



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:16 AM UTC

PDB ID : 6O61 / pdb_00006o61
Title : Tubulin-RB3_SLD-TTL in complex with compound ABI-231
Authors : Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on : 2019-03-05
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

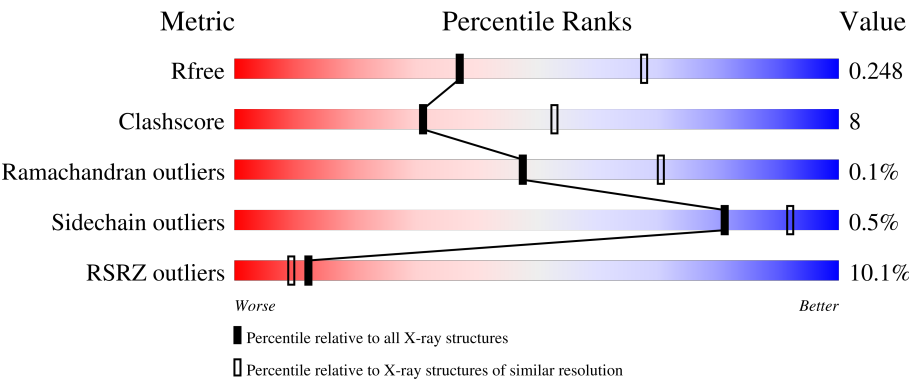
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	450	2% 83% 14%
1	C	450	2% 84% 14%
2	B	445	4% 79% 17%
2	D	445	18% 70% 24% 5%
3	E	143	8% 71% 14% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	23% 66% 16% 18%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17165 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3403	2156	579	646	22			
1	C	440	Total	C	N	O	S	0	0	0
			3427	2169	581	655	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3336	2098	570	642	26			
2	D	421	Total	C	N	O	S	0	0	0
			3156	1975	534	622	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			983	605	178	195	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

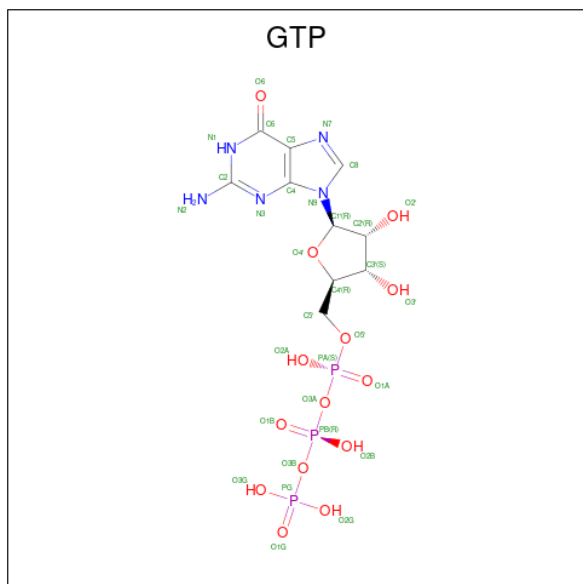
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	316	Total	C	N	O	S	0	0	0
			2390	1537	404	438	11			

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		

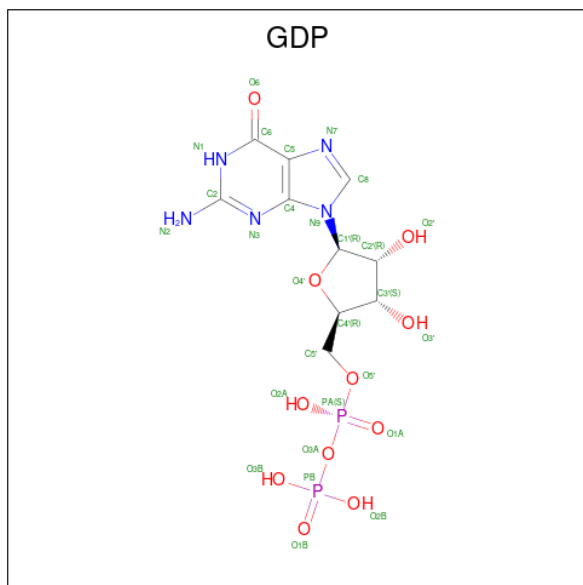
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

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

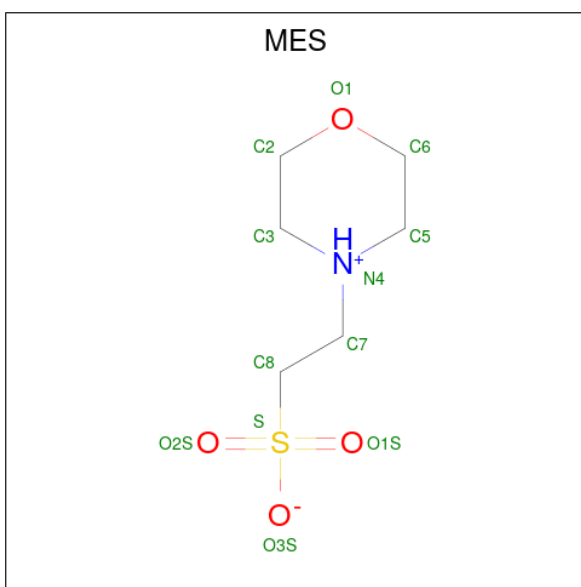
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



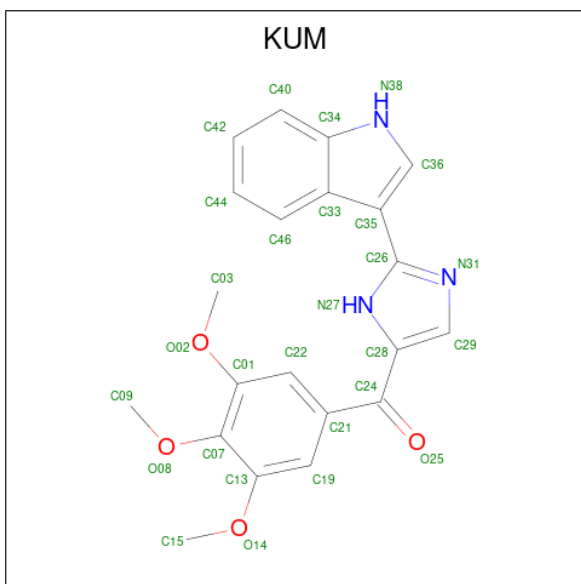
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (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-5-yl](3,4,5-trimethoxyphenyl)methanone (CCD ID: KUM) (formula: C₂₁H₁₉N₃O₄) (labeled as "Ligand of Interest" by depositor).



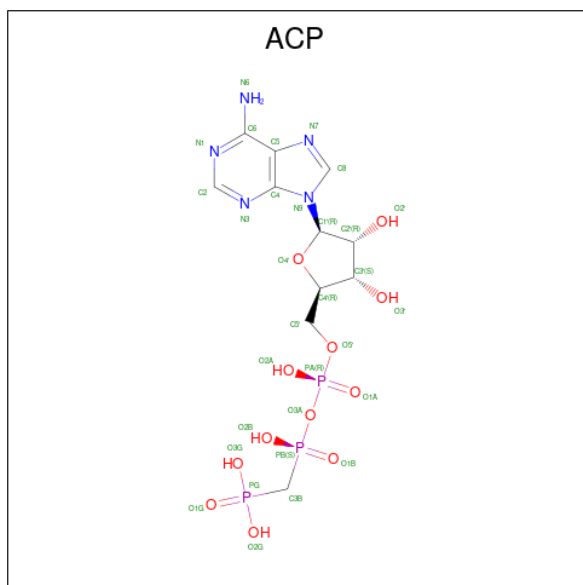
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			28	21	3	4		

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

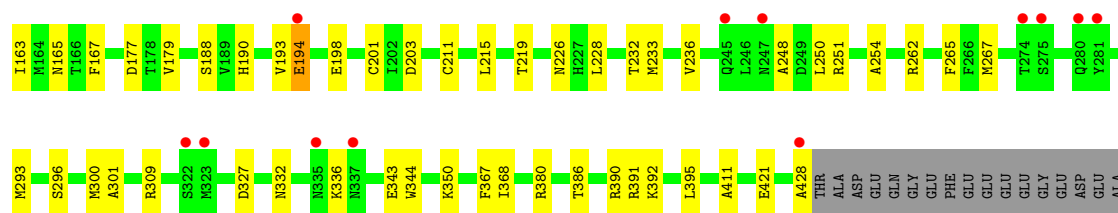
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



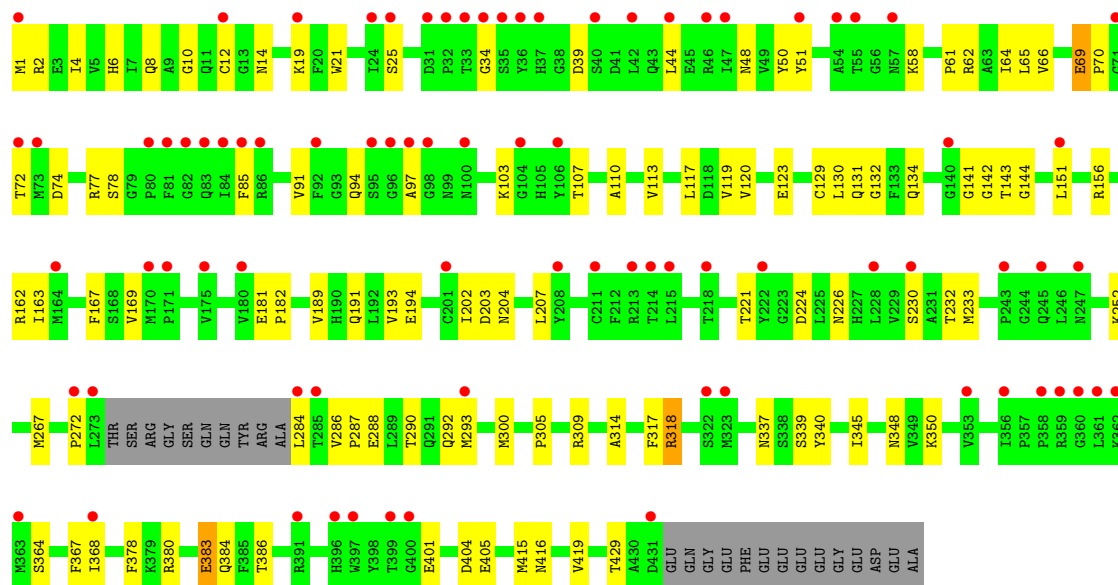
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	64	Total	O	0	0
			64	64		
12	B	38	Total	O	0	0
			38	38		
12	C	96	Total	O	0	0
			96	96		
12	D	13	Total	O	0	0
			13	13		
12	E	9	Total	O	0	0
			9	9		
12	F	14	Total	O	0	0
			14	14		



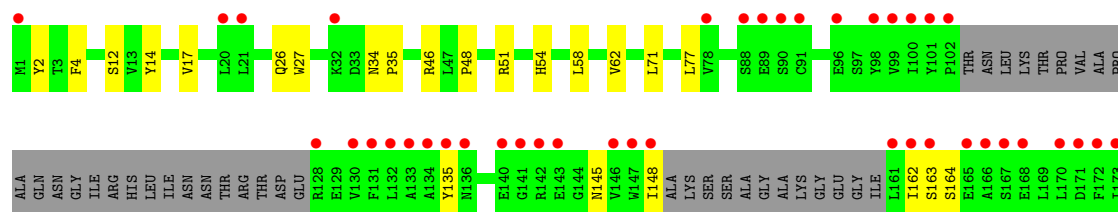
• Molecule 2: Tubulin beta-2B chain

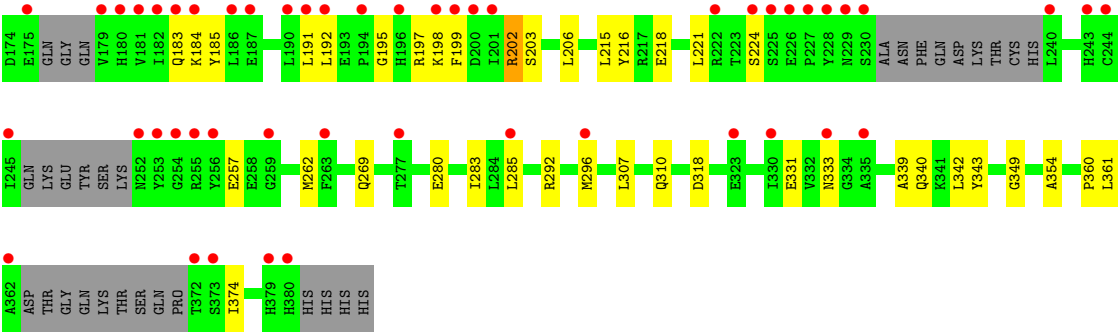


• Molecule 3: Stathmin-4



• 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	105.26Å 157.09Å 184.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.60 48.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.16-2.60) 98.0 (48.16-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.204 , 0.243 0.207 , 0.248	Depositor DCC
R_{free} test set	4627 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17165	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MG, GDP, CA, ACP, MES, GTP, KUM

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	0.18	0/3480	0.45	0/4725
1	C	0.16	0/3505	0.43	0/4759
2	B	0.19	0/3411	0.45	1/4622 (0.0%)
2	D	0.22	0/3224	0.56	4/4389 (0.1%)
3	E	0.18	0/995	0.40	0/1327
4	F	0.14	0/2442	0.38	0/3322
All	All	0.18	0/17057	0.46	5/23144 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	48	ASN	CB-CA-C	-8.35	95.19	110.63
2	B	194	GLU	CA-CB-CG	-7.62	98.86	114.10
2	D	383	GLU	CA-CB-CG	6.70	127.51	114.10
2	D	44	LEU	CB-CG-CD2	5.73	127.89	110.70
2	D	69	GLU	CA-CB-CG	5.21	124.53	114.10

There are no chirality outliers.

There are no planarity outliers.

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	3403	0	3318	42	0
1	C	3427	0	3325	39	0
2	B	3336	0	3196	59	0
2	D	3156	0	2893	79	0
3	E	983	0	966	20	0
4	F	2390	0	2188	45	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	4	0
8	D	28	0	12	6	0
9	B	24	0	24	3	0
10	B	28	0	0	3	0
10	D	28	0	0	1	0
11	F	31	0	13	3	0
12	A	64	0	0	0	0
12	B	38	0	0	0	0
12	C	96	0	0	1	0
12	D	13	0	0	0	0
12	E	9	0	0	1	0
12	F	14	0	0	1	0
All	All	17165	0	15971	268	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 8.

All (268) 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:D:226:ASN:HD21	8:D:501:GDP:HN1	1.04	0.98
4:F:280:GLU:O	4:F:285:LEU:HD13	1.65	0.95
2:D:69:GLU:HG2	2:D:72:THR:HG23	1.58	0.84
2:D:226:ASN:ND2	8:D:501:GDP:HN1	1.79	0.77
2:B:226:ASN:HD21	8:B:501:GDP:HN1	1.32	0.76
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.67	0.76
2:D:70:PRO:HG3	2:D:94:GLN:HA	1.70	0.74
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.70	0.74
1:A:206:ASN:HD21	5:A:501:GTP:HN22	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.23	0.71
2:B:66:VAL:CG1	2:B:147:MET:CE	2.69	0.71
1:C:141:PHE:HE2	1:C:203:MET:HE3	1.54	0.71
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.72	0.71
2:B:226:ASN:OD1	8:B:501:GDP:N2	2.21	0.70
2:D:309:ARG:HD2	2:D:339:SER:O	1.91	0.70
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.73	0.70
4:F:202:ARG:HH22	4:F:333:ASN:HD22	1.40	0.69
2:D:204:ASN:HA	2:D:207:LEU:HD12	1.73	0.69
3:E:61:ARG:HH12	3:E:62:LYS:HG3	1.58	0.68
3:E:115[B]:HIS:NE2	12:E:201:HOH:O	2.26	0.68
2:B:177:ASP:O	1:C:352:LYS:NZ	2.24	0.68
2:D:284:LEU:HD21	2:D:292:GLN:HE22	1.59	0.67
2:D:21:TRP:O	2:D:25:SER:OG	2.10	0.66
1:A:230:LEU:O	1:A:234:ILE:HD12	1.96	0.66
1:A:163:LYS:HG2	1:A:164:LYS:HD2	1.76	0.66
1:A:221:ARG:NH1	2:B:327:ASP:OD1	2.30	0.65
4:F:202:ARG:HH21	4:F:318:ASP:CG	2.05	0.65
4:F:292:ARG:HG2	4:F:296:MET:SD	2.37	0.65
4:F:191:LEU:H	4:F:191:LEU:HD12	1.62	0.64
2:B:165:ASN:HD22	2:B:198:GLU:HB2	1.63	0.64
1:A:2:ARG:O	1:A:133:GLN:NE2	2.29	0.64
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.62	0.64
2:D:383:GLU:HA	2:D:386:THR:HG22	1.81	0.63
2:D:404:ASP:OD1	2:D:405:GLU:N	2.32	0.63
2:D:181:GLU:OE1	8:D:501:GDP:O3'	2.16	0.62
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.81	0.62
4:F:221:LEU:HD23	4:F:262:MET:HE3	1.81	0.62
2:D:286:VAL:HG22	2:D:287:PRO:HD3	1.82	0.61
2:D:191:GLN:HE22	3:E:126:LYS:HE2	1.65	0.61
1:A:163:LYS:H	1:A:163:LYS:HD3	1.66	0.61
2:B:226:ASN:ND2	8:B:501:GDP:HN1	1.99	0.60
4:F:199:PHE:HD1	4:F:221:LEU:HD11	1.66	0.60
1:A:401:LYS:HD2	2:B:344:TRP:CD2	2.37	0.60
1:C:2:ARG:NH1	1:C:131:GLY:O	2.34	0.60
1:C:1:MET:HG2	1:C:130:THR:OG1	2.01	0.60
4:F:34:ASN:HD22	4:F:35:PRO:HD2	1.66	0.59
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.33	0.59
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.85	0.59
3:E:44:ASP:N	3:E:44:ASP:OD2	2.35	0.59
2:B:66:VAL:HG12	2:B:147:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:VAL:HG11	2:B:147:MET:HE3	1.84	0.59
2:D:10:GLY:O	2:D:14:ASN:ND2	2.22	0.58
2:D:117:LEU:HA	2:D:120:VAL:HG22	1.85	0.58
2:D:314:ALA:HB3	2:D:368:ILE:HG12	1.85	0.57
1:A:433:GLU:OE1	4:F:46:ARG:NH1	2.37	0.57
1:A:345:ASP:O	3:E:28:SER:N	2.37	0.57
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.86	0.57
2:D:97:ALA:HB2	2:D:143:THR:HG22	1.87	0.57
2:D:182:PRO:HG3	2:D:384:GLN:HE21	1.70	0.56
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.86	0.56
4:F:148:ILE:HD12	4:F:162:ILE:HG12	1.87	0.56
2:D:6:HIS:NE2	2:D:8:GLN:HG2	2.20	0.56
2:B:236:VAL:HG22	2:B:368:ILE:HD11	1.88	0.56
4:F:14:TYR:HA	4:F:17:VAL:HB	1.88	0.56
1:C:147:SER:HB2	1:C:190:THR:OG1	2.05	0.56
2:D:19:LYS:HE3	2:D:230:SER:OG	2.06	0.56
2:B:386:THR:O	2:B:390:ARG:HG2	2.05	0.56
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.88	0.55
2:D:226:ASN:O	2:D:230:SER:OG	2.23	0.55
4:F:148:ILE:N	4:F:183:GLN:O	2.37	0.54
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.89	0.54
4:F:199:PHE:CD1	4:F:221:LEU:HD11	2.42	0.54
2:D:293:MET:CG	2:D:367:PHE:HB2	2.38	0.54
1:C:1:MET:CG	1:C:130:THR:OG1	2.56	0.54
4:F:135:TYR:O	4:F:145:ASN:ND2	2.28	0.54
2:B:66:VAL:HG11	2:B:147:MET:CE	2.38	0.54
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.91	0.53
2:D:318:ARG:HG3	2:D:364:SER:HB3	1.90	0.53
2:B:228:LEU:HB3	2:B:300:MET:HE1	1.90	0.52
2:D:378:PHE:HD1	2:D:415:MET:HE2	1.72	0.52
1:C:214:ARG:HG2	1:C:219:ILE:O	2.09	0.52
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.91	0.52
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.45	0.52
2:B:262:ARG:NH2	2:B:421:GLU:OE1	2.43	0.52
2:D:66:VAL:HA	2:D:91:VAL:O	2.10	0.52
2:D:51:TYR:HE1	2:D:61:PRO:HG3	1.74	0.52
2:D:74:ASP:HA	2:D:77:ARG:HB2	1.93	0.51
3:E:61:ARG:NH1	3:E:62:LYS:HG3	2.24	0.51
2:D:97:ALA:HB2	2:D:143:THR:CG2	2.41	0.51
1:C:46:ASP:OD1	1:C:46:ASP:N	2.41	0.51
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.46	0.50
2:B:2:ARG:HA	2:B:129:CYS:O	2.11	0.50
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.93	0.50
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.94	0.50
2:B:86:ARG:NH1	2:B:123:GLU:OE2	2.45	0.50
4:F:195:GLY:C	4:F:197:ARG:HG3	2.37	0.50
1:A:180:ALA:O	1:A:183:GLU:HG3	2.12	0.50
2:D:193:VAL:HG13	2:D:194:GLU:HG2	1.94	0.50
1:C:30:ILE:HG12	1:C:36:MET:HE2	1.93	0.50
2:B:350:LYS:HB2	10:B:505:KUM:C34	2.42	0.49
2:D:151:LEU:HD13	2:D:151:LEU:C	2.37	0.49
4:F:48:PRO:HB2	4:F:51:ARG:HG3	1.93	0.49
4:F:203:SER:HB3	4:F:215:LEU:HD11	1.94	0.49
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.93	0.49
2:B:248:ALA:HB1	10:B:505:KUM:C19	2.43	0.49
2:D:50:TYR:OH	2:D:134:GLN:OE1	2.14	0.49
2:B:251:ARG:NH1	9:B:503:MES:O1S	2.45	0.49
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.48	0.49
2:B:36:TYR:C	2:B:37:HIS:HD1	2.20	0.49
3:E:10:GLU:O	3:E:10:GLU:HG2	2.13	0.49
4:F:34:ASN:HD22	4:F:35:PRO:CD	2.26	0.49
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.94	0.49
2:D:64:ILE:HD12	2:D:119:VAL:HG12	1.95	0.49
4:F:197:ARG:HB3	4:F:224:SER:O	2.13	0.48
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.49	0.48
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.93	0.48
2:D:39:ASP:OD1	2:D:39:ASP:N	2.41	0.48
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.95	0.48
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.48	0.48
1:C:401:LYS:NZ	2:D:429:THR:O	2.33	0.48
2:B:36:TYR:CD1	2:B:44:LEU:HD21	2.48	0.48
2:B:350:LYS:HD3	10:B:505:KUM:C36	2.42	0.48
2:D:132:GLY:HA3	2:D:163:ILE:O	2.13	0.48
12:C:603:HOH:O	3:E:115[B]:HIS:HE1	1.96	0.48
2:B:136:THR:HG22	2:B:167:PHE:HB2	1.95	0.48
2:D:65:LEU:HD11	2:D:85:PHE:CD1	2.49	0.48
2:B:296:SER:N	9:B:504:MES:O3S	2.30	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.48
2:B:392:LYS:HB3	2:B:395:LEU:HD12	1.96	0.48
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.29	0.47
4:F:184:LYS:O	11:F:401:ACP:N6	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.95	0.47
4:F:163:SER:OG	4:F:164:SER:N	2.47	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.50	0.47
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.97	0.47
4:F:221:LEU:HD12	4:F:221:LEU:HA	1.57	0.47
1:A:105:ARG:HG3	1:A:110:ILE:HG13	1.97	0.46
2:D:110:ALA:O	2:D:113:VAL:HG12	2.14	0.46
1:A:175:PRO:HA	1:A:178:SER:HB2	1.96	0.46
2:B:11:GLN:O	2:B:15:GLN:HG3	2.13	0.46
2:D:191:GLN:HE22	3:E:126:LYS:CE	2.27	0.46
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.97	0.46
4:F:202:ARG:HH22	4:F:333:ASN:ND2	2.08	0.46
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.46
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.45	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.51	0.46
1:C:297:GLU:CD	1:C:339:ARG:HH22	2.24	0.46
2:D:267:MET:HE1	2:D:305:PRO:HG3	1.96	0.46
4:F:2:TYR:OH	4:F:360:PRO:O	2.31	0.46
2:D:103:LYS:HA	2:D:107:THR:OG1	2.16	0.46
1:A:117:LEU:HD11	1:A:121:ARG:NH1	2.30	0.46
2:B:198:GLU:OE1	2:B:254:ALA:HB2	2.16	0.46
2:B:332:ASN:O	2:B:336:LYS:HG3	2.15	0.46
1:C:141:PHE:CE2	1:C:203:MET:HE3	2.42	0.46
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.98	0.45
4:F:4:PHE:HB3	4:F:27:TRP:CZ3	2.50	0.45
1:A:280:LYS:HD3	1:A:283:HIS:HB2	1.98	0.45
2:D:290:THR:HA	2:D:293:MET:HE2	1.98	0.45
2:D:143:THR:N	8:D:501:GDP:O1B	2.47	0.45
4:F:185:TYR:HA	11:F:401:ACP:N6	2.31	0.45
1:A:247:ALA:HB3	3:E:19:SER:OG	2.17	0.45
2:B:203:ASP:CG	2:B:380:ARG:HH22	2.23	0.45
2:B:232:THR:OG1	2:B:300:MET:HE2	2.16	0.45
3:E:56:ALA:O	3:E:59:GLU:HG3	2.16	0.45
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.81	0.45
1:A:147:SER:OG	1:A:190:THR:HB	2.17	0.45
1:A:213:CYS:O	1:A:217:LEU:HB2	2.16	0.45
1:C:100:ALA:HA	2:D:252:LYS:HE2	1.98	0.45
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:192:LEU:HB3	4:F:197:ARG:O	2.17	0.45
2:B:211:CYS:HA	2:B:215:LEU:HD12	1.98	0.45
2:D:2:ARG:HA	2:D:129:CYS:O	2.17	0.45
1:A:346:TRP:CD1	1:A:346:TRP:H	2.35	0.44
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.18	0.44
4:F:71:LEU:HD12	4:F:77:LEU:HD23	1.99	0.44
1:A:229:ARG:NE	1:A:363:VAL:HG21	2.32	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
2:D:141:GLY:HA3	8:D:501:GDP:O3A	2.17	0.44
4:F:280:GLU:O	4:F:285:LEU:CD1	2.52	0.44
9:B:504:MES:H51	9:B:504:MES:H81	1.51	0.44
2:B:219:THR:HG21	1:C:326:LYS:HA	1.98	0.44
2:D:286:VAL:O	2:D:290:THR:HG23	2.18	0.44
3:E:136:ASN:HA	3:E:139:LEU:HB2	1.99	0.44
1:A:211:ASP:OD1	1:A:304:LYS:NZ	2.34	0.44
1:C:333:ALA:O	1:C:337:THR:HG23	2.18	0.44
2:B:193:VAL:C	2:B:194:GLU:HG2	2.42	0.44
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.53	0.44
2:D:221:THR:HG23	2:D:224:ASP:H	1.82	0.44
2:D:350:LYS:HB2	10:D:502:KUM:C34	2.48	0.44
1:C:217:LEU:HD13	1:C:367:ASP:HB2	2.00	0.43
1:A:401:LYS:HE3	2:B:428:ALA:HB1	2.00	0.43
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.54	0.43
4:F:331:GLU:OE1	4:F:333:ASN:ND2	2.48	0.43
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.29	0.43
2:B:100:ASN:C	2:B:100:ASN:HD22	2.25	0.43
2:B:145:SER:OG	2:B:188:SER:OG	2.35	0.43
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.58	0.43
1:A:90:GLU:HB3	1:A:121:ARG:NE	2.33	0.43
11:F:401:ACP:H5'2	11:F:401:ACP:O1B	2.18	0.43
2:B:309:ARG:NH1	2:B:343:GLU:OE1	2.47	0.43
2:D:143:THR:OG1	2:D:144:GLY:N	2.52	0.43
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.53	0.43
3:E:136:ASN:HA	3:E:139:LEU:CB	2.49	0.43
4:F:202:ARG:NH2	4:F:333:ASN:HD22	2.13	0.43
1:A:177:VAL:O	1:A:177:VAL:HG22	2.19	0.43
1:C:90:GLU:HB3	1:C:121:ARG:HD2	2.00	0.43
2:D:232:THR:OG1	2:D:300:MET:HE3	2.19	0.43
2:D:378:PHE:CD1	2:D:415:MET:HE2	2.53	0.43
1:C:141:PHE:HB3	1:C:187:SER:OG	2.19	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:NH2	2:D:131:GLN:HB3	2.34	0.42
3:E:137:LYS:HE2	3:E:137:LYS:HB3	1.77	0.42
4:F:26:GLN:CD	4:F:361:LEU:HD23	2.44	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.42
2:D:74:ASP:O	2:D:78:SER:N	2.44	0.42
1:A:68:VAL:HA	1:A:93:ILE:O	2.19	0.42
2:B:66:VAL:HG12	2:B:147:MET:HE2	2.01	0.42
2:B:112:LEU:HD23	2:B:147:MET:HE1	2.01	0.42
2:D:189:VAL:HG11	2:D:415:MET:HG3	2.02	0.42
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.84	0.42
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.87	0.42
2:B:19:LYS:HB3	2:B:19:LYS:HE3	1.87	0.42
2:B:132:GLY:HA3	2:B:163:ILE:O	2.20	0.42
2:D:288:GLU:O	2:D:292:GLN:HB2	2.20	0.42
3:E:135:LYS:O	3:E:139:LEU:HB2	2.19	0.42
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.55	0.42
4:F:221:LEU:HB3	4:F:262:MET:HB3	2.01	0.42
4:F:198:LYS:O	4:F:224:SER:HB3	2.18	0.42
1:A:83:TYR:CD1	1:A:86:LEU:HD22	2.55	0.41
2:D:19:LYS:HD2	2:D:19:LYS:HA	1.89	0.41
2:D:203:ASP:OD2	2:D:380:ARG:NH1	2.38	0.41
2:D:34:GLY:O	2:D:58:LYS:HA	2.20	0.41
2:B:12:CYS:HB2	8:B:501:GDP:C4	2.55	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.41
1:A:187:SER:CB	1:A:391:LEU:HD21	2.50	0.41
2:B:391:ARG:HD2	2:B:391:ARG:HA	1.89	0.41
2:D:1:MET:O	2:D:129:CYS:HB3	2.20	0.41
2:D:130:LEU:HD23	2:D:162:ARG:HH11	1.85	0.41
4:F:62:VAL:HG12	4:F:310:GLN:O	2.20	0.41
2:B:104:GLY:O	2:B:109:GLY:HA3	2.20	0.41
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.03	0.41
1:A:99:ALA:HA	1:A:105:ARG:HG2	2.03	0.41
1:A:399:TYR:OH	1:A:415:GLU:HG2	2.21	0.41
2:D:4:ILE:HG12	2:D:131:GLN:HG3	2.03	0.41
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.56	0.41
2:B:67:ASP:O	2:B:92:PHE:HA	2.21	0.41
2:D:401:GLU:HA	3:E:137:LYS:HG3	2.03	0.41
2:D:416:ASN:HA	2:D:419:VAL:HG22	2.02	0.41
2:B:94:GLN:HB3	1:C:1:MET:HE1	2.02	0.41
1:C:71:GLU:CB	1:C:98:ASP:HB3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:416:ASN:HA	2:D:416:ASN:HD22	1.72	0.41
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.56	0.40
2:B:203:ASP:OD1	2:B:380:ARG:NH1	2.41	0.40
3:E:25:LYS:HA	3:E:26:PRO:HD3	1.85	0.40
1:A:297:GLU:HG3	12:F:507:HOH:O	2.21	0.40
2:D:151:LEU:HD13	2:D:151:LEU:O	2.21	0.40
2:D:293:MET:HE1	2:D:317:PHE:CZ	2.55	0.40
2:D:337:ASN:HB3	2:D:340:TYR:HD2	1.86	0.40
4:F:339:ALA:HB3	4:F:342:LEU:HD12	2.04	0.40
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.03	0.40
2:D:97:ALA:HB1	2:D:142:GLY:HA3	2.04	0.40
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.04	0.40
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	427 (98%)	7 (2%)	1 (0%)	43	66
1	C	438/450 (97%)	429 (98%)	8 (2%)	1 (0%)	43	66
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	417/445 (94%)	410 (98%)	7 (2%)	0	100	100
3	E	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
4	F	302/384 (79%)	291 (96%)	11 (4%)	0	100	100
All	All	2135/2317 (92%)	2092 (98%)	41 (2%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
1	C	162	GLY

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	365/378 (97%)	364 (100%)	1 (0%)	86	94
1	C	368/378 (97%)	366 (100%)	2 (0%)	81	92
2	B	362/383 (94%)	362 (100%)	0	100	100
2	D	326/383 (85%)	325 (100%)	1 (0%)	86	94
3	E	104/127 (82%)	104 (100%)	0	100	100
4	F	234/342 (68%)	230 (98%)	4 (2%)	53	78
All	All	1759/1991 (88%)	1751 (100%)	8 (0%)	81	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	C	2	ARG
1	C	241	SER
2	D	318	ARG
4	F	12	SER
4	F	202	ARG
4	F	269	GLN
4	F	283	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	GLN
1	A	186	ASN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	309	HIS
1	A	358	GLN
1	A	406	HIS
2	B	100	ASN
2	B	165	ASN
2	B	247	ASN
2	B	292	GLN
1	C	15	GLN
1	C	85	GLN
1	C	101	ASN
1	C	256	GLN
1	C	309	HIS
1	C	372	GLN
1	C	380	ASN
1	C	393	HIS
2	D	99	ASN
2	D	100	ASN
2	D	191	GLN
2	D	226	ASN
2	D	292	GLN
2	D	329	GLN
2	D	347	ASN
2	D	384	GLN
2	D	416	ASN
3	E	108	ASN
4	F	34	ASN
4	F	260	ASN
4	F	269	GLN
4	F	310	GLN
4	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
11	ACP	F	401	-	31,33,33	3.21	12 (38%)	47,52,52	2.02	13 (27%)
10	KUM	D	502	-	30,31,31	1.86	10 (33%)	40,44,44	1.91	14 (35%)
9	MES	B	503	-	12,12,12	2.23	1 (8%)	15,16,16	1.76	3 (20%)
8	GDP	B	501	6	29,30,30	1.96	6 (20%)	45,47,47	3.18	14 (31%)
5	GTP	A	501	6	33,34,34	1.06	2 (6%)	50,54,54	1.57	8 (16%)
8	GDP	D	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.70	8 (17%)
5	GTP	C	501	6	33,34,34	0.96	2 (6%)	50,54,54	1.52	8 (16%)
9	MES	B	504	-	12,12,12	2.34	1 (8%)	15,16,16	1.86	3 (20%)
10	KUM	B	505	-	30,31,31	1.85	8 (26%)	40,44,44	1.94	13 (32%)

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
11	ACP	F	401	-	-	3/19/38/38	0/3/3/3
10	KUM	D	502	-	-	7/18/18/18	0/4/4/4
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
8	GDP	D	501	-	-	4/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	KUM	B	505	-	-	6/18/18/18	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	O4'-C1'	8.72	1.62	1.42
9	B	504	MES	C8-S	-7.83	1.66	1.77
8	B	501	GDP	O6-C6	-7.55	1.09	1.23
9	B	503	MES	C8-S	-7.44	1.67	1.77
11	F	401	ACP	C2'-C1'	-7.06	1.31	1.53
11	F	401	ACP	PB-O3A	6.43	1.65	1.58
11	F	401	ACP	O4'-C4'	-6.42	1.30	1.45
11	F	401	ACP	PA-O3A	5.55	1.65	1.59
11	F	401	ACP	C6-N6	4.41	1.45	1.34
10	D	502	KUM	C33-C35	-4.02	1.38	1.45
10	D	502	KUM	C35-C26	4.00	1.53	1.46
10	B	505	KUM	C35-C26	3.88	1.52	1.46
10	B	505	KUM	C33-C35	-3.88	1.38	1.45
10	D	502	KUM	C33-C34	-3.84	1.36	1.41
10	B	505	KUM	C33-C34	-3.73	1.36	1.41
10	B	505	KUM	C28-N27	-3.38	1.32	1.37
10	D	502	KUM	C28-N27	-3.31	1.32	1.37
8	B	501	GDP	C2-N3	3.30	1.41	1.33
10	B	505	KUM	C29-N31	-3.22	1.31	1.37
10	D	502	KUM	C29-N31	-3.18	1.31	1.37
8	D	501	GDP	C5-C4	3.06	1.47	1.38
11	F	401	ACP	O2'-C2'	2.87	1.50	1.43
11	F	401	ACP	C5-C4	-2.86	1.34	1.39
8	B	501	GDP	C8-N7	2.71	1.40	1.32
11	F	401	ACP	O3'-C3'	-2.70	1.36	1.43
8	B	501	GDP	C5-N7	-2.56	1.33	1.39
8	D	501	GDP	C6-N1	-2.53	1.34	1.38
11	F	401	ACP	C5-N7	-2.51	1.34	1.39
5	A	501	GTP	PA-O3A	2.41	1.62	1.59
5	A	501	GTP	PB-O3B	2.39	1.62	1.59
8	B	501	GDP	C1'-N9	2.28	1.54	1.47
8	B	501	GDP	PA-O3A	2.24	1.61	1.59
8	D	501	GDP	C4-N9	-2.22	1.32	1.38
10	D	502	KUM	O02-C01	2.22	1.40	1.37
11	F	401	ACP	PB-O2B	-2.20	1.51	1.56
10	B	505	KUM	O02-C01	2.19	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	KUM	O25-C24	-2.19	1.18	1.23
5	C	501	GTP	PB-O3B	2.15	1.61	1.59
10	B	505	KUM	O14-C13	2.13	1.40	1.37
11	F	401	ACP	C8-N9	-2.11	1.34	1.37
10	D	502	KUM	O25-C24	-2.09	1.18	1.23
10	D	502	KUM	O14-C13	2.06	1.40	1.37
10	D	502	KUM	C28-C24	2.05	1.53	1.46
10	D	502	KUM	C21-C24	2.05	1.53	1.49
8	D	501	GDP	C5-N7	-2.05	1.35	1.39
5	C	501	GTP	C2-N3	2.02	1.38	1.33

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C5-C4-N3	-9.12	113.88	128.39
8	B	501	GDP	C2-N1-C6	-8.63	109.46	125.11
8	B	501	GDP	C2-N3-C4	8.28	126.56	112.30
8	B	501	GDP	O6-C6-N1	-8.05	104.97	120.11
8	B	501	GDP	C5-C6-N1	6.89	130.79	113.25
10	B	505	KUM	C29-C28-C24	-6.61	123.84	132.74
10	D	502	KUM	C29-C28-C24	-6.17	124.44	132.74
11	F	401	ACP	N3-C2-N1	-5.58	120.13	128.58
8	B	501	GDP	N9-C4-N3	5.41	136.76	125.95
8	D	501	GDP	C5-C4-N3	-5.06	120.34	128.39
11	F	401	ACP	N6-C6-N1	-4.97	107.32	118.38
11	F	401	ACP	C5-C4-N3	-4.95	119.90	126.72
8	B	501	GDP	C6-C5-N7	4.72	138.88	130.29
5	A	501	GTP	C5-C4-N3	-4.69	120.92	128.39
5	C	501	GTP	C5-C4-N3	-4.62	121.04	128.39
5	A	501	GTP	C2-N3-C4	4.61	120.24	112.30
5	C	501	GTP	C2-N3-C4	4.58	120.18	112.30
8	D	501	GDP	C2-N3-C4	4.54	120.12	112.30
11	F	401	ACP	N9-C8-N7	-4.24	107.92	113.94
9	B	504	MES	C5-N4-C3	4.00	117.45	108.84
8	D	501	GDP	N9-C4-N3	3.95	133.86	125.95
11	F	401	ACP	C5-C6-N6	3.80	132.71	123.29
10	B	505	KUM	C24-C28-N27	3.75	127.76	120.99
9	B	503	MES	C5-N4-C3	3.73	116.89	108.84
10	D	502	KUM	C24-C28-N27	3.63	127.54	120.99
8	D	501	GDP	C6-C5-N7	3.46	136.58	130.29
10	B	505	KUM	O14-C13-C07	3.37	120.92	115.14
11	F	401	ACP	C2-N3-C4	3.35	120.01	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	KUM	C33-C35-C36	3.28	107.96	106.15
10	D	502	KUM	O14-C13-C07	3.07	120.41	115.14
11	F	401	ACP	N3-C4-N9	3.03	132.31	127.17
10	D	502	KUM	C33-C35-C36	3.02	107.82	106.15
9	B	504	MES	C6-C5-N4	-3.02	105.53	110.12
10	D	502	KUM	O02-C01-C07	2.95	120.20	115.14
11	F	401	ACP	C5-N7-C8	2.94	108.08	103.45
11	F	401	ACP	C3'-C2'-C1'	2.84	106.84	101.46
8	B	501	GDP	C6-C5-C4	-2.84	114.56	118.83
5	C	501	GTP	N9-C4-N3	2.82	131.60	125.95
8	B	501	GDP	N9-C8-N7	-2.81	108.18	113.40
5	A	501	GTP	C2-N1-C6	-2.80	120.03	125.11
5	C	501	GTP	C2-N1-C6	-2.79	120.06	125.11
10	B	505	KUM	C35-C36-N38	-2.79	108.33	110.22
5	C	501	GTP	N9-C8-N7	-2.77	108.26	113.40
5	A	501	GTP	N9-C8-N7	-2.77	108.26	113.40
10	D	502	KUM	C35-C36-N38	-2.73	108.37	110.22
5	A	501	GTP	N9-C4-N3	2.72	131.39	125.95
8	B	501	GDP	N2-C2-N1	-2.68	111.11	116.76
10	D	502	KUM	C35-C26-N27	2.66	127.55	122.87
9	B	503	MES	C6-C5-N4	-2.66	106.08	110.12
10	D	502	KUM	O14-C13-C19	-2.62	119.57	124.08
10	D	502	KUM	C15-O14-C13	-2.61	113.68	117.51
8	B	501	GDP	C4-C5-N7	-2.60	106.56	110.67
10	B	505	KUM	O14-C13-C19	-2.57	119.66	124.08
5	A	501	GTP	C5-C6-N1	2.56	119.78	113.25
10	B	505	KUM	O02-C01-C07	2.54	119.50	115.14
5	A	501	GTP	C8-N7-C5	2.53	108.77	104.26
10	B	505	KUM	C15-O14-C13	-2.53	113.80	117.51
5	C	501	GTP	C8-N7-C5	2.51	108.73	104.26
9	B	503	MES	C7-N4-C5	2.49	117.88	111.24
5	C	501	GTP	C5-C6-N1	2.49	119.59	113.25
10	D	502	KUM	O02-C01-C22	-2.48	119.80	124.08
8	D	501	GDP	C2'-C3'-C4'	2.47	107.38	102.61
10	B	505	KUM	C21-C24-C28	2.45	122.88	119.52
11	F	401	ACP	C4-N9-C8	2.34	108.20	105.74
5	C	501	GTP	O6-C6-C5	-2.32	120.42	126.53
8	B	501	GDP	N2-C2-N3	2.29	124.14	119.67
8	D	501	GDP	C4-C5-N7	-2.28	107.06	110.67
5	A	501	GTP	O6-C6-C5	-2.25	120.59	126.53
11	F	401	ACP	C4-C5-N7	-2.25	108.01	110.58
10	B	505	KUM	C35-C26-N27	2.21	126.77	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	KUM	C40-C34-C33	-2.21	120.05	122.19
10	D	502	KUM	C03-O02-C01	-2.17	114.33	117.51
8	B	501	GDP	C8-N7-C5	2.16	108.11	104.26
8	D	501	GDP	O6-C6-C5	-2.16	120.84	126.53
10	D	502	KUM	C40-C34-C33	-2.14	120.11	122.19
9	B	504	MES	C7-N4-C5	2.11	116.86	111.24
11	F	401	ACP	PB-O3A-PA	-2.10	125.50	132.37
11	F	401	ACP	C6-C5-C4	2.08	120.02	117.18
8	B	501	GDP	C5-C4-N9	2.07	109.36	105.66
10	D	502	KUM	C21-C24-C28	2.07	122.36	119.52
10	D	502	KUM	C34-C33-C35	2.04	107.93	106.62
8	D	501	GDP	C2'-C1'-N9	-2.02	107.62	113.25
10	B	505	KUM	C03-O02-C01	-2.02	114.56	117.51
10	B	505	KUM	O02-C01-C22	-2.00	120.63	124.08

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
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-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O3S
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
10	B	505	KUM	C21-C24-C28-C29
10	B	505	KUM	C21-C24-C28-N27

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Mol	Chain	Res	Type	Atoms
10	B	505	KUM	O25-C24-C28-N27
10	D	502	KUM	C21-C24-C28-C29
10	D	502	KUM	C21-C24-C28-N27
10	D	502	KUM	O25-C24-C28-N27
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
10	D	502	KUM	C07-C13-O14-C15
10	D	502	KUM	C19-C13-O14-C15
10	D	502	KUM	C07-C01-O02-C03
11	F	401	ACP	C3'-C4'-C5'-O5'
10	B	505	KUM	C07-C13-O14-C15
9	B	504	MES	C7-C8-S-O3S
10	D	502	KUM	C22-C01-O02-C03
8	D	501	GDP	PA-O3A-PB-O1B
10	B	505	KUM	C19-C13-O14-C15
9	B	503	MES	C7-C8-S-O2S
10	B	505	KUM	C07-C01-O02-C03
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C3'-C4'-C5'-O5'

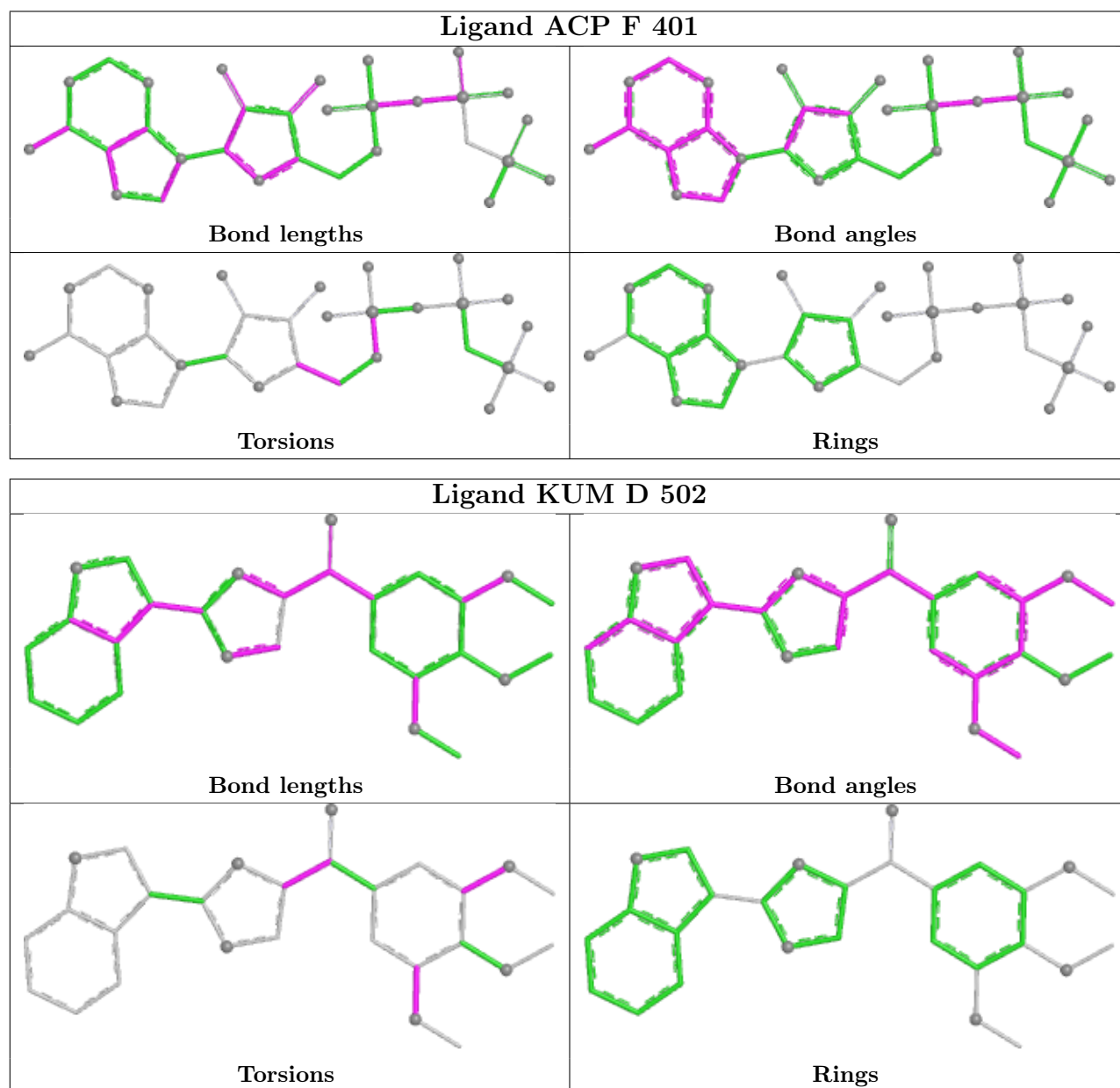
There are no ring outliers.

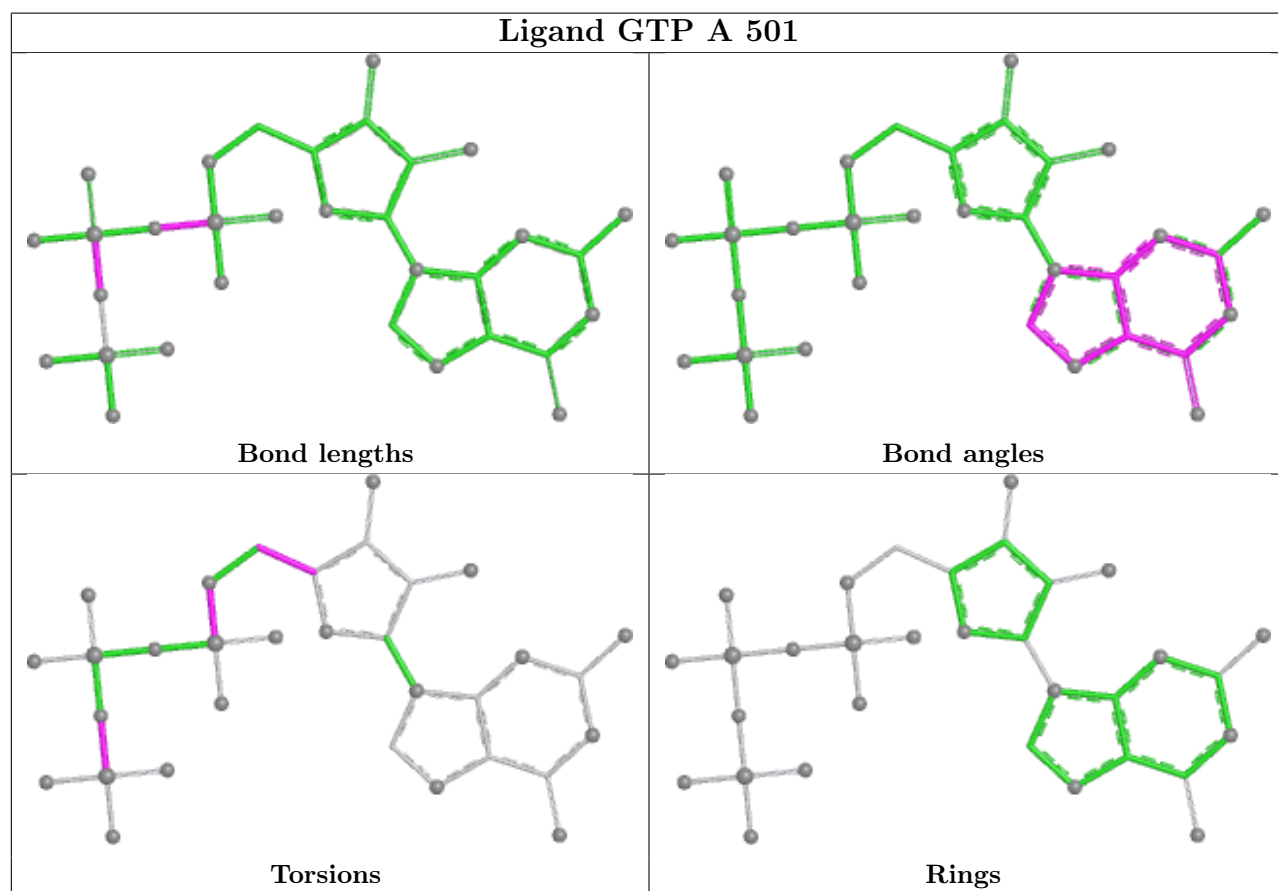
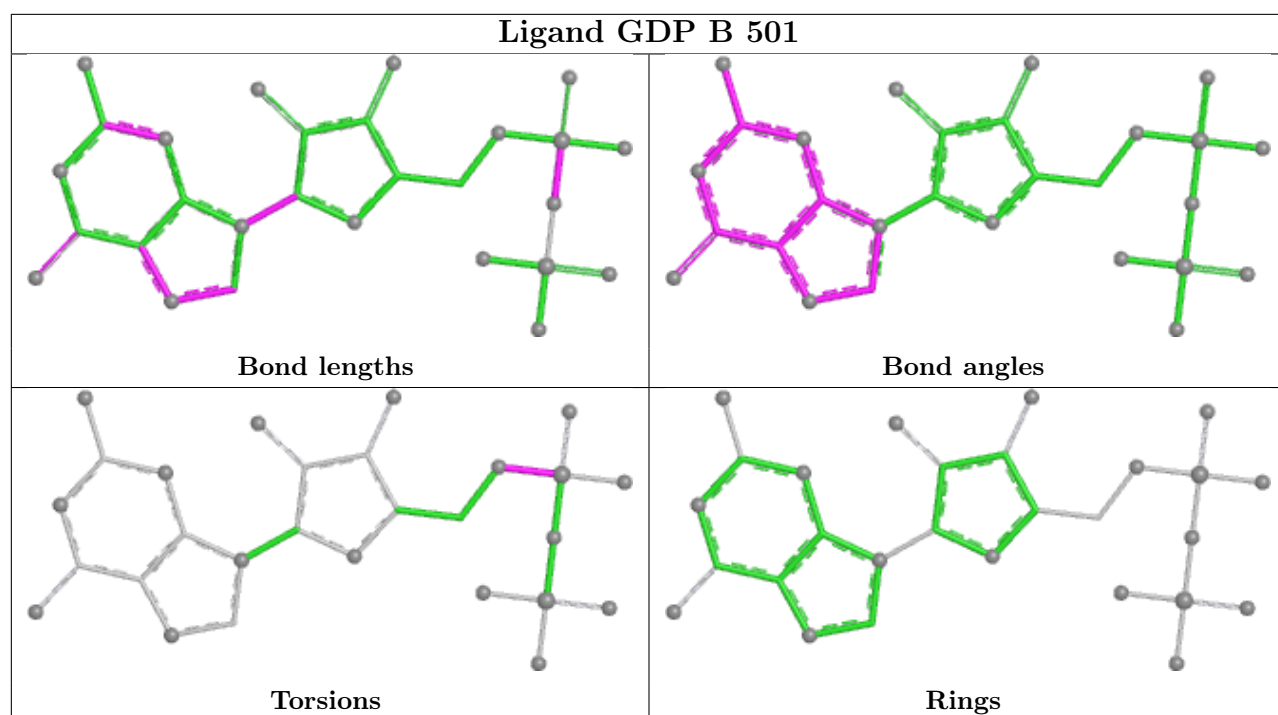
8 monomers are involved in 21 short contacts:

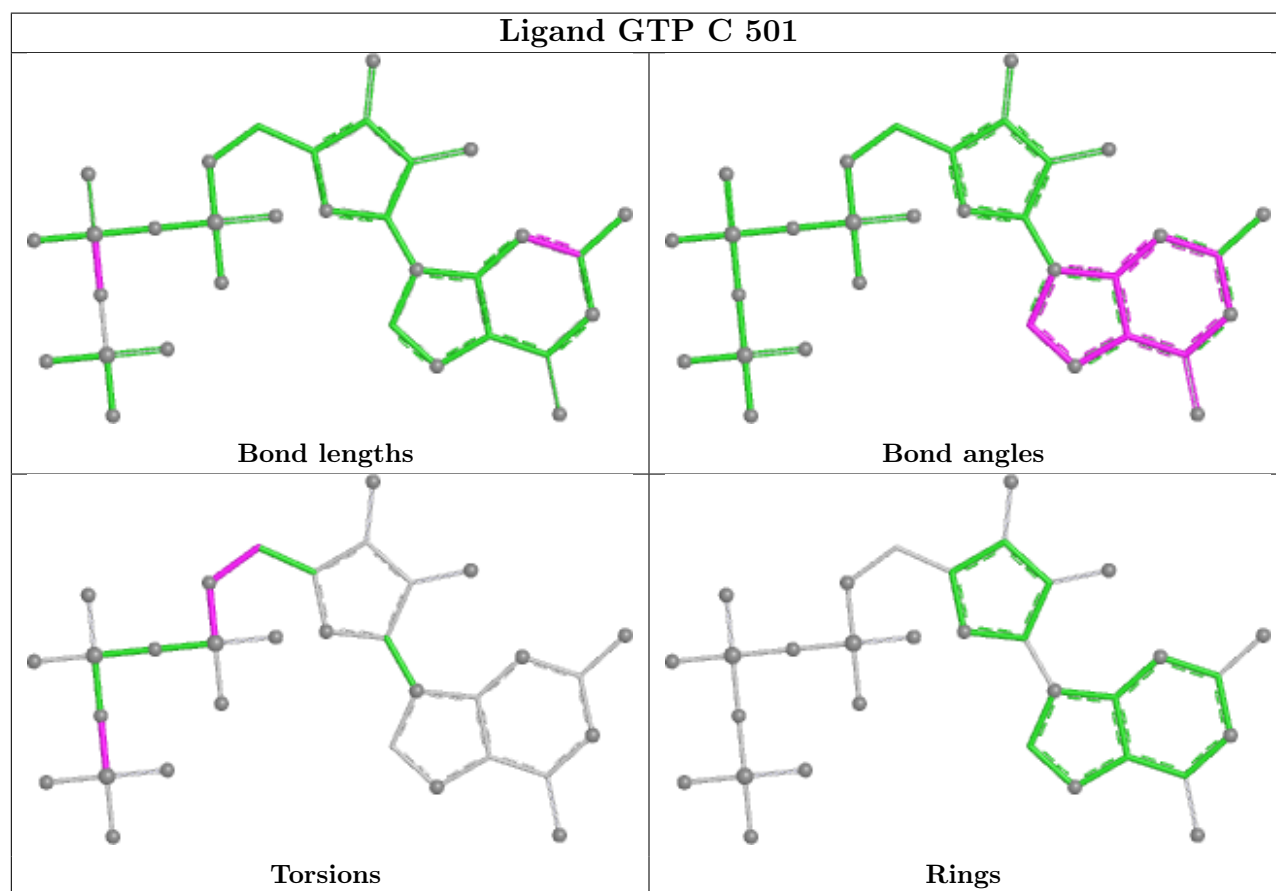
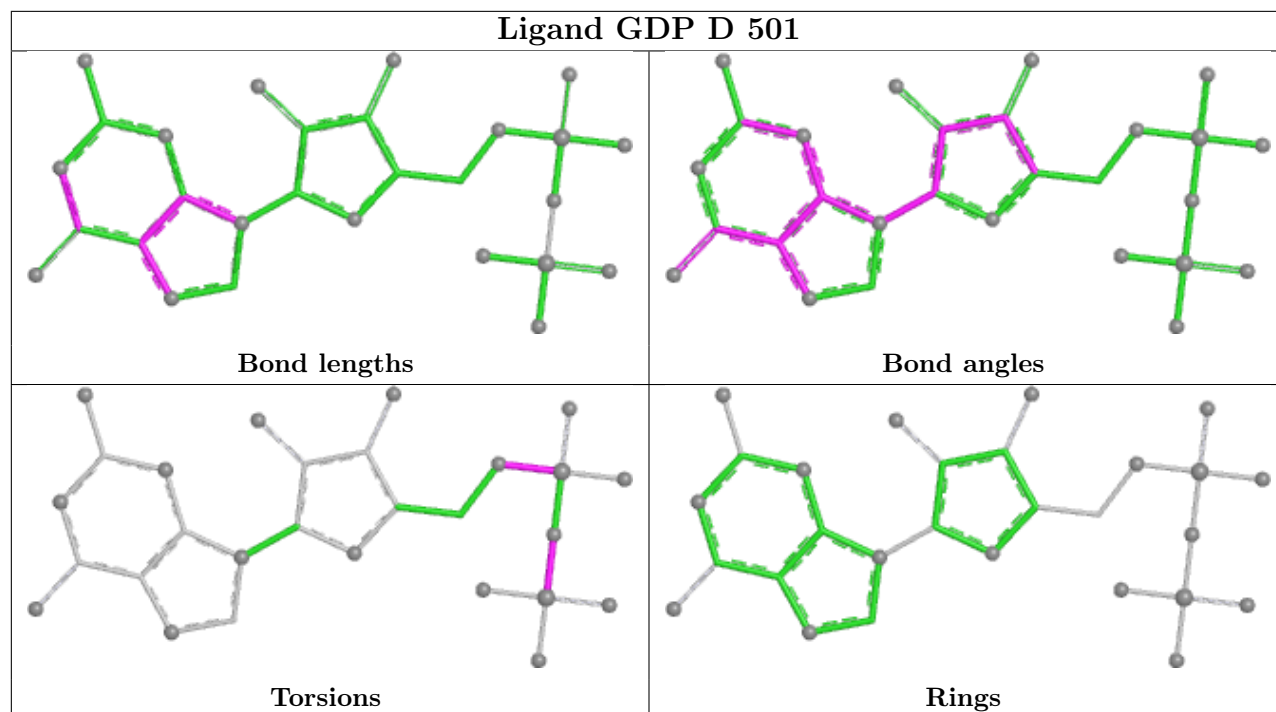
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	3	0
10	D	502	KUM	1	0
9	B	503	MES	1	0
8	B	501	GDP	4	0
5	A	501	GTP	1	0
8	D	501	GDP	6	0
9	B	504	MES	2	0
10	B	505	KUM	3	0

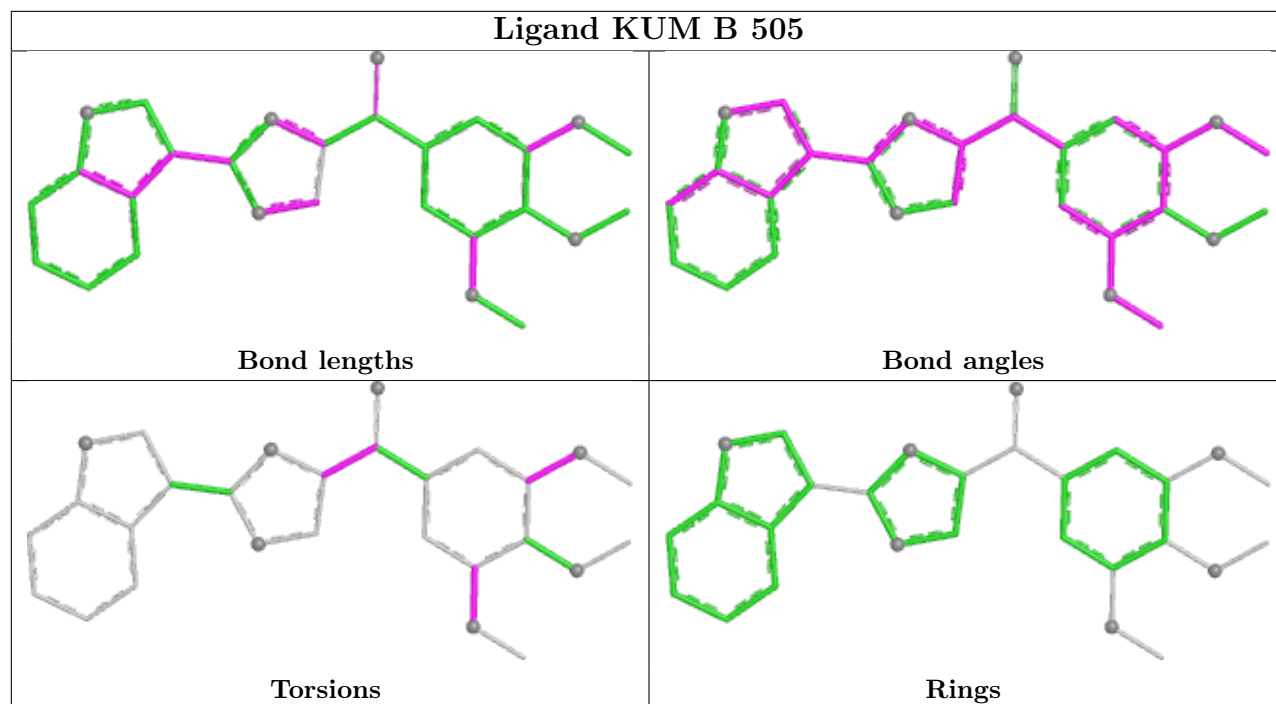
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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%)	0.16	11 (2%) 58 52	28, 46, 75, 95	0
1	C	440/450 (97%)	-0.07	7 (1%) 70 66	22, 34, 60, 86	0
2	B	427/445 (95%)	0.15	18 (4%) 40 35	20, 40, 79, 133	0
2	D	421/445 (94%)	1.15	81 (19%) 3 2	34, 71, 109, 137	0
3	E	121/143 (84%)	0.77	11 (9%) 15 11	29, 60, 102, 117	1 (0%)
4	F	316/384 (82%)	1.41	90 (28%) 1 1	31, 75, 131, 152	0
All	All	2162/2317 (93%)	0.52	218 (10%) 12 9	20, 51, 106, 152	1 (0%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	191	LEU	7.4
4	F	362	ALA	6.5
4	F	134	ALA	6.3
4	F	161	LEU	6.2
4	F	140	GLU	5.5
4	F	253	TYR	5.4
4	F	167	SER	5.3
2	D	81	PHE	5.2
4	F	99	VAL	5.1
2	D	431	ASP	4.9
2	D	1	MET	4.8
2	D	396	HIS	4.8
2	D	54	ALA	4.8
4	F	166	ALA	4.8
4	F	244	CYS	4.8
4	F	171	ASP	4.8
4	F	148	ILE	4.6
1	C	440	VAL	4.5
4	F	100	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	147	TRP	4.4
2	D	397	TRP	4.4
4	F	229	ASN	4.4
4	F	245	ILE	4.2
2	D	55	THR	4.1
1	C	163	LYS	4.0
3	E	6	MET	4.0
4	F	173	ILE	3.9
2	D	84	ILE	3.9
2	D	44	LEU	3.9
4	F	133	ALA	3.9
4	F	143	GLU	3.8
4	F	296	MET	3.7
2	D	83	GLN	3.7
4	F	101	TYR	3.7
2	D	218	THR	3.7
2	D	46	ARG	3.7
2	D	170	MET	3.5
4	F	132	LEU	3.5
4	F	102	PRO	3.5
4	F	243	HIS	3.5
4	F	135	TYR	3.5
2	D	42	LEU	3.5
2	D	32	PRO	3.4
4	F	182	ILE	3.4
2	D	85	PHE	3.4
4	F	131	PHE	3.4
2	D	356	ILE	3.4
2	D	323	MET	3.4
2	D	208	TYR	3.4
4	F	226	GLU	3.4
4	F	170	LEU	3.4
1	C	1	MET	3.3
4	F	146	VAL	3.3
2	B	274	THR	3.3
2	B	428	ALA	3.3
2	D	72	THR	3.2
2	B	55	THR	3.2
2	D	215	LEU	3.2
2	B	281	TYR	3.2
4	F	186	LEU	3.2
2	D	247	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	89	GLU	3.1
2	D	37	HIS	3.1
2	B	280	GLN	3.1
3	E	140	LYS	3.1
4	F	130	VAL	3.1
4	F	179	VAL	3.1
4	F	190	LEU	3.1
2	D	47	ILE	3.1
4	F	183	GLN	3.0
4	F	98	TYR	3.0
4	F	88	SER	3.0
4	F	230	SER	3.0
2	D	171	PRO	3.0
2	D	284	LEU	3.0
2	D	140	GLY	3.0
2	D	36	TYR	3.0
4	F	78	VAL	3.0
3	E	45	PRO	3.0
1	A	437	VAL	2.9
4	F	372	THR	2.9
2	D	82	GLY	2.9
4	F	252	ASN	2.9
1	A	179	THR	2.9
2	D	214	THR	2.9
4	F	181	VAL	2.9
2	D	362	LYS	2.9
2	B	73	MET	2.9
2	D	97	ALA	2.8
4	F	180	HIS	2.8
2	D	273	LEU	2.8
4	F	263	PHE	2.8
4	F	379	HIS	2.8
4	F	194	PRO	2.8
1	C	285	GLN	2.8
2	B	33	THR	2.8
3	E	44	ASP	2.8
2	B	322	SER	2.7
4	F	240	LEU	2.7
2	D	98	GLY	2.7
2	D	243	PRO	2.7
4	F	200	ASP	2.7
2	B	323	MET	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	213	ARG	2.7
2	D	363	MET	2.7
1	A	38	SER	2.7
2	D	31	ASP	2.6
2	D	92	PHE	2.6
2	D	96	GLY	2.6
4	F	175	GLU	2.6
2	B	245	GLN	2.6
4	F	277	THR	2.6
4	F	380	HIS	2.6
3	E	96	MET	2.6
2	D	180	VAL	2.6
2	B	95	SER	2.6
4	F	141	GLY	2.6
2	D	399	THR	2.6
2	D	86	ARG	2.5
3	E	119	MET	2.5
4	F	165	GLU	2.5
2	B	247	ASN	2.5
1	C	178	SER	2.5
3	E	28	SER	2.5
4	F	90	SER	2.5
4	F	373	SER	2.5
4	F	187	GLU	2.5
2	D	33	THR	2.5
4	F	162	ILE	2.5
4	F	142	ARG	2.5
1	A	178	SER	2.5
2	D	95	SER	2.5
4	F	224	SER	2.5
2	B	194	GLU	2.5
4	F	259	GLY	2.5
2	B	275	SER	2.5
2	D	322	SER	2.5
2	D	211	CYS	2.4
1	A	282	TYR	2.4
4	F	201	ILE	2.4
3	E	139	LEU	2.4
4	F	192	LEU	2.4
4	F	136	ASN	2.4
4	F	333	ASN	2.4
2	D	164	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	222	TYR	2.4
2	D	359	ARG	2.4
2	D	80	PRO	2.4
2	D	19	LYS	2.4
2	D	368	ILE	2.4
4	F	91	CYS	2.4
4	F	196	HIS	2.4
2	D	57	ASN	2.4
4	F	184	LYS	2.4
4	F	227	PRO	2.4
2	D	104	GLY	2.4
2	B	15	GLN	2.4
3	E	116	LEU	2.4
4	F	198	LYS	2.4
4	F	168	GLU	2.4
1	A	59	GLY	2.3
2	D	391	ARG	2.3
2	D	151	LEU	2.3
2	D	361	LEU	2.3
4	F	20	LEU	2.3
2	B	335	ASN	2.3
4	F	255	ARG	2.3
2	D	245	GLN	2.3
2	B	57	ASN	2.3
2	D	71	GLY	2.3
2	D	360	GLY	2.3
4	F	254	GLY	2.3
1	A	346	TRP	2.3
2	D	24	ILE	2.2
4	F	330	ILE	2.2
1	A	262	TYR	2.2
2	D	293	MET	2.2
1	C	341	ILE	2.2
2	D	25	SER	2.2
2	D	175	VAL	2.2
4	F	335	ALA	2.2
2	D	285	THR	2.2
4	F	21	LEU	2.2
2	D	230	SER	2.2
3	E	46	SER	2.2
4	F	256	TYR	2.2
4	F	96	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	84	ARG	2.2
2	D	272	PRO	2.2
2	D	358	PRO	2.2
1	A	177	VAL	2.1
2	D	400	GLY	2.1
2	D	51	TYR	2.1
2	D	35	SER	2.1
4	F	128	ARG	2.1
4	F	228	TYR	2.1
4	F	323	GLU	2.1
2	D	201	CYS	2.1
2	B	337	ASN	2.1
2	D	228	LEU	2.1
1	A	90	GLU	2.1
1	A	196	GLU	2.1
3	E	141	GLU	2.1
4	F	225	SER	2.1
2	D	353	VAL	2.1
4	F	199	PHE	2.1
2	D	34	GLY	2.1
2	D	73	MET	2.1
4	F	1	MET	2.1
4	F	222	ARG	2.0
2	D	100	ASN	2.0
4	F	32	LYS	2.0
2	D	40	SER	2.0
2	D	12	CYS	2.0
4	F	172	PHE	2.0
4	F	285	LEU	2.0
2	D	106	TYR	2.0
4	F	163	SER	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

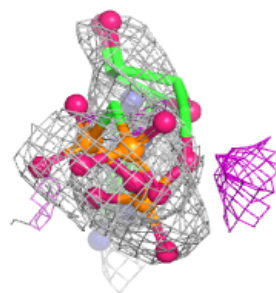
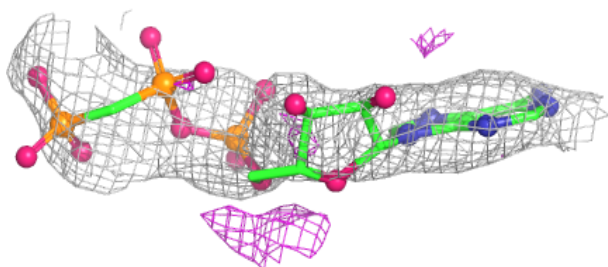
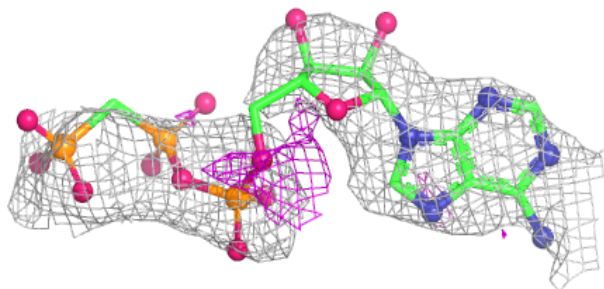
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.63	0.18	88,108,155,157	0
8	GDP	D	501	28/28	0.83	0.14	55,64,76,84	0
9	MES	B	504	12/12	0.87	0.16	82,86,93,98	0
8	GDP	B	501	28/28	0.94	0.10	19,34,47,63	0
10	KUM	D	502	28/28	0.94	0.11	38,55,76,87	0
9	MES	B	503	12/12	0.94	0.10	31,49,69,73	0
6	MG	B	502	1/1	0.95	0.09	39,39,39,39	0
10	KUM	B	505	28/28	0.95	0.09	25,38,53,58	0
7	CA	C	503	1/1	0.96	0.05	55,55,55,55	0
5	GTP	A	501	32/32	0.97	0.07	26,29,38,42	0
6	MG	C	502	1/1	0.98	0.07	39,39,39,39	0
7	CA	A	503	1/1	0.98	0.06	71,71,71,71	0
5	GTP	C	501	32/32	0.99	0.05	27,28,33,35	0
6	MG	A	502	1/1	1.00	0.04	43,43,43,43	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.

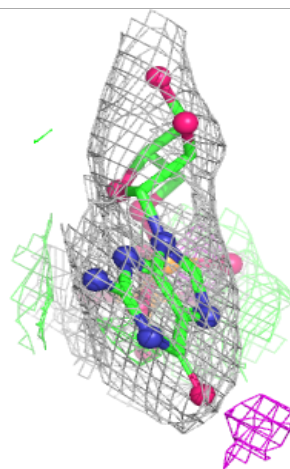
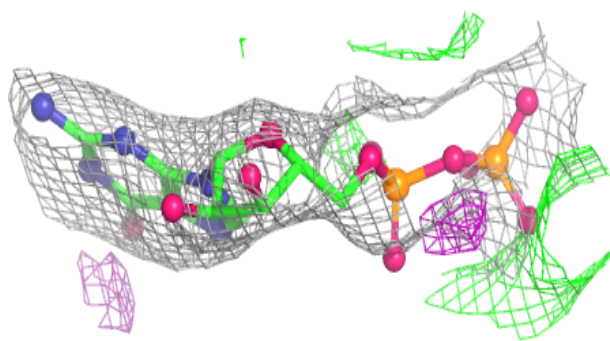
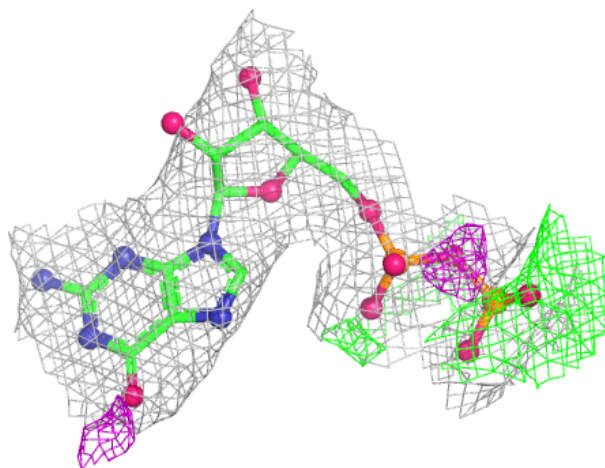
Electron density around ACP F 401:

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



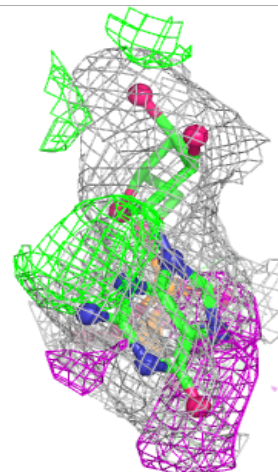
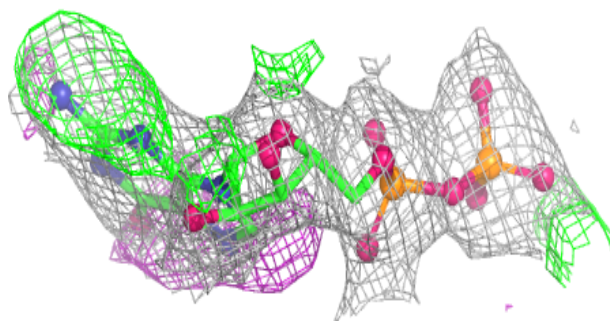
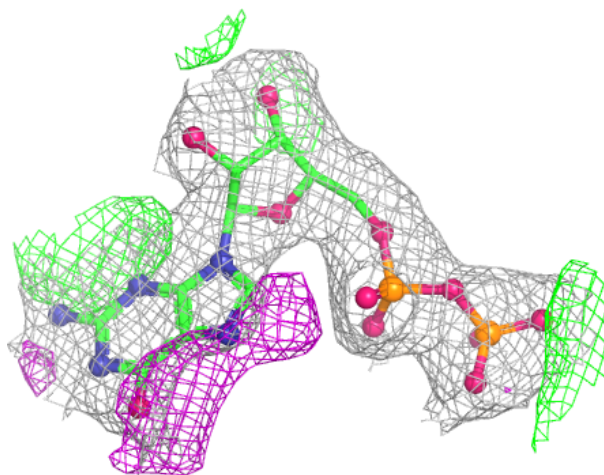
Electron density around GDP D 501:

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



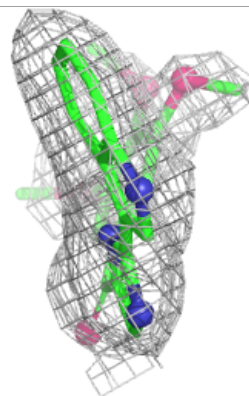
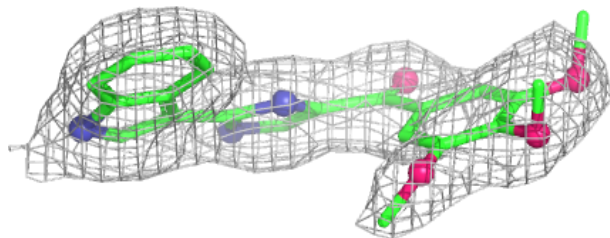
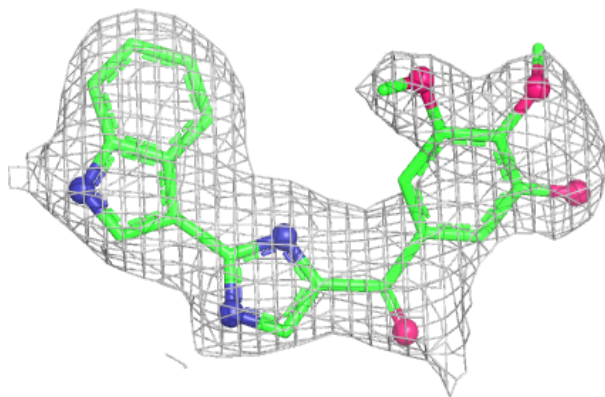
Electron density around GDP B 501:

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

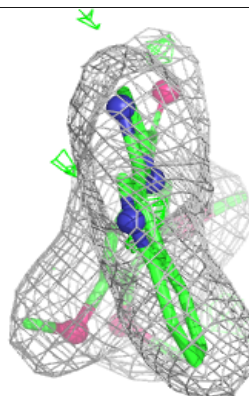
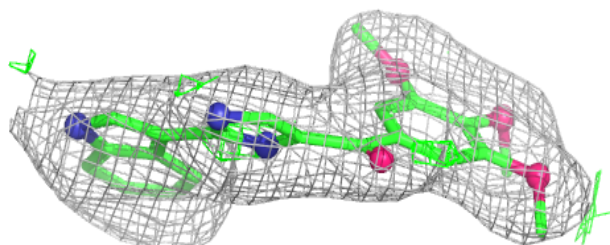
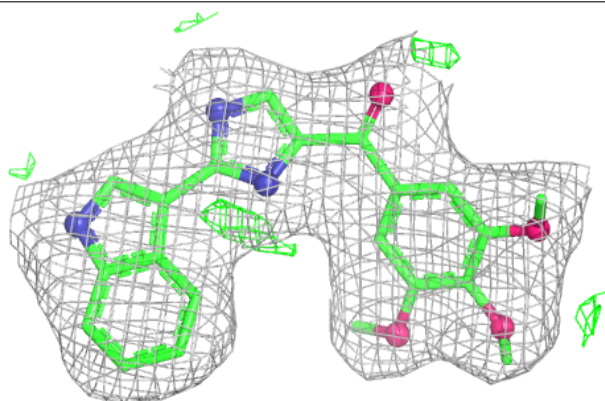


Electron density around KUM D 502:

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

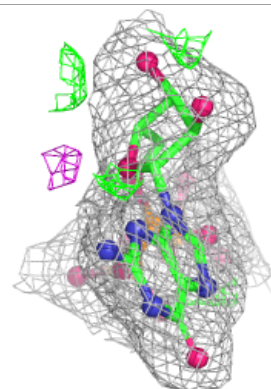
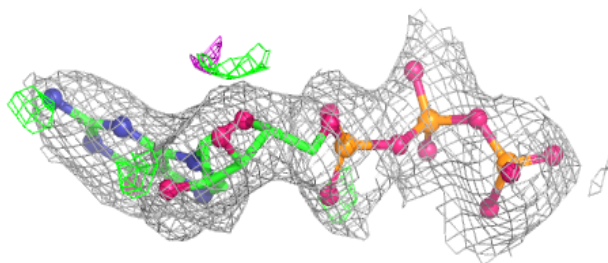
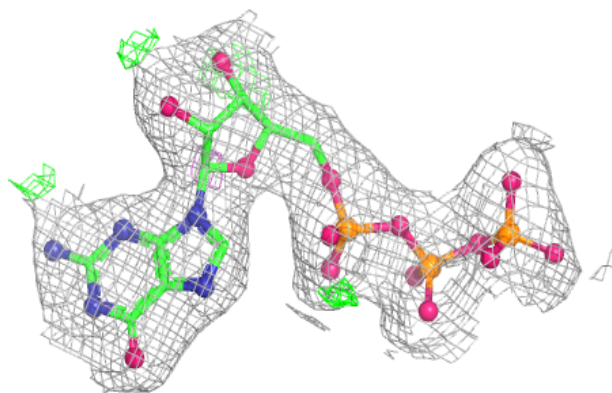
**Electron density around KUM B 505:**

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

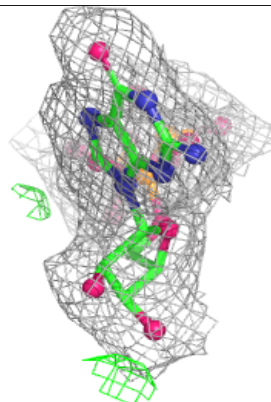
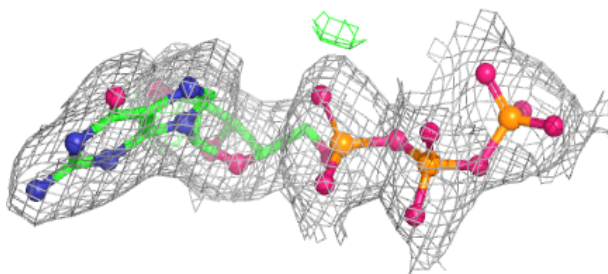
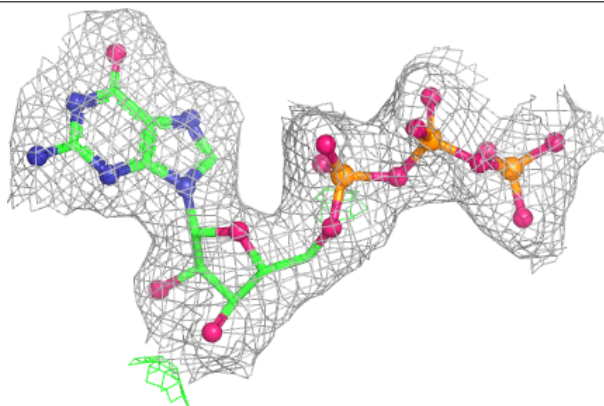


Electron density around GTP A 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.