



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:10 PM UTC

PDB ID : 6D88 / pdb_00006d88
Title : Tubulin-RB3_SLD-TTL in complex with compound 13f
Authors : Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on : 2018-04-26
Resolution : 2.85 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

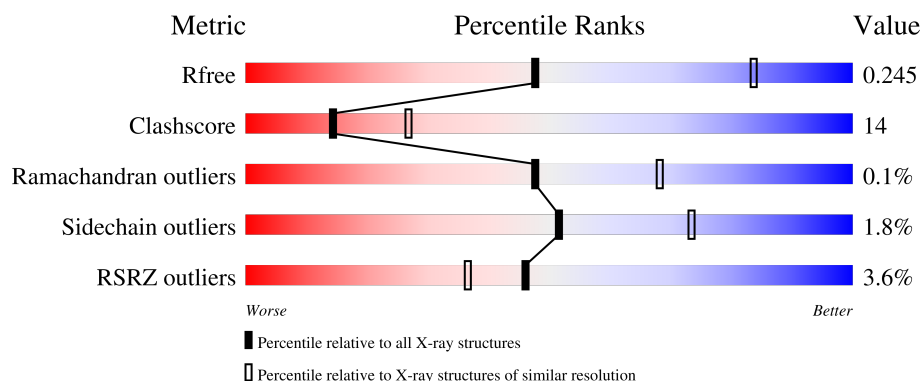
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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

Mol	Chain	Length	Quality of chain
1	A	450	0.2% 74% 23% •
1	C	450	0.2% 79% 18% •
2	B	445	2% 70% 26% •
2	D	445	6% 62% 32% 5%
3	E	143	0.2% 59% 26% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	9% 53% 32% 14%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17544 atoms, of which 14 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	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3300	2076	559	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

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

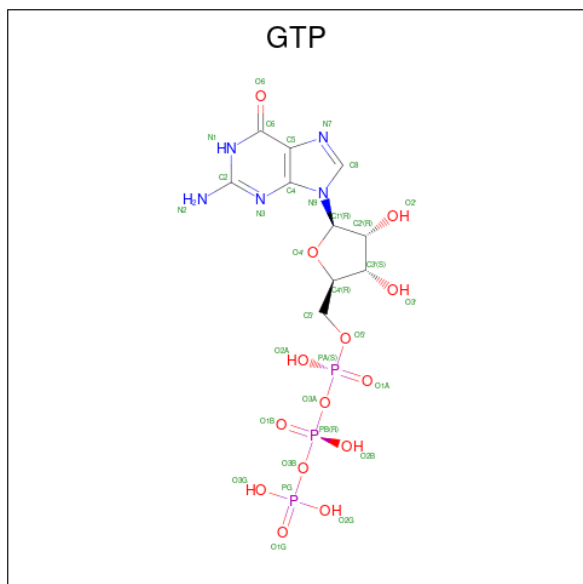
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2713	1740	466	493	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

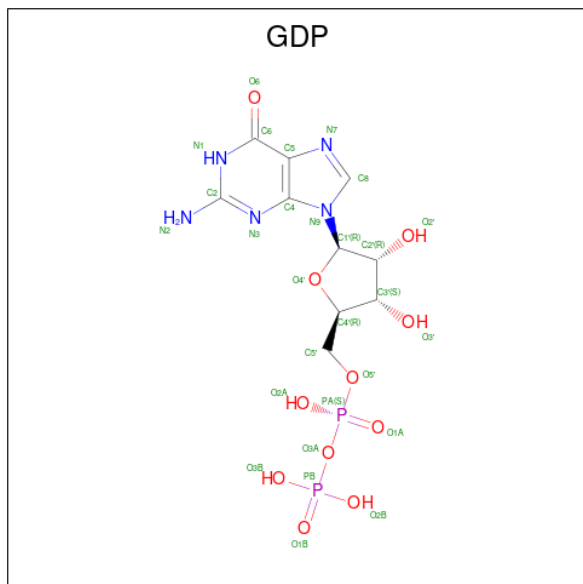
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

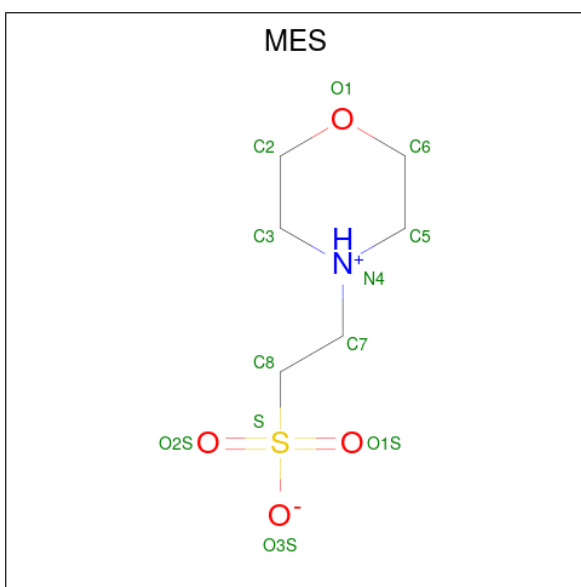
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



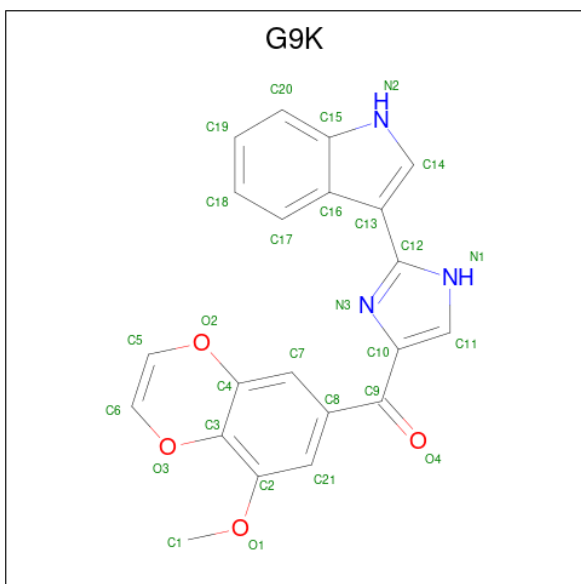
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is [2-(1H-indol-3-yl)-1H-imidazol-4-yl](8-methoxy-1,4-benzodioxin-6-yl)methanone (CCD ID: G9K) (formula: C₂₁H₁₅N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			28	21	3	4		

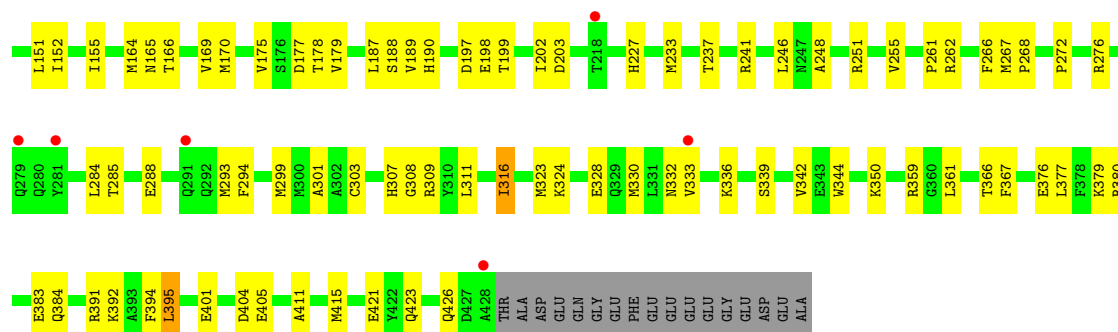
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			28	21	3	4		

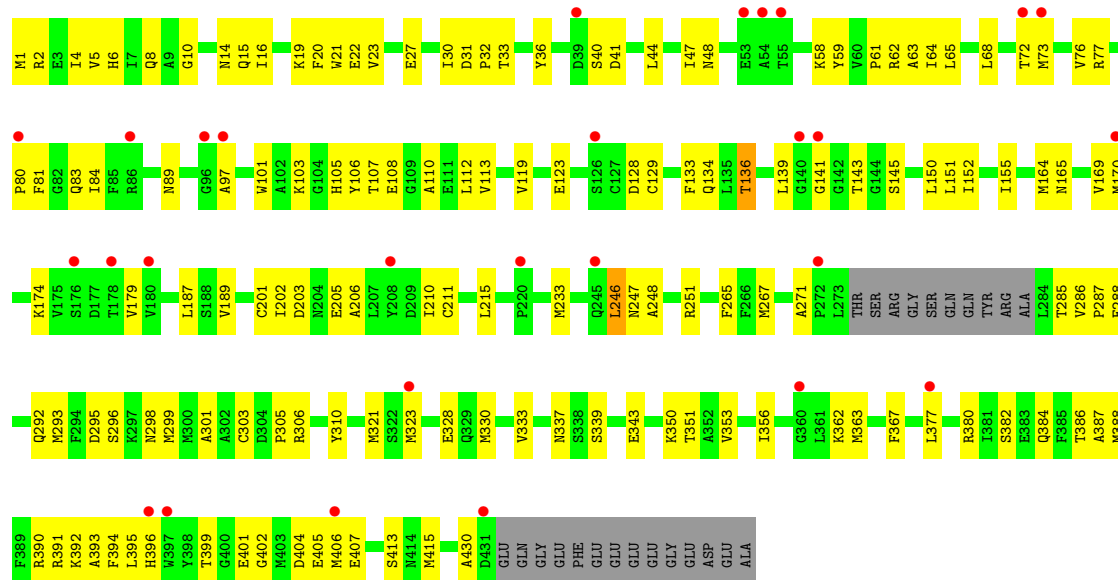
- # ACP

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

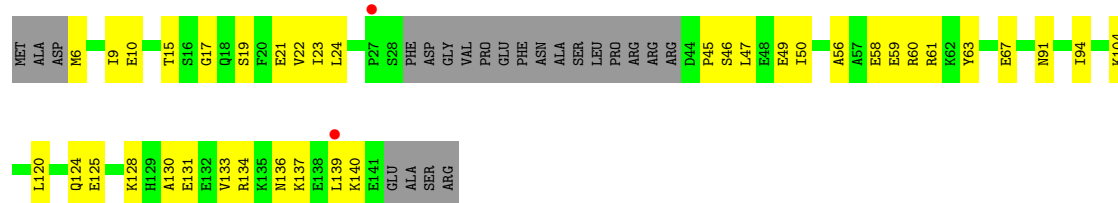
- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 12 | A | 17 | Total O
17 17 | 0 | 0 |
| 12 | B | 19 | Total O
19 19 | 0 | 0 |
| 12 | C | 29 | Total O
29 29 | 0 | 0 |
| 12 | D | 14 | Total O
14 14 | 0 | 0 |
| 12 | E | 5 | Total O
5 5 | 0 | 0 |
| 12 | F | 8 | Total O
8 8 | 0 | 0 |



• Molecule 2: Tubulin beta chain

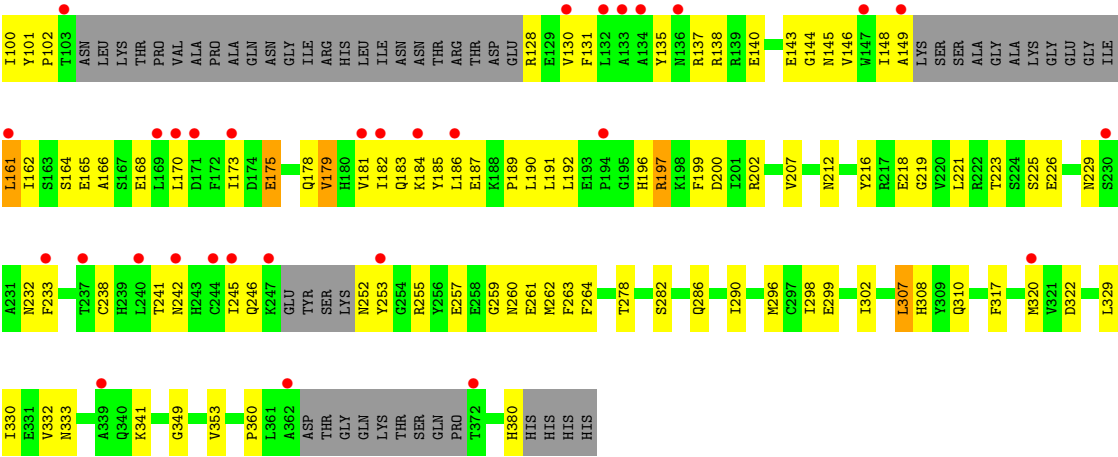


• Molecule 3: Stathmin-4



• 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	105.54Å 157.89Å 182.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 – 2.85 45.65 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (45.65-2.85) 97.2 (45.65-2.85)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.192 , 0.246 0.192 , 0.245	Depositor DCC
R_{free} test set	4083 reflections (5.71%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17544	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, CA, MES, ACP, G9K, 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	0.31	0/3482	0.51	0/4728
1	C	0.35	0/3511	0.57	0/4768
2	B	0.33	0/3426	0.54	0/4643
2	D	0.26	0/3373	0.46	0/4570
3	E	0.30	0/1008	0.40	0/1337
4	F	0.25	0/2775	0.44	0/3752
All	All	0.30	0/17575	0.50	0/23798

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3405	0	3313	84	0
1	C	3433	0	3337	51	2
2	B	3351	0	3216	94	1
2	D	3300	0	3176	125	0
3	E	1000	0	1018	36	1
4	F	2713	0	2659	109	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	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	24	0	24	3	0
10	B	28	0	0	3	0
10	D	28	0	0	2	0
11	F	31	14	13	4	0
12	A	17	0	0	0	0
12	B	19	0	0	2	0
12	C	29	0	0	0	0
12	D	14	0	0	1	0
12	E	5	0	0	0	0
12	F	8	0	0	1	0
All	All	17530	14	16804	482	2

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 14.

All (482) 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)
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.26	1.08
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.38	1.01
2:D:170:MET:HE2	2:D:377:LEU:HD11	1.48	0.96
2:B:307:HIS:O	2:B:426:GLN:NE2	1.99	0.95
4:F:100:ILE:HD12	4:F:128:ARG:N	1.91	0.85
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.51	0.84
2:D:330:MET:HG3	2:D:351:THR:HG21	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:296:MET:HE2	4:F:380:HIS:HB2	1.63	0.81
4:F:137:ARG:O	4:F:137:ARG:NH1	2.12	0.80
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.16	0.80
2:D:388:MET:HG2	2:D:391:ARG:HH21	1.46	0.79
4:F:16:GLU:O	4:F:20:LEU:HD12	1.82	0.79
2:B:308:GLY:HA2	2:B:426:GLN:HE21	1.47	0.79
2:D:285:THR:HG23	2:D:288:GLU:H	1.47	0.79
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.65	0.77
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.84	0.77
2:B:177:ASP:O	1:C:352:LYS:HE2	1.85	0.76
2:D:285:THR:HG22	2:D:288:GLU:OE2	1.85	0.76
2:D:151:LEU:O	2:D:155:ILE:HG13	1.86	0.76
1:A:221:ARG:HH11	2:B:323:MET:HB3	1.50	0.76
2:D:110:ALA:O	2:D:113:VAL:HG12	1.86	0.75
4:F:197:ARG:HH12	4:F:257:GLU:CD	1.94	0.75
2:B:324:LYS:O	2:B:328:GLU:HG3	1.86	0.75
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.69	0.75
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.68	0.74
2:D:401:GLU:HA	3:E:137:LYS:HD2	1.69	0.73
2:D:106:TYR:CD1	3:E:133:VAL:HG11	2.24	0.72
4:F:149:ALA:HB3	4:F:161:LEU:HD23	1.71	0.72
2:D:382:SER:O	2:D:386:THR:HG23	1.90	0.72
2:D:81:PHE:O	2:D:84:ILE:HG22	1.90	0.72
2:B:66:VAL:CG1	2:B:147:MET:HE1	2.20	0.71
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.55	0.71
1:A:72:PRO:CA	1:A:94:THR:HG21	2.20	0.71
2:D:106:TYR:O	3:E:134:ARG:NH1	2.23	0.71
4:F:192:LEU:HD21	4:F:262:MET:CE	2.16	0.71
11:F:401:ACP:H5'1	11:F:401:ACP:H8	1.72	0.71
2:D:16:ILE:HD11	2:D:136:THR:HG22	1.72	0.70
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.73	0.70
2:D:139:LEU:HA	2:D:145:SER:HB3	1.73	0.70
1:A:72:PRO:HA	1:A:94:THR:HG21	1.74	0.70
2:B:262:ARG:NH1	2:B:421:GLU:OE2	2.24	0.70
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.74	0.69
1:A:221:ARG:NH1	2:B:323:MET:HE2	2.07	0.69
4:F:95:PRO:HB2	4:F:183:GLN:HG2	1.75	0.69
2:D:387:ALA:HA	2:D:390:ARG:HE	1.58	0.68
4:F:148:ILE:O	4:F:182:ILE:HA	1.93	0.68
2:D:134:GLN:HA	2:D:165:ASN:O	1.93	0.68
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.29	0.68
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.24	0.68
2:D:1:MET:HG3	2:D:128:ASP:HB3	1.76	0.67
1:C:204:VAL:HG22	1:C:302:MET:CE	2.22	0.67
2:D:89:ASN:ND2	2:D:123:GLU:OE2	2.23	0.67
4:F:62:VAL:HG12	4:F:310:GLN:O	1.94	0.67
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.13	0.67
2:B:81:PHE:O	2:B:84:ILE:HG22	1.94	0.67
2:B:324:LYS:HE3	2:B:328:GLU:OE2	1.94	0.67
2:B:189:VAL:HB	2:B:415:MET:HE3	1.76	0.67
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.25	0.67
1:A:90:GLU:OE2	1:A:124:LYS:NZ	2.19	0.66
2:B:134:GLN:HA	2:B:165:ASN:O	1.96	0.66
1:A:28:HIS:O	1:A:36:MET:HE3	1.96	0.66
4:F:184:LYS:O	11:F:401:ACP:N6	2.29	0.65
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.28	0.65
2:D:141:GLY:HA3	8:D:501:GDP:O3A	1.97	0.65
1:A:72:PRO:HB3	1:A:94:THR:HG21	1.78	0.65
2:D:63:ALA:O	2:D:64:ILE:HD13	1.96	0.65
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.79	0.65
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.78	0.64
2:D:386:THR:O	2:D:390:ARG:HG2	1.97	0.64
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.32	0.64
2:D:330:MET:O	2:D:333:VAL:HG12	1.97	0.64
2:B:261:PRO:HD2	12:B:611:HOH:O	1.98	0.64
1:C:214:ARG:O	1:C:218:ASP:HA	1.97	0.64
2:D:10:GLY:O	2:D:14:ASN:ND2	2.21	0.63
4:F:242:ASN:HB2	4:F:245:ILE:HB	1.79	0.63
2:B:237:THR:HG22	2:B:241:ARG:HG3	1.79	0.63
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.34	0.62
4:F:21:LEU:HD22	4:F:27:TRP:CD1	2.35	0.62
3:E:128:LYS:HD2	3:E:128:LYS:O	1.99	0.62
1:A:175:PRO:HA	1:A:178:SER:HB3	1.82	0.62
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.35	0.61
2:D:33:THR:OG1	2:D:58:LYS:HE3	2.00	0.61
2:D:285:THR:HG22	2:D:288:GLU:CD	2.26	0.61
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.83	0.61
2:D:293:MET:CG	2:D:367:PHE:HB2	2.31	0.61
4:F:135:TYR:OH	4:F:164:SER:O	2.17	0.61
2:B:2:ARG:HA	2:B:129:CYS:O	2.01	0.61
2:B:316:ILE:HG23	2:B:366:THR:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.36	0.60
1:A:72:PRO:CB	1:A:94:THR:HG21	2.32	0.60
2:B:66:VAL:HG12	2:B:147:MET:HE1	1.83	0.60
2:B:251:ARG:O	2:B:255:VAL:HG23	2.01	0.60
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.33	0.60
4:F:1:MET:HE2	4:F:28:LYS:HG2	1.84	0.60
2:D:396:HIS:HA	2:D:399:THR:HG22	1.83	0.60
2:B:423:GLN:HG3	12:B:614:HOH:O	2.01	0.60
4:F:296:MET:HE2	4:F:380:HIS:CB	2.30	0.60
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.82	0.59
4:F:135:TYR:CD2	4:F:166:ALA:HB2	2.36	0.59
2:D:285:THR:OG1	2:D:287:PRO:HD2	2.01	0.59
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.38	0.59
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.38	0.59
2:D:1:MET:HE3	2:D:128:ASP:CB	2.33	0.59
2:D:103:LYS:HE2	2:D:108:GLU:OE2	2.03	0.59
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.37	0.59
4:F:16:GLU:OE2	4:F:20:LEU:HD11	2.02	0.59
3:E:46:SER:O	3:E:50:ILE:HG12	2.02	0.59
2:B:316:ILE:CG2	2:B:366:THR:HB	2.33	0.58
1:A:398:MET:HE3	1:A:404:PHE:CD2	2.39	0.58
2:B:309:ARG:HH21	2:B:342:VAL:HA	1.67	0.58
4:F:144:GLY:HA3	4:F:187:GLU:OE2	2.02	0.58
2:D:387:ALA:HA	2:D:390:ARG:NE	2.16	0.58
2:B:20:PHE:CD1	2:B:233:MET:HE2	2.38	0.58
2:D:251:ARG:HG3	2:D:251:ARG:HH11	1.68	0.58
2:B:145:SER:HG	2:B:188:SER:HG	1.52	0.57
2:D:251:ARG:HG3	2:D:251:ARG:NH1	2.18	0.57
1:A:72:PRO:HA	1:A:94:THR:CG2	2.33	0.57
3:E:21:GLU:HG2	3:E:23:ILE:HD11	1.85	0.57
3:E:46:SER:HB3	3:E:49:GLU:HG3	1.86	0.57
2:B:332:ASN:O	2:B:336:LYS:HG3	2.05	0.57
4:F:97:SER:OG	4:F:183:GLN:HG3	2.05	0.57
4:F:138:ARG:HD2	4:F:143:GLU:HB2	1.87	0.57
2:B:189:VAL:HB	2:B:415:MET:CE	2.35	0.56
1:C:28:HIS:O	1:C:36:MET:HE3	2.04	0.56
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.86	0.56
1:A:221:ARG:NH1	2:B:323:MET:HB3	2.17	0.56
1:A:105:ARG:NH1	1:A:411:GLU:OE1	2.36	0.56
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.41	0.56
2:B:248:ALA:HB1	10:B:505:G9K:C7	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:LEU:HD22	2:D:76:VAL:HG11	1.88	0.56
4:F:74:LYS:NZ	4:F:183:GLN:OE1	2.39	0.56
2:D:97:ALA:HB2	2:D:143:THR:OG1	2.06	0.55
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.40	0.55
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.36	0.55
1:A:96:LYS:HE3	2:B:128:ASP:OD1	2.07	0.55
1:A:247:ALA:HB3	3:E:19:SER:OG	2.07	0.55
2:D:6:HIS:NE2	2:D:8:GLN:HG2	2.21	0.55
2:D:271:ALA:HB2	2:D:298:ASN:HD22	1.70	0.55
1:A:2:ARG:HB2	1:A:133:GLN:HG3	1.87	0.55
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.15	0.55
4:F:87:LEU:O	4:F:88:SER:OG	2.17	0.55
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.72	0.55
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.17	0.55
11:F:401:ACP:H5'1	11:F:401:ACP:C8	2.37	0.55
4:F:95:PRO:HD2	4:F:183:GLN:NE2	2.22	0.55
4:F:137:ARG:NH1	4:F:140:GLU:HB3	2.21	0.55
2:D:31:ASP:CG	2:D:33:THR:HG22	2.32	0.55
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.72	0.55
3:E:45:PRO:HB2	3:E:50:ILE:HD11	1.89	0.55
4:F:2:TYR:OH	4:F:360:PRO:O	2.22	0.55
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.36	0.55
2:B:31:ASP:CG	2:B:33:THR:HG22	2.31	0.54
2:B:251:ARG:NH2	9:B:502:MES:O3S	2.41	0.54
2:B:284:LEU:N	2:B:284:LEU:HD12	2.22	0.54
2:D:169:VAL:HA	2:D:202:ILE:O	2.08	0.54
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.72	0.54
2:B:227:HIS:CG	2:B:276:ARG:HG3	2.43	0.54
4:F:199:PHE:CE2	4:F:221:LEU:HD23	2.43	0.54
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.38	0.54
2:B:266:PHE:O	2:B:268:PRO:HD3	2.08	0.54
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.73	0.54
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.90	0.54
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.90	0.53
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.89	0.53
2:B:330:MET:O	2:B:333:VAL:HG12	2.09	0.53
2:D:170:MET:HE2	2:D:377:LEU:CD1	2.31	0.53
2:D:23:VAL:O	2:D:27:GLU:HG3	2.09	0.53
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.89	0.53
4:F:99:VAL:O	4:F:100:ILE:HD13	2.09	0.53
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:TYR:OH	2:D:40:SER:O	2.27	0.53
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.44	0.52
1:C:1:MET:HB3	1:C:130:THR:OG1	2.09	0.52
4:F:74:LYS:HD2	4:F:181:VAL:HG11	1.91	0.52
1:A:31:GLN:HG3	1:A:33:ASP:OD1	2.09	0.52
2:B:67:ASP:O	2:B:92:PHE:HA	2.10	0.52
2:B:267:MET:CE	2:B:299:MET:HG3	2.39	0.52
2:B:380:ARG:O	2:B:384:GLN:HG3	2.09	0.52
3:E:9:ILE:HG13	3:E:10:GLU:HG3	1.92	0.52
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.92	0.52
2:D:64:ILE:HD12	2:D:119:VAL:CG1	2.40	0.52
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.90	0.52
2:D:101:TRP:CE3	2:D:187:LEU:HD13	2.44	0.52
4:F:86:GLU:C	4:F:87:LEU:HD23	2.35	0.52
1:A:71:GLU:HG2	1:A:72:PRO:N	2.23	0.52
2:B:350:LYS:HB2	10:B:505:G9K:C15	2.40	0.52
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.91	0.52
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.45	0.52
1:C:166:LYS:HE2	1:C:197:HIS:O	2.10	0.52
2:D:306:ARG:NH2	2:D:337:ASN:OD1	2.43	0.52
4:F:259:GLY:O	4:F:261:GLU:HG3	2.10	0.52
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.45	0.51
2:D:395:LEU:O	2:D:399:THR:HG22	2.10	0.51
2:B:203:ASP:HB3	2:B:301:ALA:HA	1.93	0.51
1:A:214:ARG:HG2	1:A:219:ILE:O	2.09	0.51
4:F:102:PRO:HG3	4:F:178:GLN:O	2.10	0.51
1:C:43:GLY:HA2	1:C:56:THR:O	2.10	0.51
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.45	0.51
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.11	0.51
4:F:138:ARG:NH1	4:F:144:GLY:O	2.44	0.51
2:D:30:ILE:HD13	2:D:59:TYR:HB2	1.92	0.51
2:D:206:ALA:O	2:D:210:ILE:HG13	2.10	0.51
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.40	0.51
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.25	0.51
1:A:192:HIS:CG	1:A:421:ALA:HA	2.47	0.50
2:D:1:MET:HB3	2:D:48:ASN:ND2	2.26	0.50
3:E:130:ALA:O	3:E:133:VAL:HG12	2.11	0.50
1:A:94:THR:HG22	1:A:95:GLY:N	2.27	0.50
2:B:31:ASP:OD1	2:B:33:THR:HG22	2.12	0.50
2:D:203:ASP:HB3	2:D:301:ALA:HA	1.93	0.50
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:16:GLU:OE1	4:F:19:ARG:HD2	2.12	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.47	0.50
1:A:287:SER:OG	1:A:290:GLU:HG3	2.11	0.50
2:D:211:CYS:HA	2:D:215:LEU:HD13	1.93	0.50
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.47	0.50
2:D:63:ALA:C	2:D:64:ILE:HD13	2.37	0.50
4:F:221:LEU:HD13	4:F:262:MET:HE3	1.94	0.50
1:A:288:VAL:HG22	1:A:323:VAL:HG22	1.93	0.49
1:A:249:ASN:N	1:A:254:GLU:OE2	2.43	0.49
2:B:151:LEU:O	2:B:155:ILE:HG13	2.12	0.49
2:D:323:MET:SD	2:D:353:VAL:HG11	2.52	0.49
4:F:138:ARG:HB3	4:F:145:ASN:OD1	2.12	0.49
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.48	0.49
2:D:393:ALA:HB1	2:D:394:PHE:CD2	2.47	0.49
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.48	0.49
2:B:66:VAL:CG1	2:B:147:MET:CE	2.90	0.48
1:A:298:PRO:HA	1:A:301:GLN:HG3	1.95	0.48
4:F:20:LEU:O	4:F:24:THR:HG23	2.13	0.48
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.95	0.48
2:D:301:ALA:O	2:D:303:CYS:N	2.44	0.48
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.95	0.48
2:D:64:ILE:HD12	2:D:119:VAL:HG12	1.95	0.48
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.31	0.48
3:E:125:GLU:OE2	3:E:128:LYS:HB3	2.12	0.48
4:F:191:LEU:N	4:F:191:LEU:HD12	2.28	0.48
4:F:202:ARG:NH1	12:F:501:HOH:O	2.41	0.48
1:A:34:GLY:O	1:A:61:HIS:N	2.40	0.48
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.96	0.48
2:D:285:THR:HG22	2:D:288:GLU:HB2	1.94	0.48
2:D:80:PRO:O	2:D:81:PHE:HB2	2.13	0.48
2:D:267:MET:HE1	2:D:305:PRO:HG3	1.95	0.48
2:D:392:LYS:HG3	2:D:395:LEU:HD12	1.96	0.48
1:A:72:PRO:CA	1:A:94:THR:CG2	2.90	0.48
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.44	0.48
1:A:241:SER:HB2	1:A:249:ASN:O	2.13	0.48
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.14	0.47
4:F:8:ASP:OD2	4:F:44:ARG:HG3	2.14	0.47
2:D:380:ARG:O	2:D:384:GLN:HG3	2.13	0.47
2:D:388:MET:HG2	2:D:391:ARG:NH2	2.21	0.47
3:E:130:ALA:HA	3:E:133:VAL:HG12	1.96	0.47
3:E:140:LYS:O	3:E:140:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.26	0.47
3:E:22:VAL:O	3:E:23:ILE:HD13	2.14	0.47
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.96	0.47
9:B:503:MES:H51	9:B:503:MES:H81	1.59	0.47
4:F:263:PHE:CZ	4:F:341:LYS:HD3	2.49	0.47
4:F:71:LEU:HD12	4:F:80:LEU:HD23	1.97	0.47
4:F:138:ARG:HB3	4:F:145:ASN:HD21	1.79	0.47
2:B:359:ARG:HE	2:B:359:ARG:HA	1.78	0.47
1:A:251:ASP:OD2	1:A:254:GLU:N	2.47	0.47
1:C:215:ARG:NH1	1:C:299:ALA:HB1	2.29	0.47
2:D:83:GLN:HB3	12:D:611:HOH:O	2.15	0.47
4:F:175:GLU:HG2	4:F:175:GLU:O	2.14	0.47
4:F:349:GLY:O	4:F:353:VAL:HG23	2.14	0.47
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.50	0.47
2:B:28:HIS:O	2:B:30:ILE:HD12	2.14	0.47
2:B:308:GLY:HA2	2:B:426:GLN:NE2	2.23	0.47
3:E:63:TYR:O	3:E:67:GLU:HG2	2.15	0.47
4:F:165:GLU:HB2	4:F:168:GLU:HG3	1.95	0.47
2:D:72:THR:O	2:D:76:VAL:HG23	2.15	0.47
4:F:98:TYR:O	4:F:181:VAL:HG23	2.14	0.47
1:C:27:GLU:OE1	1:C:236:SER:OG	2.27	0.46
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.97	0.46
2:D:330:MET:HE2	2:D:351:THR:CG2	2.45	0.46
4:F:191:LEU:HA	4:F:197:ARG:O	2.14	0.46
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.51	0.46
2:B:246:LEU:HD22	10:B:505:G9K:C11	2.45	0.46
2:B:267:MET:HE1	2:B:299:MET:HG3	1.97	0.46
1:C:282:TYR:O	1:C:283:HIS:HB2	2.14	0.46
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.46
2:B:189:VAL:CB	2:B:415:MET:CE	2.94	0.46
1:A:313:MET:HE3	1:A:380:ASN:OD1	2.14	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.46
2:D:20:PHE:CD1	2:D:233:MET:HE2	2.50	0.46
4:F:128:ARG:N	4:F:128:ARG:HD2	2.30	0.46
2:D:44:LEU:HA	2:D:47:ILE:HB	1.97	0.46
2:D:107:THR:OG1	2:D:108:GLU:N	2.48	0.46
2:D:170:MET:CE	2:D:377:LEU:HD11	2.34	0.46
2:D:285:THR:HG22	2:D:288:GLU:CG	2.46	0.46
4:F:170:LEU:O	4:F:173:ILE:HG12	2.15	0.46
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.46
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:THR:OG1	2:B:199:THR:HB	2.16	0.46
4:F:96:GLU:O	4:F:183:GLN:HG3	2.16	0.46
4:F:232:ASN:OD1	4:F:232:ASN:N	2.48	0.46
2:B:12:CYS:SG	2:B:169:VAL:HG21	2.56	0.46
1:C:216:ASN:HB3	1:C:275:VAL:O	2.15	0.46
2:D:19:LYS:O	2:D:23:VAL:HG23	2.16	0.46
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.46	0.46
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.65	0.46
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.97	0.46
2:B:7:ILE:O	2:B:135:LEU:HA	2.16	0.46
2:B:169:VAL:HA	2:B:202:ILE:O	2.16	0.46
4:F:189:PRO:O	4:F:191:LEU:HD12	2.15	0.46
1:C:265:ILE:N	1:C:265:ILE:HD12	2.31	0.45
4:F:161:LEU:N	4:F:161:LEU:HD12	2.31	0.45
2:B:391:ARG:HD2	2:B:391:ARG:HA	1.72	0.45
4:F:149:ALA:HB3	4:F:161:LEU:HB3	1.99	0.45
2:B:311:LEU:HD23	2:B:342:VAL:HG11	1.96	0.45
1:C:252:LEU:O	1:C:256:GLN:HG3	2.16	0.45
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.51	0.45
2:D:179:VAL:O	2:D:388:MET:HE1	2.16	0.45
2:D:271:ALA:HB2	2:D:298:ASN:ND2	2.32	0.45
4:F:223:THR:O	4:F:260:ASN:HB3	2.17	0.45
1:A:43:GLY:HA2	1:A:56:THR:O	2.16	0.45
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.99	0.45
4:F:189:PRO:HA	4:F:322:ASP:HA	1.97	0.45
1:A:2:ARG:O	1:A:51:THR:HG23	2.16	0.45
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.51	0.45
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.51	0.45
1:C:192:HIS:CG	1:C:421:ALA:HA	2.51	0.45
4:F:191:LEU:HD22	4:F:196:HIS:CD2	2.52	0.45
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.52	0.45
4:F:148:ILE:HG13	4:F:149:ALA:N	2.32	0.45
1:A:411:GLU:O	3:E:61:ARG:NH1	2.44	0.45
1:C:90:GLU:O	1:C:121:ARG:HD2	2.16	0.45
3:E:22:VAL:C	3:E:23:ILE:HD13	2.42	0.45
4:F:47:LEU:C	4:F:47:LEU:HD23	2.42	0.45
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.45	0.45
4:F:229:ASN:ND2	4:F:232:ASN:OD1	2.50	0.45
2:B:190:HIS:HD2	2:B:411:ALA:HA	1.82	0.45
2:D:106:TYR:OH	2:D:407:GLU:OE2	2.25	0.45
2:D:203:ASP:OD1	2:D:377:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ARG:HH11	2:D:251:ARG:CG	2.28	0.45
4:F:130:VAL:HG12	4:F:130:VAL:O	2.16	0.45
4:F:146:VAL:HG11	4:F:233:PHE:CE1	2.52	0.45
1:A:265:ILE:CG2	1:A:313:MET:HE1	2.42	0.45
2:B:394:PHE:CD1	1:C:261:PRO:HA	2.52	0.45
2:D:286:VAL:HB	2:D:287:PRO:HD3	1.98	0.45
2:D:305:PRO:HB3	2:D:310:TYR:OH	2.17	0.45
4:F:93:TRP:HZ3	4:F:329:LEU:CD2	2.29	0.45
2:B:227:HIS:HB2	2:B:276:ARG:HG3	1.98	0.44
2:B:285:THR:O	2:B:288:GLU:N	2.50	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.44
2:D:105:HIS:O	2:D:150:LEU:HD22	2.16	0.44
2:D:215:LEU:HD12	2:D:215:LEU:N	2.32	0.44
2:D:288:GLU:O	2:D:292:GLN:HG3	2.17	0.44
2:B:152:ILE:HG23	2:B:164:MET:HG2	1.99	0.44
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.99	0.44
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.48	0.44
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.44
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.52	0.44
1:A:165:SER:OG	1:A:256:GLN:OE1	2.29	0.44
1:A:187:SER:CB	1:A:391:LEU:HD21	2.48	0.44
1:A:63:PRO:HD3	1:A:86:LEU:HG	2.00	0.44
4:F:31:ARG:HG3	4:F:32:LYS:N	2.32	0.44
4:F:87:LEU:HD23	4:F:87:LEU:N	2.31	0.44
2:D:174:LYS:HE3	2:D:205:GLU:CD	2.42	0.44
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.43	0.44
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.53	0.44
2:D:8:GLN:OE1	2:D:14:ASN:HA	2.17	0.44
3:E:139:LEU:O	3:E:139:LEU:HG	2.18	0.44
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.52	0.44
2:D:4:ILE:O	2:D:62:ARG:HD2	2.18	0.44
2:D:112:LEU:O	2:D:112:LEU:HG	2.18	0.44
2:D:141:GLY:HA3	8:D:501:GDP:O5'	2.18	0.44
3:E:130:ALA:C	3:E:133:VAL:HG12	2.43	0.44
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.53	0.44
2:D:350:LYS:HB2	10:D:502:G9K:C15	2.48	0.43
1:C:108:TYR:OH	3:E:104:LYS:HD2	2.18	0.43
1:C:343:PHE:CG	1:C:349:THR:HG22	2.53	0.43
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.83	0.43
2:D:41:ASP:OD1	2:D:41:ASP:N	2.40	0.43
2:D:343:GLU:HG3	2:D:430:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:253:TYR:CE2	4:F:259:GLY:HA2	2.54	0.43
1:A:402:ARG:HG3	1:A:402:ARG:NH1	2.33	0.43
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.58	0.43
2:D:248:ALA:HA	10:D:502:G9K:O4	2.18	0.43
2:D:267:MET:CE	2:D:299:MET:HG3	2.48	0.43
4:F:100:ILE:HG23	4:F:128:ARG:N	2.33	0.43
1:A:401:LYS:HG3	2:B:344:TRP:CE3	2.53	0.43
1:C:151:SER:O	1:C:155:GLU:HG3	2.18	0.43
2:D:267:MET:SD	2:D:303:CYS:HB2	2.57	0.43
4:F:1:MET:HE2	4:F:1:MET:HB3	1.96	0.43
4:F:138:ARG:CB	4:F:145:ASN:OD1	2.67	0.43
1:A:31:GLN:HG2	1:A:35:GLN:O	2.18	0.43
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.43
2:D:404:ASP:OD1	2:D:405:GLU:N	2.51	0.43
1:A:213:CYS:O	1:A:217:LEU:HB2	2.19	0.43
1:A:7:ILE:HG23	1:A:66:VAL:CG1	2.49	0.43
4:F:138:ARG:HG3	4:F:145:ASN:OD1	2.18	0.43
1:A:336:LYS:HG2	3:E:24:LEU:HD13	2.01	0.42
2:D:246:LEU:HD13	2:D:248:ALA:HB2	1.99	0.42
4:F:101:TYR:CE2	4:F:179:VAL:HG23	2.54	0.42
4:F:135:TYR:CE1	4:F:145:ASN:HB3	2.54	0.42
4:F:190:LEU:HB2	4:F:322:ASP:O	2.19	0.42
2:B:395:LEU:HA	2:B:395:LEU:HD12	1.66	0.42
2:D:77:ARG:HG2	2:D:83:GLN:OE1	2.19	0.42
2:D:189:VAL:HG11	2:D:415:MET:HG3	2.02	0.42
2:D:402:GLY:HA2	3:E:136:ASN:HB3	2.01	0.42
3:E:47:LEU:HD12	3:E:47:LEU:O	2.19	0.42
3:E:128:LYS:HD2	3:E:128:LYS:C	2.43	0.42
4:F:226:GLU:HB2	4:F:238:CYS:HB3	2.01	0.42
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.83	0.42
4:F:278:THR:O	4:F:282:SER:OG	2.35	0.42
4:F:286:GLN:O	4:F:290:ILE:HG13	2.19	0.42
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.54	0.42
1:C:241:SER:HA	1:C:249:ASN:OD1	2.20	0.42
4:F:135:TYR:HE1	4:F:145:ASN:HB3	1.84	0.42
4:F:185:TYR:HA	11:F:401:ACP:N1	2.34	0.42
4:F:200:ASP:O	4:F:221:LEU:HA	2.19	0.42
4:F:330:ILE:HD13	4:F:330:ILE:HA	1.79	0.42
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.19	0.42
2:B:301:ALA:O	2:B:303:CYS:N	2.52	0.42
2:D:143:THR:HB	8:D:501:GDP:O1B	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:ILE:HG23	2:D:164:MET:HG2	2.00	0.42
2:D:362:LYS:HE2	2:D:362:LYS:HB3	1.88	0.42
2:B:177:ASP:O	2:B:178:THR:HG23	2.20	0.42
2:B:359:ARG:HA	2:B:359:ARG:NE	2.35	0.42
2:D:1:MET:CE	2:D:128:ASP:HB2	2.44	0.42
3:E:131:GLU:OE1	3:E:131:GLU:HA	2.20	0.42
1:A:47:ASP:O	1:A:50:ASN:HB2	2.20	0.42
1:C:88:HIS:NE2	1:C:90:GLU:HG3	2.34	0.42
4:F:202:ARG:HA	4:F:317:PHE:O	2.20	0.42
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.52	0.42
2:B:404:ASP:OD1	2:B:405:GLU:N	2.53	0.42
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.55	0.42
2:D:31:ASP:OD1	2:D:33:THR:HG22	2.19	0.42
1:A:107:HIS:O	1:A:152:LEU:HD22	2.20	0.41
1:C:174:ALA:HB2	1:C:207:GLU:N	2.34	0.41
1:A:70:LEU:HD13	1:A:110:ILE:HG21	2.02	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.41
2:D:68:LEU:HD23	2:D:68:LEU:HA	1.94	0.41
1:A:134:GLY:HA3	1:A:165:SER:O	2.21	0.41
1:C:55:GLU:HA	1:C:60:LYS:O	2.20	0.41
1:C:88:HIS:CD2	1:C:90:GLU:H	2.38	0.41
1:C:158:SER:CB	1:C:197:HIS:HD1	2.31	0.41
4:F:93:TRP:HZ3	4:F:329:LEU:HD23	1.85	0.41
1:A:301:GLN:HE22	1:A:307:PRO:HG2	1.86	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.56	0.41
4:F:225:SER:HB2	4:F:252:ASN:HB3	2.01	0.41
2:D:31:ASP:OD1	2:D:33:THR:CG2	2.68	0.41
2:D:267:MET:HE3	2:D:299:MET:CG	2.51	0.41
1:C:159:VAL:HA	3:E:94:ILE:HG23	2.02	0.41
1:C:176:GLN:NE2	1:C:207:GLU:HG3	2.35	0.41
2:D:139:LEU:CA	2:D:145:SER:HB3	2.46	0.41
2:B:267:MET:HE3	2:B:299:MET:HG3	2.02	0.41
2:D:203:ASP:CB	2:D:301:ALA:HA	2.50	0.41
2:D:363:MET:HB3	2:D:363:MET:HE2	1.77	0.41
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.55	0.41
2:B:16:ILE:HD11	2:B:136:THR:HB	2.03	0.41
2:B:203:ASP:CG	2:B:380:ARG:HH22	2.29	0.41
2:B:267:MET:HE3	2:B:299:MET:CG	2.51	0.41
2:B:309:ARG:NH2	2:B:342:VAL:HA	2.35	0.41
9:B:502:MES:H82	9:B:502:MES:H51	1.90	0.41
1:C:124:LYS:HD3	1:C:124:LYS:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:CYS:HA	1:C:386:GLU:OE2	2.21	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.93	0.41
2:D:295:ASP:OD1	2:D:296:SER:N	2.54	0.41
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.54	0.41
4:F:298:ILE:HD12	4:F:302:ILE:HD13	2.03	0.41
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.55	0.40
2:B:307:HIS:ND1	2:B:376:GLU:OE1	2.49	0.40
2:B:379:LYS:O	2:B:383:GLU:HG3	2.20	0.40
4:F:131:PHE:CZ	4:F:182:ILE:CD1	3.03	0.40
1:A:112:LYS:O	1:A:112:LYS:HG2	2.21	0.40
2:B:237:THR:HG22	2:B:237:THR:O	2.21	0.40
2:B:294:PHE:CZ	2:B:330:MET:HE1	2.56	0.40
2:D:1:MET:HE3	2:D:128:ASP:CG	2.46	0.40
3:E:120:LEU:O	3:E:124:GLN:HG3	2.22	0.40
2:B:66:VAL:HG11	2:B:147:MET:CE	2.51	0.40
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.51	0.40
1:C:141:PHE:CE2	1:C:170:SER:HB3	2.57	0.40
1:C:323:VAL:HG12	1:C:355:ILE:HD13	2.04	0.40
4:F:207:VAL:HA	4:F:212:ASN:O	2.22	0.40
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.51	0.40
2:B:197:ASP:C	2:B:198:GLU:HG3	2.47	0.40
1:A:71:GLU:OE1	1:A:73:THR:HB	2.21	0.40
2:D:233:MET:HE2	2:D:233:MET:HB3	1.99	0.40
4:F:135:TYR:HE2	4:F:166:ALA:H	1.70	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:GLU:OE1	1:C:282:TYR:OH[4_545]	1.99	0.21
1:C:285:GLN:NE2	3:E:91:ASN:OD1[4_445]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	427 (98%)	8 (2%)	0	100	100
1	C	438/450 (97%)	426 (97%)	11 (2%)	1 (0%)	43	62
2	B	425/445 (96%)	414 (97%)	10 (2%)	1 (0%)	43	62
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	117/143 (82%)	114 (97%)	3 (3%)	0	100	100
4	F	322/384 (84%)	301 (94%)	20 (6%)	1 (0%)	36	54
All	All	2154/2317 (93%)	2089 (97%)	62 (3%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	ASP
4	F	255	ARG
2	B	175	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/378 (97%)	362 (99%)	4 (1%)	65	81
1	C	370/378 (98%)	368 (100%)	2 (0%)	81	90
2	B	367/383 (96%)	362 (99%)	5 (1%)	59	78
2	D	362/383 (94%)	351 (97%)	11 (3%)	36	61
3	E	109/127 (86%)	108 (99%)	1 (1%)	70	84
4	F	295/342 (86%)	284 (96%)	11 (4%)	30	55
All	All	1869/1991 (94%)	1835 (98%)	34 (2%)	51	73

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	68	VAL
1	A	71	GLU
2	B	15	GLN
2	B	115	SER
2	B	316	ILE
2	B	339	SER
2	B	395	LEU
1	C	71	GLU
1	C	251	ASP
2	D	15	GLN
2	D	73	MET
2	D	136	THR
2	D	246	LEU
2	D	247	ASN
2	D	321	MET
2	D	328	GLU
2	D	339	SER
2	D	356	ILE
2	D	406	MET
2	D	413	SER
3	E	15	THR
4	F	12	SER
4	F	69	ASP
4	F	89	GLU
4	F	161	LEU
4	F	175	GLU
4	F	179	VAL
4	F	197	ARG
4	F	299	GLU
4	F	307	LEU
4	F	332	VAL
4	F	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	35	GLN
1	A	101	ASN
1	A	300	ASN
1	A	301	GLN

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Mol	Chain	Res	Type
1	A	309	HIS
1	A	393	HIS
2	B	99	ASN
2	B	337	ASN
2	B	423	GLN
1	C	101	ASN
1	C	356	ASN
1	C	393	HIS
2	D	11	GLN
2	D	43	GLN
2	D	298	ASN
2	D	334	GLN
2	D	426	GLN
3	E	84	GLN
4	F	260	ASN
4	F	310	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MES	B	503	-	12,12,12	2.25	1 (8%)	15,16,16	1.85	4 (26%)
5	GTP	C	501	7	33,34,34	0.89	1 (3%)	50,54,54	1.63	13 (26%)
8	GDP	D	501	-	29,30,30	1.36	4 (13%)	45,47,47	1.87	9 (20%)
5	GTP	A	501	7	33,34,34	1.00	2 (6%)	50,54,54	1.67	12 (24%)
9	MES	B	502	-	12,12,12	2.23	1 (8%)	15,16,16	1.99	5 (33%)
8	GDP	B	501	7	29,30,30	1.19	3 (10%)	45,47,47	1.79	8 (17%)
10	G9K	B	505	-	32,32,32	0.80	1 (3%)	36,46,46	0.82	2 (5%)
10	G9K	D	502	-	32,32,32	0.86	1 (3%)	36,46,46	0.79	2 (5%)
11	ACP	F	401	-	31,33,33	3.16	12 (38%)	47,52,52	2.04	12 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	C	501	7	-	7/22/38/38	0/3/3/3
8	GDP	D	501	-	-	3/16/32/32	0/3/3/3
5	GTP	A	501	7	-	7/22/38/38	0/3/3/3
9	MES	B	502	-	-	5/6/14/14	0/1/1/1
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
10	G9K	B	505	-	-	2/14/21/21	0/5/5/5
10	G9K	D	502	-	-	0/14/21/21	0/5/5/5
11	ACP	F	401	-	-	6/19/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	O4'-C1'	8.36	1.61	1.42
9	B	503	MES	C8-S	-7.46	1.67	1.77
9	B	502	MES	C8-S	-7.41	1.67	1.77
11	F	401	ACP	C2'-C1'	-7.39	1.30	1.53
11	F	401	ACP	O4'-C4'	-6.25	1.31	1.45
11	F	401	ACP	PA-O3A	5.65	1.65	1.59
11	F	401	ACP	PB-O3A	5.54	1.64	1.58
11	F	401	ACP	C6-N6	4.21	1.45	1.34
8	D	501	GDP	PA-O3A	4.02	1.63	1.59
10	D	502	G9K	C6-C5	3.25	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	G9K	C6-C5	3.20	1.41	1.32
11	F	401	ACP	C5-C4	-3.14	1.33	1.39
8	B	501	GDP	C5-C4	3.12	1.47	1.38
8	D	501	GDP	C5-C4	3.06	1.47	1.38
11	F	401	ACP	O2'-C2'	2.97	1.50	1.43
11	F	401	ACP	C5-N7	-2.96	1.33	1.39
8	B	501	GDP	C5-N7	-2.62	1.33	1.39
11	F	401	ACP	O3'-C3'	-2.56	1.36	1.43
5	A	501	GTP	PB-O3B	2.55	1.62	1.59
5	C	501	GTP	PB-O3B	2.48	1.62	1.59
8	D	501	GDP	C5-N7	-2.46	1.34	1.39
5	A	501	GTP	C2-N3	2.34	1.38	1.33
8	B	501	GDP	C6-N1	-2.20	1.34	1.38
11	F	401	ACP	C8-N9	-2.20	1.33	1.37
8	D	501	GDP	C6-N1	-2.11	1.34	1.38
11	F	401	ACP	C4-N9	-2.07	1.33	1.37

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C5-C4-N3	-6.30	118.36	128.39
8	D	501	GDP	C5-C4-N3	-6.22	118.49	128.39
11	F	401	ACP	N3-C2-N1	-5.59	120.12	128.58
8	D	501	GDP	N9-C4-N3	4.99	135.93	125.95
8	D	501	GDP	C2-N3-C4	4.93	120.79	112.30
8	B	501	GDP	N9-C4-N3	4.87	135.69	125.95
5	A	501	GTP	C5-C4-N3	-4.80	120.76	128.39
8	B	501	GDP	C2-N3-C4	4.63	120.28	112.30
11	F	401	ACP	N6-C6-N1	-4.58	108.18	118.38
11	F	401	ACP	C5-C4-N3	-4.58	120.41	126.72
5	C	501	GTP	C5-C4-N3	-4.40	121.39	128.39
5	C	501	GTP	C2-N3-C4	4.36	119.81	112.30
9	B	503	MES	C5-N4-C3	4.35	118.20	108.84
5	A	501	GTP	C2-N3-C4	4.34	119.78	112.30
9	B	502	MES	C5-N4-C3	4.09	117.66	108.84
11	F	401	ACP	C3'-C2'-C1'	4.00	109.03	101.46
11	F	401	ACP	C5-C6-N6	3.68	132.39	123.29
9	B	502	MES	C6-C5-N4	-3.61	104.64	110.12
11	F	401	ACP	N9-C8-N7	-3.59	108.84	113.94
11	F	401	ACP	PB-O3A-PA	-3.58	120.69	132.37
8	D	501	GDP	O3B-PB-O3A	3.33	115.79	104.64
5	A	501	GTP	O2B-PB-O3B	3.22	115.98	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C8-N7-C5	3.13	109.84	104.26
8	D	501	GDP	C6-C5-N7	3.08	135.89	130.29
5	A	501	GTP	N9-C4-N3	3.06	132.07	125.95
11	F	401	ACP	C2-N3-C4	3.05	119.27	111.83
5	A	501	GTP	N9-C8-N7	-3.02	107.81	113.40
5	C	501	GTP	N9-C8-N7	-3.00	107.84	113.40
8	B	501	GDP	O6-C6-C5	-2.94	118.78	126.53
5	A	501	GTP	C2-N1-C6	-2.85	119.94	125.11
5	A	501	GTP	C8-N7-C5	2.79	109.24	104.26
11	F	401	ACP	N3-C4-N9	2.79	131.91	127.17
5	C	501	GTP	C4-C5-N7	-2.75	106.31	110.67
5	C	501	GTP	N2-C2-N1	2.66	122.37	116.76
8	B	501	GDP	C6-C5-N7	2.66	135.12	130.29
10	D	502	G9K	O2-C4-C7	2.66	118.79	115.81
5	C	501	GTP	C2-N1-C6	-2.65	120.30	125.11
9	B	502	MES	O3S-S-C8	2.59	111.07	106.00
9	B	502	MES	O1S-S-C8	2.53	110.56	106.73
8	D	501	GDP	C4-C5-N7	-2.49	106.73	110.67
8	D	501	GDP	O6-C6-C5	-2.46	120.05	126.53
5	C	501	GTP	O3B-PB-O1B	-2.45	103.33	110.70
9	B	503	MES	C6-C5-N4	-2.41	106.46	110.12
10	B	505	G9K	O2-C4-C7	2.39	118.49	115.81
11	F	401	ACP	C6-C5-C4	2.38	120.43	117.18
8	B	501	GDP	C4-C5-N7	-2.38	106.91	110.67
5	A	501	GTP	O3B-PB-O1B	-2.33	103.70	110.70
9	B	502	MES	C7-N4-C5	2.32	117.43	111.24
5	A	501	GTP	C5-C6-N1	2.27	119.04	113.25
5	A	501	GTP	O2B-PB-O3A	2.23	113.30	107.27
9	B	503	MES	O2S-S-C8	2.23	110.10	106.73
11	F	401	ACP	C5-N7-C8	2.22	106.95	103.45
11	F	401	ACP	C5'-C4'-C3'	-2.21	107.25	115.21
10	D	502	G9K	O3-C3-C2	2.19	118.97	114.70
9	B	503	MES	C7-N4-C5	2.19	117.07	111.24
5	A	501	GTP	O6-C6-C5	-2.13	120.91	126.53
10	B	505	G9K	O3-C3-C2	2.13	118.85	114.70
5	C	501	GTP	N9-C4-N3	2.13	130.21	125.95
8	B	501	GDP	C2-N1-C6	-2.11	121.29	125.11
5	C	501	GTP	O3G-PG-O3B	2.09	111.66	104.64
5	A	501	GTP	O2G-PG-O3B	2.08	111.61	104.64
5	C	501	GTP	O3'-C3'-C4'	-2.07	105.15	111.08
5	C	501	GTP	C6-C5-N7	2.06	134.04	130.29
8	B	501	GDP	C5-C6-N1	2.05	118.47	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C8-N7-C5	2.05	107.91	104.26
5	C	501	GTP	O2B-PB-O3B	2.02	112.72	107.27
8	D	501	GDP	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	502	MES	C8-C7-N4-C5
9	B	502	MES	C7-C8-S-O1S
9	B	502	MES	C7-C8-S-O2S
9	B	502	MES	C7-C8-S-O3S
9	B	503	MES	C8-C7-N4-C5
10	B	505	G9K	C11-C10-C9-O4
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
11	F	401	ACP	C4'-C5'-O5'-PA
10	B	505	G9K	C11-C10-C9-C8
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	502	MES	C8-C7-N4-C3
5	A	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	O4'-C4'-C5'-O5'

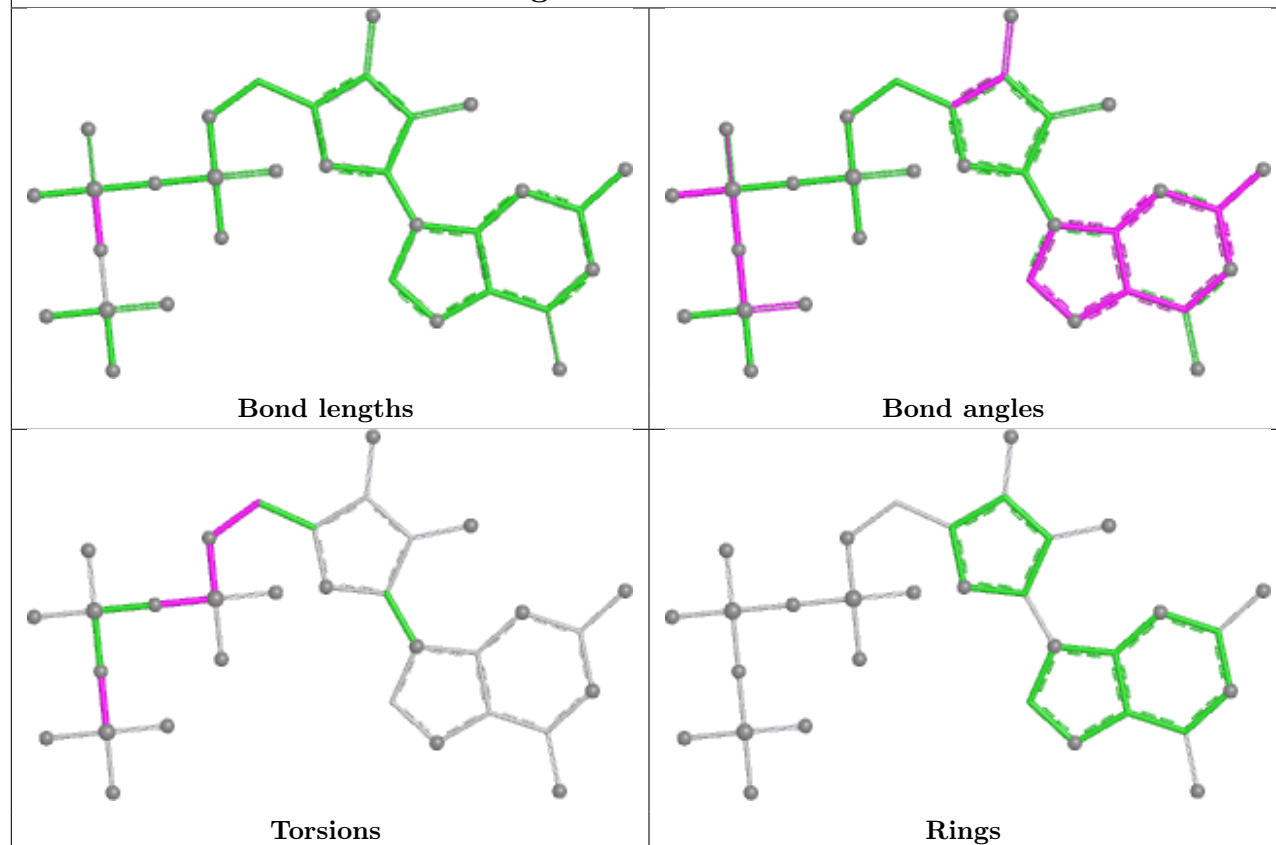
There are no ring outliers.

7 monomers are involved in 16 short contacts:

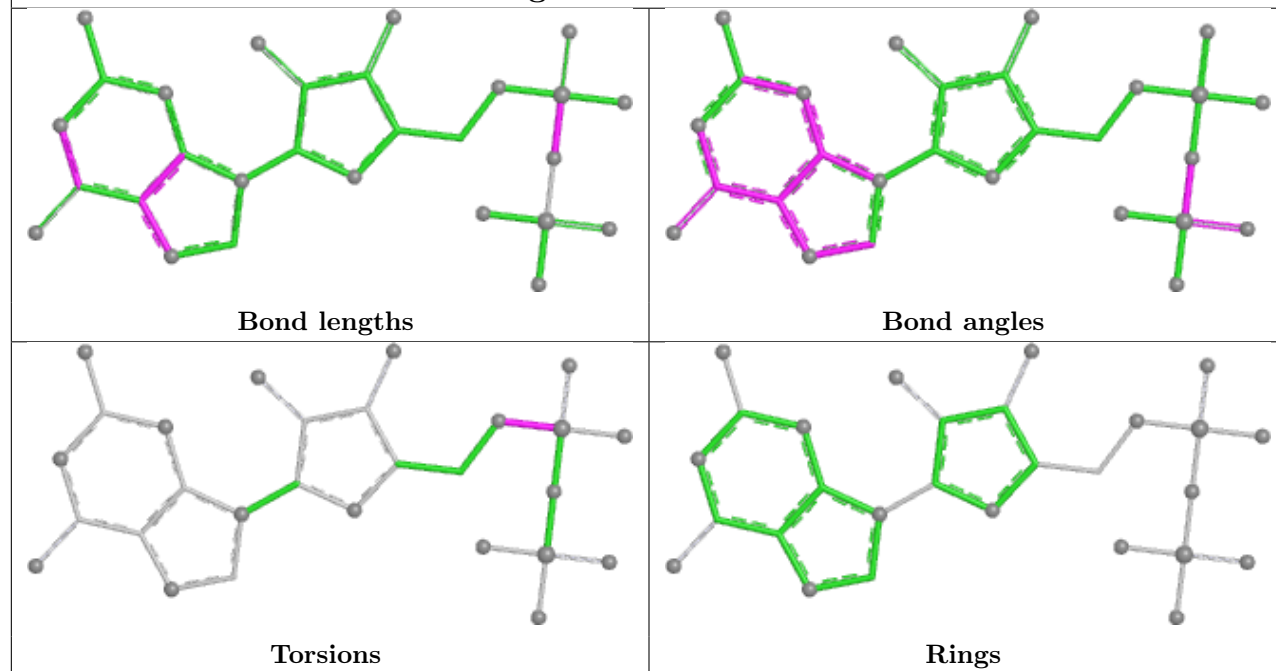
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	1	0
8	D	501	GDP	3	0
5	A	501	GTP	1	0
9	B	502	MES	2	0
10	B	505	G9K	3	0
10	D	502	G9K	2	0
11	F	401	ACP	4	0

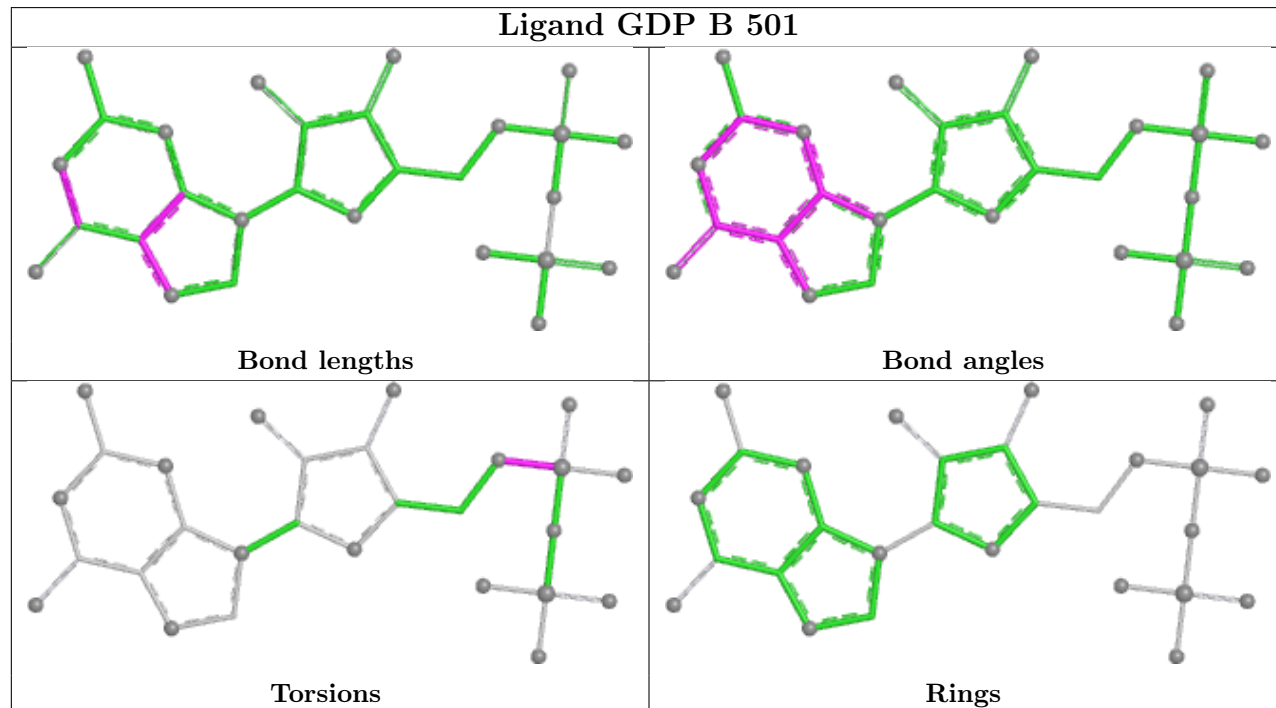
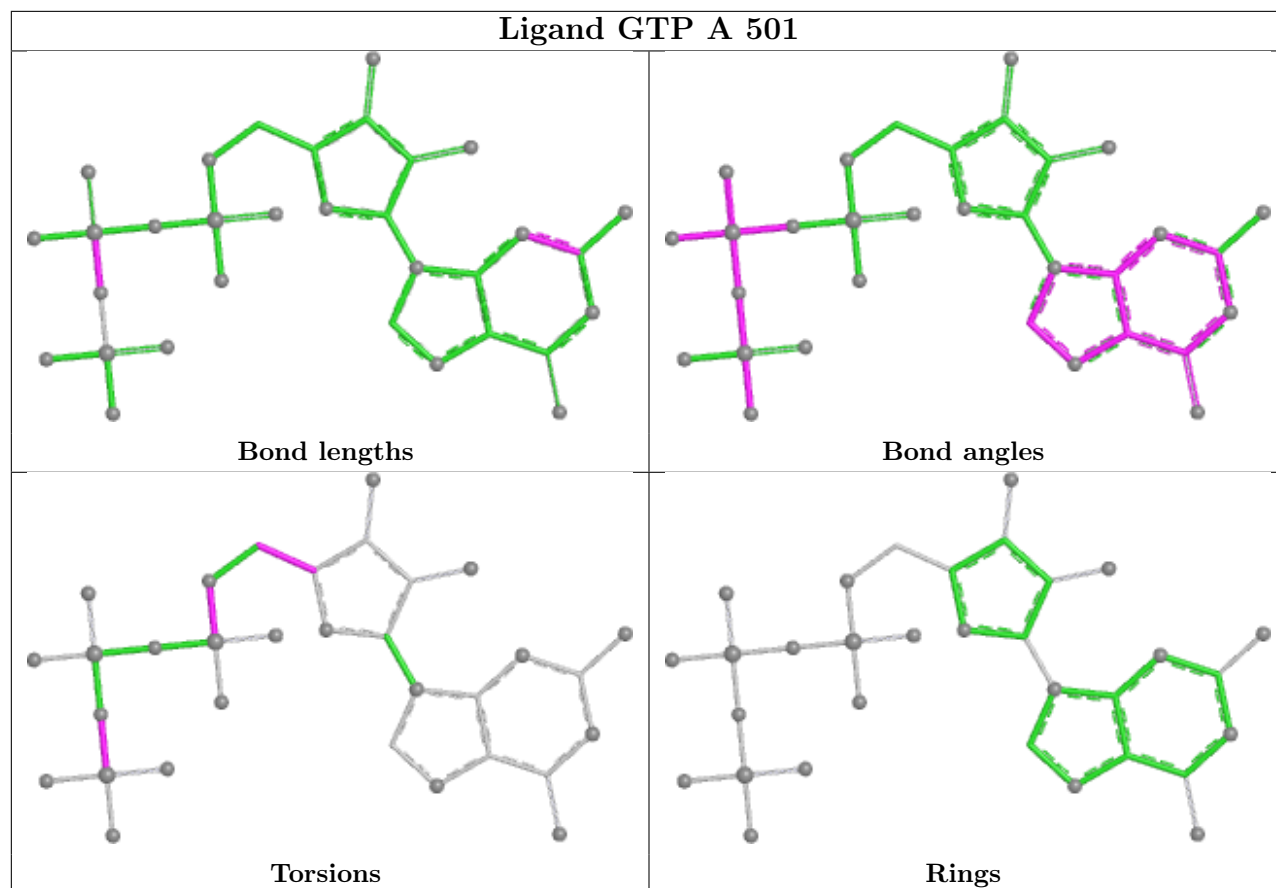
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

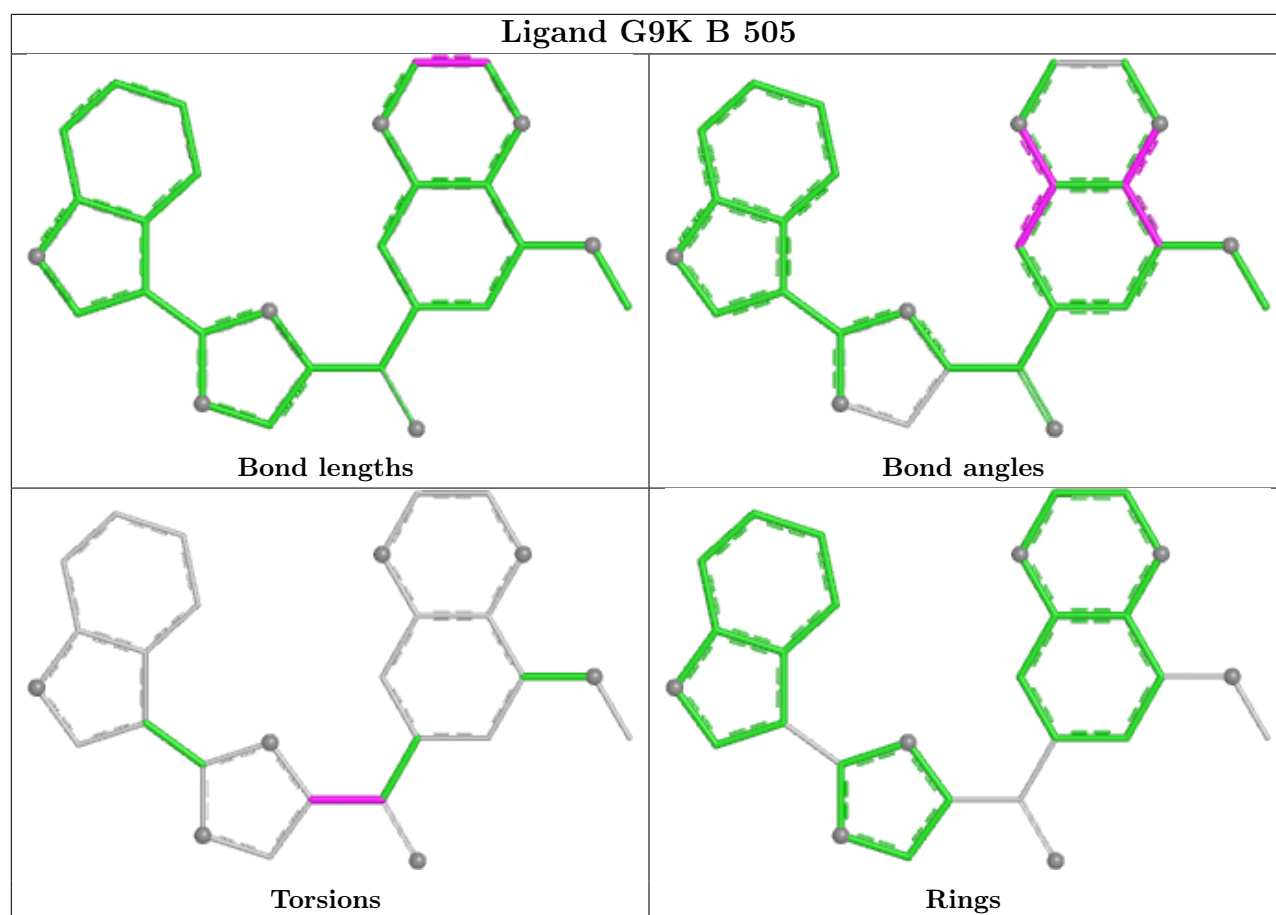
Ligand GTP C 501

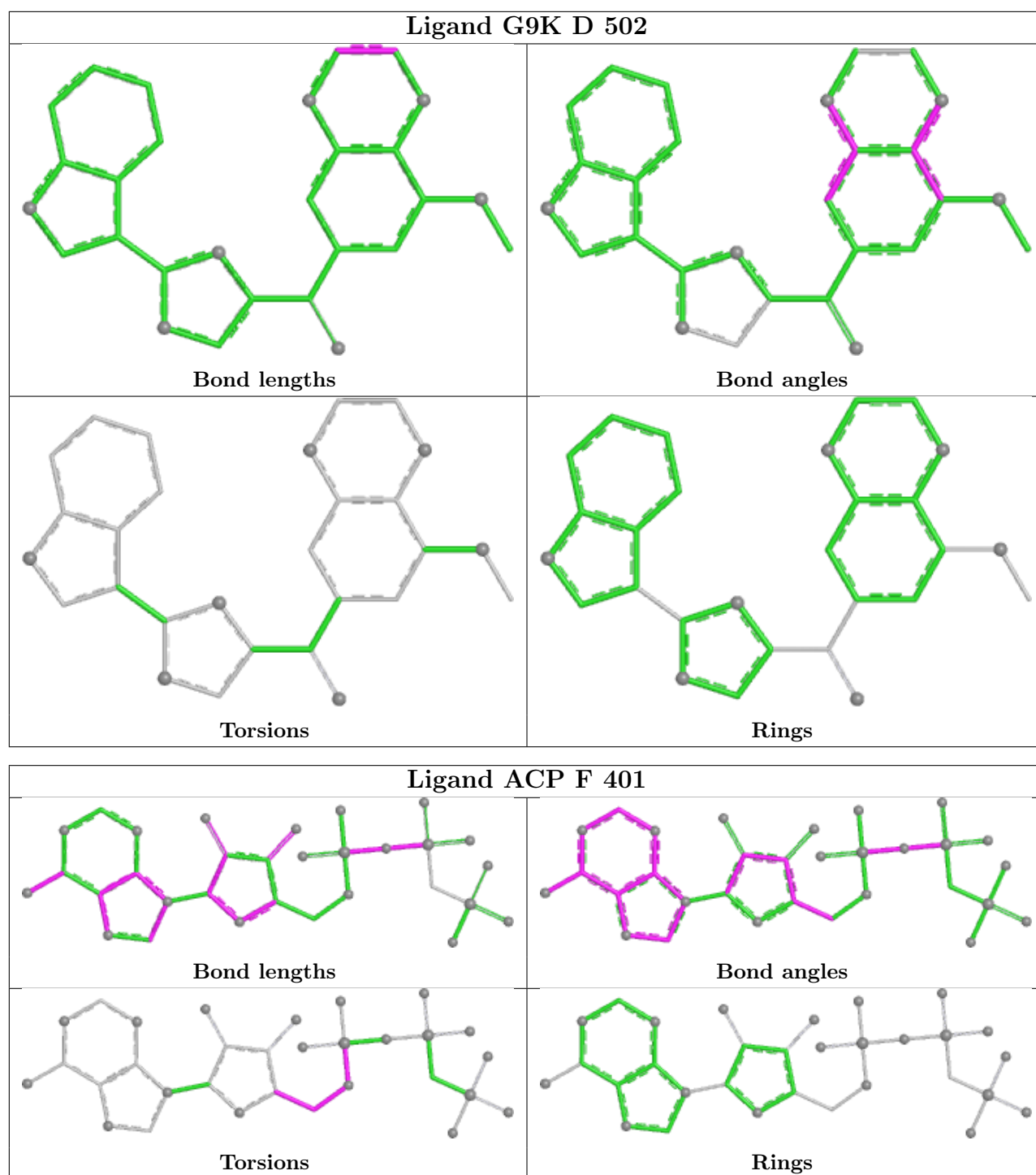


Ligand GDP D 501









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	-0.26	5 (1%) 78 73	29, 49, 79, 142	0
1	C	440/450 (97%)	-0.45	3 (0%) 84 80	21, 36, 63, 93	0
2	B	427/445 (95%)	-0.21	7 (1%) 70 64	21, 44, 84, 147	0
2	D	421/445 (94%)	0.34	28 (6%) 24 17	35, 69, 115, 152	0
3	E	121/143 (84%)	0.10	2 (1%) 69 63	30, 63, 100, 122	0
4	F	332/384 (86%)	0.64	34 (10%) 12 10	39, 81, 146, 179	0
All	All	2178/2317 (94%)	-0.02	79 (3%) 46 36	21, 53, 112, 179	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	5.1
2	B	291	GLN	4.6
4	F	173	ILE	4.2
4	F	362	ALA	3.9
4	F	161	LEU	3.8
2	D	431	ASP	3.7
2	D	360	GLY	3.7
1	A	282	TYR	3.7
4	F	136	ASN	3.6
2	D	245	GLN	3.5
2	D	141	GLY	3.5
4	F	244	CYS	3.5
4	F	133	ALA	3.4
4	F	182	ILE	3.4
4	F	245	ILE	3.4
2	D	73	MET	3.4
4	F	132	LEU	3.4
4	F	170	LEU	3.4
4	F	103	THR	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	90	SER	3.2
3	E	139	LEU	3.2
1	A	281	ALA	3.1
1	A	437	VAL	3.1
2	D	176	SER	3.1
1	C	284	GLU	3.0
2	D	396	HIS	3.0
2	D	140	GLY	3.0
1	A	113	GLU	2.9
4	F	171	ASP	2.9
2	D	323	MET	2.9
2	D	397	TRP	2.9
2	D	55	THR	2.8
2	D	406	MET	2.7
2	D	72	THR	2.7
4	F	230	SER	2.7
4	F	247	LYS	2.6
4	F	237	THR	2.6
4	F	169	LEU	2.6
2	D	272	PRO	2.6
2	B	333	VAL	2.5
2	D	180	VAL	2.5
2	B	218	THR	2.5
4	F	147	TRP	2.5
2	D	53	GLU	2.5
2	B	428	ALA	2.5
2	D	220	PRO	2.5
2	B	279	GLN	2.5
3	E	27	PRO	2.4
4	F	181	VAL	2.4
4	F	99	VAL	2.4
4	F	372	THR	2.4
2	D	39	ASP	2.4
4	F	130	VAL	2.4
2	D	126	SER	2.3
2	D	97	ALA	2.3
4	F	91	CYS	2.3
4	F	242	ASN	2.3
2	D	54	ALA	2.2
2	D	86	ARG	2.2
2	B	281	TYR	2.2
2	D	208	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	184	LYS	2.2
2	D	178	THR	2.2
2	D	96	GLY	2.2
2	D	170	MET	2.2
4	F	233	PHE	2.2
2	D	80	PRO	2.2
4	F	194	PRO	2.2
4	F	253	TYR	2.2
4	F	320	MET	2.1
4	F	339	ALA	2.1
1	A	18	ASN	2.1
2	D	377	LEU	2.1
1	C	245	ASP	2.1
4	F	240	LEU	2.0
2	B	96	GLY	2.0
4	F	134	ALA	2.0
1	C	440	VAL	2.0
4	F	186	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ACP	F	401	31/31	0.75	0.16	103,125,149,162	0
8	GDP	D	501	28/28	0.86	0.13	59,66,98,103	0
9	MES	B	503	12/12	0.91	0.14	67,73,84,87	12
10	G9K	D	502	28/28	0.92	0.11	47,62,81,81	0
7	MG	C	503	1/1	0.94	0.12	41,41,41,41	0

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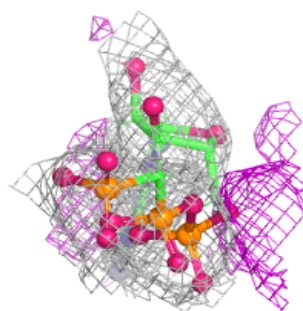
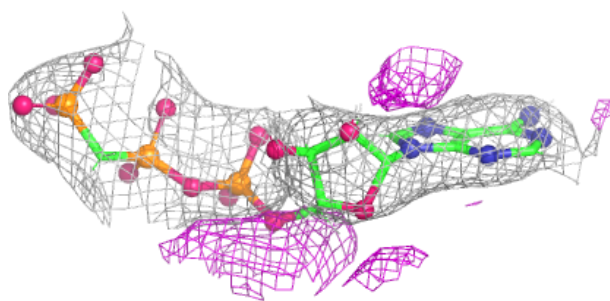
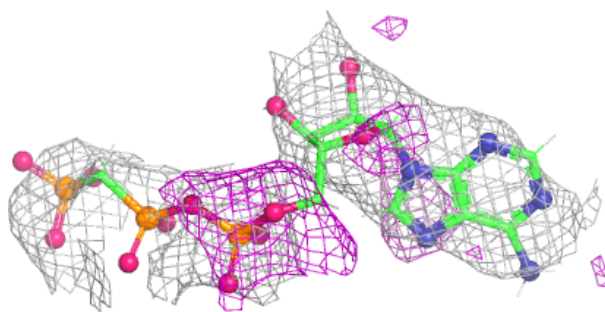
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	B	504	1/1	0.95	0.13	38,38,38,38	0
9	MES	B	502	12/12	0.96	0.11	24,40,55,58	12
10	G9K	B	505	28/28	0.96	0.07	39,44,54,54	0
6	CA	C	502	1/1	0.97	0.04	54,54,54,54	0
8	GDP	B	501	28/28	0.97	0.07	19,32,37,38	0
7	MG	A	503	1/1	0.97	0.11	41,41,41,41	0
5	GTP	C	501	32/32	0.97	0.07	27,34,38,42	0
5	GTP	A	501	32/32	0.98	0.05	27,34,41,45	0
6	CA	A	502	1/1	0.99	0.04	63,63,63,63	0

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

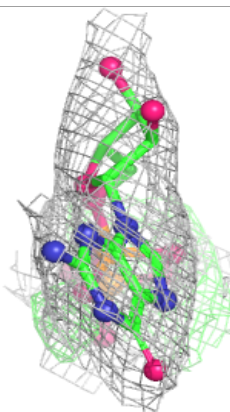
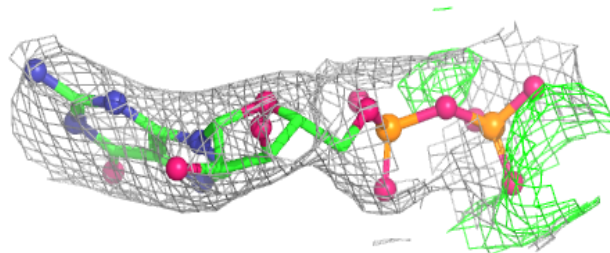
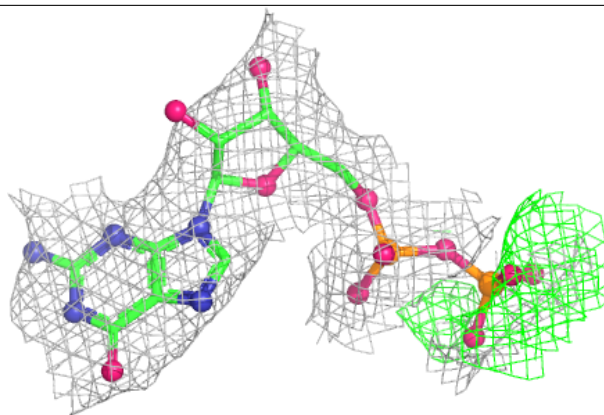
Electron density around ACP F 401:

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

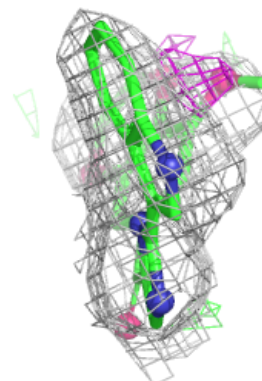
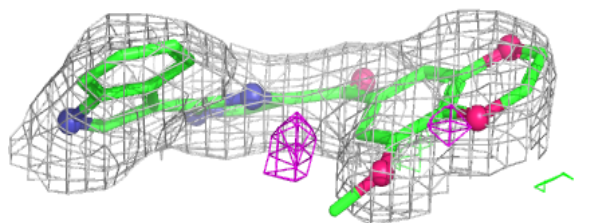
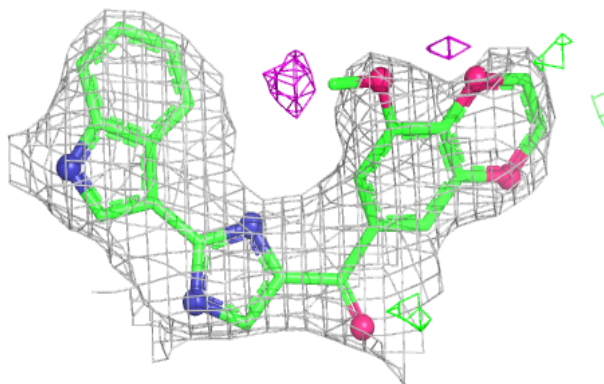


Electron density around GDP D 501:

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

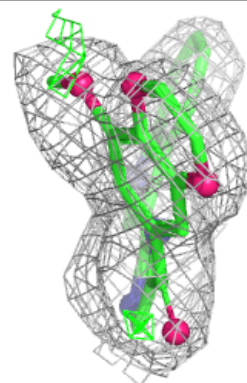
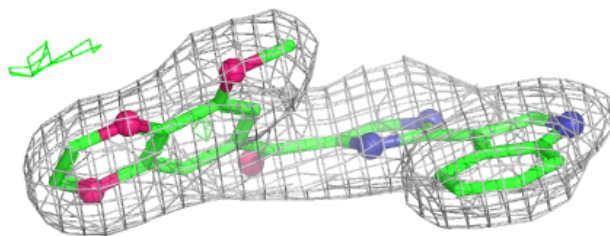
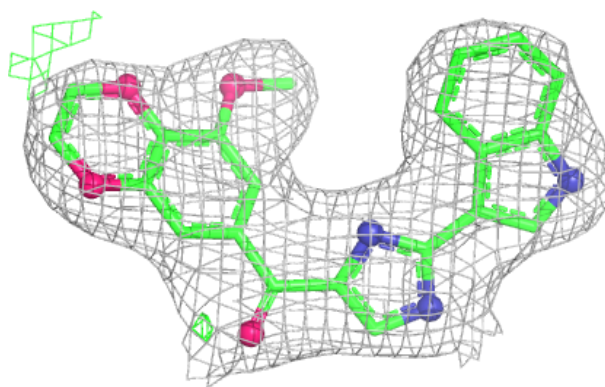
**Electron density around G9K D 502:**

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



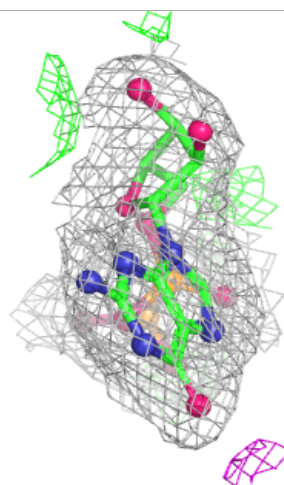
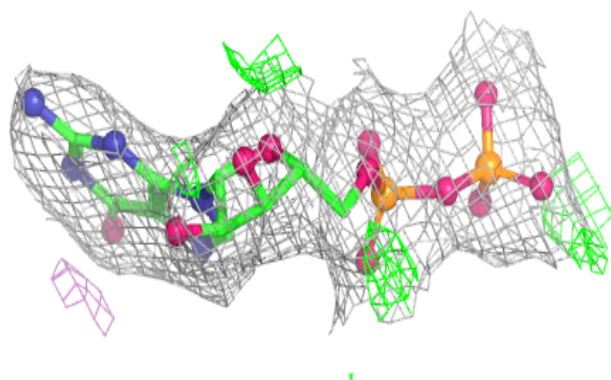
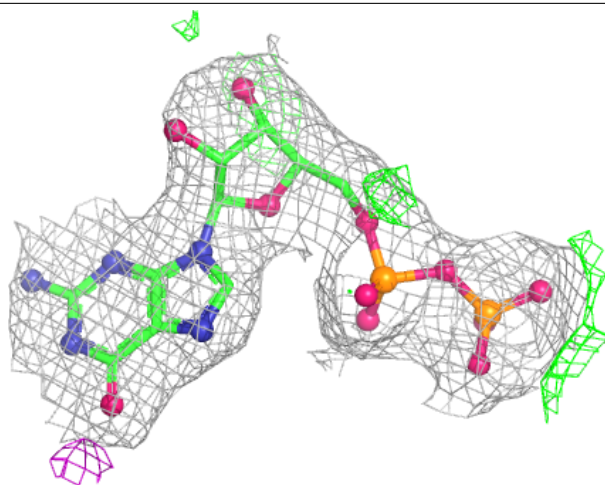
Electron density around G9K B 505:

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



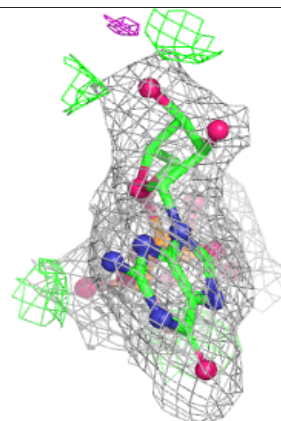
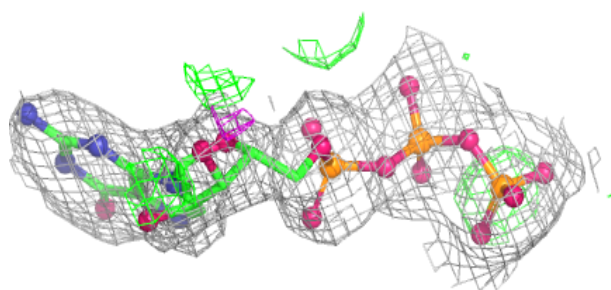
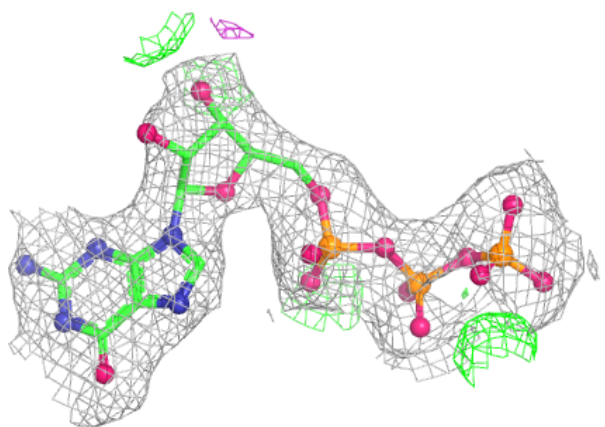
Electron density around GDP B 501:

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



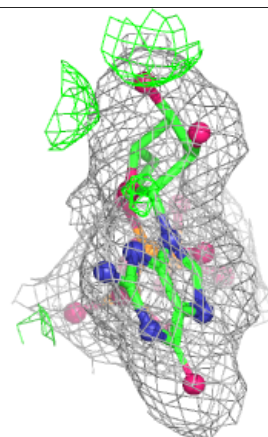
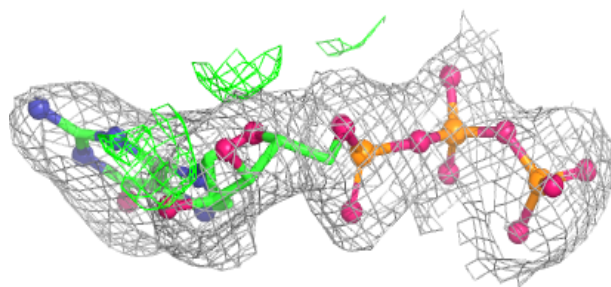
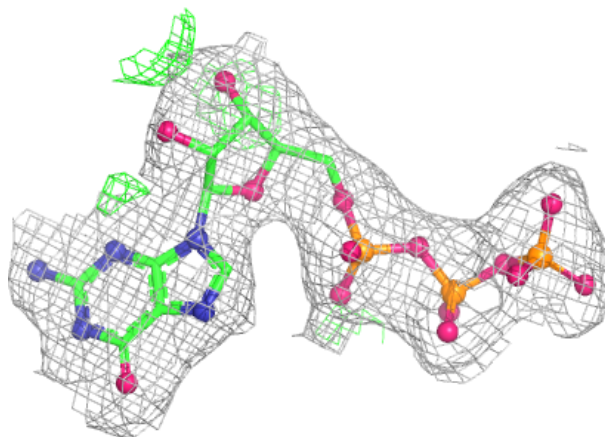
Electron density around GTP C 501:

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



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.