Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 06:55 PM EDT

PDB ID	:	4TUY
Title	:	Tubulin-Rhizoxin complex
Authors	:	Prota, A.E.; Bargsten, K.; Diaz, J.F.; Marsh, M.; Cuevas, C.; Liniger, M.; Neuhaus, C.; Andreu, J.M.; Altmann, K.H.; Steinmetz, M.O.
Deposited on	:	2014-06-25
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

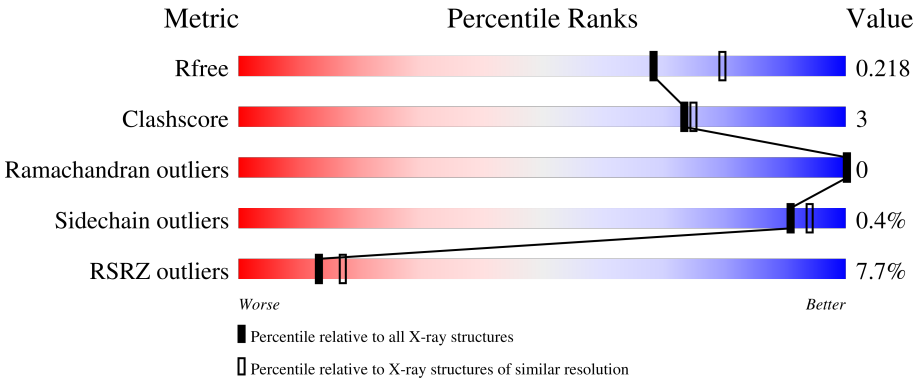
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	2% 87% 10% ·
1	C	451	90% 7% ·
2	B	445	% 88% 8% 5%
2	D	445	7% 87% 8% 5%
3	E	143	6% 80% · 16%

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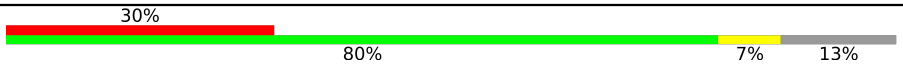
Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	12	0
			3475	2210	583	657	25			
1	C	440	Total	C	N	O	S	0	10	0
			3475	2203	585	663	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	8	0
			3372	2121	571	652	28			
2	D	422	Total	C	N	O	S	0	3	0
			3325	2090	563	644	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	2	0
			1002	619	182	196	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

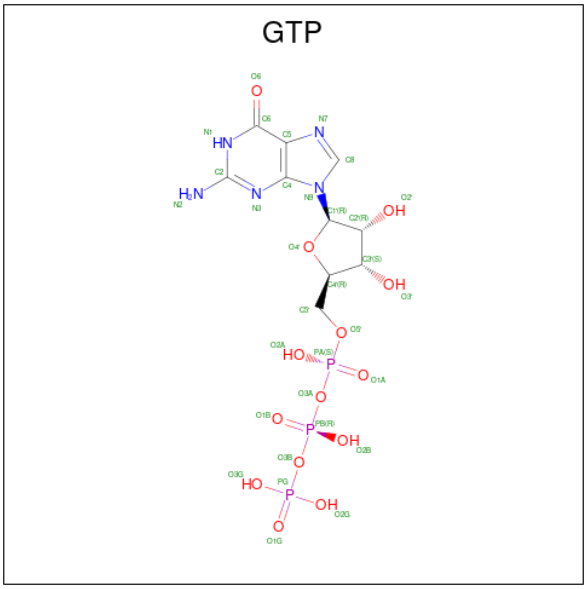
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	335	Total	C	N	O	S	0	0	0
			2749	1768	467	500	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		
6	D	1	Total	Mg	0	0
			1	1		

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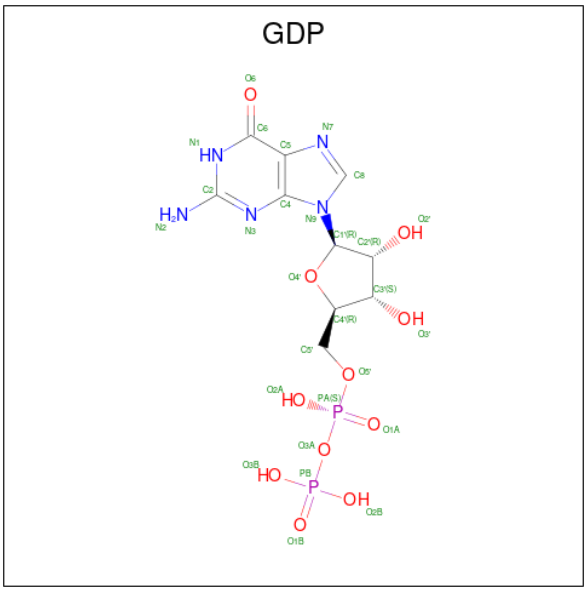
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

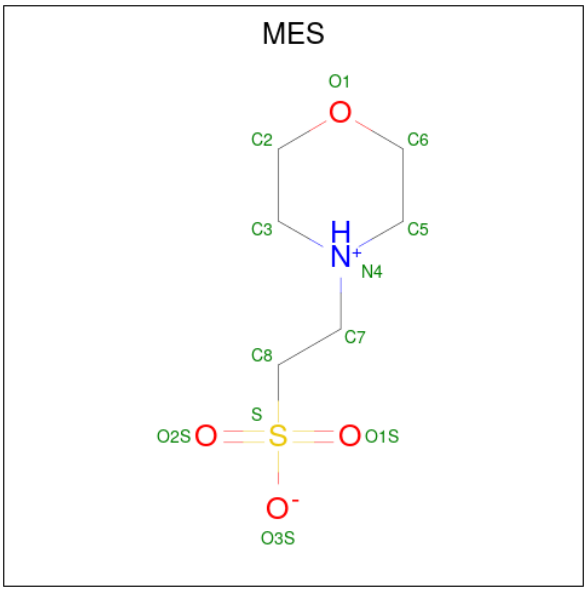
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



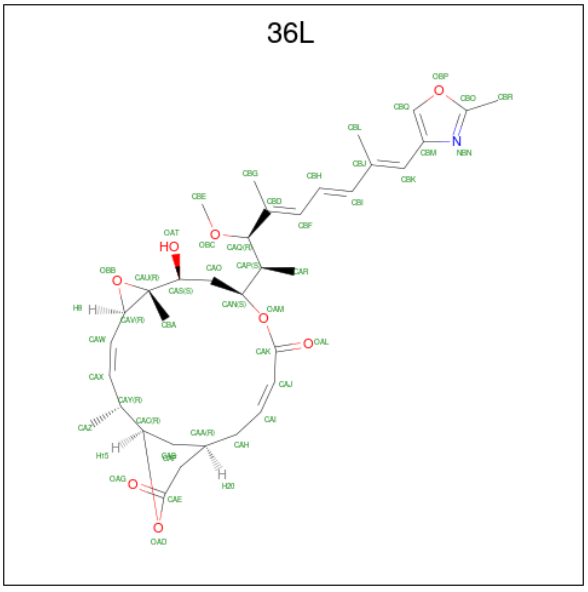
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



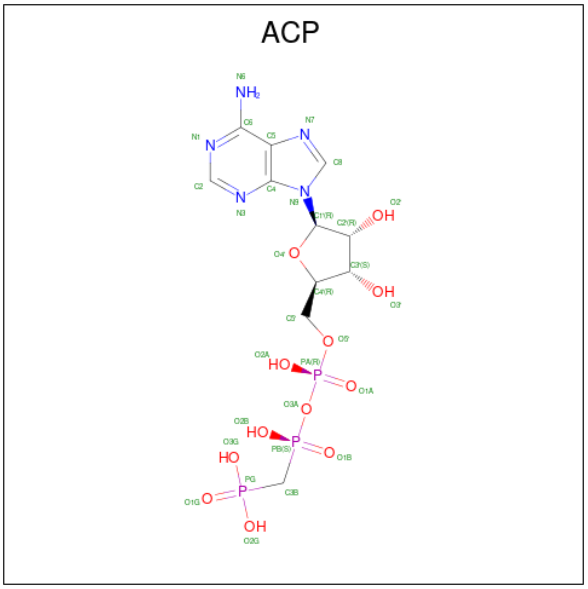
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (1R,2R,3E,5R,7R,8S,10S,13E,16R)-8-hydroxy-10-[(2S,3R,4E,6E,8E)-3-methoxy-4,8-dimethyl-9-(2-methyl-1,3-oxazol-4-yl)nona-4,6,8-trien-2-yl]-2,7-dimethyl-6,11,19-trioxatricyclo[14.3.1.0 5,7]icosa-3,13-diene-12,18-dione (three-letter code: 36L) (formula: $C_{35}H_{47}NO_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			44	35	1	8		

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

- Molecule 12 is water.

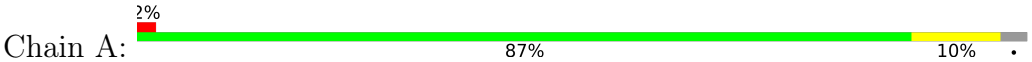
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	244	Total	O	0	0
			244	244		
12	B	226	Total	O	0	0
			226	226		
12	C	378	Total	O	0	0
			378	378		
12	D	172	Total	O	0	0
			172	172		
12	E	74	Total	O	0	0
			74	74		
12	F	95	Total	O	0	0
			95	95		

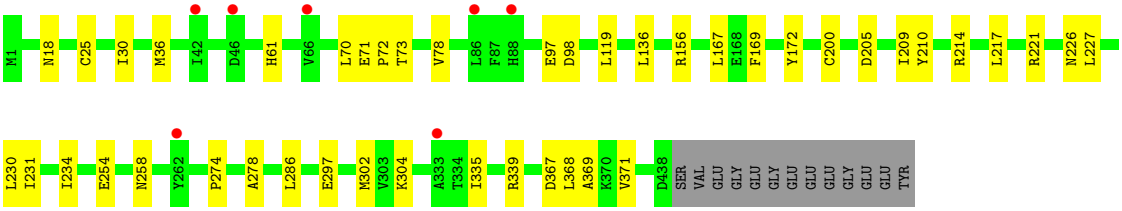
3 Residue-property plots (i)

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

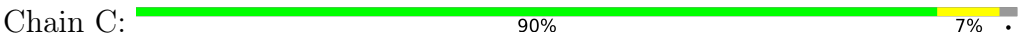
Chain A:

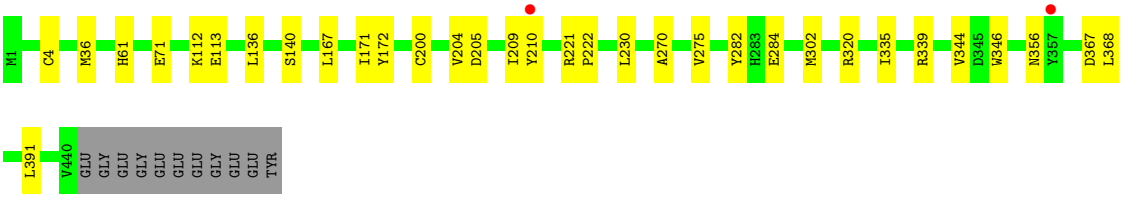




• Molecule 1: Tubulin alpha-1B chain

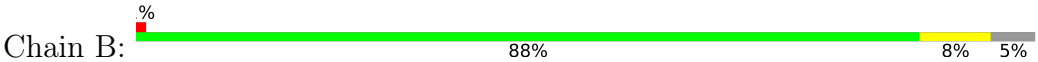
Chain C:

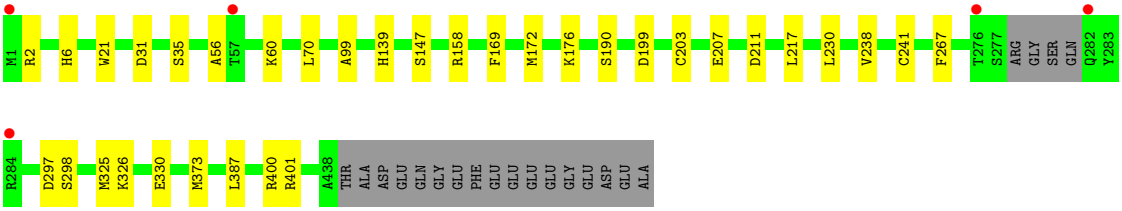




• Molecule 2: Tubulin beta-2B chain

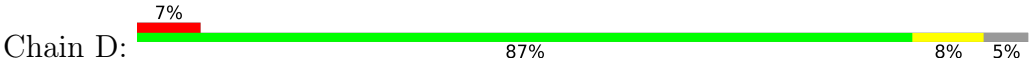
Chain B:

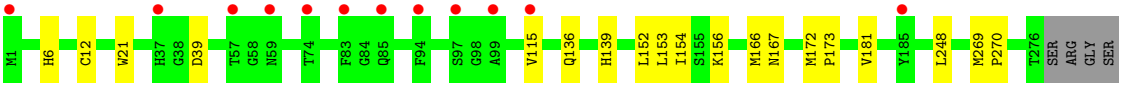




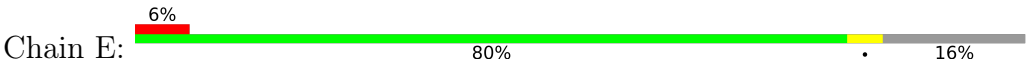
• Molecule 2: Tubulin beta-2B chain

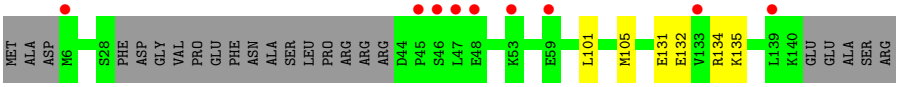
Chain D:



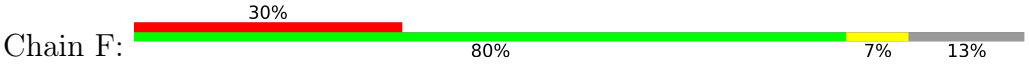


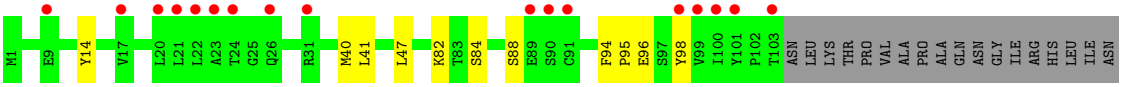
• Molecule 3: Stathmin-4

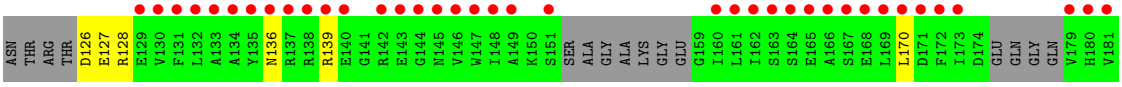


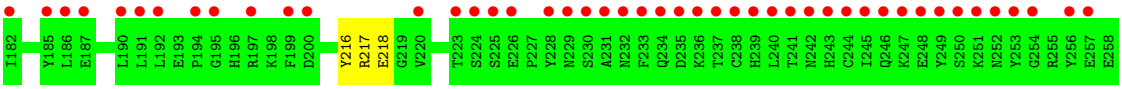


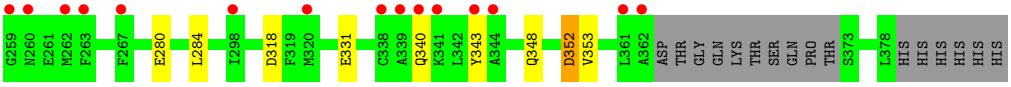
• Molecule 4: Tubulin-Tyrosine Ligase











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.31Å 156.92Å 181.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.70 – 2.10 68.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.70-2.10) 100.0 (68.38-2.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.184 , 0.217 0.187 , 0.218	Depositor DCC
R_{free} test set	8663 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.0	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	0.96	EDS
Total number of atoms	18801	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: GDP, MG, CA, MES, GTP, 36L, 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	0.22	0/3590	0.39	0/4875
1	C	0.23	0/3583	0.39	0/4867
2	B	0.22	0/3467	0.38	0/4695
2	D	0.21	0/3407	0.37	0/4615
3	E	0.21	0/1016	0.32	0/1348
4	F	0.21	0/2810	0.37	0/3794
All	All	0.22	0/17873	0.38	0/24194

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

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	3475	0	3429	30	0
1	C	3475	0	3410	18	0
2	B	3372	0	3265	21	0
2	D	3325	0	3211	24	0
3	E	1002	0	1026	3	0
4	F	2749	0	2728	16	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	12	0	13	3	0
10	D	44	0	47	10	0
11	F	31	0	14	2	0
12	A	244	0	0	2	0
12	B	226	0	0	2	0
12	C	378	0	0	1	0
12	D	172	0	0	3	0
12	E	74	0	0	0	0
12	F	95	0	0	0	0
All	All	18801	0	17191	113	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 3.

All (113) 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)
10:D:503:36L:H47	10:D:503:36L:H40	1.20	1.13
10:D:503:36L:H40	10:D:503:36L:CBQ	1.91	0.96
2:D:404:PHE:HE1	10:D:503:36L:H41	1.36	0.90
2:D:404:PHE:CE1	10:D:503:36L:H41	2.14	0.82
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.97	0.82
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.32	0.74
2:B:211:ASP:OD2	12:B:753:HOH:O	2.06	0.73
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.69	0.73
1:C:367:ASP:OD2	12:C:902:HOH:O	2.09	0.70
3:E:131:GLU:OE2	3:E:134:ARG:NH2	2.24	0.68
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.76	0.68
2:B:199:ASP:OD2	9:B:503:MES:H52	1.95	0.66
4:F:318:ASP:OD2	11:F:401:ACP:O3G	2.12	0.66
2:D:401:ARG:HD2	10:D:503:36L:H44	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:LYS:NZ	2:B:330:GLU:OE2	2.27	0.65
4:F:82:LYS:NZ	4:F:127:GLU:OE1	2.29	0.64
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.31	0.64
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.81	0.62
10:D:503:36L:OAL	10:D:503:36L:H35	2.00	0.61
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.82	0.61
2:D:181:VAL:HG21	10:D:503:36L:CBK	2.34	0.57
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.85	0.57
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.89	0.55
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.54
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.90	0.54
2:B:158:ARG:CZ	9:B:503:MES:H21	2.38	0.53
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.90	0.53
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.41	0.52
2:D:286:LEU:N	2:D:290:GLU:OE1	2.42	0.52
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.91	0.52
2:D:308:ARG:NH1	12:D:601:HOH:O	2.39	0.52
4:F:128:ARG:NH1	4:F:170:LEU:HD13	2.25	0.51
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.92	0.51
1:A:221:ARG:NH2	2:B:325:MET:SD	2.84	0.51
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.92	0.51
1:A:221:ARG:HG2	2:B:325:MET:HB3	1.93	0.51
1:A:71:GLU:O	12:A:665:HOH:O	2.19	0.51
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.50
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.46	0.50
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.94	0.50
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.94	0.50
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.12	0.49
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.95	0.49
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.95	0.49
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.95	0.49
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.95	0.48
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.79	0.48
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.44	0.48
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.96	0.47
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.47
3:E:132:GLU:HA	3:E:135:LYS:HG2	1.96	0.47
1:A:304:LYS:NZ	12:A:768:HOH:O	2.47	0.47
4:F:40:MET:HE1	4:F:47:LEU:HG	1.98	0.46
1:C:140:SER:HA	1:C:171:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:84:SER:O	4:F:88:SER:N	2.42	0.46
4:F:128:ARG:HH12	4:F:170:LEU:HD13	1.81	0.46
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.96	0.46
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.31	0.46
2:B:241[B]:CYS:SG	12:B:665:HOH:O	2.61	0.46
1:C:204:VAL:HG22	1:C:302:MET:HE3	1.96	0.45
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.98	0.45
4:F:136:ASN:HA	4:F:139:ARG:HB3	1.99	0.45
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.97	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.45
2:D:311:ARG:NH1	12:D:632:HOH:O	2.49	0.45
2:D:401:ARG:CD	10:D:503:36L:H44	2.44	0.45
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.99	0.45
2:D:39:ASP:N	2:D:39:ASP:OD1	2.49	0.44
1:A:136[B]:LEU:HD23	1:A:169:PHE:HE1	1.83	0.44
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.52	0.44
4:F:126:ASP:OD1	4:F:128:ARG:HG3	2.17	0.44
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.00	0.44
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.99	0.44
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.99	0.44
4:F:331:GLU:OE2	11:F:401:ACP:O2B	2.35	0.44
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.57	0.44
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.58	0.44
2:D:152:LEU:O	2:D:156:LYS:HG2	2.18	0.43
2:B:217:LEU:HD11	2:B:230:LEU:HD21	2.00	0.43
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.01	0.43
1:C:221:ARG:HG3	2:D:325:MET:HG2	2.00	0.43
2:B:70:LEU:HD12	2:B:99:ALA:HB2	2.01	0.42
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.24	0.42
2:B:199:ASP:OD1	9:B:503:MES:H32	2.19	0.42
10:D:503:36L:H7	10:D:503:36L:H1	1.86	0.42
1:A:25:CYS:HB3	1:A:30:ILE:O	2.20	0.42
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.01	0.42
2:D:167:ASN:ND2	12:D:648:HOH:O	2.51	0.42
3:E:101:LEU:O	3:E:105:MET:HG2	2.20	0.42
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.90	0.42
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.01	0.42
1:A:274:PRO:HG2	1:A:371:VAL:HG11	2.02	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.55	0.41
2:D:136:GLN:HA	2:D:167:ASN:O	2.20	0.41
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HA	1:C:356:ASN:O	2.20	0.41
2:D:172:MET:HA	2:D:173:PRO:HD3	1.82	0.41
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.34	0.41
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.85	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.55	0.41
1:A:70:LEU:HB2	1:A:98:ASP:HA	2.02	0.41
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.03	0.41
1:A:230:LEU:O	1:A:234:ILE:HD12	2.21	0.41
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.03	0.41
1:C:282:TYR:O	1:C:284:GLU:HG2	2.21	0.41
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.56	0.41
1:A:71:GLU:HB2	1:A:98:ASP:HB3	2.03	0.41
1:A:97:GLU:OE2	2:B:2:ARG:NH2	2.54	0.41
10:D:503:36L:CBQ	10:D:503:36L:CBL	2.76	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.57	0.40
2:B:169:PHE:HE2	2:B:238[A]:VAL:HG21	1.87	0.40
2:B:297:ASP:OD1	2:B:298:SER:N	2.54	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	448/451 (99%)	437 (98%)	11 (2%)	0	100	100
1	C	448/451 (99%)	441 (98%)	7 (2%)	0	100	100
2	B	428/445 (96%)	420 (98%)	8 (2%)	0	100	100
2	D	421/445 (95%)	414 (98%)	7 (2%)	0	100	100
3	E	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
4	F	325/384 (85%)	315 (97%)	10 (3%)	0	100	100
All	All	2188/2319 (94%)	2144 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	381/379 (100%)	381 (100%)	0	100 100
1	C	381/379 (100%)	380 (100%)	1 (0%)	92 95
2	B	375/383 (98%)	373 (100%)	2 (0%)	88 92
2	D	368/383 (96%)	367 (100%)	1 (0%)	92 95
3	E	110/127 (87%)	110 (100%)	0	100 100
4	F	302/342 (88%)	299 (99%)	3 (1%)	76 82
All	All	1917/1993 (96%)	1910 (100%)	7 (0%)	91 94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
2	B	373	MET
1	C	71	GLU
2	D	139	HIS
4	F	217	ARG
4	F	352	ASP
4	F	353	VAL

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	C	501	6	26,34,34	0.91	1 (3%)	32,54,54	1.18	3 (9%)
9	MES	B	503	-	12,12,12	2.24	1 (8%)	14,16,16	1.20	1 (7%)
8	GDP	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.14	3 (10%)
10	36L	D	503	-	41,47,47	1.08	3 (7%)	41,67,67	1.55	7 (17%)
5	GTP	A	501	6	26,34,34	0.91	1 (3%)	32,54,54	1.22	3 (9%)
8	GDP	D	501	6	24,30,30	0.92	1 (4%)	30,47,47	1.25	4 (13%)
11	ACP	F	401	6	27,33,33	1.38	5 (18%)	32,52,52	1.40	4 (12%)

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	C	501	6	-	6/18/38/38	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
10	36L	D	503	-	-	11/51/73/73	0/2/4/4
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
11	ACP	F	401	6	-	6/15/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.51	1.66	1.77
10	D	503	36L	OBB-CAU	-4.44	1.40	1.45
10	D	503	36L	OBB-CAV	-3.12	1.40	1.46
11	F	401	ACP	PG-O2G	2.87	1.61	1.54
11	F	401	ACP	PG-O3G	2.82	1.61	1.54
11	F	401	ACP	PB-O3A	2.80	1.61	1.58
11	F	401	ACP	C5-C4	2.51	1.47	1.40
10	D	503	36L	OAD-CAC	-2.36	1.43	1.46
5	A	501	GTP	C6-N1	-2.35	1.34	1.37
8	D	501	GDP	C6-N1	-2.28	1.34	1.37
8	B	501	GDP	C6-N1	-2.26	1.34	1.37
5	C	501	GTP	C6-N1	-2.18	1.34	1.37
11	F	401	ACP	PB-O2B	2.05	1.61	1.56

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	503	36L	CAU-OBB-CAV	3.82	64.23	60.90
11	F	401	ACP	PB-O3A-PA	-3.64	121.02	132.56
11	F	401	ACP	C3'-C2'-C1'	3.35	106.03	100.98
10	D	503	36L	CAB-CAC-CAY	-3.18	110.19	114.41
11	F	401	ACP	N3-C2-N1	-3.16	123.74	128.68
8	D	501	GDP	PA-O3A-PB	-3.06	122.33	132.83
10	D	503	36L	OAM-CAK-OAL	-2.75	118.88	123.35
5	A	501	GTP	PA-O3A-PB	-2.72	123.48	132.83
5	C	501	GTP	PA-O3A-PB	-2.71	123.52	132.83
9	B	503	MES	O3S-S-C8	2.68	110.10	105.77
11	F	401	ACP	C4-C5-N7	-2.59	106.70	109.40
10	D	503	36L	OBB-CAU-CBA	2.53	117.80	114.17
8	B	501	GDP	C5-C6-N1	2.42	118.22	113.95
5	C	501	GTP	C8-N7-C5	2.42	107.59	102.99
8	D	501	GDP	C8-N7-C5	2.37	107.50	102.99
10	D	503	36L	OAM-CAK-CAJ	2.33	116.66	111.38
5	A	501	GTP	C5-C6-N1	2.31	118.03	113.95
8	D	501	GDP	C5-C6-N1	2.30	118.01	113.95
8	B	501	GDP	PA-O3A-PB	-2.29	124.97	132.83
5	A	501	GTP	C8-N7-C5	2.27	107.32	102.99
5	C	501	GTP	C5-C6-N1	2.27	117.96	113.95
8	B	501	GDP	C8-N7-C5	2.22	107.22	102.99
10	D	503	36L	OAD-CAC-CAY	2.22	110.32	105.72
8	D	501	GDP	C3'-C2'-C1'	2.17	104.24	100.98
10	D	503	36L	OBB-CAV-CAU	-2.04	57.81	59.34

There are no chirality outliers.

All (35) 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	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	503	MES	C8-C7-N4-C5
10	D	503	36L	CAP-CAN-CAO-CAS
10	D	503	36L	CAO-CAS-CAU-CBA
10	D	503	36L	OAT-CAS-CAU-CBA
10	D	503	36L	OAT-CAS-CAU-CAV
10	D	503	36L	CBJ-CBK-CBM-NBN
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	C5'-O5'-PA-O3A
10	D	503	36L	CAA-CAH-CAI-CAJ
10	D	503	36L	OAM-CAN-CAO-CAS
10	D	503	36L	CAF-CAA-CAH-CAI
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
10	D	503	36L	CAN-CAO-CAS-OAT
5	C	501	GTP	PB-O3B-PG-O1G
10	D	503	36L	CAB-CAA-CAH-CAI
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
10	D	503	36L	CAO-CAS-CAU-CAV

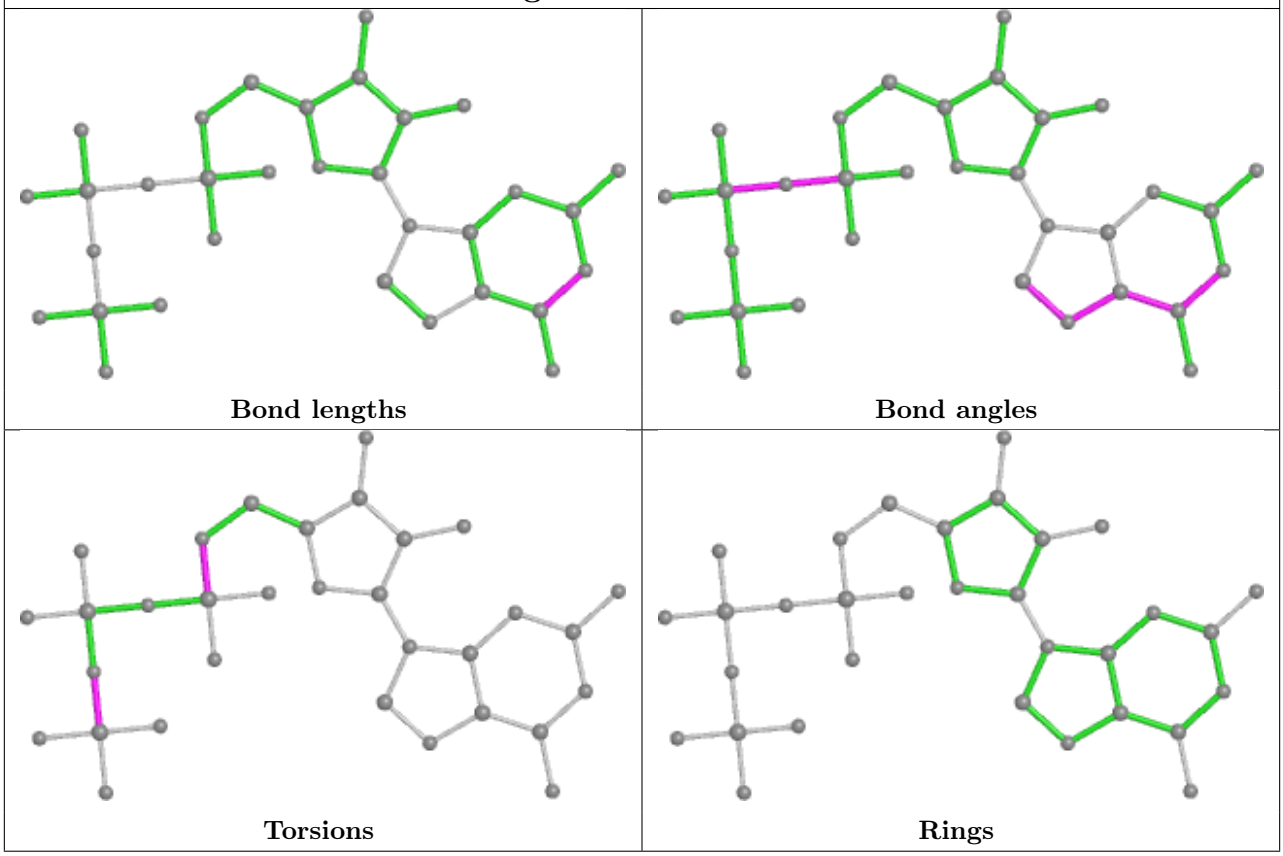
There are no ring outliers.

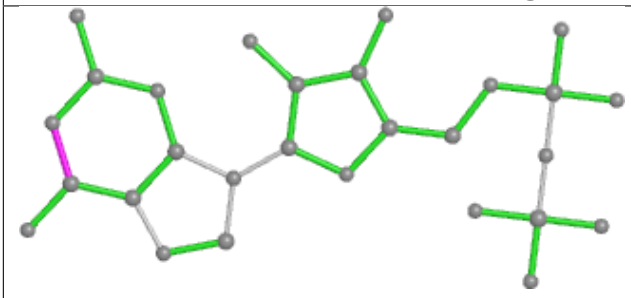
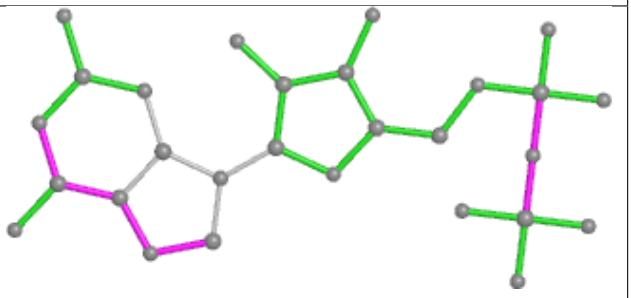
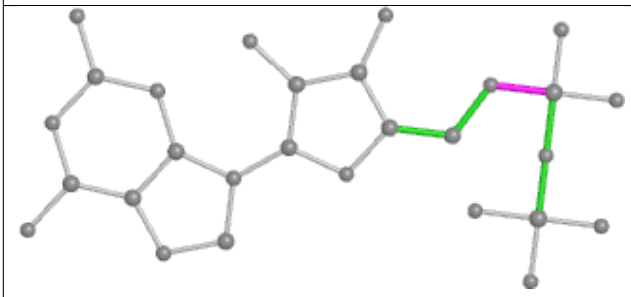
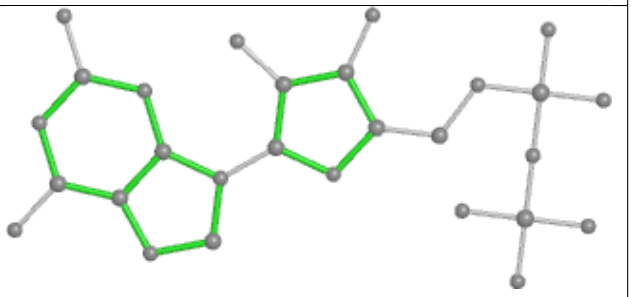
4 monomers are involved in 16 short contacts:

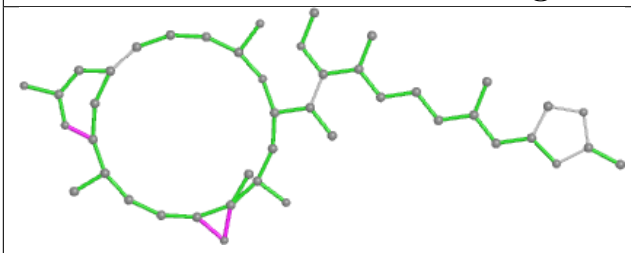
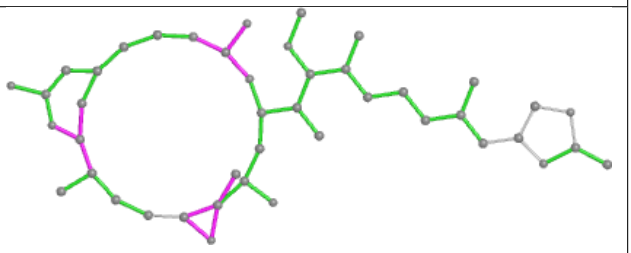
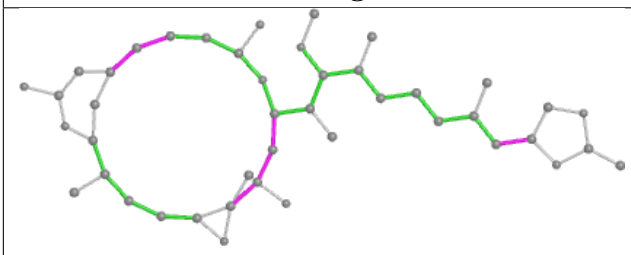
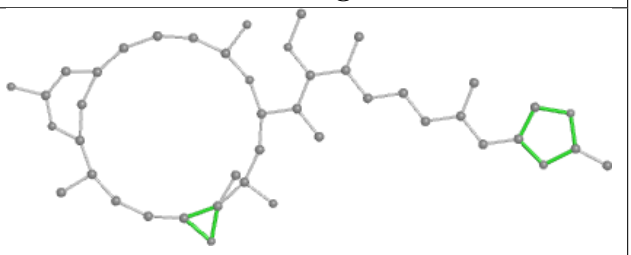
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	3	0
10	D	503	36L	10	0
8	D	501	GDP	1	0
11	F	401	ACP	2	0

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.

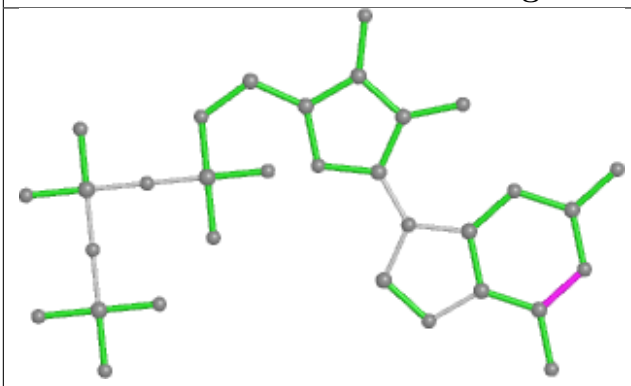
Ligand GTP C 501



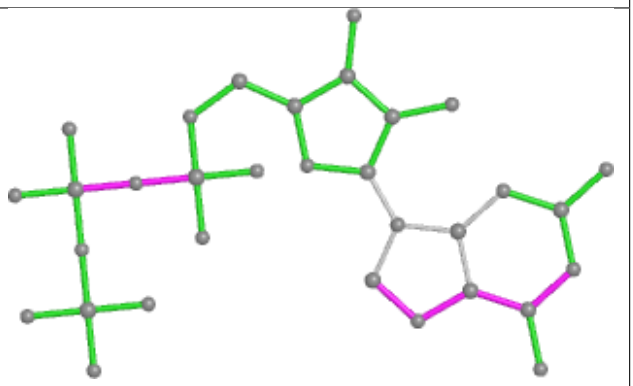
Ligand GDP B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 36L D 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

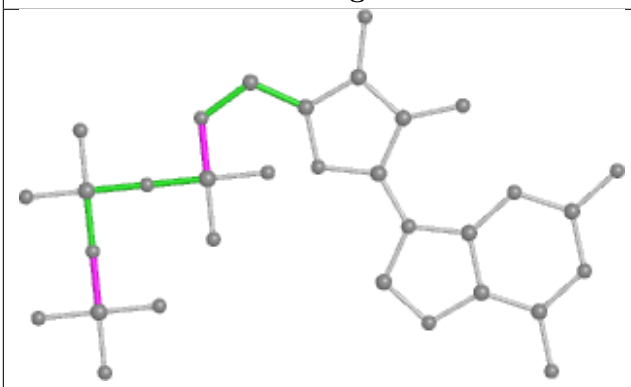
Ligand GTP A 501



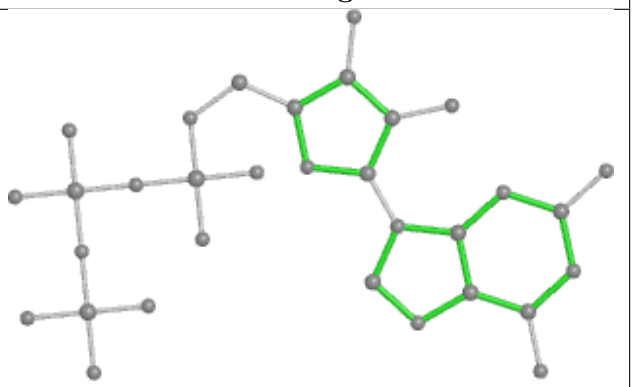
Bond lengths



Bond angles

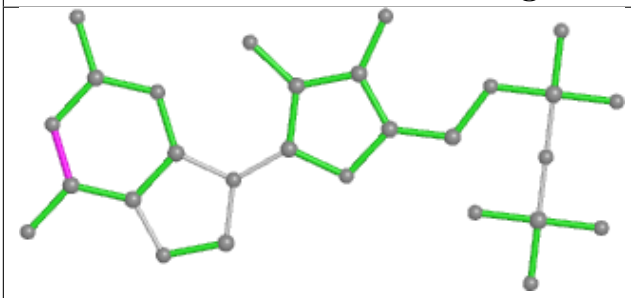


Torsions

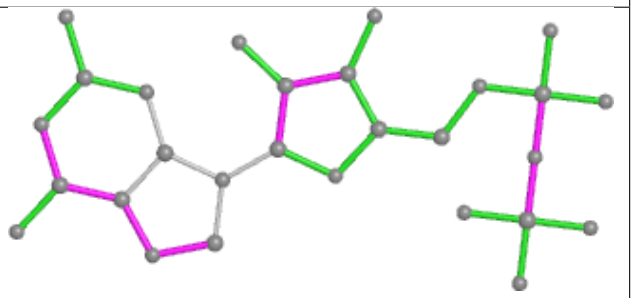


Rings

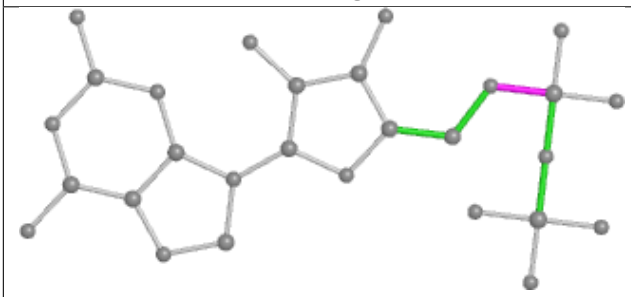
Ligand GDP D 501



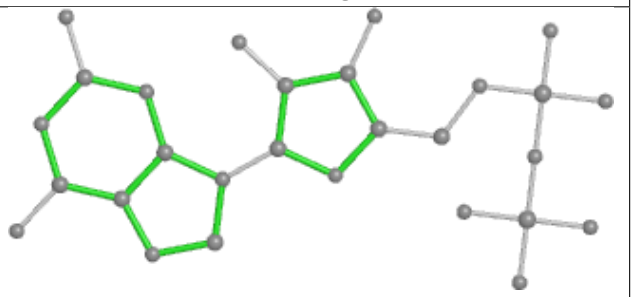
Bond lengths



Bond angles

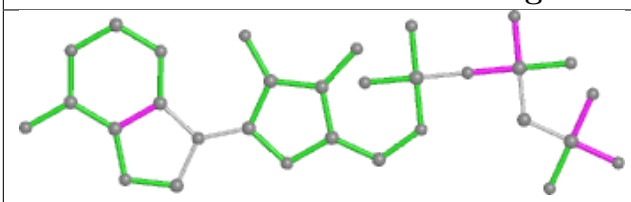


Torsions

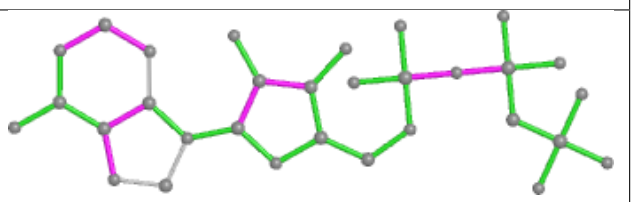


Rings

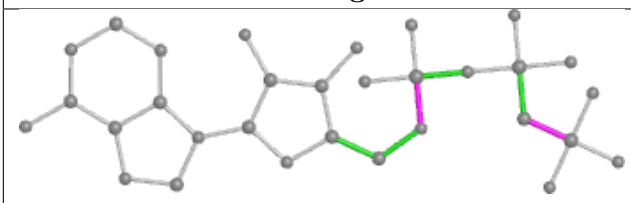
Ligand ACP F 401



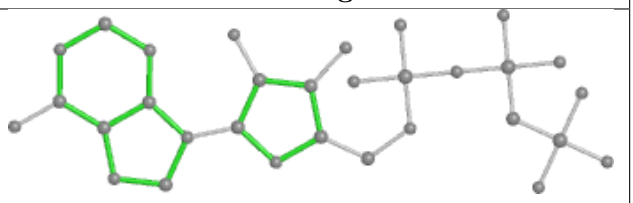
Bond lengths



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	438/451 (97%)	0.26	7 (1%) 72 75	28, 43, 76, 92	0
1	C	440/451 (97%)	0.23	2 (0%) 91 92	22, 34, 57, 106	0
2	B	424/445 (95%)	0.34	5 (1%) 79 82	24, 41, 73, 113	1 (0%)
2	D	422/445 (94%)	0.56	29 (6%) 16 21	31, 52, 83, 108	4 (0%)
3	E	120/143 (83%)	0.71	9 (7%) 14 18	35, 57, 90, 101	0
4	F	335/384 (87%)	1.64	116 (34%) 0 0	35, 68, 128, 158	0
All	All	2179/2319 (93%)	0.56	168 (7%) 13 17	22, 46, 89, 158	5 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	9.7
4	F	161	LEU	9.6
4	F	173	ILE	9.1
4	F	172	PHE	8.2
4	F	251	LYS	7.3
4	F	169	LEU	6.8
4	F	162	ILE	6.7
4	F	233	PHE	6.7
4	F	245	ILE	6.3
1	A	262	TYR	6.3
4	F	234	GLN	6.3
4	F	182	ILE	5.8
4	F	179	VAL	5.8
4	F	235	ASP	5.2
4	F	244	CYS	5.1
4	F	147	TRP	5.0
4	F	149	ALA	5.0
4	F	148	ILE	5.0
4	F	253	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
4	F	240	LEU	4.9
4	F	232	ASN	4.9
4	F	181	VAL	4.9
4	F	134	ALA	4.9
4	F	250	SER	4.9
4	F	192	LEU	4.8
4	F	130	VAL	4.6
4	F	224	SER	4.6
4	F	132	LEU	4.6
4	F	248	GLU	4.6
4	F	160	ILE	4.5
4	F	100	ILE	4.5
4	F	236	LYS	4.4
4	F	259	GLY	4.4
2	D	405	LEU	4.3
4	F	21	LEU	4.3
3	E	133	VAL	4.3
4	F	225	SER	4.2
4	F	252	ASN	4.2
2	D	57	THR	4.2
3	E	45	PRO	4.2
4	F	101	TYR	4.1
4	F	133	ALA	4.1
4	F	256	TYR	4.1
4	F	166	ALA	4.0
4	F	142	ARG	4.0
4	F	17	VAL	3.9
2	D	404	PHE	3.9
2	B	1	MET	3.8
4	F	89	GLU	3.8
4	F	135	TYR	3.8
4	F	139	ARG	3.8
4	F	163	SER	3.8
2	D	94	PHE	3.8
4	F	131	PHE	3.8
4	F	165	GLU	3.7
4	F	186	LEU	3.7
4	F	140	GLU	3.7
1	C	357	TYR	3.7
4	F	170	LEU	3.6
4	F	103	THR	3.6
4	F	129	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	246	GLN	3.6
4	F	239	HIS	3.5
2	B	284	ARG	3.5
2	D	99	ALA	3.5
4	F	199	PHE	3.5
4	F	241	THR	3.4
4	F	339	ALA	3.4
4	F	20	LEU	3.4
4	F	180	HIS	3.3
4	F	194	PRO	3.3
2	D	37	HIS	3.2
4	F	231	ALA	3.2
4	F	138	ARG	3.2
4	F	263	PHE	3.1
2	D	286	LEU	3.1
4	F	223	THR	3.0
4	F	145	ASN	3.0
2	B	57	THR	3.0
4	F	238	CYS	3.0
4	F	344	ALA	3.0
4	F	164	SER	3.0
4	F	99	VAL	3.0
2	D	400	ARG	3.0
4	F	228	TYR	2.9
3	E	48	GLU	2.9
2	D	74	THR	2.9
4	F	137	ARG	2.9
4	F	9	GLU	2.9
2	D	115	VAL	2.8
2	D	97	SER	2.8
4	F	31	ARG	2.8
4	F	243	HIS	2.8
4	F	136	ASN	2.8
2	B	282	GLN	2.8
4	F	168	GLU	2.8
4	F	146	VAL	2.8
2	D	83	PHE	2.8
4	F	320	MET	2.8
4	F	167	SER	2.8
4	F	237	THR	2.8
2	D	401	ARG	2.8
4	F	230	SER	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	197	ARG	2.8
3	E	47	LEU	2.8
4	F	143	GLU	2.7
1	A	333	ALA	2.7
4	F	195	GLY	2.7
4	F	242	ASN	2.7
4	F	229	ASN	2.7
4	F	171	ASP	2.7
4	F	26	GLN	2.6
4	F	341	LYS	2.6
4	F	185	TYR	2.6
1	A	88	HIS	2.6
1	A	42	ILE	2.6
3	E	139	LEU	2.6
4	F	260	ASN	2.5
3	E	59	GLU	2.5
2	D	289	PRO	2.5
4	F	200	ASP	2.5
1	A	86	LEU	2.5
1	A	66[A]	VAL	2.5
4	F	257	GLU	2.5
4	F	24	THR	2.5
4	F	226	GLU	2.5
4	F	362	ALA	2.5
4	F	220	VAL	2.4
4	F	144	GLY	2.4
4	F	23	ALA	2.4
4	F	90	SER	2.4
4	F	91	CYS	2.4
4	F	254	GLY	2.4
2	D	293	GLN	2.4
4	F	22	LEU	2.4
3	E	46	SER	2.4
3	E	53	LYS	2.4
2	D	414	ASP	2.4
4	F	191	LEU	2.3
2	D	317	ALA	2.3
4	F	187	GLU	2.3
4	F	343	TYR	2.3
2	D	295	MET	2.3
2	D	415	GLU	2.3
2	D	288	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	247	LYS	2.3
2	D	59	ASN	2.3
2	D	416	MET	2.3
2	D	1	MET	2.2
2	D	397	ALA	2.2
3	E	6	MET	2.2
4	F	340	GLN	2.2
4	F	361	LEU	2.2
2	D	407	TRP	2.2
4	F	298	ILE	2.2
2	D	399	PHE	2.2
2	B	276	THR	2.1
4	F	151	SER	2.1
2	D	406	HIS	2.1
1	C	210	TYR	2.1
2	D	185	TYR	2.1
1	A	46	ASP	2.1
4	F	98	TYR	2.1
2	D	85	GLN	2.1
4	F	267	PHE	2.1
4	F	190	LEU	2.1
4	F	262	MET	2.0
4	F	338	CYS	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.

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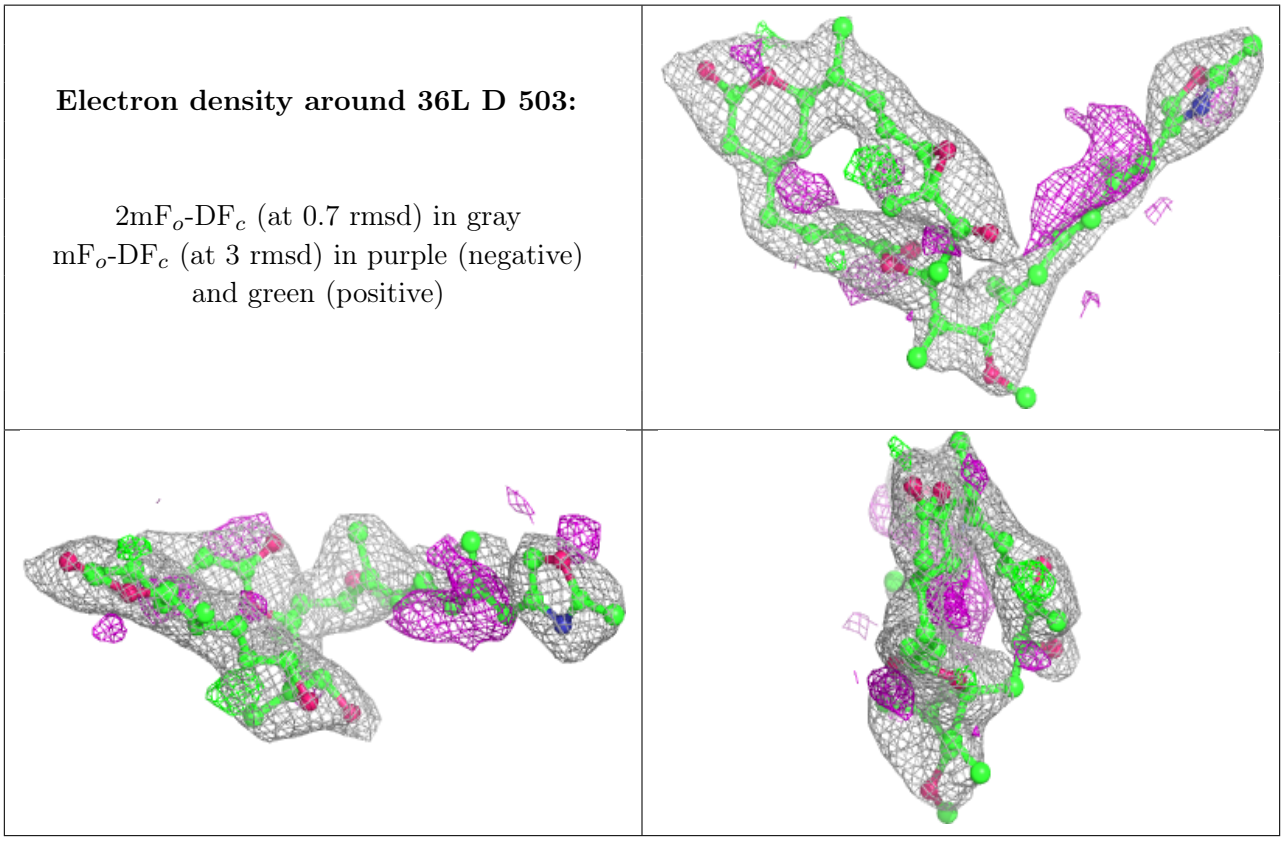
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	36L	D	503	44/44	0.84	0.30	51,64,73,74	0
6	MG	F	402	1/1	0.87	0.06	61,61,61,61	0
11	ACP	F	401	31/31	0.91	0.16	61,71,119,144	0
6	MG	D	502	1/1	0.92	0.08	45,45,45,45	0
7	CA	A	503	1/1	0.92	0.06	59,59,59,59	0
8	GDP	D	501	28/28	0.95	0.14	37,46,60,60	0
9	MES	B	503	12/12	0.95	0.15	43,52,62,64	0
6	MG	C	502	1/1	0.98	0.14	25,25,25,25	0
5	GTP	A	501	32/32	0.98	0.14	22,29,34,37	0
7	CA	C	503	1/1	0.98	0.04	43,43,43,43	0
8	GDP	B	501	28/28	0.98	0.15	23,29,34,34	0
5	GTP	C	501	32/32	0.99	0.15	18,26,29,34	0
6	MG	A	502	1/1	0.99	0.11	29,29,29,29	0
6	MG	B	502	1/1	1.00	0.15	20,20,20,20	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.

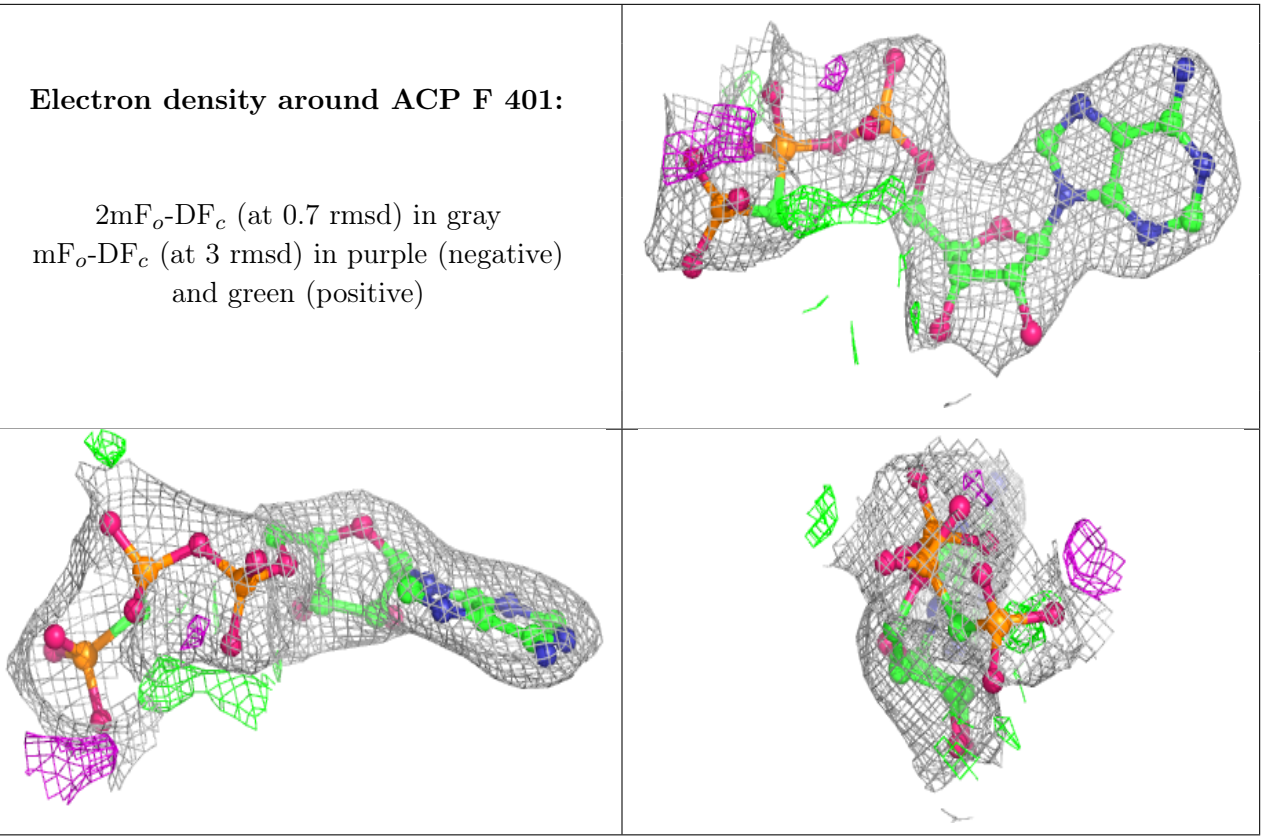
Electron density around 36L D 503:

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



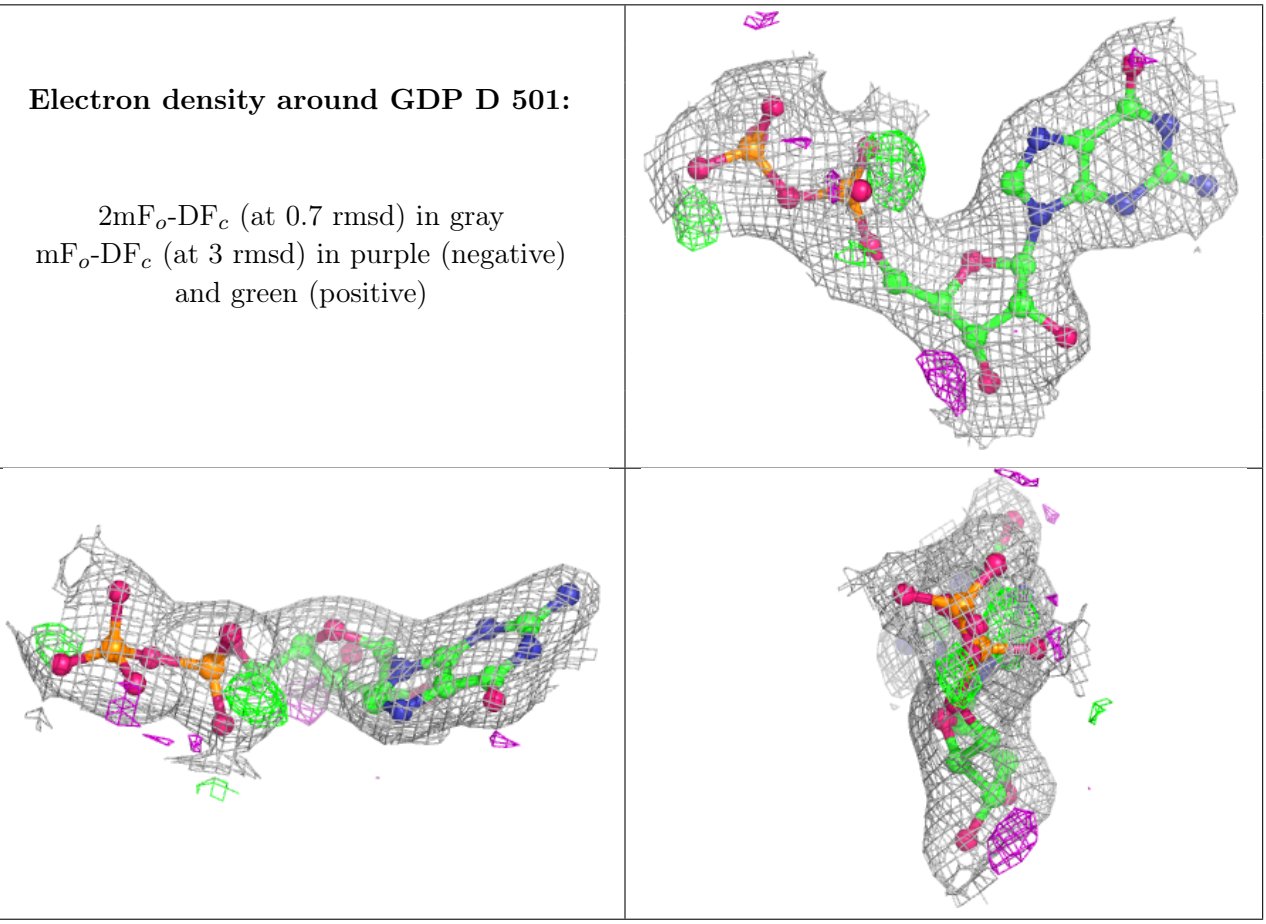
Electron density around ACP F 401:

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



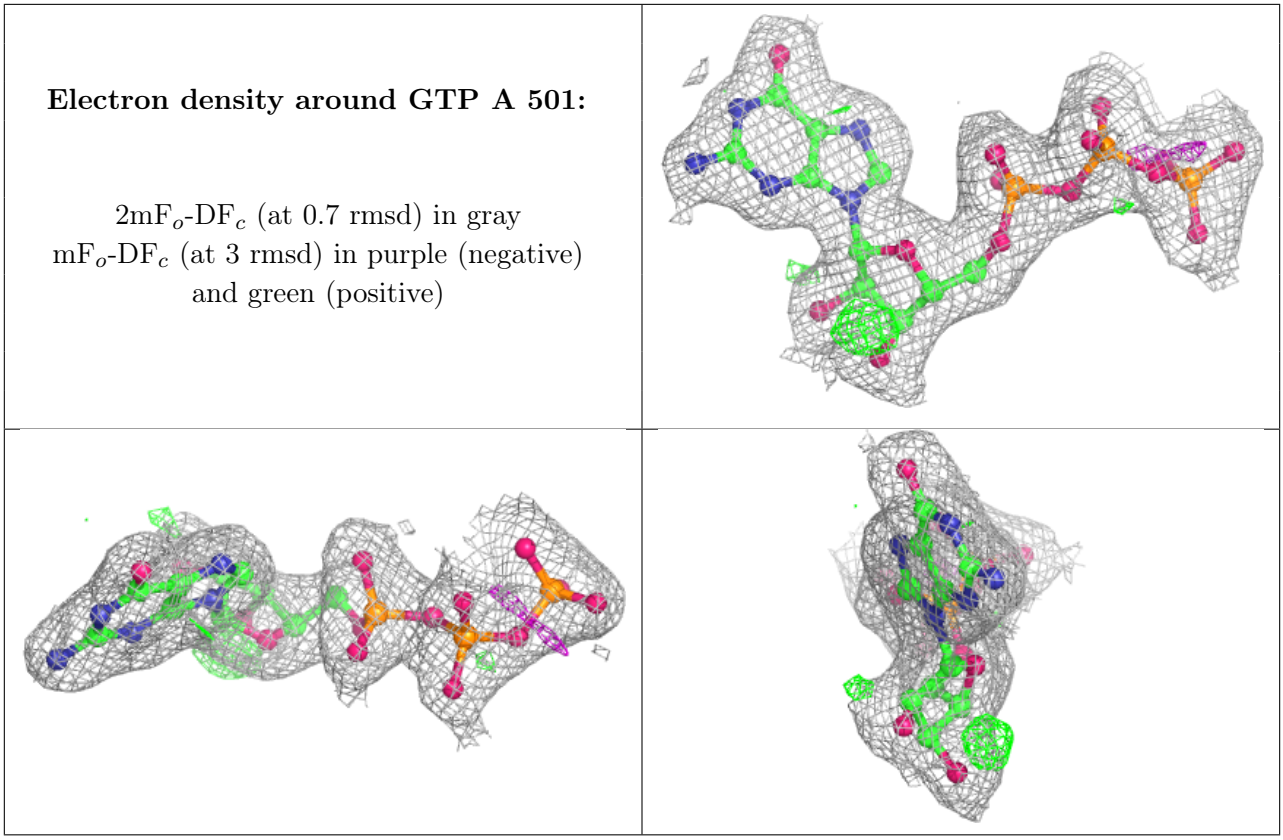
Electron density around GDP D 501:

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



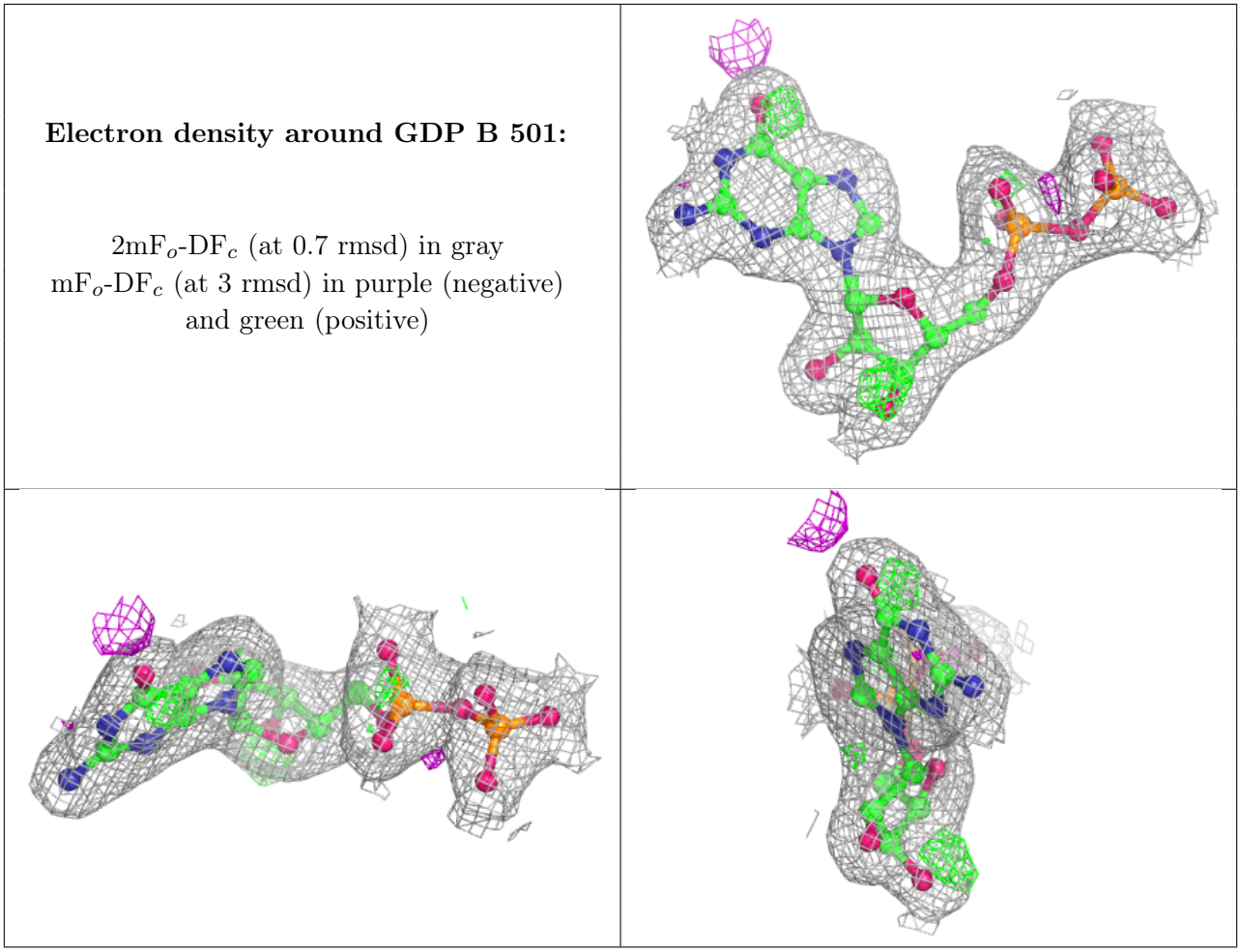
Electron density around GTP A 501:

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



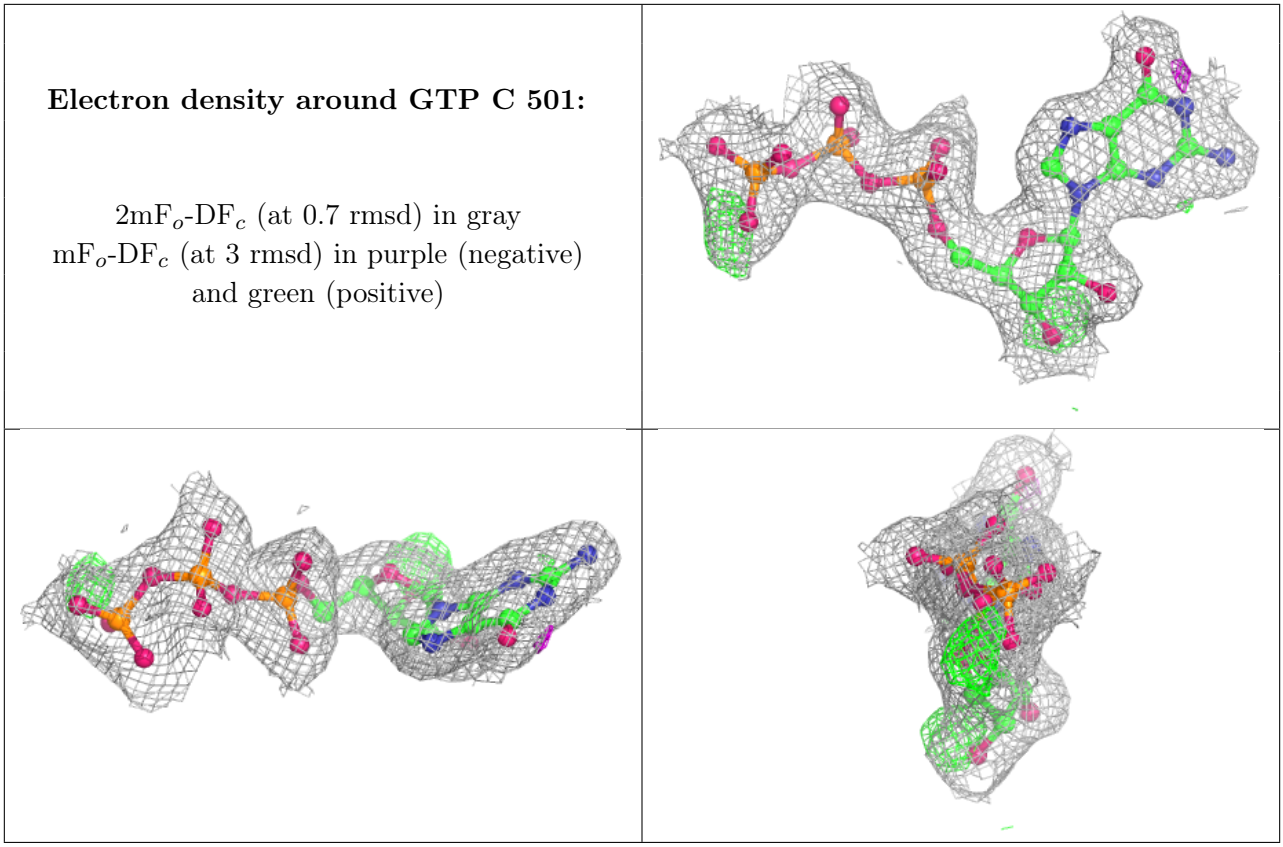
Electron density around GDP B 501:

$2mF_o$-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.