	120.78	111.83
8	D	501	GDP	C6-C5-N7	3.45	136.57	130.29
11	F	402	ACP	C4-C5-N7	-3.41	106.68	110.58
10	D	503	R3Q	C15-C1-C2	3.27	115.53	111.93
11	F	402	ACP	N3-C2-N1	-3.12	123.86	128.58
10	D	503	R3Q	C3-C8-C9	3.10	121.42	116.30
8	B	501	GDP	C6-C5-N7	3.05	135.84	130.29
10	D	503	R3Q	C31-C15-C30	-2.93	97.96	106.29
10	D	503	R3Q	C8-C9-C10	2.89	127.58	121.38
10	D	503	R3Q	O9-C9-C10	-2.83	115.88	119.28
8	B	501	GDP	O6-C6-C5	-2.82	119.08	126.53
5	C	501	GTP	N9-C4-N3	2.80	131.56	125.95
5	C	501	GTP	N9-C8-N7	-2.76	108.28	113.40
10	D	503	R3Q	C10-C11-C12	-2.75	116.38	120.29
5	A	501	GTP	N9-C8-N7	-2.71	108.38	113.40
5	C	501	GTP	C2-N1-C6	-2.71	120.20	125.11
5	A	501	GTP	N9-C4-N3	2.66	131.27	125.95
10	D	503	R3Q	C41-C4-C5	-2.65	82.65	85.38
5	A	501	GTP	C2-N1-C6	-2.55	120.49	125.11
11	F	402	ACP	C4-N9-C8	2.52	108.39	105.74
8	D	501	GDP	C4-C5-N7	-2.52	106.68	110.67
5	C	501	GTP	C5-C6-N1	2.50	119.62	113.25
11	F	402	ACP	C5-N7-C8	2.47	107.33	103.45
5	C	501	GTP	C8-N7-C5	2.41	108.55	104.26
8	D	501	GDP	O6-C6-C5	-2.39	120.23	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	O6-C6-C5	-2.36	120.31	126.53
5	A	501	GTP	C5-C6-N1	2.33	119.17	113.25
11	F	402	ACP	C3'-C2'-C1'	2.30	105.81	101.46
11	F	402	ACP	PB-O3A-PA	-2.28	124.93	132.37
5	A	501	GTP	C8-N7-C5	2.28	108.31	104.26
5	C	501	GTP	O6-C6-C5	-2.21	120.69	126.53
10	D	503	R3Q	C1-C2-C3	2.17	121.44	118.19
8	B	501	GDP	C4-C5-N7	-2.13	107.30	110.67
8	B	501	GDP	C5-C6-N1	2.05	118.46	113.25
10	D	503	R3Q	C2-O2-C22	2.03	121.51	117.80
10	D	503	R3Q	C11-C10-C9	2.03	117.72	113.31

There are no chirality outliers.

All (36) 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
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	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
10	D	503	R3Q	C33-C32-O10-C10
11	F	402	ACP	PB-C3B-PG-O2G
11	F	402	ACP	C5'-O5'-PA-O2A
10	D	503	R3Q	O11-C32-O10-C10
10	D	503	R3Q	O2-C22-C23-C28
10	D	503	R3Q	O2-C22-C23-C24
10	D	503	R3Q	O22-C22-C23-C28
10	D	503	R3Q	O22-C22-C23-C24
5	C	501	GTP	PB-O3B-PG-O3G
11	F	402	ACP	PB-C3B-PG-O3G
11	F	402	ACP	C5'-O5'-PA-O1A
11	F	402	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A

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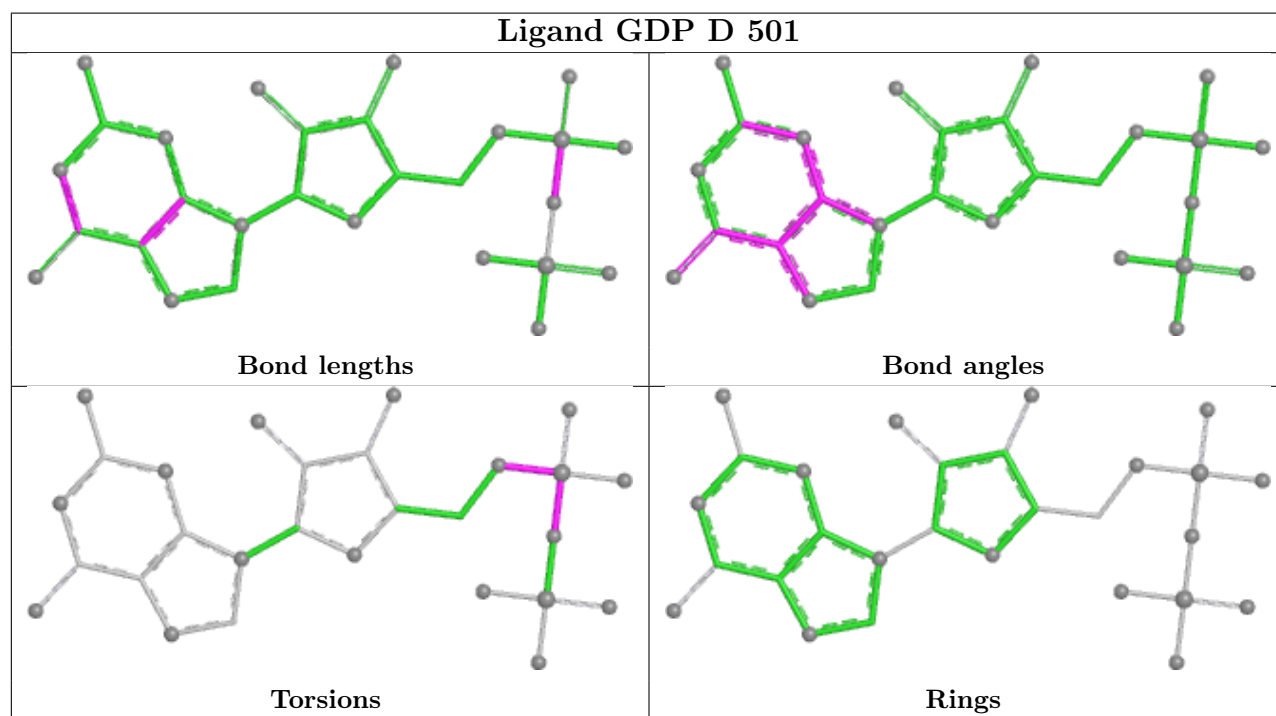
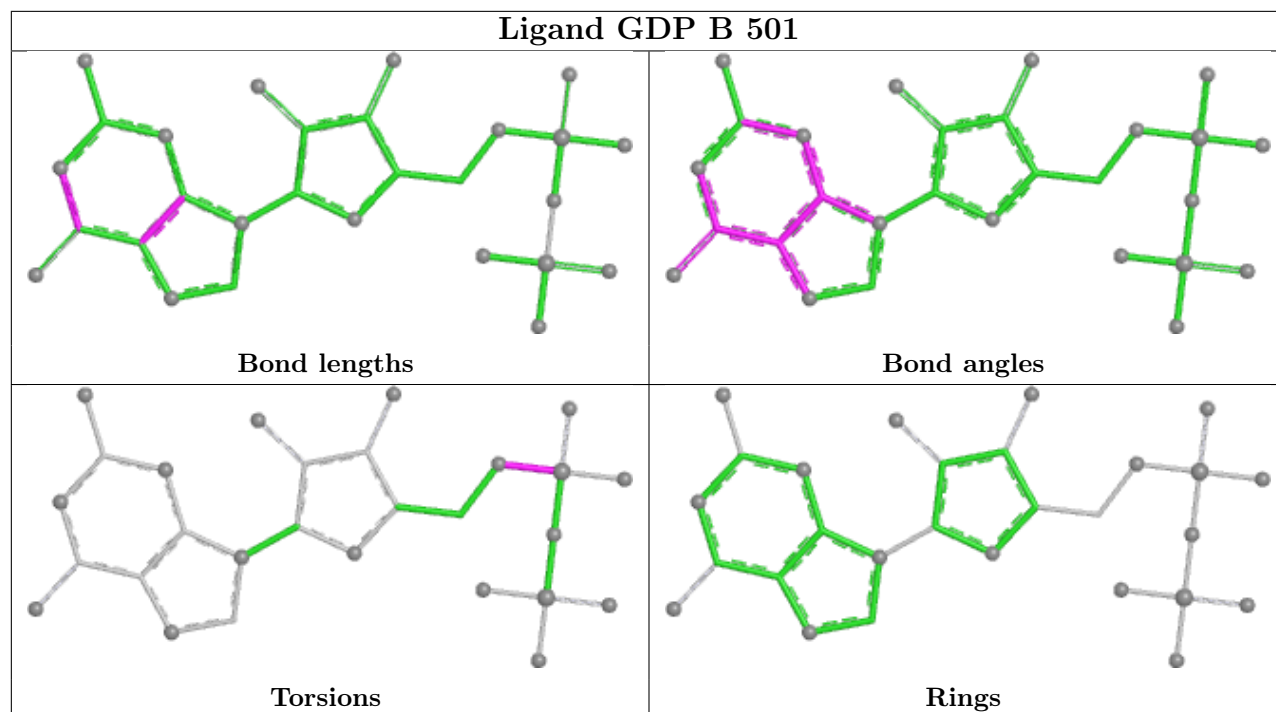
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O1G
11	F	402	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
8	D	501	GDP	PB-O3A-PA-O1A

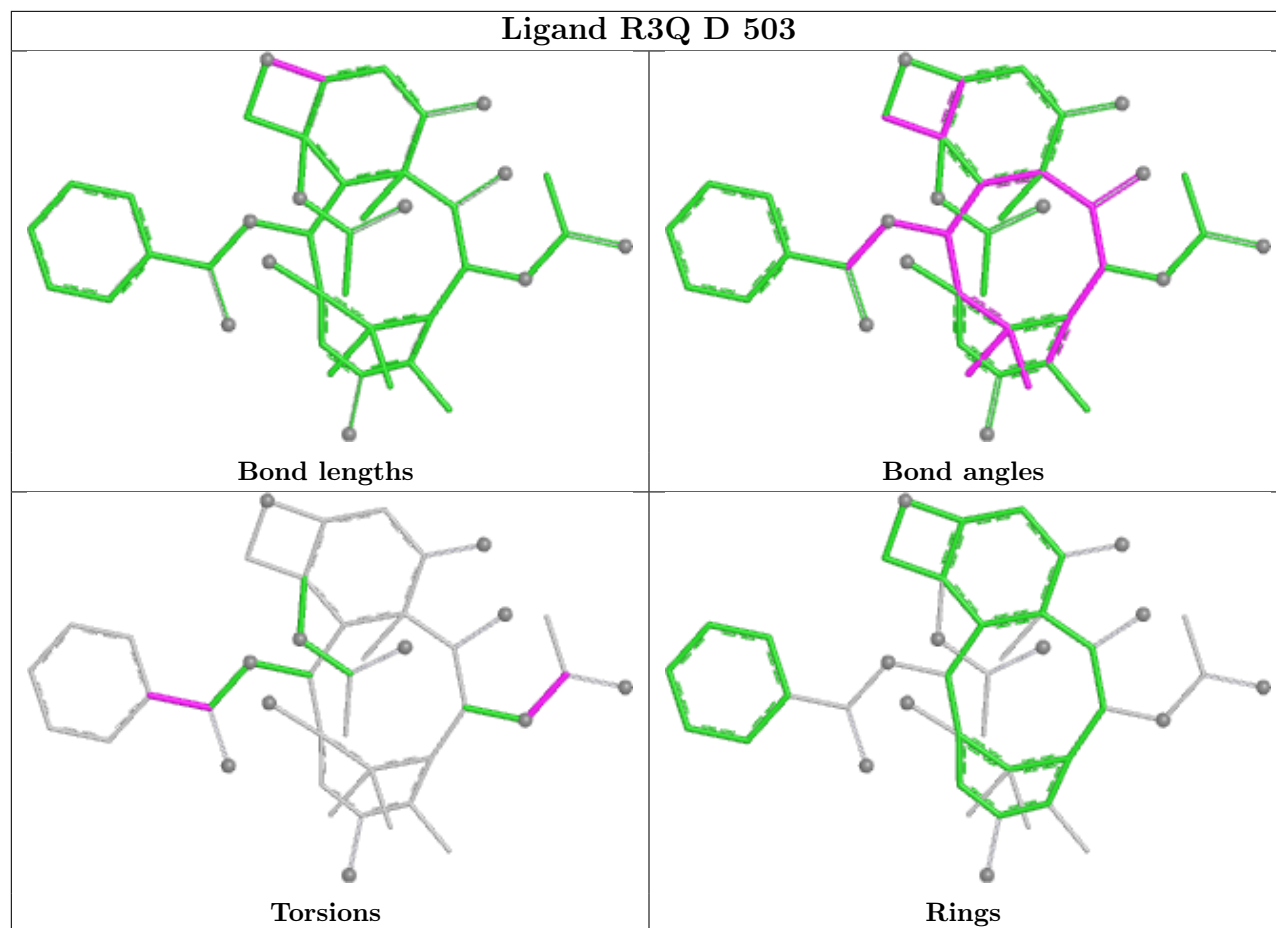
There are no ring outliers.

2 monomers are involved in 3 short contacts:

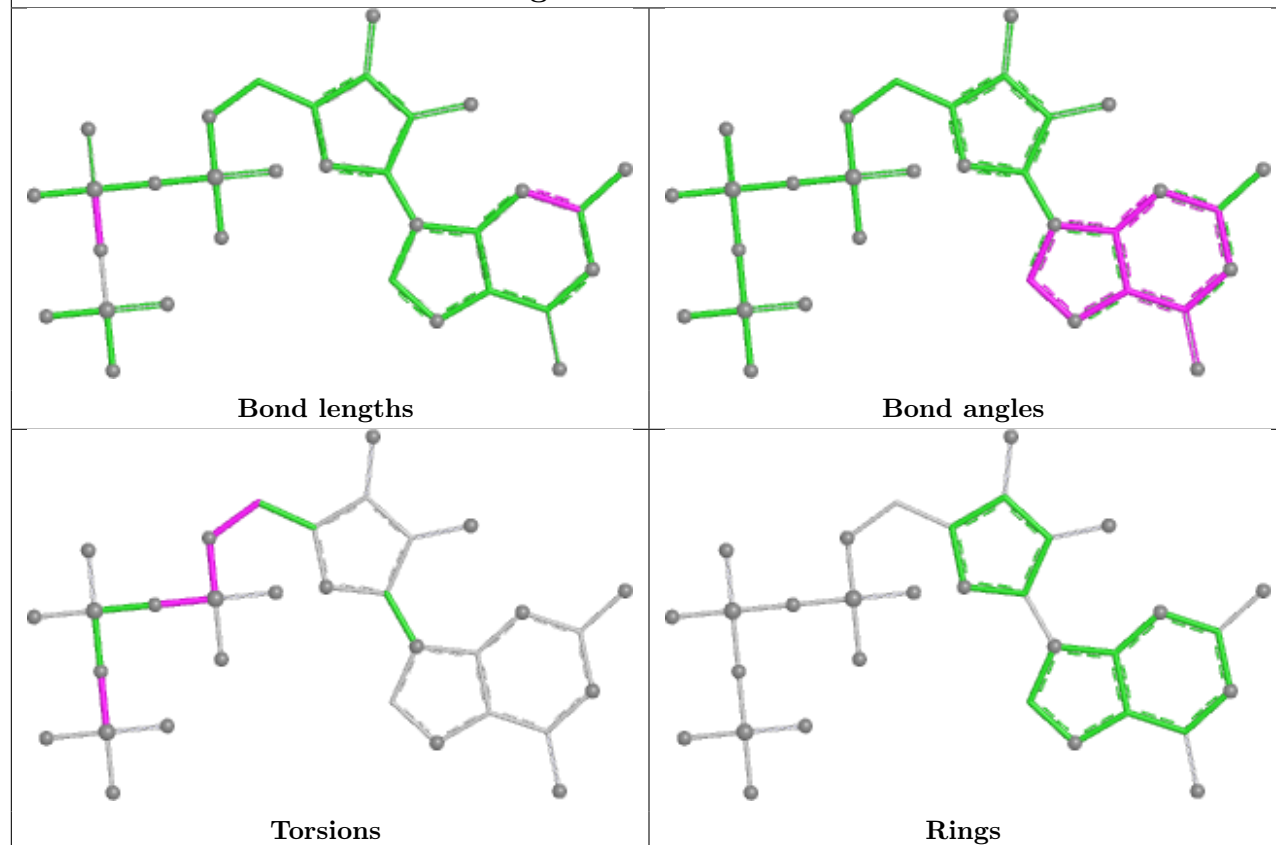
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
11	F	402	ACP	2	0

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

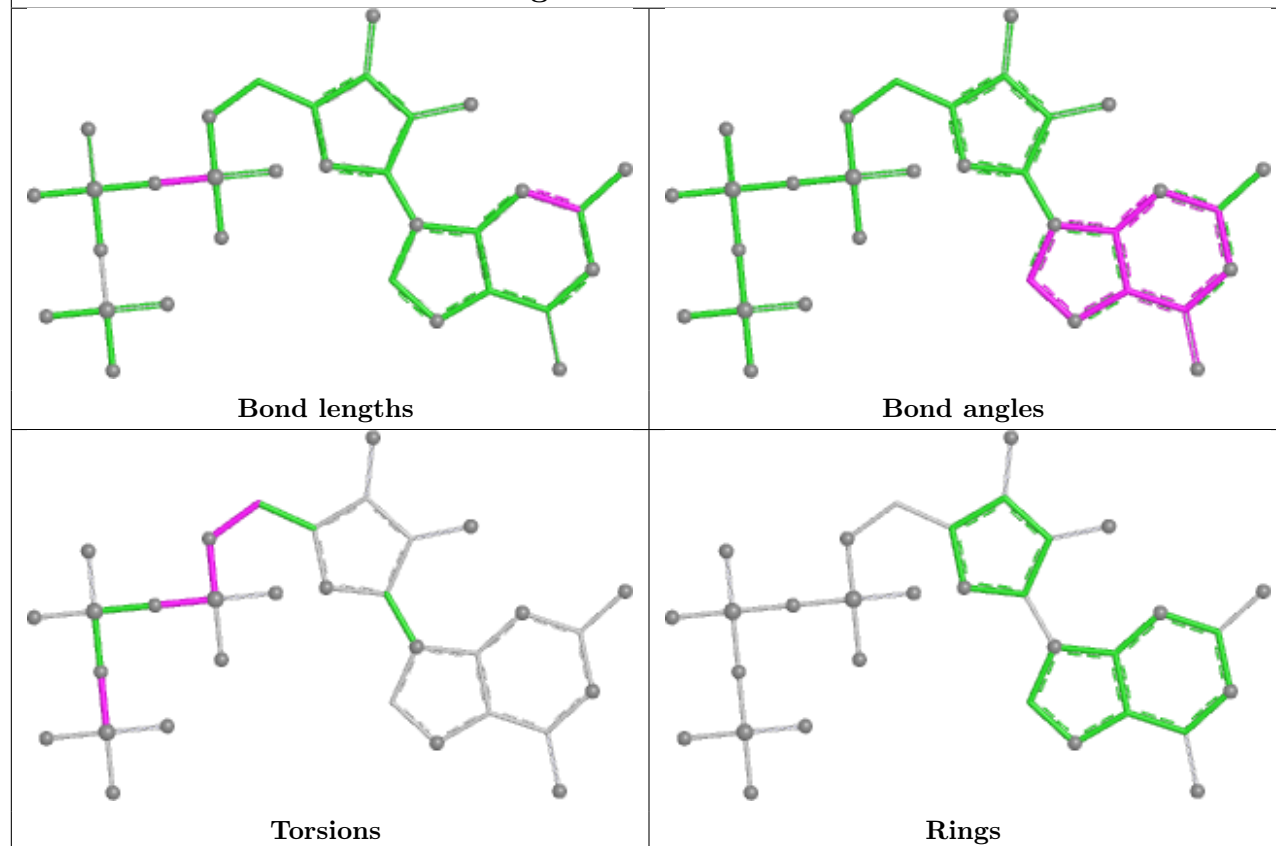


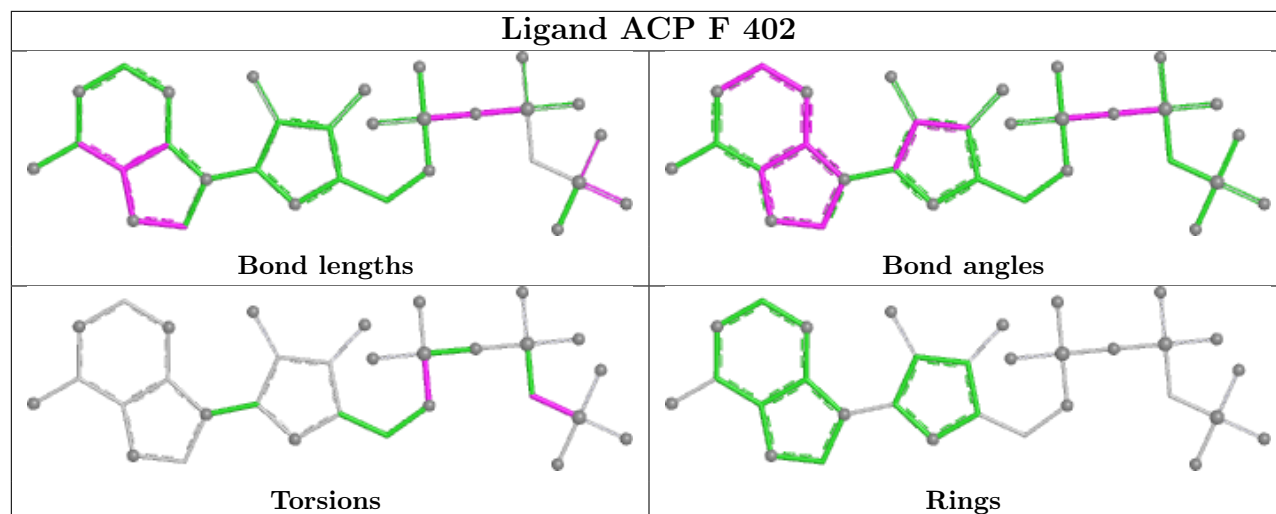


Ligand GTP A 501



Ligand GTP C 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	434/451 (96%)	0.20	15 (3%)	47	50	22, 51, 83, 107	6 (1%)
1	C	440/451 (97%)	-0.04	11 (2%)	58	62	21, 40, 68, 106	10 (2%)
2	B	425/445 (95%)	0.39	29 (6%)	23	24	21, 50, 86, 135	5 (1%)
2	D	424/445 (95%)	0.39	21 (4%)	34	36	28, 56, 89, 124	2 (0%)
3	E	121/143 (84%)	0.61	8 (6%)	24	26	38, 62, 101, 123	0
4	F	334/384 (86%)	0.95	46 (13%)	6	6	44, 75, 150, 186	0
All	All	2178/2319 (93%)	0.36	130 (5%)	27	29	21, 52, 103, 186	23 (1%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	276	THR	5.5
4	F	166	ALA	4.9
4	F	159	GLY	4.9
1	C	440	VAL	4.5
2	D	404	PHE	4.2
2	B	248	LEU	4.2
2	D	276	THR	4.1
2	D	1	MET	4.1
2	D	407	TRP	4.1
4	F	160	ILE	4.1
1	C	340	SER	4.1
2	D	172	MET	4.1
2	B	333	LEU	3.9
4	F	130	VAL	3.9
2	B	83	PHE	3.9
1	A	437	VAL	3.8
2	B	286	LEU	3.8
2	D	82	PRO	3.7
4	F	186	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	E	9	ILE	3.7
2	B	275	LEU	3.6
4	F	182	ILE	3.6
4	F	146	VAL	3.6
4	F	181	VAL	3.6
2	B	285	ALA	3.5
2	B	85	GLN	3.5
4	F	144	GLY	3.5
1	A	179	THR	3.5
2	B	82	PRO	3.5
4	F	362	ALA	3.4
2	B	220	THR	3.3
2	D	57	THR	3.3
4	F	170	LEU	3.3
1	C	341	ILE	3.2
1	C	357	TYR	3.2
4	F	237	THR	3.2
4	F	240	LEU	3.1
2	B	80	SER	3.1
1	C	1	MET	3.1
2	B	325	MET	3.1
4	F	99	VAL	3.0
4	F	173	ILE	3.0
4	F	361	LEU	3.0
2	D	277	SER	2.9
2	B	1	MET	2.9
2	B	328	VAL	2.9
1	A	262	TYR	2.8
3	E	15	THR	2.8
4	F	147	TRP	2.8
3	E	8	VAL	2.8
2	B	241	CYS	2.8
1	C	46	ASP	2.8
2	B	438	ALA	2.7
4	F	244	CYS	2.7
4	F	1	MET	2.7
4	F	137	ARG	2.7
1	A	280	LYS	2.7
2	B	400	ARG	2.7
2	D	83	PHE	2.7
1	C	286	LEU	2.7
1	C	284	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	37	HIS	2.7
4	F	179	VAL	2.7
4	F	231	ALA	2.6
3	E	6	MET	2.6
4	F	138	ARG	2.6
2	D	286	LEU	2.6
4	F	133	ALA	2.6
1	C	283	HIS	2.6
4	F	233	PHE	2.6
4	F	236	LYS	2.6
4	F	339	ALA	2.6
4	F	132	LEU	2.5
1	A	42	ILE	2.5
2	B	172	MET	2.5
3	E	26	PRO	2.5
4	F	102	PRO	2.5
2	B	337	ASN	2.5
1	A	336	LYS	2.5
2	D	219	LEU	2.4
2	D	248	LEU	2.4
2	B	86	ILE	2.4
1	C	163	LYS	2.4
4	F	33	ASP	2.4
2	D	81	GLY	2.4
1	A	346	TRP	2.4
1	A	340	SER	2.4
4	F	225	SER	2.4
2	D	334	ASN	2.4
1	A	178	SER	2.4
2	D	278	ARG	2.3
4	F	44	ARG	2.3
4	F	253	TYR	2.3
2	B	57	THR	2.3
2	B	247	GLN	2.3
2	B	339	ASN	2.3
2	B	77	SER	2.3
4	F	12	SER	2.3
1	A	284	GLU	2.3
3	E	24	LEU	2.3
4	F	379	HIS	2.3
4	F	228	TYR	2.3
3	E	45	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	376	ILE	2.3
2	D	355	VAL	2.2
2	B	79	ARG	2.2
4	F	91	CYS	2.2
1	A	176	GLN	2.2
2	B	340	SER	2.2
4	F	330	ILE	2.2
4	F	306	HIS	2.2
1	A	83	TYR	2.2
4	F	245	ILE	2.2
4	F	320	MET	2.2
3	E	14	CYS	2.2
1	A	18	ASN	2.1
4	F	98	TYR	2.1
2	B	355	VAL	2.1
1	A	45	GLY	2.1
1	C	338	LYS	2.1
4	F	194	PRO	2.1
2	B	353	THR	2.1
1	A	77	GLU	2.1
2	D	337	ASN	2.1
4	F	172	PHE	2.1
2	D	128	SER	2.1
4	F	89	GLU	2.1
2	D	317	ALA	2.1
2	D	2	ARG	2.0
2	B	335	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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,

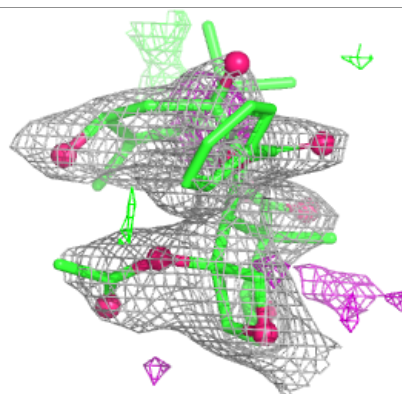
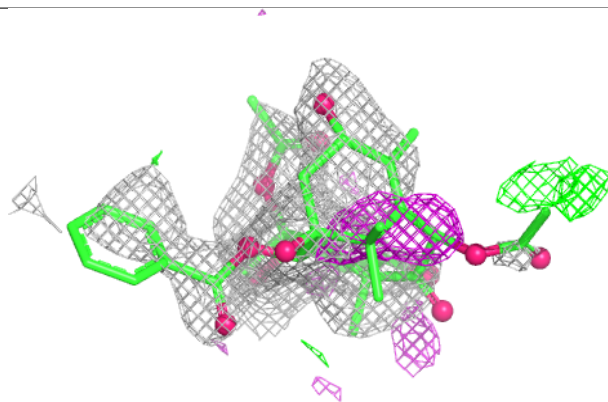
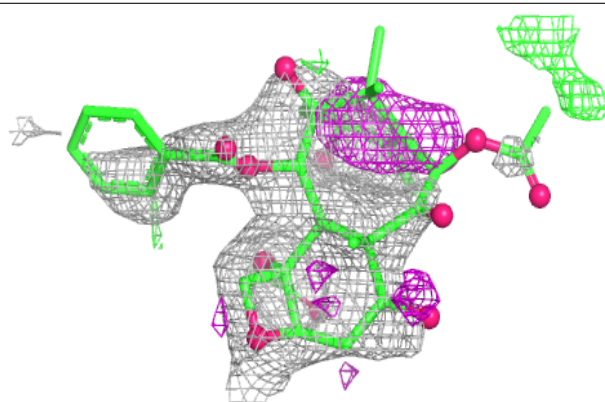
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	R3Q	D	503	42/42	0.75	0.18	94,109,117,119	0
6	MG	D	502	1/1	0.83	0.15	82,82,82,82	0
9	MES	B	503	12/12	0.88	0.14	47,60,69,71	0
11	ACP	F	402	31/31	0.89	0.10	80,96,134,135	0
6	MG	F	401	1/1	0.91	0.12	82,82,82,82	0
8	GDP	D	501	28/28	0.95	0.08	45,52,59,64	0
5	GTP	A	501	32/32	0.98	0.06	29,36,39,40	0
7	CA	A	503	1/1	0.98	0.05	63,63,63,63	0
7	CA	C	503	1/1	0.98	0.05	51,51,51,51	0
8	GDP	B	501	28/28	0.98	0.05	29,36,40,41	0
6	MG	A	502	1/1	0.99	0.02	35,35,35,35	0
6	MG	B	502	1/1	0.99	0.07	29,29,29,29	0
6	MG	C	502	1/1	0.99	0.02	32,32,32,32	0
5	GTP	C	501	32/32	0.99	0.04	26,31,34,37	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.

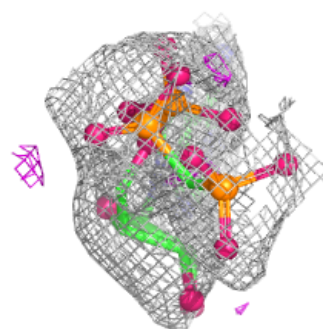
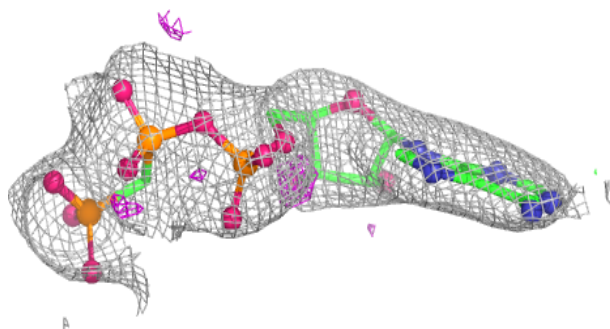
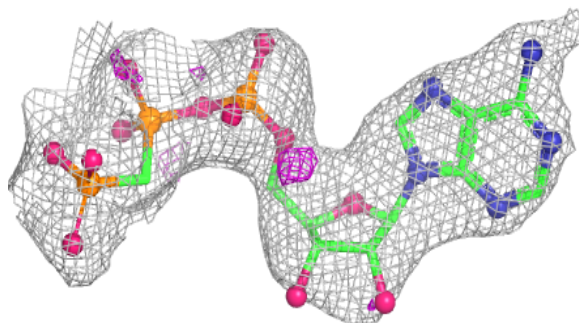
Electron density around R3Q D 503:

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

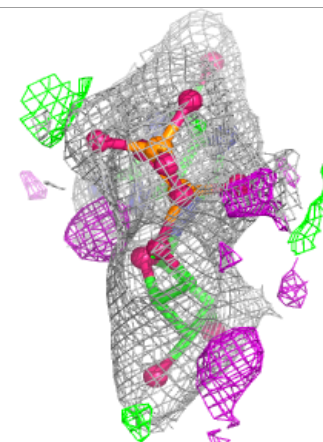
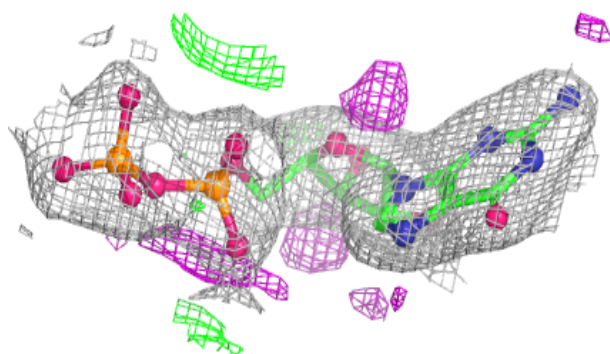
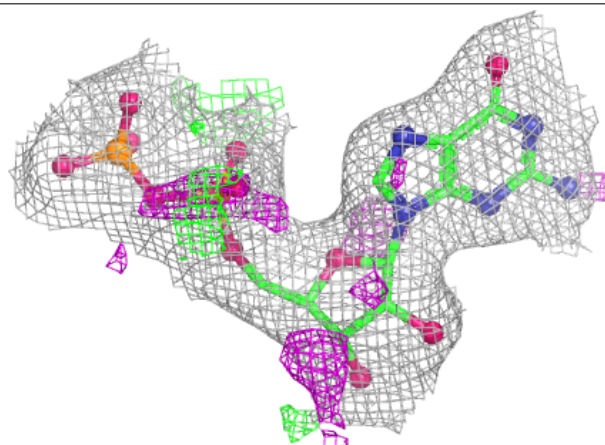


Electron density around ACP F 402:

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

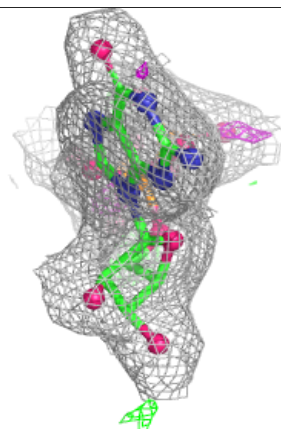
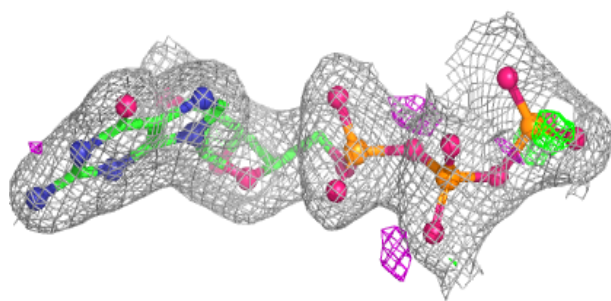
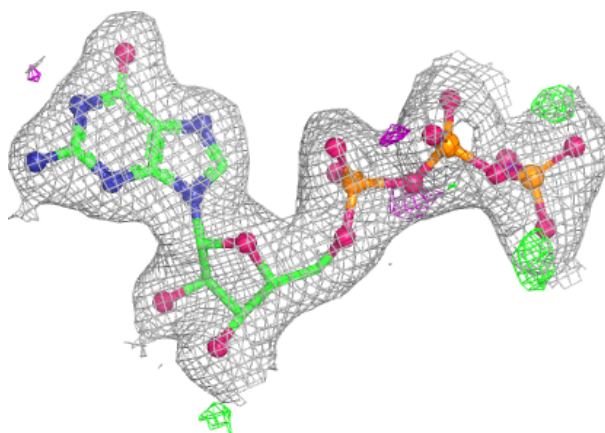
**Electron density around GDP D 501:**

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



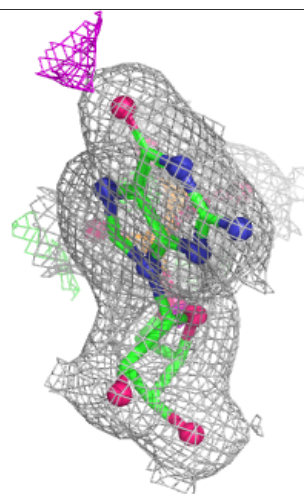
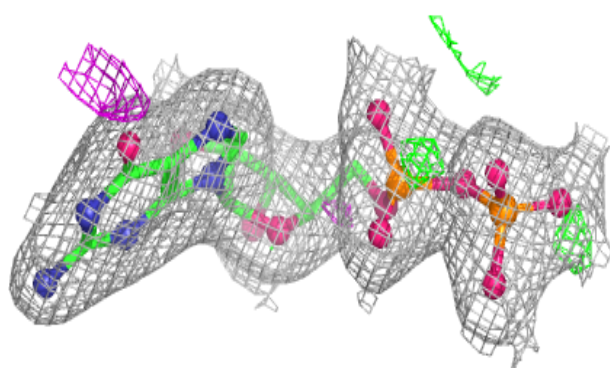
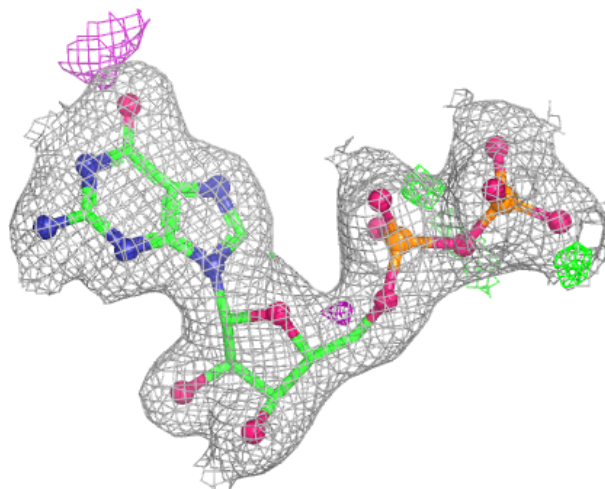
Electron density around GTP A 501:

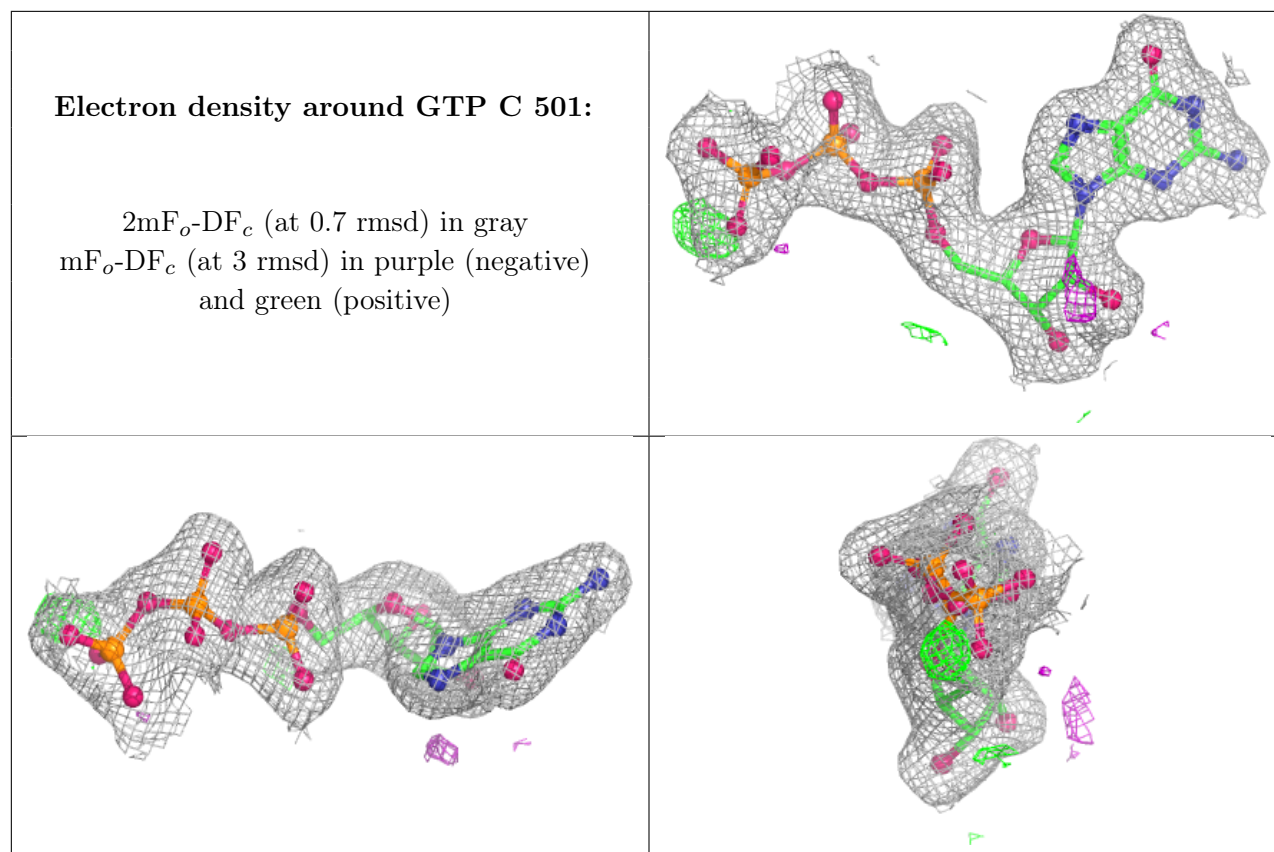
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.