



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 10:09 PM EST

PDB ID : 5S5C
Title : Tubulin-Z44592329-complex
Authors : Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

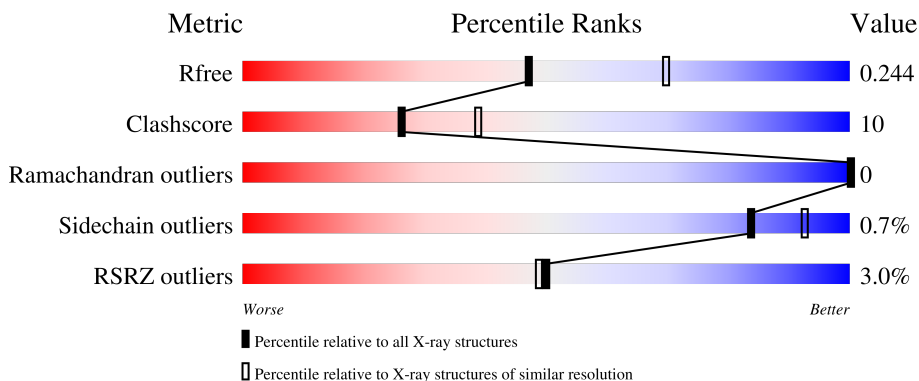
1 Overall quality at a glance i

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">2% 75% 22% .</p>
1	C	451	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">% 78% 19% .</p>
2	B	445	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">4% 68% 27% 5%</p>
2	D	445	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">3% 75% 22% .</p>
3	E	143	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">6% 73% 13% 14%</p>

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>5% 71% 21% 8%</p>

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 18033 atoms, of which 22 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	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	Total	C	N	O	S	1	1	0
			3349	2103	575	644	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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 (three-letter code: MG) (formula: Mg).

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

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

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

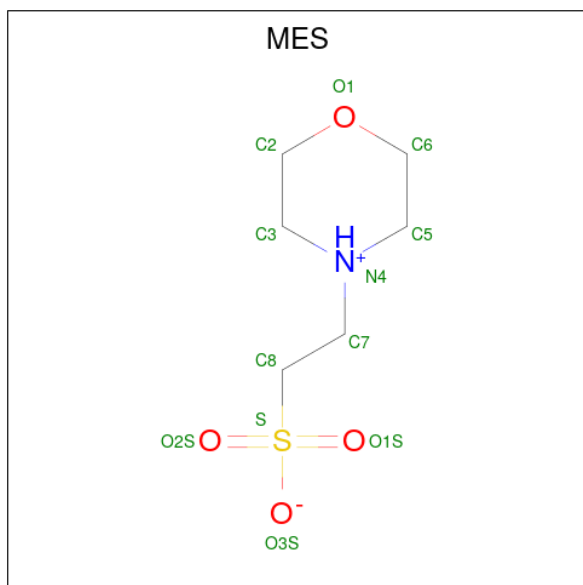
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



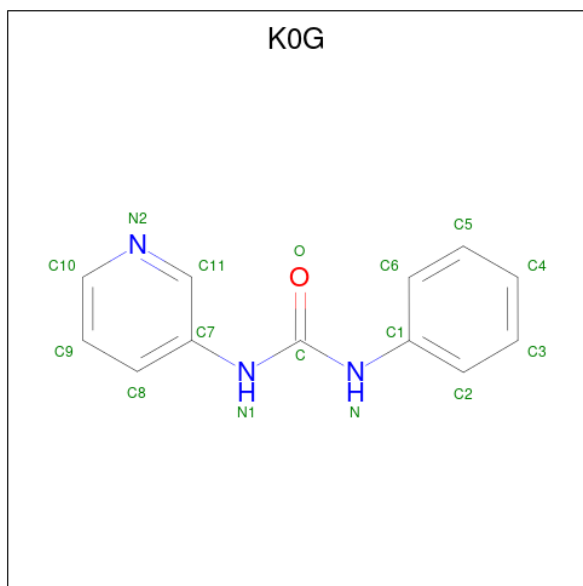
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



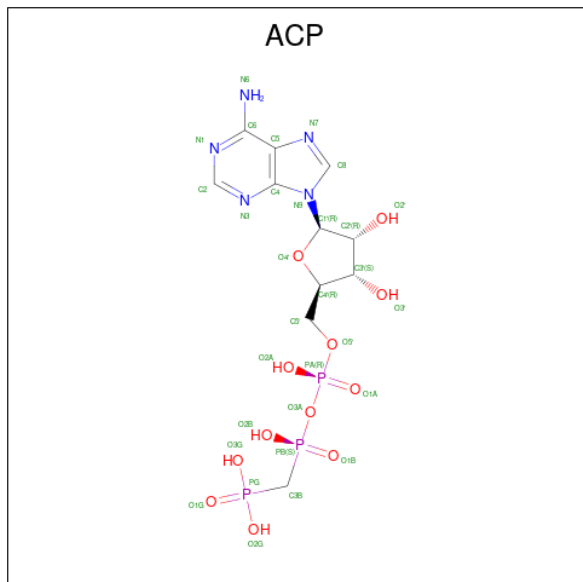
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is N-phenyl-N'-pyridin-3-ylurea (three-letter code: K0G) (formula: $C_{12}H_{11}N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
10	B	1	27	12	11	3	1	0	0
10	C	1	27	12	11	3	1	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

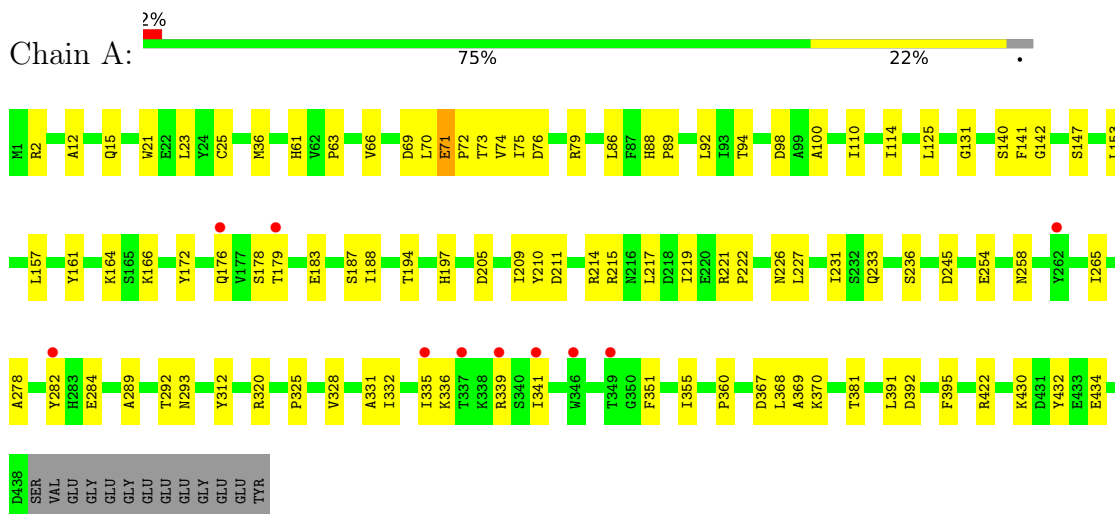
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	52	Total	O	0	0
			52	52		
12	B	78	Total	O	0	0
			78	78		
12	C	162	Total	O	0	0
			162	162		
12	D	25	Total	O	0	0
			25	25		
12	E	8	Total	O	0	0
			8	8		
12	F	7	Total	O	0	0
			7	7		

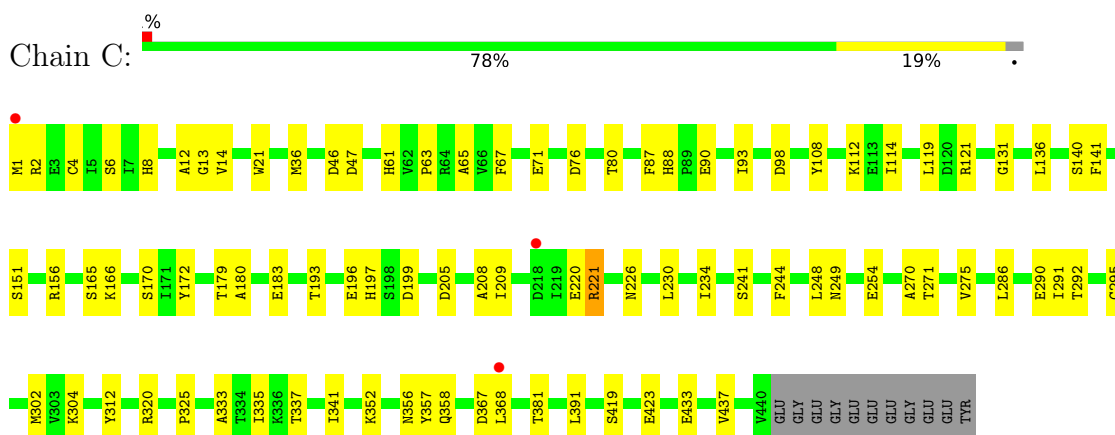
3 Residue-property plots [i](#)

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.

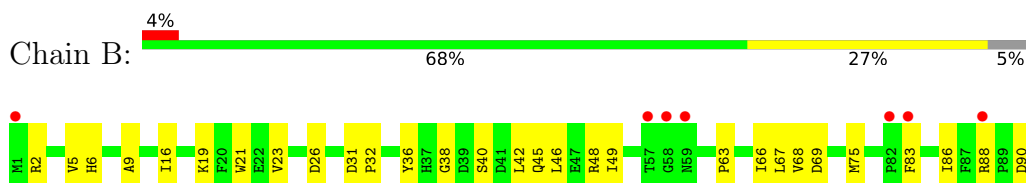
- Molecule 1: Tubulin alpha-1B chain

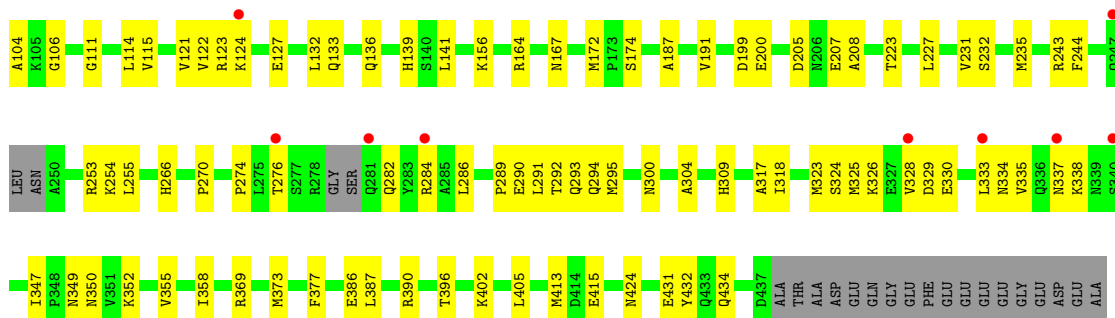


- Molecule 1: Tubulin alpha-1B chain

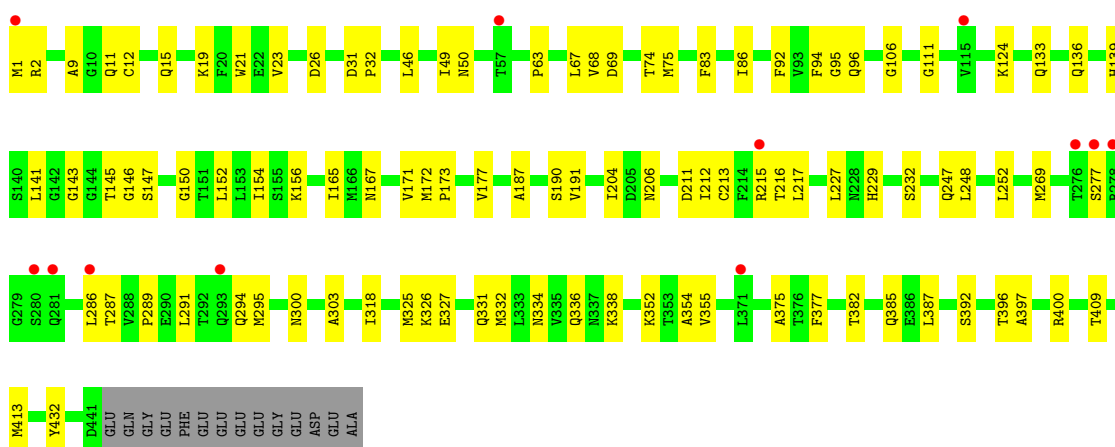
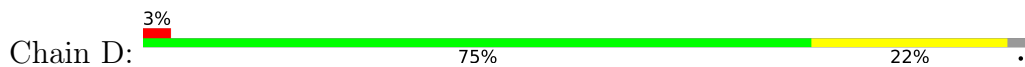


- Molecule 2: Tubulin beta-2B chain

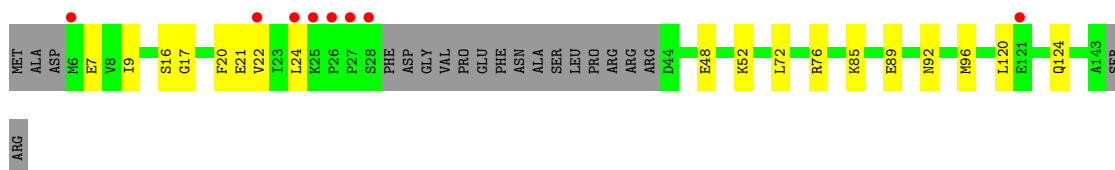
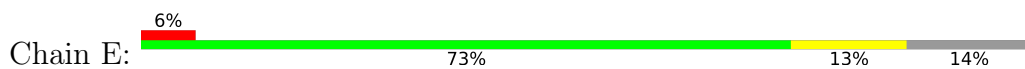




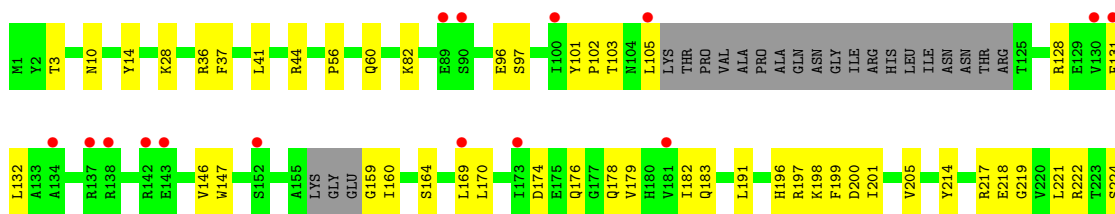
● Molecule 2: Tubulin beta-2B chain

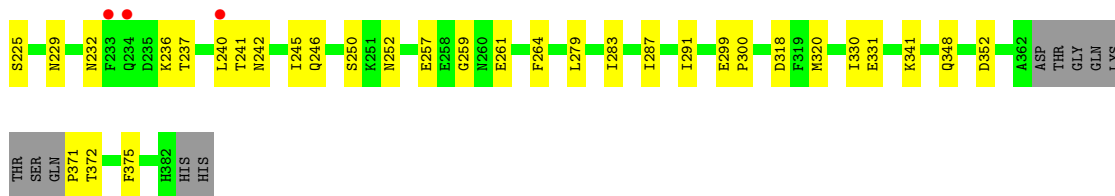


● Molecule 3: Stathmin-4



● 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	105.22Å 159.90Å 177.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.93 – 2.40 118.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.93-2.40) 99.8 (118.93-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.40Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.207 , 0.244 0.208 , 0.244	Depositor DCC
R_{free} test set	5813 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtrriage
Anisotropy	0.348	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18033	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: K0G, CA, ACP, MES, GDP, GTP, MG

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	0.25	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.26	0/3422	0.41	0/4630
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1022	0.34	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17853	0.41	0/24162

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	3424	0	3334	78	0
1	C	3443	0	3352	62	0
2	B	3349	0	3230	92	0
2	D	3368	0	3236	68	0
3	E	1014	0	1029	14	0
4	F	2877	0	2839	62	0
5	A	32	0	12	2	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	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	3	0
9	B	12	0	12	2	0
10	B	16	11	0	0	0
10	C	16	11	0	0	0
11	F	31	0	14	6	0
12	A	52	0	0	2	0
12	B	78	0	0	8	0
12	C	162	0	0	4	0
12	D	25	0	0	3	0
12	E	8	0	0	0	0
12	F	7	0	0	0	0
All	All	18011	22	17094	363	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 10.

All (363) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.38	1.03
2:D:217:LEU:HA	2:D:277:SER:HB3	1.40	1.01
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.22	0.88
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.37	0.87
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.63	0.81
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.46	0.78
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.02	0.78
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.67	0.75
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.69	0.74
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.68	0.74
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.71	0.72
2:D:2:ARG:NH1	12:D:602:HOH:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HA	2:B:167:ASN:O	1.90	0.72
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.24	0.70
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.71	0.70
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.05	0.69
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.75	0.69
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.75	0.68
1:C:270:ALA:O	1:C:302:MET:HG2	1.92	0.68
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.01	0.68
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.75	0.68
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.26	0.68
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.94	0.68
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.30	0.67
2:D:83:PHE:O	2:D:86:ILE:HG22	1.95	0.67
2:D:136:GLN:HA	2:D:167:ASN:O	1.95	0.67
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.29	0.66
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.28	0.66
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.66
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.78	0.66
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.76	0.66
1:A:166:LYS:HE2	1:A:197:HIS:O	1.96	0.65
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.37	0.65
1:C:320:ARG:HA	1:C:356:ASN:O	1.96	0.65
1:C:76:ASP:O	1:C:80:THR:HG22	1.97	0.64
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.77	0.64
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.78	0.64
3:E:85:LYS:O	3:E:89:GLU:HG3	1.96	0.64
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.78	0.63
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.81	0.63
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.10	0.63
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.29	0.62
4:F:371:PRO:HA	4:F:372:THR:O	1.99	0.62
2:B:69:ASP:O	2:B:94:PHE:HA	1.99	0.62
1:A:214:ARG:HG2	1:A:219:ILE:O	1.98	0.62
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.82	0.61
2:D:432:TYR:OH	12:D:601:HOH:O	2.16	0.61
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.00	0.61
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.81	0.61
2:D:152:LEU:O	2:D:156:LYS:HG2	2.01	0.61
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.83	0.60
1:C:271:THR:HG21	1:C:295:CYS:O	2.01	0.60
4:F:159:GLY:C	4:F:160:ILE:HD12	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:GLN:O	2:D:15:GLN:HG2	2.01	0.60
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.30	0.60
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.84	0.60
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.14	0.60
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.34	0.60
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.37	0.60
2:B:83:PHE:O	2:B:86:ILE:HG22	2.02	0.59
4:F:246:GLN:O	4:F:250:SER:HB3	2.01	0.59
4:F:371:PRO:HA	4:F:372:THR:HB	1.84	0.59
4:F:371:PRO:CA	4:F:372:THR:HB	2.33	0.59
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.38	0.58
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.38	0.58
2:D:19:LYS:O	2:D:23:VAL:HG23	2.04	0.58
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.04	0.58
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.04	0.58
2:D:106:GLY:O	2:D:111:GLY:HA3	2.04	0.58
2:D:294:GLN:HG2	2:D:300:ASN:ND2	2.18	0.58
1:C:165:SER:HA	1:C:199:ASP:OD2	2.04	0.58
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.86	0.57
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.86	0.57
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.87	0.57
2:B:40:SER:OG	2:B:42:LEU:HD13	2.05	0.56
1:C:209:ILE:CD1	1:C:302:MET:HE3	2.35	0.56
2:D:294:GLN:HG2	2:D:300:ASN:HD21	1.70	0.56
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.23	0.56
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.06	0.56
2:B:42:LEU:H	2:B:42:LEU:HD12	1.71	0.56
1:A:179:THR:HA	2:B:352:LYS:HD2	1.88	0.56
2:D:332:MET:O	2:D:336:GLN:HG3	2.06	0.56
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.69	0.56
4:F:371:PRO:HA	4:F:372:THR:C	2.26	0.55
2:B:141:LEU:HD12	2:B:172:MET:SD	2.47	0.55
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.41	0.55
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.35	0.55
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.42	0.55
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.89	0.55
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.22	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.42	0.54
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.88	0.54
2:B:396:THR:HG23	12:B:654:HOH:O	2.07	0.54
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.33	0.54
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.23	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.53
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.40	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.53
2:D:382:THR:O	2:D:385:GLN:HG2	2.07	0.53
2:D:392:SER:O	2:D:396:THR:HG22	2.07	0.53
1:A:100:ALA:CB	2:B:253[B]:ARG:HG2	2.38	0.53
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.53
2:B:123:ARG:O	2:B:127:GLU:HG3	2.09	0.53
1:C:1:MET:O	1:C:2:ARG:HB2	2.08	0.53
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.43	0.53
2:B:289:PRO:O	2:B:293:GLN:HG3	2.09	0.53
1:C:180:ALA:O	1:C:183:GLU:HG3	2.08	0.53
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.91	0.53
2:B:329:ASP:O	2:B:333:LEU:HG	2.10	0.52
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.43	0.52
1:C:333:ALA:O	1:C:337:THR:HG23	2.09	0.52
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.44	0.52
1:C:47:ASP:OD2	12:C:601:HOH:O	2.19	0.52
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.44	0.52
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.40	0.52
3:E:120:LEU:O	3:E:124:GLN:HG3	2.10	0.52
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.92	0.52
2:D:171:VAL:HA	2:D:204:ILE:O	2.10	0.52
1:C:151:SER:HB2	1:C:193:THR:CG2	2.40	0.52
2:D:145:THR:HB	8:D:501:GDP:O2B	2.10	0.52
1:A:227:LEU:O	1:A:231:ILE:HG13	2.10	0.51
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.51
1:A:178:SER:OG	1:A:183:GLU:OE1	2.18	0.51
1:A:430:LYS:O	1:A:434:GLU:HG3	2.10	0.51
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.11	0.51
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.74	0.51
1:C:367:ASP:O	12:C:602:HOH:O	2.19	0.51
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.93	0.51
2:D:318:ILE:N	2:D:318:ILE:HD12	2.26	0.51
2:B:19:LYS:O	2:B:23:VAL:HG23	2.11	0.51
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.91	0.51
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.93	0.51
1:A:312:TYR:CE2	1:A:341:ILE:HG23	2.45	0.51
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:O	1:C:112:LYS:HG2	2.11	0.51
2:D:46:LEU:HA	2:D:49:ILE:HB	1.93	0.51
2:D:124:LYS:C	2:D:124:LYS:HD3	2.31	0.51
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.93	0.51
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.41	0.51
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.46	0.50
2:D:147:SER:HB2	2:D:190:SER:OG	2.10	0.50
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.41	0.50
2:B:174:SER:OG	2:B:207:GLU:HB2	2.12	0.50
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.93	0.50
2:B:318:ILE:N	2:B:318:ILE:HD12	2.27	0.50
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.93	0.50
1:C:230:LEU:O	1:C:234:ILE:HD12	2.11	0.50
1:A:141:PHE:O	1:A:147:SER:HB3	2.12	0.50
2:B:164:ARG:HD2	12:B:659:HOH:O	2.11	0.50
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.92	0.50
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.47	0.50
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.41	0.49
1:C:166:LYS:HE2	1:C:197:HIS:O	2.13	0.49
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.12	0.49
2:D:187:ALA:O	2:D:191:VAL:HG23	2.12	0.49
1:A:187:SER:CB	1:A:391:LEU:HD21	2.42	0.49
2:D:211:ASP:O	2:D:215:ARG:HB2	2.12	0.49
2:B:276:THR:HG21	2:B:282:GLN:HA	1.94	0.49
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.43	0.49
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.48	0.49
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.77	0.49
2:B:187:ALA:O	2:B:191:VAL:HG23	2.12	0.49
2:B:9:ALA:HA	2:B:68:VAL:O	2.12	0.49
2:D:1:MET:CE	2:D:50:ASN:HB2	2.43	0.49
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.43	0.49
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.94	0.49
2:D:95:GLY:O	2:D:96:GLN:NE2	2.45	0.49
2:B:199:ASP:OD1	9:B:504:MES:H62	2.13	0.49
2:B:349:ASN:HA	12:B:646:HOH:O	2.12	0.48
2:D:212:ILE:O	2:D:216:THR:HB	2.13	0.48
1:A:289:ALA:HA	1:A:331:ALA:CB	2.44	0.48
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.13	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.48
1:A:141:PHE:HB3	1:A:187:SER:OG	2.13	0.48
1:A:320:ARG:HD2	12:A:637:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:320:MET:CG	4:F:330:ILE:HD11	2.43	0.48
2:B:324:SER:O	2:B:328:VAL:HG23	2.13	0.48
2:B:124:LYS:HD3	2:B:124:LYS:C	2.34	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.13	0.48
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.95	0.48
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.46	0.48
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.95	0.48
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.27	0.48
1:A:71:GLU:HG2	1:A:72:PRO:N	2.28	0.48
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.49	0.48
2:D:1:MET:HG3	2:D:50:ASN:CB	2.44	0.48
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.54	0.47
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.48	0.47
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.78	0.47
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.49	0.47
1:C:1:MET:CE	1:C:131:GLY:HA3	2.41	0.47
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.45	0.47
2:B:270:PRO:HA	2:B:377:PHE:O	2.14	0.47
3:E:92:ASN:O	3:E:96:MET:HG2	2.14	0.47
12:B:606:HOH:O	3:E:85:LYS:NZ	2.45	0.47
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.48	0.47
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.14	0.47
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.95	0.47
2:B:66:ILE:HD13	2:B:121:VAL:HG12	1.96	0.47
1:C:8:HIS:HB3	1:C:13:GLY:O	2.15	0.47
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.15	0.47
2:B:42:LEU:HD12	2:B:42:LEU:N	2.30	0.47
2:D:217:LEU:CA	2:D:277:SER:HB3	2.29	0.47
2:D:387:LEU:HD23	2:D:387:LEU:C	2.34	0.47
1:A:292:THR:HG22	1:A:335:ILE:HD12	1.96	0.47
2:B:333:LEU:O	2:B:337:ASN:ND2	2.48	0.47
1:C:46:ASP:N	1:C:46:ASP:OD1	2.46	0.47
4:F:287:ILE:O	4:F:291:ILE:HG13	2.15	0.47
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.47
1:A:360:PRO:O	1:A:370:LYS:NZ	2.47	0.47
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.49	0.47
2:D:141:LEU:HD12	2:D:172:MET:SD	2.54	0.47
1:A:69:ASP:O	1:A:94:THR:HA	2.16	0.46
1:A:328:VAL:O	1:A:332:ILE:HG13	2.15	0.46
2:D:173:PRO:HG3	2:D:187:ALA:HB2	1.97	0.46
3:E:9:ILE:HD11	3:E:21:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HB	12:A:601:HOH:O	2.15	0.46
1:A:114:ILE:HG12	1:A:114:ILE:O	2.16	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.97	0.46
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.51	0.46
2:B:223:THR:O	2:B:227:LEU:HD13	2.16	0.46
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.46	0.46
2:B:46:LEU:HA	2:B:49:ILE:HB	1.96	0.46
1:C:6:SER:O	1:C:65:ALA:HA	2.16	0.46
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.97	0.46
4:F:229:ASN:ND2	4:F:232:ASN:HB3	2.31	0.46
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.97	0.46
1:A:355:ILE:O	3:E:17:GLY:HA3	2.16	0.46
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.51	0.46
1:C:234:ILE:HD12	1:C:234:ILE:H	1.81	0.46
11:F:401:ACP:H5'1	11:F:401:ACP:H3B2	1.98	0.46
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.97	0.46
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.98	0.46
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.98	0.46
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.45	0.46
2:B:66:ILE:CD1	2:B:121:VAL:HG12	2.46	0.45
1:A:211:ASP:HB3	1:A:215:ARG:NH2	2.31	0.45
2:D:327:GLU:O	2:D:331:GLN:HG2	2.16	0.45
2:B:334:ASN:O	2:B:338:LYS:HG3	2.16	0.45
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.99	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.45
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.46	0.45
1:C:419:SER:O	1:C:423:GLU:HG3	2.16	0.45
4:F:3:THR:HA	4:F:28:LYS:O	2.15	0.45
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.99	0.45
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.98	0.45
2:B:68:VAL:HA	2:B:93:VAL:O	2.17	0.45
4:F:197:ARG:HB2	4:F:224:SER:O	2.17	0.45
2:B:114:LEU:O	2:B:114:LEU:HG	2.16	0.45
2:B:424:ASN:HB3	12:B:608:HOH:O	2.17	0.45
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.97	0.45
2:D:69:ASP:O	2:D:94:PHE:HA	2.17	0.45
2:D:287:THR:HB	2:D:289:PRO:HD2	1.99	0.45
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.81	0.45
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.44	0.45
2:B:432:TYR:OH	12:B:601:HOH:O	2.19	0.45
2:D:146:GLY:O	2:D:150:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.45	0.45
2:B:390:ARG:NH1	12:B:602:HOH:O	2.32	0.45
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.52	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.99	0.44
2:D:150:GLY:O	2:D:154:ILE:HG13	2.18	0.44
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.52	0.44
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.00	0.44
4:F:225:SER:HB2	4:F:252:ASN:O	2.17	0.44
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.18	0.44
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.99	0.44
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.99	0.44
1:A:75:ILE:HB	1:A:94:THR:CG2	2.47	0.44
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.48	0.44
2:B:323:MET:CE	2:B:373:MET:HB2	2.47	0.44
2:D:213:CYS:SG	2:D:227:LEU:HD23	2.57	0.44
2:B:42:LEU:H	2:B:42:LEU:CD1	2.31	0.44
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.52	0.44
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.98	0.44
2:B:42:LEU:HB2	2:B:358:ILE:HD11	2.00	0.44
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.52	0.44
4:F:200:ASP:OD2	4:F:222:ARG:NH2	2.50	0.44
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.47	0.43
1:C:1:MET:HE3	1:C:131:GLY:CA	2.43	0.43
1:C:179:THR:HG21	12:D:610:HOH:O	2.18	0.43
4:F:237:THR:O	4:F:246:GLN:NE2	2.45	0.43
1:A:284:GLU:CD	1:A:284:GLU:H	2.22	0.43
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.00	0.43
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.01	0.43
2:B:415:GLU:HG3	12:B:627:HOH:O	2.18	0.43
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.84	0.43
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.00	0.43
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.49	0.43
2:B:294:GLN:HB3	2:B:300:ASN:ND2	2.33	0.43
2:D:9:ALA:HA	2:D:68:VAL:O	2.19	0.43
2:D:11:GLN:HA	2:D:74:THR:HG21	1.99	0.43
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.41	0.43
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.54	0.43
2:B:349:ASN:O	2:B:352:LYS:HE2	2.19	0.43
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.84	0.43
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HG12	1:C:302:MET:CE	2.47	0.43
4:F:371:PRO:HA	4:F:372:THR:CB	2.46	0.43
1:A:153:LEU:O	1:A:157:LEU:HG	2.18	0.42
1:C:220:GLU:HB3	2:D:326:LYS:HD2	2.01	0.42
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.00	0.42
1:A:245:ASP:HB3	3:E:16:SER:OG	2.18	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.54	0.42
2:B:48:ARG:HB2	2:B:243:ARG:O	2.19	0.42
2:D:409:THR:HA	2:D:413:MET:O	2.19	0.42
4:F:37:PHE:O	4:F:60:GLN:HG2	2.18	0.42
2:B:199:ASP:O	2:B:266:HIS:HB2	2.19	0.42
2:D:248:LEU:HD11	2:D:352:LYS:HB3	2.01	0.42
2:D:295:MET:CE	2:D:375:ALA:HB1	2.50	0.42
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.01	0.42
1:A:194:THR:O	1:A:194:THR:HG22	2.19	0.42
1:C:151:SER:HB2	1:C:193:THR:HG22	2.02	0.42
3:E:7:GLU:O	3:E:22:VAL:HA	2.19	0.42
2:B:235:MET:HE2	2:B:235:MET:HB3	1.89	0.42
4:F:259:GLY:O	4:F:261:GLU:HG3	2.19	0.42
1:A:100:ALA:HB1	2:B:253[B]:ARG:HG2	2.02	0.42
1:C:196:GLU:HG2	12:C:647:HOH:O	2.20	0.42
2:B:431:GLU:O	2:B:434:GLN:HG2	2.20	0.42
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.55	0.42
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.42	0.42
4:F:222:ARG:O	4:F:241:THR:HB	2.20	0.42
2:B:5:VAL:HG23	2:B:132:LEU:HD13	2.01	0.41
1:C:325:PRO:HD2	12:C:613:HOH:O	2.20	0.41
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.51	0.41
2:B:295:MET:CG	2:B:377:PHE:HB2	2.50	0.41
1:C:241:SER:HA	1:C:249:ASN:OD1	2.19	0.41
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.55	0.41
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.02	0.41
2:B:205:ASP:OD1	2:B:207:GLU:N	2.42	0.41
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.01	0.41
4:F:198:LYS:HG2	4:F:199:PHE:H	1.86	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.41
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.20	0.41
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.36	0.41
4:F:341:LYS:HG2	4:F:341:LYS:O	2.20	0.41
1:A:12:ALA:CB	1:A:140:SER:HB3	2.51	0.41
1:A:176:GLN:HG3	4:F:56:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.36	0.41
2:B:104:ALA:HB2	2:B:413:MET:SD	2.61	0.41
2:B:326:LYS:O	2:B:330:GLU:HG3	2.21	0.41
2:D:325:MET:HE2	2:D:355:VAL:HG21	2.03	0.41
1:A:2:ARG:HB3	1:A:131:GLY:O	2.21	0.41
1:A:392:ASP:HB3	1:A:422:ARG:NH2	2.36	0.41
2:B:325:MET:HE1	2:B:355:VAL:HB	2.03	0.41
2:B:402:LYS:CB	2:B:405:LEU:HD12	2.49	0.41
1:C:93:ILE:HD11	1:C:121:ARG:CG	2.44	0.41
4:F:96:GLU:O	4:F:183:GLN:HA	2.20	0.41
2:B:115:VAL:HG11	2:B:156:LYS:HE3	2.02	0.41
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.37	0.41
1:C:291:ILE:HG13	1:C:292:THR:N	2.37	0.40
4:F:320:MET:HE3	4:F:320:MET:HB3	1.96	0.40
4:F:82:LYS:NZ	4:F:97:SER:O	2.51	0.40
2:B:317:ALA:C	2:B:318:ILE:HD12	2.40	0.40
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.56	0.40
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.40	0.40
2:B:292:THR:HG22	2:B:335:VAL:HG21	2.03	0.40
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.03	0.40
1:C:433:GLU:O	1:C:437:VAL:HG23	2.22	0.40
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.02	0.40
2:D:286:LEU:HD23	2:D:291:LEU:HD13	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	436/451 (97%)	427 (98%)	9 (2%)	0	100	100
1	C	439/451 (97%)	428 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	418/445 (94%)	404 (97%)	14 (3%)	0	100	100
2	D	429/445 (96%)	415 (97%)	14 (3%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	331 (96%)	13 (4%)	0	100	100
All	All	2185/2319 (94%)	2123 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	369/379 (97%)	365 (99%)	4 (1%)	73	87
1	C	372/379 (98%)	369 (99%)	3 (1%)	81	91
2	B	368/383 (96%)	366 (100%)	2 (0%)	88	95
2	D	368/383 (96%)	364 (99%)	4 (1%)	73	87
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1902/1993 (95%)	1889 (99%)	13 (1%)	84	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	282	TYR
1	A	381	THR
2	B	139	HIS
2	B	291	LEU
1	C	71	GLU
1	C	221	ARG
1	C	381	THR

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Mol	Chain	Res	Type
2	D	26	ASP
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	15	GLN
2	B	294	GLN
2	B	300	ASN
1	C	11	GLN
1	C	133	GLN
2	D	96	GLN
2	D	294	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 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	504	-	12,12,12	2.20	1 (8%)	14,16,16	2.02	6 (42%)
10	K0G	C	504	-	17,17,17	0.16	0	21,21,21	0.39	0
8	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.17	3 (10%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.34	6 (18%)
8	GDP	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.06	3 (10%)
11	ACP	F	401	6	27,33,33	1.40	5 (18%)	32,52,52	1.49	4 (12%)
10	K0G	B	505	-	17,17,17	0.18	0	21,21,21	0.41	0
5	GTP	A	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.41	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	K0G	C	504	-	-	0/8/8/8	0/2/2/2
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	ACP	F	401	6	-	12/15/38/38	0/3/3/3
10	K0G	B	505	-	-	0/8/8/8	0/2/2/2
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.33	1.67	1.77
5	A	501	GTP	C5-C6	-3.93	1.39	1.47
5	C	501	GTP	C5-C6	-3.89	1.39	1.47
11	F	401	ACP	PG-O3G	2.97	1.61	1.54
11	F	401	ACP	PG-O2G	2.93	1.61	1.54
11	F	401	ACP	PB-O3A	2.81	1.61	1.58
11	F	401	ACP	C5-C4	2.52	1.47	1.40
8	B	501	GDP	C6-N1	-2.41	1.34	1.37
8	D	501	GDP	C6-N1	-2.28	1.34	1.37
11	F	401	ACP	PB-O2B	2.19	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C2-N3	2.17	1.38	1.33
5	C	501	GTP	C2-N3	2.14	1.38	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-4.15	119.41	132.56
9	B	504	MES	C5-N4-C3	3.80	117.39	108.83
11	F	401	ACP	C3'-C2'-C1'	3.49	106.23	100.98
5	A	501	GTP	C5-C6-N1	3.26	119.71	113.95
11	F	401	ACP	N3-C2-N1	-3.16	123.75	128.68
5	C	501	GTP	C8-N7-C5	3.08	108.86	102.99
8	D	501	GDP	PA-O3A-PB	-3.06	122.33	132.83
5	A	501	GTP	PA-O3A-PB	-3.05	122.37	132.83
5	C	501	GTP	C5-C6-N1	3.01	119.28	113.95
5	A	501	GTP	C8-N7-C5	2.99	108.68	102.99
5	A	501	GTP	C2-N1-C6	-2.92	119.73	125.10
9	B	504	MES	C6-C5-N4	-2.89	105.72	110.10
5	C	501	GTP	PA-O3A-PB	-2.86	123.01	132.83
9	B	504	MES	O1S-S-C8	2.86	110.36	106.92
5	C	501	GTP	C2-N1-C6	-2.84	119.87	125.10
5	A	501	GTP	PB-O3B-PG	-2.63	123.79	132.83
8	B	501	GDP	PA-O3A-PB	-2.57	124.00	132.83
11	F	401	ACP	C4-C5-N7	-2.54	106.75	109.40
8	D	501	GDP	C8-N7-C5	2.45	107.65	102.99
8	B	501	GDP	C8-N7-C5	2.38	107.53	102.99
9	B	504	MES	O3S-S-C8	2.38	109.61	105.77
8	B	501	GDP	C5-C6-N1	2.32	118.04	113.95
8	D	501	GDP	C5-C6-N1	2.32	118.04	113.95
9	B	504	MES	C7-N4-C5	2.31	117.15	111.23
5	A	501	GTP	O6-C6-C5	-2.18	120.12	124.37
9	B	504	MES	O2S-S-C8	2.17	109.52	106.92
5	C	501	GTP	PB-O3B-PG	-2.12	125.56	132.83
5	C	501	GTP	O6-C6-C5	-2.08	120.31	124.37

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O2A
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-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3B-PG-O1G

There are no ring outliers.

5 monomers are involved in 14 short contacts:

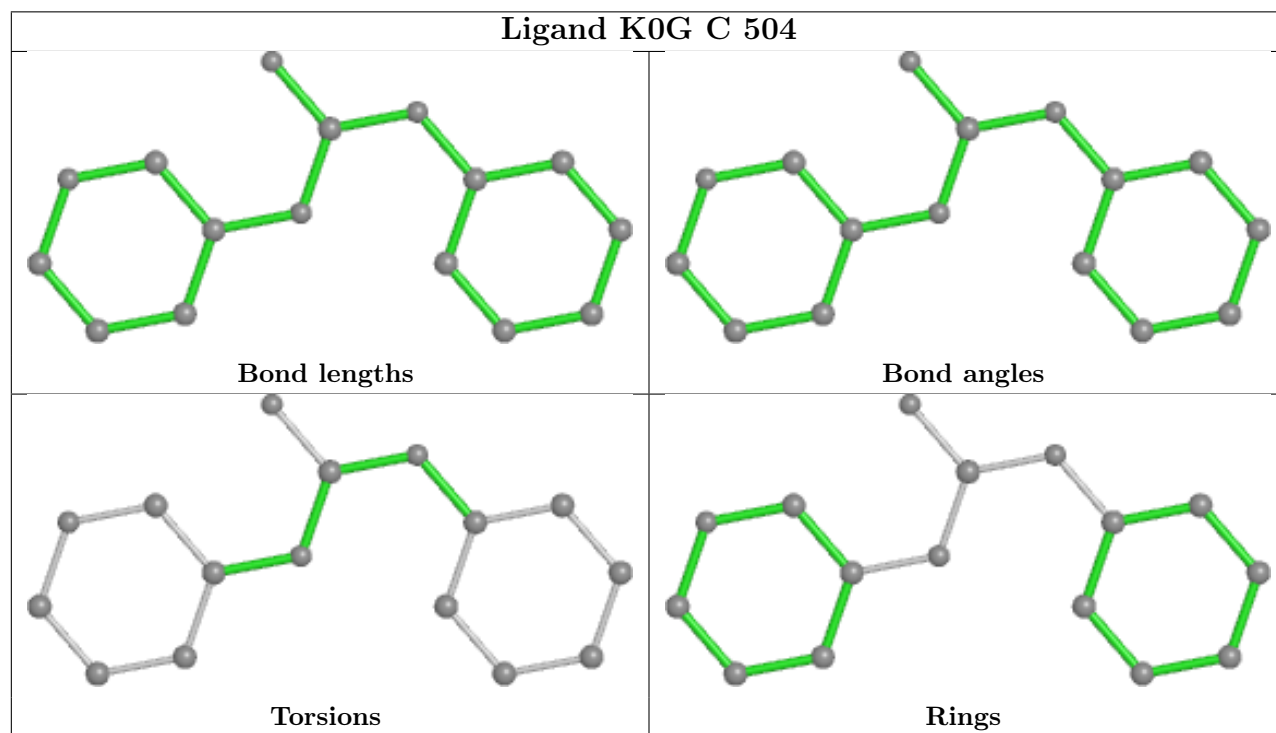
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	MES	2	0
8	D	501	GDP	3	0

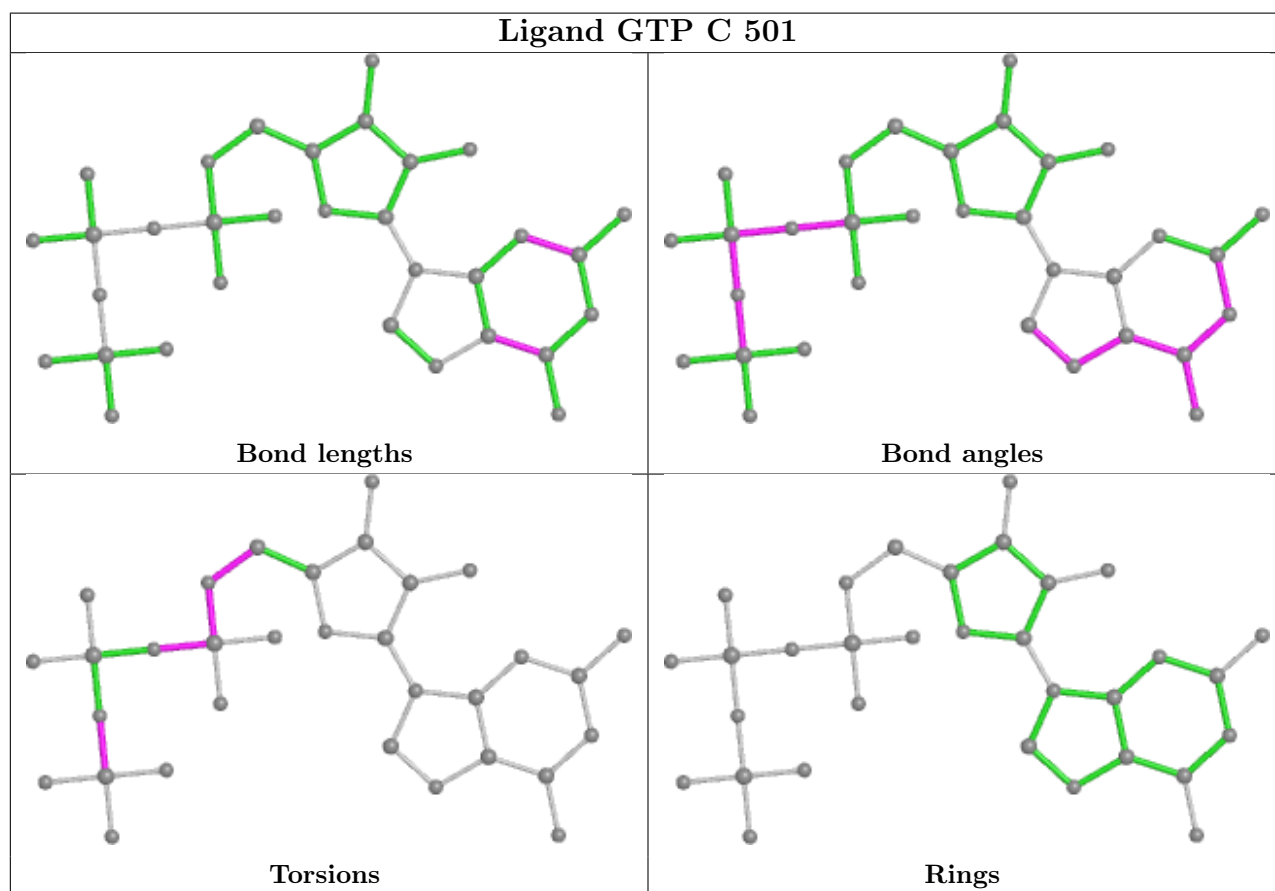
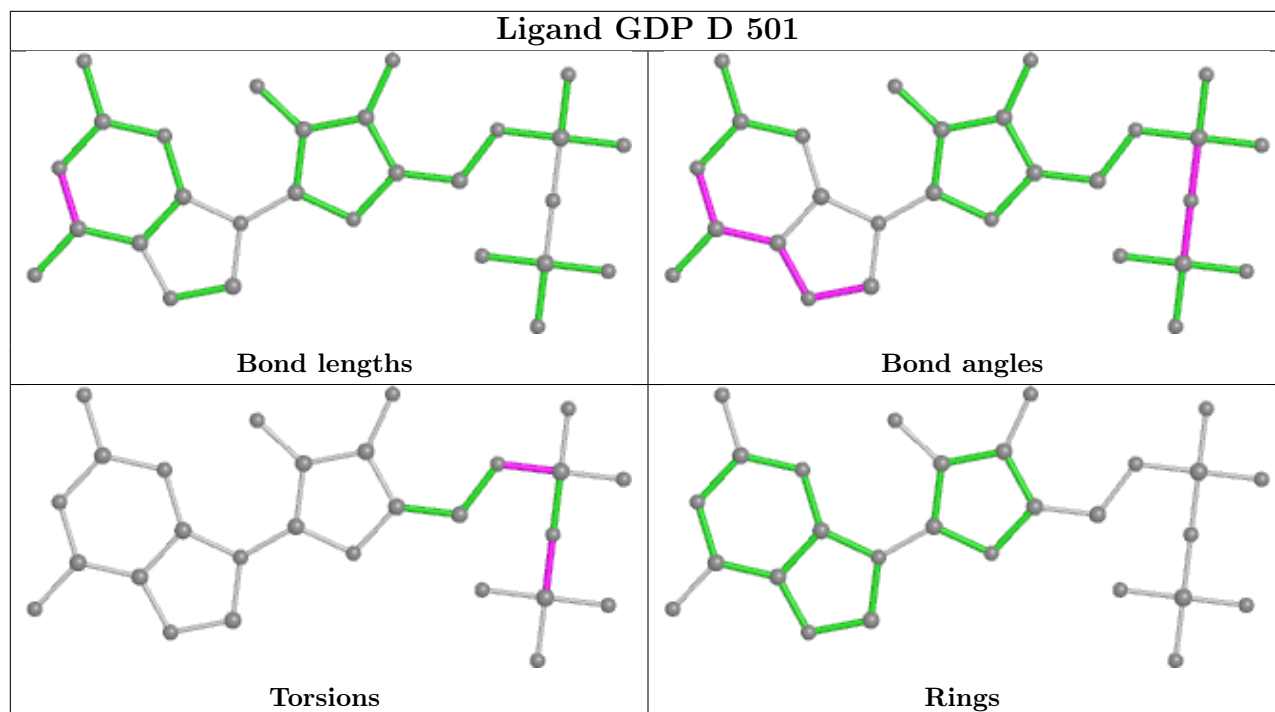
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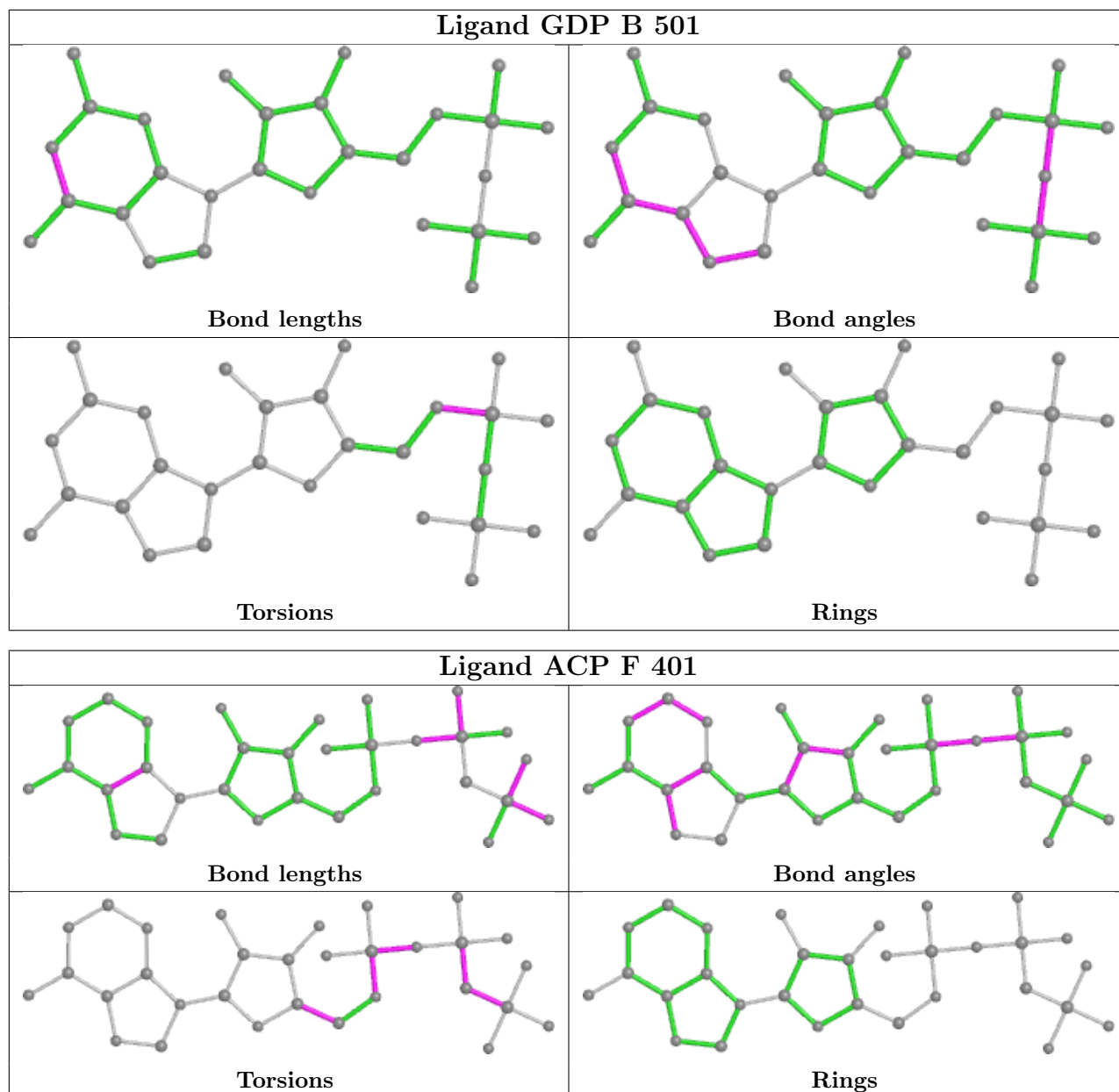
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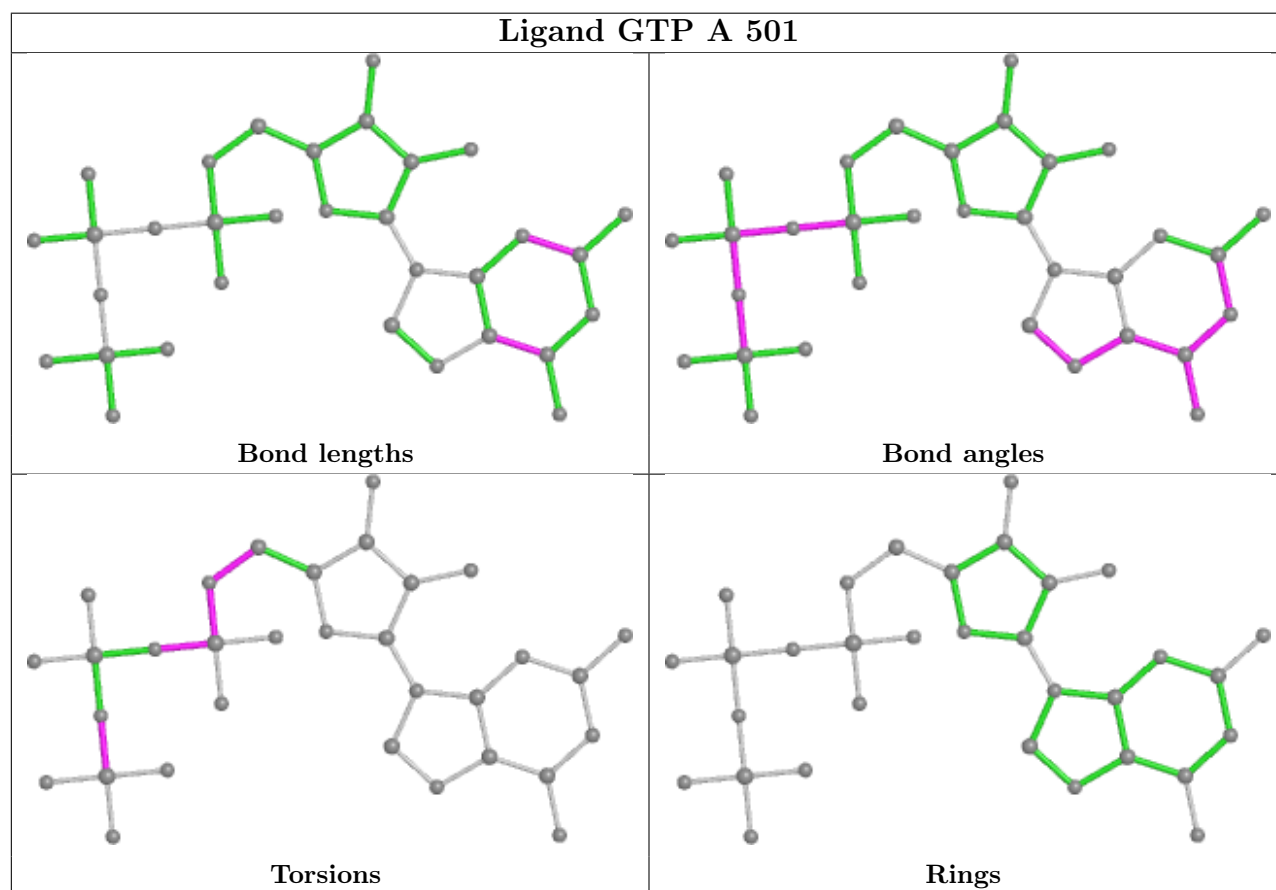
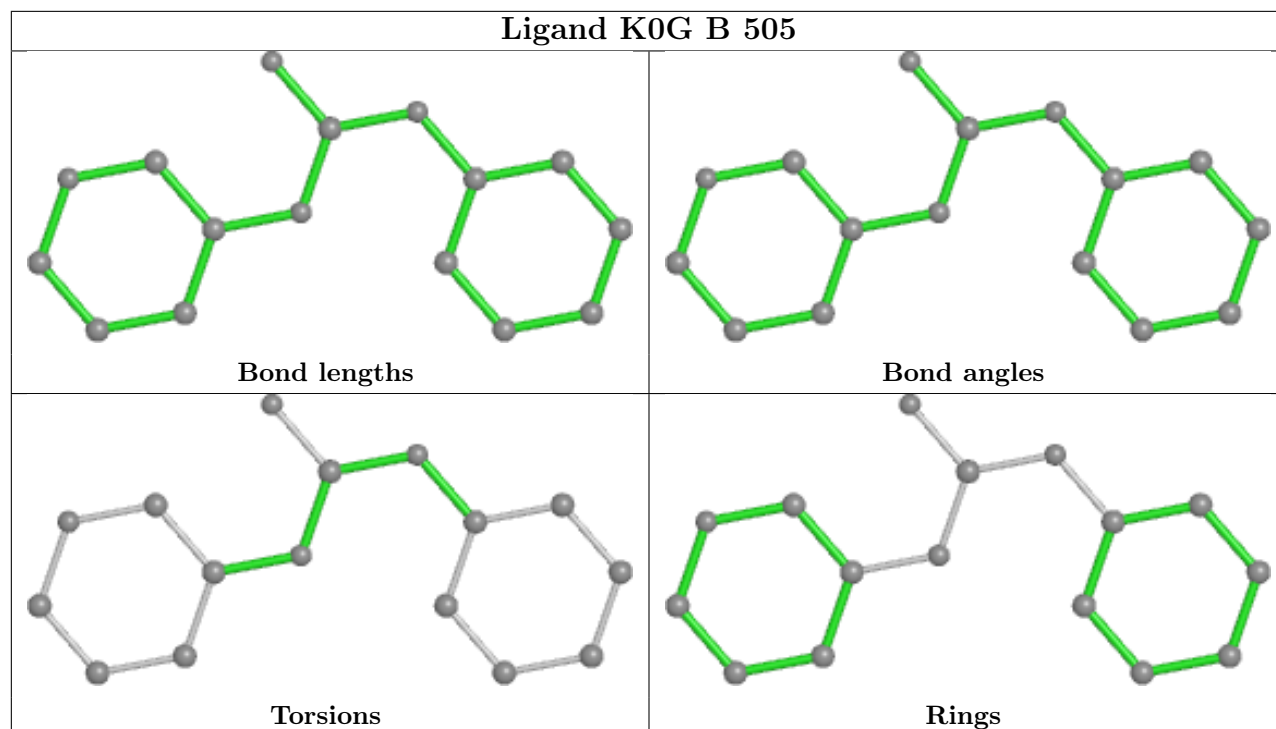
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
11	F	401	ACP	6	0
5	A	501	GTP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.16	10 (2%) 60 58	53, 70, 108, 181	0
1	C	440/451 (97%)	0.12	3 (0%) 87 86	46, 58, 82, 113	0
2	B	423/445 (95%)	0.37	16 (3%) 40 39	46, 70, 117, 151	3 (0%)
2	D	431/445 (96%)	0.18	12 (2%) 53 51	54, 75, 111, 167	4 (0%)
3	E	123/143 (86%)	0.52	8 (6%) 18 17	56, 79, 125, 156	0
4	F	352/384 (91%)	0.26	18 (5%) 28 26	66, 98, 157, 190	0
All	All	2207/2319 (95%)	0.23	67 (3%) 50 49	46, 72, 128, 190	7 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	90	SER	8.2
3	E	6	MET	7.5
4	F	89	GLU	6.4
4	F	240	LEU	6.1
4	F	169	LEU	5.3
2	B	281	GLN	5.1
2	D	278	ARG	4.8
4	F	105	LEU	4.6
3	E	27	PRO	4.3
3	E	26	PRO	4.1
2	B	57	THR	4.0
2	B	276	THR	4.0
2	D	215	ARG	4.0
2	D	277	SER	4.0
2	D	276	THR	3.9
4	F	134	ALA	3.9
3	E	24	LEU	3.8
4	F	173	ILE	3.8
4	F	138	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	137	ARG	3.6
2	B	1	MET	3.6
2	D	371	LEU	3.5
4	F	233	PHE	3.3
1	A	346	TRP	3.3
1	A	335	ILE	3.3
2	B	58	GLY	3.1
2	D	1	MET	3.1
2	D	281	GLN	3.0
2	D	280	SER	3.0
4	F	142	ARG	3.0
2	B	284	ARG	3.0
4	F	143	GLU	2.9
1	A	179	THR	2.8
4	F	131	PHE	2.8
3	E	22	VAL	2.8
2	B	124	LYS	2.7
2	B	247	GLN	2.7
2	B	59	ASN	2.6
3	E	28	SER	2.6
4	F	181	VAL	2.6
2	D	293	GLN	2.6
1	C	218	ASP	2.6
2	B	337	ASN	2.6
4	F	100	ILE	2.5
4	F	234	GLN	2.4
2	B	340	SER	2.4
3	E	25	LYS	2.4
4	F	130	VAL	2.4
1	A	337	THR	2.3
2	B	328	VAL	2.3
1	C	1	MET	2.3
2	B	88	ARG	2.3
2	B	83	PHE	2.3
2	B	82	PRO	2.2
1	A	262	TYR	2.2
4	F	152	SER	2.2
1	A	282	TYR	2.2
1	A	341	ILE	2.2
1	A	176	GLN	2.2
2	D	115	VAL	2.2
2	B	333	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	57	THR	2.1
3	E	121	GLU	2.1
1	A	349	THR	2.1
2	D	286	LEU	2.0
1	A	339	ARG	2.0
1	C	368	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

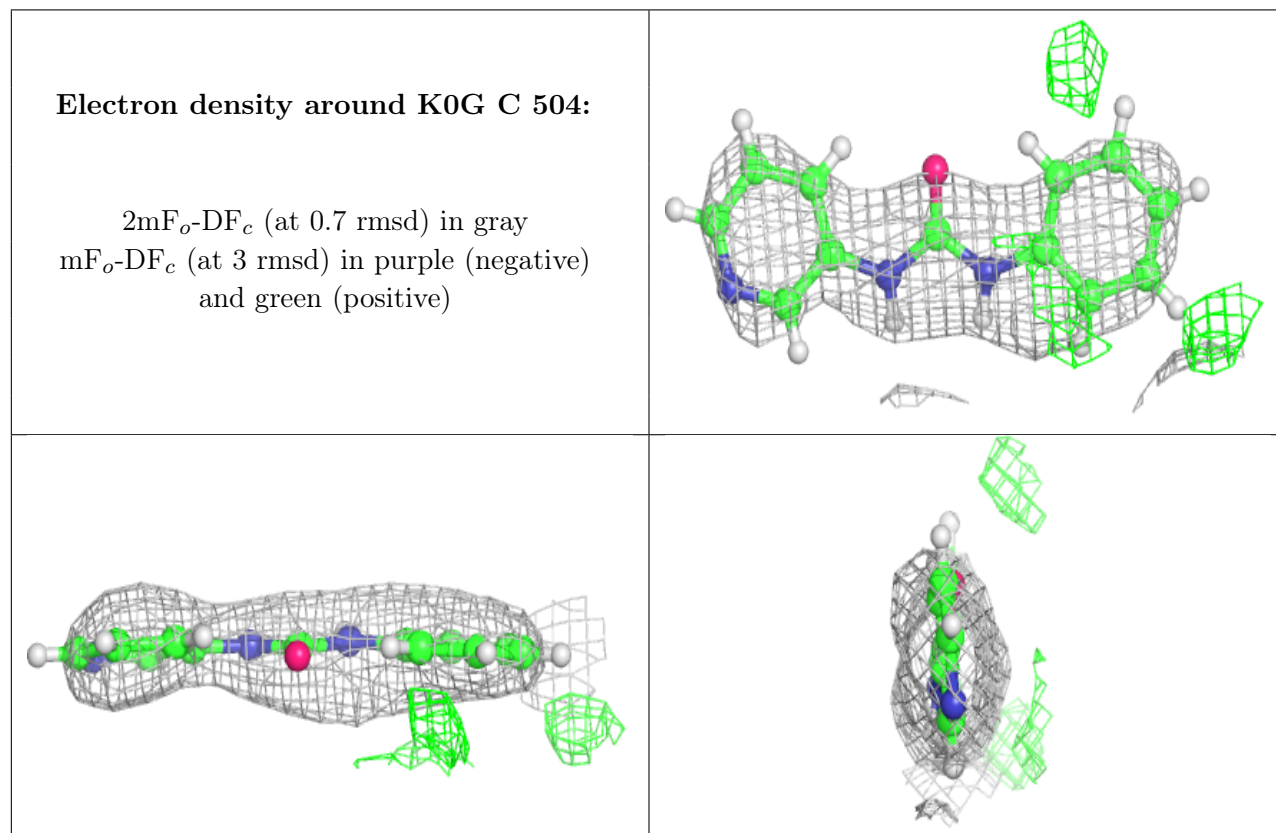
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

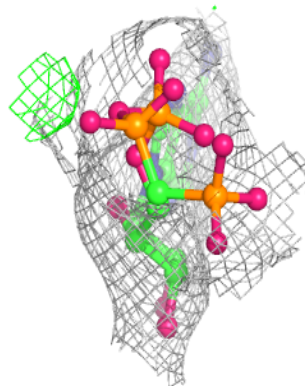
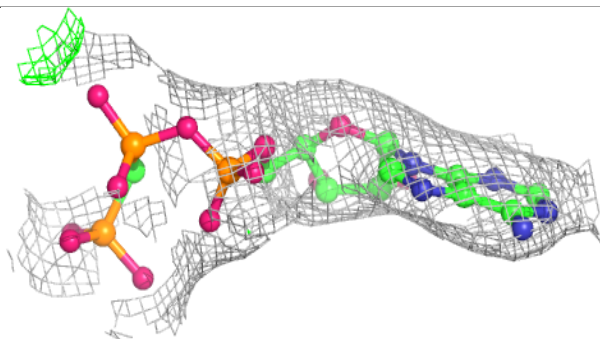
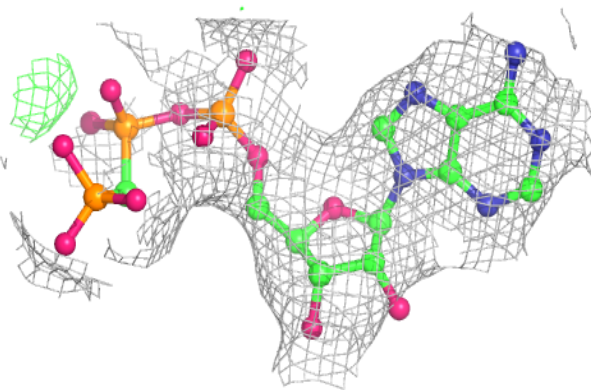
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.74	0.14	76,76,76,76	0
7	CA	B	503	1/1	0.76	0.08	118,118,118,118	0
7	CA	A	504	1/1	0.81	0.09	94,94,94,94	0
9	MES	B	504	12/12	0.88	0.19	90,96,115,122	0
10	K0G	C	504	16/16	0.88	0.25	56,69,83,85	27
11	ACP	F	401	31/31	0.89	0.13	96,109,117,122	0
10	K0G	B	505	16/16	0.93	0.19	55,66,79,80	27
6	MG	B	502	1/1	0.95	0.19	46,46,46,46	0
6	MG	F	402	1/1	0.95	0.19	95,95,95,95	0
7	CA	C	503	1/1	0.96	0.14	78,78,78,78	0
8	GDP	D	501	28/28	0.96	0.17	68,75,82,89	0
7	CA	A	503	1/1	0.96	0.10	100,100,100,100	0
6	MG	C	502	1/1	0.97	0.13	52,52,52,52	0
5	GTP	A	501	32/32	0.98	0.16	48,55,60,64	0
8	GDP	B	501	28/28	0.99	0.15	47,53,57,60	0
5	GTP	C	501	32/32	0.99	0.17	42,49,54,57	0
6	MG	A	502	1/1	0.99	0.14	53,53,53,53	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.

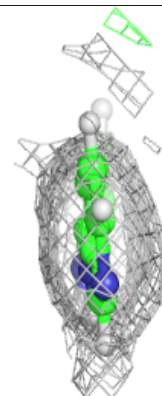
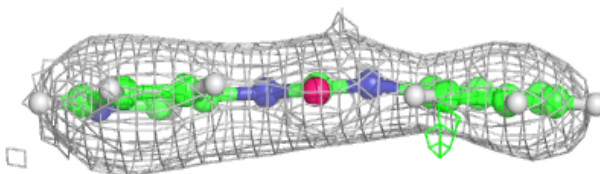
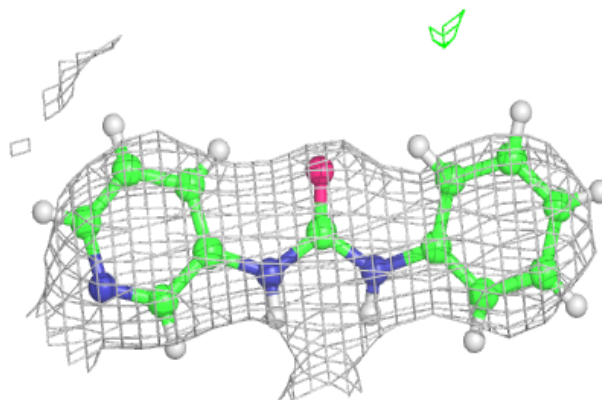


Electron density around ACP F 401:

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

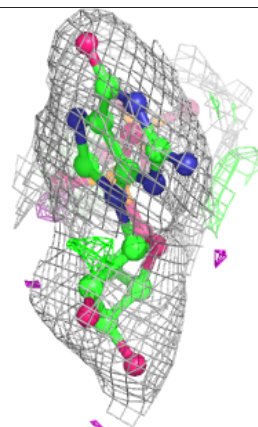
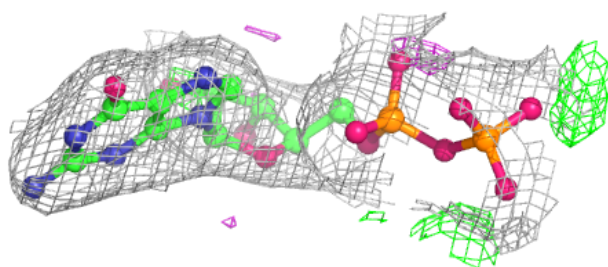
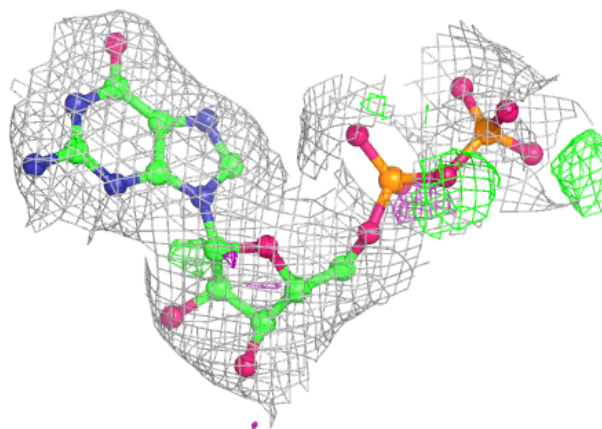
**Electron density around K0G B 505:**

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

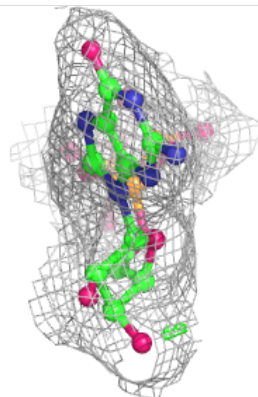
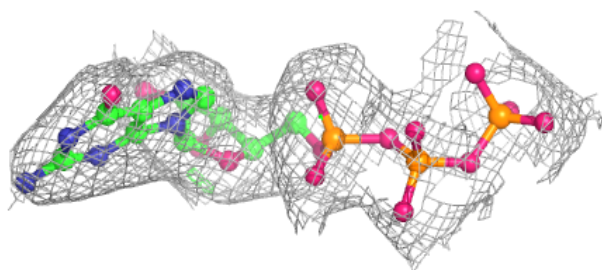
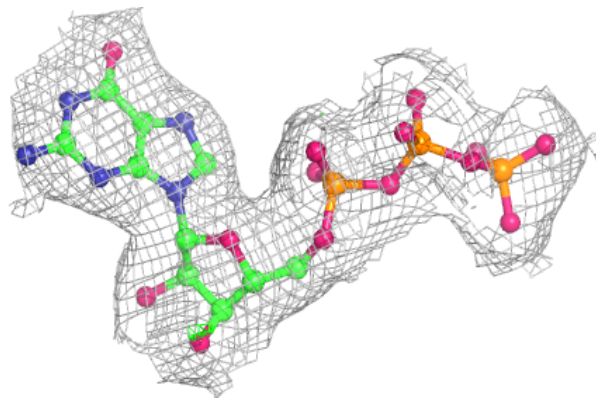


Electron density around GDP D 501:

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

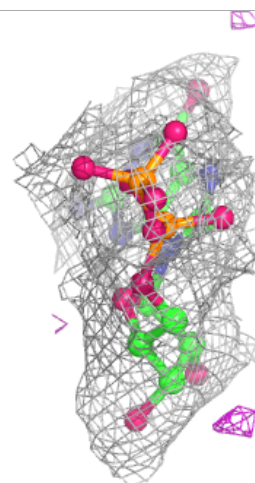
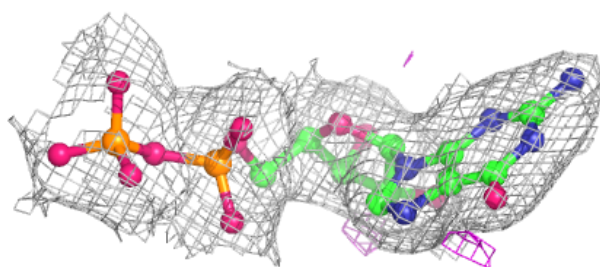
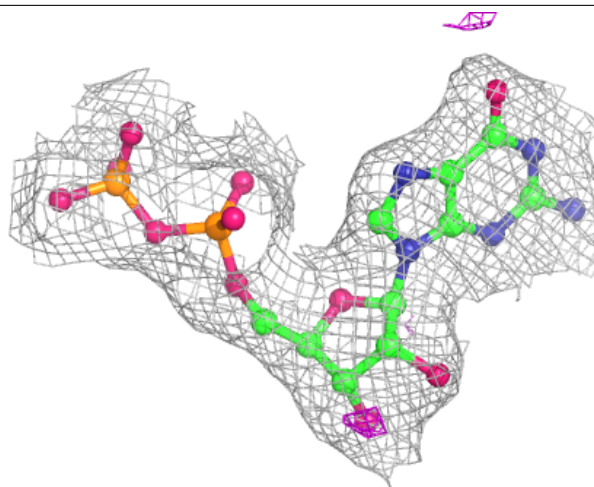
**Electron density around GTP A 501:**

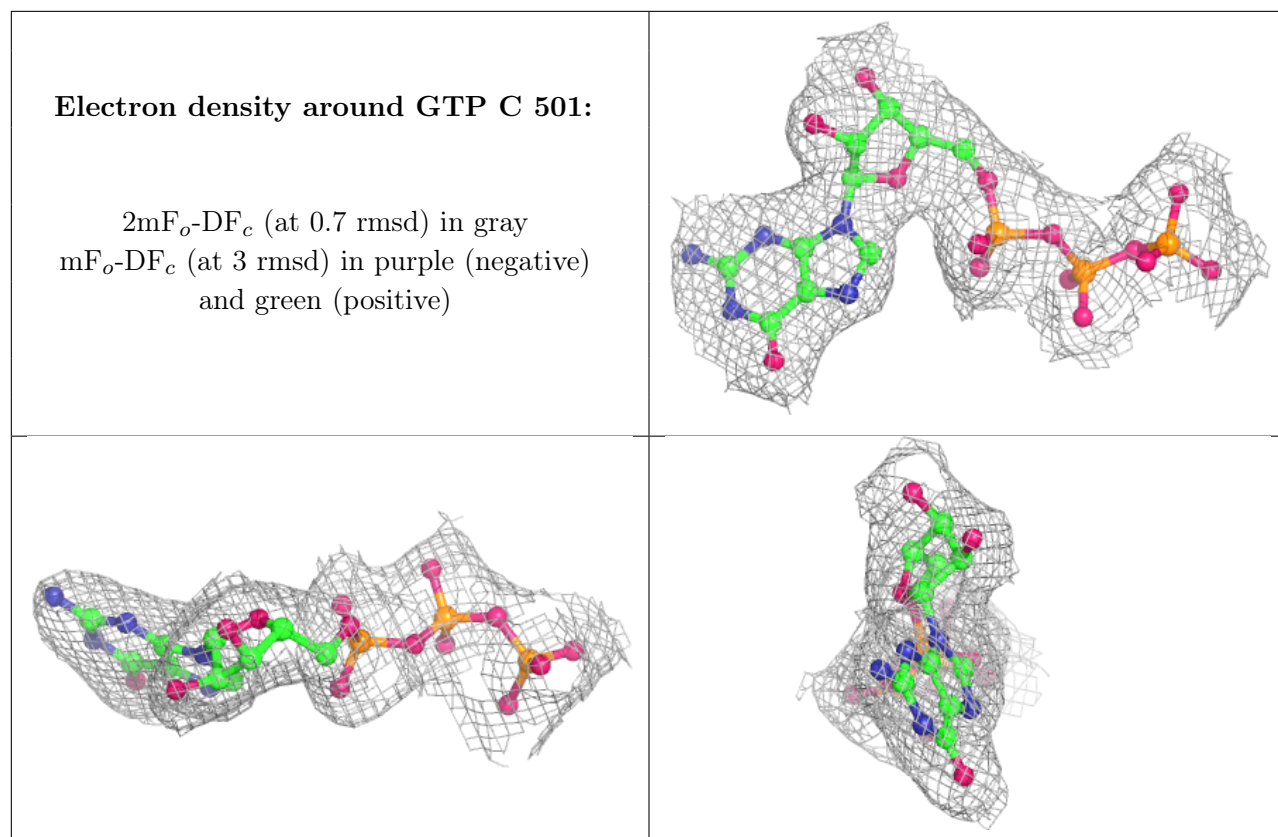
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.