



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 PM UTC

PDB ID : 6BRY / pdb_00006bry
Title : Tubulin-RB3_SLD-TTL in complex with heterocyclic pyrimidine compound 6a
Authors : Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on : 2017-12-01
Resolution : 2.70 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

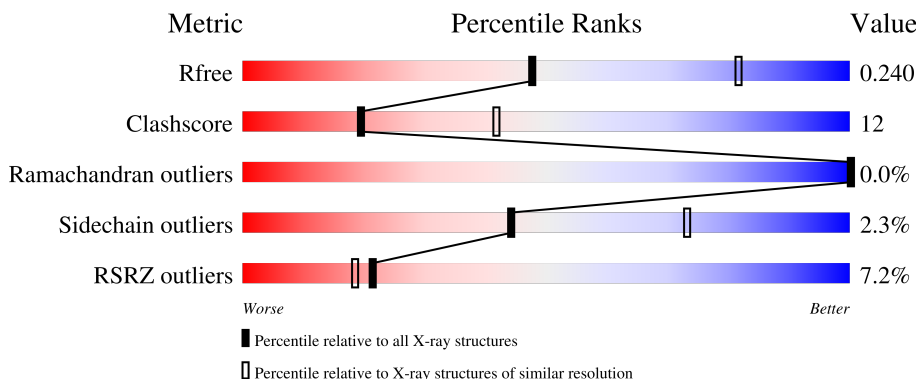
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
1	C	450	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	19% 54% 30% • 14%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17762 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
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	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 Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

- 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
			2727	1752	468	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		

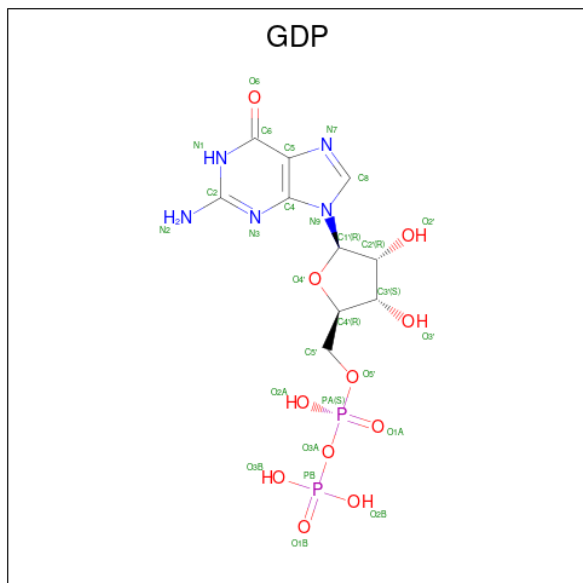
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

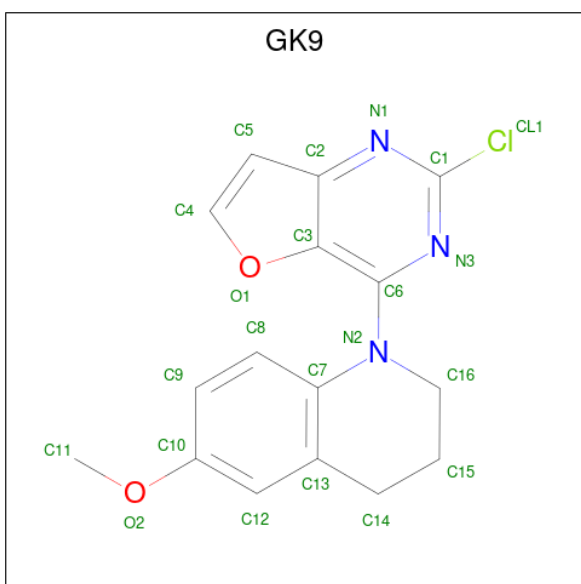
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





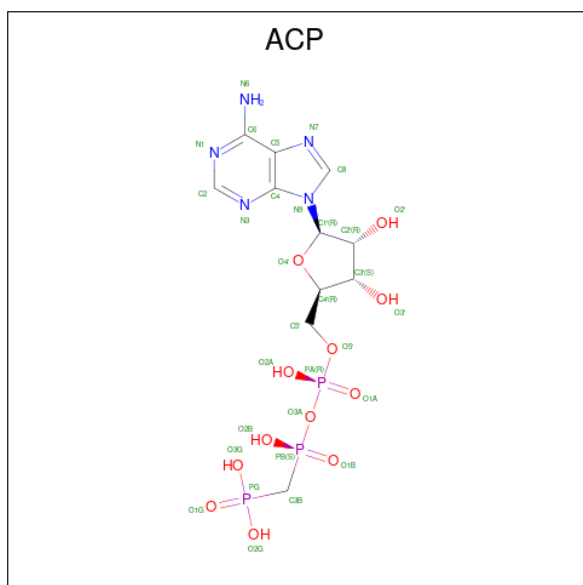
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 1-(2-chlorofuro[3,2-d]pyrimidin-4-yl)-6-methoxy-1,2,3,4-tetrahydroquinoline (CCD ID: GK9) (formula: C₁₆H₁₄ClN₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
10	D	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		

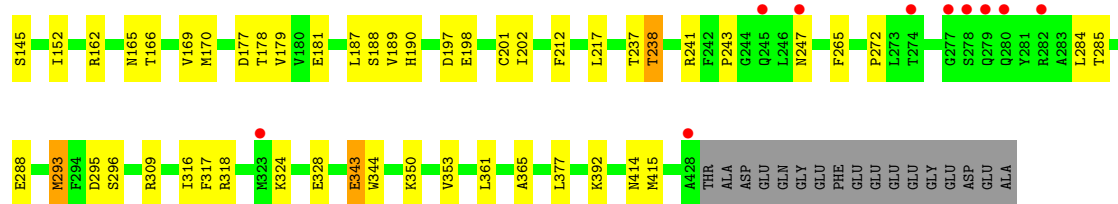
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



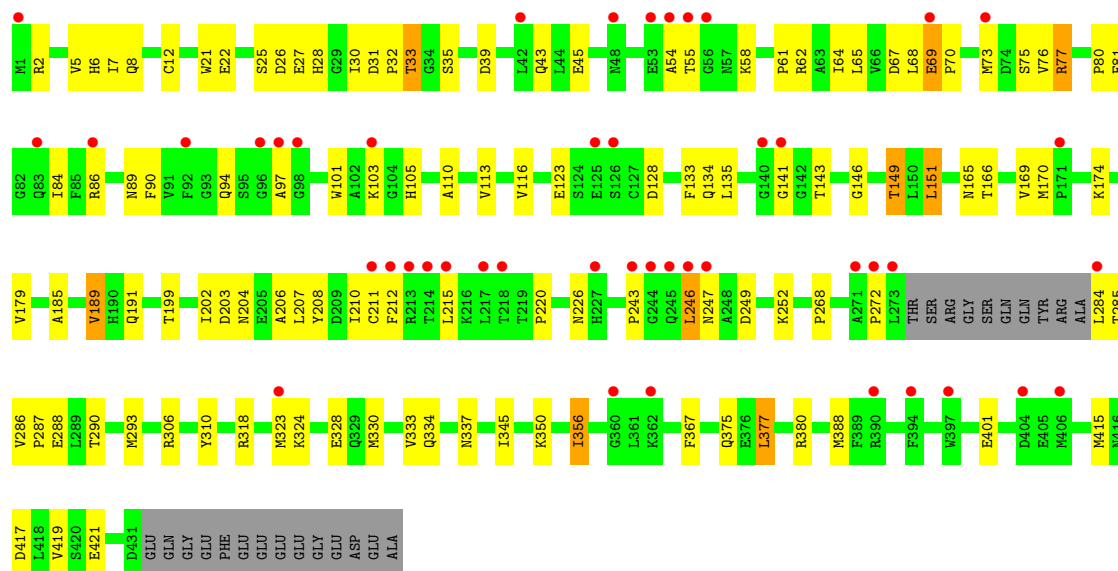
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 12 is water.

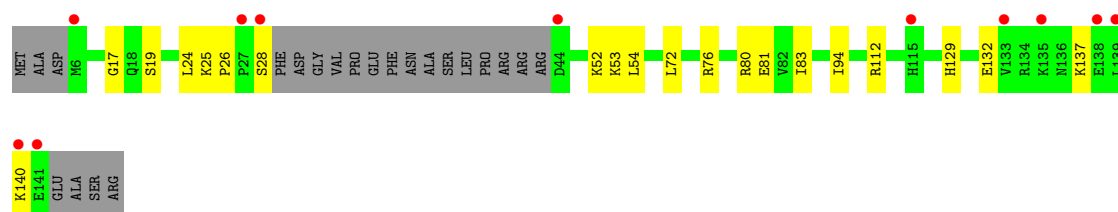
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	55	Total	O	0	0
			55	55		
12	B	52	Total	O	0	0
			52	52		
12	C	109	Total	O	0	0
			109	109		
12	D	12	Total	O	0	0
			12	12		
12	E	5	Total	O	0	0
			5	5		
12	F	20	Total	O	0	0
			20	20		



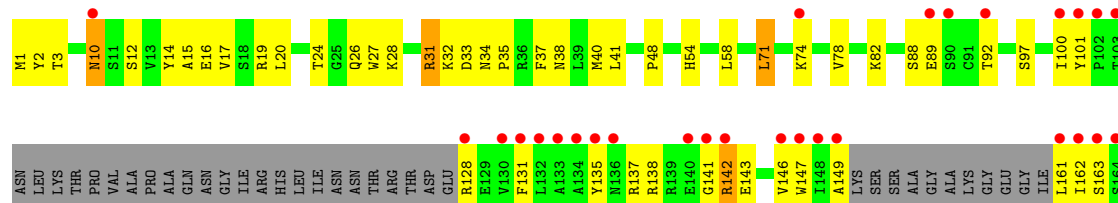
• Molecule 2: Tubulin beta-2B chain

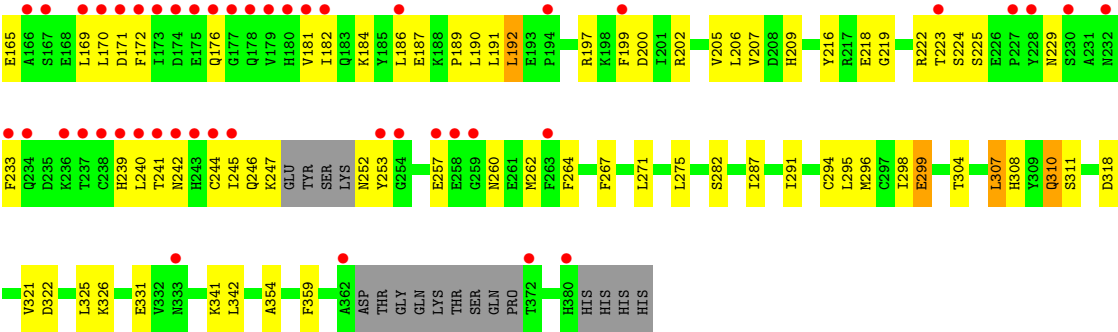


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.09Å 157.77Å 181.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.70 49.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.75-2.70) 97.3 (49.75-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.69Å)	Xtriage
Refinement program	PHENIX dev_2947	Depositor
R, R_{free}	0.191 , 0.236 0.193 , 0.240	Depositor DCC
R_{free} test set	4788 reflections (5.70%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.3	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	0.94	EDS
Total number of atoms	17762	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: GK9, MG, MES, ACP, GTP, CA, 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	0.33	0/3494	0.56	0/4743
1	C	0.37	0/3515	0.61	0/4772
2	B	0.33	0/3444	0.57	0/4664
2	D	0.29	0/3382	0.52	0/4581
3	E	0.32	0/1008	0.45	0/1337
4	F	0.28	0/2789	0.47	0/3768
All	All	0.32	0/17632	0.55	0/23865

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3331	57	0
1	C	3437	0	3348	64	0
2	B	3369	0	3250	63	0
2	D	3309	0	3189	104	0
3	E	1000	0	1018	15	0
4	F	2727	0	2699	116	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	4	0
9	B	24	0	24	6	0
9	C	12	0	12	3	0
10	B	22	0	0	0	0
10	D	22	0	0	0	0
11	F	31	14	13	6	0
12	A	55	0	0	1	0
12	B	52	0	0	0	0
12	C	109	0	0	1	0
12	D	12	0	0	0	0
12	E	5	0	0	1	0
12	F	20	0	0	0	0
All	All	17748	14	16932	400	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 12.

All (400) 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:238:THR:HG21	2:B:318:ARG:HD2	1.33	1.08
2:D:189:VAL:HG21	2:D:415:MET:HE3	1.35	1.05
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.41	1.03
1:C:264:ARG:HD3	9:C:504:MES:H81	1.37	1.01
4:F:71:LEU:HD13	4:F:298:ILE:HD13	1.49	0.95
1:C:71:GLU:OE1	1:C:73:THR:HB	1.67	0.94
2:D:189:VAL:HG21	2:D:415:MET:CE	1.97	0.93
2:D:73:MET:HE2	2:D:77:ARG:HH12	1.29	0.93
4:F:31:ARG:HD3	4:F:32:LYS:H	1.33	0.91
2:D:189:VAL:CG2	2:D:415:MET:HE3	2.00	0.91
4:F:137:ARG:O	4:F:137:ARG:NH1	2.05	0.90
2:D:375:GLN:HG3	2:D:419:VAL:HG13	1.55	0.87
1:A:71:GLU:OE1	1:A:73:THR:HB	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:THR:HG21	2:D:191:GLN:HG3	1.59	0.85
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.08	0.83
4:F:172:PHE:O	4:F:176:GLN:HG2	1.78	0.81
1:C:241:SER:HA	1:C:249:ASN:HD21	1.45	0.79
2:D:179:VAL:HB	2:D:388:MET:HE1	1.66	0.78
4:F:31:ARG:HD3	4:F:32:LYS:N	1.98	0.78
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.64	0.77
2:D:33:THR:O	2:D:58:LYS:NZ	2.13	0.76
1:C:249:ASN:ND2	1:C:356:ASN:OD1	2.19	0.76
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.21	0.76
4:F:137:ARG:HH12	4:F:141:GLY:HA3	1.49	0.76
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.16	0.76
2:B:238:THR:HG21	2:B:318:ARG:CD	2.14	0.75
2:D:67:ASP:OD1	2:D:69:GLU:HG3	1.87	0.74
4:F:223:THR:HG22	4:F:260:ASN:O	1.87	0.74
2:D:86:ARG:HD2	2:D:89:ASN:OD1	1.88	0.73
1:C:221:ARG:HD3	2:D:323:MET:HG2	1.71	0.72
2:D:285:THR:OG1	2:D:288:GLU:HG3	1.89	0.72
1:C:381:THR:HG22	1:C:383:ALA:H	1.55	0.72
2:D:134:GLN:HA	2:D:165:ASN:O	1.91	0.70
4:F:209:HIS:HB2	4:F:310:GLN:CG	2.23	0.68
2:B:324:LYS:HE2	2:B:328:GLU:OE2	1.94	0.68
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.29	0.68
2:B:177:ASP:O	1:C:352:LYS:HE2	1.94	0.68
4:F:10:ASN:O	4:F:10:ASN:ND2	2.17	0.68
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.29	0.67
2:D:105:HIS:CE1	2:D:149:THR:HG22	2.30	0.67
2:D:375:GLN:CG	2:D:419:VAL:HG13	2.24	0.67
4:F:187:GLU:O	4:F:189:PRO:HD3	1.95	0.66
4:F:225:SER:HB3	4:F:252:ASN:HB3	1.75	0.66
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.77	0.66
2:D:203:ASP:OD1	2:D:380:ARG:NH2	2.28	0.66
2:D:141:GLY:HA3	8:D:501:GDP:O3A	1.96	0.65
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.78	0.65
2:B:238:THR:OG1	2:B:316:ILE:HG21	1.97	0.65
1:A:381:THR:HG22	1:A:383:ALA:H	1.61	0.64
4:F:296:MET:HE1	4:F:299:GLU:OE2	1.97	0.64
1:C:332:ILE:HG22	1:C:336:LYS:HE2	1.77	0.64
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.27	0.64
2:B:179:VAL:HG22	1:C:258:ASN:OD1	1.98	0.64
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:222:ARG:O	4:F:241:THR:HG21	1.97	0.64
2:B:178:THR:O	2:B:181:GLU:HG3	1.98	0.63
4:F:10:ASN:HD22	4:F:10:ASN:C	2.05	0.63
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.80	0.63
4:F:246:GLN:C	4:F:247:LYS:HD2	2.24	0.63
2:D:33:THR:HG23	2:D:58:LYS:NZ	2.14	0.62
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.31	0.62
1:C:221:ARG:HD3	2:D:323:MET:CG	2.28	0.62
4:F:209:HIS:HB2	4:F:310:GLN:HG3	1.81	0.62
3:E:140:LYS:HG3	3:E:140:LYS:O	1.99	0.62
1:A:399:TYR:O	1:A:402:ARG:NH1	2.32	0.62
4:F:32:LYS:HG3	4:F:33:ASP:OD2	1.99	0.62
2:D:356:ILE:N	2:D:356:ILE:HD12	2.15	0.62
1:A:187:SER:CB	1:A:391:LEU:HD21	2.29	0.61
4:F:31:ARG:HA	4:F:31:ARG:NE	2.15	0.61
2:B:285:THR:OG1	2:B:288:GLU:HG3	2.00	0.61
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.40	0.61
2:D:105:HIS:HE1	2:D:149:THR:HG22	1.65	0.61
1:A:178:SER:O	2:B:350:LYS:NZ	2.34	0.61
2:D:97:ALA:HB2	2:D:143:THR:OG1	2.01	0.61
2:B:135:LEU:HD23	2:B:152:ILE:HD11	1.83	0.60
1:C:398:MET:HE3	2:D:345:ILE:HG23	1.82	0.60
2:D:25:SER:HB3	2:D:30:ILE:HD11	1.83	0.60
2:D:166:THR:OG1	2:D:199:THR:HG22	2.02	0.60
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.84	0.59
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.37	0.59
4:F:247:LYS:HE3	4:F:253:TYR:CD1	2.37	0.59
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.37	0.59
2:D:31:ASP:OD1	2:D:33:THR:HB	2.03	0.59
2:B:2:ARG:NH1	2:B:129:CYS:SG	2.76	0.58
4:F:197:ARG:HB3	4:F:224:SER:O	2.03	0.58
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.67	0.58
3:E:129:HIS:HA	3:E:132:GLU:HG2	1.85	0.58
2:D:185:ALA:O	2:D:189:VAL:HG13	2.03	0.58
2:B:165:ASN:HD22	2:B:198:GLU:HB2	1.69	0.58
2:D:80:PRO:O	2:D:81:PHE:HB2	2.03	0.58
3:E:81:GLU:OE2	12:E:201:HOH:O	2.17	0.58
4:F:223:THR:HG21	4:F:257:GLU:OE2	2.04	0.58
1:A:120:ASP:O	1:A:124:LYS:HG2	2.04	0.58
2:B:94:GLN:HB3	1:C:1:MET:HE2	1.84	0.57
2:D:179:VAL:HB	2:D:388:MET:CE	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:THR:HG23	4:F:38:ASN:H	1.69	0.57
4:F:88:SER:OG	4:F:89:GLU:HA	2.04	0.57
4:F:71:LEU:CD1	4:F:298:ILE:HD13	2.30	0.57
4:F:74:LYS:H	4:F:74:LYS:HD3	1.69	0.57
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.86	0.57
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
4:F:200:ASP:OD2	4:F:241:THR:HB	2.05	0.56
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.40	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.56
2:B:145:SER:HG	2:B:188:SER:HG	1.54	0.56
2:D:73:MET:HE2	2:D:77:ARG:NH1	2.10	0.56
2:B:189:VAL:HB	2:B:415:MET:CE	2.35	0.56
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.87	0.56
1:A:112:LYS:HD2	3:E:54:LEU:HB3	1.88	0.56
2:B:130:LEU:O	2:B:162:ARG:NH1	2.38	0.56
1:C:166:LYS:HE2	1:C:197:HIS:O	2.04	0.56
4:F:191:LEU:HD12	4:F:197:ARG:O	2.06	0.56
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.41	0.56
2:B:309:ARG:NH1	2:B:343:GLU:OE1	2.35	0.56
1:C:178:SER:O	2:D:350:LYS:HE2	2.06	0.56
4:F:138:ARG:HH11	4:F:143:GLU:HB3	1.70	0.56
3:E:137:LYS:O	3:E:140:LYS:HG2	2.05	0.56
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.36	0.55
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.06	0.55
2:D:81:PHE:O	2:D:84:ILE:HG22	2.06	0.55
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.88	0.55
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.89	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.41	0.55
2:B:162:ARG:O	9:B:502:MES:H71	2.06	0.55
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.88	0.55
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.42	0.55
2:D:55:THR:O	2:D:58:LYS:HG2	2.07	0.55
1:C:399:TYR:O	1:C:402:ARG:NH2	2.37	0.55
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.36	0.55
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.42	0.54
4:F:71:LEU:HD21	4:F:294:CYS:HB3	1.89	0.54
2:B:42:LEU:CD2	2:B:243:PRO:HD2	2.38	0.54
2:D:103:LYS:HG2	2:D:401:GLU:OE2	2.07	0.54
4:F:162:ILE:HD11	4:F:240:LEU:HD21	1.90	0.54
2:B:135:LEU:HB3	2:B:166:THR:HG22	1.87	0.54
2:D:25:SER:HB3	2:D:30:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.54
4:F:137:ARG:NH1	4:F:141:GLY:HA3	2.19	0.54
2:B:293:MET:HE3	2:B:365:ALA:HB1	1.89	0.54
4:F:15:ALA:O	4:F:19:ARG:HG3	2.07	0.54
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.43	0.54
2:D:293:MET:CG	2:D:367:PHE:HB2	2.37	0.54
4:F:3:THR:O	4:F:38:ASN:HB2	2.08	0.54
1:C:209:ILE:HD11	1:C:302:MET:SD	2.48	0.53
4:F:137:ARG:HH12	4:F:141:GLY:CA	2.20	0.53
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.43	0.53
2:B:33:THR:HG22	2:B:58:LYS:NZ	2.24	0.53
2:B:94:GLN:HB3	1:C:1:MET:CE	2.38	0.53
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.90	0.53
2:D:116:VAL:CG1	2:D:151:LEU:HD11	2.38	0.53
4:F:100:ILE:HG13	4:F:182:ILE:HD12	1.89	0.53
4:F:202:ARG:NE	4:F:318:ASP:OD2	2.31	0.53
2:B:35:SER:OG	2:B:58:LYS:NZ	2.36	0.53
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.90	0.53
4:F:184:LYS:O	11:F:402:ACP:N6	2.40	0.53
1:A:25:CYS:HB3	1:A:30:ILE:O	2.09	0.53
2:B:392:LYS:N	2:B:392:LYS:HD2	2.24	0.52
2:D:110:ALA:O	2:D:113:VAL:HG12	2.09	0.52
2:B:31:ASP:OD1	2:B:33:THR:HB	2.10	0.52
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.92	0.52
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.91	0.52
2:D:45:GLU:OE2	2:D:243:PRO:HG3	2.10	0.52
2:D:189:VAL:HG21	2:D:415:MET:HE2	1.90	0.52
4:F:20:LEU:O	4:F:24:THR:HG23	2.09	0.52
4:F:146:VAL:HG21	4:F:233:PHE:CZ	2.45	0.52
1:C:165:SER:HA	1:C:199:ASP:OD2	2.10	0.52
3:E:72:LEU:O	3:E:76:ARG:HG2	2.10	0.52
4:F:137:ARG:NH2	4:F:143:GLU:HG3	2.23	0.52
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.44	0.52
1:C:221:ARG:CD	2:D:323:MET:HG2	2.39	0.52
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.10	0.52
2:D:73:MET:CG	2:D:77:ARG:HH22	2.22	0.52
1:C:171:ILE:HD12	1:C:171:ILE:N	2.25	0.52
2:D:54:ALA:HB3	2:D:58:LYS:HB2	1.92	0.52
4:F:244:CYS:O	4:F:247:LYS:HG2	2.09	0.52
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.40	0.52
2:D:169:VAL:HA	2:D:202:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HG3	1:A:194:THR:HG23	1.92	0.51
1:A:261:PRO:HD2	12:A:614:HOH:O	2.10	0.51
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.45	0.51
1:A:283:HIS:HD2	1:A:285:GLN:NE2	2.07	0.51
4:F:131:PHE:CE2	4:F:182:ILE:HG21	2.47	0.50
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.18	0.50
2:B:293:MET:CE	2:B:365:ALA:HB1	2.42	0.50
1:C:171:ILE:N	1:C:171:ILE:CD1	2.74	0.50
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.47	0.50
2:D:306:ARG:NH2	2:D:337:ASN:OD1	2.45	0.50
4:F:128:ARG:HH21	4:F:170:LEU:HD13	1.76	0.50
1:C:96:LYS:NZ	2:D:128:ASP:O	2.26	0.50
4:F:192:LEU:HD12	4:F:192:LEU:H	1.75	0.50
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.44	0.50
4:F:138:ARG:NH2	4:F:184:LYS:HE2	2.27	0.50
4:F:205:VAL:HG21	4:F:291:ILE:HG21	1.92	0.50
1:C:398:MET:CE	1:C:404:PHE:CE2	2.95	0.50
2:B:2:ARG:HA	2:B:129:CYS:O	2.13	0.49
4:F:16:GLU:O	4:F:20:LEU:HG	2.11	0.49
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.49
4:F:242:ASN:HD21	11:F:402:ACP:C3B	2.25	0.49
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.76	0.49
1:A:247:ALA:HB3	3:E:19:SER:OG	2.12	0.49
4:F:74:LYS:HD3	4:F:74:LYS:N	2.28	0.49
4:F:245:ILE:HG22	4:F:245:ILE:O	2.13	0.49
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.94	0.49
2:D:377:LEU:C	2:D:377:LEU:HD23	2.37	0.49
1:C:255:PHE:CD1	1:C:352:LYS:HD3	2.48	0.49
2:D:324:LYS:O	2:D:328:GLU:HG3	2.12	0.49
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.95	0.48
2:D:73:MET:HG2	2:D:77:ARG:NH2	2.27	0.48
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.93	0.48
4:F:287:ILE:O	4:F:291:ILE:HG13	2.13	0.48
4:F:137:ARG:HH22	4:F:143:GLU:HG3	1.77	0.48
4:F:161:LEU:HD23	4:F:172:PHE:CE2	2.48	0.48
1:A:159:VAL:HG23	1:A:160:ASP:OD1	2.13	0.48
1:C:71:GLU:OE1	1:C:73:THR:CB	2.52	0.48
1:C:264:ARG:HD3	9:C:504:MES:C8	2.26	0.48
4:F:74:LYS:H	4:F:74:LYS:CD	2.25	0.48
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.48	0.48
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.49	0.48
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.47	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.48
2:D:203:ASP:CG	2:D:380:ARG:HH22	2.22	0.48
2:D:330:MET:O	2:D:334:GLN:HG3	2.12	0.48
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.44	0.48
2:D:64:ILE:HG13	2:D:89:ASN:HD22	1.78	0.48
2:D:67:ASP:CG	2:D:69:GLU:HG3	2.38	0.48
4:F:92:THR:O	4:F:326:LYS:HE2	2.14	0.47
2:B:295:ASP:HA	9:B:503:MES:O3S	2.14	0.47
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.94	0.47
1:C:324:VAL:HG22	12:C:611:HOH:O	2.13	0.47
4:F:147:TRP:O	4:F:162:ILE:HG23	2.13	0.47
4:F:242:ASN:HD21	11:F:402:ACP:H3B2	1.80	0.47
2:B:189:VAL:HB	2:B:415:MET:HE3	1.96	0.47
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.96	0.47
4:F:199:PHE:HZ	4:F:321:VAL:HB	1.78	0.47
2:B:67:ASP:O	2:B:92:PHE:HA	2.14	0.47
2:B:135:LEU:HD22	2:B:152:ILE:HD11	1.95	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.96	0.47
2:D:7:ILE:O	2:D:135:LEU:HD12	2.15	0.47
2:D:70:PRO:HG3	2:D:94:GLN:HA	1.97	0.47
2:D:204:ASN:HA	2:D:207:LEU:HD12	1.97	0.47
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.97	0.47
1:C:167:LEU:HA	1:C:200:CYS:O	2.14	0.47
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.50	0.47
1:C:398:MET:CE	1:C:404:PHE:CD2	2.98	0.47
2:D:68:LEU:H	2:D:143:THR:HG21	1.80	0.47
4:F:187:GLU:C	4:F:189:PRO:HD3	2.40	0.47
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.95	0.47
4:F:190:LEU:HB2	4:F:322:ASP:O	2.15	0.47
2:D:174:LYS:HE3	2:D:208:TYR:CD2	2.50	0.46
4:F:3:THR:HG23	4:F:37:PHE:HA	1.97	0.46
2:B:169:VAL:HA	2:B:202:ILE:O	2.16	0.46
4:F:225:SER:CB	4:F:252:ASN:HB3	2.43	0.46
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.51	0.46
2:B:197:ASP:OD1	9:B:502:MES:H62	2.15	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE3	1.97	0.46
2:D:143:THR:HB	8:D:501:GDP:O1B	2.14	0.46
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:MET:HE2	1:C:404:PHE:CD2	2.50	0.46
4:F:135:TYR:OH	4:F:165:GLU:HA	2.15	0.46
2:D:226:ASN:OD1	8:D:501:GDP:N1	2.34	0.46
4:F:247:LYS:HD2	4:F:247:LYS:N	2.29	0.46
1:C:244:PHE:HB2	1:C:356:ASN:ND2	2.31	0.46
2:D:25:SER:CB	2:D:30:ILE:HD11	2.45	0.46
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.97	0.46
2:D:268:PRO:HA	2:D:367:PHE:O	2.16	0.46
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.97	0.45
2:D:189:VAL:HG22	2:D:415:MET:HE3	1.95	0.45
1:A:147:SER:HB2	1:A:190:THR:HB	1.98	0.45
2:B:212:PHE:HA	2:B:217:LEU:O	2.16	0.45
1:C:210:TYR:CE2	1:C:214:ARG:HD3	2.52	0.45
4:F:341:LYS:HG3	4:F:342:LEU:HD23	1.97	0.45
2:B:324:LYS:O	2:B:328:GLU:HG3	2.15	0.45
4:F:88:SER:CB	4:F:89:GLU:HA	2.45	0.45
1:A:2:ARG:O	1:A:51:THR:HG23	2.16	0.45
2:D:284:LEU:HD12	2:D:284:LEU:N	2.32	0.45
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.52	0.45
2:D:73:MET:HE3	2:D:90:PHE:CB	2.47	0.45
1:A:166:LYS:HE2	1:A:197:HIS:O	2.17	0.45
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.86	0.45
1:C:43:GLY:HA2	1:C:56:THR:O	2.16	0.45
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.52	0.45
1:A:133:GLN:OE1	1:A:252:LEU:HG	2.17	0.44
1:A:262:TYR:CE1	1:A:346:TRP:CZ2	3.06	0.44
1:A:345:ASP:O	3:E:28:SER:N	2.51	0.44
1:C:398:MET:HE2	1:C:404:PHE:HD2	1.82	0.44
4:F:192:LEU:HD12	4:F:192:LEU:N	2.32	0.44
1:A:104:ALA:HB2	1:A:413:MET:SD	2.57	0.44
2:B:103:LYS:HA	2:B:107:THR:OG1	2.18	0.44
2:D:73:MET:HG2	2:D:77:ARG:HH22	1.82	0.44
4:F:207:VAL:HG21	4:F:295:LEU:HD13	2.00	0.44
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.99	0.44
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.99	0.44
4:F:163:SER:CB	4:F:169:LEU:HD21	2.30	0.44
2:B:33:THR:HG22	2:B:58:LYS:HZ3	1.82	0.44
9:B:502:MES:H81	9:B:502:MES:H51	1.63	0.44
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.44
1:A:88:HIS:O	1:A:91:GLN:HG3	2.18	0.44
1:A:401:LYS:HG3	2:B:344:TRP:CE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ASN:HB2	2:B:60:VAL:HG13	1.99	0.44
2:B:317:PHE:HB2	2:B:353:VAL:HG22	2.00	0.44
2:D:28:HIS:HA	2:D:43:GLN:HB3	2.00	0.43
4:F:162:ILE:O	4:F:163:SER:HB2	2.17	0.43
4:F:275:LEU:HD23	4:F:325:LEU:HD11	1.99	0.43
1:A:349:THR:O	3:E:24:LEU:HB2	2.18	0.43
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.47	0.43
2:B:104:GLY:O	2:B:109:GLY:HA3	2.19	0.43
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.18	0.43
2:D:318:ARG:NH2	2:D:356:ILE:O	2.49	0.43
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.48	0.43
2:B:73:MET:CE	2:B:92:PHE:HD2	2.32	0.43
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.54	0.43
2:D:249:ASP:OD2	2:D:252:LYS:HD2	2.18	0.43
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.53	0.43
2:D:62:ARG:HG3	2:D:123:GLU:OE2	2.18	0.43
4:F:142:ARG:CD	4:F:142:ARG:O	2.66	0.43
4:F:331:GLU:OE2	11:F:402:ACP:O2A	2.37	0.43
1:A:46:ASP:OD2	1:A:46:ASP:N	2.48	0.43
2:D:206:ALA:O	2:D:210:ILE:HG13	2.19	0.43
4:F:163:SER:HB3	4:F:169:LEU:CD2	2.29	0.43
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.01	0.43
3:E:52:LYS:O	3:E:53:LYS:HE2	2.19	0.43
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.18	0.43
4:F:186:LEU:H	11:F:402:ACP:C2	2.32	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
2:D:116:VAL:HG11	2:D:151:LEU:HD11	2.01	0.43
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.00	0.43
4:F:82:LYS:NZ	4:F:97:SER:O	2.27	0.43
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.49	0.42
1:A:294:ALA:HB1	1:A:300:ASN:ND2	2.34	0.42
1:C:262:TYR:CD1	9:C:504:MES:H32	2.54	0.42
1:C:291:ILE:HD13	1:C:373:ARG:HG3	2.02	0.42
3:E:80:ARG:HA	3:E:83:ILE:HG22	2.01	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.42
4:F:3:THR:HG23	4:F:38:ASN:N	2.33	0.42
1:A:229:ARG:HD2	1:A:363:VAL:HG21	2.01	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.42
1:C:343:PHE:CG	1:C:349:THR:HG22	2.55	0.42
2:D:7:ILE:HG21	2:D:151:LEU:CD2	2.50	0.42
4:F:169:LEU:N	4:F:169:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.53	0.42
4:F:267:PHE:CZ	4:F:271:LEU:HD11	2.54	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.02	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.42
2:D:212:PHE:C	2:D:212:PHE:CD2	2.95	0.42
2:D:310:TYR:CE2	2:D:367:PHE:HZ	2.38	0.42
2:D:30:ILE:HD13	2:D:84:ILE:HD11	2.00	0.42
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.50	0.42
4:F:14:TYR:HA	4:F:17:VAL:HB	2.02	0.42
4:F:240:LEU:HD22	11:F:402:ACP:O4'	2.20	0.42
2:B:6:HIS:CE1	2:B:21:TRP:HE1	2.38	0.42
2:D:33:THR:CG2	2:D:58:LYS:NZ	2.79	0.42
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.42
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.55	0.42
4:F:1:MET:HE2	4:F:28:LYS:HB2	2.01	0.42
4:F:304:THR:HG21	4:F:311:SER:HB2	2.02	0.42
3:E:25:LYS:HA	3:E:26:PRO:HD3	1.92	0.42
4:F:223:THR:HG23	4:F:260:ASN:CG	2.44	0.41
4:F:229:ASN:O	4:F:239:HIS:CE1	2.74	0.41
2:B:284:LEU:N	2:B:284:LEU:HD12	2.35	0.41
1:A:163:LYS:C	1:A:164:LYS:HD3	2.45	0.41
1:A:344:VAL:HG21	1:A:346:TRP:CE2	2.55	0.41
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.68	0.41
4:F:229:ASN:O	4:F:239:HIS:HE1	2.03	0.41
1:A:88:HIS:N	1:A:91:GLN:OE1	2.50	0.41
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.14	0.41
2:B:1:MET:HE3	2:B:1:MET:HB2	1.89	0.41
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.35	0.41
2:D:417:ASP:O	2:D:421:GLU:HG3	2.20	0.41
4:F:247:LYS:HE3	4:F:253:TYR:CE1	2.55	0.41
1:A:192:HIS:CG	1:A:421:ALA:HA	2.56	0.41
4:F:170:LEU:N	4:F:170:LEU:HD23	2.35	0.41
4:F:191:LEU:N	4:F:191:LEU:HD22	2.36	0.41
4:F:78:VAL:HG21	4:F:181:VAL:HG11	2.01	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HG2	2.02	0.41
2:B:296:SER:N	9:B:503:MES:O3S	2.47	0.41
9:B:503:MES:H81	9:B:503:MES:H51	1.47	0.41
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.03	0.41
4:F:1:MET:HE3	4:F:27:TRP:C	2.46	0.41
2:B:344:TRP:CD1	2:B:344:TRP:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:GLU:OE1	2:D:318:ARG:NH2	2.42	0.41
2:D:246:LEU:HD23	2:D:246:LEU:C	2.46	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.79	0.40
4:F:218:GLU:OE1	4:F:218:GLU:HA	2.21	0.40
2:D:22:GLU:HG3	2:D:81:PHE:CE2	2.56	0.40
2:D:149:THR:HG21	2:D:191:GLN:CG	2.40	0.40
4:F:149:ALA:HB3	4:F:161:LEU:HB3	2.02	0.40
2:B:139:LEU:HD12	2:B:170:MET:SD	2.60	0.40
1:C:409:VAL:HA	1:C:413:MET:O	2.21	0.40
2:D:211:CYS:CB	2:D:220:PRO:HG3	2.51	0.40
2:D:323:MET:SD	2:D:323:MET:N	2.92	0.40
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.04	0.40
1:A:2:ARG:HB3	1:A:133:GLN:HG3	2.03	0.40
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.21	0.40
2:D:65:LEU:HD21	2:D:76:VAL:HG11	2.02	0.40
3:E:52:LYS:HA	3:E:52:LYS:HD3	1.87	0.40
2:B:237:THR:O	2:B:241:ARG:HG3	2.21	0.40
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

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%)	423 (97%)	12 (3%)	0	100	100
1	C	438/450 (97%)	424 (97%)	14 (3%)	0	100	100
2	B	426/445 (96%)	418 (98%)	7 (2%)	1 (0%)	43	68
2	D	417/445 (94%)	409 (98%)	8 (2%)	0	100	100
3	E	117/143 (82%)	113 (97%)	4 (3%)	0	100	100
4	F	322/384 (84%)	295 (92%)	27 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2155/2317 (93%)	2082 (97%)	72 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	247	ASN

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	368/378 (97%)	367 (100%)	1 (0%)	86	94
1	C	371/378 (98%)	363 (98%)	8 (2%)	45	74
2	B	370/383 (97%)	363 (98%)	7 (2%)	50	77
2	D	364/383 (95%)	350 (96%)	14 (4%)	29	58
3	E	109/127 (86%)	108 (99%)	1 (1%)	70	87
4	F	299/342 (87%)	287 (96%)	12 (4%)	28	56
All	All	1881/1991 (94%)	1838 (98%)	43 (2%)	44	73

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
2	B	42	LEU
2	B	78	SER
2	B	115	SER
2	B	131	GLN
2	B	238	THR
2	B	293	MET
2	B	343	GLU
1	C	96	LYS
1	C	171	ILE
1	C	177	VAL

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Mol	Chain	Res	Type
1	C	241	SER
1	C	251	ASP
1	C	318	LEU
1	C	379	SER
1	C	391	LEU
2	D	26	ASP
2	D	33	THR
2	D	35	SER
2	D	39	ASP
2	D	69	GLU
2	D	75	SER
2	D	77	ARG
2	D	149	THR
2	D	151	LEU
2	D	189	VAL
2	D	246	LEU
2	D	247	ASN
2	D	356	ILE
2	D	377	LEU
3	E	112	ARG
4	F	10	ASN
4	F	12	SER
4	F	26	GLN
4	F	31	ARG
4	F	71	LEU
4	F	101	TYR
4	F	142	ARG
4	F	171	ASP
4	F	192	LEU
4	F	299	GLU
4	F	307	LEU
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	300	ASN
1	A	301	GLN
1	A	309	HIS
1	A	329	ASN
1	A	372	GLN

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Mol	Chain	Res	Type
2	B	6	HIS
2	B	11	GLN
2	B	247	ASN
2	B	329	GLN
2	B	347	ASN
1	C	85	GLN
1	C	133	GLN
1	C	249	ASN
1	C	356	ASN
2	D	11	GLN
2	D	48	ASN
2	D	134	GLN
2	D	165	ASN
2	D	329	GLN
2	D	347	ASN
4	F	242	ASN
4	F	260	ASN
4	F	269	GLN
4	F	310	GLN
4	F	379	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	C	504	-	12,12,12	2.13	1 (8%)	15,16,16	2.01	3 (20%)
5	GTP	A	501	6	33,34,34	1.17	4 (12%)	50,54,54	1.68	11 (22%)
10	GK9	B	504	-	25,25,25	1.11	2 (8%)	27,36,36	1.63	3 (11%)
8	GDP	B	501	6	29,30,30	1.28	3 (10%)	45,47,47	1.82	9 (20%)
10	GK9	D	502	-	25,25,25	1.07	2 (8%)	27,36,36	1.79	4 (14%)
5	GTP	C	501	6	33,34,34	0.90	1 (3%)	50,54,54	1.58	13 (26%)
11	ACP	F	402	6	31,33,33	3.31	12 (38%)	47,52,52	2.07	14 (29%)
8	GDP	D	501	-	29,30,30	1.28	4 (13%)	45,47,47	1.83	7 (15%)
9	MES	B	502	-	12,12,12	2.39	1 (8%)	15,16,16	1.98	3 (20%)
9	MES	B	503	-	12,12,12	2.33	1 (8%)	15,16,16	1.87	4 (26%)

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	C	504	-	-	2/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
10	GK9	B	504	-	-	3/6/16/16	0/4/4/4
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
10	GK9	D	502	-	-	2/6/16/16	0/4/4/4
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
11	ACP	F	402	6	-	1/19/38/38	0/3/3/3
8	GDP	D	501	-	-	6/16/32/32	0/3/3/3
9	MES	B	502	-	-	4/6/14/14	0/1/1/1
9	MES	B	503	-	-	1/6/14/14	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O4'-C1'	9.12	1.63	1.42
9	B	502	MES	C8-S	-7.97	1.66	1.77
9	B	503	MES	C8-S	-7.69	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	PB-O3A	7.23	1.66	1.58
9	C	504	MES	C8-S	-7.02	1.67	1.77
11	F	402	ACP	C2'-C1'	-6.82	1.32	1.53
11	F	402	ACP	PA-O3A	6.75	1.66	1.59
11	F	402	ACP	O4'-C4'	-5.80	1.32	1.45
11	F	402	ACP	C6-N6	4.43	1.45	1.34
10	D	502	GK9	C6-N2	4.12	1.43	1.37
10	B	504	GK9	C6-N2	3.87	1.42	1.37
10	B	504	GK9	C2-C5	-3.65	1.37	1.42
5	A	501	GTP	PB-O3A	3.51	1.63	1.59
8	D	501	GDP	PA-O3A	3.39	1.63	1.59
8	D	501	GDP	C5-C4	3.13	1.47	1.38
10	D	502	GK9	C2-C5	-2.93	1.38	1.42
5	A	501	GTP	PA-O3A	2.91	1.62	1.59
11	F	402	ACP	O3'-C3'	-2.85	1.35	1.43
8	B	501	GDP	C5-C4	2.84	1.46	1.38
11	F	402	ACP	O2'-C2'	2.77	1.49	1.43
11	F	402	ACP	C5-C4	-2.65	1.34	1.39
11	F	402	ACP	C5-N7	-2.64	1.34	1.39
8	B	501	GDP	PA-O3A	2.63	1.62	1.59
8	D	501	GDP	C6-N1	-2.48	1.34	1.38
8	B	501	GDP	C6-N1	-2.39	1.34	1.38
8	D	501	GDP	C5-N7	-2.27	1.34	1.39
5	C	501	GTP	PA-O3A	2.16	1.61	1.59
5	A	501	GTP	PB-O3B	2.13	1.61	1.59
5	A	501	GTP	C2-N3	2.08	1.38	1.33
11	F	402	ACP	C8-N9	-2.04	1.34	1.37
11	F	402	ACP	PB-O2B	-2.01	1.51	1.56

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	GK9	O1-C3-C6	7.54	133.85	126.46
10	B	504	GK9	O1-C3-C6	7.07	133.39	126.46
8	D	501	GDP	C5-C4-N3	-6.17	118.57	128.39
9	C	504	MES	C5-N4-C3	5.68	121.08	108.84
8	B	501	GDP	C5-C4-N3	-5.64	119.41	128.39
11	F	402	ACP	N3-C2-N1	-5.37	120.45	128.58
11	F	402	ACP	N6-C6-N1	-5.13	106.96	118.38
11	F	402	ACP	C5-C4-N3	-4.99	119.84	126.72
8	D	501	GDP	N9-C4-N3	4.98	135.91	125.95
9	B	502	MES	C5-N4-C3	4.95	119.51	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	C5-N4-C3	4.93	119.45	108.84
5	A	501	GTP	C5-C4-N3	-4.91	120.58	128.39
8	B	501	GDP	C2-N3-C4	4.88	120.71	112.30
8	D	501	GDP	C2-N3-C4	4.86	120.67	112.30
8	B	501	GDP	N9-C4-N3	4.78	135.51	125.95
5	A	501	GTP	C2-N3-C4	4.48	120.02	112.30
5	C	501	GTP	C2-N3-C4	4.41	119.89	112.30
5	C	501	GTP	C5-C4-N3	-4.14	121.79	128.39
11	F	402	ACP	C5-C6-N6	4.11	133.47	123.29
11	F	402	ACP	N9-C8-N7	-3.76	108.60	113.94
9	B	502	MES	O1S-S-C8	3.48	111.98	106.73
8	B	501	GDP	C6-C5-N7	3.34	136.37	130.29
5	A	501	GTP	N9-C8-N7	-3.21	107.45	113.40
5	A	501	GTP	O2B-PB-O3B	3.20	115.93	107.27
11	F	402	ACP	C2-N3-C4	3.18	119.61	111.83
11	F	402	ACP	O4'-C1'-N9	3.13	114.10	108.09
5	A	501	GTP	C8-N7-C5	3.10	109.79	104.26
5	A	501	GTP	C2-N1-C6	-3.05	119.58	125.11
5	A	501	GTP	N9-C4-N3	2.97	131.90	125.95
10	D	502	GK9	C7-N2-C6	2.97	124.69	119.21
5	C	501	GTP	N9-C8-N7	-2.96	107.91	113.40
11	F	402	ACP	N3-C4-N9	2.88	132.07	127.17
5	C	501	GTP	C8-N7-C5	2.86	109.35	104.26
11	F	402	ACP	C5-N7-C8	2.81	107.87	103.45
8	B	501	GDP	O6-C6-C5	-2.75	119.27	126.53
8	D	501	GDP	C6-C5-N7	2.73	135.27	130.29
10	D	502	GK9	C1-N3-C6	2.68	118.56	110.98
8	D	501	GDP	O2A-PA-O3A	2.60	114.30	107.27
9	B	503	MES	C6-C5-N4	-2.50	106.32	110.12
5	A	501	GTP	C5-C6-N1	2.50	119.61	113.25
5	C	501	GTP	N9-C4-N3	2.48	130.91	125.95
10	B	504	GK9	C1-N3-C6	2.44	117.90	110.98
5	C	501	GTP	O3G-PG-O3B	2.44	112.80	104.64
11	F	402	ACP	C6-C5-C4	2.40	120.46	117.18
8	D	501	GDP	O6-C6-C5	-2.38	120.24	126.53
5	A	501	GTP	O3B-PB-O1B	-2.38	103.56	110.70
5	C	501	GTP	O3'-C3'-C4'	-2.35	104.33	111.08
5	C	501	GTP	C5-C6-N1	2.33	119.19	113.25
11	F	402	ACP	O2G-PG-C3B	2.31	112.00	106.40
9	B	502	MES	O3S-S-C8	2.28	110.47	106.00
5	A	501	GTP	C4-C5-N7	-2.28	107.05	110.67
5	C	501	GTP	C2-N1-C6	-2.27	121.00	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C4-C5-N7	-2.25	108.01	110.58
9	C	504	MES	C7-N4-C3	2.24	117.22	111.24
9	B	503	MES	C8-C7-N4	-2.24	103.90	112.36
8	B	501	GDP	C5-C6-N1	2.23	118.94	113.25
8	B	501	GDP	C4-C5-N7	-2.21	107.17	110.67
10	D	502	GK9	C3-C6-N3	-2.20	119.09	123.81
9	C	504	MES	O3S-S-C8	2.19	110.29	106.00
5	C	501	GTP	O2B-PB-O3B	2.18	113.17	107.27
5	C	501	GTP	C4-C5-N7	-2.18	107.22	110.67
5	C	501	GTP	C6-C5-N7	2.17	134.25	130.29
8	B	501	GDP	O2B-PB-O3A	2.17	111.91	104.64
5	A	501	GTP	O6-C6-C5	-2.16	120.84	126.53
8	D	501	GDP	C4-C5-N7	-2.12	107.31	110.67
11	F	402	ACP	C5-C4-N9	2.09	108.09	105.81
8	B	501	GDP	C8-N9-C4	2.08	109.92	106.03
11	F	402	ACP	C3'-C2'-C1'	2.06	105.36	101.46
5	C	501	GTP	N1-C2-N3	-2.04	119.58	123.32
9	B	503	MES	C7-N4-C5	2.03	116.66	111.24
10	B	504	GK9	C7-N2-C6	2.02	122.94	119.21

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
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	PA-O3A-PB-O2B
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
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-O3S
9	B	503	MES	C8-C7-N4-C5
9	C	504	MES	N4-C7-C8-S

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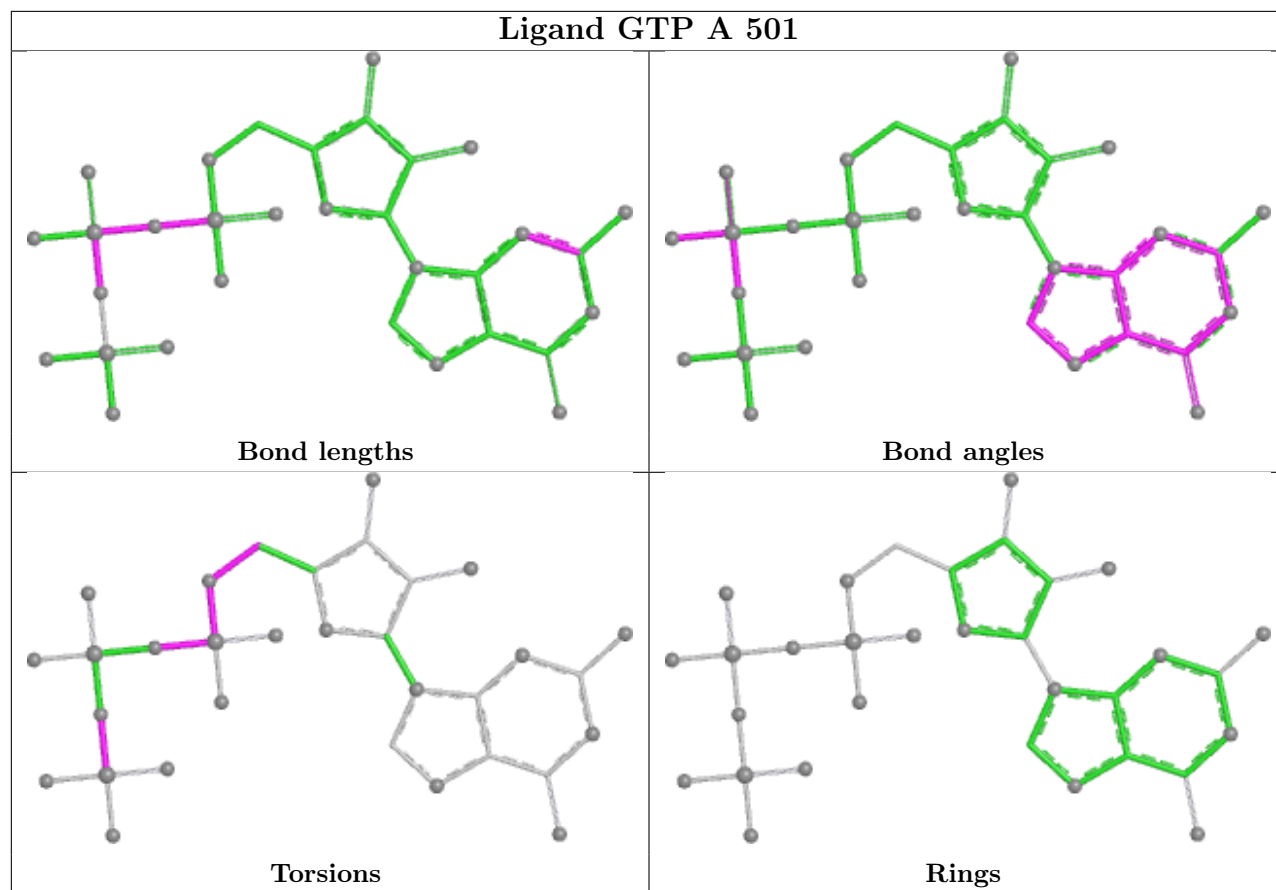
Mol	Chain	Res	Type	Atoms
10	B	504	GK9	C3-C6-N2-C7
10	D	502	GK9	C3-C6-N2-C7
10	B	504	GK9	N3-C6-N2-C16
10	D	502	GK9	N3-C6-N2-C16
10	B	504	GK9	C3-C6-N2-C16
9	B	502	MES	C7-C8-S-O2S
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
11	F	402	ACP	C5'-O5'-PA-O1A
9	C	504	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3A-PA-O1A
8	D	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
8	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

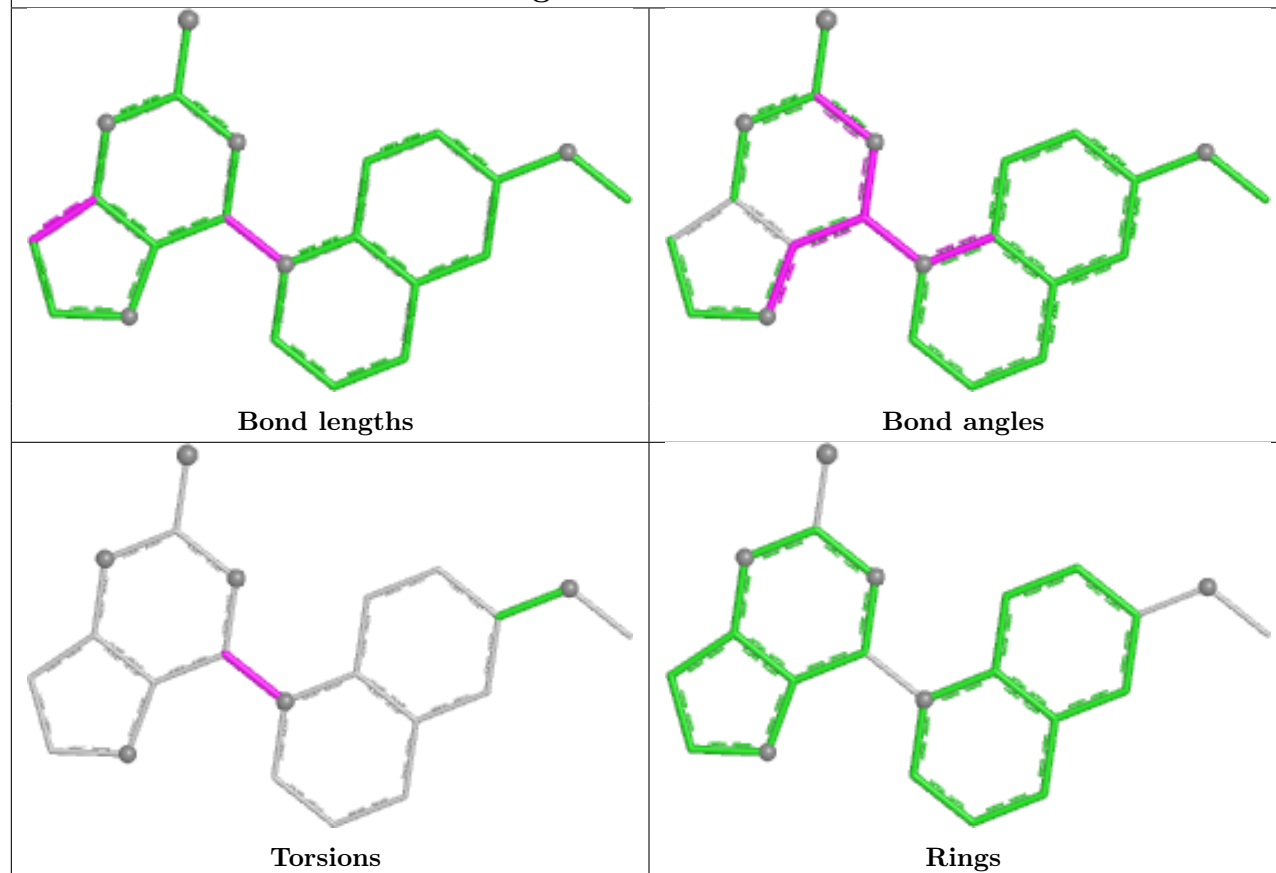
6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	504	MES	3	0
8	B	501	GDP	1	0
11	F	402	ACP	6	0
8	D	501	GDP	4	0
9	B	502	MES	3	0
9	B	503	MES	3	0

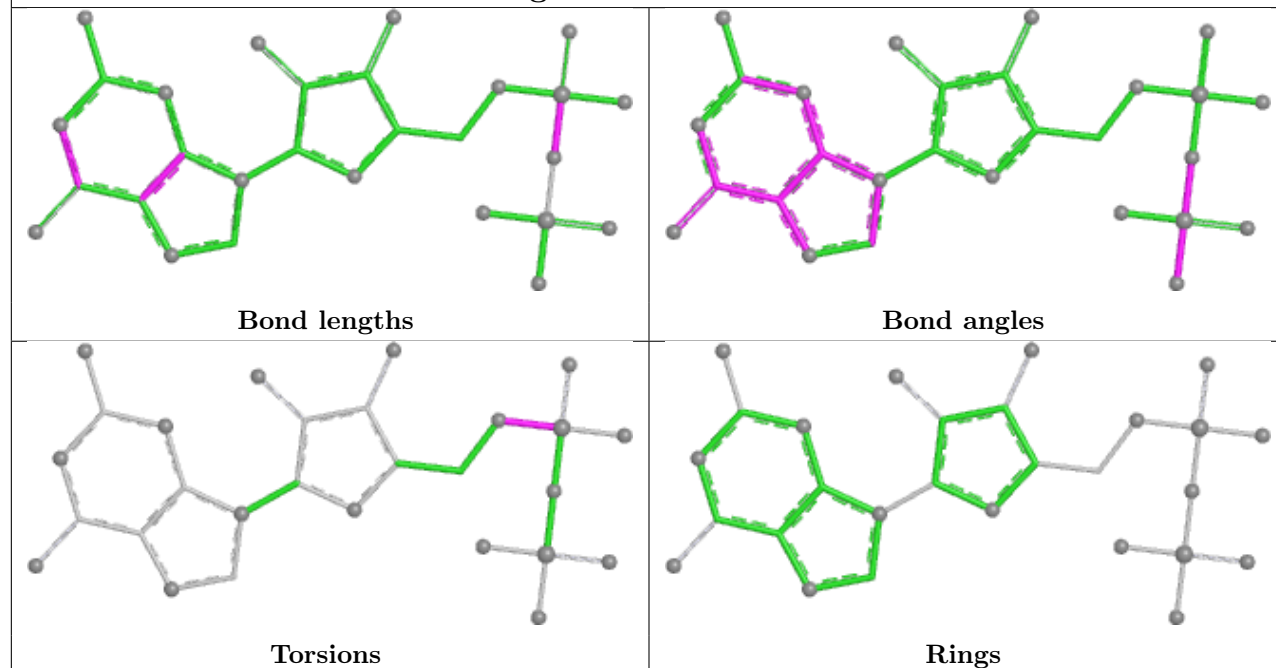
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

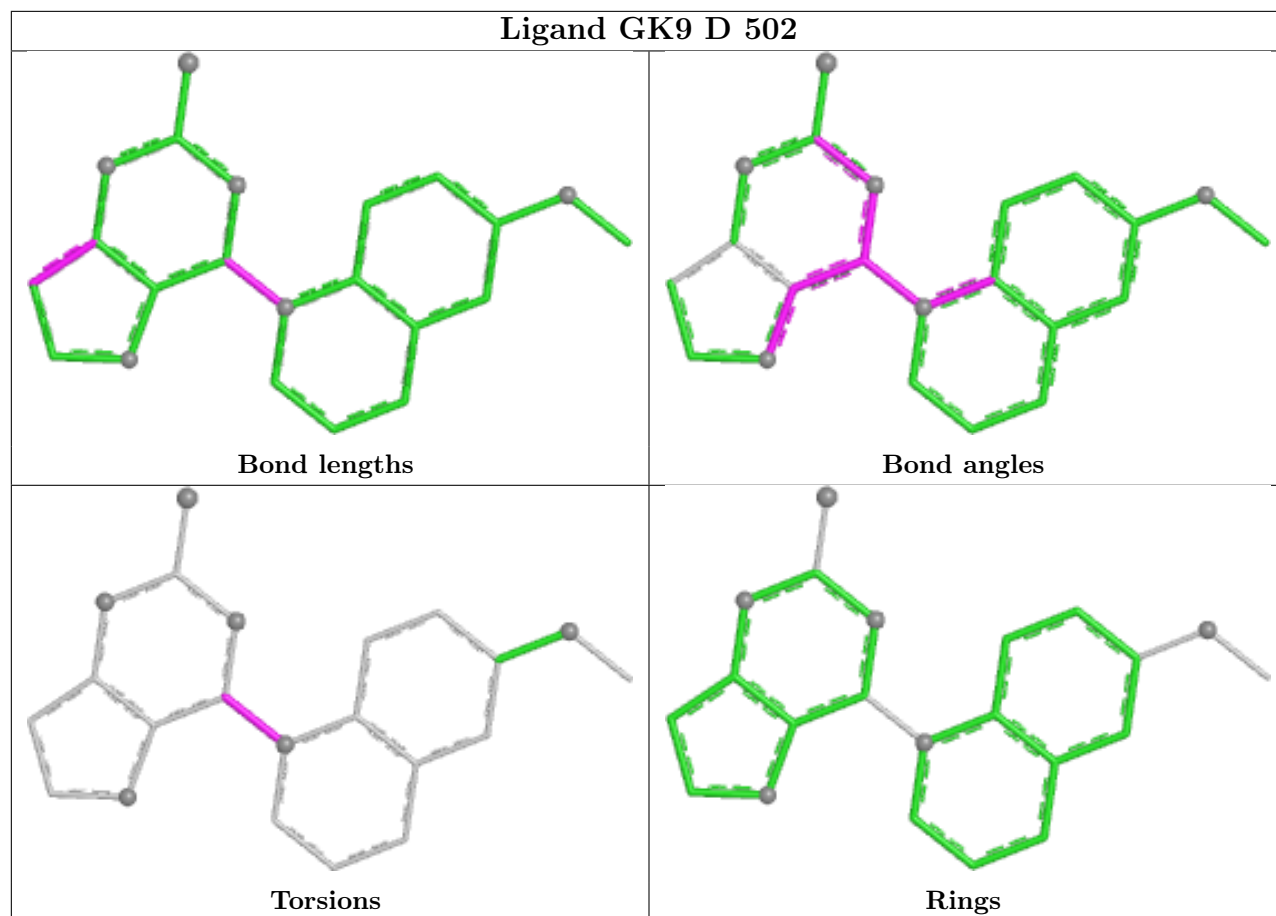


Ligand GK9 B 504

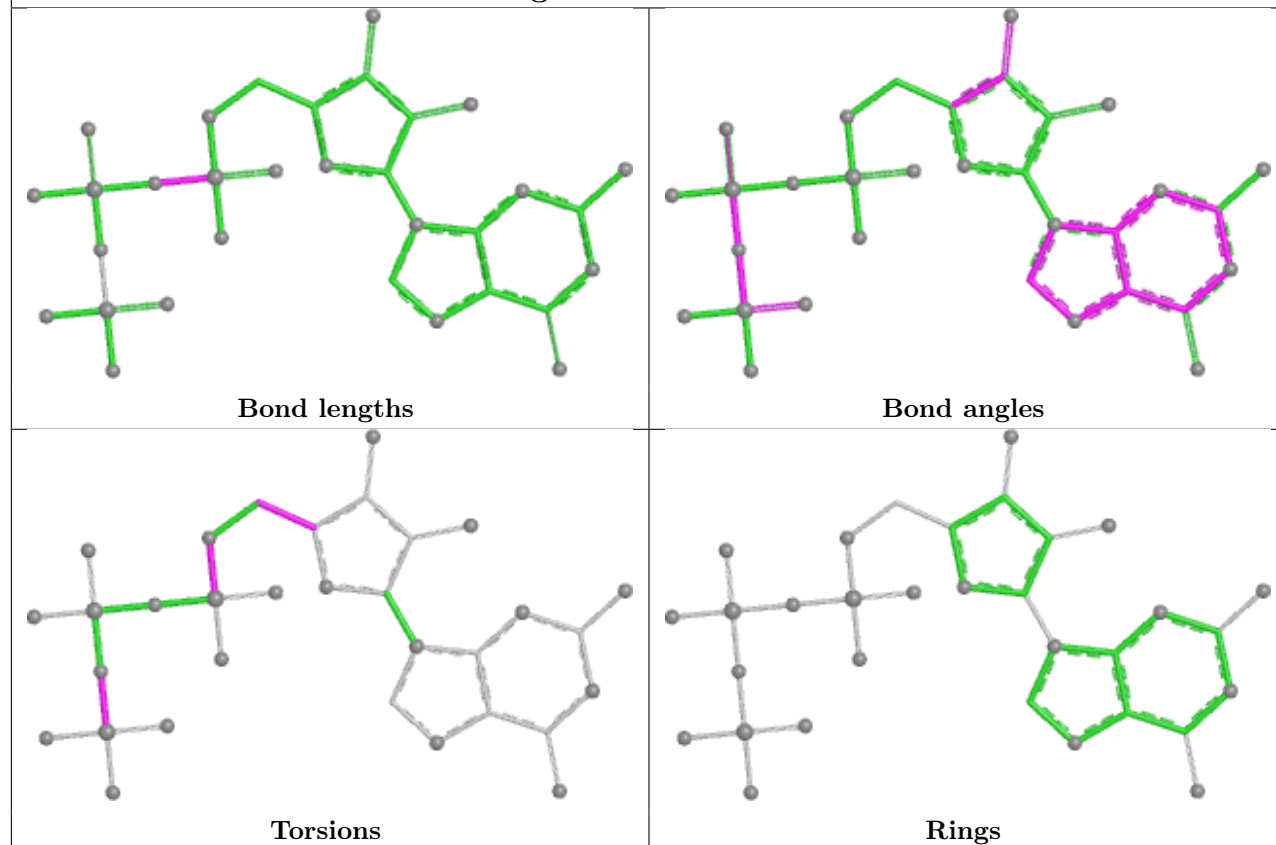


Ligand GDP B 501

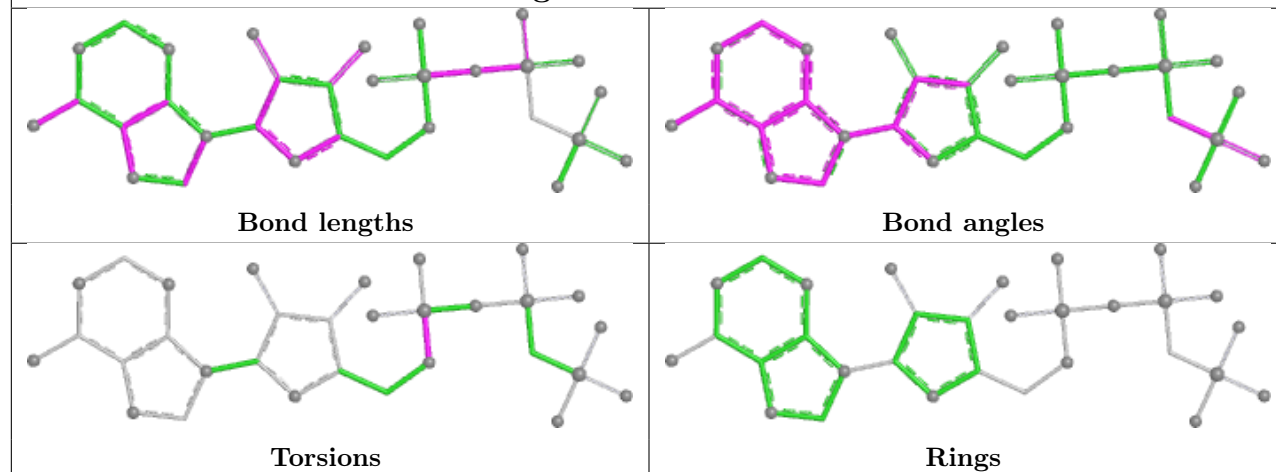


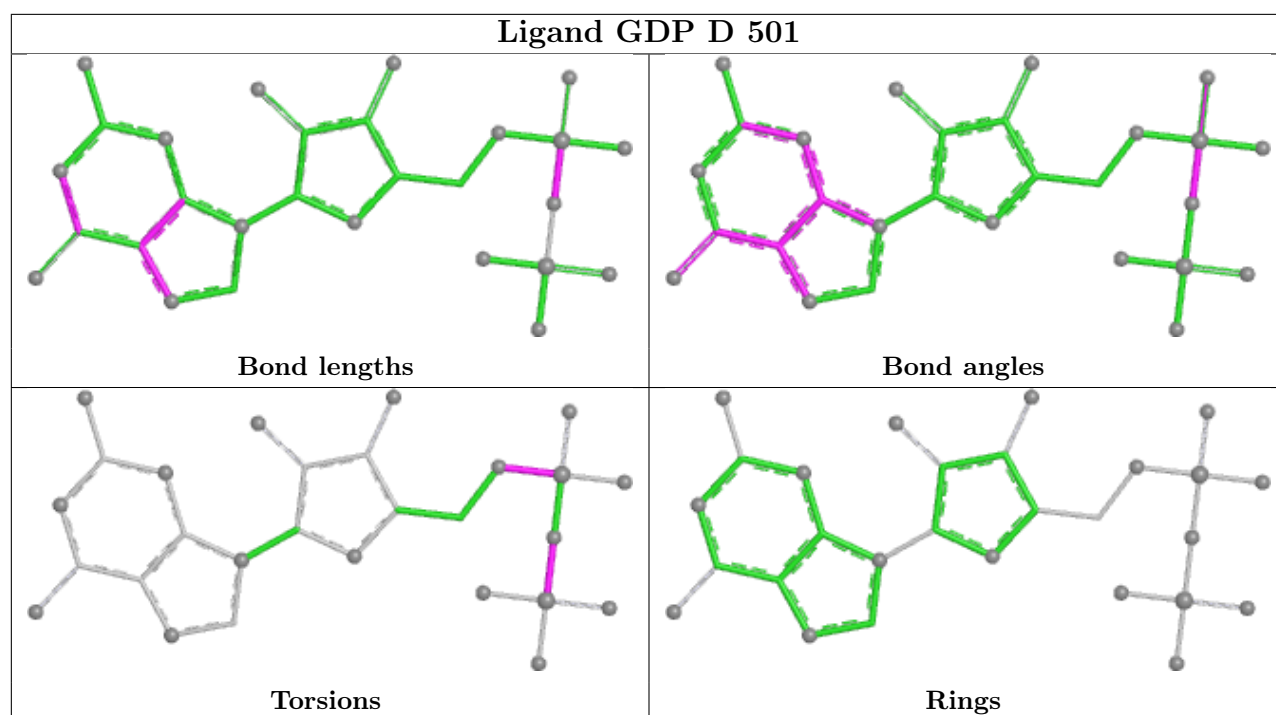


Ligand GTP C 501



Ligand ACP F 402





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%)	-0.22	6 (1%) 73 72	22, 39, 71, 95	0
1	C	440/450 (97%)	-0.43	5 (1%) 78 76	16, 28, 56, 83	0
2	B	428/445 (96%)	-0.08	15 (3%) 47 43	16, 36, 79, 115	0
2	D	421/445 (94%)	0.60	46 (10%) 10 9	25, 59, 97, 119	0
3	E	121/143 (84%)	0.35	11 (9%) 15 12	25, 53, 93, 118	0
4	F	332/384 (86%)	0.92	74 (22%) 2 2	29, 66, 128, 155	0
All	All	2179/2317 (94%)	0.13	157 (7%) 21 18	16, 45, 98, 155	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	6.2
4	F	101	TYR	5.9
2	D	323	MET	5.0
2	D	394	PHE	4.8
4	F	172	PHE	4.8
2	D	245	GLN	4.8
4	F	148	ILE	4.7
4	F	173	ILE	4.6
4	F	103	THR	4.6
2	D	55	THR	4.5
1	A	437	VAL	4.5
4	F	245	ILE	4.5
4	F	161	LEU	4.4
4	F	170	LEU	4.4
4	F	253	TYR	4.4
2	D	397	TRP	4.4
2	D	69	GLU	4.3
4	F	233	PHE	4.3
3	E	139	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	181	VAL	4.0
4	F	244	CYS	4.0
2	D	125	GLU	3.9
4	F	182	ILE	3.9
4	F	162	ILE	3.8
4	F	380	HIS	3.8
4	F	263	PHE	3.8
4	F	130	VAL	3.8
2	B	274	THR	3.6
4	F	237	THR	3.5
2	B	323	MET	3.5
2	B	279	GLN	3.5
1	A	282	TYR	3.4
4	F	174	ASP	3.3
4	F	180	HIS	3.3
4	F	171	ASP	3.3
4	F	146	VAL	3.3
2	B	245	GLN	3.3
2	B	428	ALA	3.3
2	D	217	LEU	3.2
2	D	83	GLN	3.2
2	D	97	ALA	3.2
1	C	440	VAL	3.1
4	F	179	VAL	3.1
4	F	140	GLU	3.1
2	B	55	THR	3.1
4	F	10	ASN	3.1
4	F	240	LEU	3.1
2	B	277	GLY	3.1
4	F	100	ILE	3.1
4	F	239	HIS	3.0
2	D	141	GLY	3.0
4	F	199	PHE	3.0
4	F	362	ALA	3.0
2	B	247	ASN	2.9
2	D	103	LYS	2.9
2	B	1	MET	2.9
4	F	136	ASN	2.9
4	F	135	TYR	2.9
2	D	272	PRO	2.9
2	D	247	ASN	2.9
2	B	280	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	232	ASN	2.8
4	F	241	THR	2.8
2	D	126	SER	2.8
4	F	164	SER	2.8
3	E	27	PRO	2.8
4	F	74	LYS	2.8
3	E	6	MET	2.8
1	C	284	GLU	2.8
4	F	259	GLY	2.7
4	F	102	PRO	2.7
2	D	48	ASN	2.7
4	F	147	TRP	2.7
4	F	89	GLU	2.7
2	D	54	ALA	2.7
3	E	140	LYS	2.7
4	F	230	SER	2.7
2	B	80	PRO	2.7
2	D	73	MET	2.7
4	F	177	GLY	2.7
2	D	212	PHE	2.7
2	D	1	MET	2.6
2	D	98	GLY	2.6
2	B	54	ALA	2.6
4	F	372	THR	2.6
4	F	133	ALA	2.6
4	F	92	THR	2.6
2	B	39	ASP	2.6
2	D	86	ARG	2.6
2	D	271	ALA	2.6
2	D	362	LYS	2.5
4	F	134	ALA	2.5
4	F	238	CYS	2.5
4	F	223	THR	2.5
3	E	28	SER	2.5
4	F	236	LYS	2.5
2	D	56	GLY	2.5
4	F	254	GLY	2.5
4	F	194	PRO	2.5
4	F	131	PHE	2.5
4	F	242	ASN	2.5
2	B	282	ARG	2.5
2	B	278	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	2.4
4	F	167	SER	2.4
3	E	44	ASP	2.4
4	F	234	GLN	2.4
4	F	128	ARG	2.4
3	E	115	HIS	2.4
4	F	166	ALA	2.4
1	A	262	TYR	2.3
2	D	92	PHE	2.3
4	F	243	HIS	2.3
4	F	163	SER	2.3
2	D	96	GLY	2.3
4	F	186	LEU	2.3
1	A	88	HIS	2.3
2	D	406	MET	2.3
4	F	90	SER	2.3
1	A	365	GLY	2.3
2	D	42	LEU	2.3
1	C	1	MET	2.3
3	E	135	LYS	2.3
2	D	53	GLU	2.3
2	D	215	LEU	2.3
4	F	257	GLU	2.2
1	C	340	SER	2.2
2	D	404	ASP	2.2
2	D	244	GLY	2.2
2	D	227	HIS	2.2
2	D	140	GLY	2.2
3	E	141	GLU	2.2
4	F	333	ASN	2.2
4	F	227	PRO	2.2
4	F	169	LEU	2.2
2	D	390	ARG	2.2
2	D	171	PRO	2.2
4	F	176	GLN	2.2
1	A	346	TRP	2.1
2	D	218	THR	2.1
2	D	211	CYS	2.1
1	C	232	SER	2.1
2	D	213	ARG	2.1
4	F	132	LEU	2.1
4	F	228	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	258	GLU	2.1
2	D	214	THR	2.1
4	F	178	GLN	2.1
3	E	133	VAL	2.1
2	D	243	PRO	2.0
2	D	246	LEU	2.0
2	D	284	LEU	2.0
2	D	360	GLY	2.0
3	E	138	GLU	2.0
4	F	175	GLU	2.0
2	D	273	LEU	2.0
4	F	141	GLY	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
6	MG	F	401	1/1	0.77	0.10	88,88,88,88	0
11	ACP	F	402	31/31	0.82	0.12	83,99,135,165	0
9	MES	C	504	12/12	0.88	0.22	30,34,70,77	12
8	GDP	D	501	28/28	0.89	0.10	50,56,70,72	0
6	MG	B	505	1/1	0.94	0.20	37,37,37,37	0
9	MES	B	503	12/12	0.94	0.10	53,55,66,71	0
9	MES	B	502	12/12	0.95	0.09	32,39,56,58	0
10	GK9	B	504	22/22	0.96	0.08	24,30,36,49	0
10	GK9	D	502	22/22	0.97	0.06	25,31,46,72	0
7	CA	A	503	1/1	0.98	0.06	59,59,59,59	0
5	GTP	A	501	32/32	0.98	0.05	19,22,38,41	0

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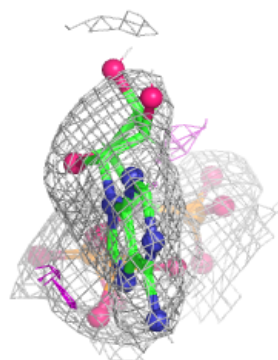
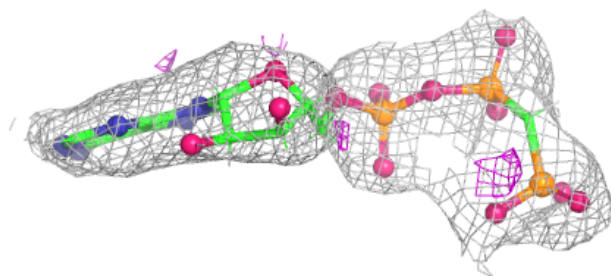
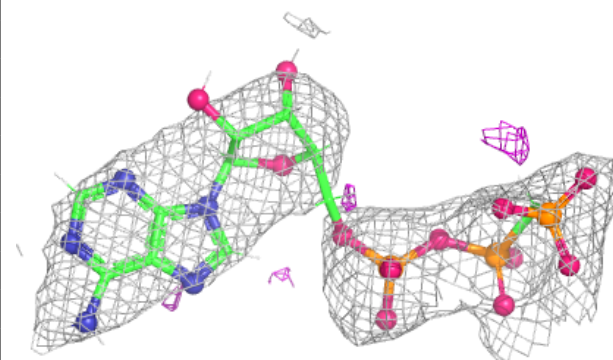
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GDP	B	501	28/28	0.99	0.05	13,21,28,28	0
5	GTP	C	501	32/32	0.99	0.04	20,22,30,33	0
6	MG	C	502	1/1	0.99	0.07	40,40,40,40	0
7	CA	C	503	1/1	0.99	0.03	36,36,36,36	0
6	MG	A	502	1/1	1.00	0.02	23,23,23,23	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.

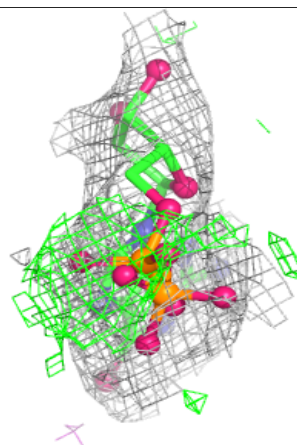
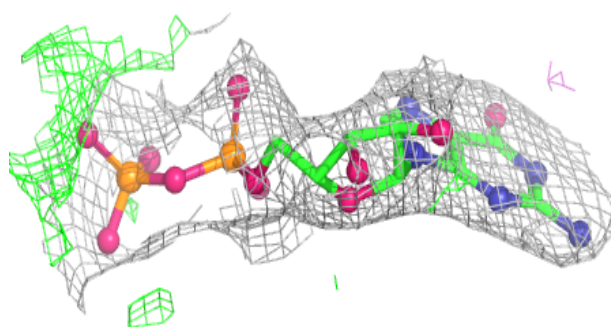
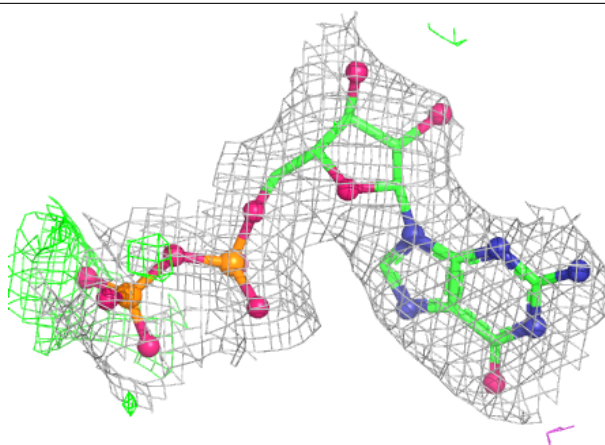
Electron density around ACP F 402:

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

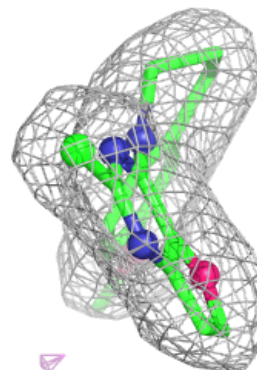
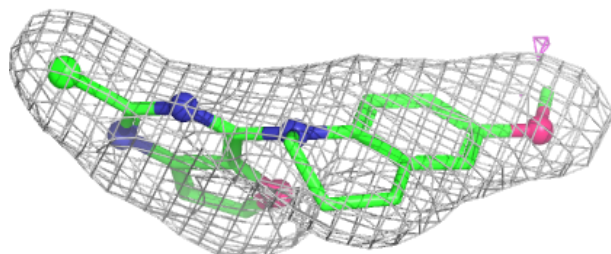
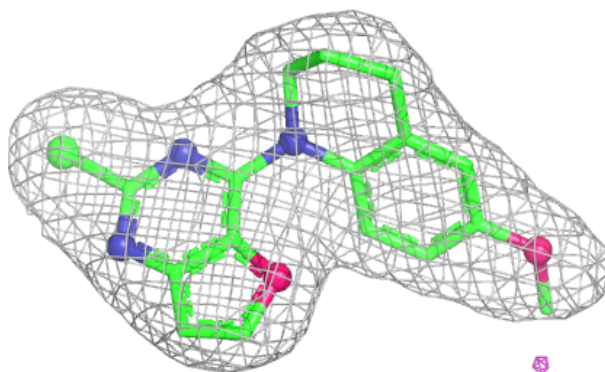


Electron density around GDP D 501:

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

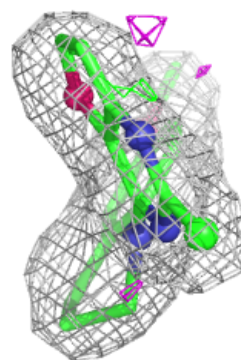
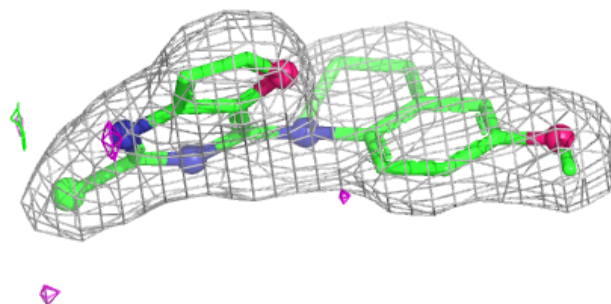
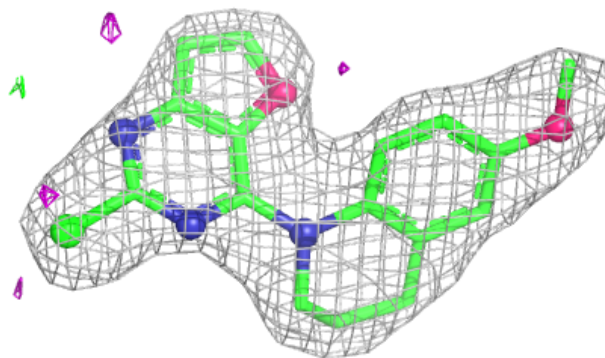
**Electron density around GK9 B 504:**

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

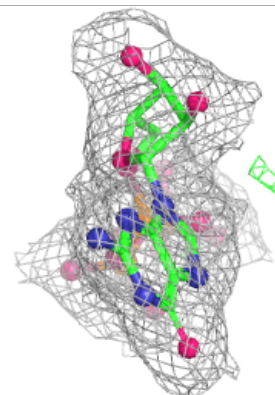
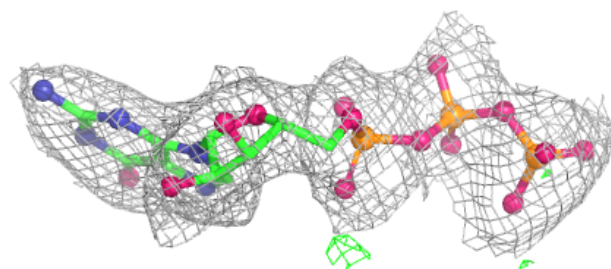
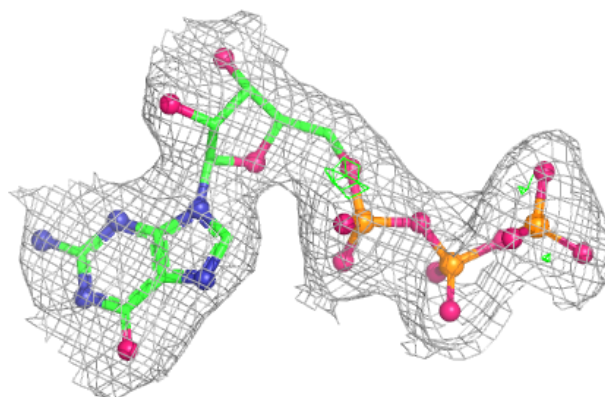


Electron density around GK9 D 502:

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

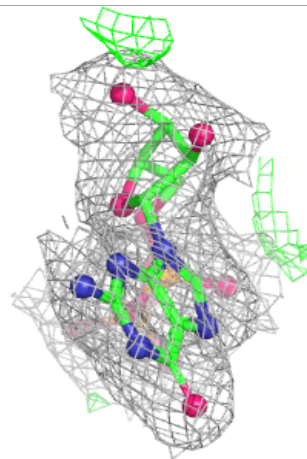
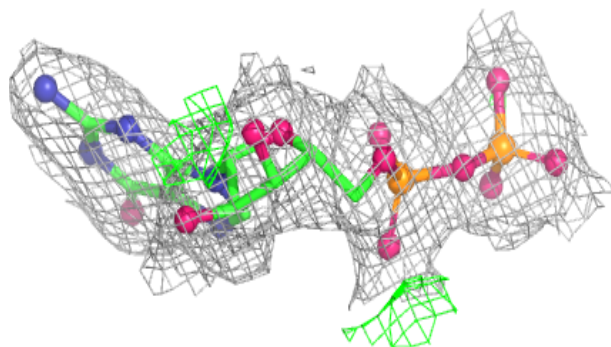
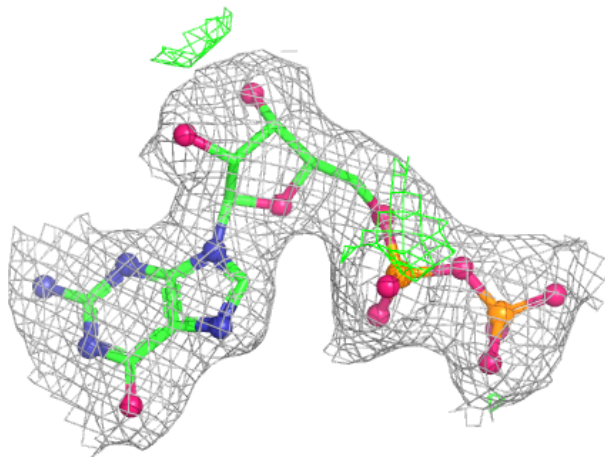
**Electron density around GTP A 501:**

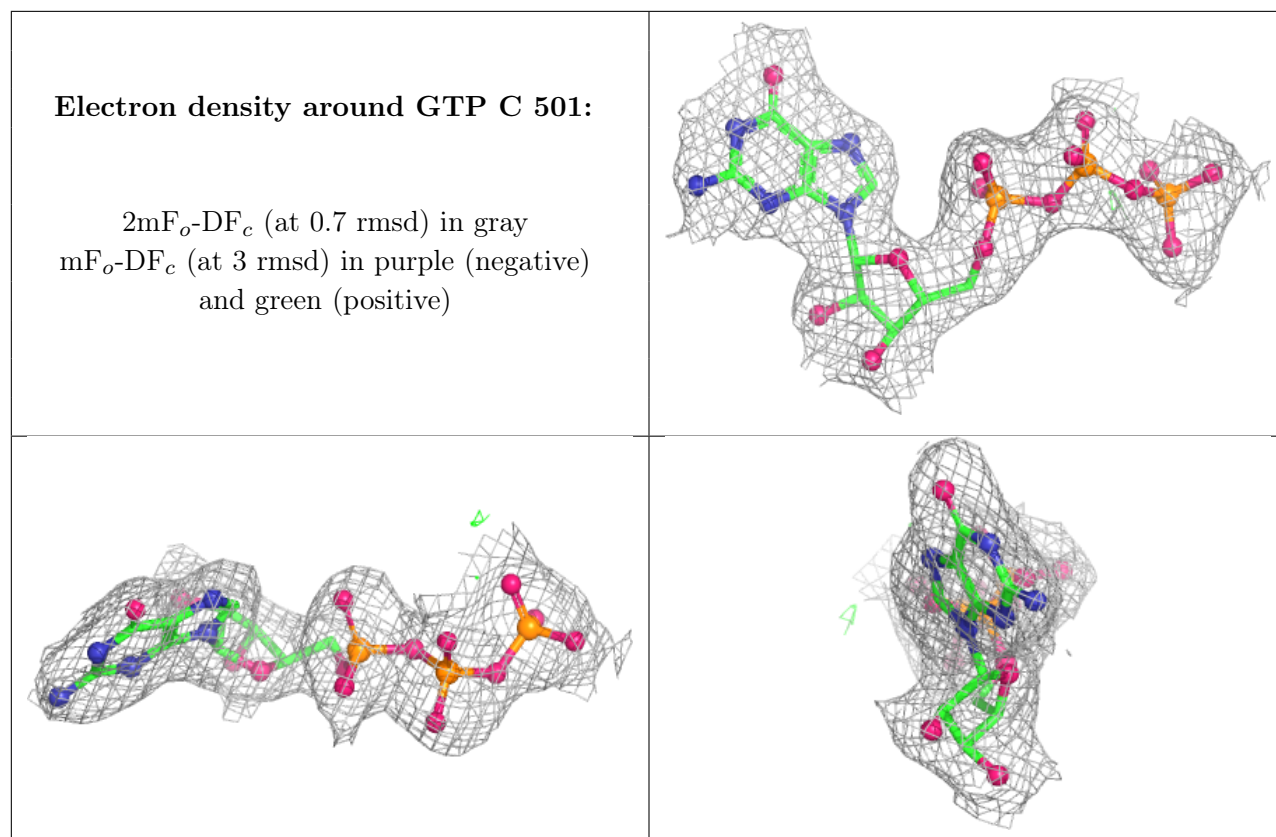
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.