Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 11:22 AM JST

PDB ID	:	5CA1
Title	:	Crystal structure of T2R-TTL-Nocodazole complex
Authors	:	Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on	:	2015-06-29
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

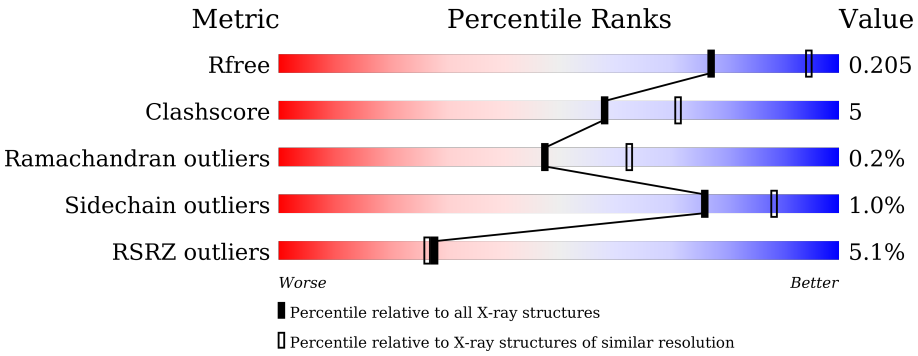
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	90% 7% •
1	C	450	91% 7% •
2	B	445	4% 87% 9% • •
2	D	445	6% 81% 13% 5%
3	E	143	7% 74% 10% 15%
4	F	384	14% 67% 17% • 13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17872 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

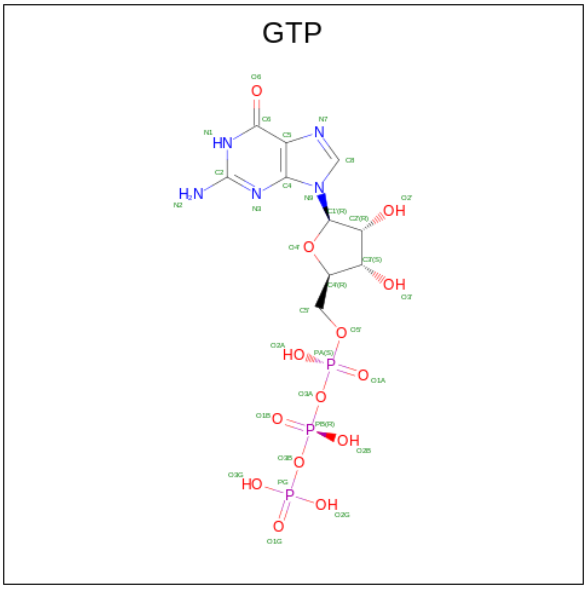
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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		

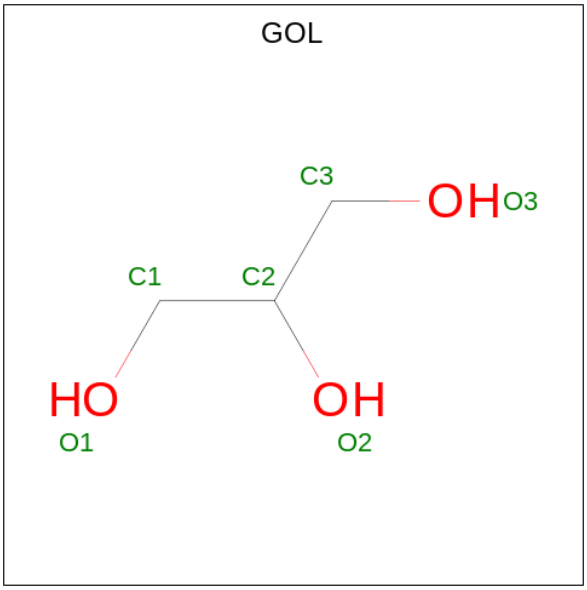
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

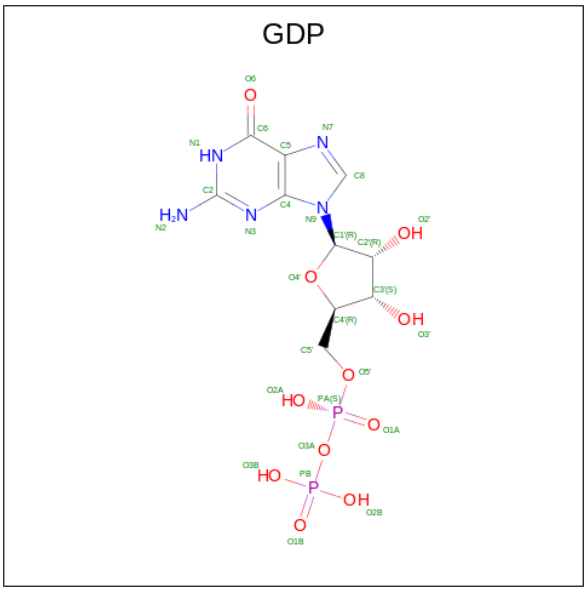
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



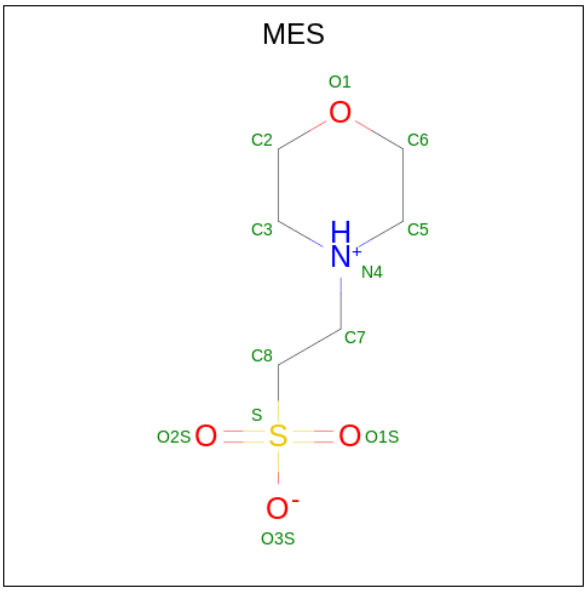
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



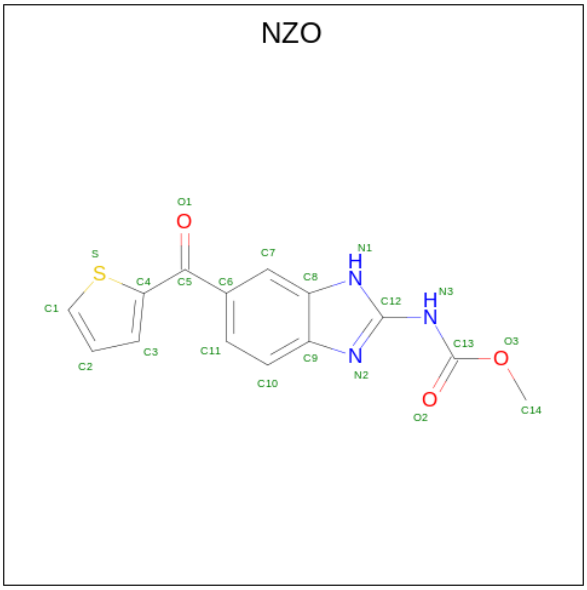
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

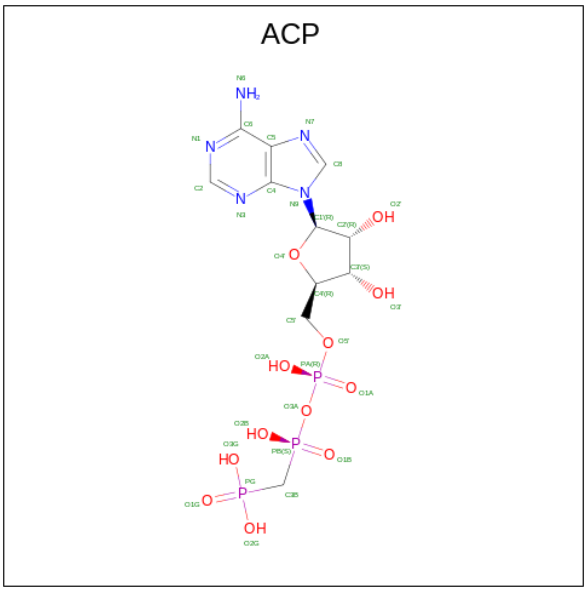
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is nocodazole (three-letter code: NZO) (formula: $C_{14}H_{11}N_3O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			21	14	3	3	1		
11	D	1	Total	C	N	O	S	0	0
			21	14	3	3	1		

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



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

- Molecule 13 is water.

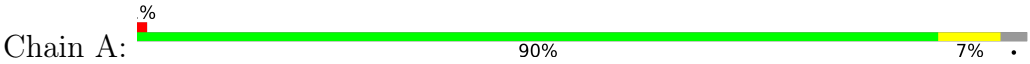
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	101	Total	O	0	0
			101	101		
13	B	74	Total	O	0	0
			74	74		
13	C	131	Total	O	0	0
			131	131		
13	D	33	Total	O	0	0
			33	33		
13	E	13	Total	O	0	0
			13	13		
13	F	25	Total	O	0	0
			25	25		

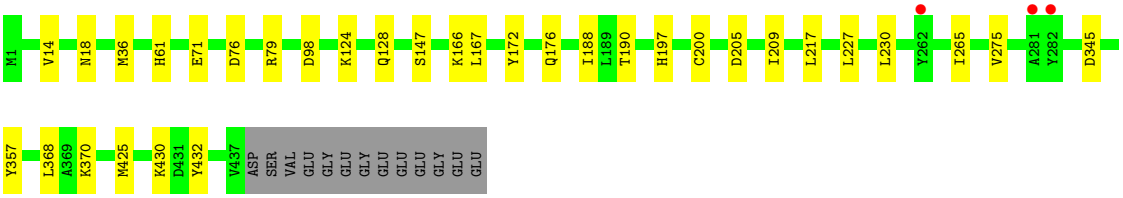
3 Residue-property plots (i)

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

• Molecule 1: Tubulin alpha

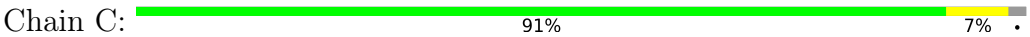
Chain A:

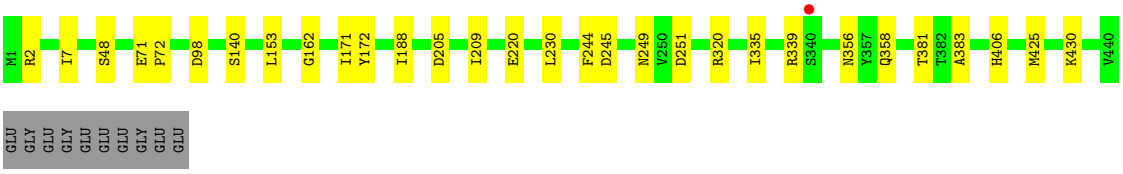




• Molecule 1: Tubulin alpha

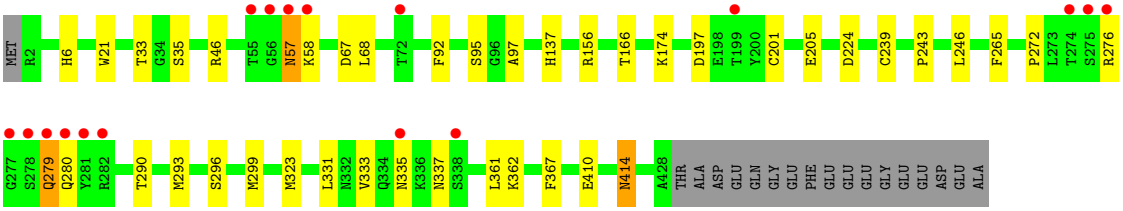
Chain C:





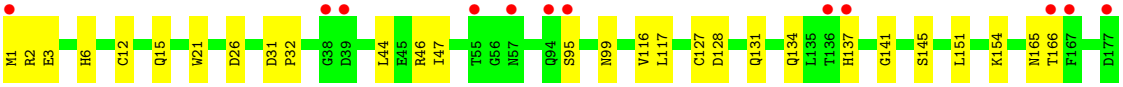
• Molecule 2: Tubulin beta-2 chain

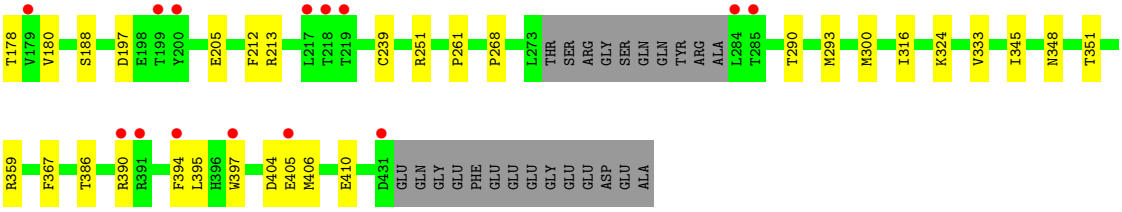
Chain B:



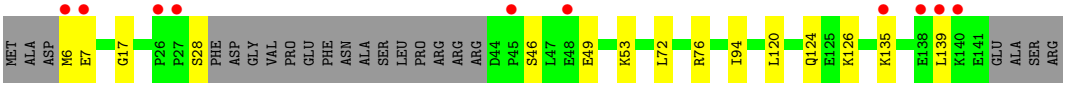
• Molecule 2: Tubulin beta-2 chain

Chain D:

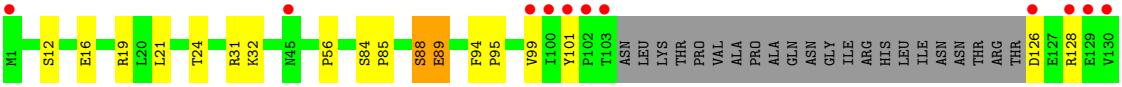


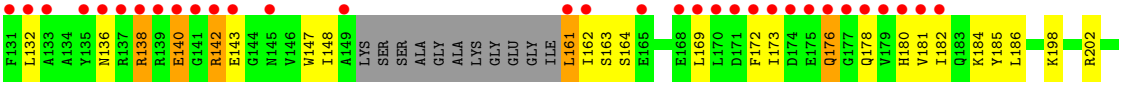


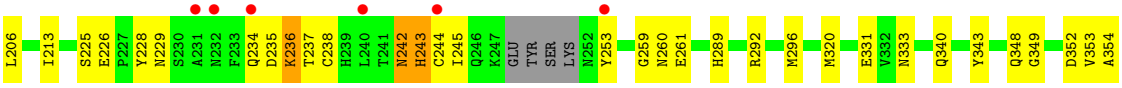
• Molecule 3: Stathmin-4

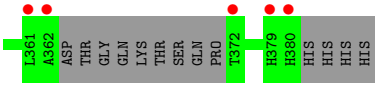


• Molecule 4: Uncharacterized protein









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.44Å 158.36Å 180.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.52 – 2.40 41.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.52-2.40) 99.8 (41.52-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.192 , 0.225 0.197 , 0.205	Depositor DCC
R_{free} test set	5924 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17872	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, CA, MES, ACP, GTP, NZO

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	0.24	0/3494	0.41	0/4743
1	C	0.25	0/3515	0.42	0/4772
2	B	0.26	0/3436	0.44	0/4654
2	D	0.24	0/3382	0.42	0/4581
3	E	0.24	0/1008	0.37	0/1337
4	F	0.32	0/2806	0.56	0/3791
All	All	0.26	0/17641	0.44	0/23878

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	138	ARG	Peptide
4	F	142	ARG	Peptide
4	F	242	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3330	20	0
1	C	3437	0	3348	19	0
2	B	3361	0	3238	26	0
2	D	3309	0	3189	38	0
3	E	1000	0	1018	10	0
4	F	2744	0	2709	57	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	A	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	2	0
10	B	12	0	12	2	0
10	D	12	0	12	3	0
11	B	21	0	11	0	0
11	D	21	0	11	2	0
12	F	31	0	14	5	0
13	A	101	0	0	0	0
13	B	74	0	0	1	0
13	C	131	0	0	0	0
13	D	33	0	0	0	0
13	E	13	0	0	0	0
13	F	25	0	0	3	0
All	All	17872	0	16948	164	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 5.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:GLU:O	2:B:414:ASN:ND2	2.00	0.93
4:F:180:HIS:O	13:F:501:HOH:O	1.92	0.87
4:F:138:ARG:HE	4:F:143:GLU:HB2	1.46	0.78
4:F:136:ASN:O	4:F:140:GLU:N	2.13	0.78
2:B:35:SER:OG	2:B:58:LYS:NZ	2.16	0.76
4:F:229:ASN:N	4:F:238:CYS:SG	2.58	0.75
2:D:268:PRO:HG2	2:D:300:MET:HB2	1.71	0.72
2:D:1:MET:HG3	2:D:2:ARG:N	2.04	0.71
2:D:116:VAL:HG11	2:D:151:LEU:HD11	1.73	0.70
4:F:235:ASP:O	4:F:237:THR:N	2.22	0.69
2:B:239:CYS:SG	13:B:618:HOH:O	2.51	0.68
2:D:251:ARG:NH1	10:D:502:MES:O3S	2.23	0.67
4:F:31:ARG:HG2	4:F:32:LYS:H	1.59	0.67
4:F:331:GLU:OE2	12:F:401:ACP:O2G	2.13	0.66
4:F:225:SER:HB3	4:F:260:ASN:HD21	1.59	0.66
4:F:184:LYS:NZ	4:F:185:TYR:O	2.30	0.64
4:F:138:ARG:HB3	4:F:143:GLU:HB3	1.79	0.64
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.81	0.63
4:F:138:ARG:HB3	4:F:143:GLU:CB	2.29	0.63
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.30	0.62
2:D:212:PHE:HD1	2:D:213:ARG:HG3	1.64	0.62
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.83	0.60
4:F:244:CYS:SG	4:F:245:ILE:N	2.75	0.60
4:F:333:ASN:ND2	12:F:401:ACP:O2G	2.32	0.60
4:F:225:SER:OG	4:F:226:GLU:OE2	2.19	0.60
4:F:88:SER:OG	4:F:89:GLU:HG2	2.01	0.59
1:A:176:GLN:HG2	4:F:56:PRO:HB3	1.85	0.59
4:F:289:HIS:HA	4:F:292:ARG:HH12	1.68	0.59
1:A:124:LYS:O	1:A:128:GLN:NE2	2.35	0.58
4:F:16:GLU:OE1	4:F:19:ARG:NH1	2.37	0.58
2:D:404:ASP:OD1	2:D:405:GLU:N	2.37	0.58
2:D:316:ILE:HG13	11:D:503:NZO:H3	1.86	0.58
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.36	0.57
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.86	0.57
2:D:3:GLU:OE1	2:D:128:ASP:N	2.37	0.57
2:D:386:THR:O	2:D:390:ARG:HG2	2.05	0.57
2:B:137:HIS:HE1	2:B:166:THR:HB	1.71	0.56
2:D:1:MET:SD	2:D:3:GLU:HG3	2.46	0.56
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.24	0.55
3:E:120:LEU:O	3:E:124:GLN:HG2	2.07	0.55
2:D:406:MET:O	2:D:410:GLU:HG3	2.07	0.55
4:F:173:ILE:HA	4:F:176:GLN:HE21	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.37	0.55
4:F:228:TYR:HA	4:F:238:CYS:SG	2.47	0.55
2:D:197:ASP:OD2	10:D:502:MES:H52	2.06	0.55
4:F:331:GLU:OE2	12:F:401:ACP:H3B2	2.06	0.55
2:D:137:HIS:HE1	2:D:166:THR:HB	1.72	0.55
2:B:156:ARG:CZ	10:B:503:MES:H21	2.36	0.55
4:F:181:VAL:HA	13:F:501:HOH:O	2.06	0.55
4:F:253:TYR:CE1	4:F:260:ASN:HB2	2.43	0.54
1:C:220:GLU:HG2	2:D:324:LYS:HD2	1.90	0.54
2:B:333:VAL:O	2:B:337:ASN:ND2	2.40	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.91	0.53
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.90	0.53
2:B:414:ASN:H	2:B:414:ASN:HD22	1.55	0.53
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.90	0.53
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.91	0.52
2:B:197:ASP:OD2	10:B:503:MES:H52	2.10	0.51
1:C:381:THR:HG22	1:C:383:ALA:H	1.75	0.51
2:B:57:ASN:N	2:B:57:ASN:OD1	2.44	0.51
4:F:138:ARG:NE	4:F:143:GLU:HB2	2.20	0.51
2:B:279:GLN:O	2:B:280:GLN:HG2	2.10	0.51
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.92	0.50
4:F:99:VAL:HA	13:F:501:HOH:O	2.11	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.11	0.50
3:E:135:LYS:O	3:E:139:LEU:HG	2.11	0.50
2:D:2:ARG:HB3	2:D:131:GLN:NE2	2.27	0.49
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.92	0.49
4:F:31:ARG:HG2	4:F:32:LYS:N	2.27	0.49
4:F:161:LEU:HD11	4:F:163:SER:HB2	1.95	0.49
4:F:163:SER:OG	4:F:164:SER:N	2.43	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.49
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.94	0.49
4:F:202:ARG:NH2	12:F:401:ACP:O1G	2.46	0.49
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.53	0.49
2:D:3:GLU:HG2	2:D:127:CYS:SG	2.53	0.49
2:D:134:GLN:HA	2:D:165:ASN:O	2.12	0.48
4:F:136:ASN:O	4:F:140:GLU:HB2	2.13	0.48
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.95	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.26	0.48
4:F:172:PHE:CD2	4:F:176:GLN:NE2	2.79	0.48
3:E:6:MET:HG3	3:E:7:GLU:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:SER:O	1:C:2:ARG:NH2	2.48	0.47
1:C:430:LYS:HD3	1:C:430:LYS:HA	1.69	0.47
4:F:289:HIS:HA	4:F:292:ARG:NH1	2.28	0.47
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.96	0.47
2:D:3:GLU:O	2:D:131:GLN:HG2	2.14	0.47
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.96	0.47
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.96	0.47
2:D:397:TRP:CD1	2:D:397:TRP:N	2.83	0.47
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.97	0.47
10:D:502:MES:H51	10:D:502:MES:H81	1.72	0.47
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.96	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.46
2:D:46:ARG:NH1	2:D:239:CYS:O	2.49	0.46
4:F:176:GLN:HG3	4:F:180:HIS:CE1	2.51	0.46
4:F:213:ILE:CD1	4:F:296:MET:HE2	2.46	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.52	0.45
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.99	0.45
4:F:101:TYR:HD2	4:F:126:ASP:HB2	1.81	0.45
4:F:138:ARG:HB3	4:F:143:GLU:HB2	1.97	0.45
2:D:3:GLU:OE2	2:D:3:GLU:N	2.44	0.45
4:F:331:GLU:OE2	12:F:401:ACP:C3B	2.64	0.45
4:F:213:ILE:HD11	4:F:296:MET:HE2	1.98	0.45
2:D:293:MET:HE2	2:D:367:PHE:HB2	1.98	0.45
1:C:140:SER:HA	1:C:171:ILE:HB	1.99	0.44
3:E:53:LYS:HA	3:E:53:LYS:HD2	1.70	0.44
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.00	0.44
4:F:161:LEU:HD23	4:F:172:PHE:CD2	2.53	0.44
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.99	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.44
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.53	0.44
2:D:1:MET:HG2	2:D:3:GLU:OE1	2.18	0.44
3:E:46:SER:OG	3:E:49:GLU:HG3	2.18	0.44
4:F:243:HIS:CE1	4:F:253:TYR:OH	2.70	0.44
2:D:44:LEU:HA	2:D:47:ILE:HB	2.00	0.43
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.99	0.43
2:D:394:PHE:HD2	2:D:397:TRP:CZ2	2.35	0.43
2:D:395:LEU:HD21	2:D:405:GLU:HG2	2.00	0.43
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.84	0.43
4:F:243:HIS:ND1	4:F:243:HIS:O	2.52	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:SER:OG	1:C:245:ASP:OD2	2.34	0.43
1:C:71:GLU:HB2	1:C:98:ASP:HB3	2.00	0.43
2:D:290:THR:HG22	2:D:333:VAL:HG21	2.01	0.43
1:A:14:VAL:O	1:A:18:ASN:ND2	2.52	0.43
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.42
2:D:26:ASP:OD2	2:D:359:ARG:HD3	2.19	0.42
2:B:362:LYS:HE2	2:B:362:LYS:HB3	1.88	0.42
3:E:126:LYS:HB3	3:E:126:LYS:HE3	1.66	0.42
4:F:178:GLN:HB2	4:F:180:HIS:CD2	2.54	0.42
2:B:46:ARG:HH21	2:B:243:PRO:HA	1.85	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.42
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.00	0.42
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.19	0.42
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.54	0.42
1:A:98:ASP:HB2	5:A:501:GTP:O3G	2.19	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.42
1:C:406:HIS:CD2	2:D:261:PRO:HD3	2.55	0.42
4:F:176:GLN:HG3	4:F:180:HIS:NE2	2.35	0.42
2:B:33:THR:O	2:B:58:LYS:HE3	2.20	0.42
2:B:239:CYS:SG	2:B:246:LEU:HD23	2.60	0.42
2:D:145:SER:OG	2:D:188:SER:OG	2.29	0.42
2:D:117:LEU:HD11	2:D:154:LYS:HB3	2.02	0.42
4:F:259:GLY:O	4:F:261:GLU:HG3	2.19	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
4:F:348:GLN:NE2	4:F:352:ASP:OD2	2.51	0.42
4:F:349:GLY:O	4:F:353:VAL:HG22	2.20	0.42
4:F:128:ARG:O	4:F:132:LEU:HD12	2.19	0.41
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.79	0.41
1:C:2:ARG:HD2	1:C:2:ARG:HA	1.91	0.41
2:B:331:LEU:O	2:B:335:ASN:ND2	2.54	0.41
1:C:320:ARG:HA	1:C:356:ASN:O	2.21	0.41
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.50	0.41
2:B:296:SER:HA	2:B:299:MET:HG2	2.01	0.41
4:F:84:SER:HA	4:F:85:PRO:HD3	1.95	0.41
2:D:351:THR:C	11:D:503:NZO:H2	2.40	0.41
3:E:72:LEU:O	3:E:76:ARG:HG2	2.20	0.41
1:A:430:LYS:HD2	1:A:430:LYS:HA	1.66	0.41
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.95	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.40
2:B:290:THR:HG22	2:B:333:VAL:HG21	2.02	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%)	425 (98%)	10 (2%)	0	100 100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100 100
2	B	425/445 (96%)	413 (97%)	11 (3%)	1 (0%)	47 62
2	D	417/445 (94%)	399 (96%)	18 (4%)	0	100 100
3	E	117/143 (82%)	114 (97%)	3 (3%)	0	100 100
4	F	324/384 (84%)	308 (95%)	13 (4%)	3 (1%)	17 25
All	All	2156/2317 (93%)	2086 (97%)	66 (3%)	4 (0%)	47 62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	ASN
4	F	236	LYS
4	F	142	ARG
4	F	140	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	368/378 (97%)	367 (100%)	1 (0%)	92 97
1	C	371/378 (98%)	370 (100%)	1 (0%)	92 97
2	B	369/383 (96%)	366 (99%)	3 (1%)	81 91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	364/383 (95%)	360 (99%)	4 (1%)	73 87
3	E	109/127 (86%)	109 (100%)	0	100 100
4	F	301/342 (88%)	292 (97%)	9 (3%)	41 61
All	All	1882/1991 (94%)	1864 (99%)	18 (1%)	76 88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
2	B	279	GLN
2	B	323	MET
2	B	414	ASN
1	C	251	ASP
2	D	15	GLN
2	D	95	SER
2	D	180	VAL
2	D	205	GLU
4	F	12	SER
4	F	88	SER
4	F	89	GLU
4	F	161	LEU
4	F	176	GLN
4	F	234	GLN
4	F	236	LYS
4	F	242	ASN
4	F	243	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	414	ASN
4	F	243	HIS
4	F	260	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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	ACP	F	401	-	27,33,33	1.69	5 (18%)	32,52,52	1.58	5 (15%)
10	MES	B	503	-	12,12,12	2.16	1 (8%)	14,16,16	2.06	6 (42%)
11	NZO	B	504	-	23,23,23	1.61	5 (21%)	20,32,32	3.01	5 (25%)
11	NZO	D	503	-	23,23,23	1.65	5 (21%)	20,32,32	3.12	6 (30%)
9	GDP	D	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.13	4 (13%)
9	GDP	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.13	4 (13%)
5	GTP	A	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.43	6 (18%)
8	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.21	0
10	MES	D	502	-	12,12,12	2.29	1 (8%)	14,16,16	2.00	2 (14%)
5	GTP	C	501	6	26,34,34	1.10	2 (7%)	32,54,54	1.39	5 (15%)

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
12	ACP	F	401	-	-	4/15/38/38	0/3/3/3
10	MES	B	503	-	-	5/6/14/14	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NZO	B	504	-	-	0/8/14/14	0/3/3/3
11	NZO	D	503	-	-	0/8/14/14	0/3/3/3
9	GDP	D	501	-	-	5/12/32/32	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
8	GOL	A	504	-	-	4/4/4/4	-
10	MES	D	502	-	-	3/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	MES	C8-S	-7.66	1.66	1.77
10	B	503	MES	C8-S	-7.17	1.67	1.77
12	F	401	ACP	PG-O3G	-4.24	1.45	1.54
5	A	501	GTP	C5-C6	-3.94	1.39	1.47
12	F	401	ACP	PG-O1G	3.91	1.58	1.50
5	C	501	GTP	C5-C6	-3.89	1.39	1.47
11	D	503	NZO	C4-S	-3.65	1.67	1.72
11	D	503	NZO	O3-C13	3.63	1.40	1.34
11	B	504	NZO	O3-C13	3.53	1.40	1.34
11	B	504	NZO	C4-S	-3.36	1.68	1.72
12	F	401	ACP	C2'-C1'	-3.03	1.49	1.53
11	D	503	NZO	C13-N3	3.02	1.42	1.36
11	B	504	NZO	C13-N3	2.89	1.42	1.36
11	B	504	NZO	C12-N3	2.50	1.42	1.38
11	D	503	NZO	C12-N3	2.48	1.42	1.38
9	B	501	GDP	C6-N1	-2.40	1.34	1.37
11	D	503	NZO	C2-C1	2.28	1.41	1.34
11	B	504	NZO	C2-C1	2.28	1.41	1.34
9	D	501	GDP	C6-N1	-2.22	1.34	1.37
12	F	401	ACP	C5-N7	-2.11	1.32	1.39
5	C	501	GTP	C2-N3	2.10	1.38	1.33
12	F	401	ACP	PB-O1B	-2.09	1.46	1.51
5	A	501	GTP	C2-N3	2.03	1.38	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	503	NZO	C2-C1-S	-9.86	104.98	112.98
11	B	504	NZO	C2-C1-S	-9.44	105.32	112.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	504	NZO	O3-C13-N3	6.92	118.94	109.25
11	D	503	NZO	O3-C13-N3	6.29	118.06	109.25
10	D	502	MES	C5-N4-C3	5.46	121.12	108.83
10	B	503	MES	C5-N4-C3	4.05	117.95	108.83
11	D	503	NZO	O3-C13-O2	-3.92	118.81	124.58
11	D	503	NZO	C12-N3-C13	-3.92	121.89	127.67
12	F	401	ACP	PB-O3A-PA	-3.81	120.49	132.56
10	B	503	MES	O2S-S-C8	3.49	111.12	106.92
12	F	401	ACP	C3'-C2'-C1'	3.45	106.17	100.98
11	B	504	NZO	O3-C13-O2	-3.41	119.56	124.58
10	D	502	MES	O1S-S-C8	3.36	110.96	106.92
11	B	504	NZO	C12-N3-C13	-3.24	122.89	127.67
12	F	401	ACP	N3-C2-N1	-3.16	123.73	128.68
5	A	501	GTP	C5-C6-N1	3.08	119.39	113.95
5	A	501	GTP	PB-O3B-PG	-3.08	122.26	132.83
5	C	501	GTP	C8-N7-C5	3.06	108.82	102.99
5	C	501	GTP	C5-C6-N1	3.04	119.31	113.95
5	A	501	GTP	C8-N7-C5	3.00	108.71	102.99
12	F	401	ACP	C4-C5-N7	-2.97	106.30	109.40
5	C	501	GTP	PB-O3B-PG	-2.82	123.16	132.83
5	C	501	GTP	C2-N1-C6	-2.74	120.06	125.10
5	A	501	GTP	C2-N1-C6	-2.73	120.06	125.10
5	C	501	GTP	PA-O3A-PB	-2.62	123.84	132.83
5	A	501	GTP	PA-O3A-PB	-2.58	123.96	132.83
12	F	401	ACP	O3G-PG-O1G	-2.56	105.63	112.39
9	B	501	GDP	PA-O3A-PB	-2.55	124.07	132.83
9	B	501	GDP	C5-C6-N1	2.47	118.31	113.95
10	B	503	MES	C7-N4-C5	2.46	117.53	111.23
9	D	501	GDP	C8-N7-C5	2.44	107.64	102.99
10	B	503	MES	C6-C5-N4	-2.42	106.44	110.10
10	B	503	MES	O3S-S-C8	2.39	109.64	105.77
9	B	501	GDP	C8-N7-C5	2.39	107.54	102.99
9	D	501	GDP	C5-C6-N1	2.33	118.07	113.95
11	D	503	NZO	O2-C13-N3	-2.33	121.04	126.11
9	D	501	GDP	PA-O3A-PB	-2.31	124.90	132.83
11	D	503	NZO	C7-C6-C5	-2.19	116.31	120.58
10	B	503	MES	C7-N4-C3	2.15	116.72	111.23
11	B	504	NZO	O2-C13-N3	-2.14	121.47	126.11
5	A	501	GTP	O6-C6-C5	-2.05	120.36	124.37
9	B	501	GDP	O2B-PB-O3A	2.05	111.50	104.64
9	D	501	GDP	O2B-PB-O3A	2.02	111.42	104.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	C1-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	PA-O3A-PB-O2B
9	D	501	GDP	PA-O3A-PB-O3B
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
10	B	503	MES	C7-C8-S-O3S
10	D	502	MES	C7-C8-S-O1S
10	D	502	MES	C7-C8-S-O2S
10	D	502	MES	C7-C8-S-O3S
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O3A
8	A	504	GOL	O1-C1-C2-O2
8	A	504	GOL	O2-C2-C3-O3
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G

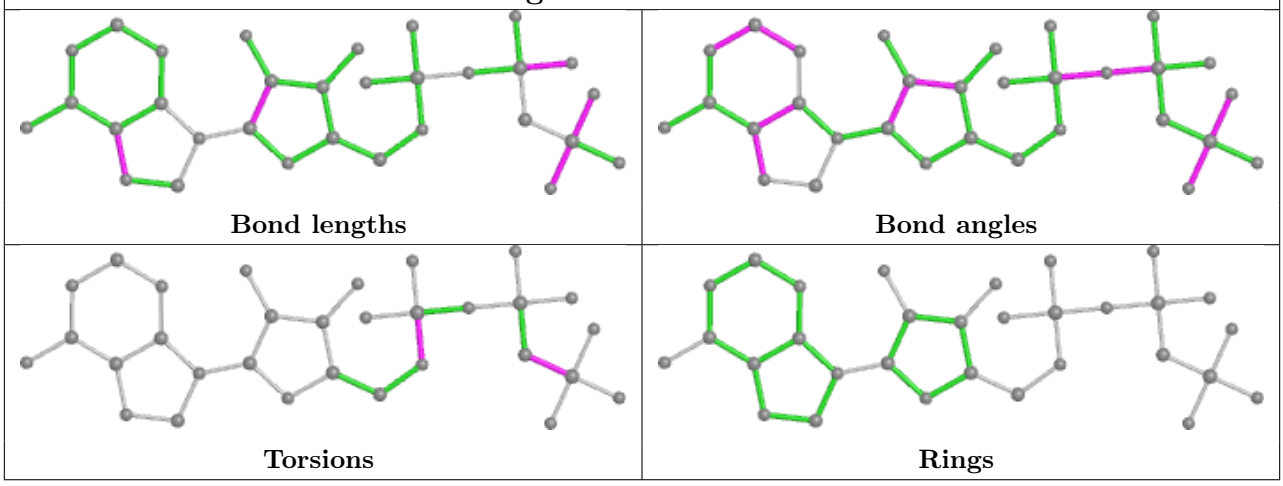
There are no ring outliers.

6 monomers are involved in 15 short contacts:

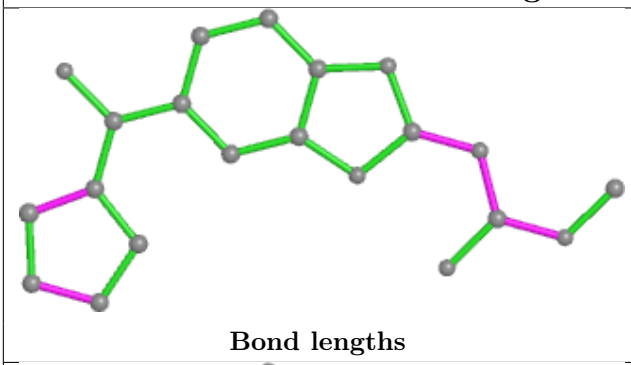
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	5	0
10	B	503	MES	2	0
11	D	503	NZO	2	0
9	D	501	GDP	2	0
5	A	501	GTP	1	0
10	D	502	MES	3	0

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

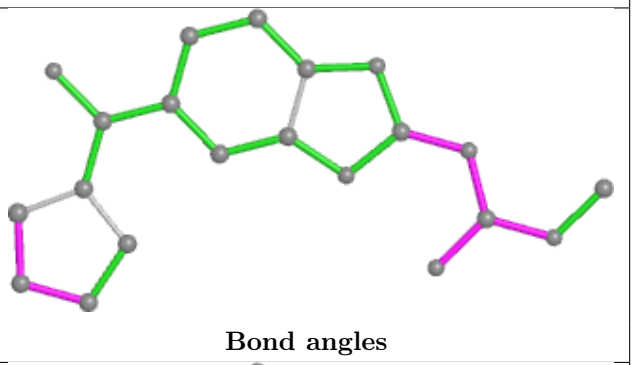
Ligand ACP F 401



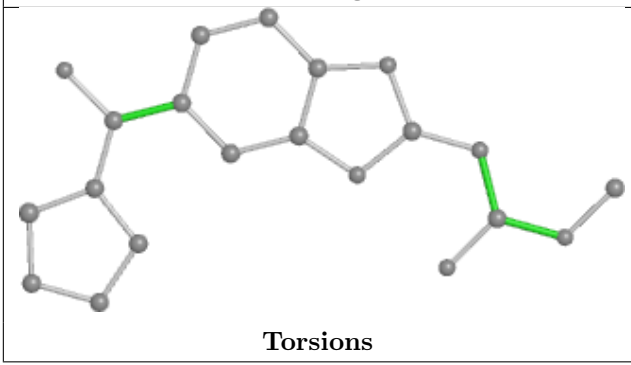
Ligand NZO B 504



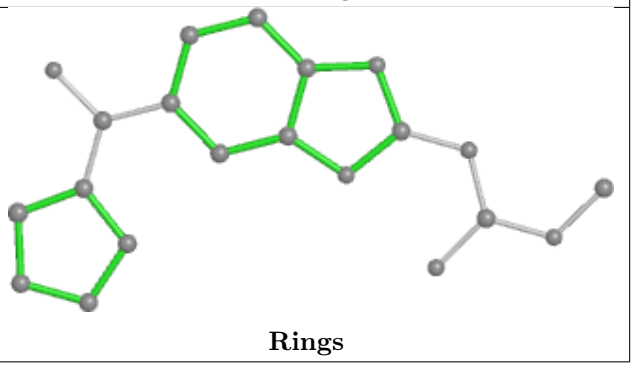
Bond lengths



Bond angles

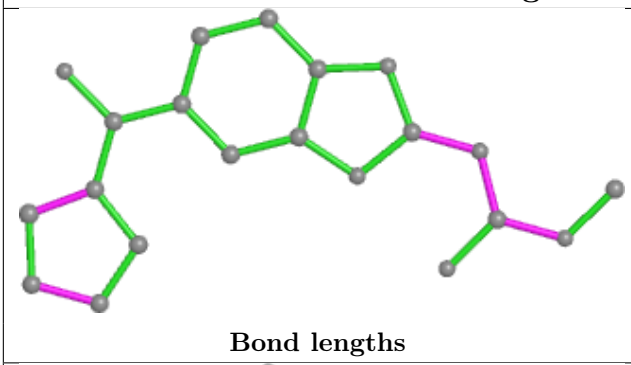


Torsions

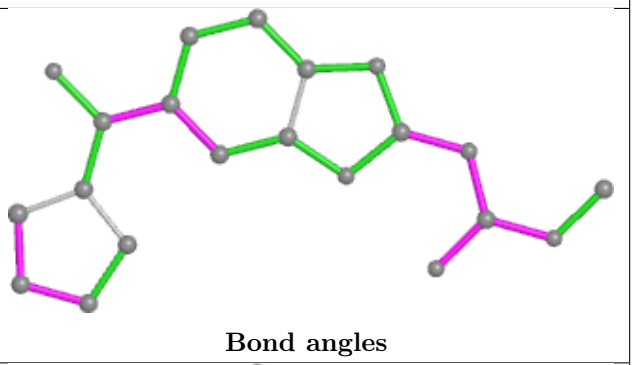


Rings

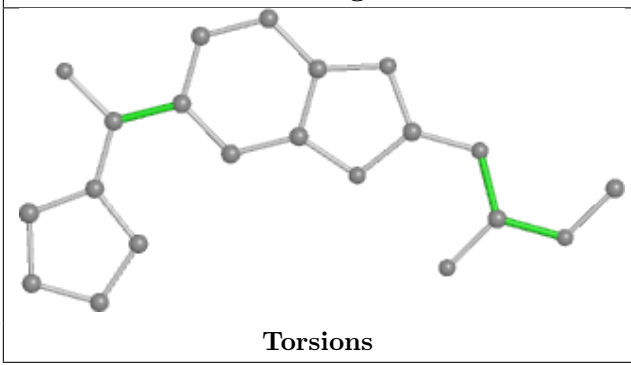
Ligand NZO D 503



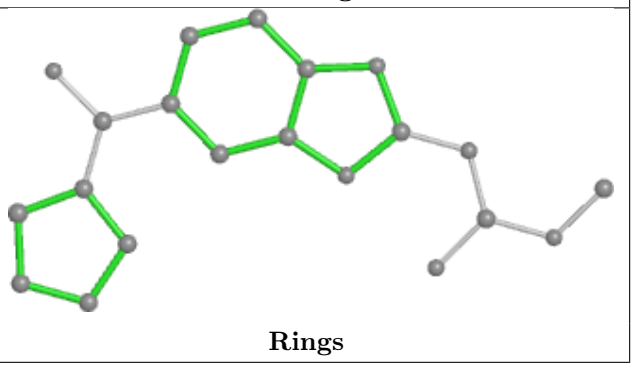
Bond lengths



Bond angles

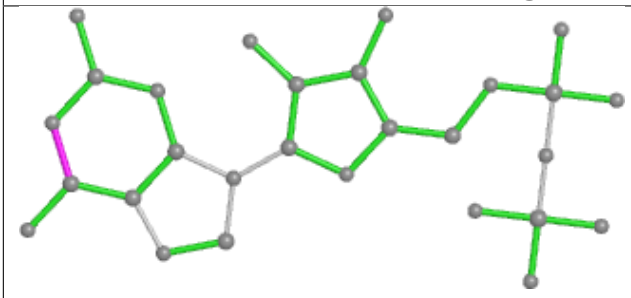


Torsions

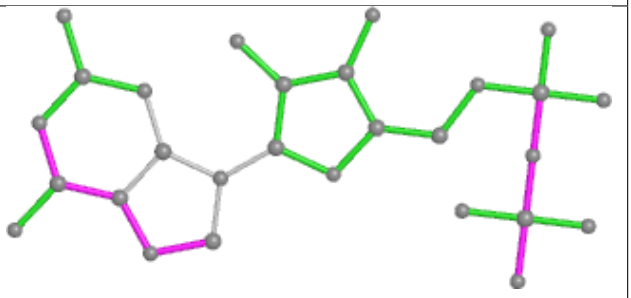


Rings

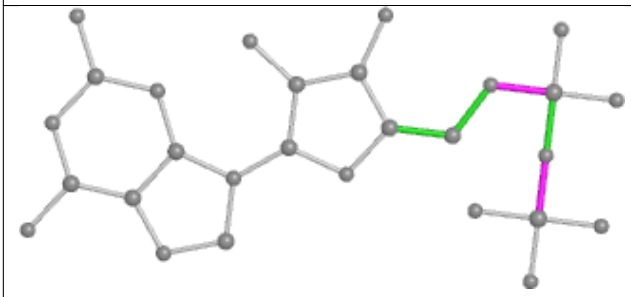
Ligand GDP D 501



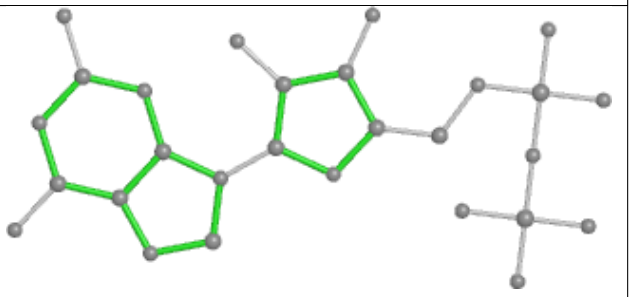
Bond lengths



Bond angles

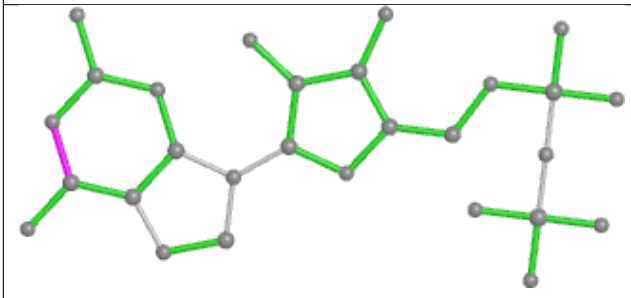


Torsions

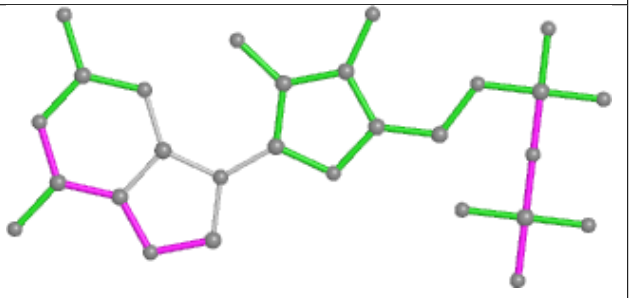


Rings

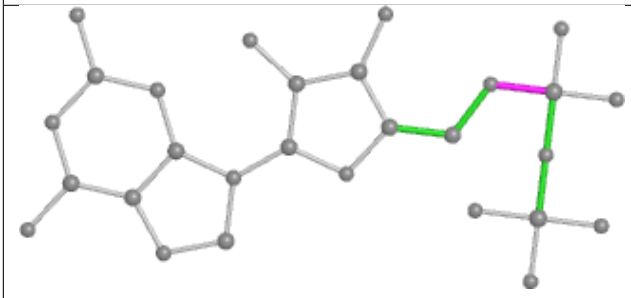
Ligand GDP B 501



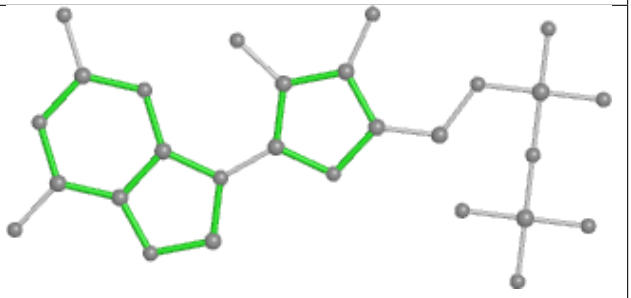
Bond lengths



Bond angles

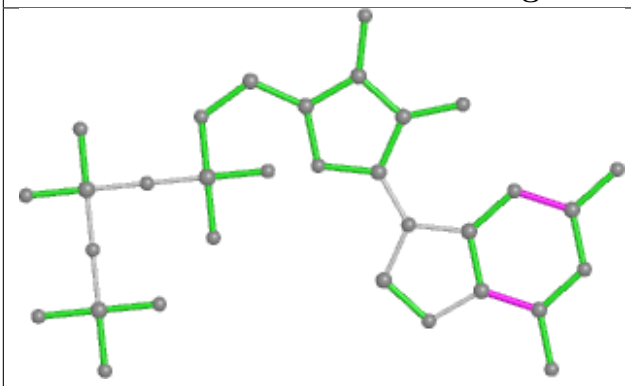


Torsions

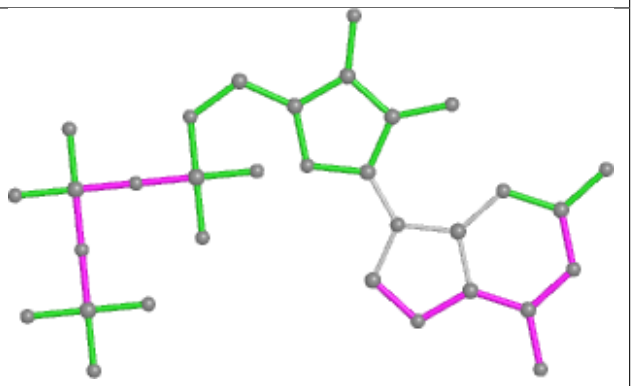


Rings

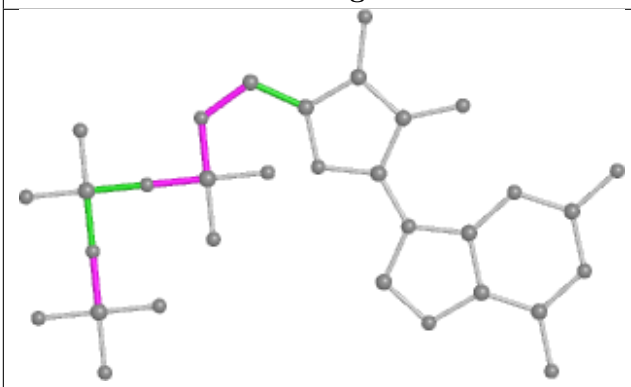
Ligand GTP A 501



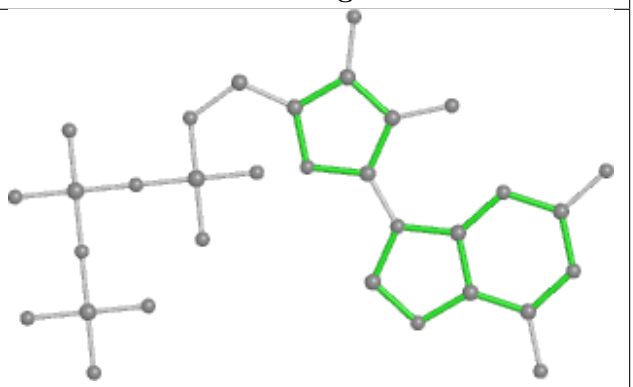
Bond lengths



Bond angles

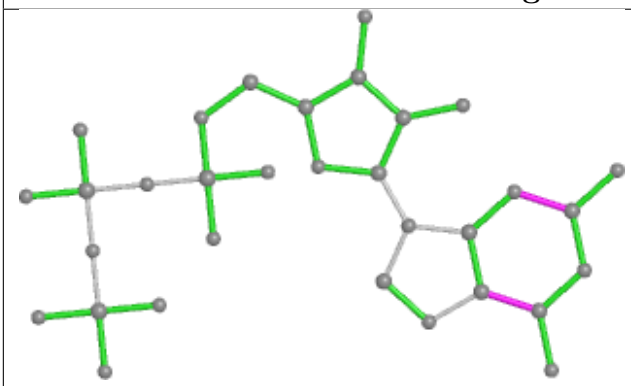


Torsions

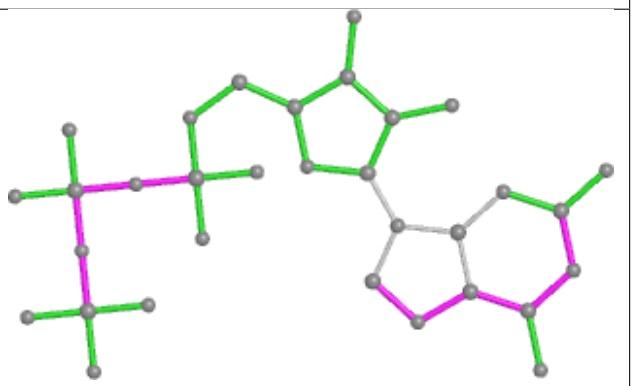


Rings

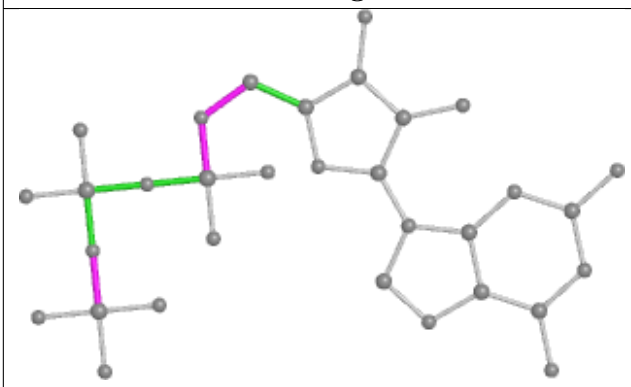
Ligand GTP C 501



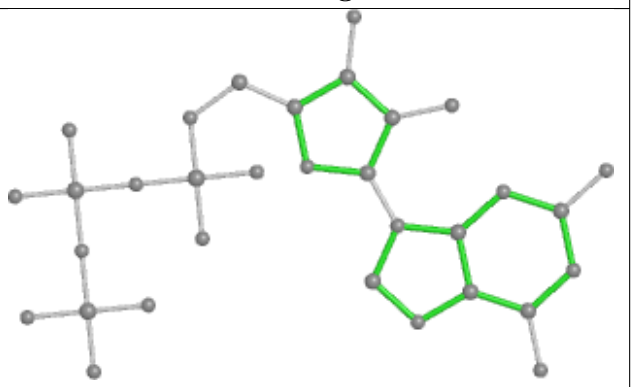
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	3 (0%) 87 86	24, 39, 62, 87	0
1	C	440/450 (97%)	-0.38	1 (0%) 95 94	19, 31, 53, 69	0
2	B	427/445 (95%)	0.03	17 (3%) 38 37	22, 38, 69, 103	0
2	D	421/445 (94%)	0.21	26 (6%) 20 19	26, 48, 78, 101	0
3	E	121/143 (84%)	0.34	10 (8%) 11 10	29, 53, 83, 94	0
4	F	334/384 (86%)	0.53	54 (16%) 1 1	32, 59, 116, 135	0
All	All	2180/2317 (94%)	0.04	111 (5%) 28 26	19, 42, 82, 135	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	7.5
4	F	173	ILE	7.4
4	F	176	GLN	6.4
4	F	132	LEU	6.1
4	F	135	TYR	5.4
4	F	172	PHE	5.4
2	D	57	ASN	5.3
4	F	372	THR	5.2
2	B	55	THR	5.1
4	F	130	VAL	5.1
4	F	177	GLY	5.1
4	F	169	LEU	4.8
4	F	178	GLN	4.7
3	E	48	GLU	4.7
2	B	276	ARG	4.6
4	F	161	LEU	4.6
4	F	174	ASP	4.6
4	F	138	ARG	4.4
4	F	234	GLN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	4.2
2	D	390	ARG	4.1
4	F	380	HIS	4.1
3	E	6	MET	4.1
2	B	282	ARG	4.0
4	F	131	PHE	4.0
4	F	101	TYR	4.0
3	E	7	GLU	4.0
2	B	275	SER	3.9
4	F	143	GLU	3.8
4	F	180	HIS	3.8
2	B	335	ASN	3.8
4	F	103	THR	3.8
3	E	139	LEU	3.7
2	B	57	ASN	3.7
1	A	281	ALA	3.7
4	F	175	GLU	3.7
4	F	253	TYR	3.6
2	D	391	ARG	3.5
2	B	278	SER	3.5
2	B	279	GLN	3.4
2	D	55	THR	3.2
2	D	219	THR	3.2
4	F	231	ALA	3.2
4	F	232	ASN	3.2
2	B	274	THR	3.2
2	D	167	PHE	3.2
4	F	99	VAL	3.2
4	F	170	LEU	3.2
2	D	137	HIS	3.1
4	F	171	ASP	3.0
4	F	100	ILE	3.0
2	B	277	GLY	3.0
1	C	340	SER	3.0
4	F	133	ALA	2.9
2	D	394	PHE	2.9
4	F	361	LEU	2.9
4	F	168	GLU	2.9
4	F	244	CYS	2.9
4	F	165	GLU	2.9
4	F	140	GLU	2.8
4	F	136	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	2.8
2	D	39	ASP	2.8
4	F	137	ARG	2.8
2	D	199	THR	2.8
4	F	129	GLU	2.7
3	E	26	PRO	2.7
3	E	27	PRO	2.7
3	E	45	PRO	2.7
2	B	56	GLY	2.7
4	F	379	HIS	2.7
4	F	139	ARG	2.7
2	D	431	ASP	2.7
4	F	362	ALA	2.7
4	F	128	ARG	2.7
4	F	179	VAL	2.6
4	F	102	PRO	2.6
1	A	282	TYR	2.6
4	F	126	ASP	2.5
4	F	1	MET	2.5
2	D	285	THR	2.5
2	D	38	GLY	2.5
3	E	138	GLU	2.5
3	E	135	LYS	2.4
2	D	284	LEU	2.4
4	F	181	VAL	2.4
4	F	45	ASN	2.4
4	F	141	GLY	2.4
2	D	166	THR	2.4
2	B	281	TYR	2.3
2	D	200	TYR	2.3
4	F	240	LEU	2.3
3	E	140	LYS	2.3
2	B	280	GLN	2.3
2	D	94	GLN	2.2
2	D	405	GLU	2.2
4	F	145	ASN	2.2
2	B	199	THR	2.2
2	D	397	TRP	2.2
2	D	179	VAL	2.1
2	D	217	LEU	2.1
2	D	95	SER	2.1
4	F	149	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	218	THR	2.1
1	A	262	TYR	2.1
2	D	177	ASP	2.1
2	B	338	SER	2.1
2	B	58	LYS	2.1
2	B	72	THR	2.0
2	D	136	THR	2.0
4	F	162	ILE	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)

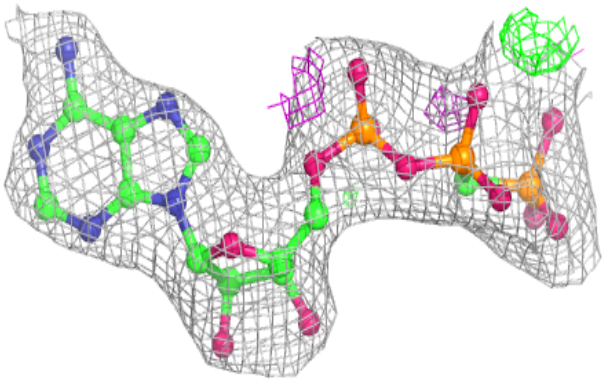
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

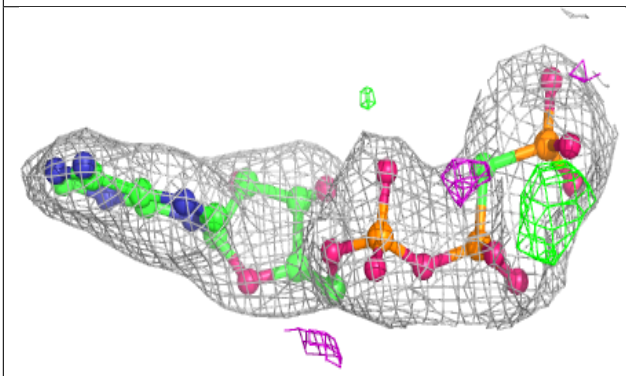
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	A	504	6/6	0.91	0.20	45,54,59,59	0
10	MES	D	502	12/12	0.92	0.18	50,58,63,66	0
12	ACP	F	401	31/31	0.92	0.13	73,81,94,97	0
7	CA	C	503	1/1	0.94	0.07	45,45,45,45	0
11	NZO	D	503	21/21	0.94	0.15	25,40,50,69	0
9	GDP	D	501	28/28	0.94	0.12	37,43,57,63	0
10	MES	B	503	12/12	0.95	0.16	32,43,51,53	0
6	MG	B	502	1/1	0.95	0.19	26,26,26,26	0
7	CA	A	503	1/1	0.96	0.05	54,54,54,54	0
11	NZO	B	504	21/21	0.97	0.21	14,29,35,50	0
5	GTP	A	501	32/32	0.98	0.17	21,29,33,36	0
6	MG	A	502	1/1	0.98	0.14	28,28,28,28	0
5	GTP	C	501	32/32	0.99	0.15	19,24,30,30	0
9	GDP	B	501	28/28	0.99	0.13	23,29,31,40	0
6	MG	C	502	1/1	1.00	0.17	24,24,24,24	0

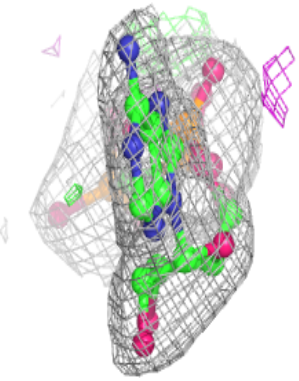
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

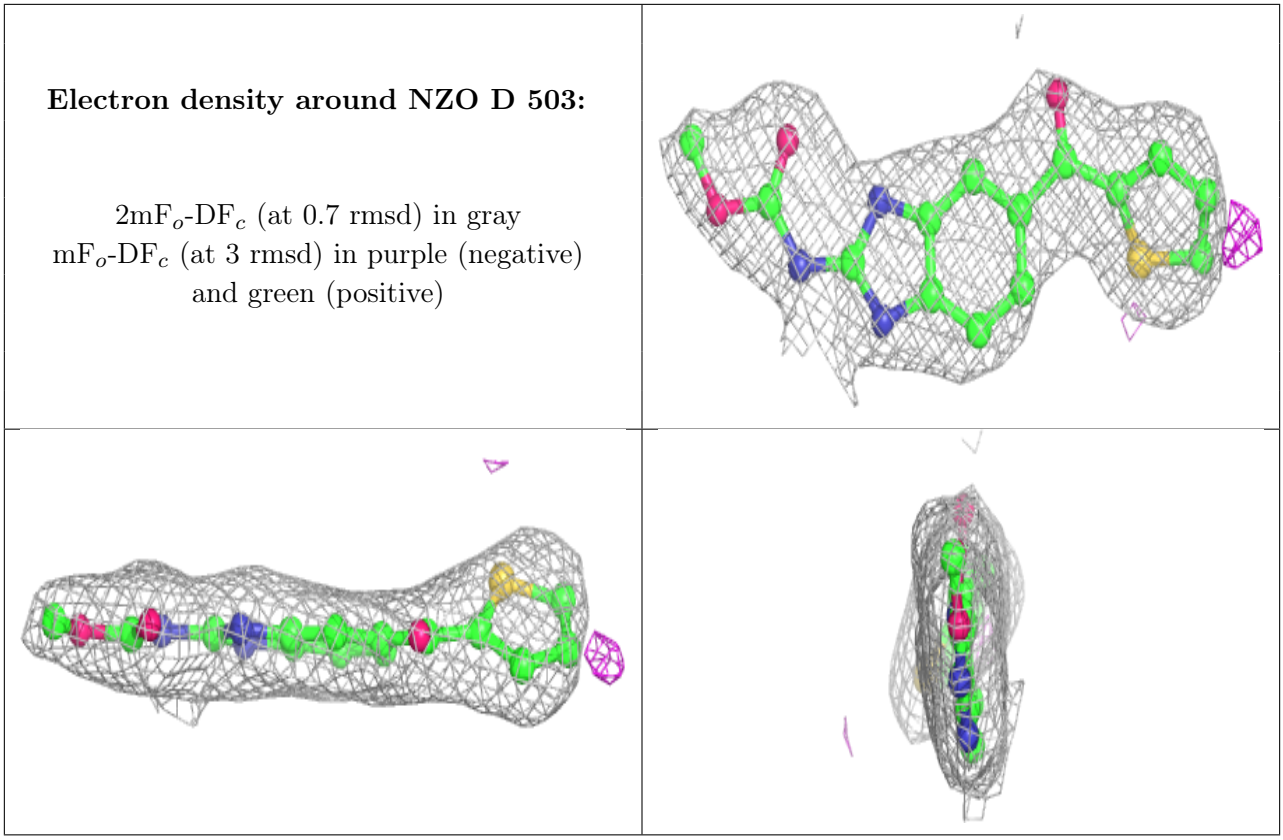






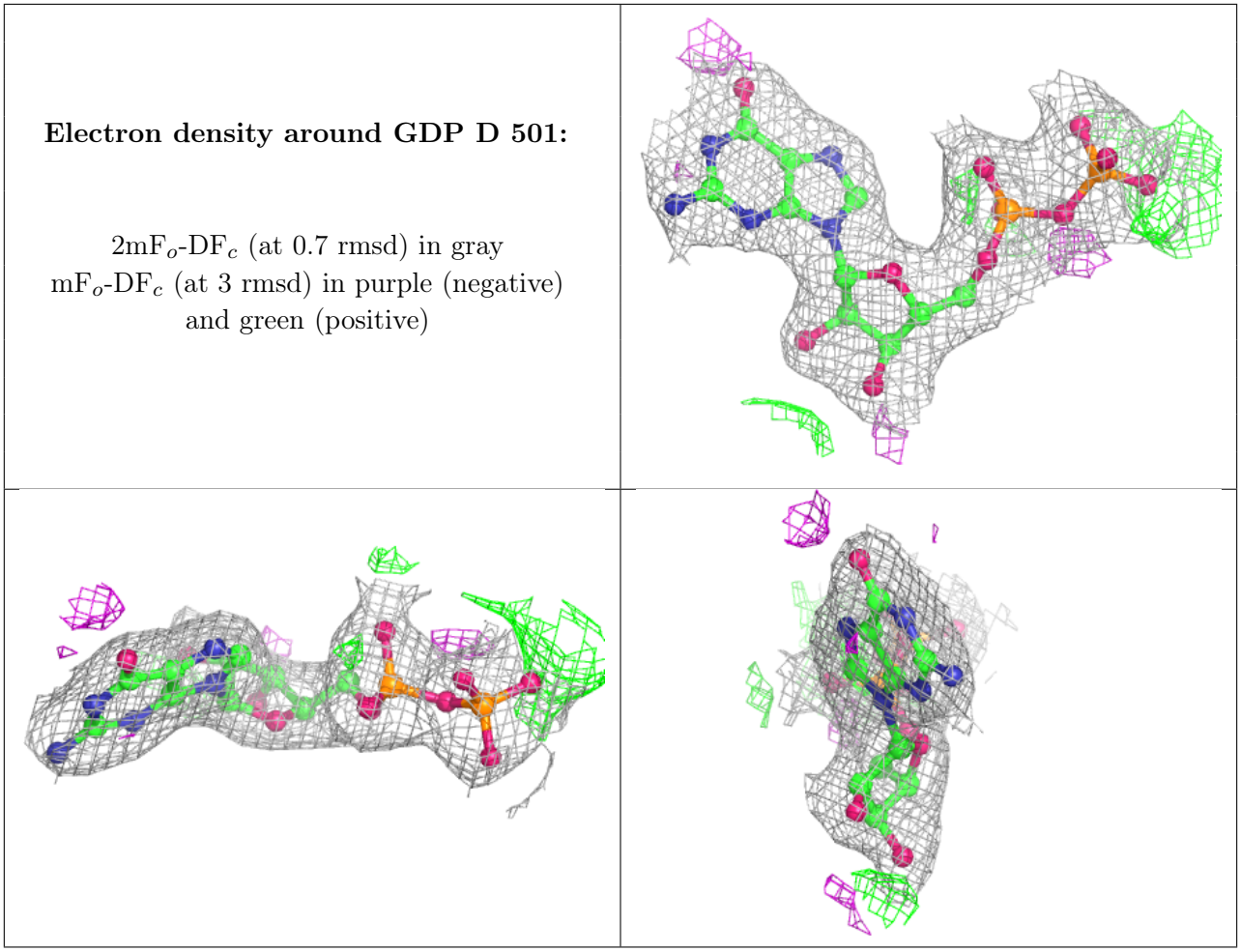
Electron density around NZO D 503:

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



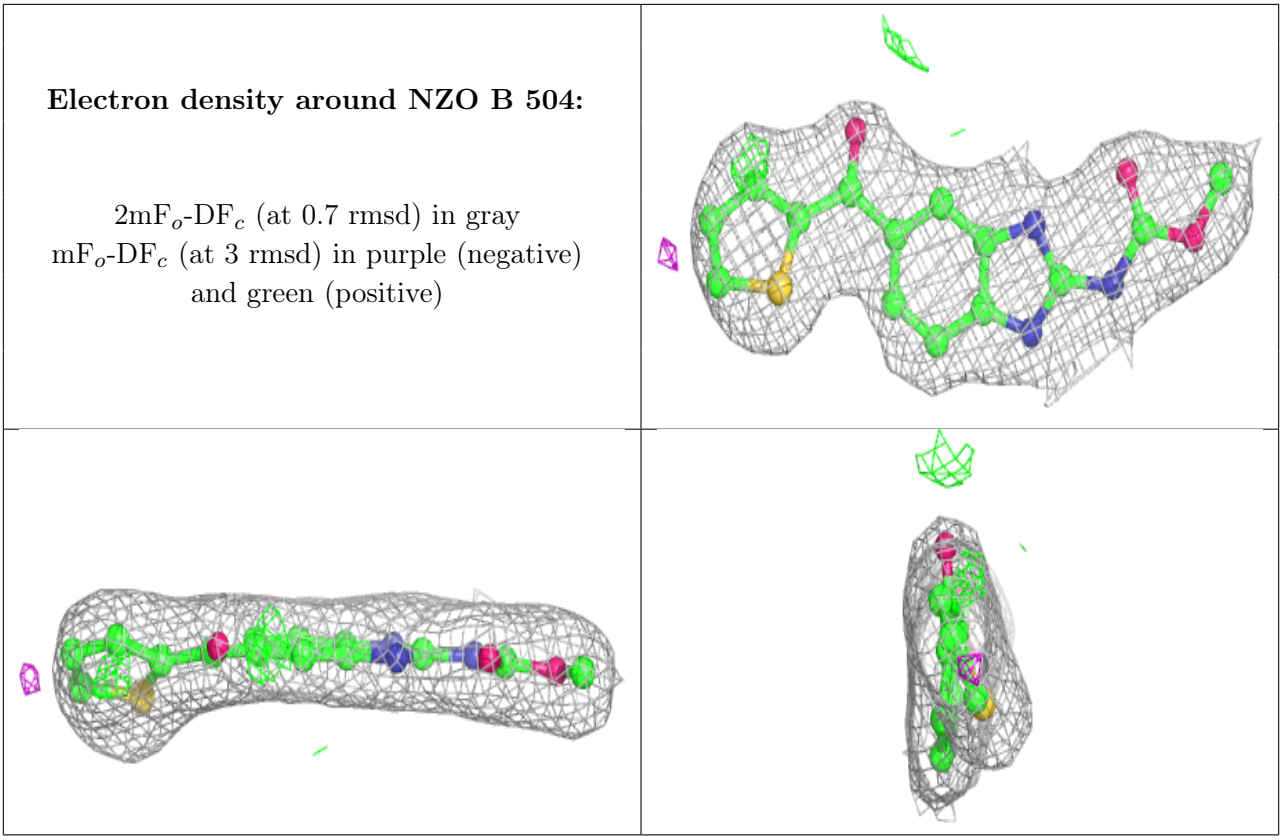
Electron density around GDP D 501:

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



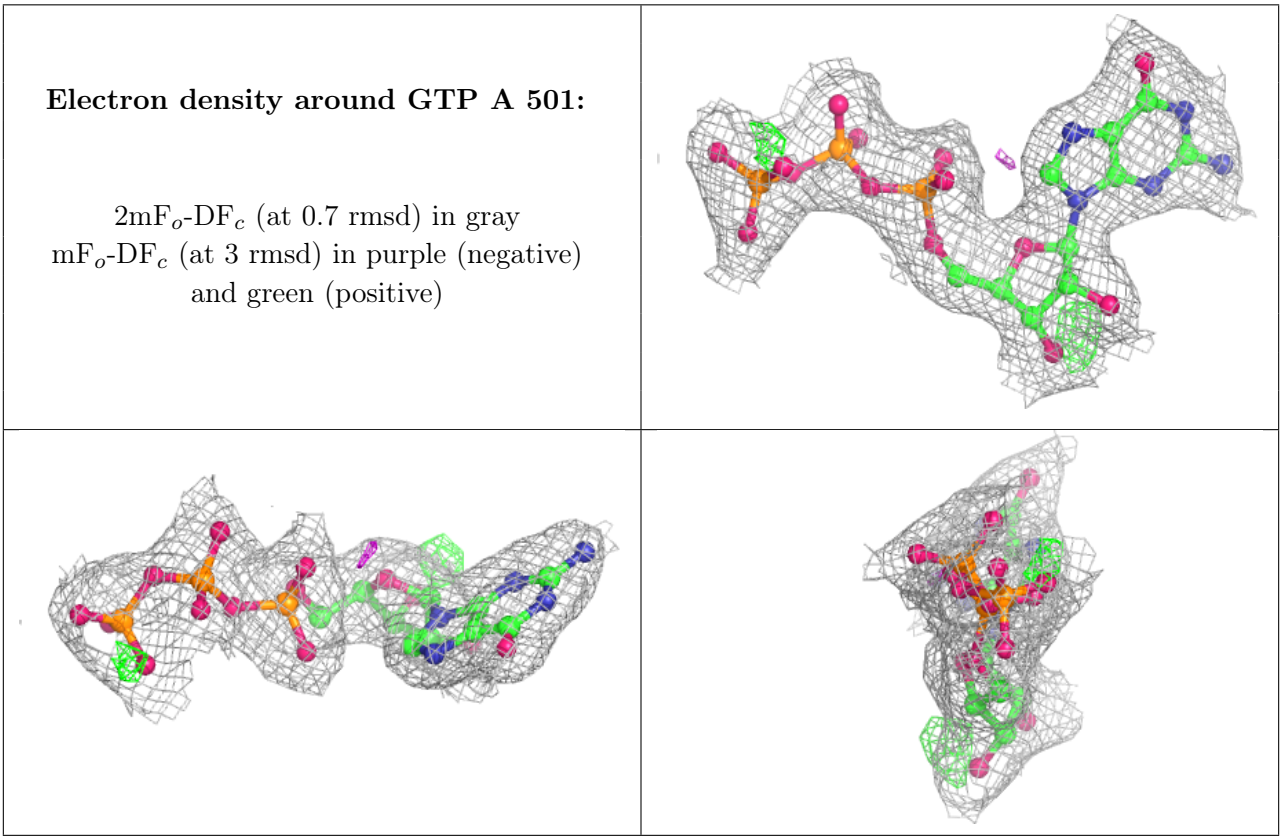
Electron density around NZO B 504:

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



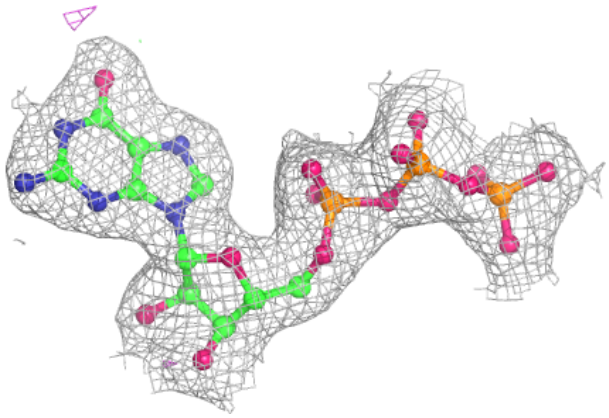
Electron density around GTP A 501:

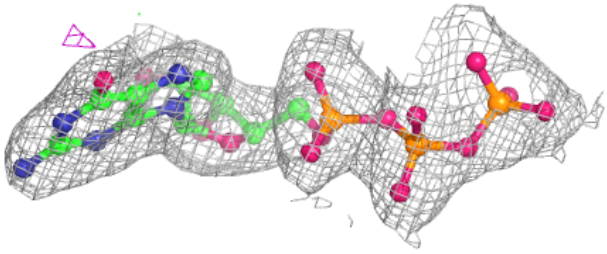
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

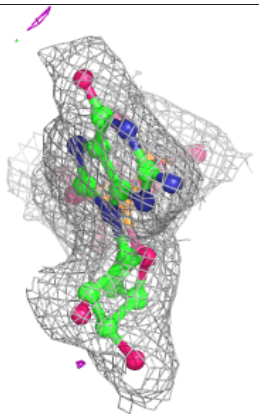


Electron density around GTP C 501:

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

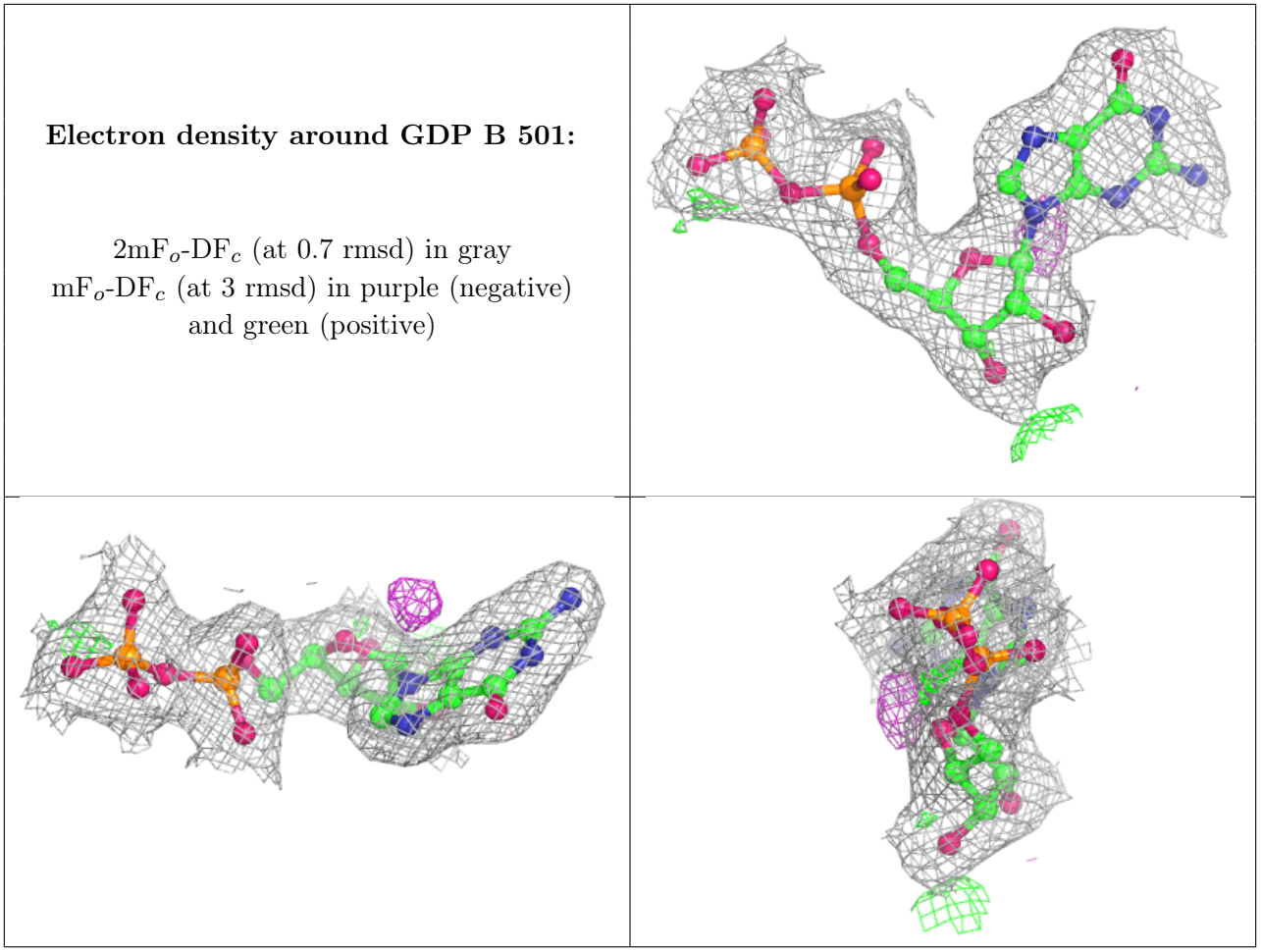






Electron density around GDP B 501:

$2mF_o$-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.