Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 06:39 pm BST

PDB ID	:	5O7A
Title	:	Quinolin-6-yloxyacetamides are microtubule destabilizing agents that bind to the colchicine site of tubulin
Authors	:	Sharma, A.; Olieric, N.; Steinmetz, M.O.
Deposited on	:	2017-06-08
Resolution	:	2.50 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:

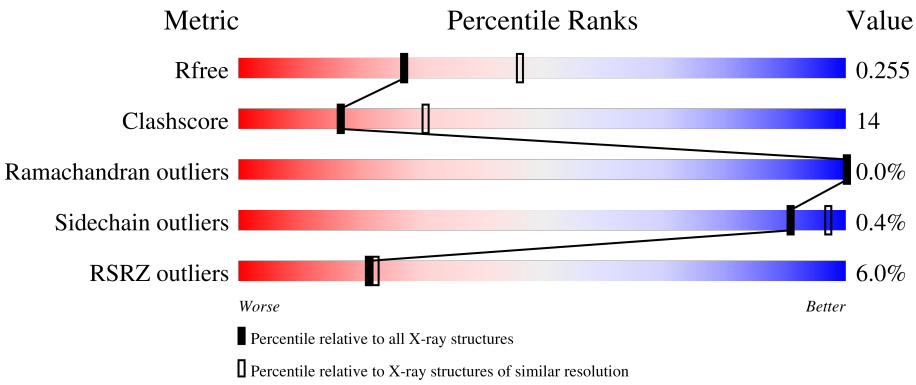
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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%, 72%, 25%, •
1	C	451	%, 77%, 20%, •
2	B	445	4%, 67%, 28%, 5%
2	D	445	6%, 67%, 28%, 6%
3	E	143	7%, 63%, 20%, 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	14% 46% 20% 34%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 17086 atoms, of which 104 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	437	3460	2198	582	655	25	0	10	0
1	C	440	3461	2191	585	663	22	0	5	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	421	3346	2107	568	644	27	0	6	0
2	D	419	3298	2075	560	636	27	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	118	985	609	179	192	5	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

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

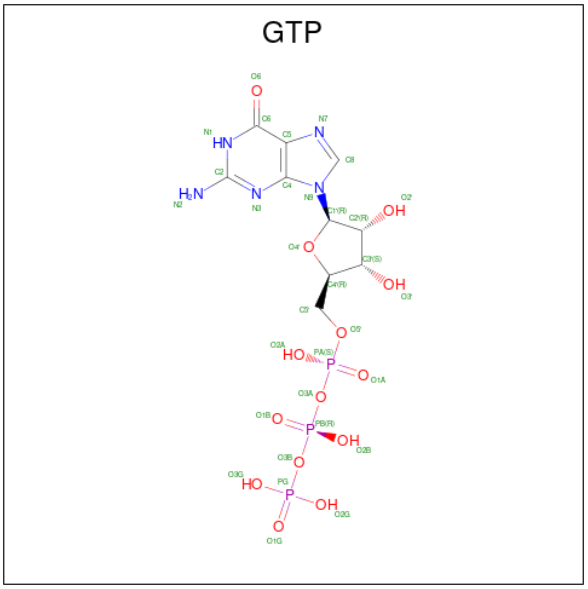
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	254	2093	1364	349	367	13	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

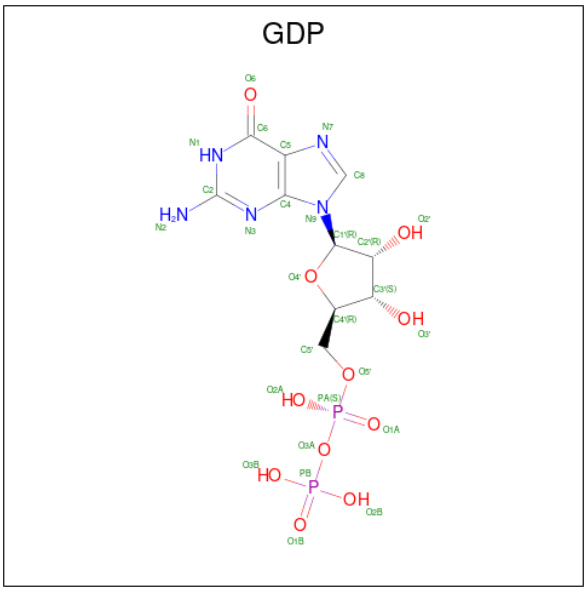
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- 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
			Total	C	H	N	O	P		
5	A	1	44	10	12	5	14	3	0	0
			Total	C	H	N	O	P		
5	C	1	44	10	12	5	14	3	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

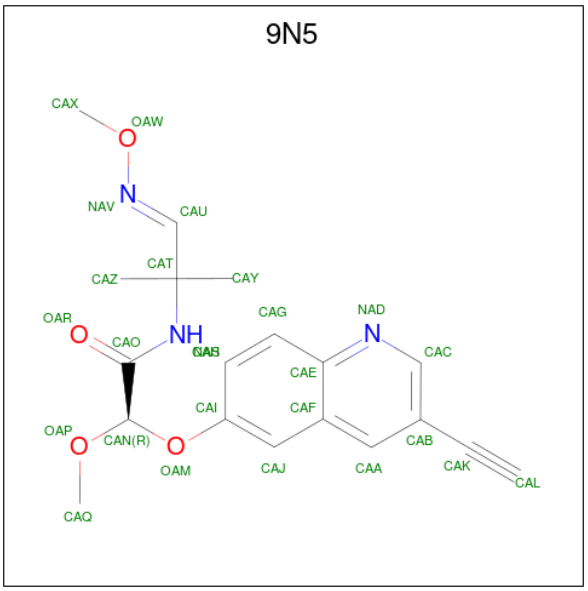


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
6	B	1	40	10	12	5	11	2	0	0
			Total	C	H	N	O	P		
6	D	1	40	10	12	5	11	2	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

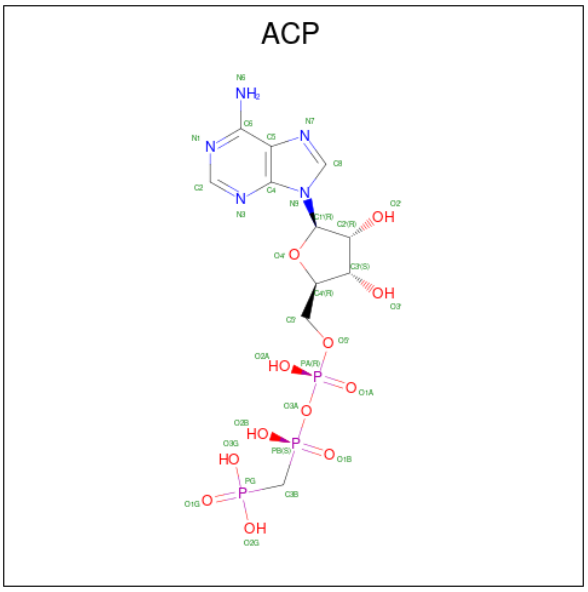
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	B	2	2	2	0	0
			Total	Mg		
7	D	2	2	2	0	0

- Molecule 8 is (2 {R})-2-(3-ethynylquinolin-6-yl)oxy-2-methoxy- {N}-[(1 {E})-1-methoxyimino-2-methyl-propan-2-yl]ethanamide (three-letter code: 9N5) (formula: $C_{19}H_{21}N_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	B	1	47	19	21	3	4	0	0
			Total	C	H	N	O		
8	D	1	47	19	21	3	4	0	0

- Molecule 9 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	H	N	O	P		
9	F	1	45	11	14	5	12	3	0	0

- Molecule 10 is water.

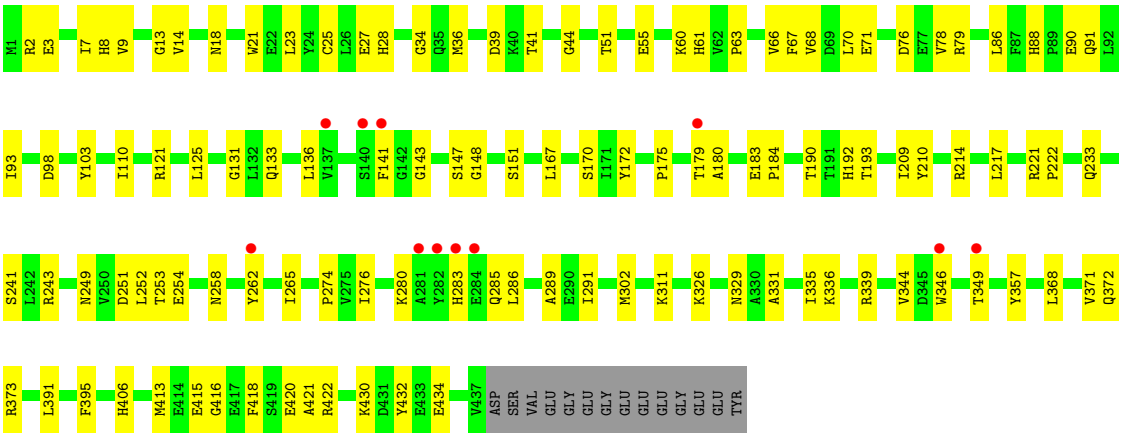
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	30	30	30	0	0
			Total	O		
10	B	25	25	25	0	0
			Total	O		
10	C	43	43	43	0	0
			Total	O		
10	D	18	18	18	0	0
			Total	O		
10	E	6	6	6	0	0
			Total	O		
10	F	10	10	10	0	0

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.

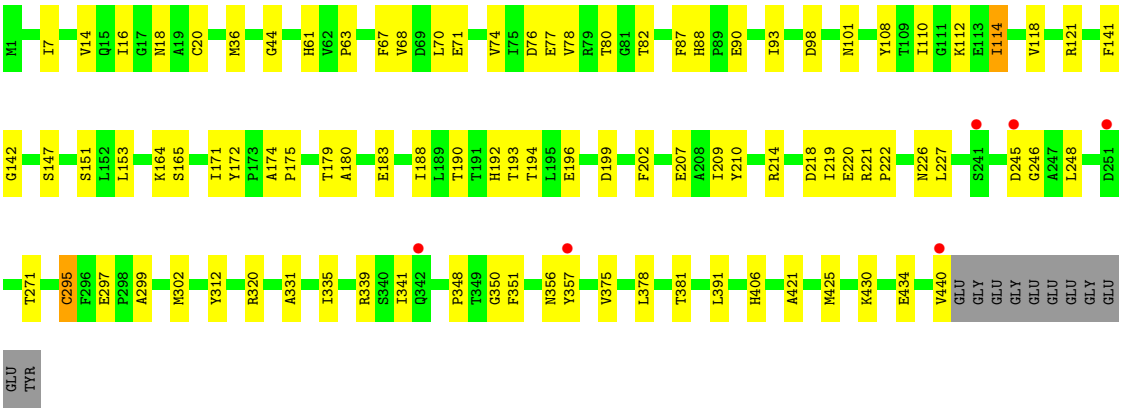
• Molecule 1: Tubulin alpha-1B chain

Chain A: 2% 72% 25%



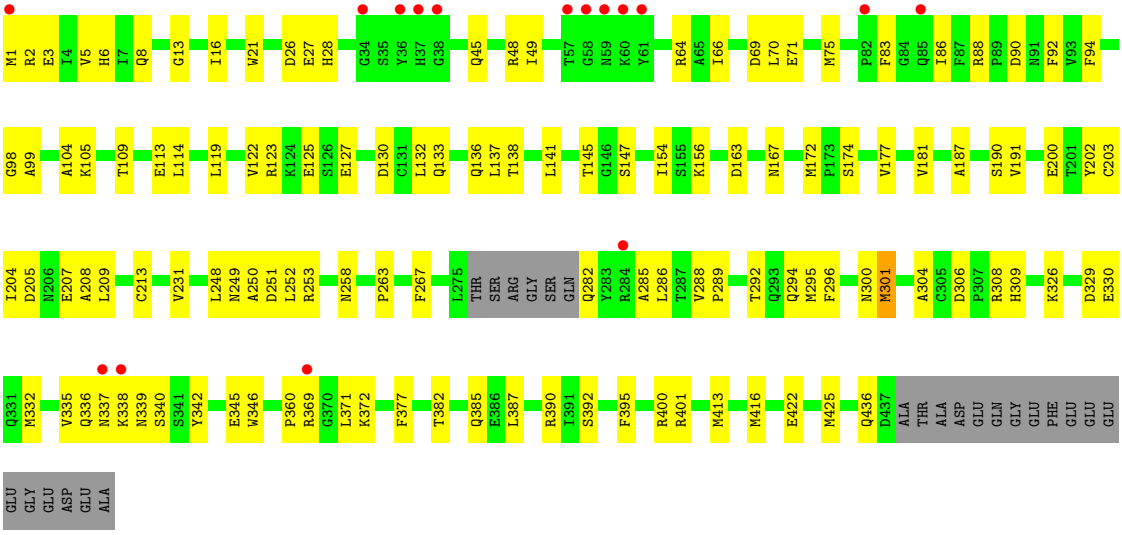
• Molecule 1: Tubulin alpha-1B chain

Chain C: % 77% 20%



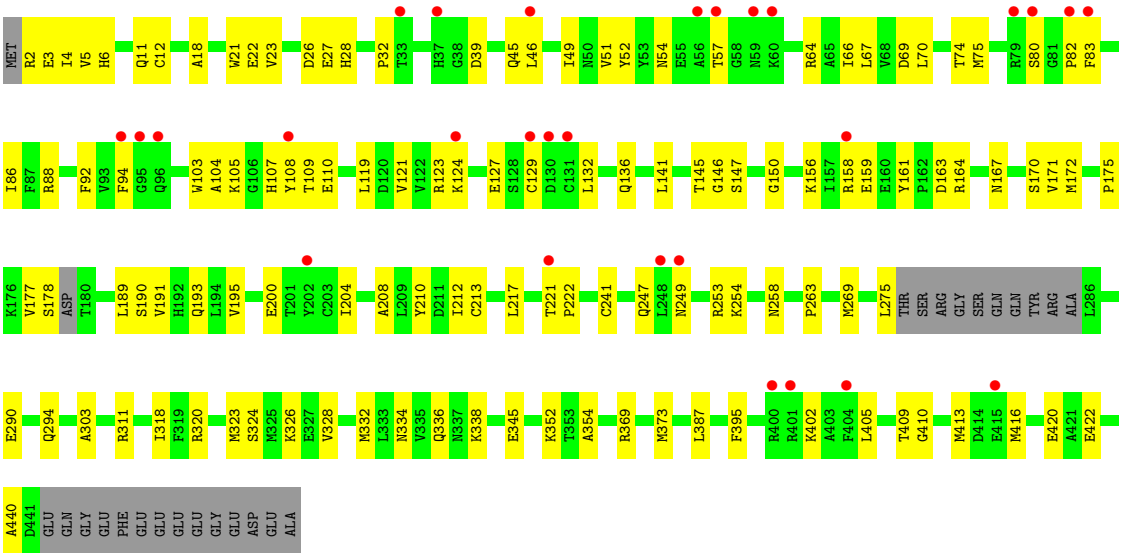
• Molecule 2: Tubulin beta-2B chain

Chain B: 4% 67% 28% 5%



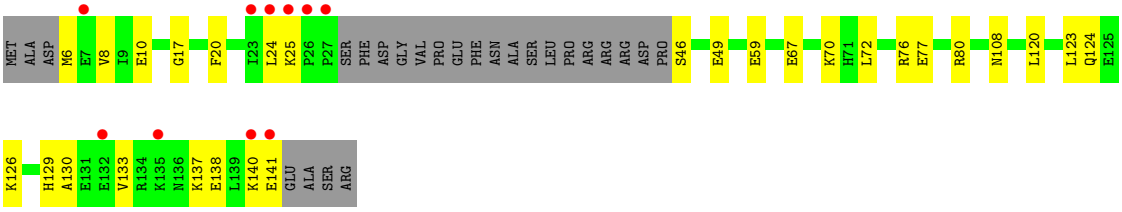
- Molecule 2: Tubulin beta-2B chain

Chain D:



- Molecule 3: Stathmin-4

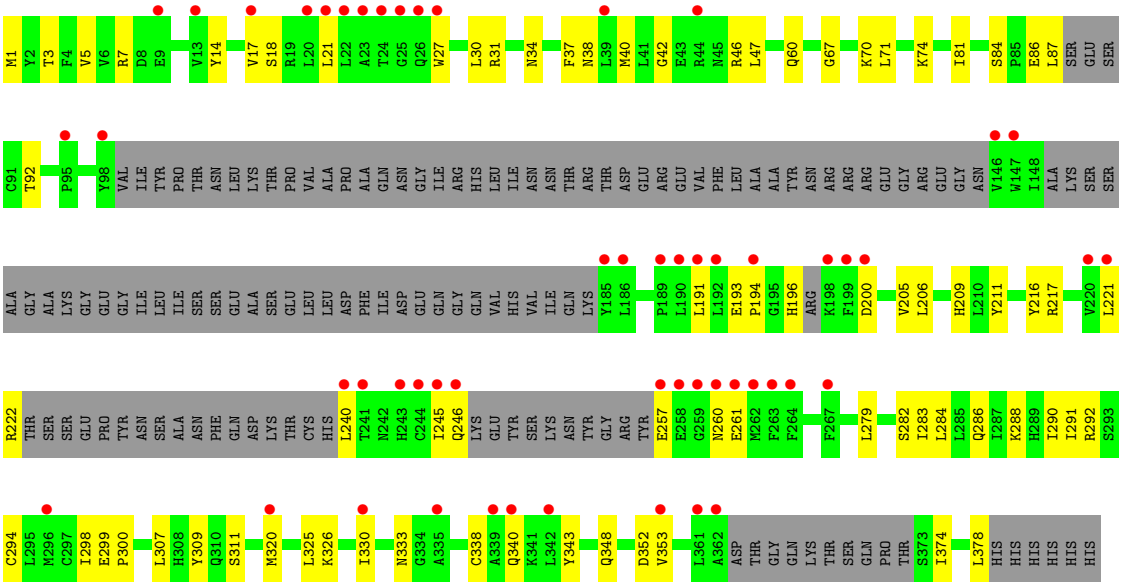
Chain E:



- Molecule 4: Uncharacterized protein

Chain F:

14%
46%
20%
34%


M1 Y2 T3 F4 V5 V6 R7 D8 E9 V13 Y14 V17 S18 R19 L20 L21 L22 A23 T24 G25 Q26 W27 L30 R31 N34 F37 N38 L39 M40 L41 G42 E43 R44 N45 R46 L47 Q60 G67 K70 L71 K74 I81 S84 P85 E86 L87 SER GLU SER
C91 T92 P95 Y98 VAL ILE TYR PRO THR ASN LEU LYS THR PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG THR ASP GLU ARG GLU VAL PHE LEU ALA ALA TYR ASN ARG ARG ARG GLU GLY ARG GLU GLY ASN V146 W147 I148 ALA LYS SER SER
ALA GLY ALA LYS GLY GLU GLY ILE LEU ILE SER SER GLU ALA SER GLU LEU LEU ASP PHE ILE ASP GLU GLN GLY GLN VAL HIS VAL ILE GLN LYS Y185 L186 P189 L190 L191 L192 E193 P194 G195 H196 ARG K198 F199 D200 V205 L206 H209 L210 Y211 Y216 R217 V220 L221
R222 THR SER SER GLU PRO TYR ASN SER ALA ASN PHE GLN ASP LYS THR CYS HIS L240 T241 N242 H243 C244 I245 Q246 LYS GLU TYR SER LYS ASN TYR GLY ARG TYR E257 E258 G259 N260 E261 M262 F263 F264 F267 L279 S282 I283 L284 L285 Q286 I287 K288 H289 I290 I291 R292 S293
C294 L295 M296 C297 I298 E299 P300 L307 H308 Y309 Q310 S311 M320 L325 K326 I330 N333 G334 A335 C338 A339 Q340 K341 L342 Y343 Q348 D352 V353 L361 A362 ASP THR GLY GLN LYS THR SER GLN PRO THR S373 I374 L378 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.91Å 157.47Å 180.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.98 – 2.50 47.98 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.98-2.50) 99.6 (47.98-2.49)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.48Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, R_{free}	0.204 , 0.256 0.204 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.6	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	17086	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

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

[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, MG, 9N5, GDP, 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	0.45	0/3568	0.58	0/4844
1	C	0.57	2/3551 (0.1%)	0.65	0/4822
2	B	0.54	1/3438 (0.0%)	0.65	0/4656
2	D	0.42	0/3373	0.58	0/4568
3	E	0.57	0/995	0.56	0/1318
4	F	0.41	0/2141	0.53	0/2889
All	All	0.49	3/17066 (0.0%)	0.60	0/23097

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	20	CYS	CB-SG	-6.20	1.71	1.82
1	C	295	CYS	CB-SG	-5.79	1.72	1.81
2	B	213	CYS	CB-SG	-5.04	1.73	1.81

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	3460	0	3407	99	0
1	C	3461	0	3377	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3346	0	3243	100	0
2	D	3298	0	3181	120	0
3	E	985	0	1010	36	0
4	F	2093	0	2105	76	0
5	A	32	12	12	1	0
5	C	32	12	12	0	0
6	B	28	12	12	0	0
6	D	28	12	12	3	0
7	B	2	0	0	0	0
7	D	2	0	0	0	0
8	B	26	21	0	1	0
8	D	26	21	0	1	0
9	F	31	14	14	3	0
10	A	30	0	0	0	0
10	B	25	0	0	3	0
10	C	43	0	0	4	0
10	D	18	0	0	3	0
10	E	6	0	0	1	0
10	F	10	0	0	0	0
All	All	16982	104	16385	469	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 14.

All (469) 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)
4:F:67:GLY:O	4:F:70:LYS:HD3	1.39	1.21
1:C:331:ALA:O	1:C:335:ILE:HD13	1.47	1.15
2:D:5:VAL:HG23	2:D:132:LEU:HD11	1.31	1.13
1:C:331:ALA:O	1:C:335:ILE:CD1	2.04	1.04
1:C:172:TYR:CE2	1:C:391:LEU:HD11	1.94	1.02
1:A:336:LYS:HD3	3:E:24:LEU:CD1	1.90	1.00
2:D:107:HIS:HD2	2:D:108:TYR:CE2	1.81	0.98
2:D:323:MET:SD	2:D:373:MET:HE3	2.03	0.97
2:D:2:ARG:NH1	2:D:249:ASN:OD1	1.98	0.95
2:B:205:ASP:OD2	2:B:390:ARG:NH2	1.98	0.94
1:C:71:GLU:OE1	2:D:249:ASN:ND2	2.01	0.94
1:C:175:PRO:HA	1:C:179:THR:HG21	1.53	0.90
1:C:175:PRO:HA	1:C:179:THR:CG2	2.05	0.87
2:D:345:GLU:OE2	2:D:345:GLU:N	2.07	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:CG	2:B:390:ARG:HH22	1.77	0.86
4:F:31:ARG:HB2	4:F:31:ARG:NH1	1.91	0.86
1:A:336:LYS:CD	3:E:24:LEU:HD13	2.07	0.84
1:A:3:GLU:OE2	1:A:131:GLY:O	1.95	0.84
4:F:46:ARG:HA	4:F:46:ARG:HH11	1.41	0.84
1:A:336:LYS:HD3	3:E:24:LEU:HD11	1.59	0.84
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.60	0.83
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.60	0.83
2:D:158:ARG:HG3	3:E:123:LEU:HD11	1.61	0.82
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.61	0.82
1:C:221:ARG:HH11	2:D:326:LYS:HG3	1.45	0.82
2:D:323:MET:SD	2:D:373:MET:CE	2.68	0.82
1:C:172:TYR:CE2	1:C:391:LEU:CD1	2.63	0.81
2:D:3:GLU:O	2:D:132:LEU:HD12	1.80	0.81
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.62	0.81
1:C:71:GLU:CD	2:D:249:ASN:HD21	1.84	0.81
2:B:338:LYS:HE2	4:F:1:MET:HB3	1.63	0.80
1:A:336:LYS:CD	3:E:24:LEU:CD1	2.59	0.80
2:B:1:MET:HG3	2:B:130:ASP:OD2	1.82	0.79
4:F:14:TYR:HA	4:F:17:VAL:HG23	1.66	0.78
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.65	0.77
2:B:338:LYS:CE	4:F:1:MET:HB3	2.13	0.77
2:B:207:GLU:OE1	2:B:390:ARG:NH1	2.18	0.77
2:D:3:GLU:OE2	2:D:3:GLU:N	2.18	0.76
2:B:1:MET:HB2	2:B:3:GLU:OE1	1.86	0.76
4:F:257:GLU:OE1	4:F:257:GLU:N	2.19	0.75
2:B:71:GLU:HG3	2:B:98:GLY:HA2	1.68	0.75
2:D:107:HIS:CD2	2:D:108:TYR:CE2	2.72	0.74
1:C:335:ILE:HD12	1:C:335:ILE:H	1.52	0.74
3:E:129:HIS:O	3:E:133:VAL:HG23	1.88	0.74
2:B:360:PRO:HG2	2:B:371:LEU:HB2	1.71	0.73
1:C:381:THR:OG1	10:C:601:HOH:O	2.07	0.72
2:D:409:THR:O	3:E:140:LYS:HE3	1.89	0.72
2:B:337:ASN:OD1	10:B:601:HOH:O	2.07	0.71
2:D:141:LEU:HD12	2:D:172:MET:SD	2.30	0.71
2:D:5:VAL:HG23	2:D:132:LEU:CD1	2.17	0.71
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.71	0.71
1:C:335:ILE:HD12	1:C:335:ILE:N	2.06	0.71
2:D:4:ILE:O	2:D:64:ARG:HD2	1.91	0.70
1:A:2:ARG:HB2	1:A:133:GLN:HG3	1.72	0.70
1:A:179:THR:HG22	1:A:183:GLU:OE2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TYR:CD2	1:C:391:LEU:HD11	2.26	0.70
2:D:18:ALA:O	2:D:22:GLU:HG3	1.91	0.70
2:D:416:MET:O	2:D:420:GLU:HG3	1.91	0.70
2:D:80:SER:OG	10:D:601:HOH:O	2.09	0.70
1:C:440:VAL:HG12	1:C:440:VAL:O	1.92	0.69
1:A:336:LYS:CE	3:E:24:LEU:HD13	2.21	0.69
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.57	0.69
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.73	0.69
2:D:290:GLU:O	2:D:294:GLN:HG3	1.93	0.69
1:A:23:LEU:O	1:A:27:GLU:HG3	1.93	0.69
4:F:86:GLU:O	4:F:87:LEU:HG	1.93	0.68
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.75	0.68
2:D:5:VAL:CG2	2:D:132:LEU:HD11	2.19	0.68
1:C:44:GLY:O	10:C:602:HOH:O	2.11	0.68
4:F:217:ARG:HE	4:F:374:ILE:HA	1.59	0.68
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	1.76	0.68
1:C:71:GLU:CD	2:D:249:ASN:ND2	2.47	0.68
1:A:336:LYS:HE2	3:E:24:LEU:HD13	1.74	0.68
1:C:221:ARG:HH11	2:D:326:LYS:CG	2.07	0.67
1:C:221:ARG:NH1	2:D:326:LYS:HG3	2.09	0.67
2:D:54:ASN:OD1	2:D:64:ARG:NH2	2.28	0.67
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.28	0.67
2:D:147:SER:HB2	2:D:190:SER:OG	1.95	0.67
2:B:332:MET:O	2:B:336:GLN:HG3	1.94	0.66
1:C:245:ASP:OD1	1:C:246:GLY:N	2.28	0.66
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.30	0.66
2:B:167:ASN:HD21	2:B:252:LEU:HD22	1.61	0.66
2:B:163:ASP:O	2:B:253:ARG:NH2	2.28	0.66
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.28	0.66
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.78	0.65
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.11	0.65
1:C:142:GLY:CA	1:C:183:GLU:HG2	2.27	0.65
2:D:345:GLU:H	2:D:345:GLU:CD	1.99	0.65
2:B:113:GLU:OE1	10:B:602:HOH:O	2.15	0.65
4:F:70:LYS:N	4:F:70:LYS:HD2	2.11	0.65
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.78	0.65
4:F:3:THR:HG22	4:F:30:LEU:HD11	1.79	0.65
2:D:123:ARG:O	2:D:127:GLU:HG3	1.97	0.64
2:B:285:ALA:HB2	2:B:372:LYS:HD2	1.79	0.64
1:A:88:HIS:N	1:A:91:GLN:OE1	2.31	0.63
2:D:323:MET:HB3	2:D:373:MET:HE3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.28	0.63
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.79	0.63
1:C:76:ASP:O	1:C:80:THR:HG22	1.99	0.63
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.80	0.63
1:C:335:ILE:CD1	1:C:335:ILE:H	2.11	0.63
1:A:336:LYS:CE	3:E:24:LEU:CD1	2.77	0.63
2:D:108:TYR:HE1	3:E:130:ALA:HB2	1.64	0.63
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.79	0.62
1:C:101:ASN:ND2	2:D:254:LYS:HE2	2.14	0.62
2:D:159:GLU:HG3	3:E:123:LEU:HD13	1.81	0.62
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.34	0.62
2:D:11:GLN:HB3	6:D:501:GDP:O2A	1.99	0.62
4:F:240:LEU:HB3	4:F:245:ILE:HD12	1.82	0.62
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.34	0.62
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.82	0.62
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.30	0.62
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	1.80	0.61
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.65	0.61
2:D:175:PRO:HA	2:D:178:SER:OG	2.01	0.61
4:F:92:THR:HG22	4:F:92:THR:O	2.00	0.61
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.17	0.61
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.82	0.61
4:F:70:LYS:HD2	4:F:70:LYS:H	1.66	0.61
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.82	0.60
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.83	0.60
2:D:241:CYS:HA	2:D:247:GLN:HG3	1.82	0.60
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.83	0.60
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.37	0.60
2:B:295:MET:CG	2:B:377:PHE:HB2	2.32	0.60
1:C:297:GLU:OE1	1:C:299:ALA:N	2.31	0.60
4:F:31:ARG:HB2	4:F:31:ARG:HH11	1.64	0.60
2:B:123:ARG:O	2:B:127:GLU:HG3	2.02	0.60
2:D:67:LEU:N	2:D:67:LEU:HD12	2.17	0.60
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.37	0.59
2:B:147[B]:SER:OG	2:B:190:SER:OG	2.18	0.59
2:D:108:TYR:CE1	3:E:130:ALA:HB2	2.37	0.59
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.84	0.59
2:D:28:HIS:HA	2:D:45:GLN:HB3	1.83	0.59
2:B:296:PHE:CD1	2:B:335:VAL:HG11	2.38	0.59
2:D:208:ALA:O	2:D:212:ILE:HG13	2.01	0.59
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:ARG:NE	2:D:129:CYS:SG	2.76	0.59
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.85	0.59
4:F:31:ARG:HB2	4:F:31:ARG:CZ	2.31	0.59
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.84	0.59
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.84	0.58
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.43	0.58
4:F:216:TYR:CE1	4:F:374:ILE:HD12	2.39	0.58
2:B:340:SER:HB3	4:F:34:ASN:HD21	1.69	0.58
3:E:67:GLU:OE2	3:E:70:LYS:HE2	2.03	0.58
2:D:158:ARG:CG	3:E:123:LEU:HD11	2.31	0.58
2:B:26:ASP:OD2	2:B:369:ARG:CD	2.52	0.57
4:F:7:ARG:HD3	4:F:40:MET:CE	2.34	0.57
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.04	0.57
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.86	0.57
4:F:46:ARG:HH11	4:F:46:ARG:CA	2.16	0.57
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.39	0.57
2:B:83:PHE:O	2:B:86:ILE:HG22	2.05	0.57
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.85	0.57
3:E:46:SER:OG	3:E:49:GLU:OE1	2.20	0.57
1:A:7:ILE:HG12	1:A:66[B]:VAL:CG1	2.36	0.56
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.88	0.56
4:F:18:SER:HA	4:F:21:LEU:HD12	1.88	0.56
2:B:26:ASP:OD2	2:B:369:ARG:HD3	2.05	0.56
2:B:282:GLN:N	10:B:603:HOH:O	2.38	0.56
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.88	0.56
1:A:329:ASN:HB3	3:E:6:MET:CE	2.36	0.56
1:C:172:TYR:HE2	1:C:391:LEU:CD1	2.16	0.56
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.88	0.56
2:D:345:GLU:CG	2:D:440:ALA:HB2	2.36	0.56
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.88	0.56
2:D:323:MET:CE	2:D:373:MET:HE3	2.36	0.56
1:C:175:PRO:HA	1:C:179:THR:HG22	1.84	0.55
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.36	0.55
4:F:333:ASN:ND2	9:F:401:ACP:O1G	2.40	0.55
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.06	0.55
1:A:44:GLY:O	1:A:55:GLU:OE2	2.25	0.55
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.40	0.55
4:F:70:LYS:H	4:F:70:LYS:CD	2.19	0.55
1:C:341:ILE:HD12	1:C:351:PHE:HZ	1.72	0.55
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.36	0.55
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLN:HG2	2:B:252:LEU:HD12	1.89	0.55
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.41	0.55
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.89	0.55
2:B:28:HIS:HB3	2:B:49:ILE:CD1	2.37	0.55
2:D:177:VAL:HG12	2:D:177:VAL:O	2.07	0.54
2:D:64:ARG:HD3	2:D:129:CYS:SG	2.47	0.54
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.56	0.54
1:C:271:THR:HG21	1:C:295:CYS:O	2.08	0.54
1:A:93:ILE:HD11	1:A:121:ARG:CG	2.35	0.54
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.89	0.54
2:D:107:HIS:HD2	2:D:108:TYR:CZ	2.24	0.54
2:D:110:GLU:OE1	2:D:110:GLU:HA	2.08	0.54
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.73	0.54
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.90	0.54
4:F:14:TYR:HA	4:F:17:VAL:CG2	2.35	0.54
2:B:137:LEU:CD2	2:B:154:ILE:HD11	2.38	0.53
1:A:416:GLY:O	1:A:420[B]:GLU:HG3	2.08	0.53
1:A:136[A]:LEU:CD2	1:A:167:LEU:HB2	2.34	0.53
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.90	0.53
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.44	0.53
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.38	0.53
2:B:167:ASN:ND2	2:B:252:LEU:HD22	2.24	0.53
2:D:210:TYR:CE1	2:D:222:PRO:HG2	2.44	0.53
4:F:86:GLU:O	4:F:87:LEU:CB	2.56	0.53
2:B:69:ASP:O	2:B:94:PHE:HA	2.09	0.53
4:F:3:THR:CG2	4:F:30:LEU:HD11	2.39	0.53
4:F:38:ASN:O	4:F:60:GLN:HA	2.09	0.53
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.09	0.53
2:D:191:VAL:O	2:D:195:VAL:HG23	2.09	0.53
1:C:331:ALA:O	1:C:335:ILE:HD12	2.03	0.52
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.08	0.52
2:D:39:ASP:N	2:D:39:ASP:OD1	2.42	0.52
2:D:323:MET:HB3	2:D:373:MET:CE	2.38	0.52
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.91	0.52
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.39	0.52
3:E:108:ASN:ND2	10:E:201:HOH:O	2.43	0.52
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.10	0.51
1:A:151:SER:HB2	1:A:193:THR:HG22	1.92	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.11	0.51
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.46	0.51
2:D:2:ARG:CZ	2:D:249:ASN:OD1	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.28	0.51
2:D:69:ASP:O	2:D:94:PHE:HA	2.10	0.51
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.22	0.51
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.45	0.51
1:C:221:ARG:HH11	2:D:326:LYS:CB	2.23	0.51
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.92	0.51
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.51
1:A:285:GLN:OE1	1:A:372[B]:GLN:HG3	2.11	0.51
1:C:350:GLY:O	1:C:351:PHE:HD1	1.94	0.50
1:A:39:ASP:OD1	1:A:41:THR:OG1	2.18	0.50
3:E:120:LEU:O	3:E:124:GLN:HG3	2.11	0.50
1:A:430:LYS:O	1:A:434:GLU:HG3	2.11	0.50
2:B:2:ARG:HD2	2:B:48:ARG:HH22	1.76	0.50
2:D:70:LEU:HD13	2:D:110:GLU:HB2	1.94	0.50
2:B:248:LEU:HG	2:B:250:ALA:HB2	1.93	0.50
2:B:326:LYS:O	2:B:330:GLU:HG3	2.12	0.50
2:D:332:MET:O	2:D:336:GLN:HG3	2.11	0.50
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.46	0.50
2:B:416:MET:HA	2:B:416:MET:HE2	1.93	0.50
2:B:205:ASP:OD2	2:B:390:ARG:CZ	2.58	0.50
1:C:108:TYR:O	1:C:112:LYS:HG2	2.12	0.50
2:B:172:MET:HE3	2:B:203:CYS:CB	2.42	0.49
2:D:88:ARG:HH12	2:D:124:LYS:HE2	1.76	0.49
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.95	0.49
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.77	0.49
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.46	0.49
1:A:151:SER:HB2	1:A:193:THR:CG2	2.42	0.49
1:A:285:GLN:HA	1:A:285:GLN:NE2	2.27	0.49
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.47	0.49
4:F:333:ASN:HD21	9:F:401:ACP:PG	2.35	0.49
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.12	0.49
1:A:241:SER:HB2	1:A:249:ASN:O	2.13	0.49
2:D:22:GLU:OE1	2:D:82:PRO:HG2	2.13	0.49
2:D:320:ARG:O	2:D:373:MET:HA	2.13	0.49
2:B:392:SER:HB2	2:B:425:MET:HE3	1.95	0.48
4:F:84:SER:O	4:F:86:GLU:O	2.31	0.48
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.95	0.48
1:A:192:HIS:NE2	1:A:420[A]:GLU:HG2	2.28	0.48
1:A:2:ARG:HB2	1:A:133:GLN:CG	2.42	0.48
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.33	0.48
1:C:180:ALA:HB1	2:D:258:ASN:OD1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:N	1:A:184:PRO:CD	2.77	0.48
2:B:137:LEU:HD22	2:B:154:ILE:HD11	1.95	0.48
1:C:209:ILE:HD11	1:C:302:MET:SD	2.53	0.48
2:D:70:LEU:HD13	2:D:110:GLU:CB	2.43	0.48
4:F:307:LEU:HD13	4:F:309:TYR:CE1	2.48	0.48
2:B:119:LEU:HD11	2:B:156:LYS:CB	2.44	0.48
2:D:75:MET:CE	2:D:92:PHE:HB3	2.43	0.48
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.44	0.48
1:A:90:GLU:O	1:A:121:ARG:HD2	2.14	0.48
1:A:276:ILE:HD12	1:A:283:HIS:NE2	2.29	0.48
1:C:77:GLU:HA	1:C:80:THR:HG22	1.95	0.48
1:A:175:PRO:HA	1:A:179:THR:OG1	2.13	0.47
2:D:88:ARG:HH12	2:D:124:LYS:CE	2.27	0.47
2:D:108:TYR:CE1	3:E:130:ALA:CB	2.97	0.47
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.95	0.47
4:F:70:LYS:N	4:F:70:LYS:CD	2.75	0.47
2:B:70:LEU:HD23	2:B:114:LEU:HD22	1.96	0.47
2:D:318:ILE:HD13	2:D:354:ALA:HB3	1.95	0.47
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.14	0.47
4:F:209:HIS:HA	4:F:311:SER:O	2.15	0.47
1:A:336:LYS:HE2	3:E:24:LEU:CD1	2.40	0.47
3:E:80:ARG:NH1	3:E:80:ARG:HB3	2.29	0.47
1:A:289:ALA:HA	1:A:331:ALA:HB2	1.97	0.47
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.47
1:C:221:ARG:HH11	2:D:326:LYS:CA	2.28	0.47
2:D:23:VAL:O	2:D:27:GLU:HG3	2.15	0.47
3:E:80:ARG:HB3	3:E:80:ARG:HH11	1.79	0.47
2:D:83:PHE:O	2:D:86:ILE:HG22	2.15	0.47
1:C:221:ARG:HH11	2:D:326:LYS:HA	1.80	0.47
2:D:124:LYS:C	2:D:124:LYS:HD3	2.35	0.47
4:F:191:LEU:HD13	4:F:196:HIS:C	2.35	0.47
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.55	0.46
2:D:167:ASN:ND2	2:D:200:GLU:HB2	2.30	0.46
2:D:212:ILE:CG2	2:D:275:LEU:HD13	2.45	0.46
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.45	0.46
1:A:8:HIS:HB3	1:A:13:GLY:O	2.16	0.46
1:C:221:ARG:NH1	2:D:326:LYS:HA	2.29	0.46
3:E:72:LEU:O	3:E:76:ARG:HG2	2.15	0.46
4:F:81:ILE:HA	4:F:87:LEU:CD1	2.44	0.46
1:A:66[A]:VAL:HG23	1:A:125:LEU:HD12	1.97	0.46
1:A:254:GLU:O	1:A:258:ASN:N	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.46
3:E:67:GLU:OE2	3:E:70:LYS:CE	2.63	0.46
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.96	0.46
1:C:36:MET:HG2	1:C:36:MET:O	2.16	0.46
4:F:221:LEU:O	4:F:261:GLU:HA	2.15	0.46
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.50	0.46
2:B:2:ARG:HE	2:B:251:ASP:HB3	1.81	0.46
2:D:105:LYS:HA	2:D:109:THR:HB	1.98	0.46
2:D:410:GLY:O	3:E:137:LYS:HG3	2.15	0.46
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.46	0.46
1:A:326:LYS:HB3	1:A:326:LYS:HE2	1.56	0.46
1:A:349:THR:HB	3:E:25:LYS:HB3	1.97	0.46
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.15	0.46
2:B:248:LEU:HD12	2:B:249:ASN:N	2.29	0.46
4:F:292:ARG:HG3	4:F:378:LEU:HD13	1.97	0.46
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.31	0.46
2:B:416:MET:HA	2:B:416:MET:CE	2.46	0.46
1:C:14:VAL:HG11	1:C:74:VAL:HG12	1.98	0.46
2:B:282:GLN:HA	2:B:282:GLN:OE1	2.16	0.46
1:C:192:HIS:CG	1:C:421:ALA:HA	2.51	0.46
4:F:3:THR:O	4:F:38:ASN:HB2	2.16	0.46
2:B:141:LEU:HD12	2:B:172:MET:SD	2.56	0.45
2:B:345:GLU:OE2	2:B:346:TRP:HD1	1.98	0.45
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.40	0.45
2:D:12:CYS:HB2	6:D:501:GDP:C8	2.51	0.45
4:F:205:VAL:HG21	4:F:291:ILE:HG21	1.98	0.45
1:C:142:GLY:HA3	1:C:183:GLU:HG2	1.97	0.45
4:F:200:ASP:OD1	4:F:222:ARG:HD3	2.17	0.45
4:F:286:GLN:O	4:F:290:ILE:HG13	2.17	0.45
2:B:174:SER:CB	2:B:207:GLU:HB2	2.47	0.45
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.52	0.45
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	1.99	0.45
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.99	0.45
2:D:311:ARG:NH1	2:D:345:GLU:OE2	2.42	0.45
1:A:9:VAL:HA	1:A:68[B]:VAL:HG13	1.99	0.45
1:A:289:ALA:HA	1:A:331:ALA:CB	2.46	0.45
1:C:172:TYR:CE2	1:C:391:LEU:CG	3.00	0.45
2:D:324:SER:O	2:D:328:VAL:HG23	2.17	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.52	0.44
2:D:163:ASP:O	2:D:253:ARG:NH2	2.50	0.44
4:F:92:THR:O	4:F:326:LYS:NZ	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:CG	1:A:421:ALA:HA	2.52	0.44
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.52	0.44
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.44
2:B:187:ALA:O	2:B:191:VAL:HG23	2.17	0.44
2:B:286:LEU:N	2:B:286:LEU:HD12	2.33	0.44
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.99	0.44
4:F:338:CYS:HB3	4:F:343:TYR:CZ	2.52	0.44
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.81	0.44
4:F:193:GLU:HA	4:F:194:PRO:C	2.38	0.44
4:F:31:ARG:HH11	4:F:31:ARG:CB	2.29	0.44
1:C:141:PHE:O	1:C:147:SER:HB3	2.18	0.44
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.52	0.44
3:E:8:VAL:O	3:E:8:VAL:HG12	2.18	0.44
4:F:240:LEU:HD13	4:F:245:ILE:HD11	1.99	0.44
1:A:311:LYS:HB3	1:A:344:VAL:HG13	1.99	0.43
1:A:415:GLU:O	1:A:418:PHE:HB2	2.18	0.43
2:B:71:GLU:HG3	2:B:98:GLY:CA	2.43	0.43
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.48	0.43
2:B:286:LEU:HD21	2:B:294:GLN:OE1	2.18	0.43
2:D:108:TYR:CD1	3:E:130:ALA:CB	3.02	0.43
2:D:141:LEU:HD21	2:D:170:SER:HB3	2.00	0.43
2:B:75:MET:CE	2:B:94:PHE:HD1	2.31	0.43
2:B:251:ASP:OD1	2:B:251:ASP:N	2.40	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.18	0.43
2:D:323:MET:CB	2:D:373:MET:HE3	2.47	0.43
4:F:47:LEU:C	4:F:47:LEU:HD23	2.39	0.43
1:A:329:ASN:HB3	3:E:6:MET:HE1	1.99	0.43
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.53	0.43
2:D:64:ARG:CD	2:D:129:CYS:SG	3.06	0.43
2:B:181:VAL:HG12	1:C:348:PRO:HD2	2.00	0.43
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.42	0.43
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.49	0.43
1:C:63:PRO:HG2	1:C:87:PHE:CE2	2.53	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.43
2:D:145:THR:HB	6:D:501:GDP:O2B	2.18	0.43
2:D:247:GLN:HA	2:D:247:GLN:OE1	2.19	0.43
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.99	0.43
1:A:251:ASP:OD1	1:A:253:THR:HB	2.18	0.43
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.82	0.43
4:F:3:THR:HB	4:F:30:LEU:CD2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.43
2:B:105:LYS:HA	2:B:109:THR:OG1	2.18	0.43
1:A:221:ARG:HH21	2:B:329:ASP:HB2	1.84	0.43
4:F:299:GLU:N	4:F:300:PRO:HD2	2.34	0.43
2:B:16[B]:ILE:HG21	2:B:231:VAL:HG11	2.01	0.43
2:D:334:ASN:O	2:D:338:LYS:HG3	2.19	0.43
4:F:74:LYS:NZ	9:F:401:ACP:H3B1	2.33	0.43
2:B:141:LEU:HD22	2:B:190:SER:HB3	2.00	0.43
1:C:214:ARG:NE	10:C:607:HOH:O	2.47	0.43
1:C:430:LYS:O	1:C:434:GLU:HG3	2.19	0.42
2:D:146:GLY:O	2:D:150:GLY:HA3	2.19	0.42
2:D:395:PHE:CE1	2:D:422:GLU:HB2	2.54	0.42
4:F:86:GLU:C	4:F:87:LEU:HG	2.39	0.42
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.50	0.42
2:B:136:GLN:HA	2:B:167:ASN:O	2.19	0.42
2:B:300:ASN:N	2:B:300:ASN:HD22	2.18	0.42
2:D:161:TYR:HB3	2:D:164:ARG:CG	2.49	0.42
4:F:46:ARG:HA	4:F:46:ARG:NH1	2.21	0.42
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	2.01	0.42
2:B:382:THR:O	2:B:385:GLN:HG2	2.20	0.42
1:C:196:GLU:HG3	10:C:617:HOH:O	2.19	0.42
2:D:221:THR:O	2:D:221:THR:OG1	2.35	0.42
4:F:67:GLY:HA2	4:F:70:LYS:HE2	2.02	0.42
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.02	0.42
4:F:298:ILE:HD12	4:F:298:ILE:HA	1.80	0.42
2:D:3:GLU:N	2:D:3:GLU:CD	2.73	0.42
2:B:27:GLU:O	2:B:45:GLN:HG2	2.20	0.42
1:C:214:ARG:HD3	1:C:220:GLU:O	2.20	0.42
2:D:200:GLU:OE2	8:D:504:9N5:NAD	2.53	0.42
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.19	0.42
2:D:212:ILE:HG21	2:D:275:LEU:HD13	2.01	0.42
4:F:40:MET:HE3	4:F:42:GLY:HA2	2.02	0.42
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.55	0.42
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.59	0.42
1:A:276:ILE:HD12	1:A:283:HIS:CD2	2.55	0.42
2:D:46:LEU:HA	2:D:49:ILE:HB	2.02	0.42
4:F:21:LEU:O	4:F:27:TRP:HB2	2.20	0.42
3:E:10:GLU:O	3:E:20:PHE:HA	2.20	0.42
3:E:77:GLU:O	3:E:80:ARG:HG2	2.20	0.42
1:A:280:LYS:HE2	1:A:283:HIS:ND1	2.35	0.42
2:B:382:THR:OG1	2:B:436:GLN:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:VAL:HG12	2:D:52:TYR:CD2	2.55	0.42
4:F:206:LEU:HD23	4:F:353[A]:VAL:HG21	2.01	0.42
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
2:B:69:ASP:HA	2:B:145:THR:HG21	2.02	0.41
1:C:210:TYR:OH	1:C:221:ARG:NH2	2.52	0.41
2:D:352:LYS:HA	2:D:352:LYS:HD3	1.85	0.41
1:A:413:MET:CE	1:A:418:PHE:CE1	3.03	0.41
2:B:301:MET:HE3	2:B:301:MET:HA	2.02	0.41
4:F:5:VAL:HG13	4:F:37:PHE:HB3	2.02	0.41
1:A:41:THR:OG1	1:A:44:GLY:O	2.38	0.41
2:B:208:ALA:HB2	2:B:304:ALA:HB2	2.01	0.41
2:D:2:ARG:NH2	2:D:249:ASN:OD1	2.53	0.41
2:D:136:GLN:HA	2:D:167:ASN:O	2.21	0.41
2:D:409:THR:HA	2:D:413:MET:O	2.21	0.41
1:A:39:ASP:OD2	1:A:55:GLU:OE2	2.37	0.41
2:B:202:TYR:CD1	2:B:202:TYR:N	2.87	0.41
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.85	0.41
1:A:262:TYR:CE2	1:A:346:TRP:CH2	3.08	0.41
2:B:248:LEU:HG	2:B:250:ALA:CB	2.50	0.41
4:F:86:GLU:O	4:F:87:LEU:CG	2.65	0.41
1:A:9:VAL:HG22	1:A:68[B]:VAL:HG11	2.01	0.41
2:B:172:MET:HE3	2:B:203:CYS:HA	2.02	0.41
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.55	0.41
2:D:253:ARG:NH2	10:D:603:HOH:O	2.51	0.41
1:A:28:HIS:NE2	1:A:243:ARG:HD2	2.35	0.41
4:F:284:LEU:O	4:F:288:LYS:HG3	2.20	0.41
1:A:93:ILE:HD11	1:A:121:ARG:CB	2.51	0.41
1:A:180:ALA:HB1	2:B:258:ASN:OD1	2.21	0.41
2:B:8:GLN:HB3	2:B:138[A]:THR:OG1	2.21	0.41
2:B:200:GLU:OE2	8:B:504:9N5:NAD	2.54	0.41
2:D:82:PRO:O	2:D:83:PHE:HB2	2.21	0.41
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.51	0.41
1:C:295:CYS:SG	1:C:375:VAL:HG13	2.61	0.40
2:D:119:LEU:HD11	2:D:156:LYS:HB3	2.02	0.40
4:F:240:LEU:HB3	4:F:245:ILE:CD1	2.49	0.40
2:B:172:MET:CE	2:B:203:CYS:SG	3.09	0.40
2:B:288:VAL:N	2:B:289:PRO:CD	2.84	0.40
1:C:202:PHE:HE1	1:C:378:LEU:HD22	1.87	0.40
1:C:219:ILE:HD13	1:C:226:ASN:ND2	2.35	0.40
4:F:240:LEU:HD23	4:F:240:LEU:HA	1.90	0.40
4:F:257:GLU:N	4:F:257:GLU:CD	2.73	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	3.10	0.40
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.04	0.40
3:E:138:GLU:HA	3:E:141:GLU:HG2	2.04	0.40
2:D:253:ARG:NH1	10:D:603:HOH:O	2.29	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	445/451 (99%)	423 (95%)	22 (5%)	0	100	100
1	C	443/451 (98%)	432 (98%)	11 (2%)	0	100	100
2	B	423/445 (95%)	404 (96%)	18 (4%)	1 (0%)	47	68
2	D	414/445 (93%)	402 (97%)	12 (3%)	0	100	100
3	E	115/143 (80%)	112 (97%)	3 (3%)	0	100	100
4	F	239/384 (62%)	227 (95%)	12 (5%)	0	100	100
All	All	2079/2319 (90%)	2000 (96%)	78 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	177	VAL

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	378/379 (100%)	378 (100%)	0	100	100
1	C	376/379 (99%)	373 (99%)	3 (1%)	81	93
2	B	371/383 (97%)	370 (100%)	1 (0%)	92	97
2	D	363/383 (95%)	362 (100%)	1 (0%)	92	97
3	E	107/127 (84%)	106 (99%)	1 (1%)	78	92
4	F	231/342 (68%)	230 (100%)	1 (0%)	91	97
All	All	1826/1993 (92%)	1819 (100%)	7 (0%)	91	97

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

Mol	Chain	Res	Type
2	B	301	MET
1	C	82	THR
1	C	114	ILE
1	C	218	ASP
2	D	57	THR
3	E	59	GLU
4	F	211	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	256	GLN
2	B	101	ASN
2	B	139	HIS
2	B	167	ASN
2	B	258	ASN
2	D	50	ASN
2	D	91	ASN
2	D	107	HIS
2	D	139	HIS
2	D	167	ASN
2	D	197	ASN
3	E	108	ASN
4	F	246	GLN
4	F	260	ASN
4	F	333	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	348	GLN

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 11 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
8	9N5	B	504	-	25,27,27	2.74	7 (28%)	33,37,37	2.12	8 (24%)
9	ACP	F	401	-	27,33,33	1.53	6 (22%)	32,52,52	1.67	7 (21%)
6	GDP	D	501	7	24,30,30	2.52	7 (29%)	30,47,47	1.48	6 (20%)
6	GDP	B	501	7	24,30,30	2.50	6 (25%)	30,47,47	1.44	6 (20%)
5	GTP	C	501	7	26,34,34	2.48	7 (26%)	32,54,54	1.44	7 (21%)
5	GTP	A	501	7	26,34,34	2.40	7 (26%)	32,54,54	1.41	3 (9%)
8	9N5	D	504	-	25,27,27	2.78	8 (32%)	33,37,37	1.87	6 (18%)

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
8	9N5	B	504	-	-	6/18/22/22	0/2/2/2
9	ACP	F	401	-	-	6/15/38/38	0/3/3/3
6	GDP	D	501	7	-	4/12/32/32	0/3/3/3
6	GDP	B	501	7	-	4/12/32/32	0/3/3/3
5	GTP	C	501	7	-	7/18/38/38	0/3/3/3
5	GTP	A	501	7	-	5/18/38/38	0/3/3/3
8	9N5	D	504	-	-	5/18/22/22	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	O6-C6	8.60	1.40	1.23
6	D	501	GDP	O6-C6	8.55	1.40	1.23
8	D	504	9N5	CAU-NAV	8.42	1.33	1.26
5	A	501	GTP	O6-C6	8.33	1.40	1.23
8	B	504	9N5	OAW-NAV	-8.13	1.29	1.40
6	B	501	GDP	O6-C6	8.10	1.39	1.23
8	D	504	9N5	OAW-NAV	-7.99	1.29	1.40
8	B	504	9N5	CAU-NAV	7.80	1.33	1.26
6	B	501	GDP	C2'-C1'	-5.07	1.46	1.53
8	D	504	9N5	CAC-NAD	4.89	1.39	1.31
6	D	501	GDP	C2'-C1'	-4.84	1.46	1.53
8	B	504	9N5	CAC-NAD	4.14	1.38	1.31
5	C	501	GTP	C2'-C1'	-4.01	1.47	1.53
5	C	501	GTP	C2-N2	3.83	1.43	1.34
5	A	501	GTP	C2-N2	3.83	1.43	1.34
5	A	501	GTP	C2'-C1'	-3.77	1.48	1.53
9	F	401	ACP	O4'-C1'	3.74	1.46	1.41
6	B	501	GDP	O4'-C1'	3.34	1.45	1.41
6	D	501	GDP	O4'-C1'	3.27	1.45	1.41
6	B	501	GDP	C8-N7	3.18	1.40	1.35
8	B	504	9N5	CAF-CAE	-3.08	1.37	1.42
6	D	501	GDP	C8-N7	3.06	1.40	1.35
6	B	501	GDP	C3'-C4'	-2.99	1.45	1.53
9	F	401	ACP	C2'-C1'	-2.82	1.49	1.53
5	A	501	GTP	O4'-C1'	2.76	1.44	1.41
6	D	501	GDP	C3'-C4'	-2.75	1.46	1.53
6	D	501	GDP	C2-N2	2.71	1.40	1.34
8	B	504	9N5	CAK-CAL	-2.69	1.08	1.17
5	A	501	GTP	C2'-C3'	-2.68	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	504	9N5	CAK-CAL	-2.55	1.08	1.17
6	B	501	GDP	C2-N2	2.53	1.40	1.34
5	C	501	GTP	C2'-C3'	-2.50	1.46	1.53
8	D	504	9N5	CAB-CAK	-2.44	1.39	1.44
8	B	504	9N5	CAB-CAK	-2.36	1.39	1.44
8	B	504	9N5	CAE-NAD	-2.34	1.33	1.37
9	F	401	ACP	C2'-C3'	-2.33	1.47	1.53
5	A	501	GTP	PG-O2G	-2.27	1.46	1.54
9	F	401	ACP	PB-O2B	-2.26	1.51	1.56
5	C	501	GTP	O3'-C3'	2.22	1.48	1.43
5	A	501	GTP	C8-N7	2.20	1.38	1.35
8	D	504	9N5	CAJ-CAF	-2.20	1.37	1.42
6	D	501	GDP	C5-C4	2.17	1.48	1.43
5	C	501	GTP	PB-O2B	-2.09	1.45	1.55
8	D	504	9N5	CAE-NAD	-2.09	1.33	1.37
9	F	401	ACP	C6-N6	2.09	1.41	1.34
9	F	401	ACP	C5-C4	2.08	1.46	1.40
8	D	504	9N5	CAF-CAE	-2.03	1.39	1.42
5	C	501	GTP	O4'-C1'	2.01	1.43	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	504	9N5	CAB-CAC-NAD	-7.73	120.14	124.36
8	D	504	9N5	CAB-CAC-NAD	-6.18	120.98	124.36
9	F	401	ACP	C3'-C2'-C1'	4.42	107.63	100.98
8	D	504	9N5	OAP-CAN-OAM	-4.31	95.94	111.81
8	B	504	9N5	CAC-NAD-CAE	3.73	121.41	116.91
6	B	501	GDP	O3B-PB-O3A	3.68	116.97	104.64
6	B	501	GDP	C5-C6-N1	3.47	120.09	113.95
9	F	401	ACP	N3-C2-N1	-3.45	123.28	128.68
9	F	401	ACP	PB-O3A-PA	-3.30	122.08	132.56
9	F	401	ACP	C4-C5-N7	-3.25	106.01	109.40
8	B	504	9N5	OAP-CAN-OAM	-3.18	100.10	111.81
5	A	501	GTP	C5-C6-N1	3.18	119.56	113.95
5	A	501	GTP	C2-N1-C6	-3.08	119.43	125.10
5	C	501	GTP	C5-C6-N1	2.94	119.15	113.95
5	A	501	GTP	O2G-PG-O3B	2.94	114.49	104.64
8	D	504	9N5	CAI-OAM-CAN	2.87	124.27	118.76
6	D	501	GDP	C5-C6-N1	2.85	118.99	113.95
6	D	501	GDP	O2B-PB-O3A	2.81	114.05	104.64
6	D	501	GDP	C3'-C2'-C1'	2.79	105.17	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	504	9N5	CAU-CAT-NAS	-2.74	105.53	113.23
6	D	501	GDP	O3B-PB-O3A	2.70	113.69	104.64
5	C	501	GTP	O3G-PG-O3B	2.69	113.66	104.64
8	D	504	9N5	CAA-CAF-CAE	2.68	121.77	118.27
8	B	504	9N5	CAQ-OAP-CAN	2.66	118.38	113.24
6	B	501	GDP	C2-N1-C6	-2.66	120.20	125.10
5	C	501	GTP	PB-O3B-PG	-2.60	123.89	132.83
5	C	501	GTP	C2-N1-C6	-2.57	120.37	125.10
8	B	504	9N5	CAN-CAO-NAS	-2.51	112.53	116.30
6	D	501	GDP	C2-N1-C6	-2.43	120.62	125.10
8	B	504	9N5	CAA-CAF-CAE	2.37	121.37	118.27
5	C	501	GTP	O2B-PB-O1B	-2.35	100.61	112.24
8	D	504	9N5	CAC-NAD-CAE	2.34	119.72	116.91
5	C	501	GTP	C3'-C2'-C1'	2.31	104.45	100.98
9	F	401	ACP	C2'-C3'-C4'	2.27	107.05	102.64
6	B	501	GDP	O6-C6-N1	-2.21	118.04	120.65
8	B	504	9N5	CAA-CAB-CAK	2.19	123.36	120.32
9	F	401	ACP	O2G-PG-C3B	2.12	111.55	106.40
5	C	501	GTP	O2G-PG-O3B	2.12	111.76	104.64
6	D	501	GDP	O6-C6-N1	-2.11	118.16	120.65
8	D	504	9N5	CAZ-CAT-NAS	2.08	114.78	108.06
6	B	501	GDP	C3'-C2'-C1'	2.06	104.08	100.98
6	B	501	GDP	O2B-PB-O3A	2.06	111.54	104.64
9	F	401	ACP	C2-N1-C6	2.01	122.20	118.75

There are no chirality outliers.

All (37) 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
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
6	D	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O1A
6	D	501	GDP	C5'-O5'-PA-O2A
8	B	504	9N5	CAO-CAN-OAP-CAQ
8	B	504	9N5	CAU-NAV-OAW-CAX
9	F	401	ACP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	F	401	ACP	O4'-C4'-C5'-O5'
9	F	401	ACP	C3'-C4'-C5'-O5'
8	D	504	9N5	OAP-CAN-CAO-OAR
8	D	504	9N5	OAP-CAN-CAO-NAS
9	F	401	ACP	C5'-O5'-PA-O3A
6	B	501	GDP	PB-O3A-PA-O2A
9	F	401	ACP	C5'-O5'-PA-O2A
6	D	501	GDP	C3'-C4'-C5'-O5'
8	B	504	9N5	CAU-CAT-NAS-CAO
8	D	504	9N5	CAU-CAT-NAS-CAO
5	C	501	GTP	PB-O3B-PG-O1G
8	B	504	9N5	OAM-CAN-OAP-CAQ
8	D	504	9N5	CAO-CAN-OAP-CAQ
8	B	504	9N5	OAP-CAN-CAO-NAS
9	F	401	ACP	PG-C3B-PB-O1B
8	D	504	9N5	CAA-CAB-CAK-CAL
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
8	B	504	9N5	OAP-CAN-CAO-OAR
5	C	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

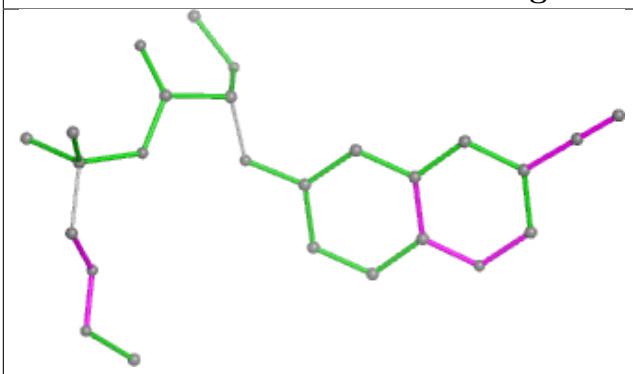
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	504	9N5	1	0
9	F	401	ACP	3	0
6	D	501	GDP	3	0
5	A	501	GTP	1	0
8	D	504	9N5	1	0

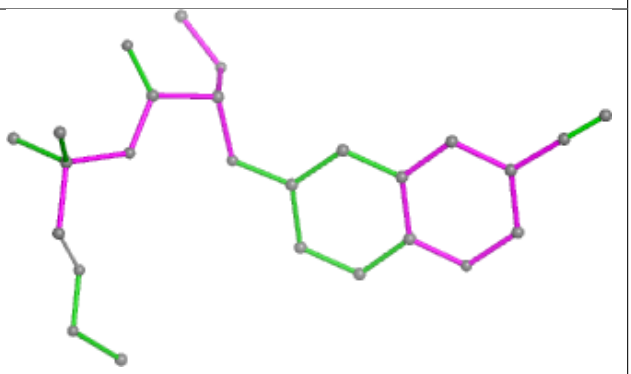
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

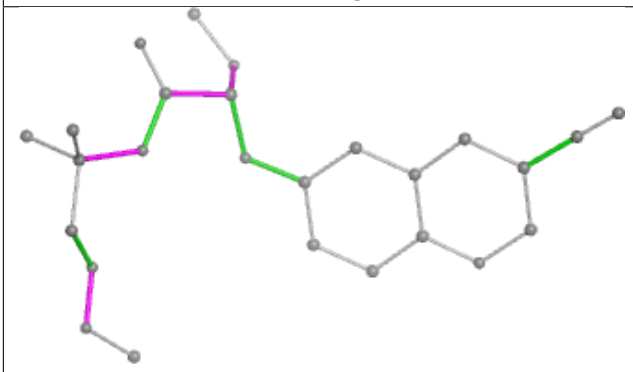
Ligand 9N5 B 504



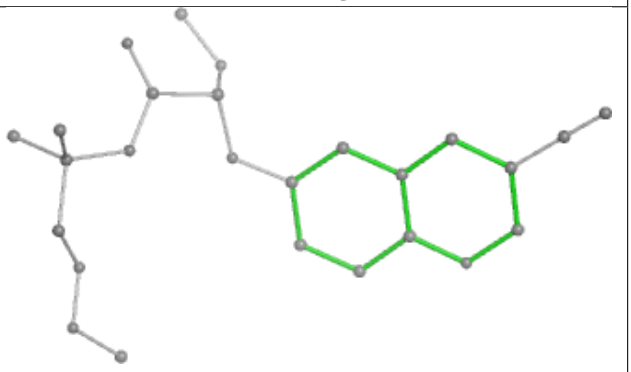
Bond lengths



Bond angles

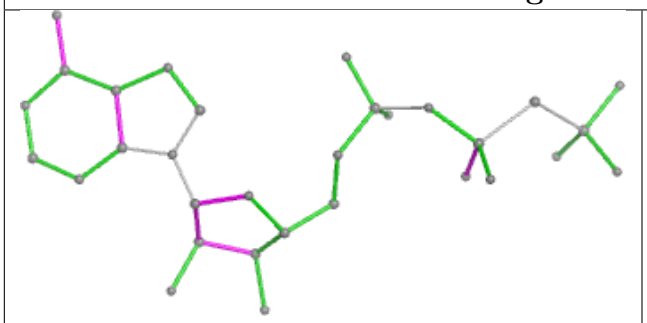


Torsions

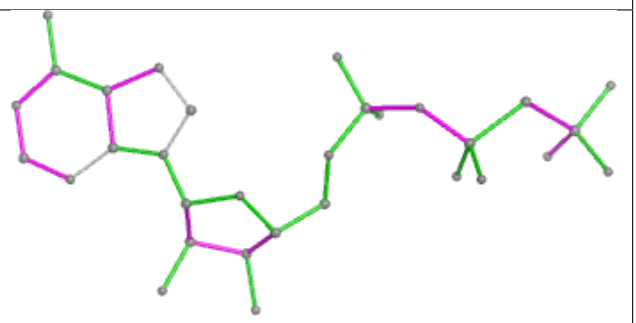


Rings

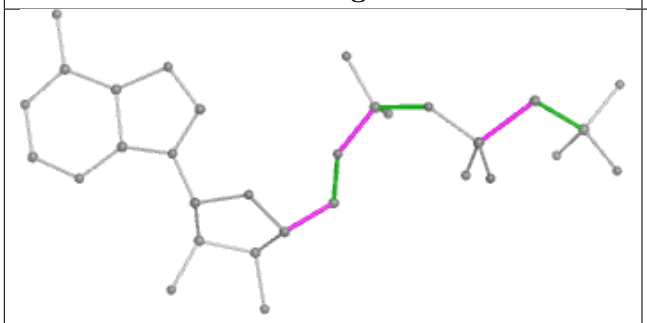
Ligand ACP F 401



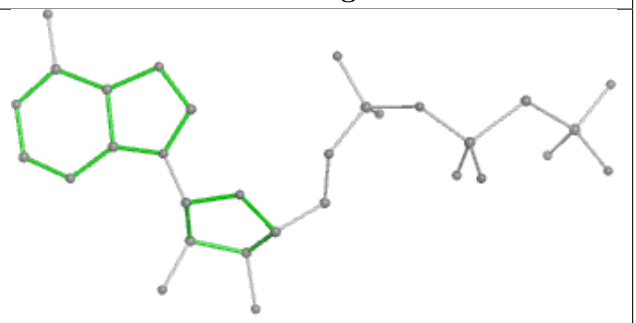
Bond lengths



Bond angles

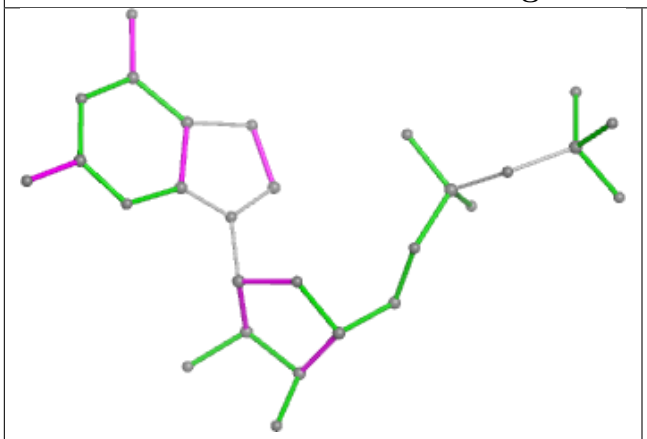


Torsions

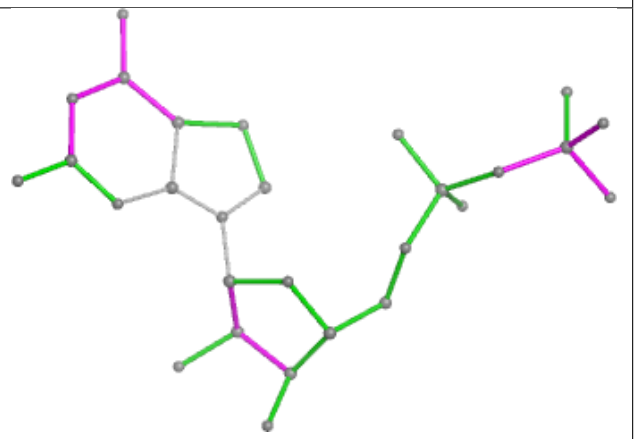


Rings

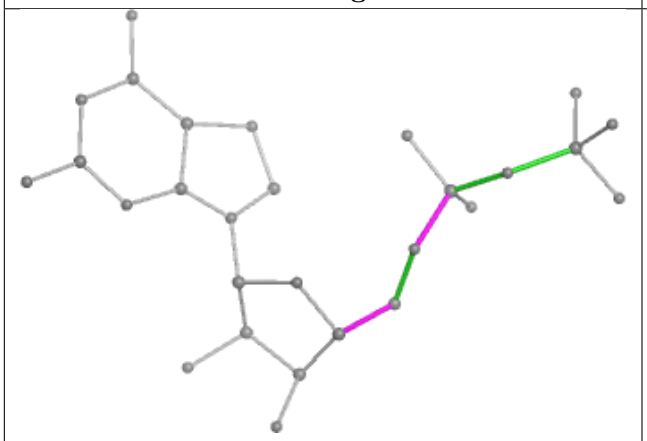
Ligand GDP D 501



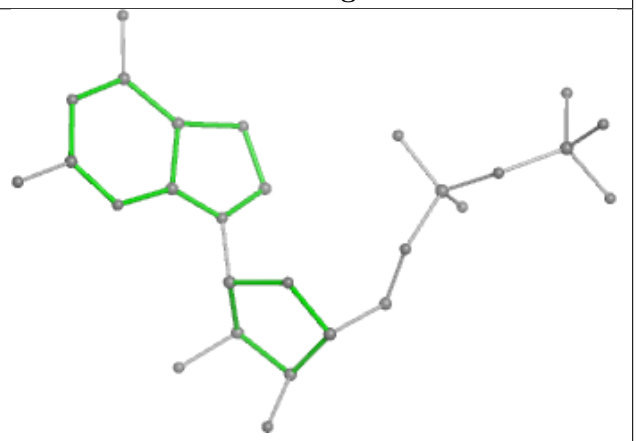
Bond lengths



Bond angles

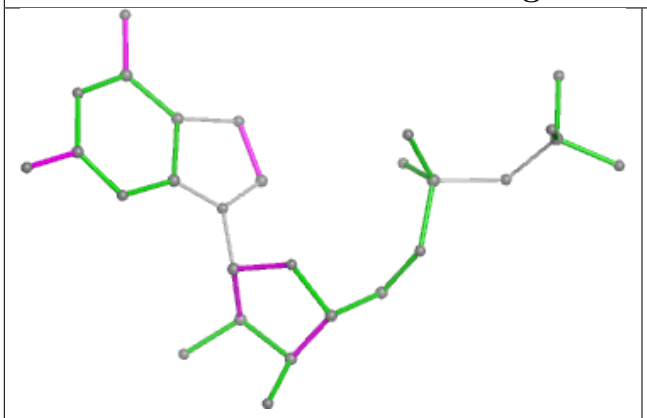


Torsions

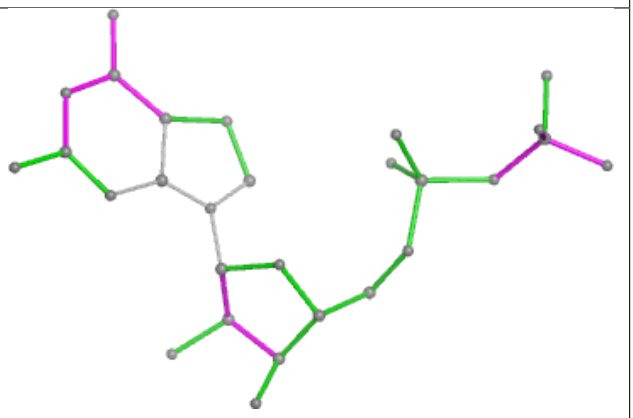


Rings

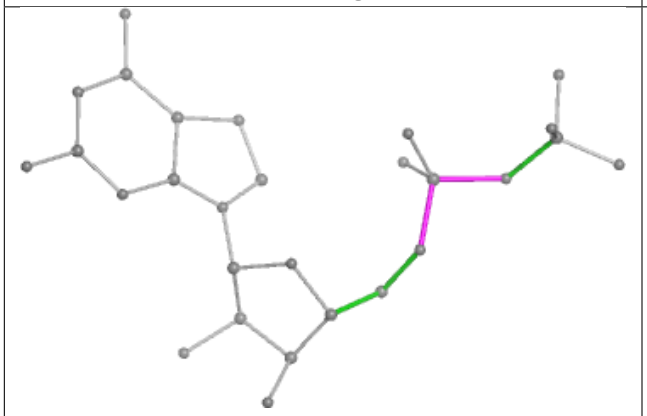
Ligand GDP B 501



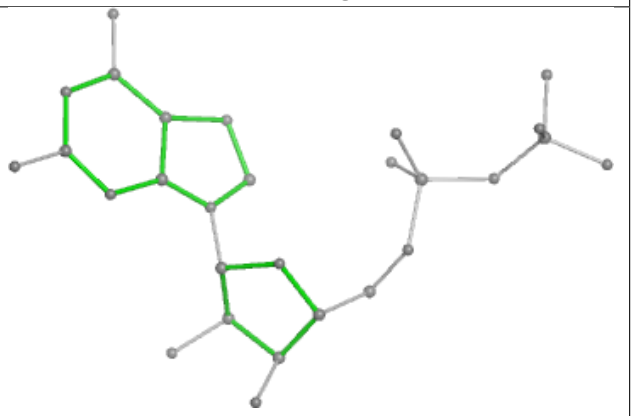
Bond lengths



Bond angles

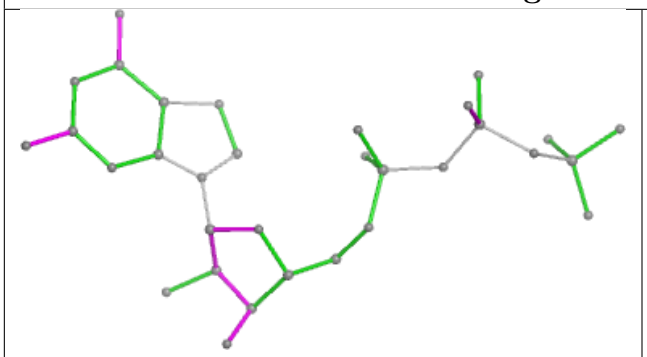


Torsions

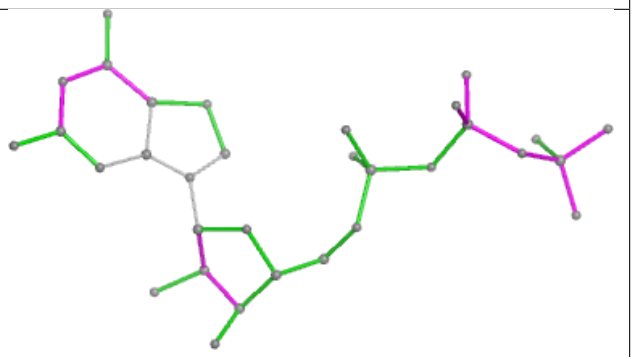


Rings

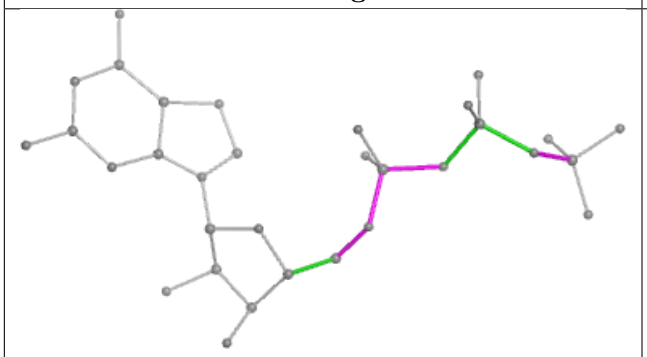
Ligand GTP C 501



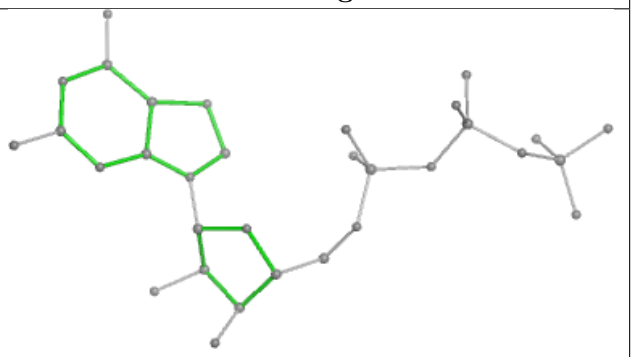
Bond lengths



Bond angles

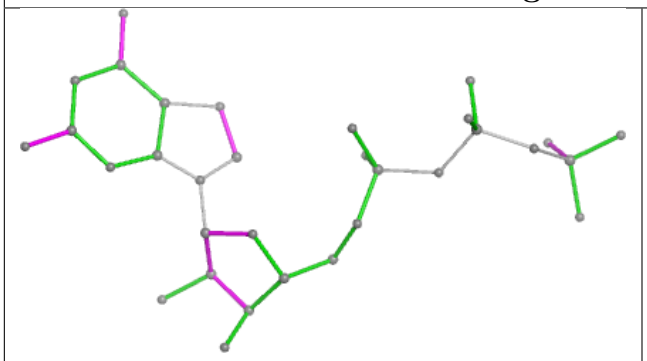


Torsions

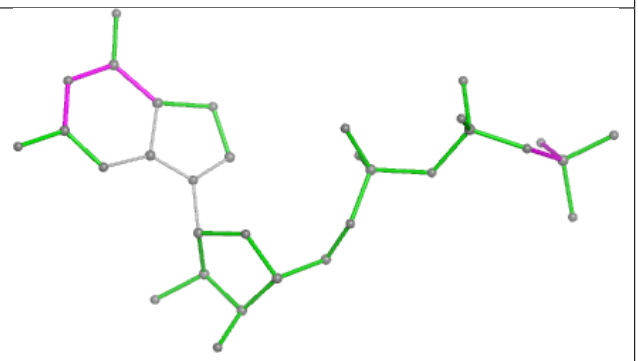


Rings

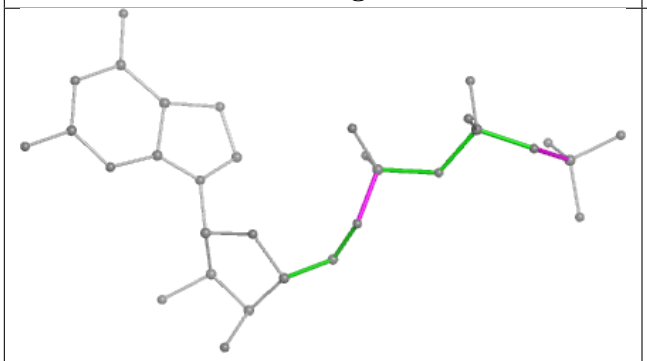
Ligand GTP A 501



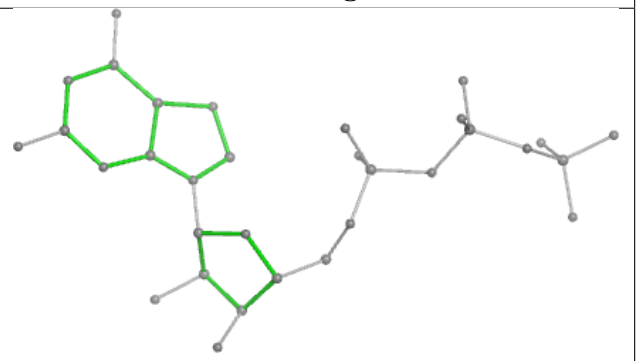
Bond lengths



Bond angles

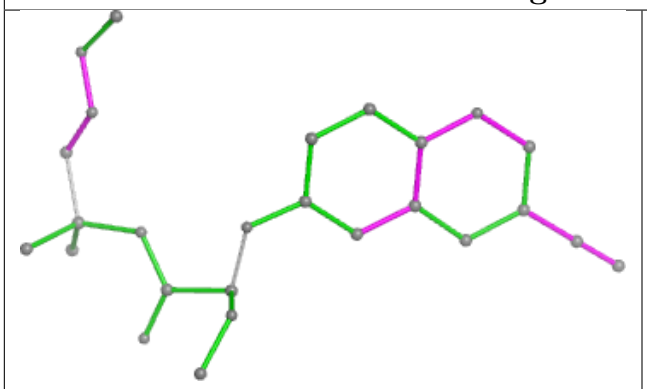


Torsions

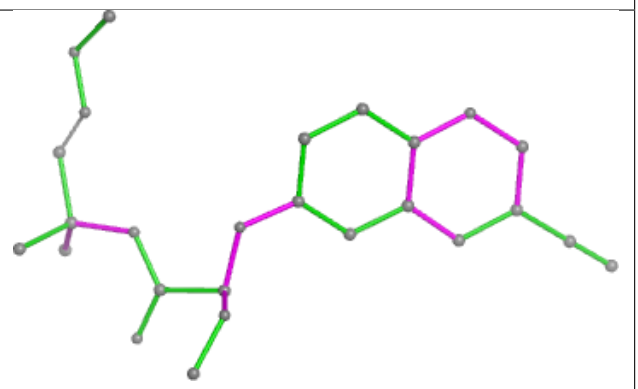


Rings

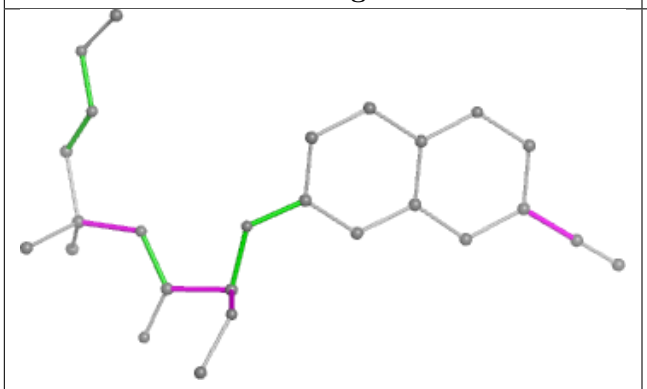
Ligand 9N5 D 504



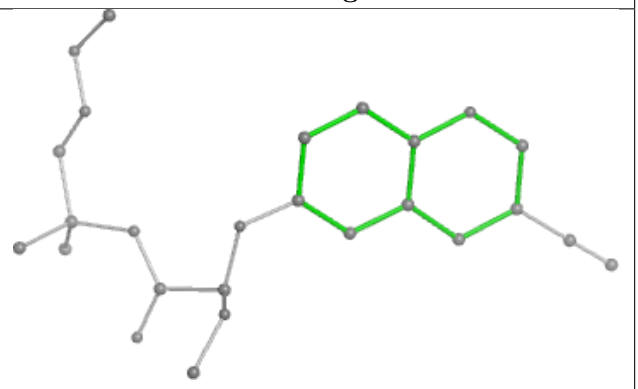
Bond lengths



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	437/451 (96%)	0.25	11 (2%)	57	61	44, 67, 100, 141	0
1	C	440/451 (97%)	0.00	6 (1%)	75	77	39, 54, 86, 125	0
2	B	421/445 (94%)	0.24	16 (3%)	40	43	38, 61, 96, 143	1 (0%)
2	D	419/445 (94%)	0.43	28 (6%)	17	18	47, 78, 114, 136	4 (0%)
3	E	118/143 (82%)	0.44	10 (8%)	10	10	50, 80, 120, 139	0
4	F	254/384 (66%)	1.02	54 (21%)	0	0	54, 87, 128, 171	0
All	All	2089/2319 (90%)	0.34	125 (5%)	21	22	38, 68, 111, 171	5 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	21	LEU	6.8
4	F	244	CYS	6.6
4	F	240	LEU	6.5
4	F	259	GLY	5.6
2	D	57	THR	5.6
2	B	59	ASN	5.6
4	F	20	LEU	5.2
3	E	27	PRO	5.0
3	E	24	LEU	5.0
2	D	129	CYS	5.0
4	F	245	ILE	4.8
2	D	108	TYR	4.7
4	F	147	TRP	4.6
4	F	199	PHE	4.5
3	E	26	PRO	4.5
4	F	362	ALA	4.3
2	D	96	GLN	4.2
2	D	82	PRO	4.1
4	F	243	HIS	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	57	THR	4.0
1	C	440	VAL	4.0
4	F	98	TYR	3.9
4	F	263	PHE	3.9
4	F	186	LEU	3.8
1	A	282	TYR	3.7
4	F	192	LEU	3.6
4	F	23	ALA	3.5
2	D	94	PHE	3.5
2	D	80	SER	3.5
2	D	400	ARG	3.5
4	F	17	VAL	3.4
3	E	25	LYS	3.4
4	F	330	ILE	3.4
4	F	27	TRP	3.4
2	D	131	CYS	3.3
4	F	24	THR	3.3
4	F	260	ASN	3.3
2	D	248	LEU	3.3
2	B	1	MET	3.2
2	B	284	ARG	3.2
2	B	58	GLY	3.2
4	F	262	MET	3.1
4	F	26	GLN	3.1
4	F	146	VAL	3.1
2	D	401	ARG	3.1
1	C	245	ASP	3.1
2	D	46	LEU	3.1
4	F	220	VAL	3.1
4	F	258	GLU	3.0
4	F	246	GLN	3.0
2	B	36	TYR	3.0
4	F	95	PRO	3.0
4	F	22	LEU	3.0
4	F	257	GLU	2.9
4	F	191	LEU	2.9
4	F	9	GLU	2.9
4	F	340	GLN	2.9
2	D	95	GLY	2.9
4	F	261	GLU	2.9
4	F	361	LEU	2.9
2	D	37	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	37	HIS	2.8
1	A	262	TYR	2.8
4	F	320	MET	2.8
1	A	283	HIS	2.8
3	E	141	GLU	2.7
2	D	33	THR	2.7
2	D	124	LYS	2.7
4	F	267	PHE	2.7
2	D	79	ARG	2.7
4	F	296	MET	2.7
2	D	60	LYS	2.7
2	D	130	ASP	2.6
2	B	82	PRO	2.6
4	F	221	LEU	2.6
2	D	404	PHE	2.6
2	D	158	ARG	2.6
4	F	241	THR	2.6
2	B	61	TYR	2.6
2	B	38	GLY	2.5
4	F	25	GLY	2.5
2	B	338	LYS	2.5
4	F	190	LEU	2.5
1	C	251	ASP	2.5
3	E	7	GLU	2.5
4	F	198	LYS	2.5
4	F	200	ASP	2.5
3	E	140	LYS	2.5
4	F	194	PRO	2.5
1	A	179	THR	2.4
1	C	241	SER	2.4
2	D	56	ALA	2.4
2	D	221	THR	2.4
2	B	85	GLN	2.4
2	D	415	GLU	2.4
1	C	357	TYR	2.4
1	A	140	SER	2.4
3	E	23	ILE	2.3
2	D	202	TYR	2.3
2	B	34	GLY	2.3
3	E	132	GLU	2.3
1	A	349	THR	2.3
4	F	13	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	335	ALA	2.2
1	A	284	GLU	2.2
4	F	44	ARG	2.2
1	A	281	ALA	2.2
1	A	346	TRP	2.2
2	B	60	LYS	2.2
4	F	342	LEU	2.2
3	E	135	LYS	2.1
2	D	59	ASN	2.1
4	F	185	TYR	2.1
2	B	369	ARG	2.1
4	F	189	PRO	2.1
2	B	337	ASN	2.1
2	D	249	ASN	2.1
4	F	353[A]	VAL	2.1
2	D	83	PHE	2.1
4	F	264	PHE	2.1
4	F	339	ALA	2.1
1	A	141	PHE	2.1
4	F	39	LEU	2.1
1	A	137	VAL	2.0
1	C	342	GLN	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
9	ACP	F	401	31/31	0.87	0.19	85,115,148,161	0

Continued on next page...

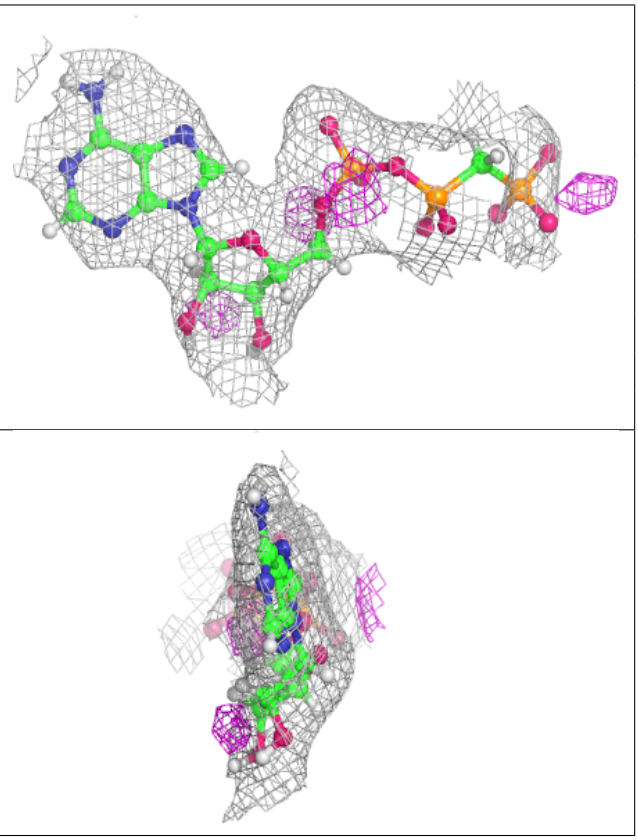
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	B	503	1/1	0.91	0.44	49,49,49,49	0
7	MG	B	502	1/1	0.94	0.28	56,56,56,56	0
7	MG	D	503	1/1	0.95	0.13	31,31,31,31	0
7	MG	D	502	1/1	0.95	0.19	56,56,56,56	0
8	9N5	B	504	26/26	0.97	0.17	54,65,73,79	0
8	9N5	D	504	26/26	0.97	0.18	59,71,85,86	0
6	GDP	D	501	28/28	0.97	0.12	64,76,99,105	0
5	GTP	C	501	32/32	0.98	0.16	36,46,58,64	0
6	GDP	B	501	28/28	0.98	0.20	40,50,64,66	0
5	GTP	A	501	32/32	0.99	0.21	43,53,62,74	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.

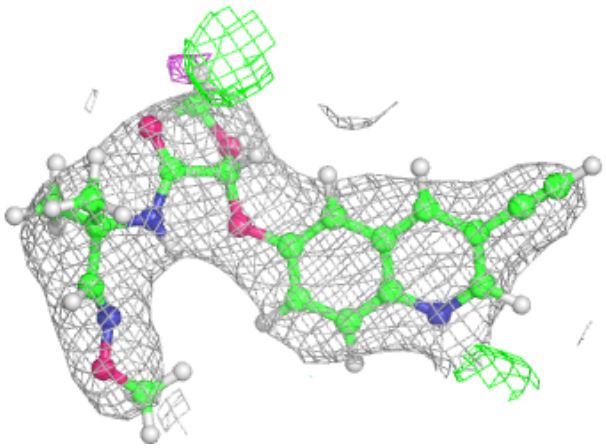
Electron density around ACP F 401:

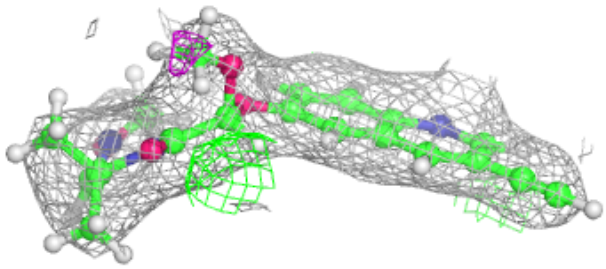
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

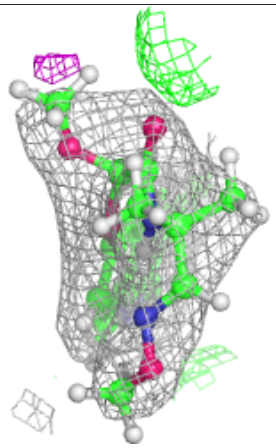


Electron density around 9N5 B 504:

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

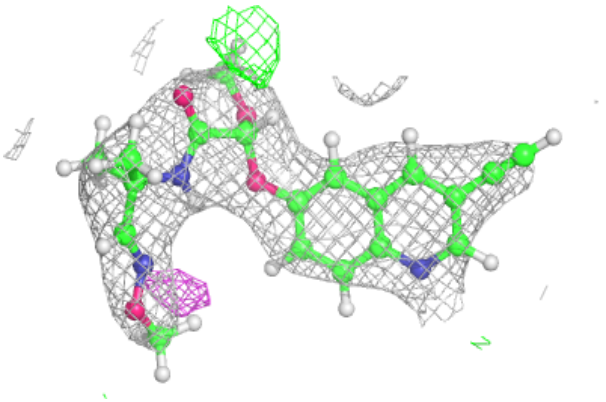


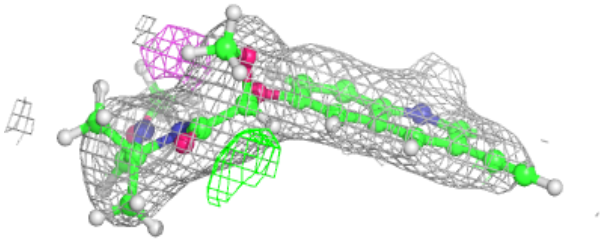


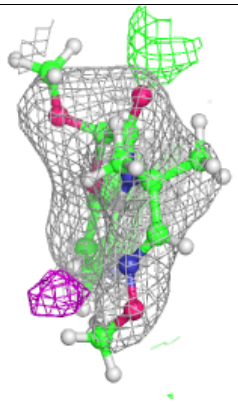


Electron density around 9N5 D 504:

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

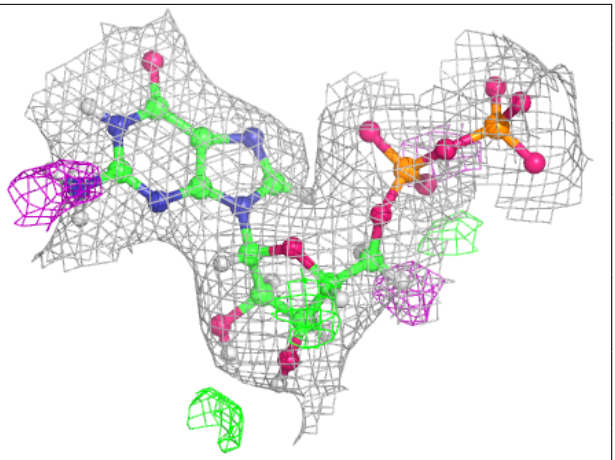


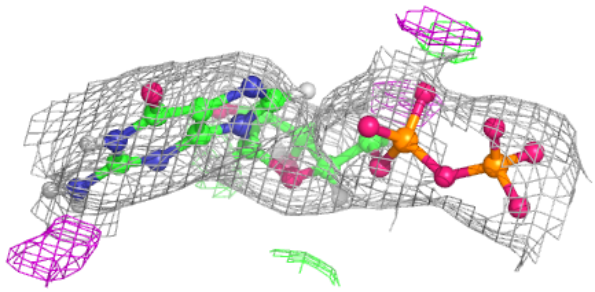


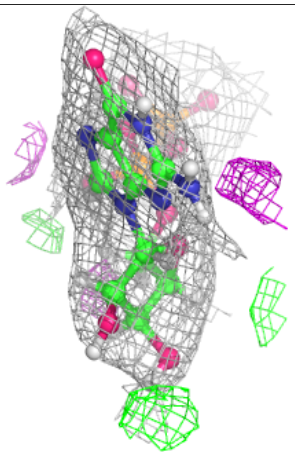


Electron density around GDP D 501:

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

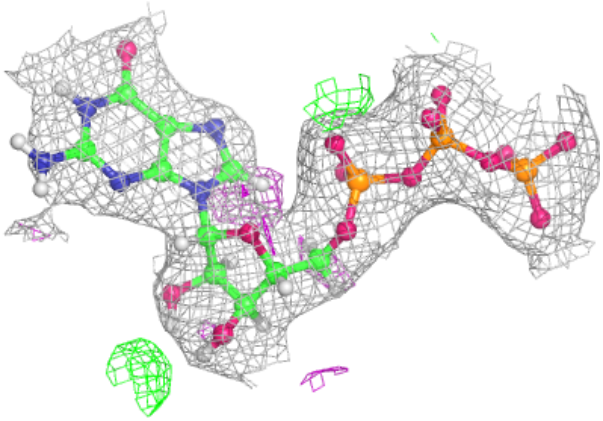


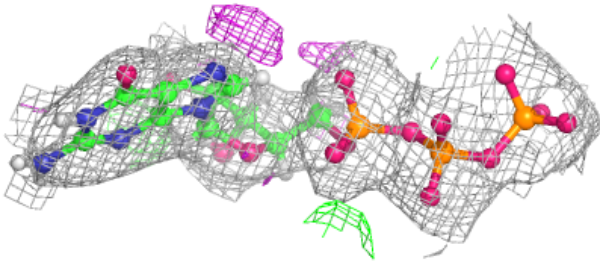


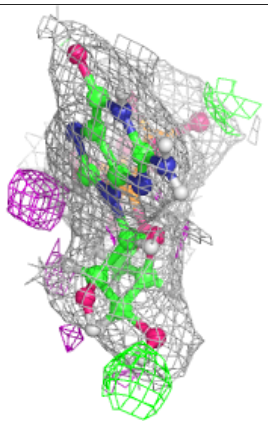


Electron density around GTP C 501:

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

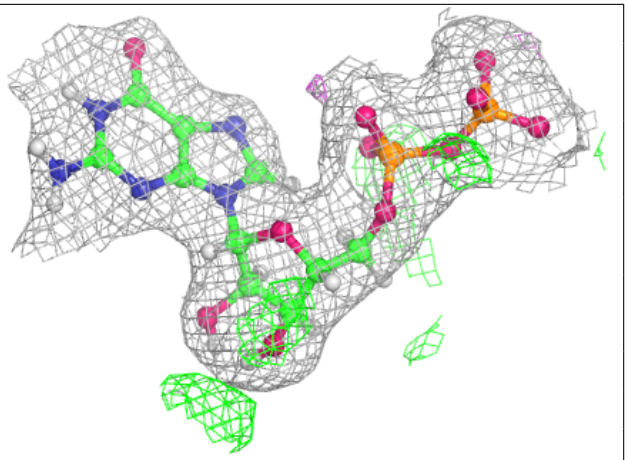


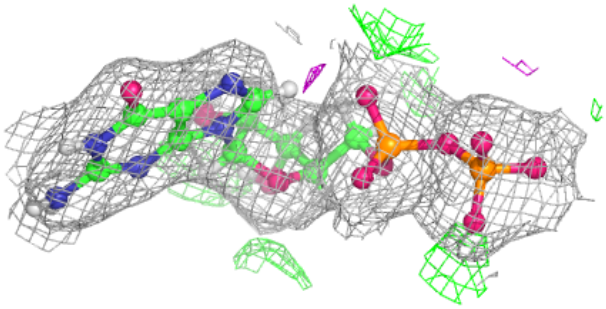


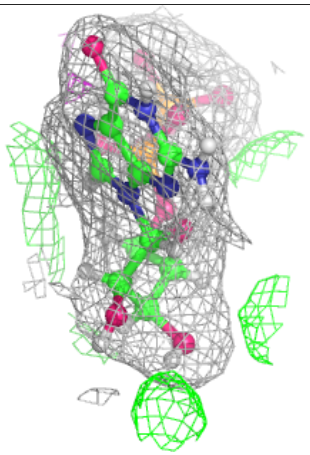


Electron density around GDP B 501:

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

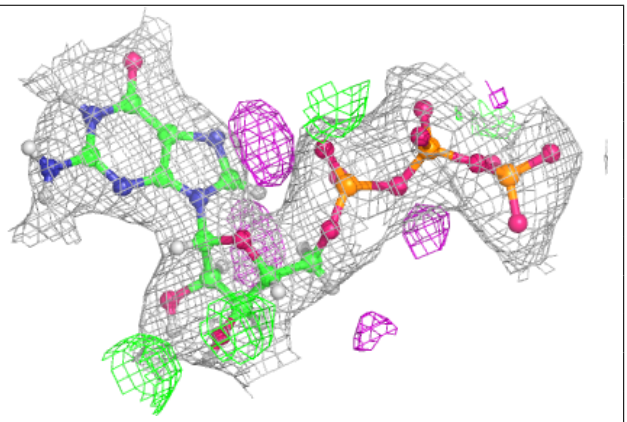


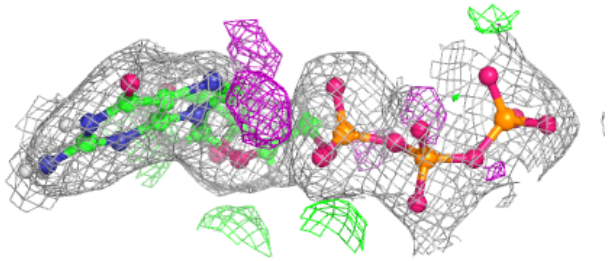


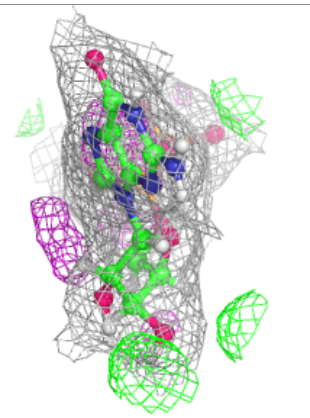


Electron density around GTP A 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.