



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:10 PM JST

PDB ID : 7DB9
Title : IC1 in complex with tubulin
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2020-10-19
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

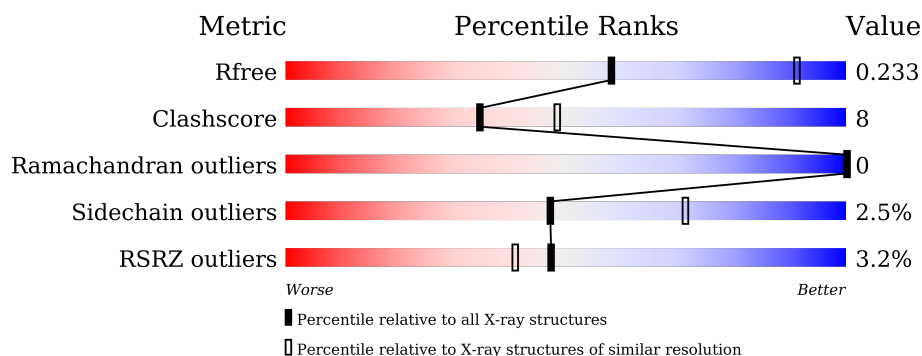
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	C	451	<div> <div>84%</div> <div>12%</div> <div>..</div> </div>
2	B	445	<div> <div>%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
2	D	445	<div> <div>4%</div> <div>70%</div> <div>24%</div> <div>5%</div> </div>
3	E	143	<div> <div>3%</div> <div>72%</div> <div>14%</div> <div>.</div> <div>13%</div> </div>
4	F	384	<div> <div>10%</div> <div>64%</div> <div>26%</div> <div>.</div> <div>8%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17750 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	439	Total	C	N	O	S	0	6	0
			3458	2188	587	659	24			
1	C	440	Total	C	N	O	S	0	6	0
			3454	2187	584	659	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	2	0
			3389	2129	579	654	27			
2	D	422	Total	C	N	O	S	0	2	0
			3318	2085	563	643	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	2	0
			1032	636	187	204	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	2	0
			2869	1838	491	525	15			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

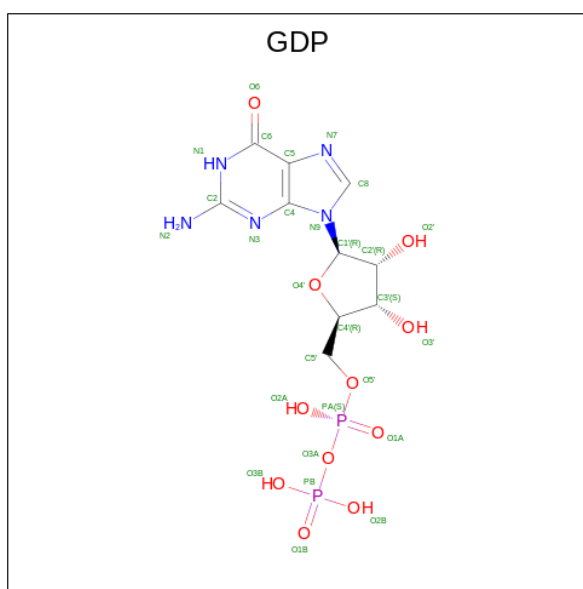
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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

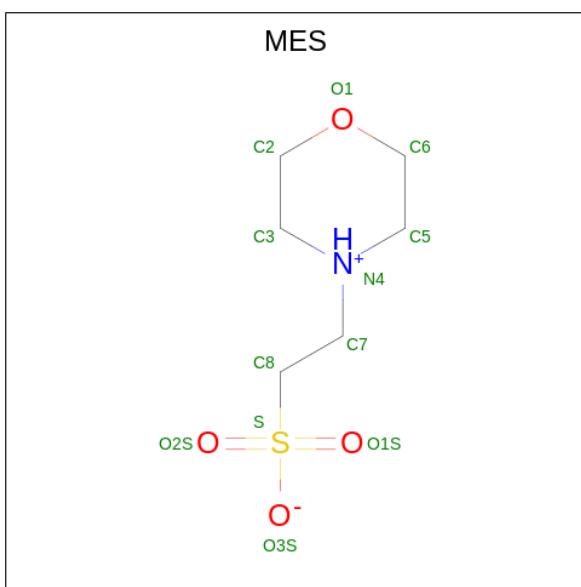
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



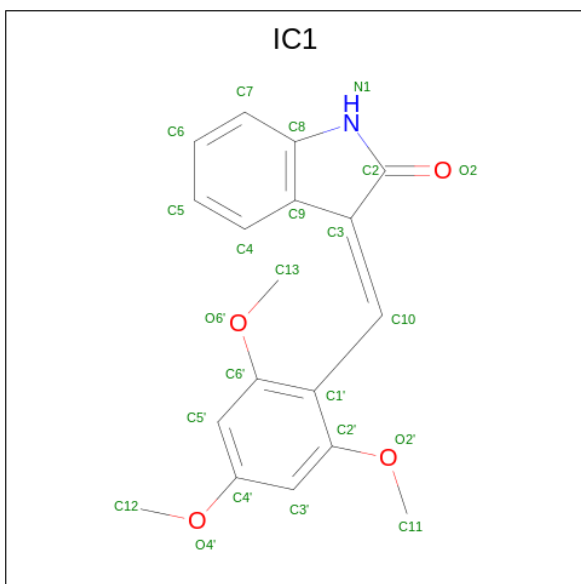
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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 3-[(2,4,6-TRIMETHOXY-PHENYL)-METHYLENE]-INDOLIN-2-ONE (three-letter code: IC1) (formula: C₁₈H₁₇NO₄) (labeled as "Ligand of Interest" by depositor).



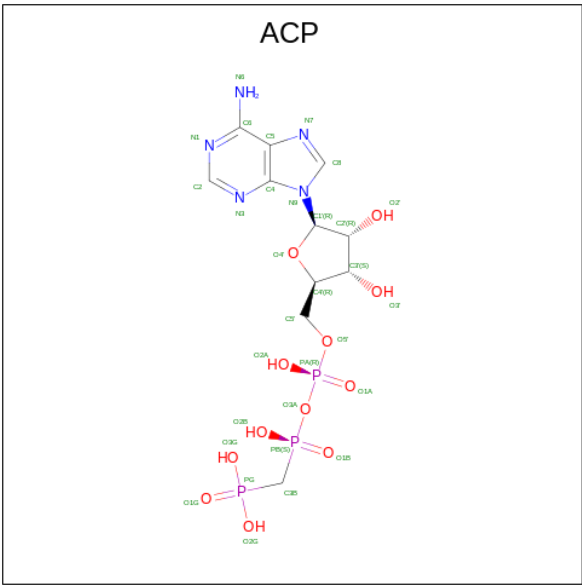
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			23	18	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			23	18	1	4		

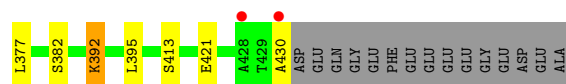
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



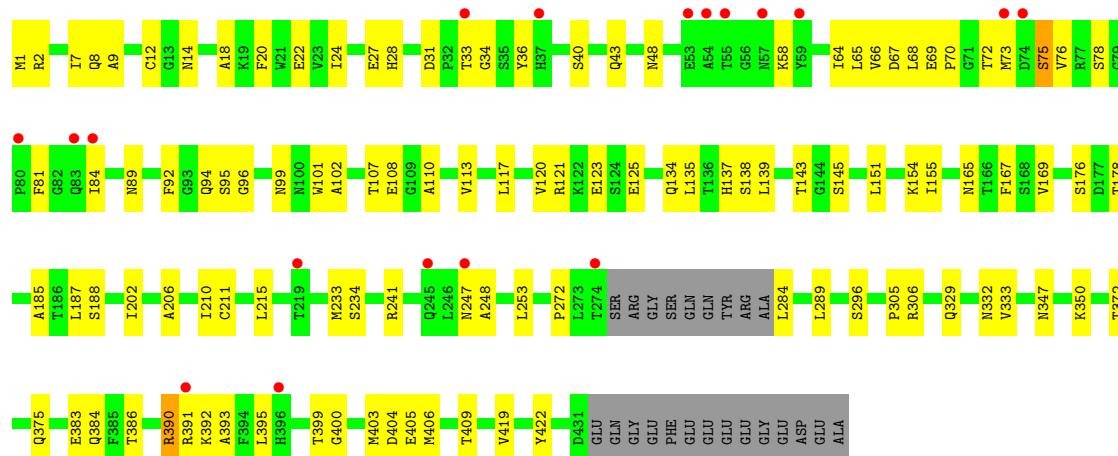
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 1: Tubulin alpha-1B chain

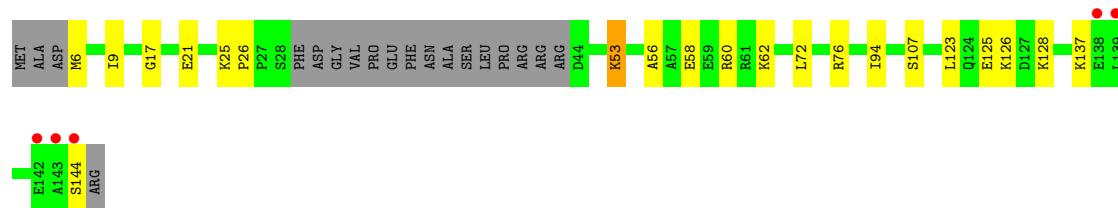




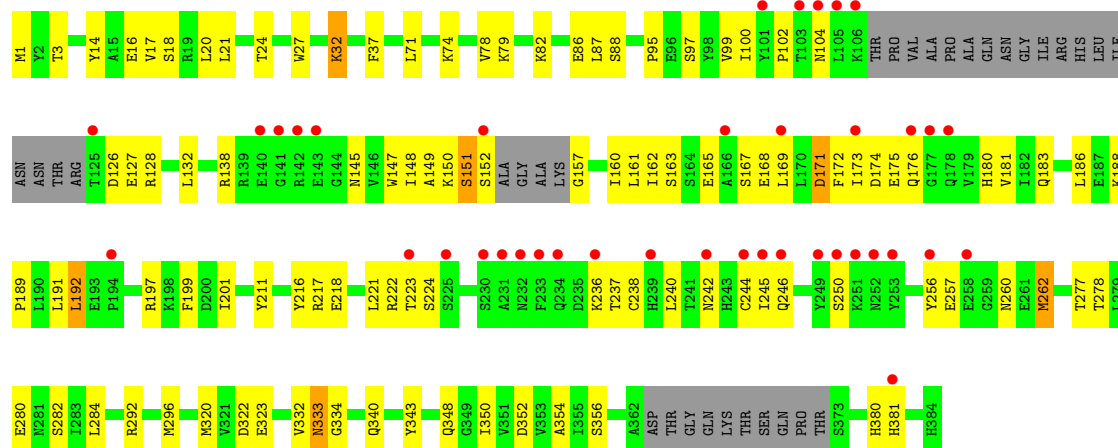
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.12Å 157.68Å 182.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 2.85 49.87 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.87-2.85) 99.0 (49.87-2.84)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.185 , 0.233 0.186 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.6	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	0.94	EDS
Total number of atoms	17750	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ACP, CA, GDP, MES, MG, IC1

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	0.49	0/3554	0.65	1/4824 (0.0%)
1	C	0.55	2/3547 (0.1%)	0.66	1/4815 (0.0%)
2	B	0.50	0/3470	0.63	0/4700
2	D	0.44	0/3396	0.61	0/4600
3	E	0.58	0/1047	0.68	0/1390
4	F	0.44	0/2942	0.63	0/3979
All	All	0.49	2/17956 (0.0%)	0.64	2/24308 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	420	GLU	CD-OE2	5.24	1.31	1.25
1	C	295	CYS	CB-SG	-5.16	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	98	ASP	CB-CG-OD1	5.29	123.06	118.30

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	3458	0	3379	46	0
1	C	3454	0	3370	43	0
2	B	3389	0	3278	44	0
2	D	3318	0	3193	76	0
3	E	1032	0	1047	14	0
4	F	2869	0	2803	75	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	24	0	24	3	0
10	B	23	0	17	2	0
10	D	23	0	17	2	0
11	F	31	0	13	1	0
All	All	17750	0	17189	289	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 (289) 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:391:ARG:NH1	2:D:393:ALA:HB2	2.00	0.77
2:D:64:ILE:HD13	2:D:120:VAL:HG12	1.66	0.77
4:F:242:ASN:HB2	4:F:245:ILE:HD12	1.68	0.76
1:C:132:LEU:O	1:C:164:LYS:NZ	2.20	0.74
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.21	0.74
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.21	0.72
2:B:284:LEU:HD23	2:B:289:LEU:HD23	1.70	0.72
2:D:296:SER:HB3	2:D:305:PRO:HD2	1.72	0.72
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.71	0.71
2:D:75:SER:O	2:D:78:SER:HB3	1.91	0.70
2:B:137:HIS:NE2	2:B:168:SER:HB3	2.07	0.70
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.30	0.70
3:E:25:LYS:HD3	3:E:26:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.74	0.69
2:D:94:GLN:HE21	2:D:95:SER:HB3	1.58	0.69
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.58	0.69
1:A:72:PRO:HG2	2:B:2:ARG:HH22	1.58	0.68
2:B:251:ARG:NH1	9:B:504:MES:O2S	2.25	0.68
2:D:134:GLN:HA	2:D:165:ASN:O	1.94	0.68
4:F:176:GLN:HA	4:F:176:GLN:NE2	2.09	0.68
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.29	0.67
4:F:167:SER:O	4:F:171:ASP:HB2	1.96	0.65
4:F:157:GLY:HA2	4:F:245:ILE:HD11	1.78	0.65
4:F:277:THR:HG22	4:F:278:THR:H	1.62	0.65
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.32	0.64
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.79	0.64
2:B:251:ARG:O	2:B:255:VAL:HG23	1.98	0.63
1:A:72:PRO:HB3	1:A:94:THR:HG21	1.78	0.63
1:A:94:THR:HG22	1:A:95:GLY:O	1.99	0.62
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.34	0.62
2:B:262:ARG:NE	2:B:421:GLU:OE2	2.31	0.62
2:D:248:ALA:HA	10:D:503:IC1:O2	1.99	0.62
2:D:390:ARG:HG3	2:D:391:ARG:N	2.14	0.62
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.81	0.62
4:F:172:PHE:O	4:F:175:GLU:HB2	2.01	0.61
4:F:186:LEU:HD23	4:F:320[B]:MET:HE1	1.82	0.61
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.40	0.61
4:F:74:LYS:O	4:F:78:VAL:HG23	2.00	0.61
4:F:236:LYS:HB2	4:F:240:LEU:HG	1.82	0.61
2:B:272:PRO:HB3	2:B:284:LEU:HD22	1.82	0.60
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.36	0.60
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.32	0.60
2:D:70:PRO:HD3	2:D:94:GLN:HA	1.84	0.60
2:B:134:GLN:HA	2:B:165:ASN:O	2.02	0.59
4:F:150:LYS:CG	4:F:160:ILE:HD13	2.32	0.59
4:F:126:ASP:OD1	4:F:127:GLU:N	2.35	0.59
2:B:40:SER:OG	2:B:42:LEU:HB2	2.03	0.59
4:F:148:ILE:HD12	4:F:162:ILE:HG12	1.85	0.58
2:B:344:TRP:HB3	2:B:430:ALA:HB2	1.85	0.58
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.69	0.58
1:C:255:PHE:CZ	1:C:318:LEU:CD2	2.87	0.58
4:F:149:ALA:CB	4:F:169:LEU:HD22	2.33	0.58
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.04	0.58
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ALA:HB1	10:B:507:IC1:H101	1.86	0.57
2:D:391:ARG:O	2:D:392:LYS:HB2	2.04	0.57
2:D:206:ALA:O	2:D:210:ILE:HG13	2.04	0.57
2:D:386:THR:O	2:D:390:ARG:HG2	2.05	0.57
4:F:16:GLU:O	4:F:20:LEU:HD12	2.04	0.57
4:F:151:SER:OG	4:F:152:SER:N	2.38	0.57
4:F:242:ASN:HD21	11:F:401:ACP:H5'2	1.69	0.57
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.41	0.56
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.40	0.56
2:D:36:TYR:OH	2:D:40:SER:O	2.22	0.56
4:F:78:VAL:HG12	4:F:82:LYS:HD2	1.87	0.56
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.88	0.56
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.40	0.56
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.86	0.56
2:D:40:SER:HB3	2:D:43:GLN:HG3	1.86	0.56
1:A:68:VAL:HG11	1:A:149:PHE:HE2	1.71	0.56
4:F:128:ARG:O	4:F:132:LEU:HD12	2.06	0.56
2:D:73:MET:HG3	2:D:92:PHE:CD2	2.42	0.55
4:F:244:CYS:SG	4:F:245:ILE:N	2.79	0.55
2:B:1:MET:SD	2:B:131:GLN:HB3	2.46	0.55
2:D:143:THR:N	8:D:501:GDP:O3B	2.38	0.55
4:F:157:GLY:CA	4:F:245:ILE:HD11	2.37	0.55
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.88	0.54
1:C:71:GLU:OE1	2:D:247:ASN:ND2	2.37	0.54
2:D:139:LEU:HB3	2:D:185:ALA:HA	1.89	0.54
4:F:145:ASN:ND2	4:F:147:TRP:HE1	2.05	0.54
4:F:237:THR:HG21	4:F:250:SER:HB2	1.89	0.54
4:F:188:LYS:HD2	4:F:323:GLU:OE2	2.07	0.54
4:F:148:ILE:CG2	4:F:183:GLN:HB3	2.37	0.54
4:F:333:ASN:HD22	4:F:334:GLY:N	2.05	0.54
2:B:30:ILE:HD11	2:B:47:ILE:HD11	1.89	0.54
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.90	0.54
4:F:145:ASN:CG	4:F:147:TRP:HE1	2.11	0.54
4:F:150:LYS:HG2	4:F:160:ILE:HD13	1.89	0.54
1:C:209:ILE:HD11	1:C:302[A]:MET:HG3	1.89	0.53
2:D:391:ARG:NH1	2:D:393:ALA:CB	2.71	0.53
3:E:72:LEU:O	3:E:76:ARG:HG2	2.08	0.53
1:C:211[A]:ASP:OD1	1:C:214:ARG:NH1	2.42	0.52
2:D:139:LEU:HG	2:D:188:SER:HB2	1.90	0.52
2:D:383:GLU:O	2:D:386:THR:HG22	2.09	0.52
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.75	0.52
4:F:14:TYR:HA	4:F:17:VAL:HB	1.90	0.52
2:D:390:ARG:HG3	2:D:391:ARG:H	1.75	0.52
4:F:99:VAL:O	4:F:100:ILE:HD13	2.09	0.52
1:A:141:PHE:HB3	1:A:187:SER:OG	2.10	0.51
1:C:230:LEU:O	1:C:234:ILE:HD12	2.09	0.51
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.45	0.51
1:C:186:ASN:O	1:C:190:THR:HG22	2.11	0.51
4:F:149:ALA:HB2	4:F:169:LEU:HD22	1.92	0.51
1:A:248:LEU:HD21	1:A:316[B]:CYS:SG	2.51	0.51
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.76	0.51
2:D:69:GLU:HG2	2:D:96:GLY:HA2	1.92	0.51
2:B:117:LEU:HD11	2:B:154:LYS:HD3	1.93	0.50
4:F:74:LYS:HD2	4:F:151:SER:O	2.11	0.50
1:C:255:PHE:CE2	1:C:318:LEU:CD2	2.95	0.50
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.92	0.50
4:F:256:TYR:HB2	4:F:257:GLU:OE2	2.11	0.50
2:B:392:LYS:O	2:B:395:LEU:HB2	2.10	0.50
2:D:8:GLN:NE2	2:D:65:LEU:HD23	2.26	0.50
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.94	0.50
2:B:45:GLU:HB3	2:B:243:PRO:HG3	1.94	0.50
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.77	0.50
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.26	0.50
2:D:107:THR:OG1	2:D:108:GLU:N	2.44	0.50
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.94	0.50
1:C:97:GLU:OE2	2:D:1:MET:HG3	2.11	0.49
4:F:3:THR:OG1	4:F:37:PHE:HA	2.12	0.49
4:F:32:LYS:HE2	4:F:32:LYS:H	1.77	0.49
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.94	0.49
1:A:107:HIS:NE2	3:E:53:LYS:HE2	2.28	0.49
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.95	0.49
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.95	0.49
2:D:121:ARG:O	2:D:125:GLU:HG2	2.12	0.49
2:D:391:ARG:HH12	2:D:393:ALA:CB	2.24	0.49
4:F:150:LYS:HG3	4:F:160:ILE:CD1	2.43	0.48
1:C:344:VAL:HG23	1:C:347:CYS:HB2	1.94	0.48
2:D:95:SER:OG	2:D:108:GLU:OE2	2.31	0.48
4:F:102:PRO:HA	4:F:174:ASP:OD1	2.12	0.48
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.44	0.48
4:F:150:LYS:HG3	4:F:160:ILE:HD13	1.94	0.48
4:F:189:PRO:HA	4:F:322:ASP:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ALA:O	1:C:337:THR:HG23	2.13	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.22	0.48
4:F:104:ASN:OD1	4:F:104:ASN:N	2.46	0.48
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.96	0.48
2:D:372:THR:HA	2:D:422:TYR:CD1	2.49	0.48
1:A:156:ARG:HA	1:A:159:VAL:HG22	1.96	0.47
4:F:176:GLN:NE2	4:F:176:GLN:CA	2.72	0.47
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.44	0.47
1:A:154:MET:HG3	1:A:194:THR:HG23	1.97	0.47
2:D:73:MET:CG	2:D:92:PHE:HB3	2.44	0.47
2:D:110:ALA:O	2:D:113:VAL:HG12	2.14	0.47
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.48	0.47
1:A:72:PRO:HG2	2:B:2:ARG:NH2	2.28	0.47
2:B:1:MET:N	2:B:129:CYS:SG	2.76	0.47
2:B:214:THR:HG22	2:B:215:LEU:HD23	1.96	0.47
2:D:400:GLY:O	3:E:137:LYS:HG3	2.14	0.47
2:B:36:TYR:CE1	2:B:44:LEU:HD21	2.50	0.47
2:D:72:THR:O	2:D:76:VAL:HG23	2.15	0.47
4:F:87:LEU:O	4:F:88:SER:OG	2.31	0.47
1:C:271:THR:HG21	1:C:295:CYS:O	2.14	0.47
4:F:223:THR:HG21	4:F:257:GLU:OE1	2.15	0.47
2:B:16[A]:ILE:HD11	2:B:136:THR:HB	1.97	0.46
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.50	0.46
4:F:21:LEU:HD22	4:F:27:TRP:CD1	2.50	0.46
4:F:82:LYS:NZ	4:F:97:SER:O	2.41	0.46
4:F:278:THR:O	4:F:282:SER:OG	2.25	0.46
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.46
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.96	0.46
1:A:46:ASP:N	1:A:46:ASP:OD1	2.48	0.46
1:A:283:HIS:HD2	1:A:285:GLN:OE1	1.99	0.46
1:C:317:LEU:HD23	1:C:377:MET:HB2	1.98	0.46
2:D:101:TRP:HD1	2:D:145[A]:SER:OG	1.98	0.46
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.97	0.46
1:C:255:PHE:CE2	1:C:318:LEU:HD21	2.50	0.46
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.46
3:E:25:LYS:HE2	3:E:25:LYS:HA	1.98	0.46
2:D:68:LEU:HA	2:D:68:LEU:HD23	1.73	0.46
2:D:94:GLN:NE2	2:D:95:SER:HB3	2.28	0.46
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.46
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ILE:HG21	2:B:229:VAL:HG22	1.98	0.46
1:A:100:ALA:HA	2:B:252:LYS:HG2	1.98	0.45
1:C:204:VAL:HG13	1:C:302[B]:MET:HE3	1.98	0.45
1:C:140:SER:HA	1:C:171:ILE:HB	1.98	0.45
4:F:149:ALA:HB3	4:F:169:LEU:HD22	1.97	0.45
2:B:2:ARG:O	2:B:49:VAL:HG13	2.16	0.45
2:D:67:ASP:HB3	2:D:73:MET:HE2	1.99	0.45
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.99	0.45
4:F:71:LEU:HD23	4:F:332:VAL:HG11	1.97	0.45
2:B:2:ARG:O	2:B:131:GLN:NE2	2.42	0.45
2:B:395:LEU:HD12	2:B:395:LEU:HA	1.80	0.45
4:F:350:ILE:O	4:F:354:ALA:HB3	2.16	0.45
2:D:101:TRP:CE3	2:D:187:LEU:HD13	2.52	0.45
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.32	0.45
1:A:298:PRO:HA	1:A:301:GLN:CD	2.36	0.45
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.99	0.44
4:F:237:THR:CG2	4:F:250:SER:HB2	2.48	0.44
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.99	0.44
2:D:18:ALA:O	2:D:22:GLU:HG3	2.18	0.44
2:D:347:ASN:O	2:D:350:LYS:HE2	2.18	0.44
4:F:292:ARG:NH2	4:F:380:HIS:HB3	2.33	0.44
1:C:292:THR:O	1:C:295:CYS:HB2	2.17	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.48	0.44
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.52	0.44
2:B:245:GLN:HG3	2:B:246:LEU:N	2.33	0.44
2:B:296:SER:HA	2:B:299:MET:HG3	1.99	0.43
2:D:253:LEU:HD13	10:D:503:IC1:C2'	2.48	0.43
4:F:86:GLU:OE1	4:F:86:GLU:N	2.39	0.43
2:D:7:ILE:O	2:D:135:LEU:HA	2.18	0.43
2:D:81:PHE:O	2:D:84:ILE:HG22	2.18	0.43
2:B:35:SER:OG	2:B:58:LYS:HE2	2.19	0.43
2:B:322:SER:HB3	2:B:325:GLU:HB2	2.00	0.43
1:A:116:ASP:OD1	1:A:156:ARG:NH2	2.47	0.43
1:C:255:PHE:CE2	1:C:318:LEU:HD22	2.53	0.43
2:D:406:MET:O	2:D:409:THR:HB	2.18	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.54	0.43
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.53	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.43
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.01	0.43
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.00	0.43
1:C:105:ARG:NH1	1:C:411:GLU:OE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:LEU:HD12	2:D:395:LEU:HA	1.74	0.43
4:F:173:ILE:O	4:F:176:GLN:O	2.37	0.43
2:D:33:THR:OG1	2:D:58:LYS:NZ	2.52	0.42
2:D:151:LEU:HD22	2:D:155:ILE:HD11	2.01	0.42
2:D:404:ASP:OD1	2:D:405:GLU:N	2.52	0.42
3:E:9:ILE:HG12	3:E:21:GLU:HB3	2.00	0.42
1:A:79:ARG:NH2	1:A:94:THR:OG1	2.52	0.42
1:A:71:GLU:HB3	1:A:98:ASP:HB3	2.01	0.42
2:B:156:ARG:HG3	9:B:504:MES:H51	2.00	0.42
2:B:315:ALA:HB3	2:B:351:THR:HG23	2.01	0.42
2:D:9:ALA:HA	2:D:66:VAL:O	2.19	0.42
2:D:12:CYS:HB3	2:D:138:SER:OG	2.20	0.42
1:C:225:THR:O	1:C:229:ARG:HG3	2.20	0.42
4:F:138:ARG:CB	4:F:145:ASN:HD22	2.32	0.42
1:A:209:ILE:HD11	1:A:302:MET:SD	2.59	0.42
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.55	0.42
2:B:273:LEU:HD11	2:B:298:ASN:HA	2.01	0.42
2:D:89:ASN:ND2	2:D:123:GLU:OE2	2.47	0.42
1:A:158:SER:OG	1:A:166:LYS:NZ	2.53	0.42
4:F:280:GLU:HA	4:F:284:LEU:CB	2.50	0.42
1:A:132:LEU:HD23	1:A:164:LYS:HZ1	1.85	0.42
1:A:132:LEU:HD23	1:A:164:LYS:NZ	2.35	0.42
1:C:12:ALA:O	1:C:16:ILE:HD12	2.20	0.42
2:D:117:LEU:HD23	2:D:117:LEU:HA	1.84	0.42
2:D:289:LEU:HD23	2:D:289:LEU:HA	1.92	0.42
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.02	0.42
1:C:48:SER:OG	1:C:245:ASP:OD2	2.37	0.42
2:D:27:GLU:OE1	2:D:234:SER:OG	2.37	0.42
1:A:355:ILE:O	3:E:17:GLY:HA3	2.20	0.41
2:D:67:ASP:CB	2:D:73:MET:CE	2.98	0.41
4:F:257:GLU:HG2	4:F:262:MET:HB2	2.02	0.41
10:B:507:IC1:H41	10:B:507:IC1:C6'	2.50	0.41
1:C:63:PRO:HD3	1:C:86:LEU:HG	2.01	0.41
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.36	0.41
2:D:102:ALA:HB2	2:D:403:MET:SD	2.60	0.41
4:F:217:ARG:HG3	4:F:218:GLU:N	2.35	0.41
1:A:249:ASN:OD1	1:A:258:ASN:ND2	2.46	0.41
2:D:399:THR:HG23	2:D:403:MET:O	2.21	0.41
3:E:6:MET:SD	3:E:6:MET:N	2.94	0.41
2:D:329:GLN:O	2:D:333:VAL:HG23	2.19	0.41
4:F:224:SER:HA	4:F:246:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:165:GLU:O	4:F:168:GLU:HB3	2.20	0.41
1:A:174:ALA:O	1:A:178:SER:HB2	2.21	0.41
2:B:227:HIS:CG	2:B:276:ARG:HG2	2.55	0.41
2:D:84:ILE:HD12	2:D:84:ILE:HA	1.75	0.41
1:A:188:ILE:HG22	1:A:421:ALA:HB1	2.03	0.41
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.56	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.56	0.41
2:D:28:HIS:NE2	2:D:241:ARG:HD2	2.36	0.41
2:D:31:ASP:OD1	2:D:34:GLY:N	2.54	0.41
2:D:391:ARG:HH11	2:D:393:ALA:HB2	1.81	0.41
4:F:169:LEU:O	4:F:172:PHE:N	2.54	0.41
4:F:197:ARG:HD2	4:F:224:SER:O	2.21	0.41
2:B:156:ARG:HG3	9:B:504:MES:C6	2.51	0.41
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.03	0.41
1:C:293[A]:ASN:CG	1:C:339:ARG:HH21	2.24	0.41
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.56	0.41
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.56	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.41
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.55	0.40
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.40
2:D:384:GLN:H	2:D:384:GLN:HG3	1.68	0.40
3:E:125:GLU:OE1	3:E:128:LYS:HD3	2.21	0.40
1:A:134:GLY:HA3	1:A:165:SER:O	2.22	0.40
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.56	0.40
1:C:344:VAL:CG2	1:C:347:CYS:HB2	2.52	0.40
3:E:123:LEU:O	3:E:126:LYS:HB2	2.21	0.40
2:B:284:LEU:HD12	2:B:284:LEU:HA	1.89	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.40
2:D:272:PRO:HB3	2:D:284:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/451 (98%)	432 (98%)	11 (2%)	0	100	100
1	C	443/451 (98%)	432 (98%)	11 (2%)	0	100	100
2	B	430/445 (97%)	417 (97%)	13 (3%)	0	100	100
2	D	419/445 (94%)	400 (96%)	19 (4%)	0	100	100
3	E	122/143 (85%)	120 (98%)	2 (2%)	0	100	100
4	F	346/384 (90%)	332 (96%)	14 (4%)	0	100	100
All	All	2203/2319 (95%)	2133 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	376/379 (99%)	374 (100%)	2 (0%)	88	94
1	C	375/379 (99%)	369 (98%)	6 (2%)	62	81
2	B	373/383 (97%)	361 (97%)	12 (3%)	39	63
2	D	365/383 (95%)	357 (98%)	8 (2%)	52	75
3	E	113/127 (89%)	110 (97%)	3 (3%)	44	69
4	F	313/342 (92%)	295 (94%)	18 (6%)	20	38
All	All	1915/1993 (96%)	1866 (97%)	49 (3%)	47	70

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LYS
1	A	221	ARG
2	B	2	ARG
2	B	35	SER

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Mol	Chain	Res	Type
2	B	137	HIS
2	B	145	SER
2	B	162	ARG
2	B	190	HIS
2	B	296	SER
2	B	323	MET
2	B	359	ARG
2	B	382	SER
2	B	392	LYS
2	B	413	SER
1	C	71	GLU
1	C	218	ASP
1	C	245	ASP
1	C	302[A]	MET
1	C	302[B]	MET
1	C	347	CYS
2	D	2	ARG
2	D	48	ASN
2	D	75	SER
2	D	137	HIS
2	D	176	SER
2	D	306	ARG
2	D	332	ASN
2	D	390	ARG
3	E	53	LYS
3	E	107	SER
3	E	144	SER
4	F	1	MET
4	F	18	SER
4	F	32	LYS
4	F	79	LYS
4	F	151	SER
4	F	161	LEU
4	F	163	SER
4	F	171	ASP
4	F	192	LEU
4	F	211	TYR
4	F	222	ARG
4	F	238	CYS
4	F	260	ASN
4	F	262	MET
4	F	296	MET

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Mol	Chain	Res	Type
4	F	333	ASN
4	F	356	SER
4	F	381	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	94	GLN
2	D	99	ASN
2	D	335	ASN
4	F	10	ASN
4	F	145	ASN
4	F	176	GLN
4	F	242	ASN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 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
10	IC1	D	503	-	25,25,25	2.64	6 (24%)	35,35,35	1.92	8 (22%)
5	GTP	A	501	6	26,34,34	1.16	1 (3%)	33,54,54	1.54	6 (18%)
5	GTP	C	501	6	26,34,34	1.26	3 (11%)	33,54,54	1.72	9 (27%)
9	MES	B	504	-	12,12,12	5.21	7 (58%)	14,16,16	2.56	5 (35%)
10	IC1	B	507	-	25,25,25	2.59	8 (32%)	35,35,35	1.88	10 (28%)
8	GDP	D	501	6	24,30,30	1.36	2 (8%)	31,47,47	2.02	8 (25%)
11	ACP	F	401	-	27,33,33	4.81	9 (33%)	32,52,52	2.02	4 (12%)
9	MES	B	505	-	12,12,12	4.66	7 (58%)	14,16,16	1.93	4 (28%)
8	GDP	B	501	6	24,30,30	1.56	5 (20%)	31,47,47	2.00	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	IC1	D	503	-	-	4/10/22/22	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
10	IC1	B	507	-	-	4/10/22/22	0/3/3/3
8	GDP	D	501	6	-	6/12/32/32	0/3/3/3
11	ACP	F	401	-	-	3/15/38/38	0/3/3/3
9	MES	B	505	-	-	1/6/14/14	0/1/1/1
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	C2'-C1'	-15.15	1.30	1.53
11	F	401	ACP	O4'-C1'	15.12	1.62	1.41
9	B	504	MES	C7-N4	-8.97	1.26	1.47
9	B	505	MES	C7-N4	-8.56	1.27	1.47
11	F	401	ACP	PB-O3A	8.33	1.67	1.58
9	B	504	MES	O1S-S	8.21	1.69	1.45
9	B	504	MES	C8-S	8.14	1.89	1.77
9	B	505	MES	O1S-S	7.40	1.66	1.45
9	B	505	MES	O2S-S	7.31	1.66	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	O2S-S	7.08	1.65	1.45
10	D	503	IC1	C8-N1	6.71	1.51	1.38
10	B	507	IC1	C8-N1	6.65	1.50	1.38
10	B	507	IC1	C2-N1	6.27	1.42	1.36
10	D	503	IC1	C2-N1	6.15	1.42	1.36
11	F	401	ACP	O4'-C4'	-6.14	1.31	1.45
9	B	504	MES	O3S-S	5.96	1.68	1.47
10	D	503	IC1	C1'-C10	5.62	1.59	1.47
9	B	505	MES	O3S-S	5.59	1.67	1.47
10	B	507	IC1	C1'-C10	5.26	1.58	1.47
9	B	505	MES	C8-S	4.84	1.84	1.77
8	D	501	GDP	C6-C5	4.36	1.48	1.41
10	D	503	IC1	C9-C3	4.21	1.53	1.45
8	B	501	GDP	C5-C4	3.84	1.51	1.40
8	B	501	GDP	C6-C5	3.80	1.47	1.41
10	B	507	IC1	C9-C3	3.68	1.52	1.45
9	B	504	MES	C5-N4	-3.65	1.36	1.46
10	D	503	IC1	O2-C2	-3.62	1.16	1.23
10	B	507	IC1	O2-C2	-3.57	1.16	1.23
9	B	505	MES	C3-N4	-3.41	1.37	1.46
9	B	504	MES	C3-N4	-3.35	1.37	1.46
5	A	501	GTP	C6-N1	3.30	1.38	1.33
9	B	505	MES	C5-N4	-3.27	1.37	1.46
11	F	401	ACP	C6-N6	3.24	1.45	1.34
5	C	501	GTP	C6-N1	3.22	1.38	1.33
10	B	507	IC1	O2'-C2'	3.15	1.42	1.37
8	B	501	GDP	C2'-C1'	-3.05	1.49	1.53
10	D	503	IC1	O2'-C2'	2.97	1.41	1.37
8	D	501	GDP	C5-C4	2.89	1.48	1.40
11	F	401	ACP	O3'-C3'	-2.84	1.36	1.43
11	F	401	ACP	O2'-C2'	2.74	1.49	1.43
11	F	401	ACP	C5-C4	-2.60	1.34	1.40
5	C	501	GTP	C2-N1	2.49	1.39	1.35
11	F	401	ACP	C2-N3	2.41	1.36	1.32
8	B	501	GDP	O4'-C1'	2.36	1.44	1.41
5	C	501	GTP	C6-C5	-2.23	1.37	1.41
10	B	507	IC1	C1'-C2'	-2.21	1.37	1.41
10	B	507	IC1	O6'-C6'	2.17	1.40	1.37
8	B	501	GDP	O6-C6	2.12	1.29	1.24

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C5-C6-N6	7.15	131.22	120.35
11	F	401	ACP	N3-C2-N1	-5.49	120.10	128.68
10	D	503	IC1	C11-O2'-C2'	-5.09	109.85	117.53
8	D	501	GDP	C6-N1-C2	5.03	123.92	115.93
9	B	504	MES	O1S-S-C8	4.68	112.55	106.92
8	B	501	GDP	C6-C5-C4	-4.60	116.41	120.80
10	B	507	IC1	C8-N1-C2	-4.52	108.54	111.38
8	B	501	GDP	C2-N3-C4	4.52	120.52	115.36
8	B	501	GDP	C6-N1-C2	4.50	123.07	115.93
11	F	401	ACP	N6-C6-N1	-4.48	109.28	118.57
8	D	501	GDP	C5-C6-N1	-4.41	117.39	123.43
8	D	501	GDP	C6-C5-C4	-4.39	116.61	120.80
9	B	504	MES	C2-C3-N4	4.37	116.73	110.10
10	D	503	IC1	C8-N1-C2	-4.35	108.65	111.38
8	B	501	GDP	C5-C6-N1	-4.28	117.58	123.43
5	C	501	GTP	N3-C2-N1	-4.13	121.72	127.22
10	B	507	IC1	O2-C2-C3	-3.96	122.52	127.71
5	C	501	GTP	O3'-C3'-C4'	-3.79	100.09	111.05
5	A	501	GTP	N3-C2-N1	-3.77	122.19	127.22
8	D	501	GDP	N3-C2-N1	-3.70	122.28	127.22
9	B	504	MES	O2S-S-C8	3.67	111.34	106.92
10	D	503	IC1	O2-C2-C3	-3.67	122.89	127.71
9	B	505	MES	C6-C5-N4	3.55	115.49	110.10
9	B	504	MES	C5-N4-C3	3.54	116.80	108.83
5	C	501	GTP	C5-C6-N1	-3.54	118.59	123.43
5	A	501	GTP	C2-N3-C4	3.53	119.39	115.36
10	D	503	IC1	C3-C2-N1	3.53	108.86	106.88
8	D	501	GDP	C2-N3-C4	3.46	119.30	115.36
9	B	504	MES	C7-N4-C3	-3.44	102.43	111.23
10	D	503	IC1	C13-O6'-C6'	-3.38	112.42	117.53
5	A	501	GTP	C5-C6-N1	-3.29	118.94	123.43
9	B	505	MES	C5-N4-C3	3.18	115.99	108.83
8	B	501	GDP	N3-C2-N1	-3.15	123.02	127.22
5	C	501	GTP	C2-N3-C4	3.13	118.93	115.36
5	C	501	GTP	PB-O3B-PG	-3.10	122.20	132.83
10	B	507	IC1	C3-C2-N1	3.08	108.61	106.88
10	B	507	IC1	O6'-C6'-C1'	3.03	121.13	115.26
8	B	501	GDP	C4-C5-N7	-3.03	106.24	109.40
10	D	503	IC1	O2'-C2'-C3'	-3.03	118.91	124.12
9	B	505	MES	O2S-S-C8	3.00	110.52	106.92
8	D	501	GDP	C4-C5-N7	-2.98	106.29	109.40
10	B	507	IC1	C13-O6'-C6'	-2.91	113.14	117.53
9	B	505	MES	C2-C3-N4	2.91	114.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C4-C5-N7	-2.87	106.41	109.40
11	F	401	ACP	C3'-C2'-C1'	2.81	105.21	100.98
10	B	507	IC1	O6'-C6'-C5'	-2.80	119.30	124.12
10	B	507	IC1	C11-O2'-C2'	-2.70	113.46	117.53
8	B	501	GDP	C1'-N9-C4	-2.66	121.97	126.64
10	B	507	IC1	C8-C9-C3	2.61	108.35	106.64
5	A	501	GTP	PB-O3B-PG	-2.57	124.02	132.83
10	B	507	IC1	C6'-C1'-C2'	2.54	120.78	117.37
8	B	501	GDP	PA-O3A-PB	-2.52	124.16	132.83
5	C	501	GTP	O4'-C1'-C2'	-2.51	103.25	106.93
8	D	501	GDP	C1'-N9-C4	-2.43	122.38	126.64
10	B	507	IC1	C7-C8-C9	-2.31	119.88	122.19
5	C	501	GTP	C4-C5-N7	-2.21	107.10	109.40
8	D	501	GDP	C2'-C3'-C4'	2.21	106.93	102.64
10	D	503	IC1	O6'-C6'-C1'	2.20	119.51	115.26
5	C	501	GTP	C6-N1-C2	2.18	119.39	115.93
10	D	503	IC1	O2'-C2'-C1'	2.13	119.38	115.26
5	C	501	GTP	N2-C2-N1	2.07	120.46	117.25
5	A	501	GTP	C1'-N9-C4	-2.01	123.11	126.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	PA-O3A-PB-O3B
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
10	D	503	IC1	C1'-C2'-O2'-C11
10	D	503	IC1	C3'-C2'-O2'-C11
10	B	507	IC1	C3'-C4'-O4'-C12
10	B	507	IC1	C5'-C4'-O4'-C12
9	B	504	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
9	B	504	MES	C8-C7-N4-C3
9	B	505	MES	C8-C7-N4-C5
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
10	B	507	IC1	C2'-C1'-C10-C3
10	B	507	IC1	C6'-C1'-C10-C3
10	D	503	IC1	C2'-C1'-C10-C3
9	B	504	MES	N4-C7-C8-S
10	D	503	IC1	C3'-C4'-O4'-C12

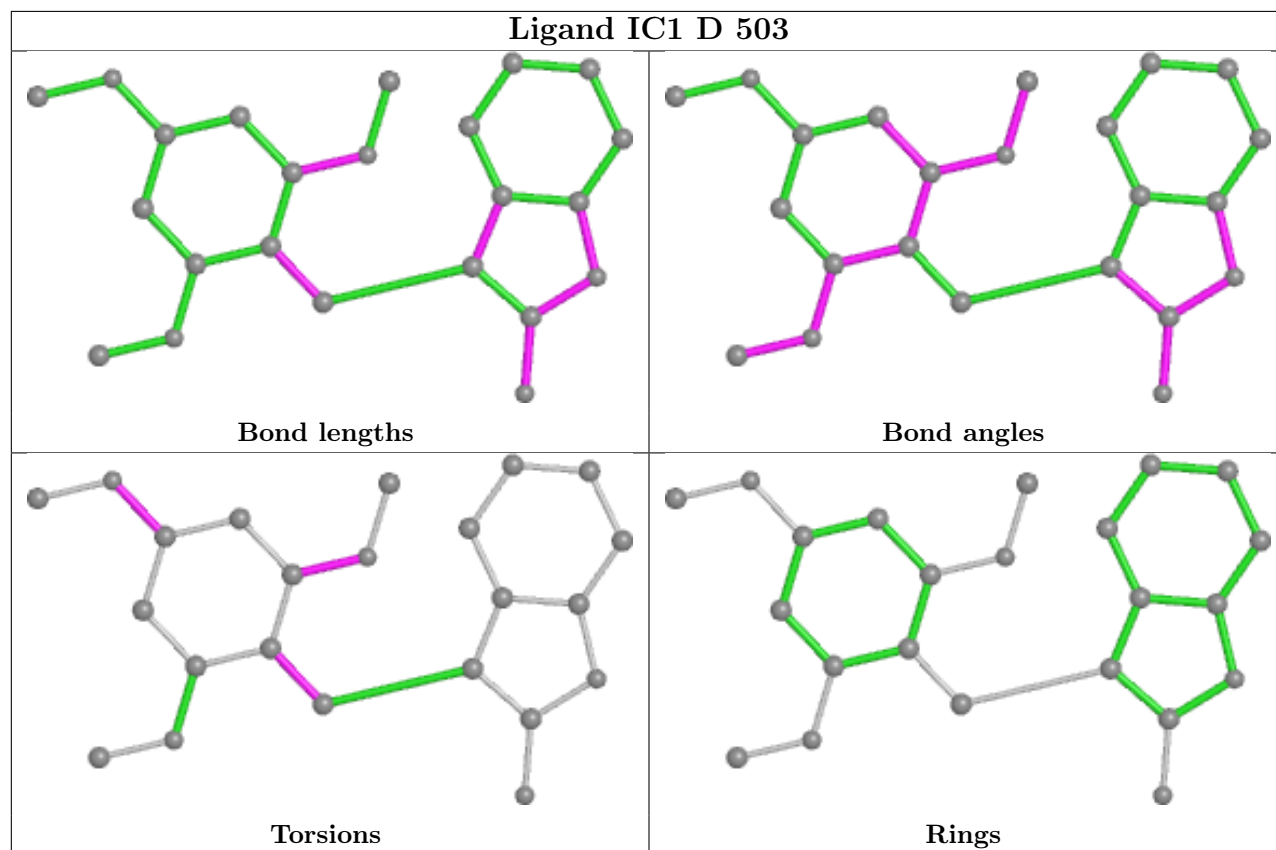
There are no ring outliers.

6 monomers are involved in 11 short contacts:

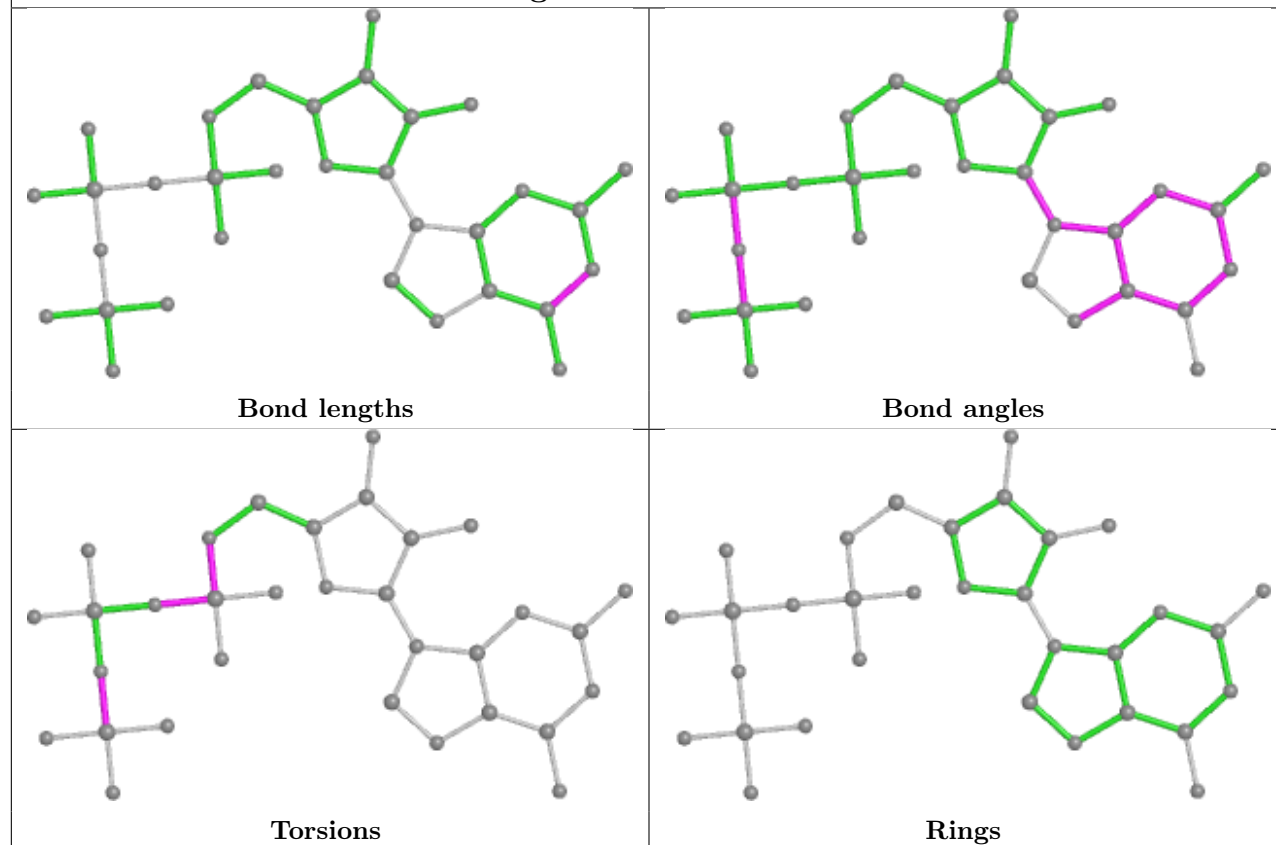
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	IC1	2	0
9	B	504	MES	3	0
10	B	507	IC1	2	0
8	D	501	GDP	2	0
11	F	401	ACP	1	0
8	B	501	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

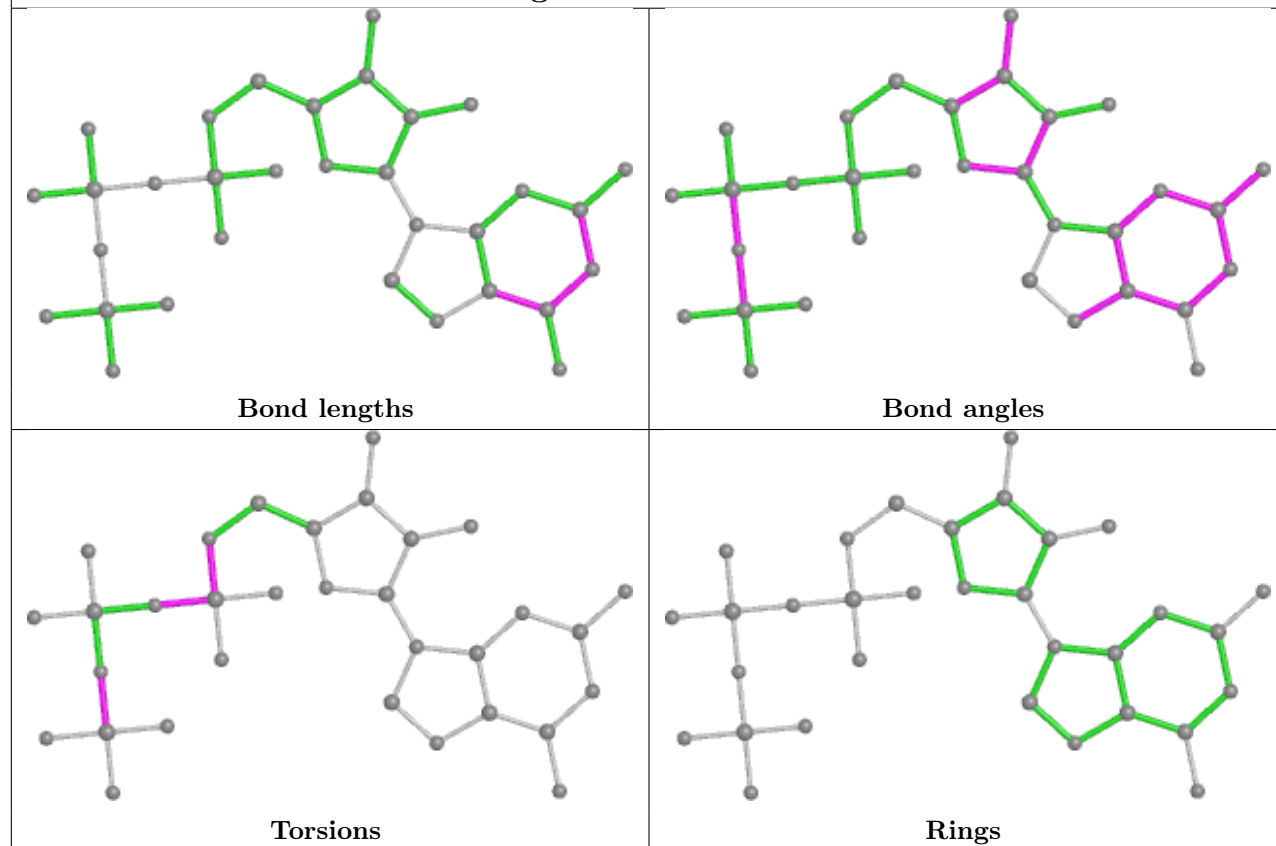
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

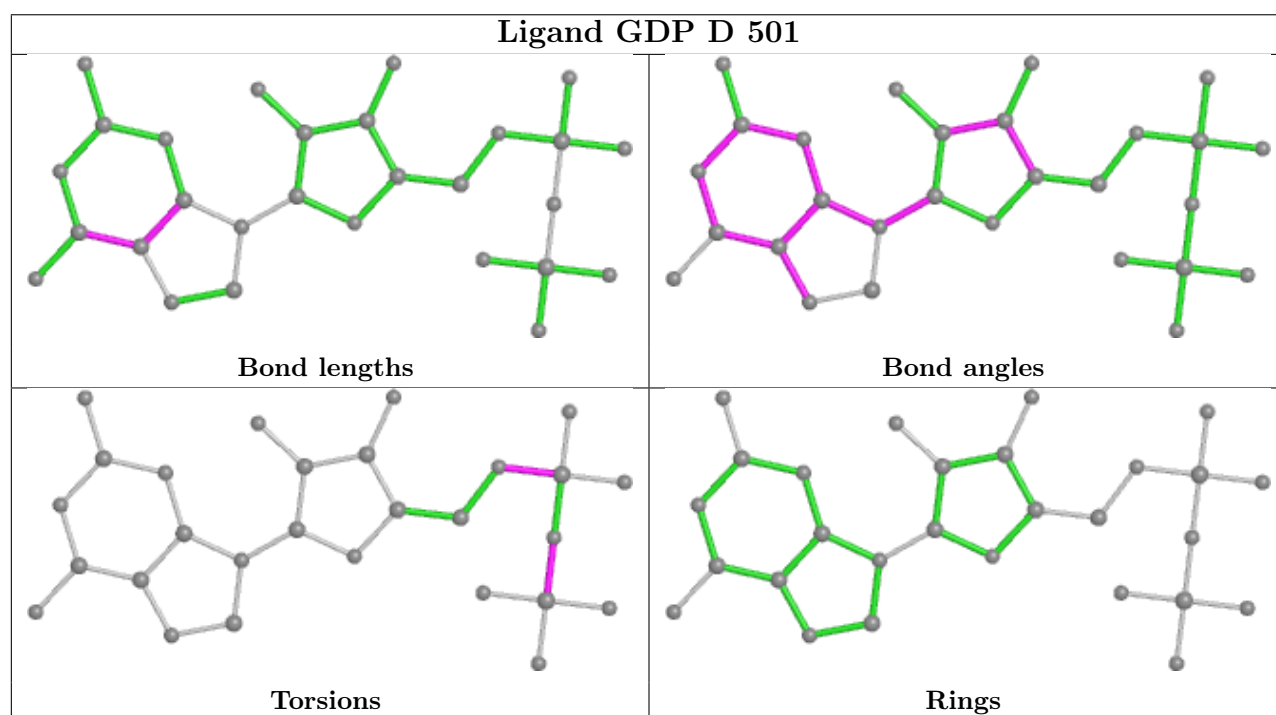
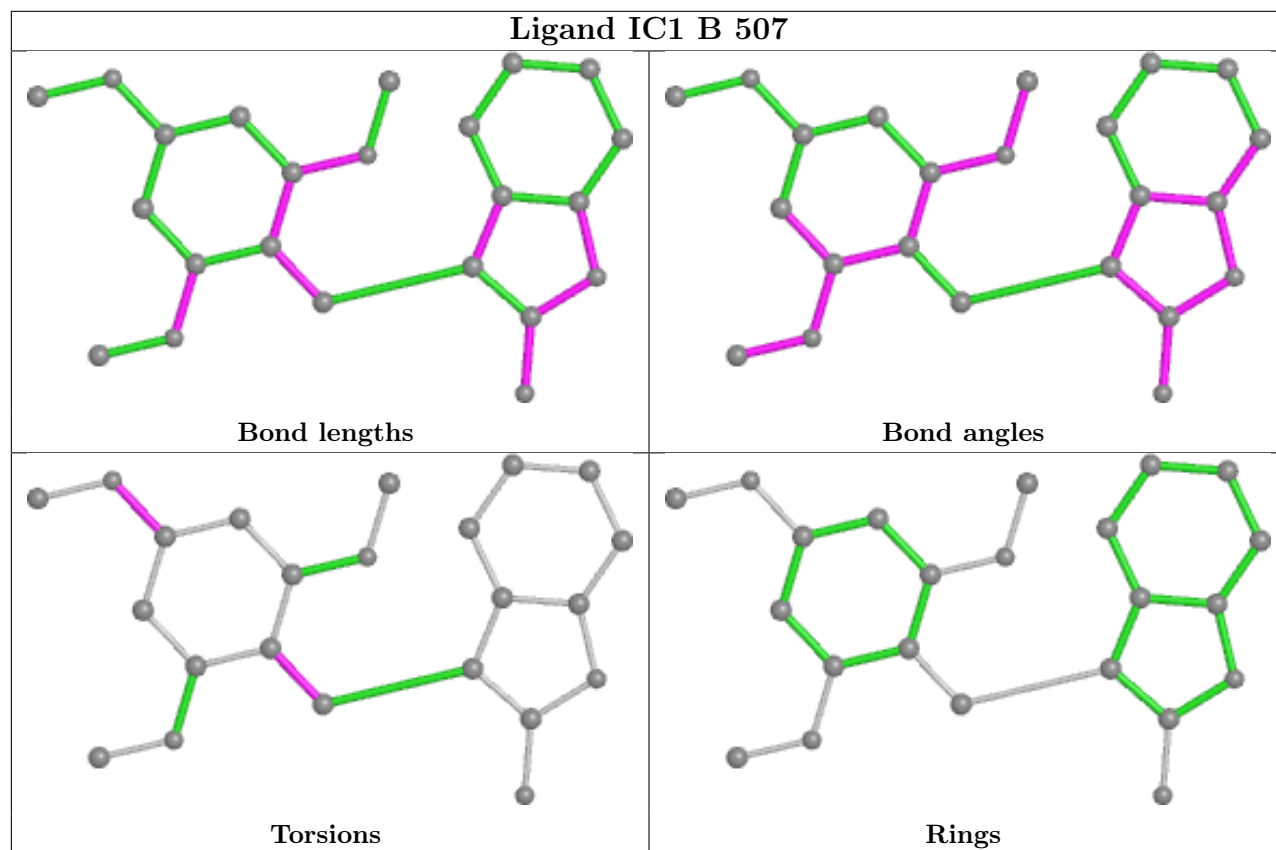


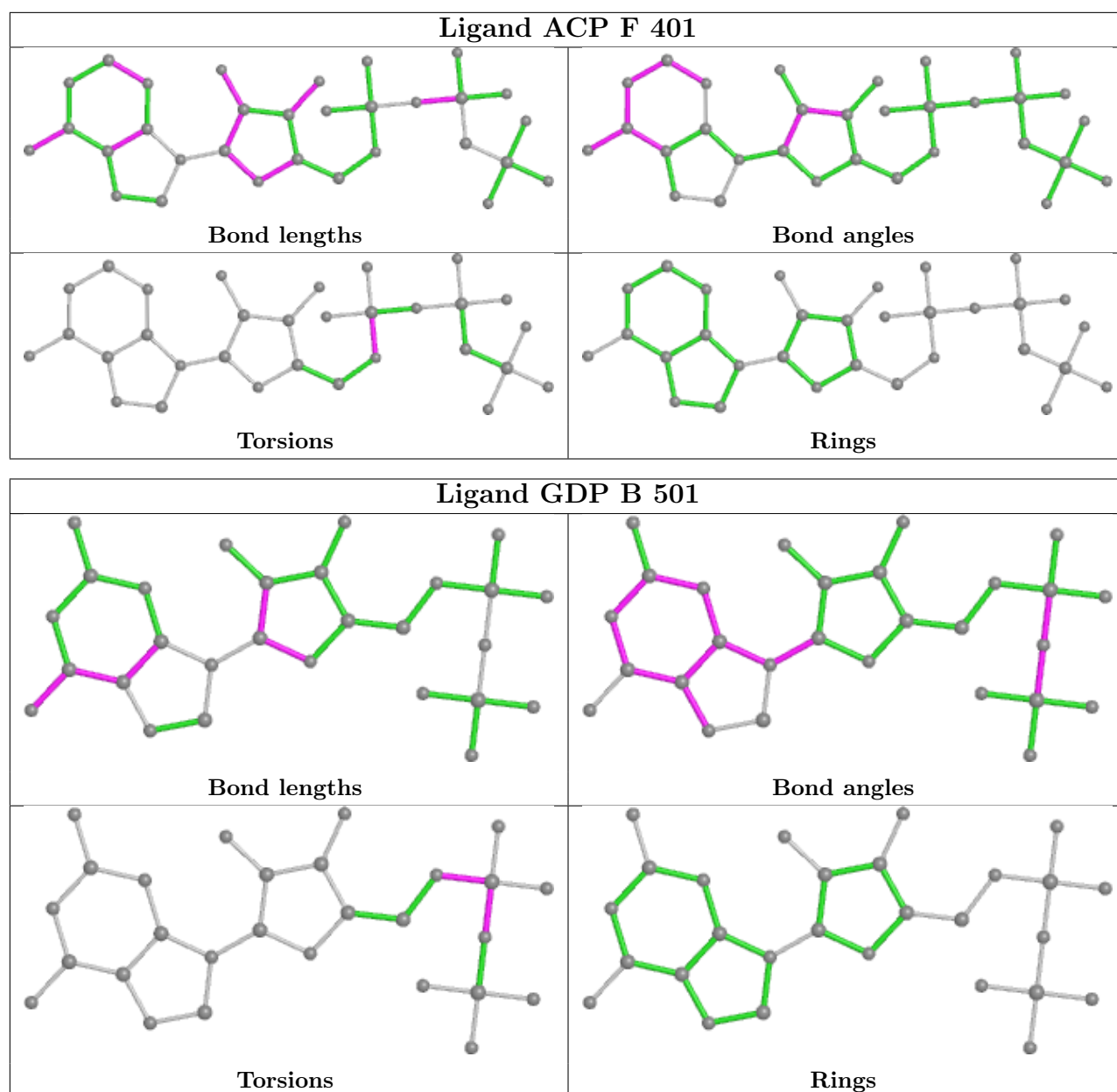
Ligand GTP A 501



Ligand GTP C 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	439/451 (97%)	-0.34	2 (0%)	91 89	24, 41, 66, 100	0
1	C	440/451 (97%)	-0.55	2 (0%)	91 89	14, 31, 55, 72	1 (0%)
2	B	430/445 (96%)	-0.32	4 (0%)	84 83	19, 39, 71, 112	0
2	D	422/445 (94%)	0.02	18 (4%)	35 27	30, 59, 86, 107	4 (0%)
3	E	124/143 (86%)	-0.04	5 (4%)	38 30	24, 54, 87, 104	0
4	F	352/384 (91%)	0.41	39 (11%)	5 3	30, 67, 107, 116	0
All	All	2207/2319 (95%)	-0.17	70 (3%)	47 41	14, 47, 91, 116	5 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	5.4
1	A	439	SER	5.2
4	F	232	ASN	4.5
4	F	249	TYR	4.5
4	F	233	PHE	4.4
4	F	225	SER	4.4
4	F	231	ALA	4.4
4	F	105	LEU	4.3
2	D	247	ASN	4.3
4	F	173	ILE	4.2
2	B	279	GLN	3.9
4	F	140	GLU	3.8
4	F	152	SER	3.7
4	F	177	GLY	3.7
3	E	144	SER	3.6
4	F	239	HIS	3.4
4	F	250	SER	3.3
2	D	219	THR	3.2
2	D	55	THR	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	246	GLN	3.1
4	F	106	LYS	3.1
4	F	252	ASN	3.0
4	F	245	ILE	3.0
2	D	245	GLN	2.9
3	E	142	GLU	2.9
4	F	244	CYS	2.8
4	F	381	HIS	2.8
4	F	258	GLU	2.7
4	F	143	GLU	2.7
2	D	54	ALA	2.7
4	F	253	TYR	2.7
1	C	340	SER	2.6
4	F	169	LEU	2.5
4	F	142	ARG	2.5
4	F	104	ASN	2.5
4	F	103	THR	2.4
4	F	101	TYR	2.4
4	F	176	GLN	2.4
4	F	178	GLN	2.4
4	F	234	GLN	2.4
2	D	80	PRO	2.3
2	B	37	HIS	2.3
4	F	141	GLY	2.3
1	A	281	ALA	2.3
4	F	230	SER	2.3
3	E	139	LEU	2.3
2	D	53	GLU	2.3
2	D	37	HIS	2.2
2	B	430	ALA	2.2
2	D	83	GLN	2.2
4	F	251	LYS	2.2
2	D	84	ILE	2.2
4	F	166	ALA	2.2
2	B	428	ALA	2.2
1	C	1	MET	2.2
4	F	256	TYR	2.2
2	D	57	ASN	2.1
2	D	391	ARG	2.1
4	F	242	ASN	2.1
2	D	274	THR	2.1
2	D	59	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	74	ASP	2.1
2	D	396	HIS	2.1
4	F	125	THR	2.1
2	D	73	MET	2.1
4	F	223	THR	2.1
4	F	194	PRO	2.0
3	E	138	GLU	2.0
2	D	33	THR	2.0
4	F	236	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

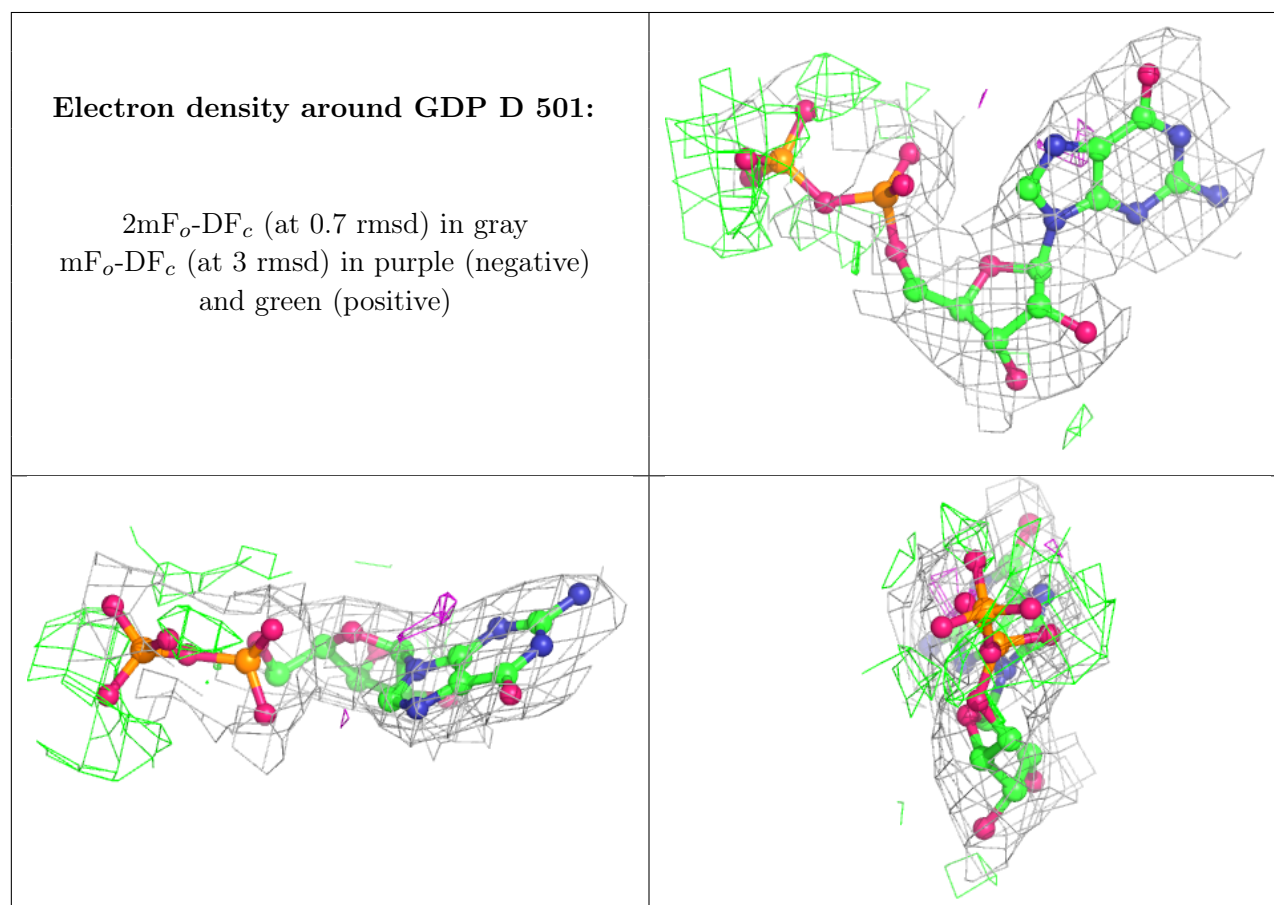
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.74	0.12	66,66,66,66	0
6	MG	B	506	1/1	0.84	0.49	82,82,82,82	0
7	CA	B	503	1/1	0.88	0.25	88,88,88,88	0
9	MES	B	504	12/12	0.88	0.27	35,51,78,82	0
8	GDP	D	501	28/28	0.91	0.16	47,56,78,80	0
7	CA	A	504	1/1	0.92	0.14	85,85,85,85	0
11	ACP	F	401	31/31	0.92	0.18	72,88,117,132	0
10	IC1	D	503	23/23	0.93	0.24	54,74,92,96	0
6	MG	B	502	1/1	0.95	0.36	43,43,43,43	0
9	MES	B	505	12/12	0.96	0.20	58,61,69,91	0
10	IC1	B	507	23/23	0.96	0.17	37,55,63,66	0
6	MG	C	502	1/1	0.97	0.39	35,35,35,35	0
7	CA	C	503	1/1	0.97	0.08	45,45,45,45	0
6	MG	A	502	1/1	0.98	0.45	29,29,29,29	0

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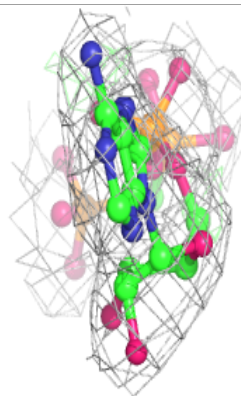
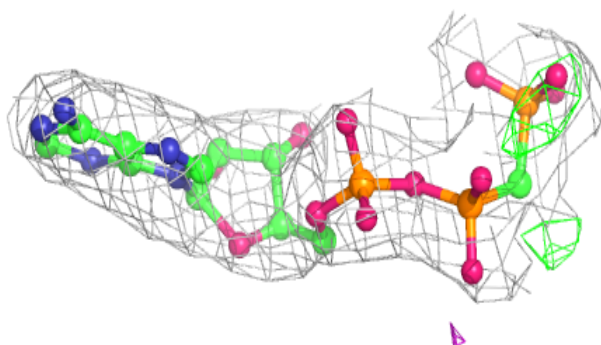
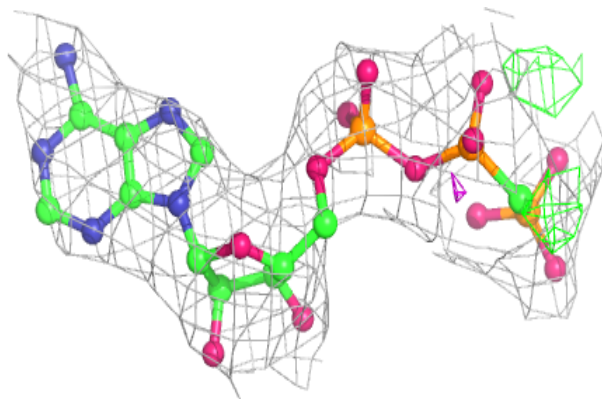
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	A	501	32/32	0.98	0.19	25,33,43,45	0
7	CA	A	503	1/1	0.98	0.04	76,76,76,76	0
5	GTP	C	501	32/32	0.98	0.14	21,27,36,50	0
8	GDP	B	501	28/28	0.99	0.15	15,28,36,40	0

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.



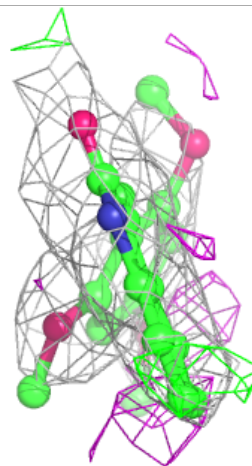
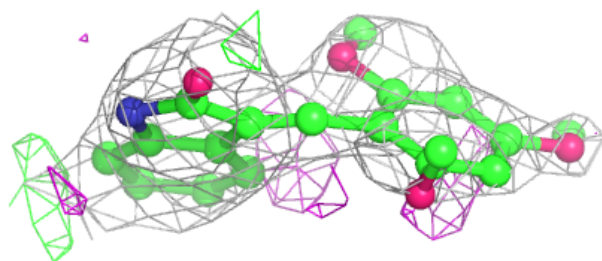
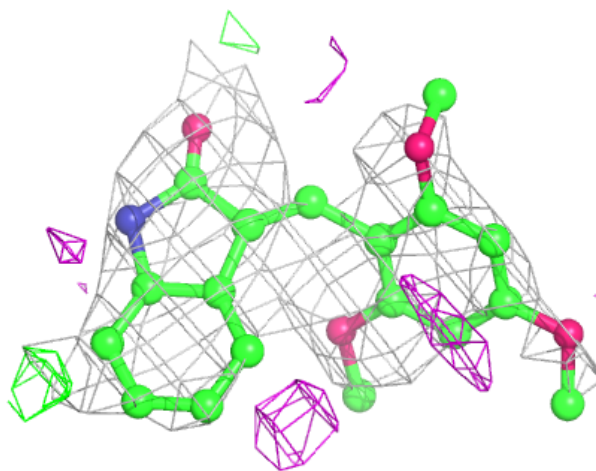
Electron density around ACP F 401:

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



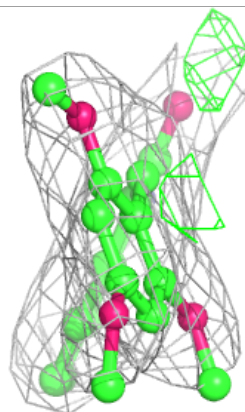
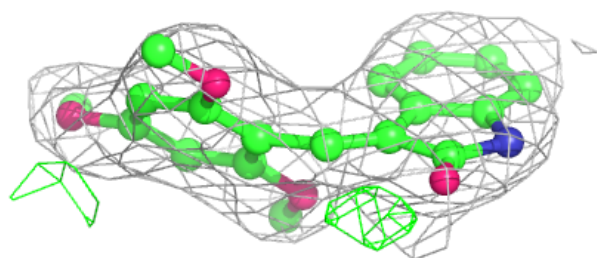
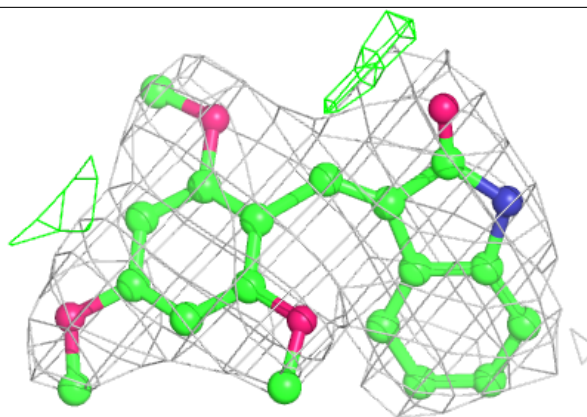
Electron density around IC1 D 503:

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

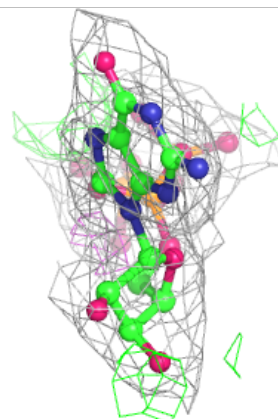
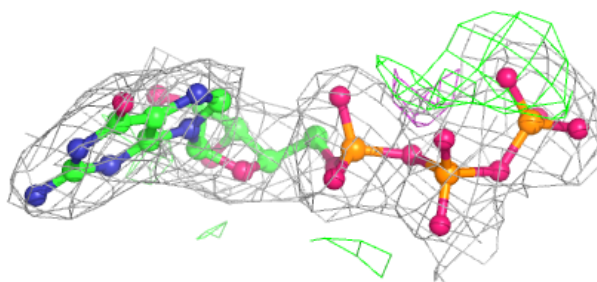
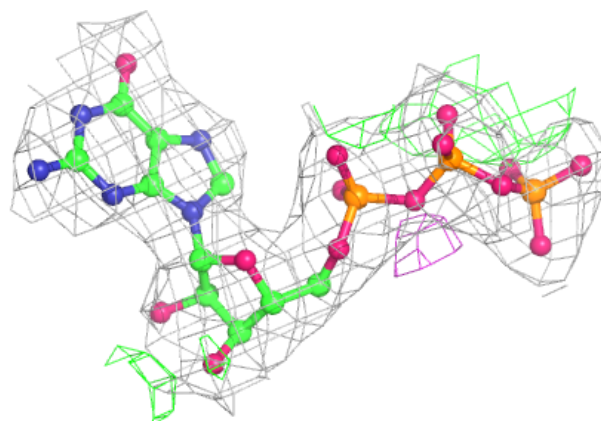


Electron density around IC1 B 507:

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

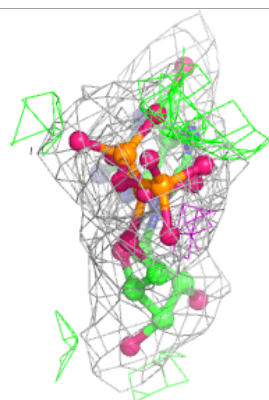
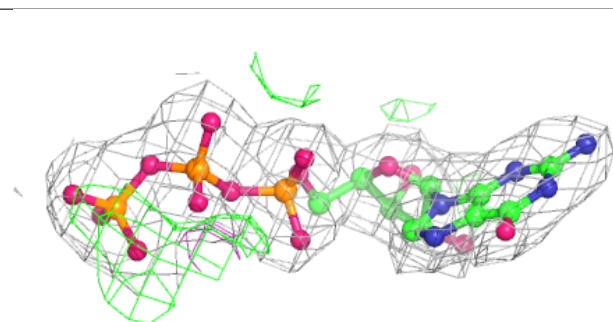
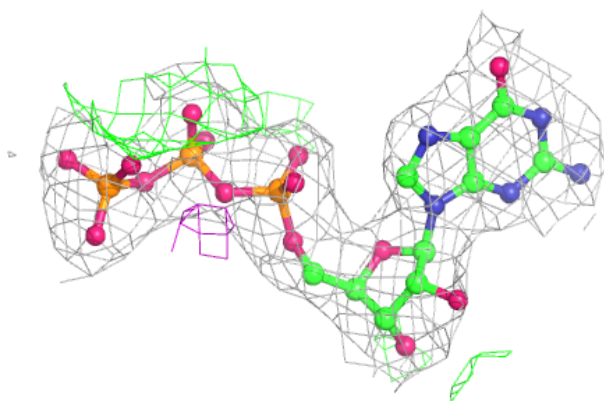
**Electron density around GTP A 501:**

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



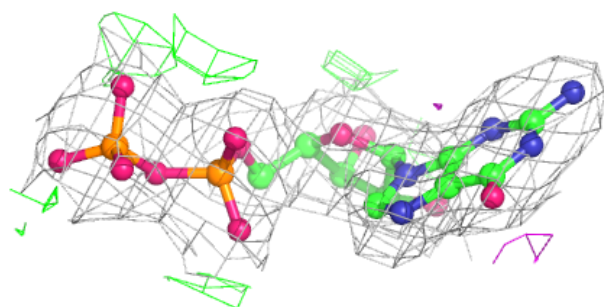
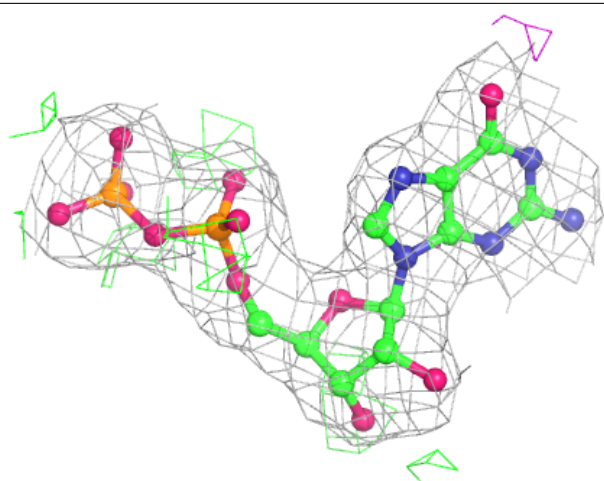
Electron density around GTP C 501:

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



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.