Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 11:42 AM EDT

PDB ID	:	4O4J
Title	:	Tubulin-Peloruside A complex
Authors	:	Prota, A.E.; Bargsten, K.; Northcote, P.T.; Marsh, M.; Altmann, K.H.; Miller, J.H.; Diaz, J.F.; Steinmetz, M.O.
Deposited on	:	2013-12-18
Resolution	:	2.20 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:

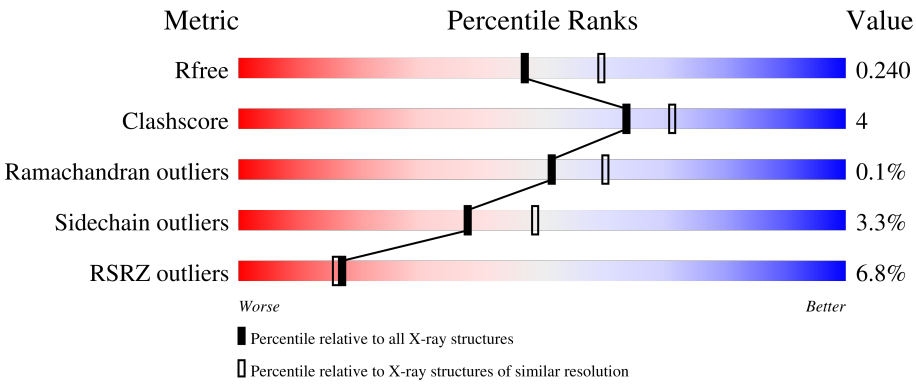
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	451	.% 90% 7% • •
1	C	451	90% 6% • •
2	B	445	.% 86% 9% • •
2	D	445	3% 83% 14% •
3	E	143	.% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	32% 50% 16% • 31%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18124 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
			Total	C	N	O	S			
1	A	439	3485	2213	587	661	24	0	12	0
1	C	440	3496	2218	585	667	26	0	15	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3424	2151	581	664	28	0	12	0
2	D	431	3413	2145	580	659	29	0	6	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1044	645	188	206	5	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

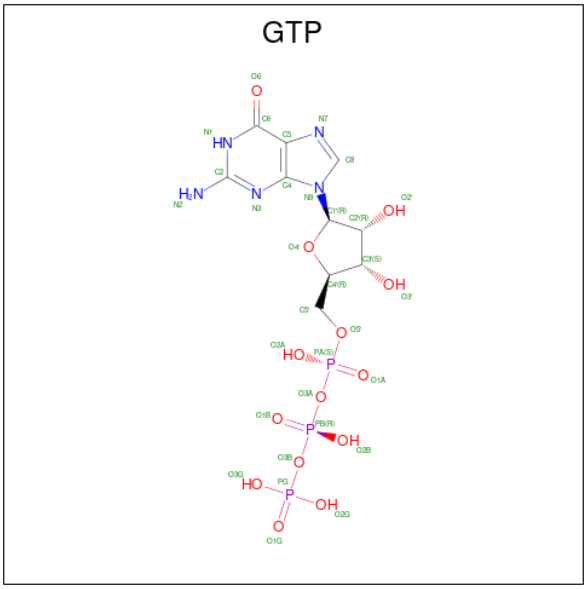
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	265	2179	1409	370	386	14	0	1	0

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		

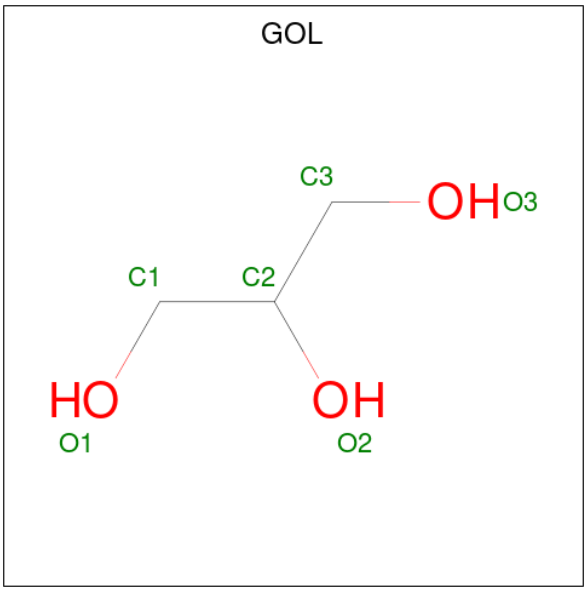
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		
6	D	1	Total	Mg	0	0
			1	1		

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

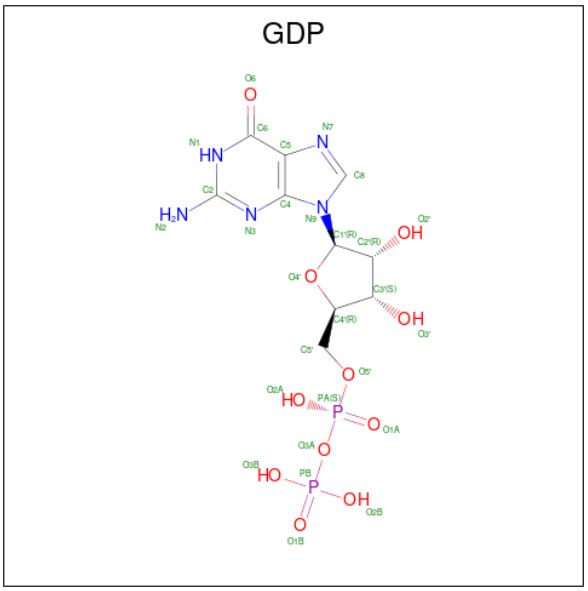
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0

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



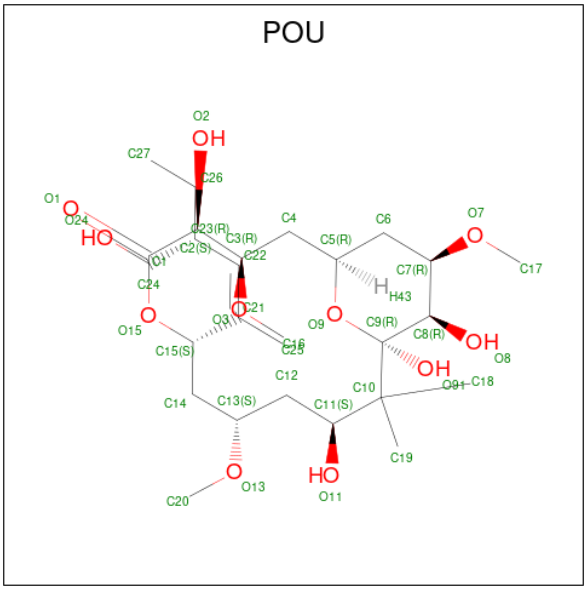
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0

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



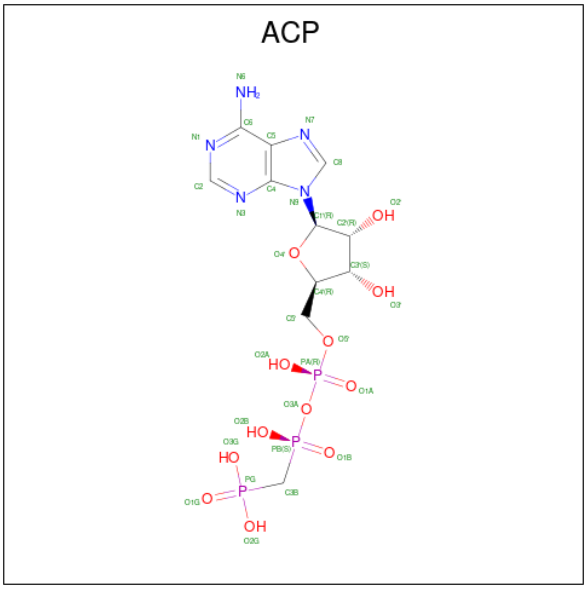
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
9	D	1	28	10	5	11	2	0	0

- Molecule 10 is Peloruside A (three-letter code: POU) (formula: $C_{27}H_{48}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	B	1	38	27	11	0	0
			Total	C	O		
10	D	1	38	27	11	0	0

- Molecule 11 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
			Total	C	N	O	P		
11	F	1	31	11	5	12	3	0	0

- Molecule 12 is water.

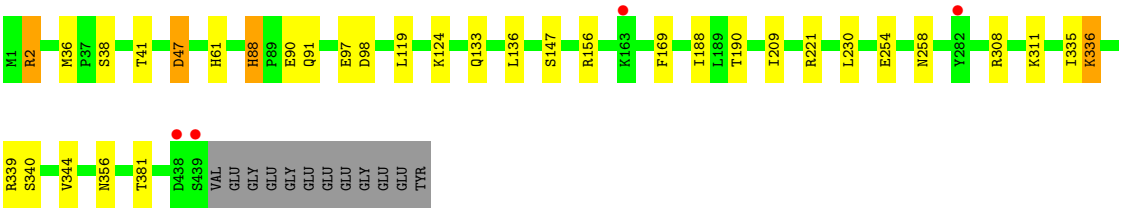
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	191	191	191	0	0
12	B	210	210	210	0	0
12	C	264	264	264	0	0
12	D	116	116	116	0	0
12	E	43	43	43	0	0
12	F	21	21	21	0	0

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.

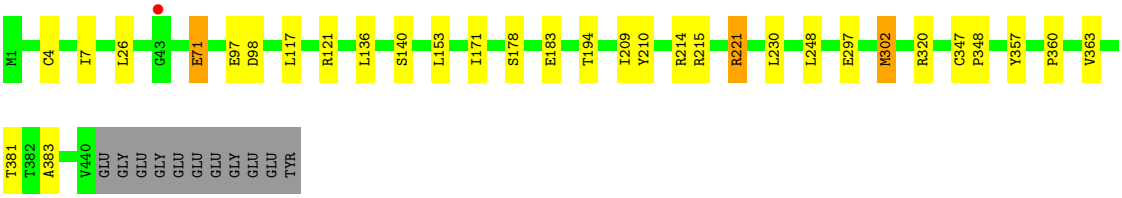
• Molecule 1: Tubulin alpha-1B chain

Chain A:



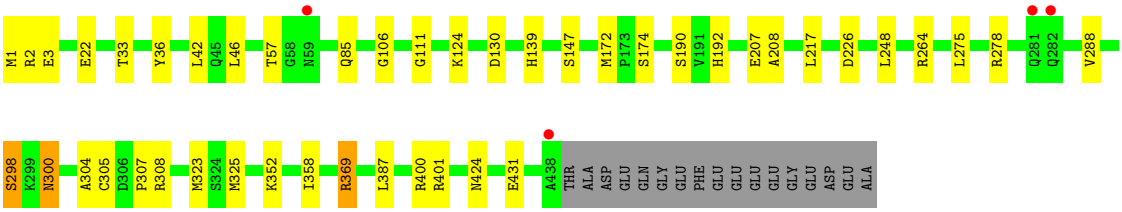
• Molecule 1: Tubulin alpha-1B chain

Chain C:



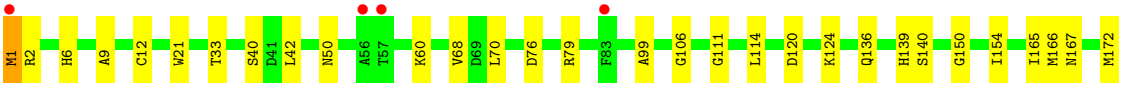
• Molecule 2: Tubulin beta-2B chain

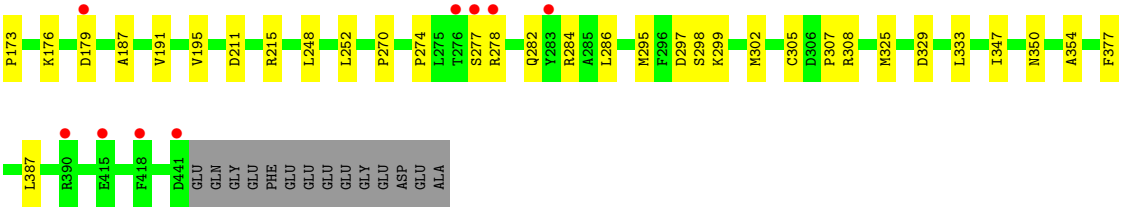
Chain B:



• Molecule 2: Tubulin beta-2B chain

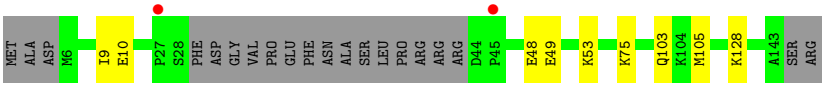
Chain D:





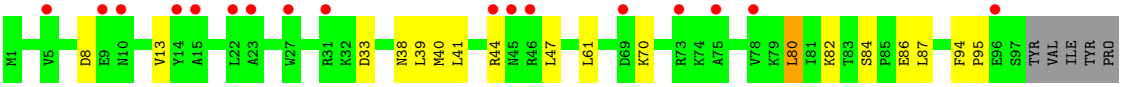
- Molecule 3: Stathmin-4

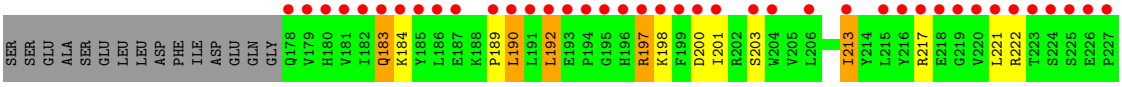
Chain E:

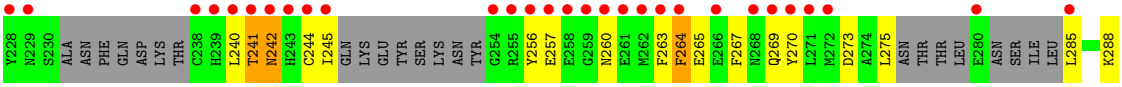


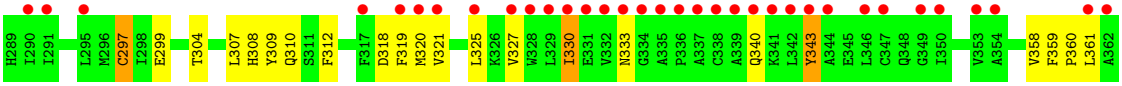
- Molecule 4: Tubulin-tyrosine ligase

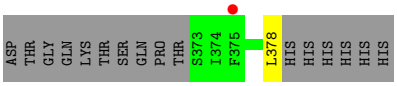
Chain F:











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.37Å 157.84Å 180.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.30 – 2.20 72.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.30-2.20) 99.7 (72.30-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.201 , 0.239 0.201 , 0.240	Depositor DCC
R_{free} test set	7568 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18124	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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 (i)

5.1 Standard geometry (i)

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

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	0.29	0/3599	0.47	0/4887
1	C	0.35	0/3619	0.51	0/4917
2	B	0.31	0/3532	0.48	0/4783
2	D	0.27	0/3506	0.45	0/4751
3	E	0.28	0/1071	0.38	0/1423
4	F	0.25	0/2230	0.46	0/3006
All	All	0.30	0/17557	0.47	0/23767

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3485	0	3436	17	0
1	C	3496	0	3440	22	0
2	B	3424	0	3319	29	0
2	D	3413	0	3310	35	0
3	E	1044	0	1068	4	0
4	F	2179	0	2178	36	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	38	0	48	3	0
10	D	38	0	48	2	0
11	F	31	0	14	1	0
12	A	191	0	0	1	0
12	B	210	0	0	5	0
12	C	264	0	0	4	0
12	D	116	0	0	2	0
12	E	43	0	0	1	0
12	F	21	0	0	0	0
All	All	18124	0	16917	143	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 4.

All (143) 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)
3:E:9:ILE:HG22	3:E:10:GLU:HG3	1.70	0.74
1:C:381:THR:HG22	1:C:383:ALA:H	1.51	0.73
2:B:298:SER:HB3	2:B:307:PRO:HD2	1.71	0.71
2:B:22:GLU:OE2	12:B:802:HOH:O	2.09	0.70
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.23	0.70
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.73	0.68
4:F:61[B]:LEU:HG	4:F:310:GLN:HB2	1.76	0.68
2:D:2:ARG:HH21	2:D:50:ASN:HB2	1.63	0.64
4:F:318:ASP:HB3	4:F:330:ILE:HD12	1.79	0.64
2:D:176:LYS:NZ	2:D:211:ASP:OD1	2.24	0.63
4:F:321:VAL:HG12	4:F:327:VAL:HG22	1.80	0.62
1:A:356:ASN:ND2	12:A:664:HOH:O	2.31	0.62
1:C:297:GLU:OE2	12:C:755:HOH:O	2.16	0.61
3:E:53:LYS:NZ	12:E:217:HOH:O	2.34	0.60
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.84	0.59
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.20	0.59
1:A:47:ASP:N	1:A:47:ASP:OD1	2.35	0.58
2:B:217:LEU:O	12:B:795:HOH:O	2.17	0.58
4:F:13:VAL:HA	4:F:343:TYR:HE1	1.69	0.57
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.51	0.57
4:F:269:GLN:O	4:F:273:ASP:N	2.32	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.57
4:F:263:PHE:O	4:F:265:GLU:N	2.39	0.56
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.87	0.55
4:F:201:ILE:O	4:F:319:PHE:N	2.32	0.55
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.89	0.55
4:F:242:ASN:N	4:F:242:ASN:OD1	2.40	0.53
2:B:264:ARG:NE	2:B:431[A]:GLU:OE2	2.34	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.52
2:D:76:ASP:OD1	2:D:79:ARG:NH1	2.40	0.52
4:F:242:ASN:O	4:F:245:ILE:N	2.38	0.52
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.92	0.51
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.92	0.51
4:F:201:ILE:HB	4:F:319:PHE:HB2	1.92	0.51
2:D:215:ARG:NH1	12:D:652:HOH:O	2.40	0.51
1:A:97:GLU:HB2	2:B:1:MET:HG2	1.93	0.50
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.50
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.94	0.50
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.94	0.50
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.49
4:F:190:LEU:HB2	4:F:321:VAL:HG23	1.94	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.49
2:B:208:ALA:HB2	2:B:304:ALA:N	2.26	0.49
2:D:120:ASP:O	2:D:124:LYS:HG2	2.12	0.49
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.94	0.49
2:B:305:CYS:O	2:B:307:PRO:HD3	2.11	0.49
2:B:300:ASN:O	12:B:798:HOH:O	2.20	0.49
4:F:61[A]:LEU:HD11	4:F:312:PHE:HD2	1.77	0.49
1:A:308:ARG:HG2	1:A:340:SER:HB3	1.95	0.48
2:D:173:PRO:HG2	2:D:187:ALA:HB2	1.95	0.48
2:B:42:LEU:HB3	2:B:358:ILE:HD11	1.96	0.48
2:B:226:ASP:HA	2:B:278:ARG:HD2	1.95	0.48
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.53	0.48
2:B:304:ALA:N	12:B:616:HOH:O	2.46	0.48
1:C:360:PRO:HB2	12:C:787:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:213:ILE:HB	4:F:378:LEU:HB2	1.96	0.48
12:B:649:HOH:O	3:E:75:LYS:HD2	2.15	0.47
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.96	0.47
2:B:226:ASP:OD1	2:B:278:ARG:NH2	2.40	0.47
2:B:248:LEU:HD11	2:B:352:LYS:HB3	1.96	0.47
1:C:221:ARG:HD2	2:D:329:ASP:OD2	2.15	0.47
2:D:277:SER:O	2:D:278:ARG:HB3	2.14	0.47
1:C:97:GLU:HG3	2:D:1:MET:HE3	1.97	0.47
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.15	0.47
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.30	0.46
1:C:381:THR:HG23	12:C:626:HOH:O	2.15	0.46
4:F:86:GLU:OE2	4:F:297:CYS:HA	2.15	0.46
4:F:257:GLU:HB2	4:F:260:ASN:HA	1.98	0.46
2:D:297:ASP:OD2	2:D:299:LYS:NZ	2.37	0.46
4:F:221:LEU:HD21	4:F:267:PHE:CG	2.50	0.46
4:F:80:LEU:O	4:F:84:SER:OG	2.22	0.46
10:D:503:POU:H27	10:D:503:POU:O15	2.16	0.45
10:D:503:POU:H46	10:D:503:POU:H40	1.80	0.45
3:E:128:LYS:HA	3:E:128:LYS:HD3	1.72	0.45
2:D:33:THR:O	2:D:60:LYS:NZ	2.35	0.45
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.71	0.45
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.99	0.45
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.45
1:A:136[B]:LEU:HD23	1:A:169:PHE:HE2	1.82	0.44
1:A:221:ARG:HG3	2:B:325:MET:HB3	1.99	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.44
11:F:401:ACP:O2G	11:F:401:ACP:O2B	2.35	0.44
4:F:192:LEU:HA	4:F:270:TYR:CZ	2.53	0.44
1:C:26:LEU:HD12	1:C:363[B]:VAL:HG12	2.00	0.44
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.17	0.44
4:F:61[B]:LEU:CD1	4:F:358:VAL:HG11	2.48	0.44
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
4:F:94:PHE:HA	4:F:95:PRO:HD2	1.88	0.43
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.00	0.43
2:B:33:THR:HG22	2:B:85:GLN:NE2	2.33	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.00	0.43
2:B:275:LEU:HD23	2:B:275:LEU:HA	1.88	0.43
2:D:172:MET:HA	2:D:173:PRO:HD3	1.85	0.43
2:D:305:CYS:SG	2:D:387:LEU:HB2	2.57	0.43
4:F:222:ARG:HB3	4:F:241:THR:OG1	2.17	0.43
2:B:2:ARG:HD2	2:B:130:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:61[B]:LEU:HD11	4:F:358:VAL:HG11	1.99	0.43
2:B:192:HIS:CE1	2:B:424:ASN:HD22	2.36	0.43
4:F:82:LYS:HE3	4:F:82:LYS:HB2	1.71	0.43
10:B:503:POU:H40	10:B:503:POU:H46	1.91	0.43
4:F:8:ASP:OD2	4:F:44:ARG:NH1	2.52	0.43
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.00	0.43
1:C:209:ILE:HD11	1:C:302:MET:HG3	2.00	0.43
2:D:40:SER:OG	2:D:42:LEU:HB2	2.19	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.43
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.01	0.42
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.53	0.42
1:C:97:GLU:HG3	2:D:1:MET:HB2	2.02	0.42
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.55	0.42
2:D:333:LEU:HG	12:D:642:HOH:O	2.20	0.42
1:C:347[A]:CYS:HA	1:C:348:PRO:HD3	1.93	0.42
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.50	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.19	0.42
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.02	0.42
2:D:150:GLY:O	2:D:154:ILE:HG12	2.20	0.42
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.55	0.42
2:B:2:ARG:HG3	2:B:3:GLU:OE2	2.20	0.42
4:F:330:ILE:H	4:F:330:ILE:HG13	1.64	0.42
1:C:194[B]:THR:HG21	12:C:617:HOH:O	2.19	0.42
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.02	0.42
1:A:311:LYS:HD3	1:A:344:VAL:HA	2.02	0.41
2:B:124:LYS:HB2	2:B:124:LYS:HE3	1.86	0.41
10:B:503:POU:H27	10:B:503:POU:O15	2.20	0.41
4:F:358:VAL:O	4:F:360:PRO:HD3	2.21	0.41
1:C:221:ARG:HD3	2:D:325:MET:SD	2.61	0.41
4:F:40:MET:HE1	4:F:47:LEU:HG	2.03	0.41
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.03	0.41
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.21	0.41
2:D:298:SER:OG	2:D:307:PRO:HD2	2.21	0.41
4:F:84:SER:OG	4:F:87:LEU:HB3	2.20	0.41
2:D:9:ALA:HA	2:D:68:VAL:O	2.21	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.04	0.40
10:B:503:POU:H32	10:B:503:POU:H8	1.89	0.40
4:F:183:GLN:HG2	4:F:184:LYS:N	2.36	0.40
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.21	0.40
2:B:369:ARG:HE	2:B:369:ARG:HB2	1.49	0.40
2:D:70:LEU:HD23	2:D:114:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:274:PRO:HB3	2:D:286:LEU:HD21	2.03	0.40
2:D:297:ASP:OD1	2:D:298:SER:N	2.55	0.40
4:F:318:ASP:HB2	4:F:330:ILE:O	2.21	0.40
4:F:307:LEU:HD13	4:F:309:TYR:CE1	2.56	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	449/451 (100%)	440 (98%)	9 (2%)	0	100	100
1	C	453/451 (100%)	441 (97%)	12 (3%)	0	100	100
2	B	438/445 (98%)	430 (98%)	8 (2%)	0	100	100
2	D	435/445 (98%)	421 (97%)	14 (3%)	0	100	100
3	E	125/143 (87%)	123 (98%)	2 (2%)	0	100	100
4	F	253/384 (66%)	239 (94%)	12 (5%)	2 (1%)	19	19
All	All	2153/2319 (93%)	2094 (97%)	57 (3%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	264	PHE
4	F	189	PRO

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	382/379 (101%)	372 (97%)	10 (3%)	46	58
1	C	386/379 (102%)	382 (99%)	4 (1%)	76	86
2	B	382/383 (100%)	376 (98%)	6 (2%)	62	76
2	D	378/383 (99%)	372 (98%)	6 (2%)	62	76
3	E	116/127 (91%)	112 (97%)	4 (3%)	37	47
4	F	241/342 (70%)	211 (88%)	30 (12%)	4	4
All	All	1885/1993 (95%)	1825 (97%)	60 (3%)	38	50

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	38	SER
1	A	41	THR
1	A	47	ASP
1	A	88	HIS
1	A	90	GLU
1	A	124	LYS
1	A	188	ILE
1	A	336	LYS
1	A	381	THR
2	B	57	THR
2	B	139	HIS
2	B	298	SER
2	B	300	ASN
2	B	308	ARG
2	B	369	ARG
1	C	71	GLU
1	C	215	ARG
1	C	221	ARG
1	C	302	MET
2	D	1	MET
2	D	139	HIS
2	D	179	ASP
2	D	282	GLN
2	D	284	ARG
2	D	308	ARG
3	E	48	GLU

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Mol	Chain	Res	Type
3	E	49	GLU
3	E	103	GLN
3	E	105	MET
4	F	33	ASP
4	F	70	LYS
4	F	80	LEU
4	F	183	GLN
4	F	190	LEU
4	F	192	LEU
4	F	197	ARG
4	F	198	LYS
4	F	203	SER
4	F	213	ILE
4	F	217	ARG
4	F	240	LEU
4	F	241	THR
4	F	242	ASN
4	F	244	CYS
4	F	256	TYR
4	F	264	PHE
4	F	275	LEU
4	F	285	LEU
4	F	288	LYS
4	F	297	CYS
4	F	299	GLU
4	F	308	HIS
4	F	320	MET
4	F	325	LEU
4	F	330	ILE
4	F	333	ASN
4	F	340	GLN
4	F	343	TYR
4	F	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.48	7 (21%)
11	ACP	F	401	-	27,33,33	1.42	5 (18%)	32,52,52	1.44	4 (12%)
9	GDP	D	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.07	3 (10%)
8	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.28	0
5	GTP	C	501	6	26,34,34	1.14	1 (3%)	32,54,54	1.39	6 (18%)
10	POU	B	503	-	37,39,39	2.39	8 (21%)	44,57,57	2.08	11 (25%)
10	POU	D	503	-	37,39,39	2.21	6 (16%)	44,57,57	1.93	10 (22%)
9	GDP	B	501	6	24,30,30	1.00	1 (4%)	30,47,47	1.06	2 (6%)

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
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
11	ACP	F	401	-	-	10/15/38/38	0/3/3/3
9	GDP	D	501	-	-	3/12/32/32	0/3/3/3
8	GOL	A	504	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
10	POU	B	503	-	-	6/54/76/76	0/1/2/2
10	POU	D	503	-	-	6/54/76/76	0/1/2/2
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	POU	C22-C21	10.97	1.56	1.33
10	D	503	POU	C22-C21	9.81	1.54	1.33
10	B	503	POU	C2-C1	-5.21	1.39	1.52
10	D	503	POU	C2-C1	-5.05	1.39	1.52
5	C	501	GTP	C5-C6	-4.17	1.38	1.47
10	D	503	POU	C14-C15	4.14	1.60	1.53
5	A	501	GTP	C5-C6	-3.96	1.39	1.47
11	F	401	ACP	PB-O3A	3.04	1.61	1.58
11	F	401	ACP	PG-O2G	2.94	1.61	1.54
10	D	503	POU	C14-C13	2.81	1.59	1.52
11	F	401	ACP	PG-O3G	2.80	1.61	1.54
10	B	503	POU	O91-C9	2.79	1.44	1.39
10	D	503	POU	O91-C9	2.77	1.44	1.39
10	B	503	POU	C23-C22	2.63	1.54	1.50
9	B	501	GDP	C6-N1	-2.62	1.34	1.37
11	F	401	ACP	C5-C4	2.51	1.47	1.40
10	D	503	POU	C23-C22	2.29	1.53	1.50
9	D	501	GDP	C6-N1	-2.28	1.34	1.37
11	F	401	ACP	PB-O2B	2.25	1.61	1.56
10	B	503	POU	C14-C15	2.22	1.56	1.53
10	B	503	POU	C14-C13	2.22	1.57	1.52
10	B	503	POU	O11-C11	2.15	1.47	1.43
10	B	503	POU	C9-C8	-2.10	1.51	1.53
5	A	501	GTP	C2-N3	2.07	1.38	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	503	POU	C13-C12-C11	-6.36	104.62	114.37
10	D	503	POU	C13-C12-C11	-6.12	104.98	114.37
10	B	503	POU	C15-O15-C1	5.39	126.93	116.67
10	B	503	POU	O9-C9-C8	5.09	112.89	105.50
10	D	503	POU	O9-C9-C8	4.66	112.27	105.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	503	POU	C15-O15-C1	4.26	124.79	116.67
10	B	503	POU	O15-C15-C21	3.69	119.58	109.48
10	D	503	POU	C3-C4-C5	-3.52	106.62	114.76
11	F	401	ACP	PB-O3A-PA	-3.34	121.97	132.56
10	D	503	POU	O15-C15-C14	3.27	113.87	106.64
11	F	401	ACP	N3-C2-N1	-3.26	123.58	128.68
5	C	501	GTP	C5-C6-N1	3.19	119.58	113.95
5	A	501	GTP	C8-N7-C5	3.14	108.97	102.99
10	B	503	POU	C3-C4-C5	-3.04	107.72	114.76
11	F	401	ACP	C4-C5-N7	-3.02	106.25	109.40
10	B	503	POU	O15-C15-C14	2.92	113.09	106.64
5	C	501	GTP	C2-N1-C6	-2.85	119.85	125.10
5	A	501	GTP	PB-O3B-PG	-2.73	123.46	132.83
10	D	503	POU	O13-C13-C12	2.71	114.87	108.27
10	D	503	POU	O15-C15-C21	2.68	116.81	109.48
9	D	501	GDP	PA-O3A-PB	-2.63	123.79	132.83
9	B	501	GDP	C8-N7-C5	2.59	107.92	102.99
10	D	503	POU	O91-C9-O9	-2.58	103.20	109.54
5	A	501	GTP	O2G-PG-O3B	2.57	113.25	104.64
5	A	501	GTP	C5-C6-N1	2.56	118.48	113.95
5	C	501	GTP	C8-N7-C5	2.52	107.78	102.99
5	A	501	GTP	O5'-PA-O1A	-2.51	99.27	109.07
5	C	501	GTP	O6-C6-C5	-2.48	119.54	124.37
9	B	501	GDP	C5-C6-N1	2.47	118.32	113.95
5	C	501	GTP	PA-O3A-PB	-2.44	124.45	132.83
5	A	501	GTP	PA-O3A-PB	-2.43	124.48	132.83
5	C	501	GTP	PB-O3B-PG	-2.43	124.49	132.83
9	D	501	GDP	C8-N7-C5	2.39	107.54	102.99
10	B	503	POU	O91-C9-O9	-2.28	103.94	109.54
10	B	503	POU	C4-C3-C2	-2.28	108.00	113.27
10	B	503	POU	C25-C21-C22	-2.22	117.60	123.45
10	B	503	POU	O13-C13-C12	2.22	113.66	108.27
9	D	501	GDP	C5-C6-N1	2.16	117.77	113.95
11	F	401	ACP	C2'-C3'-C4'	-2.16	98.44	102.64
10	B	503	POU	O9-C5-C6	2.08	112.84	108.94
5	A	501	GTP	C2-N1-C6	-2.06	121.30	125.10
10	D	503	POU	O9-C5-C6	2.05	112.80	108.94
10	D	503	POU	C13-C14-C15	-2.04	109.87	114.56

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
8	A	504	GOL	O1-C1-C2-O2
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	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	POU	C8-C7-O7-C17
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
8	A	504	GOL	O2-C2-C3-O3
10	B	503	POU	C15-C21-C22-C23
10	D	503	POU	C15-C21-C22-C23
10	D	503	POU	C8-C7-O7-C17
10	B	503	POU	C25-C21-C22-C23
10	D	503	POU	C25-C21-C22-C23
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
10	B	503	POU	C14-C13-O13-C20
11	F	401	ACP	C5'-O5'-PA-O3A
10	D	503	POU	C21-C15-O15-C1
5	C	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
10	D	503	POU	C6-C7-O7-C17
10	B	503	POU	C6-C7-O7-C17
5	A	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
10	D	503	POU	C12-C13-O13-C20
5	A	501	GTP	C4'-C5'-O5'-PA
9	B	501	GDP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O2A
10	B	503	POU	C21-C15-O15-C1

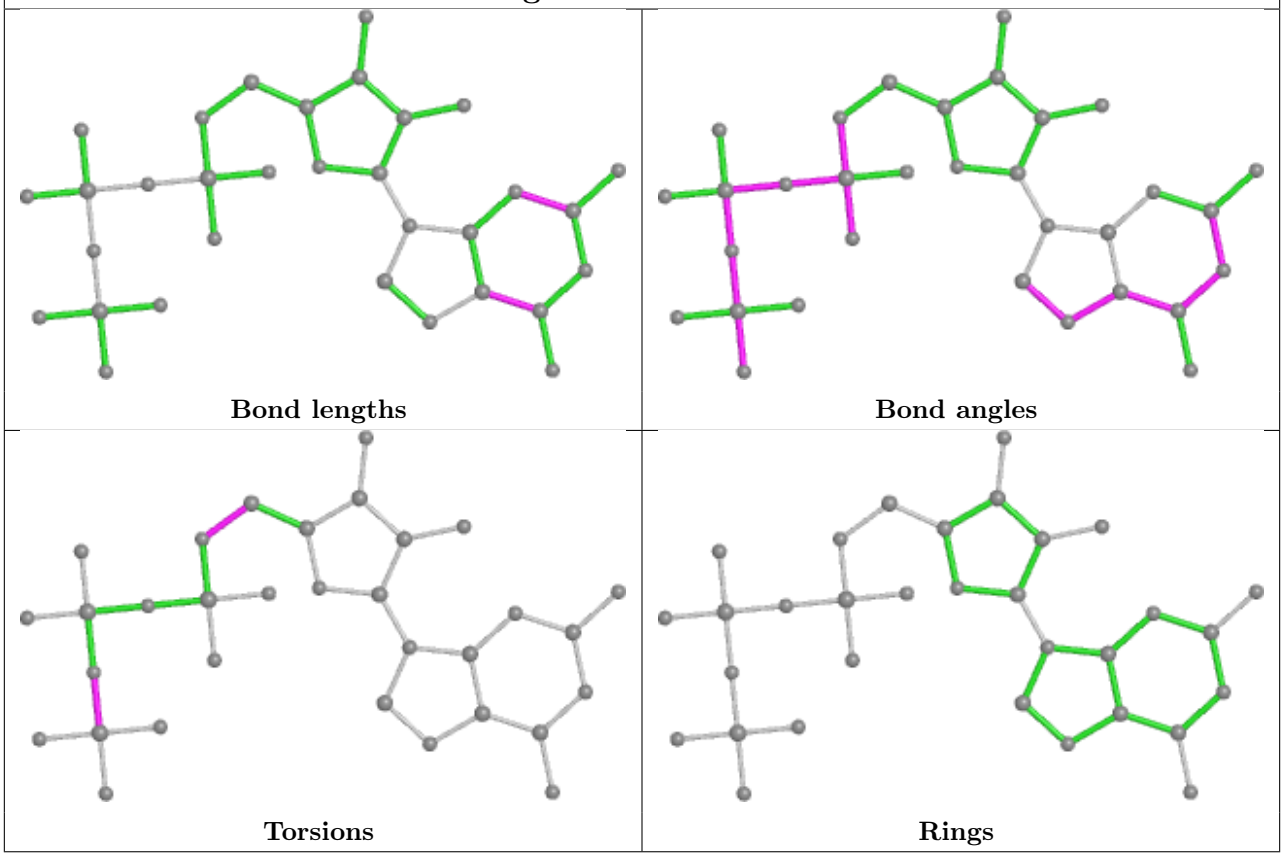
There are no ring outliers.

4 monomers are involved in 7 short contacts:

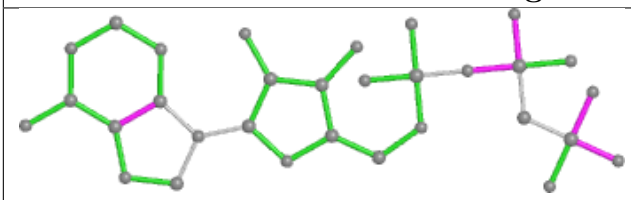
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
11	F	401	ACP	1	0
10	B	503	POU	3	0
10	D	503	POU	2	0

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.

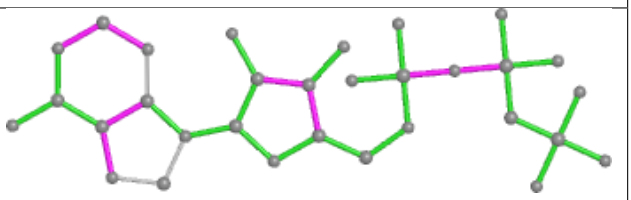
Ligand GTP A 501



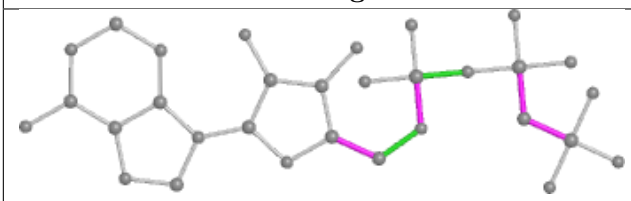
Ligand ACP F 401



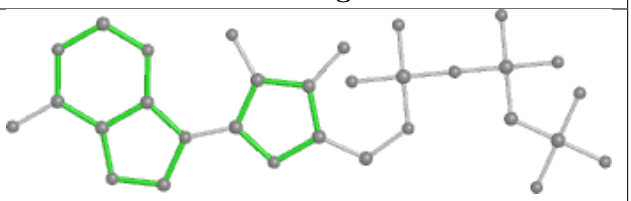
Bond lengths



Bond angles

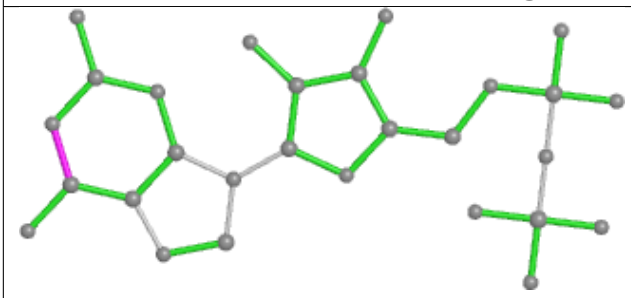


Torsions

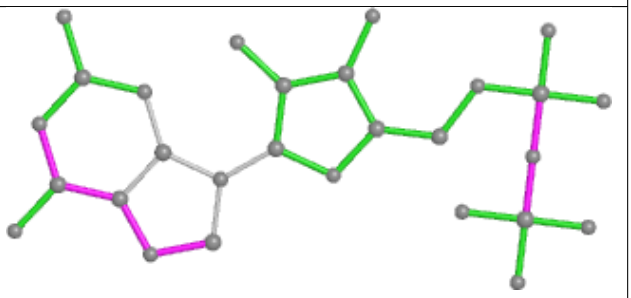


Rings

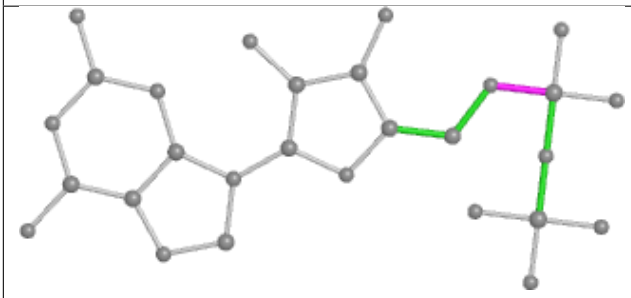
Ligand GDP D 501



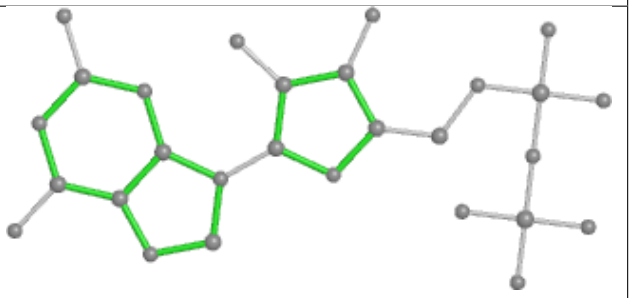
Bond lengths



Bond angles

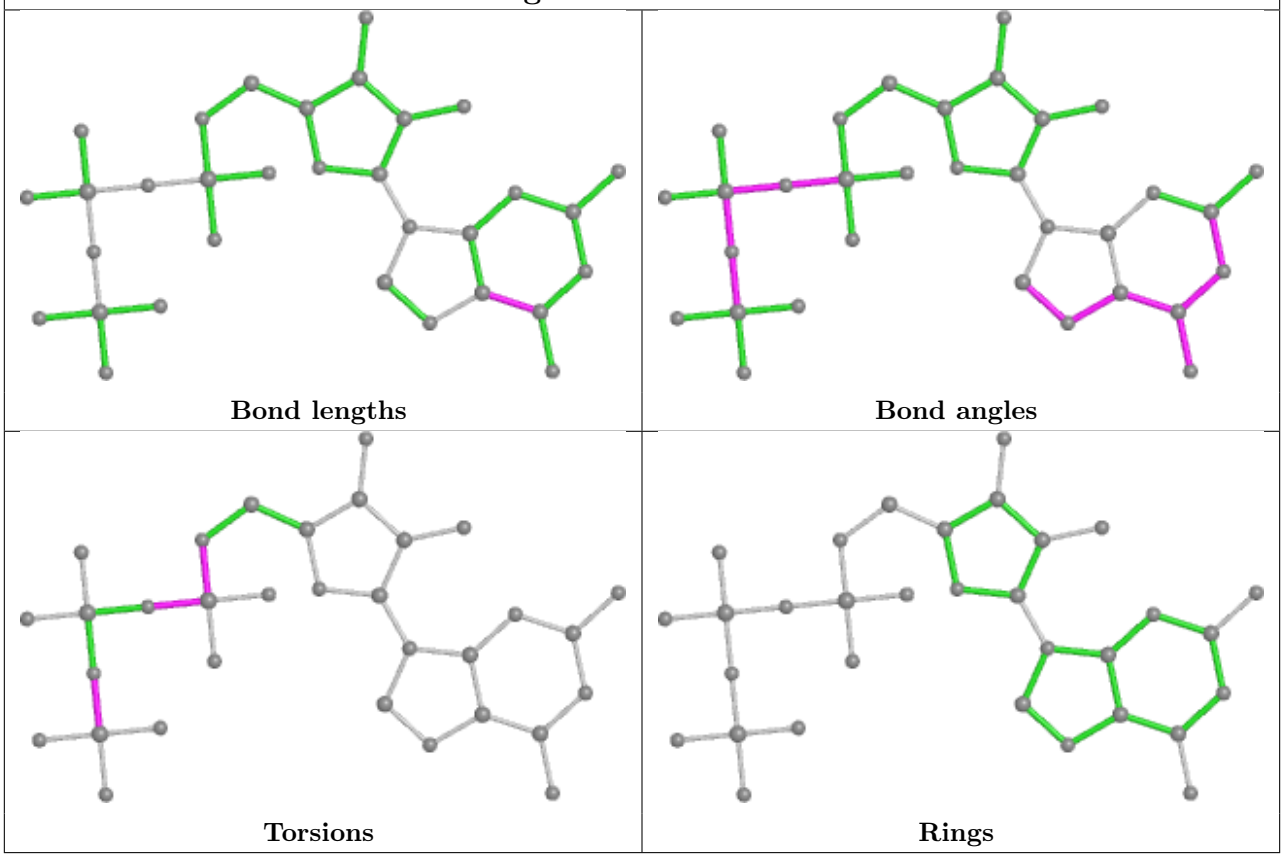


Torsions

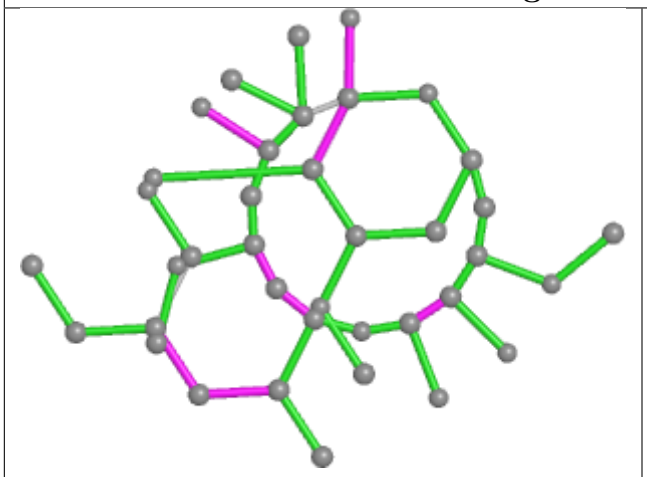


Rings

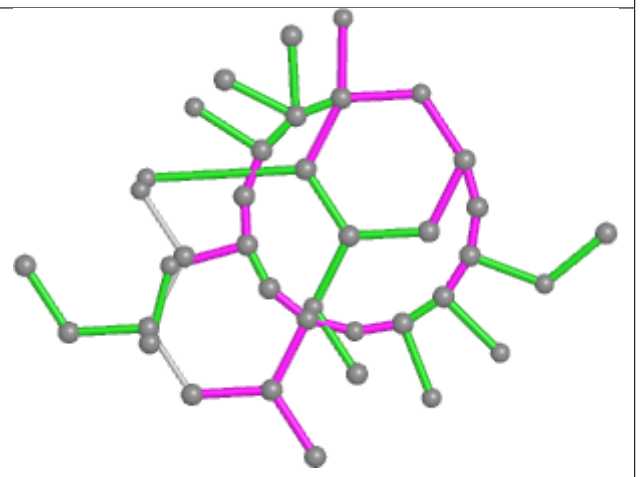
Ligand GTP C 501



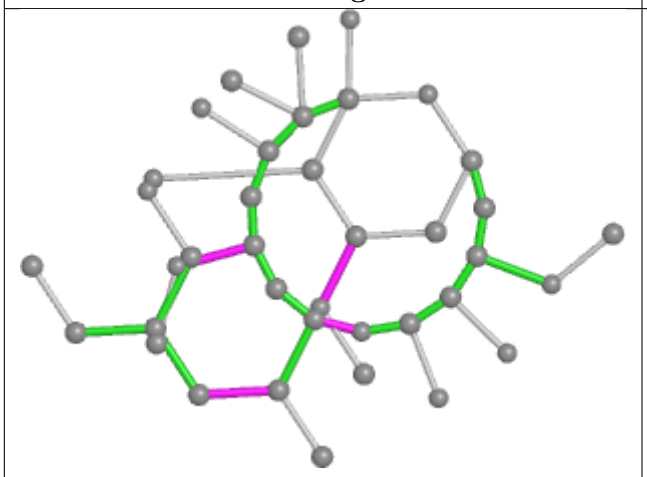
Ligand POU B 503



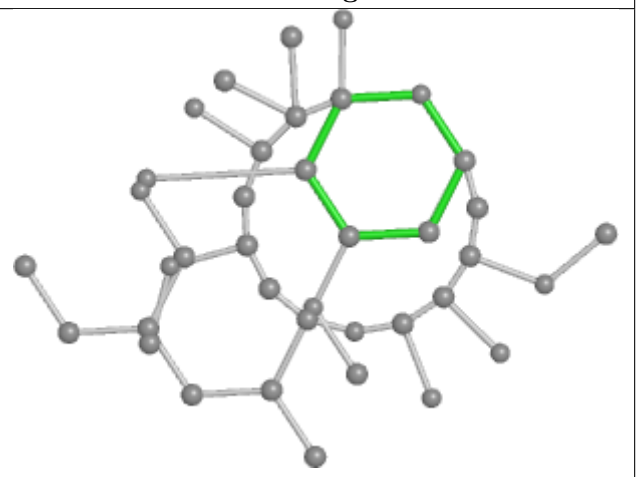
Bond lengths



Bond angles

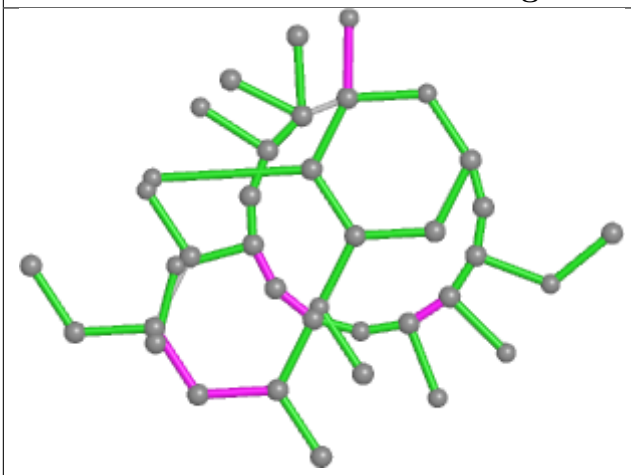


Torsions

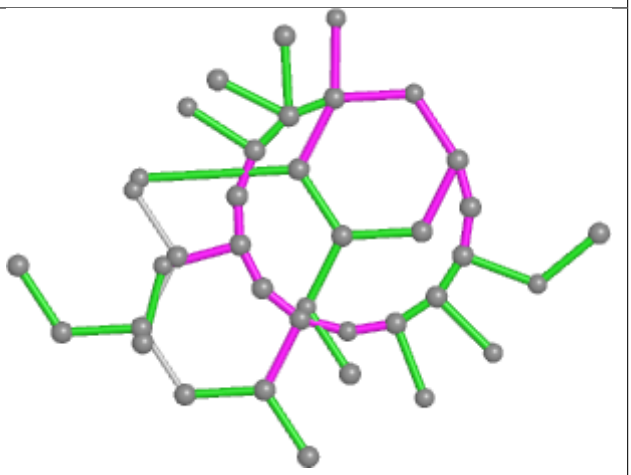


Rings

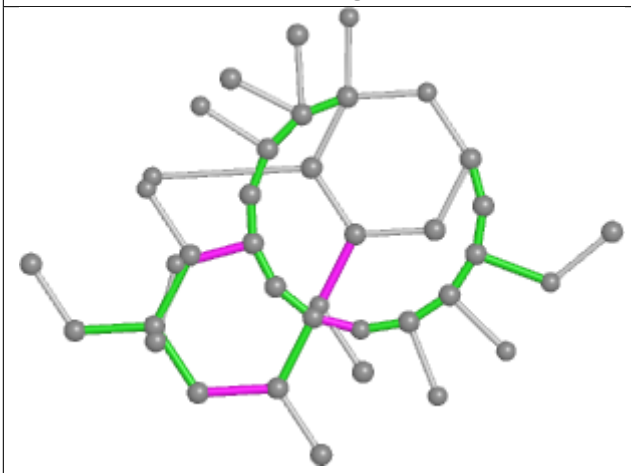
Ligand POU D 503



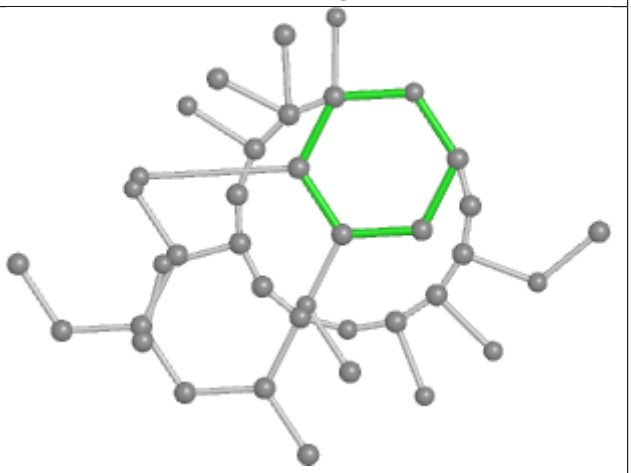
Bond lengths



Bond angles

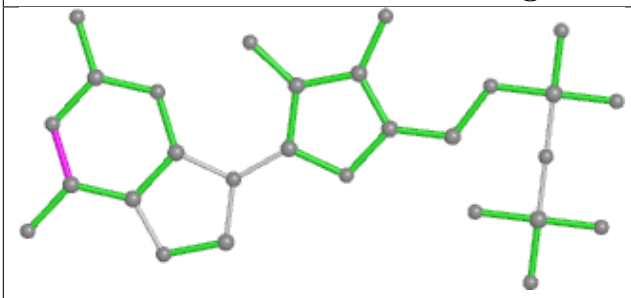


Torsions

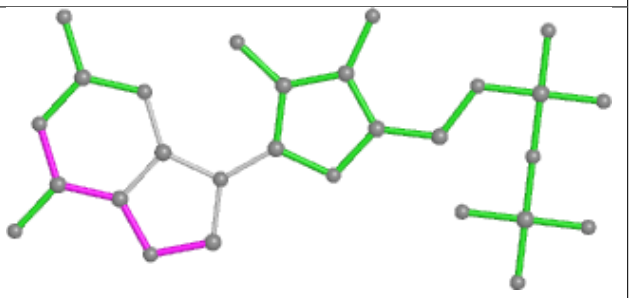


Rings

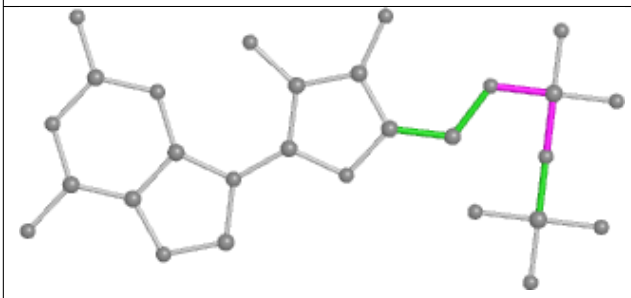
Ligand GDP B 501



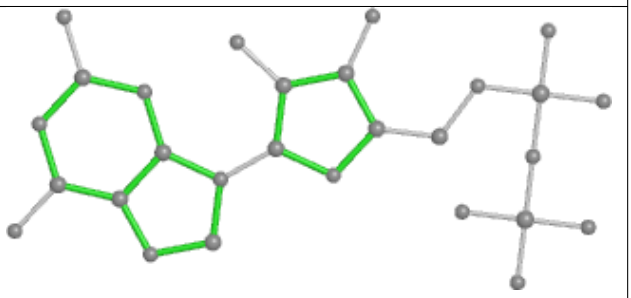
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.21	4 (0%)	84	83	17, 32, 66, 112	0
1	C	440/451 (97%)	-0.27	1 (0%)	95	94	11, 22, 45, 68	0
2	B	428/445 (96%)	-0.17	4 (0%)	84	83	13, 27, 60, 112	2 (0%)
2	D	431/445 (96%)	-0.01	13 (3%)	50	48	18, 44, 77, 102	6 (1%)
3	E	123/143 (86%)	0.11	2 (1%)	72	70	25, 44, 85, 121	0
4	F	265/384 (69%)	2.29	121 (45%)	0	0	39, 79, 123, 153	0
All	All	2126/2319 (91%)	0.15	145 (6%)	17	16	11, 35, 92, 153	8 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	12.4
4	F	182	ILE	10.5
4	F	240	LEU	9.2
4	F	241	THR	9.2
4	F	227	PRO	8.1
4	F	195	GLY	8.0
4	F	179	VAL	7.9
4	F	245	ILE	7.8
1	A	439	SER	7.3
4	F	178	GLN	7.1
4	F	244	CYS	7.0
4	F	192	LEU	6.8
4	F	243	HIS	6.7
4	F	338	CYS	6.6
4	F	44	ARG	6.5
4	F	375	PHE	6.4
4	F	238	CYS	6.4
4	F	184	LYS	6.1
1	A	282	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
4	F	255	ARG	6.0
4	F	258	GLU	5.9
4	F	199	PHE	5.7
4	F	271	LEU	5.7
4	F	201	ILE	5.7
4	F	183	GLN	5.4
4	F	229	ASN	5.4
4	F	362	ALA	5.4
4	F	198	LYS	5.3
4	F	346	LEU	5.2
4	F	75	ALA	5.2
4	F	190	LEU	5.1
4	F	330	ILE	5.0
4	F	216	TYR	5.0
4	F	180	HIS	5.0
4	F	181	VAL	4.9
4	F	221	LEU	4.9
4	F	319	PHE	4.8
4	F	225	SER	4.7
4	F	186	LEU	4.7
4	F	361	LEU	4.7
2	D	1	MET	4.6
4	F	269	GLN	4.6
2	B	282	GLN	4.6
4	F	223	THR	4.5
4	F	261	GLU	4.5
4	F	333	ASN	4.5
4	F	343	TYR	4.5
4	F	242	ASN	4.4
2	B	281	GLN	4.4
4	F	340	GLN	4.4
4	F	73	ARG	4.4
4	F	280	GLU	4.4
4	F	268	ASN	4.4
4	F	339	ALA	4.3
4	F	206	LEU	4.3
4	F	353	VAL	4.3
4	F	332	VAL	4.2
4	F	350	ILE	4.2
4	F	341	LYS	4.2
4	F	189	PRO	4.1
4	F	259	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	239	HIS	4.0
4	F	256	TYR	4.0
4	F	219	GLY	3.9
2	B	438	ALA	3.9
4	F	226	GLU	3.9
4	F	354	ALA	3.9
4	F	204	TRP	3.9
4	F	45	ASN	3.8
4	F	185	TYR	3.8
4	F	224	SER	3.7
4	F	257	GLU	3.7
4	F	263	PHE	3.6
4	F	329	LEU	3.6
4	F	218	GLU	3.6
4	F	337	ALA	3.6
2	D	57	THR	3.4
4	F	291	ILE	3.4
4	F	191	LEU	3.3
4	F	328	TRP	3.3
2	D	441	ASP	3.2
4	F	196	HIS	3.2
4	F	342	LEU	3.2
4	F	213	ILE	3.2
4	F	266	GLU	3.1
4	F	78	VAL	3.1
4	F	321	VAL	3.0
4	F	262	MET	3.0
4	F	46	ARG	3.0
4	F	325	LEU	3.0
4	F	193	GLU	3.0
4	F	9	GLU	3.0
4	F	327	VAL	2.9
4	F	200	ASP	2.8
4	F	187	GLU	2.8
4	F	23	ALA	2.8
4	F	290	ILE	2.8
3	E	27	PRO	2.8
4	F	320	MET	2.7
4	F	5	VAL	2.7
2	D	276	THR	2.7
4	F	220	VAL	2.7
4	F	15	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	179	ASP	2.6
4	F	27	TRP	2.6
2	B	59	ASN	2.6
4	F	96	GLU	2.6
4	F	336	PRO	2.6
2	D	83	PHE	2.5
2	D	277	SER	2.5
4	F	317	PHE	2.5
4	F	349	GLY	2.5
4	F	270	TYR	2.5
4	F	222	ARG	2.5
1	A	438	ASP	2.5
2	D	418	PHE	2.5
4	F	334	GLY	2.5
4	F	264	PHE	2.4
4	F	217	ARG	2.4
4	F	254	GLY	2.4
4	F	22	LEU	2.4
4	F	347	CYS	2.4
4	F	335	ALA	2.3
2	D	390	ARG	2.3
4	F	260	ASN	2.3
1	C	43	GLY	2.3
4	F	285	LEU	2.3
4	F	331	GLU	2.3
3	E	45	PRO	2.3
4	F	31	ARG	2.2
4	F	14	TYR	2.2
4	F	344	ALA	2.2
4	F	295	LEU	2.2
4	F	215	LEU	2.2
2	D	283	TYR	2.2
4	F	228	TYR	2.2
4	F	10	ASN	2.2
4	F	272	MET	2.2
1	A	163	LYS	2.2
2	D	415	GLU	2.2
2	D	56	ALA	2.1
4	F	197	ARG	2.1
4	F	203	SER	2.1
2	D	278	ARG	2.0
4	F	69	ASP	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)

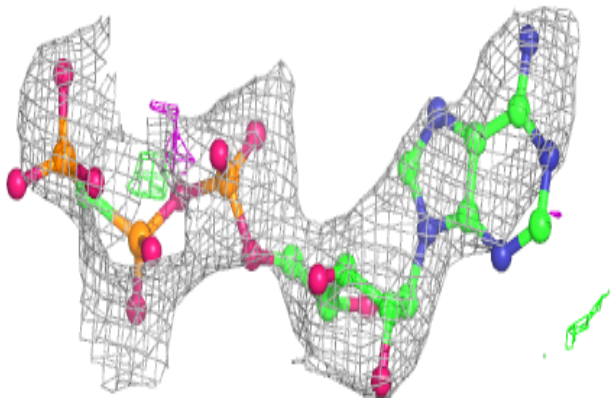
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

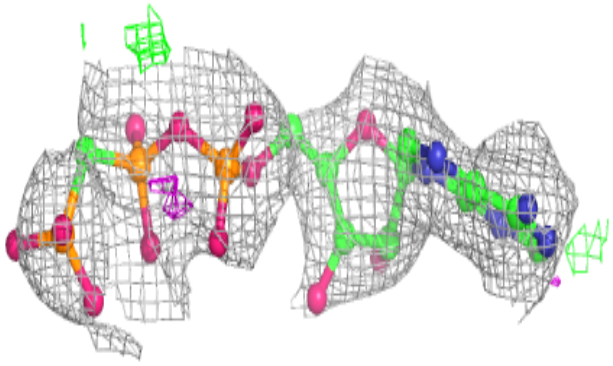
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	502	1/1	0.55	0.19	67,67,67,67	0
7	CA	A	503	1/1	0.56	0.14	68,68,68,68	0
11	ACP	F	401	31/31	0.78	0.29	67,106,145,166	0
8	GOL	A	504	6/6	0.88	0.23	57,60,60,62	0
10	POU	D	503	38/38	0.89	0.16	35,59,74,77	0
10	POU	B	503	38/38	0.89	0.13	23,44,77,81	0
6	MG	C	502	1/1	0.95	0.14	18,18,18,18	0
6	MG	A	502	1/1	0.96	0.10	14,14,14,14	0
9	GDP	D	501	28/28	0.97	0.11	27,36,45,53	0
5	GTP	A	501	32/32	0.98	0.12	10,17,22,41	0
6	MG	B	502	1/1	0.99	0.14	9,9,9,9	0
9	GDP	B	501	28/28	0.99	0.14	11,16,20,22	0
5	GTP	C	501	32/32	0.99	0.13	4,13,19,30	0

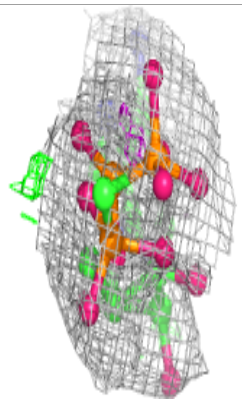
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

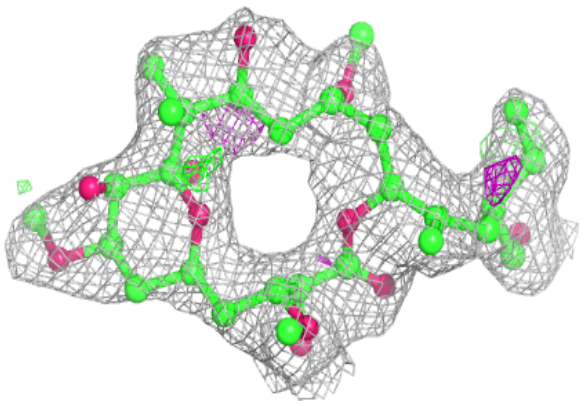


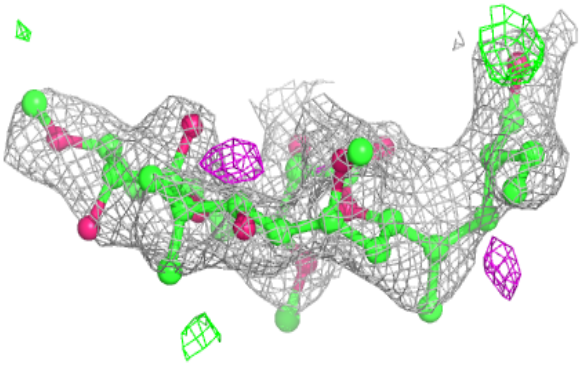


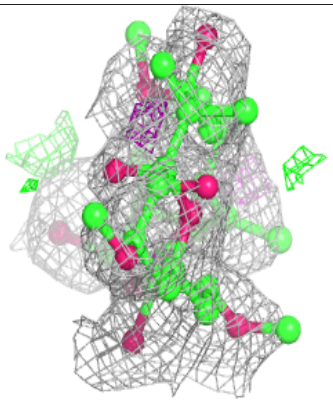


Electron density around POU D 503:

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

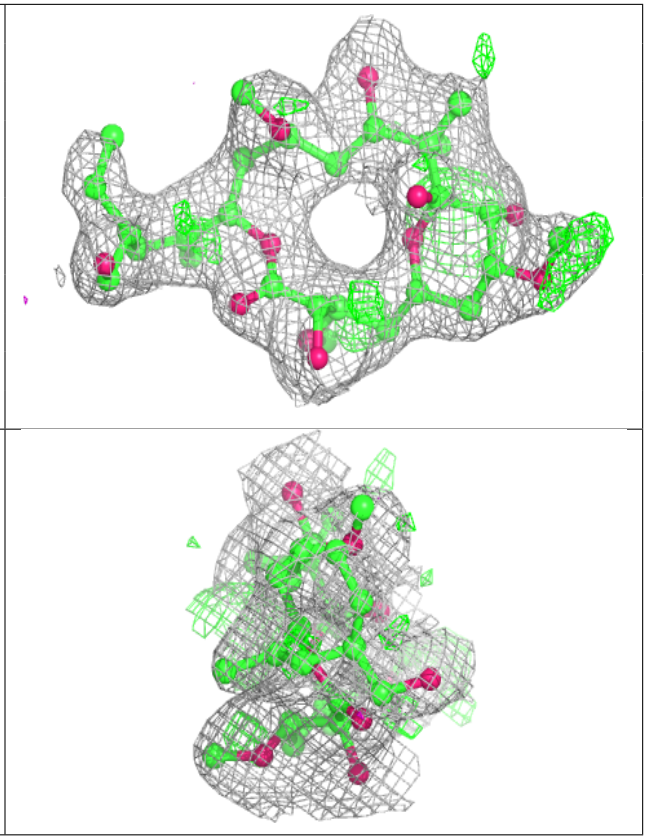






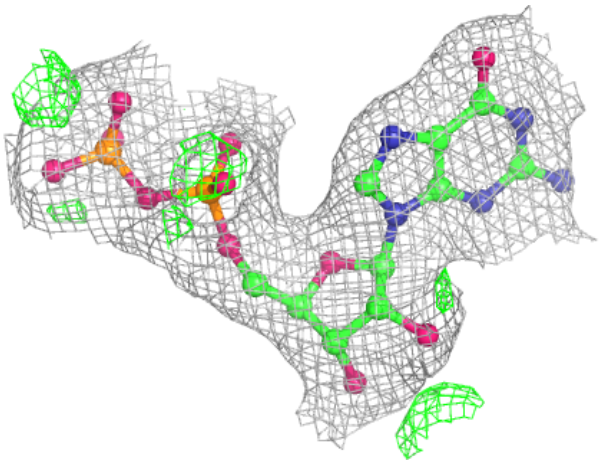
Electron density around POU B 503:

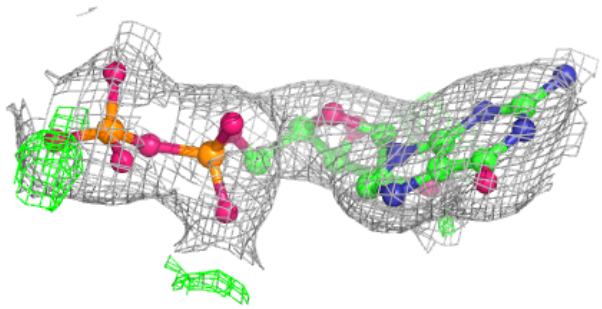
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP D 501:

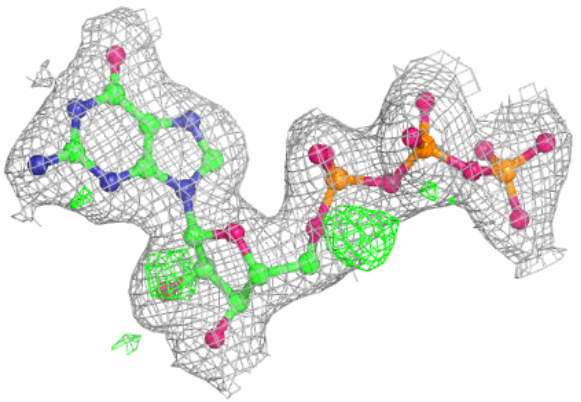
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

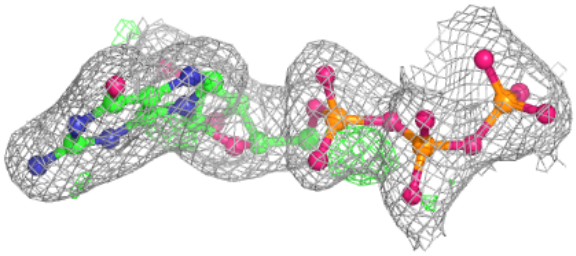


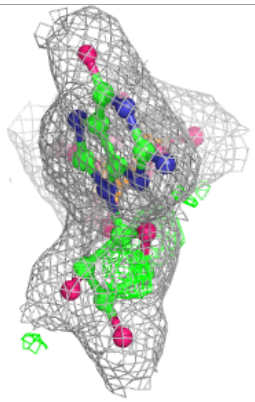


Electron density around GTP A 501:

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

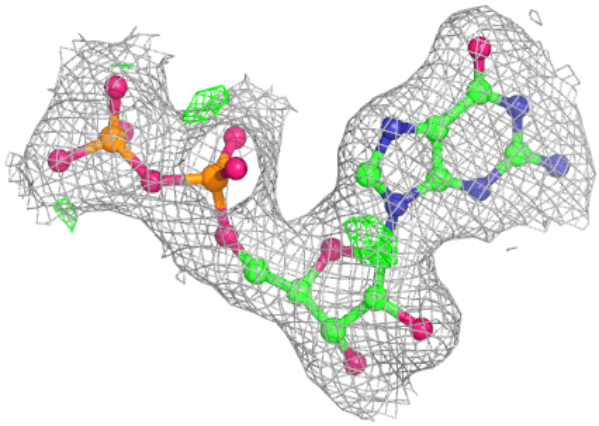


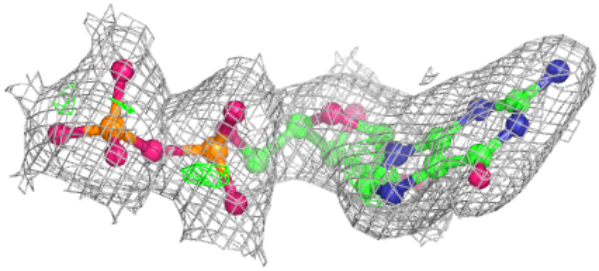


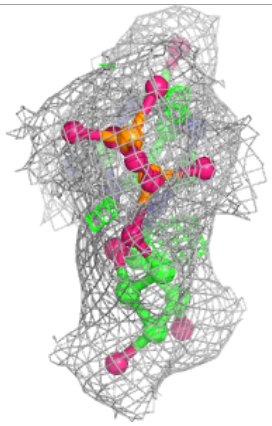


Electron density around GDP B 501:

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

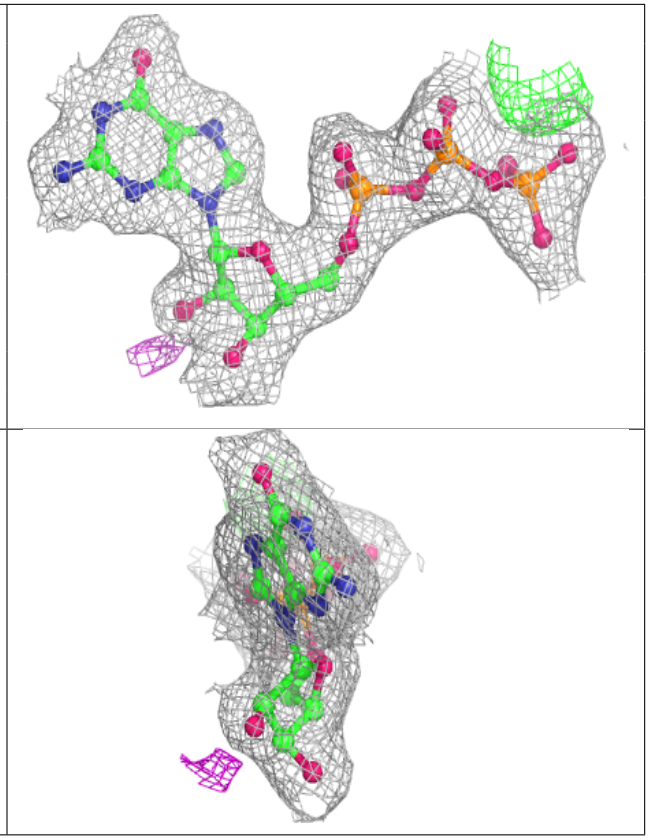






Electron density around GTP C 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.