



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:05 PM UTC

PDB ID : 7YHN / pdb_00007yhn
Title : ANTI-TUMOR AGENT Y48 IN COMPLEX WITH TUBULIN
Authors : Du, T.; Ji, M.; Hou, Z.; Lin, S.; Zhang, J.; Wu, D.; Zhang, K.; Lu, D.; Xu, H.;
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Deposited on : 2022-07-14
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

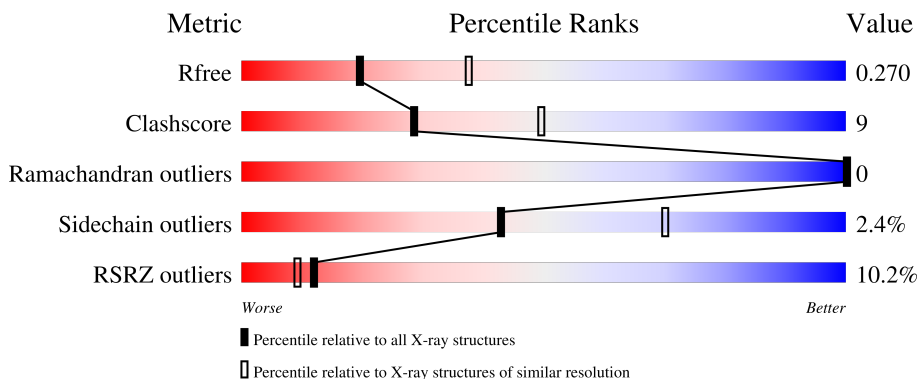
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	451	16% 75% 17% 8%
1	C	451	6% 78% 17% .
2	B	445	9% 72% 22% 6%
2	D	445	7% 72% 21% 6%
3	E	152	9% 62% 18% 19%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13868 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	415	Total	C	N	O	S	0	0	0
			3013	1902	505	587	19			
1	C	433	Total	C	N	O	S	0	0	0
			3316	2102	561	631	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3164	1990	528	622	24			
2	D	420	Total	C	N	O	S	0	0	0
			3201	2015	536	625	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	55	THR	ALA	conflict	UNP P02554
B	170	MET	VAL	conflict	UNP P02554
B	296	SER	ALA	conflict	UNP P02554
B	316	ILE	VAL	conflict	UNP P02554
D	55	THR	ALA	conflict	UNP P02554
D	170	MET	VAL	conflict	UNP P02554
D	296	SER	ALA	conflict	UNP P02554
D	316	ILE	VAL	conflict	UNP P02554

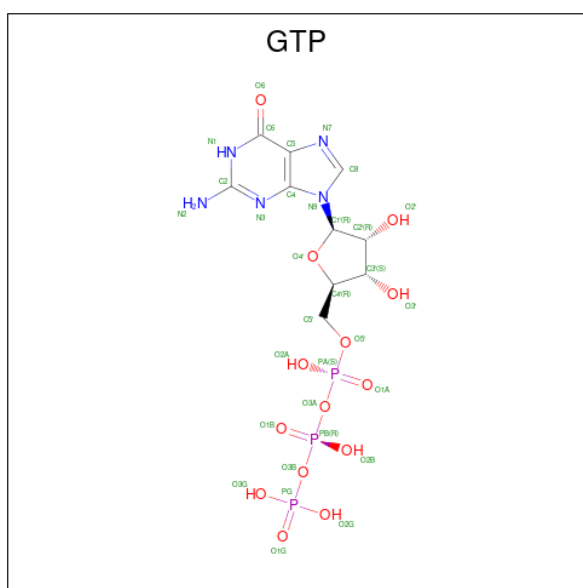
- Molecule 3 is a protein called Stathmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			952	587	171	190	4			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ALA	-	expression tag	UNP F2Z508
E	143	LEU	-	expression tag	UNP F2Z508
E	144	GLU	-	expression tag	UNP F2Z508
E	145	HIS	-	expression tag	UNP F2Z508
E	146	HIS	-	expression tag	UNP F2Z508
E	147	HIS	-	expression tag	UNP F2Z508
E	148	HIS	-	expression tag	UNP F2Z508
E	149	HIS	-	expression tag	UNP F2Z508
E	150	HIS	-	expression tag	UNP F2Z508
E	151	HIS	-	expression tag	UNP F2Z508
E	152	HIS	-	expression tag	UNP F2Z508

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

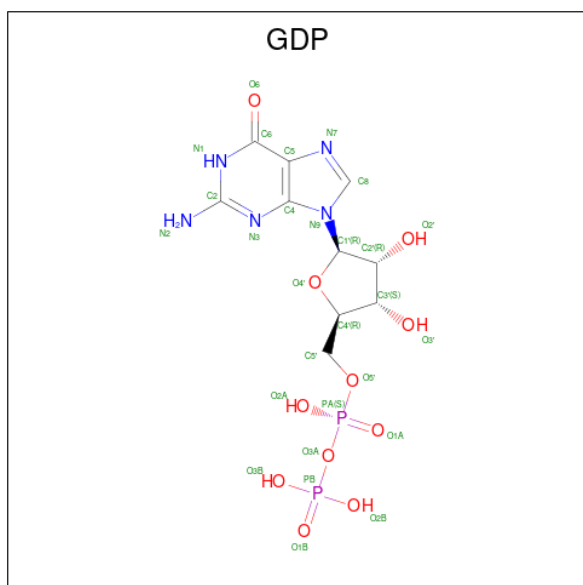
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	3	Total	Mg	0	0
			3	3		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



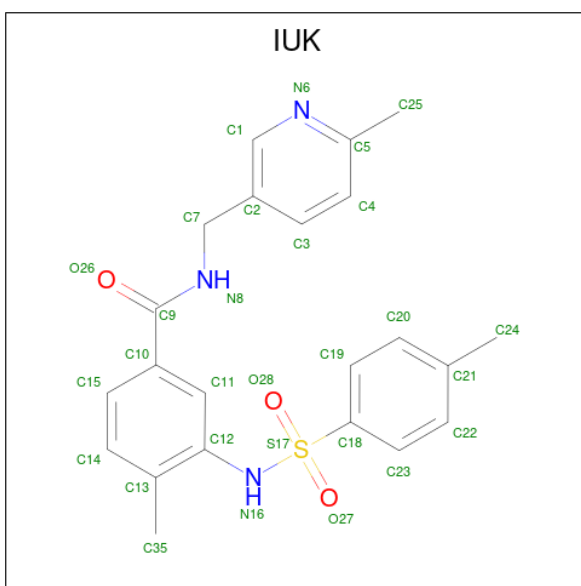
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 8 is 4-methyl-3-[(4-methylphenyl)sulfonylamino]- {N}-[(6-methylpyridin-3-yl)methyl]benzamide (CCD ID: IUK) (formula: $C_{22}H_{23}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			29	22	3	3	1		
8	D	1	Total	C	N	O	S	0	0
			29	22	3	3	1		

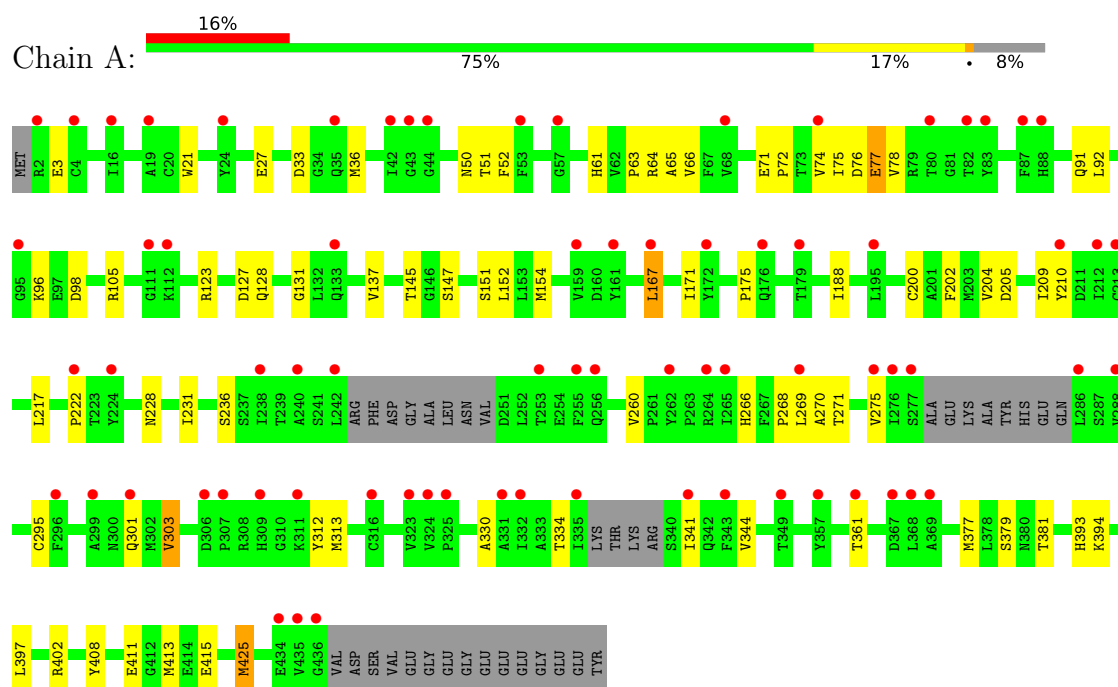
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total 2	O 2	0	0
9	B	6	Total 6	O 6	0	0
9	C	9	Total 9	O 9	0	0
9	D	5	Total 5	O 5	0	0

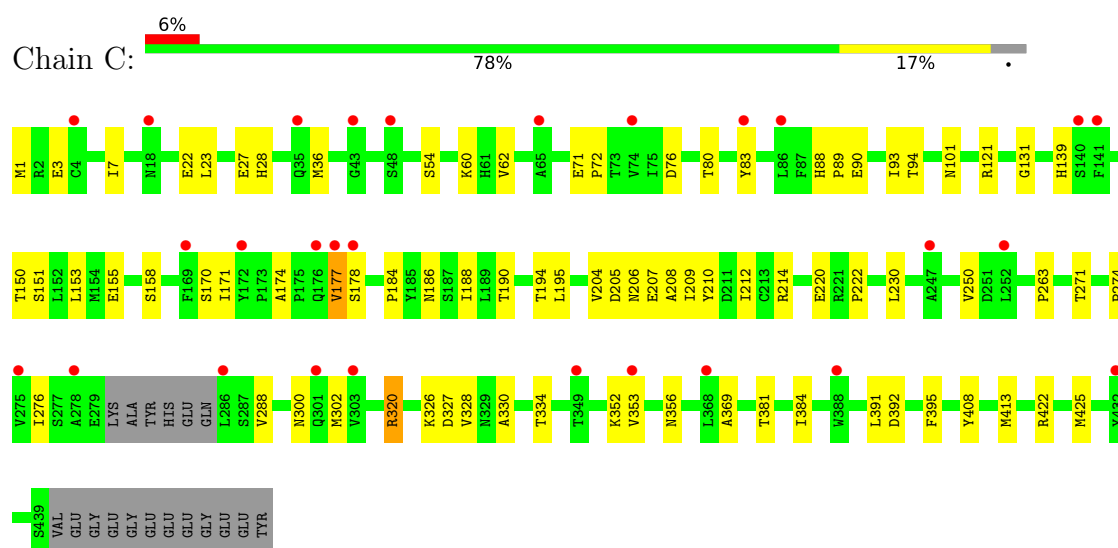
3 Residue-property plots

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

• Molecule 1: Tubulin alpha-1B chain



• Molecule 1: Tubulin alpha-1B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.87Å 102.03Å 131.13Å 90.00° 106.91° 90.00°	Depositor
Resolution (Å)	78.33 – 2.60 78.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (78.33-2.60) 99.1 (78.33-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.230 , 0.272 0.227 , 0.270	Depositor DCC
R_{free} test set	3216 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13868	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.54% 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: GTP, IUK, MG, MES, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/3079	0.46	0/4209
1	C	0.24	0/3390	0.46	0/4611
2	B	0.28	0/3236	0.47	0/4406
2	D	0.25	1/3272 (0.0%)	0.41	0/4448
3	E	0.21	0/960	0.39	0/1284
All	All	0.26	1/13937 (0.0%)	0.45	0/18958

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	107	THR	CA-C	5.16	1.55	1.52

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	3013	0	2720	45	0
1	C	3316	0	3188	50	0
2	B	3164	0	2897	64	0
2	D	3201	0	2984	64	0
3	E	952	0	907	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	12	1	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0
5	A	2	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
6	B	28	0	12	1	0
7	B	12	0	13	1	0
8	B	29	0	0	0	0
8	D	29	0	0	0	0
9	A	2	0	0	0	0
9	B	6	0	0	0	0
9	C	9	0	0	0	0
9	D	5	0	0	0	0
All	All	13868	0	12757	235	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 9.

All (235) 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:73:MET:HE2	2:B:92:PHE:HB3	1.63	0.78
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.72	0.71
2:D:180:VAL:HA	2:D:388:MET:HE1	1.75	0.67
2:B:152:ILE:HG12	2:B:164:MET:HE3	1.76	0.66
3:E:128:GLU:HG3	3:E:131:ARG:HH21	1.60	0.66
1:A:408:TYR:HB3	1:A:413:MET:HE2	1.78	0.65
1:C:88:HIS:CD2	1:C:90:GLU:HB2	2.32	0.64
1:C:250:VAL:HG22	1:C:352:LYS:HE2	1.79	0.64
2:D:267:MET:HE2	2:D:299:MET:HE3	1.80	0.63
1:A:397:LEU:HD12	2:B:346:PRO:HG3	1.81	0.63
2:B:343:GLU:H	2:B:343:GLU:CD	2.07	0.62
2:D:154:LYS:NZ	3:E:124:ASP:OD2	2.35	0.60
1:A:27:GLU:HA	1:A:361:THR:HG21	1.83	0.59
2:D:189:VAL:HG11	2:D:415:MET:HE3	1.86	0.58
2:D:378:PHE:HD1	2:D:415:MET:HE2	1.69	0.57
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.87	0.57
2:B:316:ILE:HB	2:B:366:THR:HG23	1.86	0.57
2:D:157:GLU:HG2	3:E:120:LEU:HD13	1.87	0.56
3:E:43:SER:HB3	3:E:46:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:MET:HE3	1:A:344:VAL:HG21	1.86	0.56
1:C:320:ARG:HA	1:C:356:ASN:O	2.06	0.55
2:D:267:MET:HG2	2:D:374:ILE:HD12	1.87	0.55
2:B:299:MET:HA	2:B:299:MET:HE2	1.89	0.55
2:B:293:MET:CG	2:B:367:PHE:HB2	2.35	0.55
1:A:295:CYS:HB3	1:A:377:MET:HE2	1.89	0.54
1:A:3:GLU:N	1:A:131:GLY:O	2.40	0.54
2:D:290:THR:HA	2:D:293:MET:HE2	1.89	0.54
2:B:318:ARG:HB3	2:B:357:PRO:HA	1.89	0.54
2:B:44:LEU:HA	2:B:47:ILE:HB	1.90	0.54
1:A:202:PHE:CE1	1:A:268:PRO:HG2	2.43	0.53
2:B:42:LEU:HA	2:B:45:GLU:HG3	1.91	0.53
1:C:208:ALA:O	1:C:212:ILE:HG13	2.09	0.53
1:C:214:ARG:HD3	1:C:220:GLU:O	2.09	0.52
2:D:161:ASP:OD1	2:D:161:ASP:N	2.40	0.52
2:D:296:SER:H	2:D:306:ARG:NH2	2.06	0.52
2:B:197:ASP:CG	7:B:502:MES:HN4	2.16	0.52
1:C:204:VAL:HG12	1:C:302:MET:HB3	1.91	0.52
2:D:28:HIS:HE1	2:D:241:ARG:HH11	1.56	0.52
3:E:99:ALA:O	3:E:103:GLU:HG3	2.09	0.52
1:A:312:TYR:HE1	1:A:341:ILE:HG12	1.74	0.52
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.91	0.52
1:C:23:LEU:O	1:C:27:GLU:HG3	2.08	0.52
2:D:299:MET:HE1	2:D:367:PHE:CE1	2.44	0.52
1:A:271:THR:HG23	1:A:301:GLN:HA	1.92	0.52
2:B:395:LEU:HD21	2:B:405:GLU:HG2	1.91	0.52
2:B:51:TYR:O	2:B:62:ARG:NH2	2.43	0.52
2:D:61:PRO:HD3	2:D:84:ILE:HG13	1.90	0.52
2:D:295:ASP:OD1	2:D:297:LYS:HD2	2.10	0.52
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.44	0.52
2:B:286:VAL:O	2:B:290:THR:HG23	2.10	0.51
2:B:290:THR:HG21	2:B:329:GLN:HB3	1.90	0.51
1:C:330:ALA:O	1:C:334:THR:HG23	2.11	0.51
2:D:327:ASP:O	2:D:331:LEU:HD13	2.11	0.51
2:B:309:ARG:NH2	2:B:426:GLN:O	2.44	0.51
2:B:375:GLN:OE1	2:B:423:GLN:HG2	2.09	0.51
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.92	0.51
2:B:249:ASP:OD2	2:B:252:LYS:HD2	2.10	0.51
1:A:217:LEU:HD21	1:A:275:VAL:HG12	1.92	0.51
2:B:155:ILE:HD11	2:B:164:MET:HE2	1.93	0.51
2:D:293:MET:HG3	2:D:367:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LEU:HD23	2:B:365:ALA:HB2	1.93	0.50
1:C:76:ASP:O	1:C:80:THR:HG23	2.11	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.47	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
2:B:293:MET:HE2	2:B:365:ALA:HB1	1.94	0.50
2:B:169:VAL:HA	2:B:202:ILE:O	2.11	0.50
2:D:3:GLU:OE1	2:D:3:GLU:N	2.45	0.50
3:E:62:GLU:O	3:E:66:LEU:HG	2.12	0.50
1:C:395:PHE:CD1	1:C:422:ARG:HD3	2.46	0.49
2:D:379:LYS:O	2:D:383:GLU:HG3	2.12	0.49
2:B:68:LEU:HG	2:B:147:MET:HE2	1.94	0.49
2:B:251:ARG:O	2:B:255:VAL:HG13	2.12	0.49
1:C:392:ASP:HB3	1:C:422:ARG:CZ	2.42	0.49
3:E:127:ALA:HB1	3:E:131:ARG:HH12	1.78	0.49
2:D:45:GLU:HB2	2:D:243:PRO:HG3	1.95	0.49
1:C:88:HIS:NE2	1:C:90:GLU:HB2	2.27	0.48
2:D:382:SER:O	2:D:386:THR:OG1	2.25	0.48
3:E:43:SER:CB	3:E:46:GLU:HG2	2.44	0.48
1:A:312:TYR:CE1	1:A:341:ILE:HG12	2.49	0.48
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.93	0.48
1:A:171:ILE:HD13	1:A:204:VAL:HG13	1.95	0.48
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.96	0.48
1:C:93:ILE:HD11	1:C:121:ARG:HD3	1.96	0.48
1:A:123:ARG:NH1	1:A:127:ASP:OD1	2.46	0.48
2:D:375:GLN:O	2:D:379:LYS:HG3	2.14	0.48
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.48	0.48
1:C:151:SER:O	1:C:155:GLU:HG3	2.14	0.48
1:C:171:ILE:HD13	1:C:204:VAL:HG23	1.94	0.48
2:D:232:THR:HG21	2:D:300:MET:HG3	1.96	0.48
2:D:293:MET:HE1	2:D:317:PHE:CZ	2.49	0.47
3:E:41:ASP:OD1	3:E:41:ASP:N	2.47	0.47
2:D:131:GLN:HB3	2:D:250:LEU:HD12	1.97	0.47
1:A:63:PRO:O	1:A:91:GLN:NE2	2.47	0.47
2:B:252:LYS:O	2:B:255:VAL:HG22	2.13	0.47
2:D:4:ILE:HD12	2:D:49:VAL:HG12	1.95	0.47
2:D:112:LEU:HD23	2:D:147:MET:HE1	1.96	0.47
2:D:171:PRO:HB3	2:D:181:GLU:OE1	2.14	0.47
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.96	0.47
2:D:134:GLN:HA	2:D:165:ASN:O	2.13	0.47
1:A:27:GLU:OE2	1:A:236:SER:OG	2.27	0.47
1:A:312:TYR:CD2	1:A:379:SER:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:ND1	1:C:89:PRO:HD2	2.30	0.47
1:C:177:VAL:HG21	1:C:206:ASN:HB3	1.97	0.47
1:C:274:PRO:HB2	1:C:276:ILE:HD13	1.96	0.47
2:D:296:SER:HB3	2:D:305:PRO:HD2	1.95	0.47
1:C:54:SER:HB3	1:C:62:VAL:HG22	1.97	0.47
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.49	0.47
2:D:228:LEU:O	2:D:232:THR:HG23	2.14	0.47
1:C:271:THR:HG23	1:C:300:ASN:O	2.15	0.47
2:D:12:CYS:O	2:D:16:ILE:HG12	2.15	0.47
1:A:65:ALA:O	1:A:91:GLN:HG2	2.14	0.47
2:B:189:VAL:HG11	2:B:415:MET:HG3	1.96	0.47
2:B:396:HIS:CG	1:C:263:PRO:HD3	2.50	0.47
2:B:189:VAL:O	2:B:193:VAL:HG23	2.14	0.46
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.98	0.46
1:A:152:LEU:HD11	3:E:51:LEU:HD11	1.98	0.46
3:E:67:LYS:O	3:E:71:GLU:HG3	2.15	0.46
2:B:36:TYR:CE2	2:B:44:LEU:HD11	2.51	0.46
2:B:237:THR:O	2:B:241:ARG:HG3	2.16	0.45
2:D:43:GLN:O	2:D:47:ILE:HD12	2.17	0.45
1:A:402:ARG:NE	1:A:415:GLU:OE2	2.38	0.45
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.52	0.45
1:C:209:ILE:H	1:C:209:ILE:HD12	1.82	0.45
3:E:97:LYS:HG3	3:E:98:LEU:N	2.31	0.45
1:A:145:THR:HG23	4:A:501:GTP:O2G	2.16	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.52	0.45
1:C:302:MET:N	1:C:302:MET:HE2	2.32	0.45
2:D:107:THR:OG1	2:D:108:GLU:N	2.50	0.45
1:A:330:ALA:O	1:A:334:THR:HG23	2.17	0.45
2:B:31:ASP:OD1	2:B:33:THR:HG22	2.17	0.45
2:B:203:ASP:CG	2:B:380:ARG:HH22	2.24	0.45
1:C:408:TYR:O	1:C:413:MET:HB2	2.17	0.45
2:D:237:THR:O	2:D:241:ARG:HG3	2.17	0.45
3:E:133:ASN:O	3:E:137:LYS:HG3	2.17	0.45
2:D:156:ARG:HH12	2:D:194:GLU:CD	2.25	0.45
2:D:238:THR:OG1	2:D:316:ILE:HG21	2.16	0.45
3:E:69:LEU:O	3:E:73:ARG:HG2	2.17	0.45
2:B:48:ASN:O	2:B:62:ARG:NH2	2.41	0.44
2:B:134:GLN:HA	2:B:165:ASN:O	2.18	0.44
2:B:245:GLN:CB	2:B:248:ALA:HB2	2.47	0.44
2:D:7:ILE:O	2:D:135:LEU:HA	2.17	0.44
1:A:105:ARG:NH1	1:A:411:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PRO:HG3	1:A:394:LYS:NZ	2.33	0.44
2:B:11:GLN:HA	2:B:72:THR:HG21	1.99	0.44
1:C:384:ILE:H	1:C:384:ILE:HG13	1.58	0.44
2:D:81:PHE:O	2:D:84:ILE:HG22	2.18	0.44
3:E:125:LYS:O	3:E:129:GLU:HG3	2.18	0.44
1:A:393:HIS:O	1:A:397:LEU:HG	2.18	0.44
1:A:204:VAL:HG23	1:A:209:ILE:HD11	2.00	0.44
3:E:9:ASN:N	3:E:9:ASN:OD1	2.50	0.44
1:A:175:PRO:HG3	1:A:394:LYS:HZ1	1.83	0.44
2:D:28:HIS:CE1	2:D:241:ARG:HH11	2.36	0.44
1:C:276:ILE:HG22	1:C:369:ALA:HB3	2.00	0.43
2:D:392:LYS:HG2	2:D:395:LEU:HD12	1.99	0.43
1:A:74:VAL:O	1:A:77:GLU:HG2	2.18	0.43
1:C:184:PRO:O	1:C:188:ILE:HG12	2.18	0.43
1:C:190:THR:O	1:C:194:THR:HG23	2.18	0.43
2:B:330:MET:HE2	2:B:330:MET:HB2	1.59	0.43
1:C:174:ALA:O	1:C:178:SER:N	2.51	0.43
2:B:345:ILE:HG22	2:B:348:ASN:HB3	2.01	0.43
1:C:28:HIS:HB3	1:C:36:MET:HE3	2.01	0.43
1:C:60:LYS:HE2	1:C:60:LYS:HB3	1.53	0.43
2:D:156:ARG:NE	3:E:116:MET:HE3	2.34	0.43
2:B:325:GLU:O	2:B:329:GLN:HG2	2.19	0.43
2:D:68:LEU:HD21	2:D:109:GLY:HA2	2.00	0.43
1:A:91:GLN:C	1:A:92:LEU:HD23	2.44	0.43
2:B:12:CYS:HB3	2:B:138:SER:HB3	2.01	0.43
2:D:189:VAL:O	2:D:193:VAL:HG23	2.18	0.43
2:B:46:ARG:HH11	2:B:46:ARG:HG2	1.84	0.43
1:A:50:ASN:O	1:A:64:ARG:NH1	2.52	0.43
2:D:350:LYS:HA	2:D:350:LYS:HD3	1.79	0.43
1:A:188:ILE:HG23	1:A:425:MET:HG3	2.00	0.43
1:A:269:LEU:HD22	1:A:270:ALA:H	1.84	0.43
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.54	0.43
2:B:179:VAL:O	2:B:388:MET:HE1	2.18	0.43
1:C:205:ASP:O	1:C:209:ILE:HD12	2.19	0.43
2:D:130:LEU:HD21	2:D:133:PHE:CZ	2.54	0.43
2:B:267:MET:HG2	2:B:374:ILE:HD12	2.01	0.42
1:A:3:GLU:HA	1:A:51:THR:HA	2.02	0.42
1:A:64:ARG:NH2	1:A:128:GLN:O	2.52	0.42
1:C:158:SER:HB3	3:E:90:PHE:CZ	2.54	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.42
1:A:52:PHE:C	1:A:64:ARG:HG3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:THR:HA	2:B:422:TYR:CD1	2.55	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.01	0.42
2:B:132:GLY:HA3	2:B:163:ILE:O	2.20	0.42
2:B:257:MET:HE3	2:B:257:MET:HB3	1.87	0.42
2:B:317:PHE:CZ	2:B:330:MET:HE1	2.54	0.42
1:C:1:MET:HG3	1:C:131:GLY:HA3	2.01	0.42
2:B:120:VAL:O	2:B:124:SER:OG	2.28	0.42
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.01	0.42
1:C:158:SER:HB3	3:E:90:PHE:CE2	2.54	0.42
1:C:186:ASN:O	1:C:190:THR:HG22	2.19	0.42
1:A:72:PRO:HB2	1:A:76:ASP:OD2	2.19	0.42
1:C:90:GLU:N	1:C:90:GLU:OE1	2.53	0.42
2:D:156:ARG:HG2	3:E:120:LEU:HD11	2.01	0.42
2:B:65:LEU:HD22	2:B:90:PHE:CE2	2.55	0.42
2:B:348:ASN:OD1	2:B:348:ASN:N	2.42	0.42
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.90	0.42
1:A:52:PHE:O	1:A:64:ARG:HG3	2.20	0.41
2:B:172:SER:HB2	2:B:205:GLU:HB2	2.02	0.41
2:B:203:ASP:O	2:B:207:LEU:HG	2.19	0.41
3:E:57:ARG:HA	3:E:57:ARG:HD2	1.78	0.41
2:D:149:THR:HG21	2:D:188:SER:HA	2.01	0.41
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.01	0.41
2:B:54:ALA:N	2:B:58:LYS:O	2.51	0.41
1:A:228:ASN:HA	1:A:231:ILE:HD12	2.03	0.41
2:B:101:TRP:HB2	2:B:184:ASN:OD1	2.20	0.41
2:B:379:LYS:O	2:B:383:GLU:HG3	2.20	0.41
2:D:87:PRO:HA	2:D:90:PHE:CD1	2.55	0.41
2:D:203:ASP:HB2	2:D:301:ALA:HA	2.02	0.41
1:C:90:GLU:HG3	1:C:121:ARG:HH21	1.85	0.41
2:B:293:MET:CE	2:B:365:ALA:HB1	2.50	0.41
2:B:311:LEU:HD11	2:B:372:THR:HG22	2.02	0.41
1:C:3:GLU:H	1:C:3:GLU:CD	2.27	0.41
2:D:167:PHE:CD1	2:D:233:MET:HE3	2.56	0.41
1:C:101:ASN:ND2	2:D:252:LYS:HE2	2.36	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.41
2:D:295:ASP:HB3	2:D:298:ASN:HD22	1.85	0.41
1:C:22:GLU:HG3	1:C:83:TYR:CE2	2.56	0.41
2:D:159:TYR:HB3	2:D:162:ARG:HG3	2.03	0.41
2:D:403:MET:HE2	2:D:403:MET:HB3	1.84	0.41
3:E:128:GLU:O	3:E:132:LYS:HG3	2.21	0.41
1:C:328:VAL:HG11	1:C:353:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:HIS:HE1	2:D:241:ARG:HD2	1.86	0.40
2:D:304:ASP:HB3	2:D:307:HIS:HD1	1.86	0.40
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.55	0.40
1:C:326:LYS:HG3	1:C:327:ASP:N	2.36	0.40
1:A:147:SER:O	1:A:151:SER:OG	2.38	0.40
2:B:91:VAL:HG12	2:B:112:LEU:HD11	2.04	0.40
2:B:212:PHE:CD1	2:B:218:THR:O	2.75	0.40
2:D:87:PRO:HA	2:D:90:PHE:CE1	2.56	0.40
2:B:293:MET:HG3	2:B:367:PHE:HB2	2.02	0.40
2:D:156:ARG:NH1	2:D:194:GLU:OE1	2.54	0.40
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.61	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	407/451 (90%)	385 (95%)	22 (5%)	0	100	100
1	C	429/451 (95%)	413 (96%)	16 (4%)	0	100	100
2	B	415/445 (93%)	394 (95%)	21 (5%)	0	100	100
2	D	414/445 (93%)	400 (97%)	14 (3%)	0	100	100
3	E	119/152 (78%)	118 (99%)	1 (1%)	0	100	100
All	All	1784/1944 (92%)	1710 (96%)	74 (4%)	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	294/379 (78%)	282 (96%)	12 (4%)	27	54
1	C	350/379 (92%)	342 (98%)	8 (2%)	44	71
2	B	328/383 (86%)	324 (99%)	4 (1%)	63	83
2	D	337/383 (88%)	331 (98%)	6 (2%)	51	76
3	E	94/136 (69%)	91 (97%)	3 (3%)	34	62
All	All	1403/1660 (84%)	1370 (98%)	33 (2%)	43	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	66	VAL
1	A	75	ILE
1	A	77	GLU
1	A	78	VAL
1	A	96	LYS
1	A	137	VAL
1	A	154	MET
1	A	167	LEU
1	A	303	VAL
1	A	381	THR
1	A	425	MET
2	B	219	THR
2	B	338	SER
2	B	348	ASN
2	B	423	GLN
1	C	94	THR
1	C	170	SER
1	C	177	VAL
1	C	195	LEU
1	C	230	LEU
1	C	288	VAL
1	C	320	ARG
1	C	381	THR
2	D	84	ILE
2	D	267	MET
2	D	322	SER

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Mol	Chain	Res	Type
2	D	350	LYS
2	D	364	SER
2	D	399	THR
3	E	9	ASN
3	E	49	LYS
3	E	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	393	HIS
2	B	423	GLN
1	C	50	ASN
1	C	101	ASN
1	C	329	ASN
2	D	11	GLN
2	D	99	ASN
2	D	256	ASN
2	D	384	GLN
3	E	89	ASN
3	E	112	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 13 ligands modelled in this entry, 6 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	$\# Z > 2$
7	MES	B	502	-	12,12,12	0.69	0	15,16,16	0.30	0
8	IUK	D	503	-	31,31,31	4.42	17 (54%)	44,44,44	2.59	6 (13%)
8	IUK	B	503	-	31,31,31	4.33	17 (54%)	44,44,44	2.64	8 (18%)
4	GTP	C	502	5	33,34,34	0.58	0	50,54,54	0.50	0
4	GTP	D	501	5	33,34,34	0.56	0	50,54,54	0.49	0
4	GTP	A	501	5	33,34,34	0.59	0	50,54,54	0.49	0
6	GDP	B	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.72	5 (11%)

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
7	MES	B	502	-	-	0/6/14/14	0/1/1/1
8	IUK	D	503	-	-	0/20/20/20	0/3/3/3
8	IUK	B	503	-	-	0/20/20/20	0/3/3/3
4	GTP	C	502	5	-	8/22/38/38	0/3/3/3
4	GTP	D	501	5	-	8/22/38/38	0/3/3/3
4	GTP	A	501	5	-	7/22/38/38	0/3/3/3
6	GDP	B	501	-	-	4/16/32/32	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	IUK	C23-C18	9.31	1.53	1.38
8	D	503	IUK	C15-C10	9.05	1.53	1.39
8	D	503	IUK	C19-C20	8.91	1.53	1.38
8	B	503	IUK	C19-C20	8.90	1.53	1.38
8	B	503	IUK	C23-C18	8.81	1.52	1.38
8	B	503	IUK	C15-C10	8.70	1.52	1.39
8	D	503	IUK	C11-C12	8.37	1.52	1.39
8	B	503	IUK	C11-C12	8.24	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	IUK	C14-C13	6.78	1.53	1.39
8	B	503	IUK	C14-C13	6.60	1.53	1.39
8	D	503	IUK	C22-C21	5.95	1.53	1.38
8	B	503	IUK	C22-C21	5.94	1.52	1.38
8	D	503	IUK	S17-N16	5.20	1.71	1.63
8	D	503	IUK	C9-N8	5.19	1.45	1.33
8	D	503	IUK	C11-C10	-5.14	1.31	1.39
8	B	503	IUK	C11-C10	-5.13	1.31	1.39
8	B	503	IUK	C9-N8	4.94	1.44	1.33
8	B	503	IUK	S17-N16	4.94	1.71	1.63
8	B	503	IUK	C15-C14	-4.33	1.31	1.38
8	B	503	IUK	C19-C18	-4.32	1.32	1.38
8	D	503	IUK	C12-C13	-4.32	1.31	1.40
8	D	503	IUK	C19-C18	-4.29	1.32	1.38
8	B	503	IUK	C23-C22	-4.28	1.31	1.38
8	B	503	IUK	C12-C13	-4.24	1.32	1.40
8	D	503	IUK	C15-C14	-4.17	1.32	1.38
8	D	503	IUK	C23-C22	-4.12	1.32	1.38
8	D	503	IUK	C18-S17	3.49	1.81	1.76
8	D	503	IUK	O27-S17	3.25	1.47	1.43
8	B	503	IUK	C18-S17	3.23	1.81	1.76
6	B	501	GDP	C5-C4	3.05	1.47	1.38
8	B	503	IUK	O27-S17	2.99	1.47	1.43
8	B	503	IUK	O28-S17	2.98	1.47	1.43
8	B	503	IUK	C20-C21	-2.81	1.32	1.38
8	D	503	IUK	O28-S17	2.78	1.46	1.43
8	D	503	IUK	C20-C21	-2.73	1.32	1.38
6	B	501	GDP	C6-N1	-2.24	1.34	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	IUK	O28-S17-O27	-14.87	101.46	119.52
8	D	503	IUK	O28-S17-O27	-14.82	101.53	119.52
6	B	501	GDP	C5-C4-N3	-5.48	119.67	128.39
6	B	501	GDP	C2-N3-C4	5.06	121.02	112.30
6	B	501	GDP	C6-C5-N7	3.99	137.55	130.29
6	B	501	GDP	N9-C4-N3	3.85	133.66	125.95
8	B	503	IUK	C14-C13-C12	3.45	120.73	117.50
8	B	503	IUK	O27-S17-C18	3.36	112.22	107.98
8	D	503	IUK	C14-C13-C12	3.31	120.60	117.50
8	B	503	IUK	O28-S17-C18	3.15	111.95	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	IUK	O28-S17-C18	2.79	111.50	107.98
6	B	501	GDP	C4-C5-N7	-2.77	106.28	110.67
8	B	503	IUK	C2-C1-N6	-2.77	119.88	123.99
8	D	503	IUK	O27-S17-C18	2.75	111.44	107.98
8	D	503	IUK	C2-C1-N6	-2.59	120.14	123.99
8	D	503	IUK	O27-S17-N16	2.12	111.91	106.74
8	B	503	IUK	O28-S17-N16	2.09	111.84	106.74
8	B	503	IUK	C1-N6-C5	2.08	119.99	117.53
8	B	503	IUK	C3-C2-C1	2.04	120.10	117.10

There are no chirality outliers.

All (27) torsion outliers are listed below:

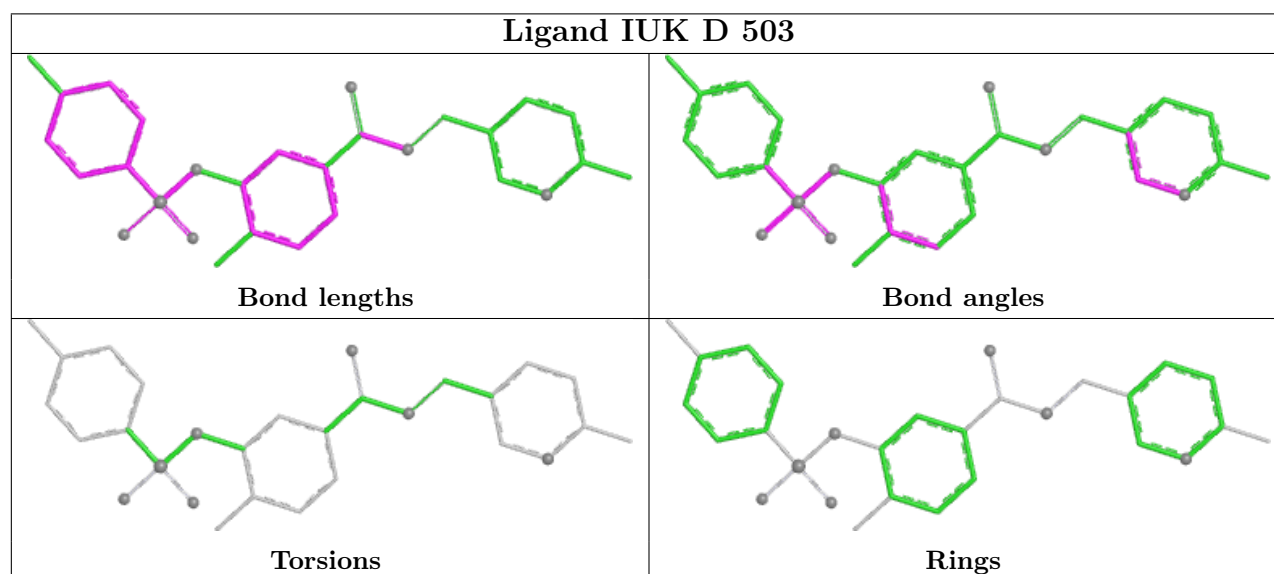
Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	C	502	GTP	C5'-O5'-PA-O3A
4	C	502	GTP	C5'-O5'-PA-O1A
4	C	502	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O3G
4	D	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	PB-O3B-PG-O1G
4	C	502	GTP	PB-O3B-PG-O1G
4	C	502	GTP	PB-O3A-PA-O2A
4	A	501	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O1G
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3B-PG-O3G
4	C	502	GTP	PB-O3B-PG-O2G
4	C	502	GTP	PB-O3B-PG-O3G
4	D	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3A-PA-O2A
4	C	502	GTP	PB-O3A-PA-O1A
4	D	501	GTP	PB-O3A-PA-O1A
4	D	501	GTP	PB-O3A-PA-O2A
6	B	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

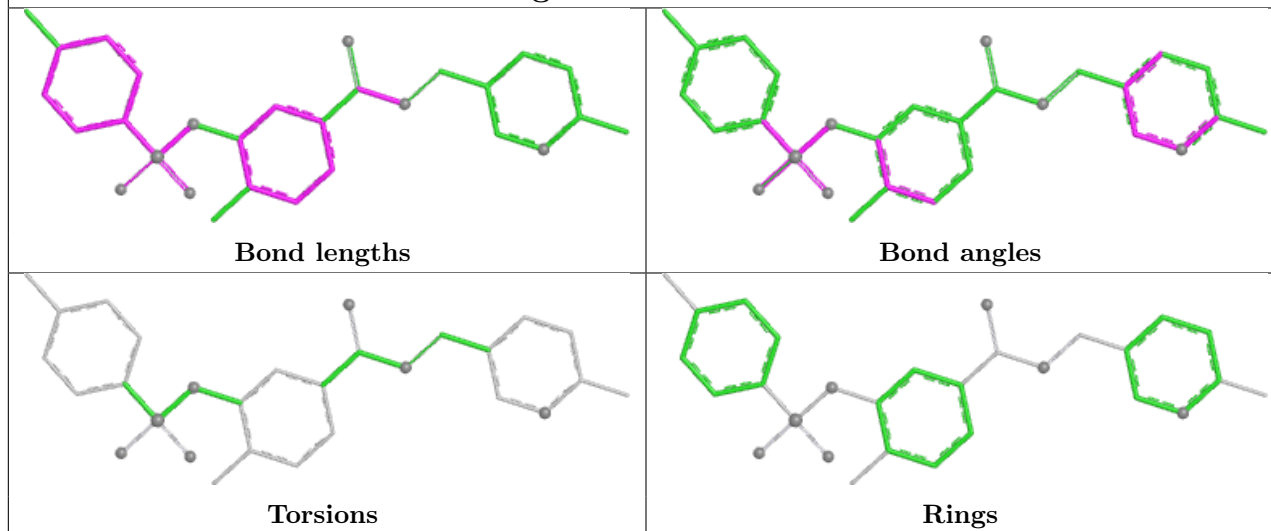
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	MES	1	0
4	A	501	GTP	1	0
6	B	501	GDP	1	0

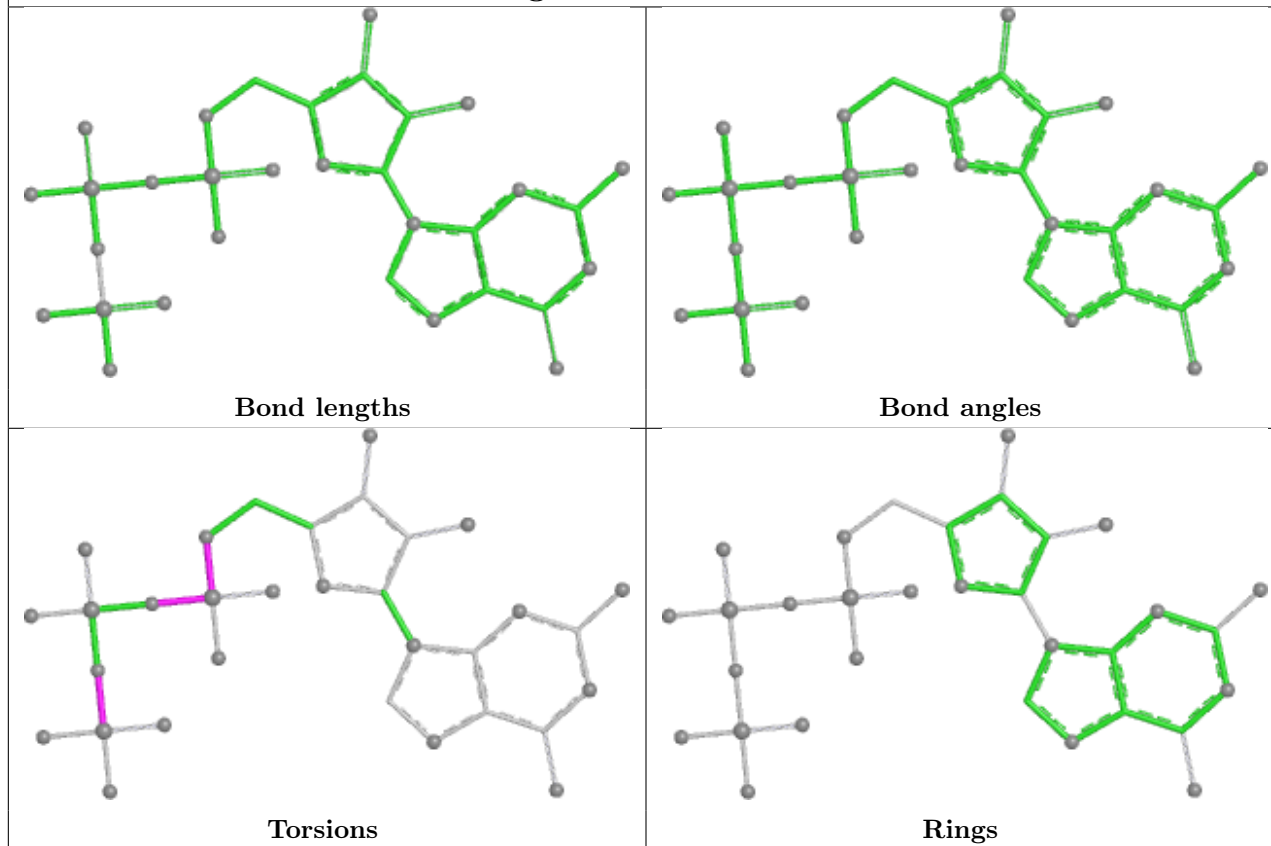
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

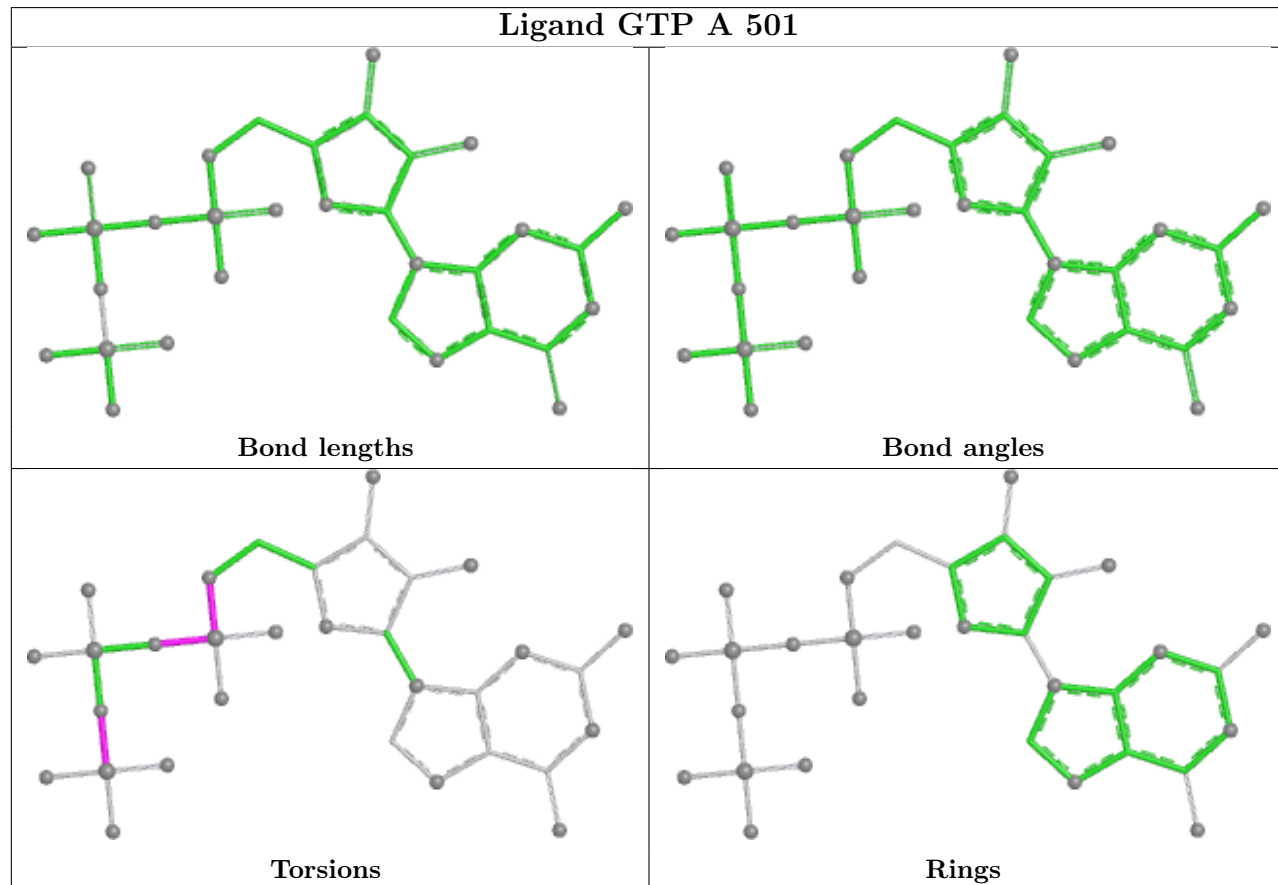
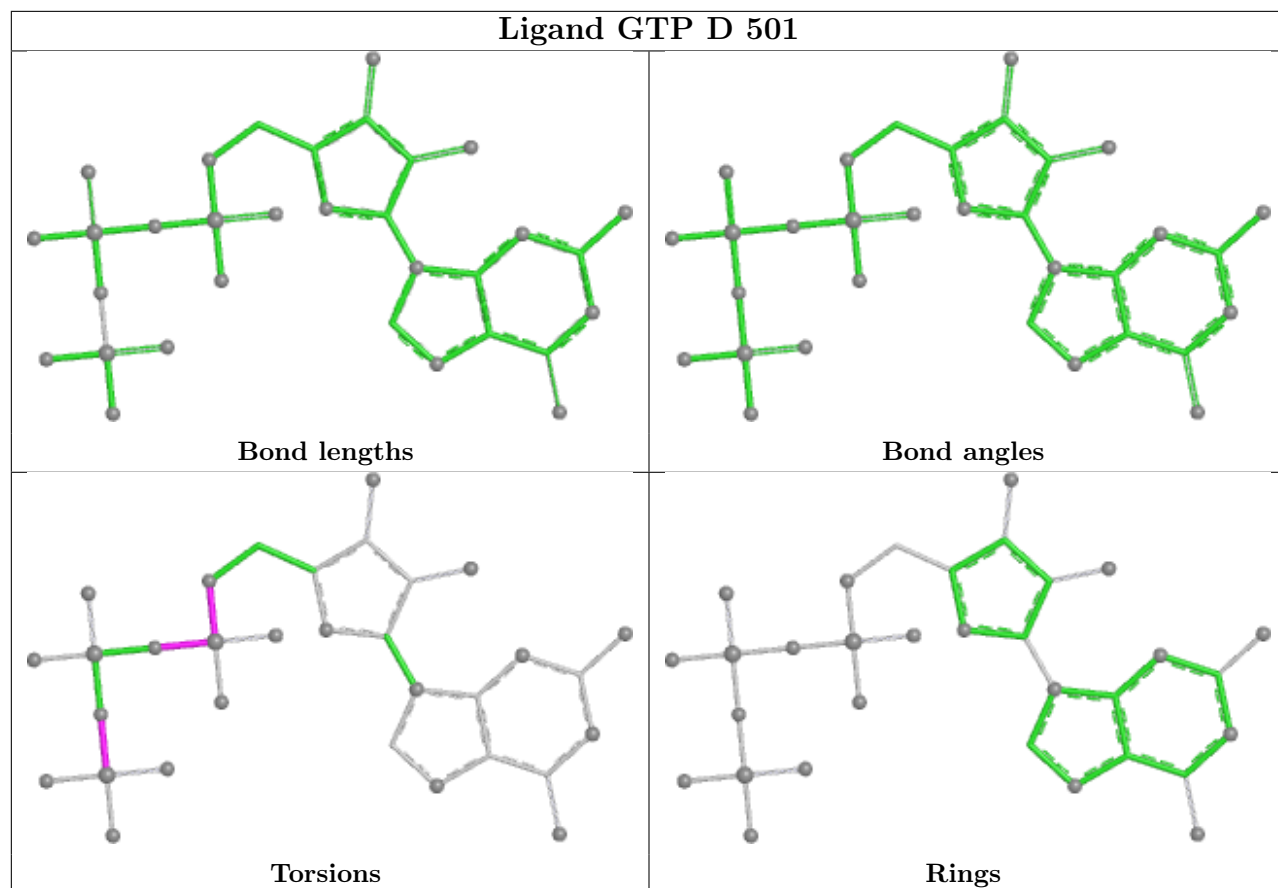


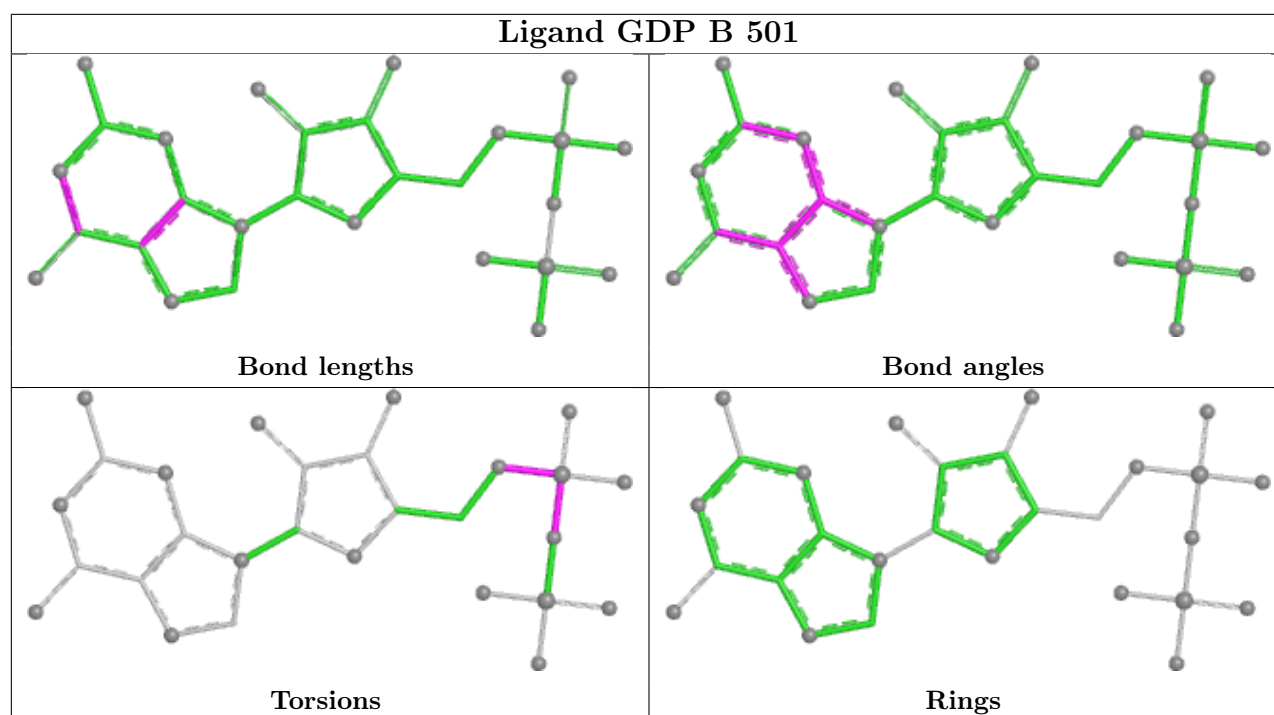
Ligand IUK B 503



Ligand GTP C 502







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	415/451 (92%)	1.33	74 (17%) 4 3	73, 102, 121, 134	0
1	C	433/451 (96%)	0.90	28 (6%) 25 19	60, 81, 104, 113	0
2	B	419/445 (94%)	0.92	39 (9%) 14 11	62, 82, 105, 124	0
2	D	420/445 (94%)	0.98	30 (7%) 22 17	63, 85, 114, 132	0
3	E	123/152 (80%)	1.01	14 (11%) 10 7	71, 89, 125, 139	0
All	All	1810/1944 (93%)	1.03	185 (10%) 12 9	60, 87, 116, 139	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	THR	4.4
2	B	247	ASN	4.2
1	C	18	ASN	4.1
1	C	178	SER	4.0
2	D	282	ARG	3.7
3	E	2	ASP	3.6
3	E	15	GLN	3.6
2	B	246	LEU	3.6
1	A	242	LEU	3.6
1	A	4	CYS	3.5
1	A	306	ASP	3.5
2	B	214	THR	3.4
2	B	285	THR	3.4
1	A	256	GLN	3.4
1	A	255	PHE	3.4
1	A	435	VAL	3.4
1	A	277	SER	3.3
1	A	80	THR	3.3
2	D	245	GLN	3.3
1	A	369	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	428	ALA	3.2
3	E	6	ILE	3.2
1	C	286	LEU	3.2
2	D	218	THR	3.2
2	D	81	PHE	3.2
1	C	275	VAL	3.1
1	A	436	GLY	3.0
1	A	301	GLN	3.0
1	A	42	ILE	3.0
1	A	335	ILE	3.0
2	B	215	LEU	2.9
1	C	35	GLN	2.9
1	A	57	GLY	2.9
1	A	331	ALA	2.9
1	A	309	HIS	2.9
1	A	159	VAL	2.9
2	D	42	LEU	2.9
2	B	248	ALA	2.8
2	D	360	GLY	2.8
1	A	112	LYS	2.8
1	A	238	ILE	2.7
1	C	349	THR	2.7
1	A	265	ILE	2.7
3	E	20	ILE	2.7
3	E	140	ALA	2.7
2	B	84	ILE	2.7
1	C	86	LEU	2.7
1	A	2	ARG	2.7
3	E	23	PRO	2.7
1	A	262	TYR	2.7
1	C	368	LEU	2.7
2	B	217	LEU	2.7
2	B	72	THR	2.7
1	A	357	TYR	2.6
2	B	360	GLY	2.6
1	A	296	PHE	2.6
2	B	284	LEU	2.6
1	C	4	CYS	2.6
2	D	89	ASN	2.6
1	A	195	LEU	2.6
1	A	368	LEU	2.6
2	B	359	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	111	GLY	2.6
2	D	430	ALA	2.6
1	A	276	ILE	2.6
1	C	301	GLN	2.6
1	C	278	ALA	2.5
1	A	16	ILE	2.5
1	C	172	TYR	2.5
1	C	247	ALA	2.5
1	A	316	CYS	2.5
1	A	24	TYR	2.5
2	D	40	SER	2.5
2	B	319	GLY	2.5
1	A	361	THR	2.4
2	D	195	ASN	2.4
1	A	167	LEU	2.4
2	B	2	ARG	2.4
1	A	68	VAL	2.4
2	D	77	ARG	2.4
2	D	395	LEU	2.4
2	B	216	LYS	2.4
1	A	95	GLY	2.4
2	B	425	TYR	2.3
2	D	35	SER	2.3
2	D	293	MET	2.3
1	A	275	VAL	2.3
1	A	286	LEU	2.3
2	D	361	LEU	2.3
2	B	176	SER	2.3
2	B	83	GLN	2.3
1	A	288	VAL	2.3
1	A	19	ALA	2.3
2	B	110	ALA	2.3
2	D	44	LEU	2.3
1	A	161	TYR	2.3
1	A	311	LYS	2.3
1	A	222	PRO	2.3
1	C	177	VAL	2.3
1	C	303	VAL	2.3
1	C	141	PHE	2.3
3	E	66	LEU	2.3
1	A	299	ALA	2.3
2	B	271	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	43	GLY	2.3
1	C	169	PHE	2.3
2	B	270	PHE	2.3
1	A	332	ILE	2.2
2	D	54	ALA	2.2
3	E	12	THR	2.2
1	C	48	SER	2.2
3	E	19	VAL	2.2
2	B	302	ALA	2.2
2	B	363	MET	2.2
1	A	83	TYR	2.2
1	A	172	TYR	2.2
2	D	80	PRO	2.2
2	D	171	PRO	2.2
1	A	323	VAL	2.2
1	C	353	VAL	2.2
1	A	87	PHE	2.2
2	D	274	THR	2.2
2	D	429	THR	2.2
1	A	35	GLN	2.2
1	A	367	ASP	2.2
1	C	252	LEU	2.2
1	A	53	PHE	2.2
1	A	341	ILE	2.2
1	A	349	THR	2.2
1	A	210	TYR	2.2
1	A	307	PRO	2.2
1	A	176	GLN	2.2
2	D	217	LEU	2.2
2	D	175	VAL	2.2
1	A	240	ALA	2.1
2	D	243	PRO	2.1
1	C	432	TYR	2.1
1	A	269	LEU	2.1
2	B	286	VAL	2.1
2	B	365	ALA	2.1
3	E	18	GLU	2.1
1	A	325	PRO	2.1
2	B	131	GLN	2.1
2	D	73	MET	2.1
1	A	224	TYR	2.1
2	D	130	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	HIS	2.1
2	D	67	ASP	2.1
2	D	177	ASP	2.1
1	A	434	GLU	2.1
1	A	179	THR	2.1
2	B	218	THR	2.1
2	B	340	TYR	2.1
1	A	74	VAL	2.1
1	A	324	VAL	2.1
1	C	140	SER	2.1
2	B	78	SER	2.1
3	E	43	SER	2.1
1	A	253	THR	2.1
2	B	323	MET	2.1
1	A	133	GLN	2.1
1	C	176	GLN	2.1
2	B	361	LEU	2.1
1	A	213	CYS	2.1
1	A	212	ILE	2.1
1	C	83	TYR	2.1
1	C	65	ALA	2.0
2	B	275	SER	2.0
1	C	388	TRP	2.0
2	B	293	MET	2.0
3	E	21	LEU	2.0
3	E	113	LEU	2.0
1	A	43	GLY	2.0
1	C	74	VAL	2.0
1	A	343	PHE	2.0
2	B	92	PHE	2.0
2	D	86	ARG	2.0
2	B	364	SER	2.0
3	E	3	MET	2.0
2	B	287	PRO	2.0
2	D	65	LEU	2.0
1	A	44	GLY	2.0
2	B	38	GLY	2.0
2	B	244	GLY	2.0
1	A	264	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

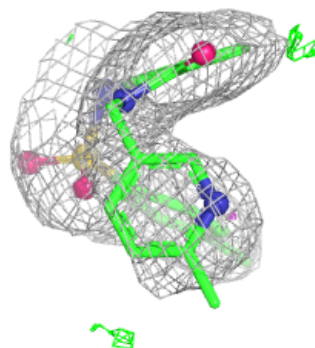
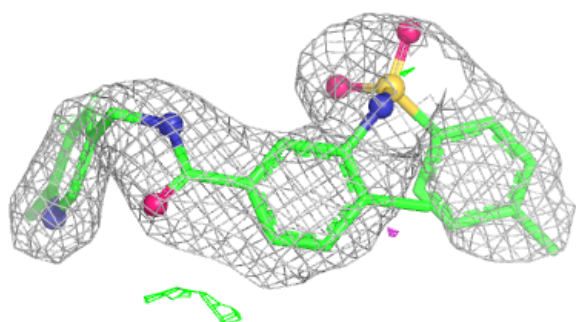
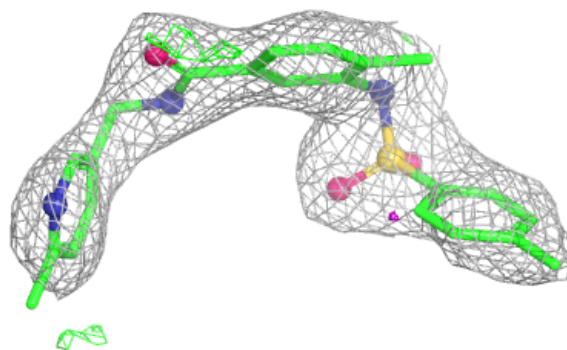
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	C	501	1/1	0.75	0.19	73,73,73,73	0
5	MG	D	502	1/1	0.82	0.26	82,82,82,82	0
5	MG	A	502	1/1	0.84	0.20	85,85,85,85	0
5	MG	A	503	1/1	0.85	0.15	106,106,106,106	0
8	IUK	D	503	29/29	0.89	0.15	77,85,90,94	0
8	IUK	B	503	29/29	0.92	0.12	76,81,87,88	0
4	GTP	D	501	32/32	0.92	0.10	58,79,84,85	0
4	GTP	C	502	32/32	0.93	0.12	67,80,87,92	0
7	MES	B	502	12/12	0.94	0.09	74,79,88,97	0
5	MG	C	504	1/1	0.95	0.10	93,93,93,93	0
5	MG	C	503	1/1	0.95	0.09	70,70,70,70	0
6	GDP	B	501	28/28	0.95	0.09	63,71,76,78	0
4	GTP	A	501	32/32	0.96	0.09	71,84,88,90	0

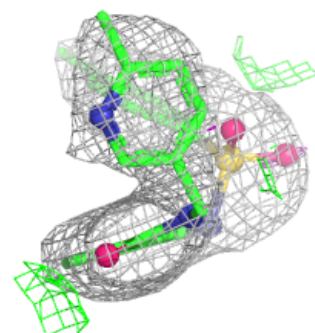
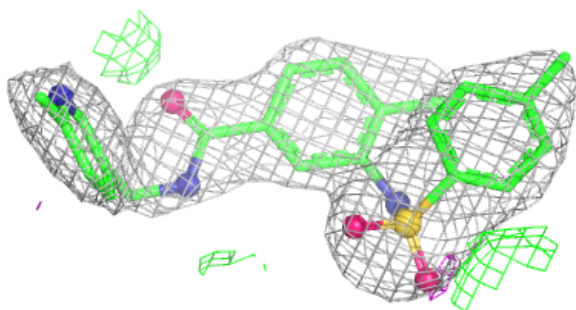
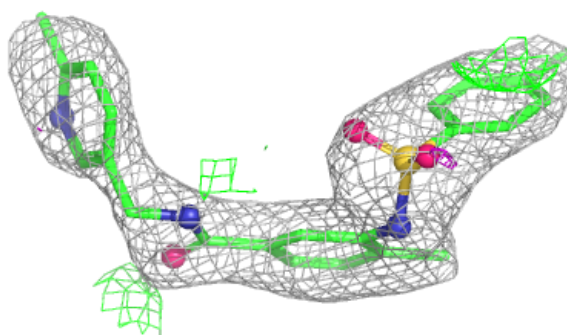
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around IUK 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)

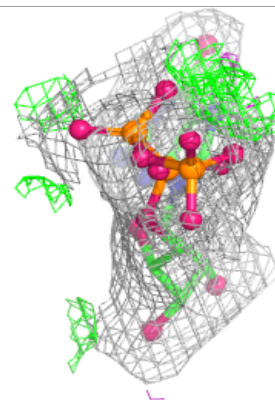
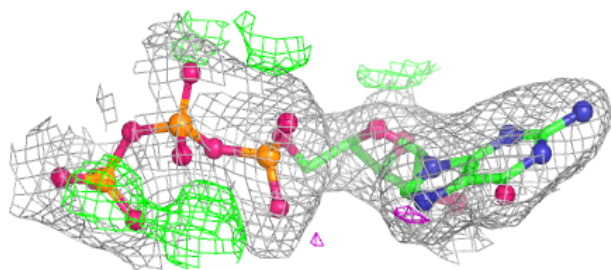
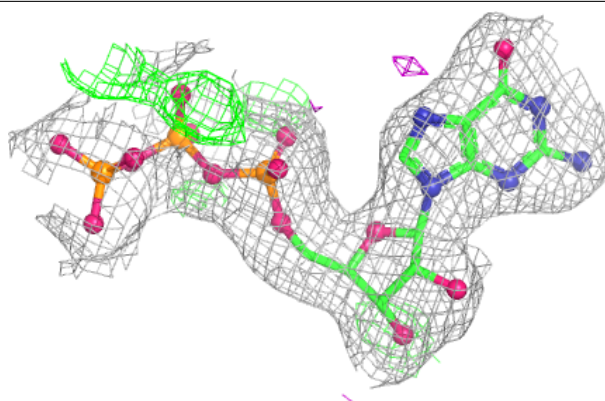
**Electron density around IUK B 503:**

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

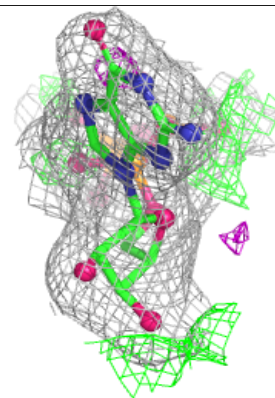
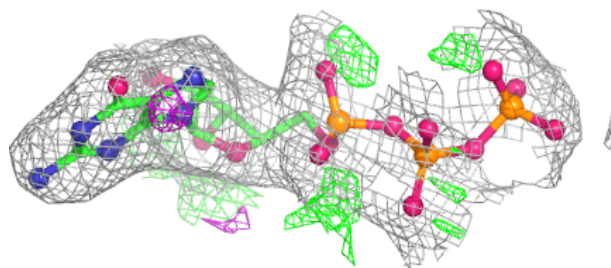
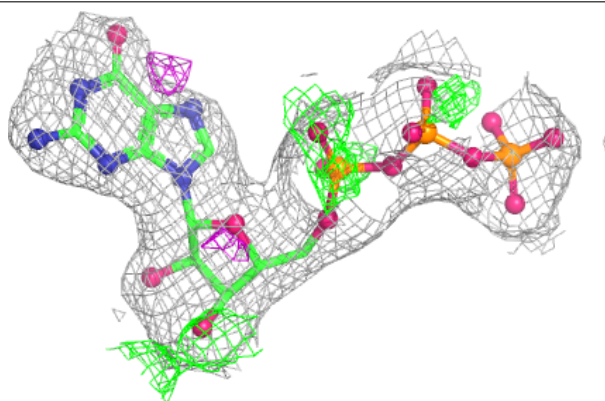


Electron density around GTP D 501:

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

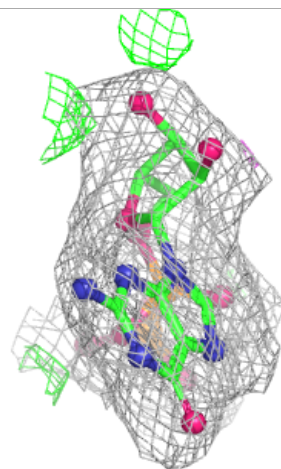
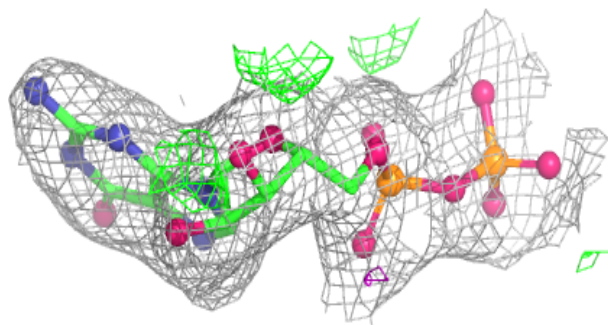
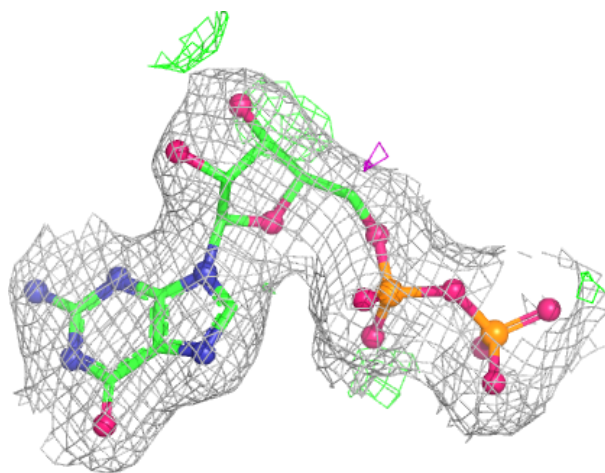
**Electron density around GTP C 502:**

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



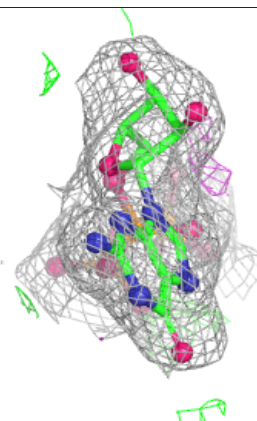
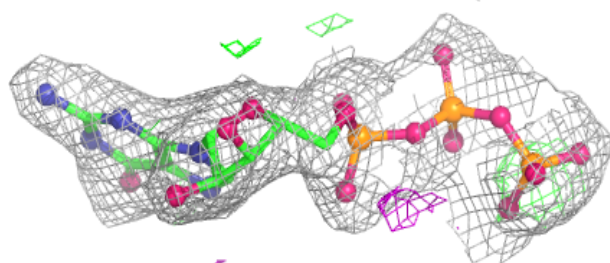
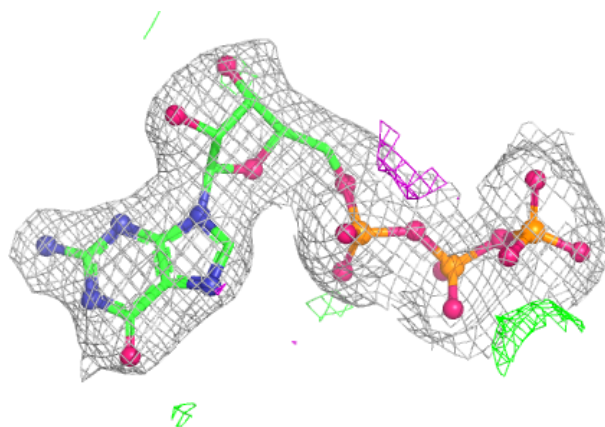
Electron density around GDP B 501:

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



Electron density around GTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.