Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2024 – 09:44 PM EST

PDB ID	:	5S63
Title	:	Tubulin-Z2241115980-complex
Authors	:	Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on	:	2020-11-08
Resolution	:	2.60 Å(reported)

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

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

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

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

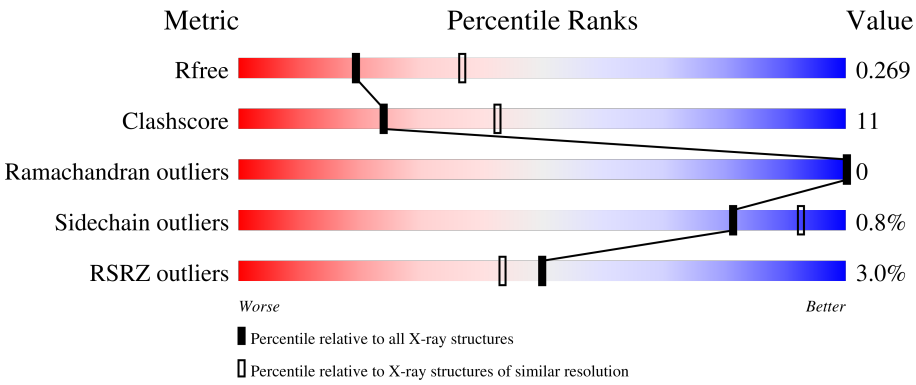
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	.% 72% 25% •
1	C	451	2% 79% 18% •
2	B	445	2% 69% 26% •
2	D	445	5% 69% 27% •
3	E	143	8% 72% 14% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	3% 67% 24% 9%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17882 atoms, of which 16 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	438	3424	2167	582	653	22	0	0	0
1	C	440	3443	2178	585	657	23	0	1	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	425	3359	2109	577	646	27	13	1	0
2	D	427	3348	2101	571	649	27	5	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1014	625	183	201	5	0	0	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

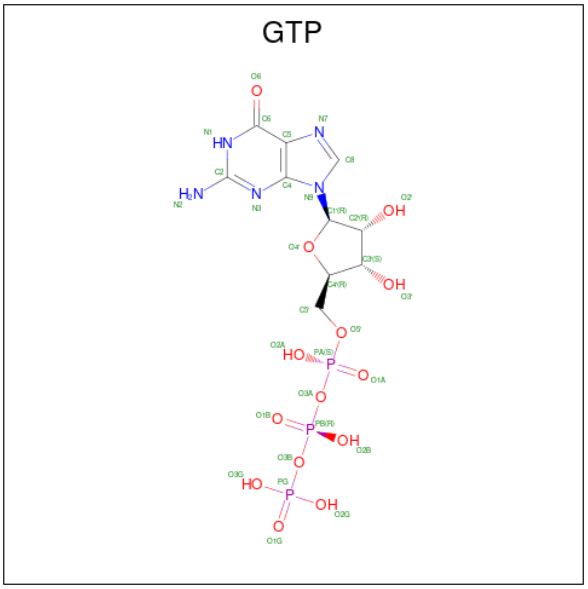
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	349	2863	1835	492	522	14	0	0	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	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0

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

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

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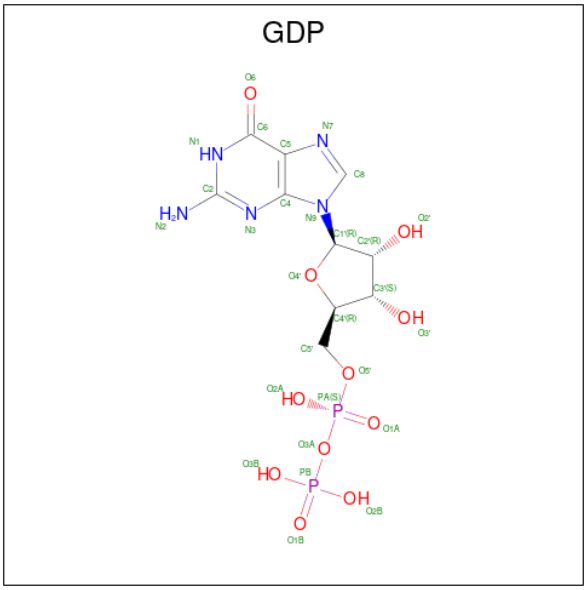
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

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

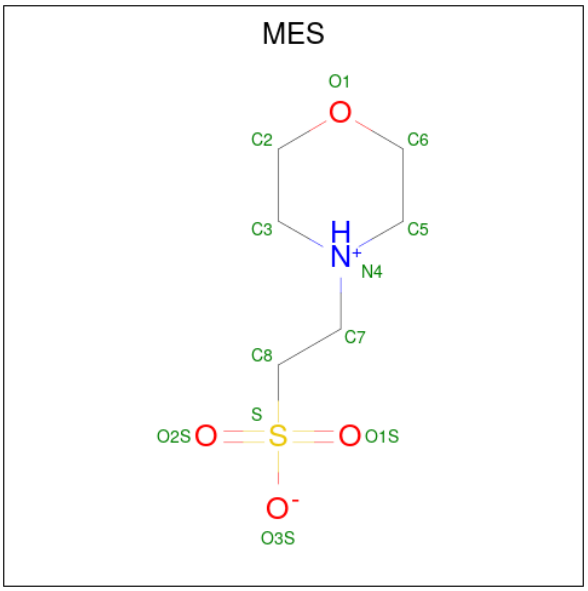
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	B	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0
			Total	Ca		
7	E	1	1	1	0	0

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



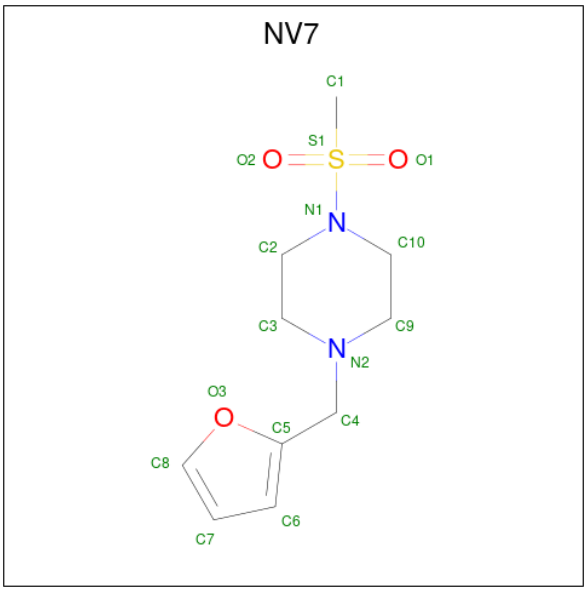
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
8	D	1	28	10	5	11	2	0	0

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



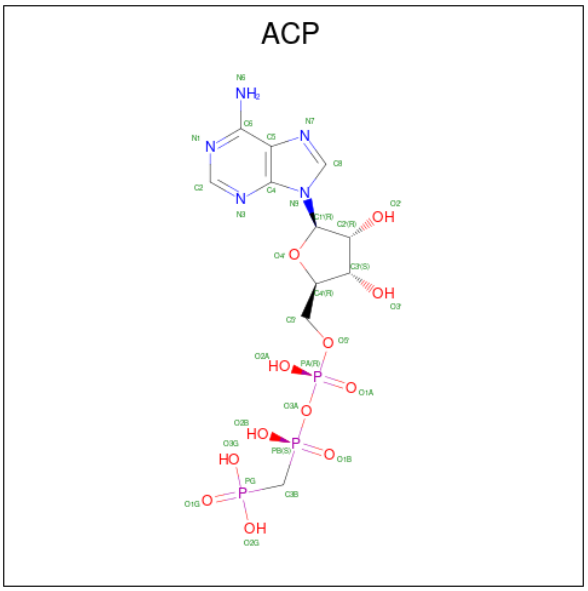
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is 1-[(furan-2-yl)methyl]-4-(methylsulfonyl)piperazine (three-letter code: NV7) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
10	C	1	32	10	16	2	3	1	0	0

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



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	35	35	35	0	0
12	B	39	39	39	0	0
12	C	124	124	124	0	0
12	D	17	17	17	0	0
12	E	6	6	6	0	0
12	F	6	6	6	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: %
72% 25% •

M1 R2 E3 G10 Q11 A12 G13 V14 W21 C25 M36 D39 K40 T41 T51 S54 E55 K60 H61 V62 P63 R64 A65 V66 D69 L70 E71 P72 T73 V74 I75 D76 R79 L86 F87 H88 P89 E90 I93 T94 D98 A99 A100 Y103 I114

R121 L125 G131 L132 Q133 G134 F135 L136 S140 F141 G142 S147 G148 K166 S170 I171 Y172 S178 T179 A180 E183 P184 Y185 I188 H197 D205 I209 Y210 R214 L217 D218 I219 E220 R221 P222 N226 L227 L230 I231 S232 Q233 I234 V235

L252 P274 V275 A278 Y282 H283 E284 Q285 L286 S287 I291 T292 N293 N300 Q301 M302 C305 D306 P307 K311 R320 P325 K326 I335 K336 R339 Q342 D345 T349 N356 V362 D367 L368 A369 T381 T382 A383 D392 M398

V409 M413 S419 E423 K430 D431 E434 V435 D438 SER VAL GLU GLY GLU GLY GLU GLU GLU GLY GLU GLU TYR

• Molecule 1: Tubulin alpha-1B chain

Chain C: 2%
79% 18% •

M1 C4 G10 Q11 V14 Q15 D39 S48 H61 V66 F67 V68 D69 D76 T80 I93 T94 G95 K96 E97 I114 R121 L125 L132 L136 T150 M154 G162 K163 K164 S165 K166 Y172 P173 A174 S178 T179 A180 T194

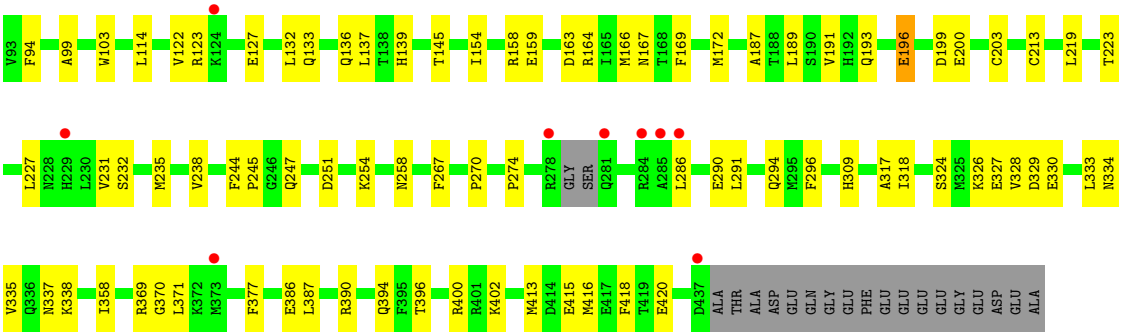
L195 E196 H197 S198 D199 V204 E207 A208 I209 Y210 R221 P222 L227 N228 R229 L230 Q233 I234 S241 F244 D245 L248 N249 V250 D251 L252 T253 E254 F255 Q256 A270 T271 P274 A281 Y282 H283 T292 C295 F296 E297 P298 M302 C305 D306 P307

R308 Y312 R320 P325 I335 R339 S340 I341 V344 D345 W346 C347 K352 N356 Y357 Q358 G366 D367 L368 V371 A385 W388 L391 V440 GLU GLY GLU GLY GLU GLU GLU GLY GLU GLU TYR

• Molecule 2: Tubulin beta-2B chain

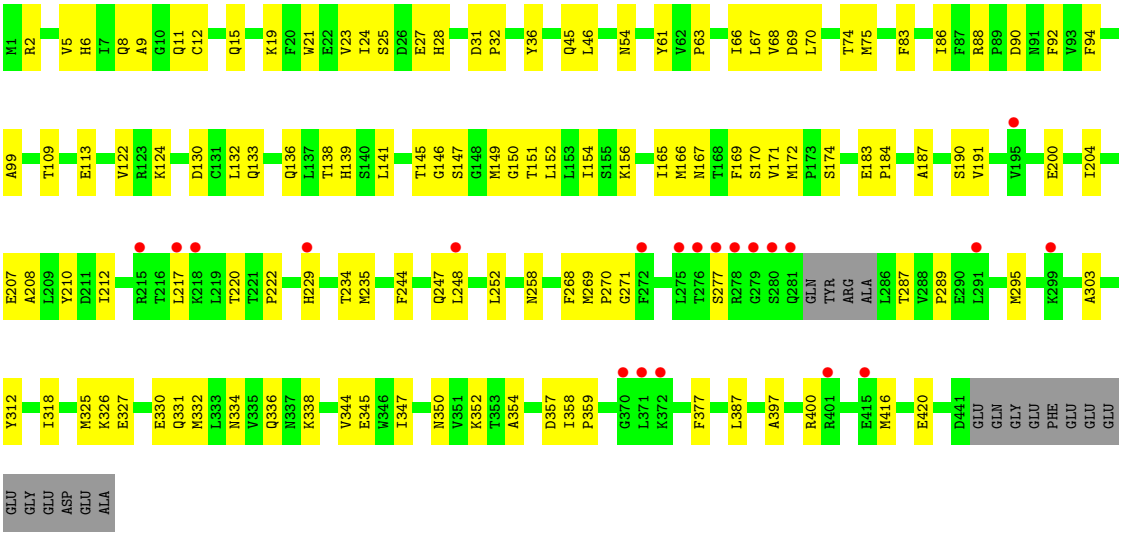
Chain B: 2%
69% 26% •

M1 R2 V5 H6 I7 Q15 I16 F20 W21 E22 V23 I24 S25 D26 E27 H28 D31 P32 Y36 L46 E47 R48 I49 N50 V51 N59 V62 P63 I66 L67 V68 D69 L70 M75 D76 S77 V78 G81 P82 F83 G84 Q85 I86 F87 R88 P89 D90 N91 F92



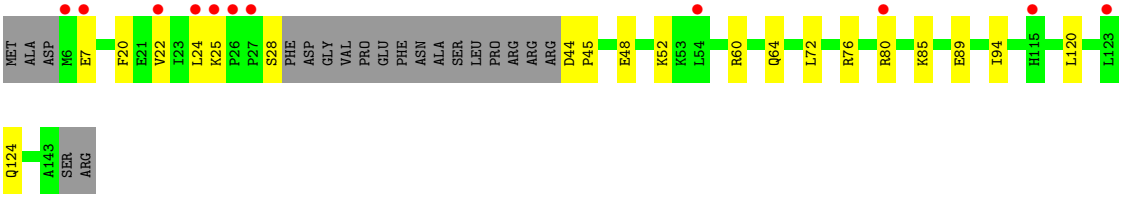
- Molecule 2: Tubulin beta-2B chain

Chain D:



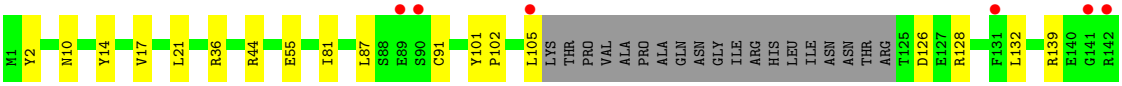
- Molecule 3: Stathmin-4

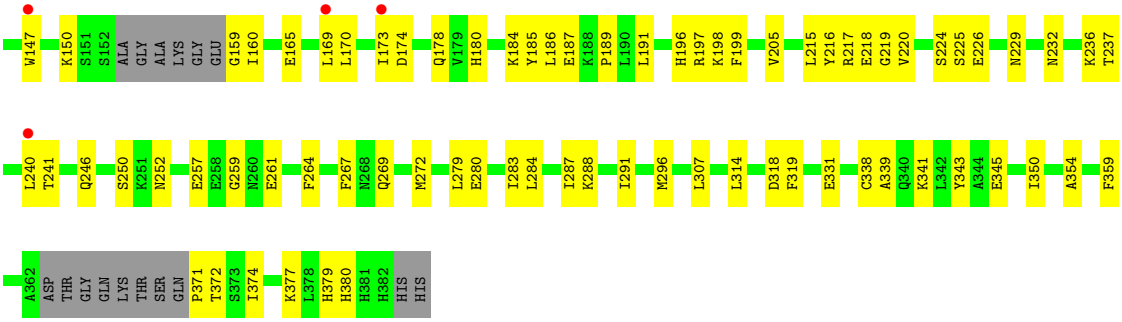
Chain E:



- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:




W147
K150
S151
S152
ALA
GLY
ALA
LYS
GLY
GLU
G159
I160
E165
L169
L170
I173
D174
Q178
V179
H180
K184
Y185
L186
E187
K188
P189
L190
L191
H196
R197
K198
F199
V205
L215
Y216
R217
E218
G219
V220
S224
S225
E226
N229
N232
K236
T237
L240
T241
Q246
S250
K251
N252
E257
E258
G259
N260
E261
F264
F267
N268
Q269
M272
L279
E280
I283
L284
I287
K288
I291
M296
L307
L314
D318
F319
E331
C338
A339
Q340
K341
L342
Y343
A344
E345
I350
A354
F359
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
P371
T372
S373
I374
K377
L378
H379
H380
H381
H382
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	105.22Å 159.10Å 179.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.78 – 2.60 119.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.78-2.60) 98.3 (119.11-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.213 , 0.268 0.215 , 0.269	Depositor DCC
R_{free} test set	4496 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17882	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: NV7, GTP, MG, MES, CA, ACP, GDP

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	0.26	0/3502	0.41	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.26	0/3433	0.42	0/4647
2	D	0.25	0/3421	0.41	0/4633
3	E	0.24	0/1022	0.34	0/1356
4	F	0.24	0/2930	0.40	0/3959
All	All	0.25	0/17829	0.41	0/24129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3335	84	0
1	C	3443	0	3352	63	1
2	B	3359	0	3235	82	0
2	D	3348	0	3224	85	0
3	E	1014	0	1029	17	1
4	F	2863	0	2826	69	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	4	0
9	B	12	0	12	4	0
10	C	16	16	0	1	0
11	F	31	0	14	4	0
12	A	35	0	0	4	0
12	B	39	0	0	1	0
12	C	124	0	0	4	0
12	D	17	0	0	0	0
12	E	6	0	0	1	0
12	F	6	0	0	1	0
All	All	17866	16	17075	386	1

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 11.

All (386) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:LEU:HA	2:D:277:SER:HB3	1.43	1.00
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.57	0.86
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.58	0.84
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.60	0.83
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.63	0.81
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.64	0.80
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.64	0.79
2:B:83:PHE:O	2:B:86:ILE:HG22	1.84	0.78
2:B:136:GLN:HA	2:B:167:ASN:O	1.85	0.77
1:C:76:ASP:O	1:C:80:THR:HG22	1.85	0.76
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.68	0.76
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HG13	1:C:302:MET:HE3	1.68	0.75
1:A:381:THR:HG22	1:A:383:ALA:H	1.50	0.74
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.52	0.74
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.68	0.73
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.20	0.72
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.72	0.70
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.74	0.70
2:D:136:GLN:HA	2:D:167:ASN:O	1.91	0.70
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.25	0.70
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.10	0.69
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.28	0.69
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.33	0.69
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.74	0.69
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.74	0.69
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.57	0.68
1:A:166:LYS:HE2	1:A:197:HIS:O	1.93	0.68
1:C:234:ILE:HD13	1:C:302:MET:CE	2.23	0.68
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.75	0.68
2:B:231:VAL:O	2:B:235:MET:HG3	1.94	0.67
2:D:174:SER:OG	2:D:207:GLU:OE1	2.09	0.67
1:C:209:ILE:HD11	1:C:302:MET:CE	2.24	0.66
4:F:101:TYR:N	4:F:126:ASP:OD1	2.21	0.66
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.31	0.66
1:A:178:SER:HB2	1:A:183:GLU:OE1	1.97	0.65
4:F:160:ILE:O	4:F:236:LYS:NZ	2.27	0.65
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.32	0.65
2:D:332:MET:O	2:D:336:GLN:HG3	1.96	0.65
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.78	0.64
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.79	0.64
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.33	0.64
4:F:371:PRO:HA	4:F:372:THR:O	1.97	0.64
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.80	0.64
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.30	0.64
2:D:312:TYR:O	2:D:344:VAL:HG22	1.98	0.64
2:D:217:LEU:CA	2:D:277:SER:HB3	2.26	0.63
2:B:158:ARG:NH1	2:B:196:GLU:O	2.32	0.63
2:D:83:PHE:O	2:D:86:ILE:HG22	1.99	0.63
1:A:10:GLY:O	1:A:14:VAL:HG23	1.98	0.62
1:C:165:SER:HA	1:C:199:ASP:OD2	1.99	0.62
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.29	0.62
4:F:91:CYS:HA	12:F:505:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.82	0.62
2:D:141:LEU:HA	2:D:147:SER:HB3	1.82	0.62
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.30	0.61
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.33	0.61
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.15	0.61
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.31	0.60
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.33	0.60
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.16	0.60
1:A:419:SER:O	1:A:423:GLU:HG3	2.02	0.60
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.84	0.60
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.85	0.59
1:C:270:ALA:O	1:C:302:MET:HG2	2.02	0.59
4:F:184:LYS:NZ	4:F:185:TYR:O	2.34	0.59
1:C:234:ILE:HD13	1:C:302:MET:HE1	1.83	0.59
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.37	0.59
1:C:234:ILE:HD13	1:C:302:MET:SD	2.43	0.58
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.86	0.58
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.36	0.58
1:A:66:VAL:HG23	1:A:125:LEU:CD1	2.33	0.58
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.21	0.58
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.84	0.58
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.85	0.58
1:C:248:LEU:HD22	10:C:601:NV7:C1	2.33	0.58
4:F:371:PRO:HA	4:F:372:THR:C	2.22	0.58
1:A:431:ASP:O	1:A:435:VAL:HG23	2.04	0.58
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.39	0.58
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.19	0.57
4:F:178:GLN:N	4:F:178:GLN:OE1	2.36	0.57
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.86	0.57
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.85	0.57
2:B:7:ILE:O	2:B:137:LEU:HD12	2.04	0.57
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.40	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.57
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.85	0.57
1:C:256:GLN:NE2	12:C:703:HOH:O	2.37	0.57
2:D:145:THR:HB	8:D:501:GDP:O2B	2.05	0.56
2:D:271:GLY:HA3	2:D:377:PHE:HB3	1.86	0.56
2:B:223:THR:O	2:B:227:LEU:HD13	2.05	0.56
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.86	0.56
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.40	0.56
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.20	0.56
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.40	0.56
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.41	0.56
2:D:152:LEU:O	2:D:156:LYS:HG2	2.04	0.56
4:F:150:LYS:HB3	4:F:160:ILE:HG13	1.87	0.56
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.35	0.56
2:D:11:GLN:O	2:D:15:GLN:HG2	2.06	0.56
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.38	0.56
4:F:371:PRO:CA	4:F:372:THR:HB	2.35	0.56
4:F:159:GLY:C	4:F:160:ILE:HD12	2.26	0.56
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.41	0.55
2:D:147:SER:O	2:D:151:THR:HG23	2.06	0.55
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.41	0.55
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.71	0.55
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.07	0.55
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.42	0.55
3:E:120:LEU:O	3:E:124:GLN:HG3	2.06	0.55
4:F:229:ASN:ND2	4:F:232:ASN:HB3	2.22	0.55
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.87	0.55
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.05	0.55
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.42	0.55
2:D:146:GLY:N	8:D:501:GDP:O2B	2.37	0.55
4:F:269:GLN:HA	4:F:272:MET:HE2	1.89	0.55
2:D:11:GLN:HA	2:D:74:THR:HG21	1.89	0.55
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.55
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.18	0.55
1:C:97:GLU:HG3	2:D:2:ARG:NH2	2.22	0.54
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.42	0.54
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.88	0.54
2:B:329:ASP:O	2:B:333:LEU:HG	2.08	0.54
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.90	0.54
3:E:7:GLU:O	3:E:22:VAL:HA	2.07	0.54
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.38	0.54
2:D:147:SER:HB2	2:D:190:SER:OG	2.07	0.54
2:B:213:CYS:HB3	2:B:219:LEU:HD12	1.89	0.54
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.73	0.53
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.38	0.53
4:F:269:GLN:HA	4:F:272:MET:CE	2.38	0.53
1:A:214:ARG:HG2	1:A:219:ILE:O	2.09	0.53
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.36	0.53
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.38	0.53
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.43	0.53
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.90	0.53
2:D:318:ILE:N	2:D:318:ILE:HD12	2.23	0.53
4:F:17:VAL:O	4:F:21:LEU:HG	2.09	0.53
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.44	0.53
2:B:193:GLN:HB3	12:B:616:HOH:O	2.08	0.53
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.44	0.53
2:B:187:ALA:O	2:B:191:VAL:HG23	2.09	0.52
1:C:241:SER:HA	1:C:249:ASN:OD1	2.09	0.52
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.24	0.52
1:A:2:ARG:HB3	1:A:131:GLY:O	2.09	0.52
4:F:350:ILE:O	4:F:354:ALA:HB3	2.09	0.52
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.45	0.52
1:A:305:CYS:O	1:A:307:PRO:HD3	2.09	0.52
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.25	0.52
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.92	0.52
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.45	0.52
2:B:370:GLY:O	2:B:371:LEU:HD23	2.09	0.52
3:E:85:LYS:NZ	12:E:301:HOH:O	2.43	0.52
2:D:200:GLU:HB2	2:D:268:PHE:CE2	2.45	0.52
1:A:345:ASP:O	3:E:28:SER:N	2.26	0.52
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.37	0.52
2:D:187:ALA:O	2:D:191:VAL:HG23	2.10	0.52
2:B:413:MET:HE1	2:B:418:PHE:CE1	2.45	0.51
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.76	0.51
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.92	0.51
4:F:371:PRO:HA	4:F:372:THR:HB	1.90	0.51
1:A:227:LEU:O	1:A:231:ILE:HG13	2.11	0.51
1:C:196:GLU:HG2	12:C:765:HOH:O	2.11	0.51
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.92	0.51
2:B:46:LEU:HA	2:B:49:ILE:HB	1.93	0.51
2:B:199:ASP:O	2:B:200:GLU:HG3	2.11	0.51
4:F:226:GLU:HG3	4:F:237:THR:HG22	1.92	0.51
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.76	0.51
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.42	0.51
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.92	0.51
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.11	0.50
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.29	0.50
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.12	0.50
2:D:8:GLN:HB3	2:D:138:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ARG:O	2:B:51:VAL:HG23	2.12	0.50
3:E:60:ARG:O	3:E:64:GLN:HG3	2.12	0.50
2:B:318:ILE:N	2:B:318:ILE:HD12	2.27	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.50
1:C:320:ARG:HA	1:C:356:ASN:O	2.12	0.50
2:D:416:MET:O	2:D:420:GLU:HG3	2.12	0.50
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.42	0.49
2:D:145:THR:O	2:D:149:MET:HB3	2.12	0.49
4:F:296:MET:SD	4:F:380:HIS:HB2	2.52	0.49
2:D:124:LYS:C	2:D:124:LYS:HD3	2.33	0.49
1:C:204:VAL:HG13	1:C:302:MET:CE	2.40	0.49
4:F:246:GLN:O	4:F:250:SER:HB3	2.12	0.49
1:A:287:SER:O	1:A:291:ILE:HG23	2.12	0.49
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.94	0.49
1:A:349:THR:HB	3:E:25:LYS:HB3	1.95	0.49
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.95	0.49
1:A:320:ARG:HD2	12:A:627:HOH:O	2.12	0.49
2:B:199:ASP:OD1	9:B:504:MES:H62	2.12	0.48
1:C:305:CYS:O	1:C:307:PRO:HD3	2.13	0.48
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.42	0.48
2:B:167:ASN:ND2	2:B:200:GLU:OE1	2.46	0.48
1:C:178:SER:OG	2:D:352:LYS:NZ	2.46	0.48
1:C:271:THR:HG21	1:C:295:CYS:O	2.12	0.48
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.95	0.48
2:D:9:ALA:HA	2:D:68:VAL:O	2.14	0.48
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.95	0.48
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.43	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.48
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.96	0.48
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.95	0.48
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.96	0.48
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.96	0.48
4:F:341:LYS:HG2	4:F:341:LYS:O	2.14	0.48
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.49	0.48
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.79	0.48
4:F:259:GLY:O	4:F:261:GLU:HG3	2.14	0.48
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.95	0.48
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.49	0.47
4:F:267:PHE:HE2	4:F:279:LEU:HD13	1.79	0.47
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.50	0.47
1:C:297:GLU:OE2	1:C:298:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:O	1:A:147:SER:HB3	2.14	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.47
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.46	0.47
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.49	0.47
2:B:114:LEU:O	2:B:114:LEU:HG	2.14	0.47
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.45	0.47
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.15	0.47
1:C:166:LYS:HE2	1:C:197:HIS:O	2.13	0.47
1:C:282:TYR:O	1:C:283:HIS:HB2	2.15	0.47
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.49	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.47
1:A:135:PHE:C	1:A:136:LEU:HD23	2.35	0.47
1:A:430:LYS:O	1:A:434:GLU:HG3	2.15	0.47
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.46
1:C:341:ILE:HD12	1:C:341:ILE:N	2.30	0.46
4:F:377:LYS:HD3	4:F:379:HIS:CE1	2.50	0.46
2:D:54:ASN:O	2:D:61:TYR:HA	2.15	0.46
2:D:141:LEU:HD12	2:D:172:MET:SD	2.54	0.46
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.97	0.46
4:F:197:ARG:HD2	4:F:224:SER:O	2.15	0.46
1:A:1:MET:HG2	1:A:51:THR:HG22	1.97	0.46
1:A:284:GLU:CD	1:A:284:GLU:H	2.19	0.46
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.46	0.46
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.16	0.46
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.50	0.46
4:F:198:LYS:HG2	4:F:199:PHE:H	1.81	0.46
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.97	0.46
1:A:349:THR:O	3:E:24:LEU:HB2	2.16	0.46
2:B:123:ARG:O	2:B:127:GLU:HG3	2.15	0.46
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.97	0.46
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.50	0.46
2:D:220:THR:C	2:D:222:PRO:HD3	2.36	0.46
2:B:32:PRO:HA	2:B:83:PHE:CD2	2.50	0.46
1:A:98:ASP:OD1	1:A:100:ALA:N	2.38	0.46
2:B:164:ARG:O	9:B:504:MES:H31	2.16	0.46
4:F:55:GLU:HA	4:F:55:GLU:OE1	2.15	0.46
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.97	0.46
1:C:229:ARG:HG3	12:C:724:HOH:O	2.15	0.46
4:F:14:TYR:HA	4:F:17:VAL:HB	1.98	0.46
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.98	0.45
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:O	2:D:94:PHE:HA	2.17	0.45
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.51	0.45
4:F:184:LYS:NZ	4:F:187:GLU:HG3	2.30	0.45
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.49	0.45
1:A:185:TYR:OH	1:A:398:MET:HB3	2.17	0.45
2:B:396:THR:O	2:B:400:ARG:HG2	2.16	0.45
2:B:416:MET:O	2:B:420:GLU:HG3	2.16	0.45
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.17	0.45
2:D:326:LYS:O	2:D:330:GLU:HG3	2.17	0.45
2:D:208:ALA:O	2:D:212:ILE:HG13	2.15	0.45
1:A:136:LEU:HD21	1:A:252:LEU:HD21	1.99	0.45
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.99	0.45
2:B:5:VAL:HG23	2:B:132:LEU:HD11	1.97	0.45
2:B:270:PRO:HA	2:B:377:PHE:O	2.17	0.45
2:D:28:HIS:HA	2:D:45:GLN:HB3	1.99	0.45
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.31	0.45
1:C:11:GLN:O	1:C:15:GLN:HG3	2.17	0.45
4:F:178:GLN:NE2	4:F:180:HIS:HE1	2.15	0.45
1:A:88:HIS:NE2	12:A:601:HOH:O	2.35	0.44
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.52	0.44
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.47	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.44
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.96	0.44
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.44
2:B:69:ASP:HA	2:B:145:THR:HG21	1.99	0.44
2:B:78:VAL:O	2:B:84:GLY:HA3	2.17	0.44
2:D:220:THR:O	2:D:222:PRO:HD3	2.18	0.44
4:F:240:LEU:HD12	4:F:240:LEU:N	2.32	0.44
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.79	0.44
2:D:23:VAL:O	2:D:27:GLU:HG3	2.18	0.44
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.44
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.44
1:A:362:VAL:HG22	12:A:606:HOH:O	2.17	0.44
1:C:325:PRO:HD2	12:C:760:HOH:O	2.18	0.44
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.44
1:A:320:ARG:HA	1:A:356:ASN:O	2.18	0.44
1:A:114:ILE:HG12	1:A:114:ILE:O	2.18	0.44
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.53	0.44
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.43
1:C:150:THR:O	1:C:154:MET:HG2	2.18	0.43
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:215:LEU:HD22	4:F:288:LYS:HG2	1.99	0.43
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.52	0.43
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.58	0.43
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.00	0.43
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.01	0.43
2:D:287:THR:HB	2:D:289:PRO:HD2	1.99	0.43
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.49	0.43
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.43
1:C:69:ASP:O	1:C:94:THR:HA	2.19	0.43
1:C:132:LEU:HG	1:C:164:LYS:HD3	2.00	0.43
4:F:186:LEU:O	4:F:189:PRO:HD3	2.18	0.43
2:B:199:ASP:C	2:B:200:GLU:HG3	2.39	0.43
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.58	0.43
1:A:55:GLU:HA	1:A:60:LYS:O	2.19	0.43
2:B:163:ASP:HA	9:B:504:MES:O1S	2.19	0.43
2:B:324:SER:OG	2:B:327:GLU:HB2	2.18	0.43
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.54	0.43
1:A:220:GLU:OE1	2:B:326:LYS:HD3	2.19	0.42
2:B:387:LEU:C	2:B:387:LEU:HD23	2.39	0.42
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.59	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.55	0.42
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.37	0.42
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.00	0.42
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.01	0.42
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.53	0.42
2:B:390:ARG:O	2:B:394:GLN:HG3	2.20	0.42
1:A:69:ASP:O	1:A:94:THR:HA	2.20	0.42
2:D:357:ASP:O	2:D:359:PRO:HD3	2.19	0.42
4:F:307:LEU:HD12	4:F:307:LEU:HA	1.92	0.42
2:B:28:HIS:HB3	2:B:49:ILE:HD13	2.02	0.42
2:B:326:LYS:O	2:B:330:GLU:HG3	2.19	0.42
2:B:324:SER:O	2:B:328:VAL:HG23	2.20	0.42
2:D:5:VAL:HG23	2:D:132:LEU:CD1	2.50	0.42
2:D:109:THR:O	2:D:113:GLU:HG2	2.20	0.42
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.42
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.54	0.42
1:C:252:LEU:O	1:C:256:GLN:HG3	2.19	0.42
4:F:173:ILE:HD13	4:F:180:HIS:HB2	2.01	0.42
1:A:54:SER:O	1:A:61:HIS:HA	2.20	0.42
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.55	0.42
1:A:188:ILE:HD11	1:A:392:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:O	1:A:235:VAL:HG23	2.19	0.41
1:A:275:VAL:HG13	1:A:368:LEU:HD22	2.01	0.41
2:D:11:GLN:HB3	8:D:501:GDP:O2A	2.20	0.41
2:D:295:MET:HE3	2:D:295:MET:HB2	1.86	0.41
2:D:345:GLU:H	2:D:345:GLU:HG2	1.67	0.41
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.02	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.02	0.41
1:C:194:THR:O	1:C:194:THR:HG22	2.20	0.41
1:A:2:ARG:O	1:A:133:GLN:NE2	2.48	0.41
2:B:77:SER:O	2:B:81:GLY:N	2.53	0.41
2:B:369:ARG:HD3	2:B:369:ARG:HA	1.87	0.41
9:B:504:MES:H51	9:B:504:MES:H81	1.65	0.41
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.40	0.41
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.54	0.41
2:B:317:ALA:C	2:B:318:ILE:HD12	2.41	0.41
4:F:198:LYS:HG2	4:F:199:PHE:N	2.35	0.41
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.55	0.41
1:A:71:GLU:HB2	1:A:98:ASP:HB3	2.02	0.41
1:A:74:VAL:HB	12:A:602:HOH:O	2.20	0.41
2:B:159:GLU:HB2	3:E:72:LEU:HD13	2.02	0.41
1:A:88:HIS:HD2	1:A:90:GLU:OE1	2.04	0.41
2:B:290:GLU:O	2:B:294:GLN:HG3	2.20	0.41
2:D:234:THR:HG21	2:D:270:PRO:CB	2.50	0.41
1:A:135:PHE:O	1:A:136:LEU:HD23	2.20	0.41
2:B:296:PHE:CE2	2:B:335:VAL:HG11	2.56	0.41
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.21	0.41
2:D:19:LYS:O	2:D:23:VAL:HG23	2.21	0.41
4:F:225:SER:O	4:F:252:ASN:HB2	2.21	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.36	0.41
1:A:292:THR:HG22	1:A:335:ILE:HD12	2.02	0.41
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.42	0.41
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.56	0.40
2:D:183:GLU:N	2:D:184:PRO:CD	2.84	0.40
2:D:327:GLU:O	2:D:331:GLN:HG2	2.21	0.40
1:A:311:LYS:HA	1:A:342:GLN:O	2.21	0.40
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.40
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.56	0.40
2:D:24:ILE:HG13	2:D:25:SER:N	2.36	0.40
2:B:169:PHE:CE2	2:B:238:VAL:HG21	2.56	0.40
1:C:10:GLY:O	1:C:14:VAL:HG23	2.21	0.40
2:D:146:GLY:O	2:D:150:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ILE:HG12	2:B:86:ILE:O	2.21	0.40
2:B:133:GLN:O	2:B:164:ARG:HD3	2.20	0.40
4:F:191:LEU:HA	4:F:197:ARG:O	2.22	0.40
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.84	0.40
2:D:66:ILE:CD1	2:D:122:VAL:HG22	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:GLY:O	3:E:80:ARG:NH1[4_455]	2.14	0.06

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	436/451 (97%)	419 (96%)	17 (4%)	0	100	100
1	C	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
2	B	422/445 (95%)	409 (97%)	13 (3%)	0	100	100
2	D	423/445 (95%)	408 (96%)	15 (4%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	341/384 (89%)	321 (94%)	20 (6%)	0	100	100
All	All	2180/2319 (94%)	2104 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	369/379 (97%)	365 (99%)	4 (1%)	73	88
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	88
2	B	368/383 (96%)	364 (99%)	4 (1%)	73	88
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	92
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1902/1993 (95%)	1887 (99%)	15 (1%)	81	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	221	ARG
1	A	282	TYR
1	A	300	ASN
2	B	139	HIS
2	B	196	GLU
2	B	247	GLN
2	B	291	LEU
1	C	48	SER
1	C	221	ARG
1	C	251	ASP
1	C	347	CYS
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN

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	11	GLN
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	88	HIS
1	A	128	GLN
1	A	300	ASN
2	B	15	GLN
2	B	282	GLN
2	B	294	GLN
1	C	11	GLN
1	C	85	GLN
1	C	372	GLN
2	D	294	GLN
4	F	180	HIS
4	F	196	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 9 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	602	6	26,34,34	1.11	2 (7%)	32,54,54	1.37	5 (15%)
11	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.50	4 (12%)
8	GDP	B	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.12	3 (10%)
9	MES	B	504	-	12,12,12	2.26	1 (8%)	14,16,16	2.00	6 (42%)
8	GDP	D	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.16	4 (13%)
10	NV7	C	601	-	14,17,17	1.12	2 (14%)	20,24,24	0.74	1 (5%)
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.45	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	602	6	-	9/18/38/38	0/3/3/3
11	ACP	F	401	6	-	11/15/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
10	NV7	C	601	-	-	4/9/20/20	0/2/2/2
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.55	1.66	1.77
5	A	501	GTP	C5-C6	-3.81	1.39	1.47
5	C	602	GTP	C5-C6	-3.73	1.39	1.47
10	C	601	NV7	C6-C5	-3.37	1.35	1.39
11	F	401	ACP	PG-O2G	2.95	1.61	1.54
11	F	401	ACP	PG-O3G	2.94	1.61	1.54
11	F	401	ACP	PB-O3A	2.61	1.61	1.58
11	F	401	ACP	C5-C4	2.52	1.47	1.40
8	D	501	GDP	C6-N1	-2.39	1.34	1.37
11	F	401	ACP	PB-O2B	2.31	1.61	1.56
10	C	601	NV7	C4-C5	-2.28	1.49	1.51
5	C	602	GTP	C2-N3	2.20	1.38	1.33
8	B	501	GDP	C6-N1	-2.17	1.34	1.37
5	A	501	GTP	C2-N3	2.04	1.38	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	401	ACP	PB-O3A-PA	-4.38	118.67	132.56
9	B	504	MES	C5-N4-C3	3.74	117.25	108.83
11	F	401	ACP	C3'-C2'-C1'	3.47	106.21	100.98
5	A	501	GTP	PA-O3A-PB	-3.42	121.08	132.83
5	C	602	GTP	PA-O3A-PB	-3.26	121.65	132.83
9	B	504	MES	C6-C5-N4	-3.24	105.19	110.10
5	C	602	GTP	C8-N7-C5	3.24	109.16	102.99
8	D	501	GDP	PA-O3A-PB	-3.13	122.08	132.83
8	B	501	GDP	PA-O3A-PB	-3.10	122.20	132.83
11	F	401	ACP	N3-C2-N1	-3.07	123.88	128.68
5	A	501	GTP	C5-C6-N1	3.07	119.37	113.95
5	A	501	GTP	C8-N7-C5	3.05	108.80	102.99
5	C	602	GTP	C5-C6-N1	2.98	119.21	113.95
5	A	501	GTP	C2-N1-C6	-2.82	119.90	125.10
9	B	504	MES	O1S-S-C8	2.78	110.26	106.92
5	C	602	GTP	C2-N1-C6	-2.77	120.00	125.10
5	A	501	GTP	PB-O3B-PG	-2.69	123.60	132.83
11	F	401	ACP	C4-C5-N7	-2.57	106.72	109.40
5	C	602	GTP	PB-O3B-PG	-2.46	124.37	132.83
8	B	501	GDP	C8-N7-C5	2.40	107.56	102.99
8	D	501	GDP	C8-N7-C5	2.34	107.44	102.99
10	C	601	NV7	C4-C5-C6	2.30	132.81	129.06
8	B	501	GDP	C5-C6-N1	2.29	118.00	113.95
9	B	504	MES	O3S-S-C8	2.19	109.31	105.77
9	B	504	MES	C7-N4-C5	2.19	116.84	111.23
8	D	501	GDP	C5-C6-N1	2.16	117.77	113.95
8	D	501	GDP	C3'-C2'-C1'	2.05	104.06	100.98
9	B	504	MES	C7-N4-C3	2.00	116.35	111.23

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	602	GTP	C5'-O5'-PA-O1A
5	C	602	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-O3A
9	B	504	MES	C8-C7-N4-C5
10	C	601	NV7	C10-N1-S1-C1

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Mol	Chain	Res	Type	Atoms
10	C	601	NV7	C10-N1-S1-O1
10	C	601	NV7	C2-N1-S1-O1
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
5	C	602	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	602	GTP	PB-O3A-PA-O2A
5	C	602	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	C	602	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	C	602	GTP	PB-O3B-PG-O2G
5	C	602	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	602	GTP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
10	C	601	NV7	C2-N1-S1-C1

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	4	0
8	B	501	GDP	1	0
9	B	504	MES	4	0
8	D	501	GDP	4	0

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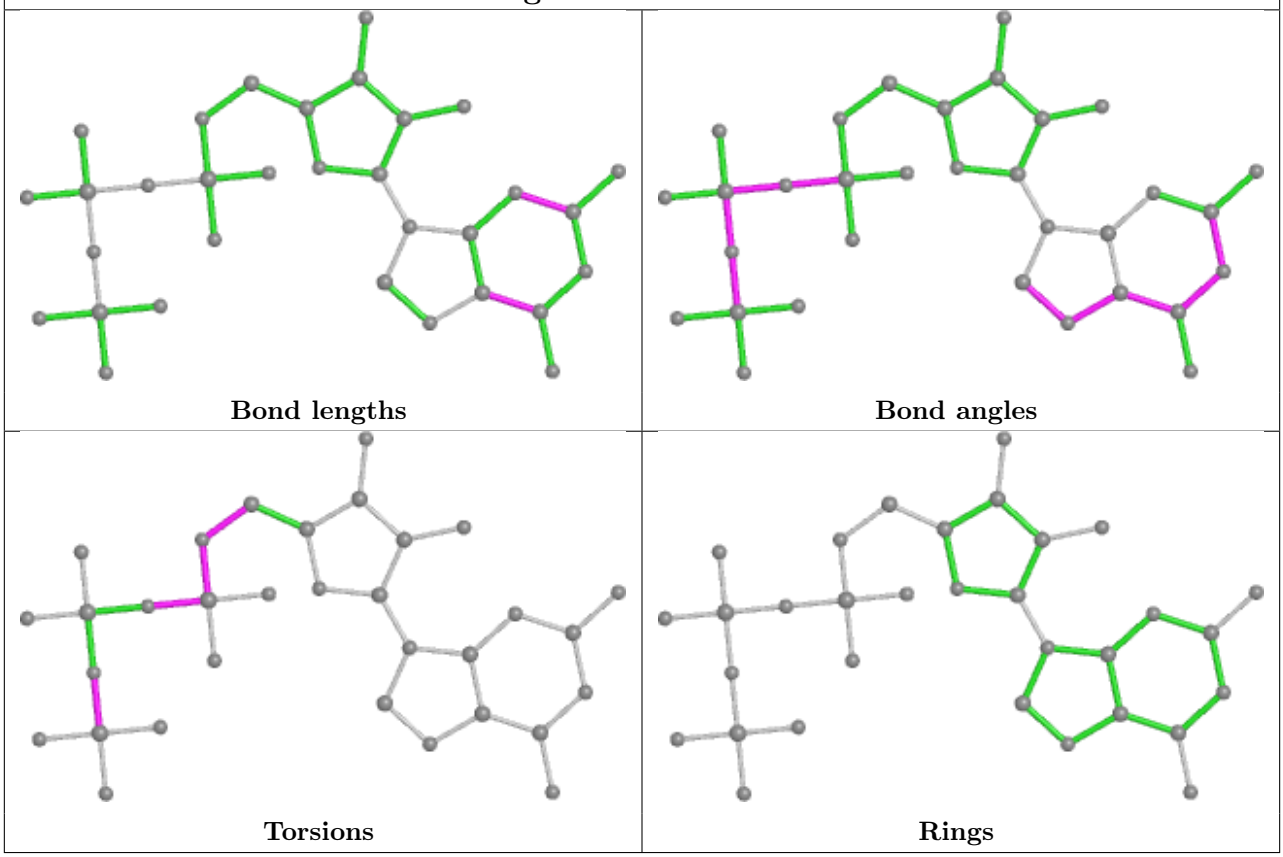
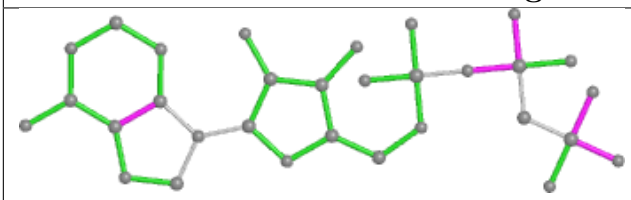
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	601	NV7	1	0
5	A	501	GTP	1	0

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.

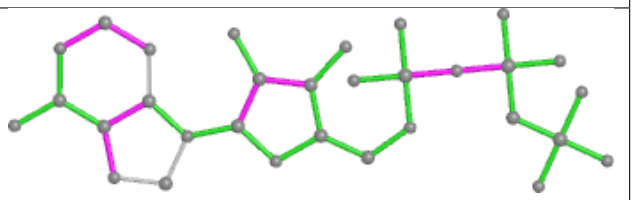
Ligand GTP C 602



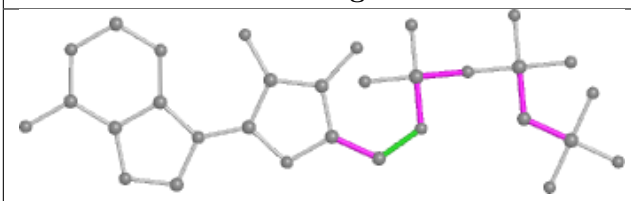
Ligand ACP F 401



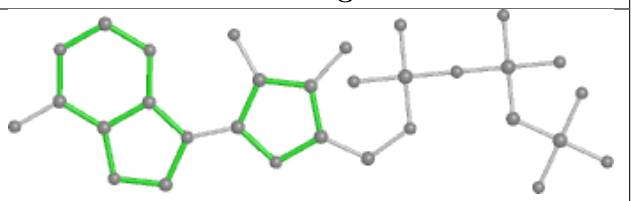
Bond lengths



Bond angles

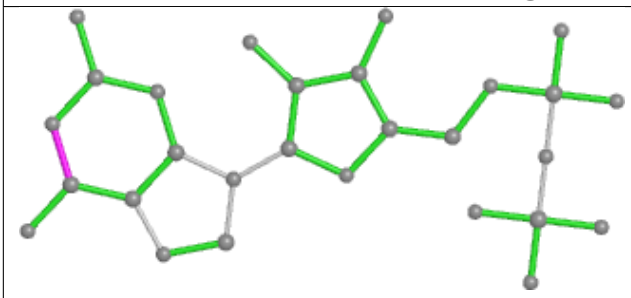


Torsions

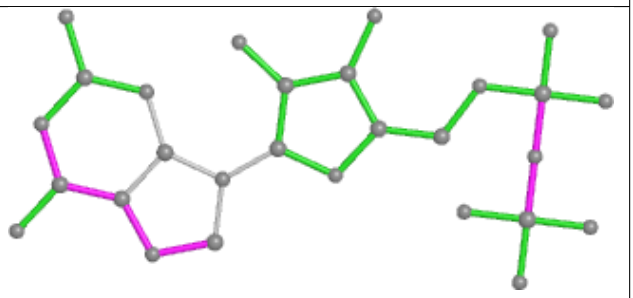


Rings

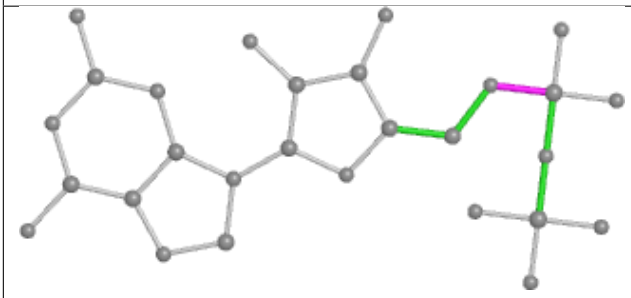
Ligand GDP B 501



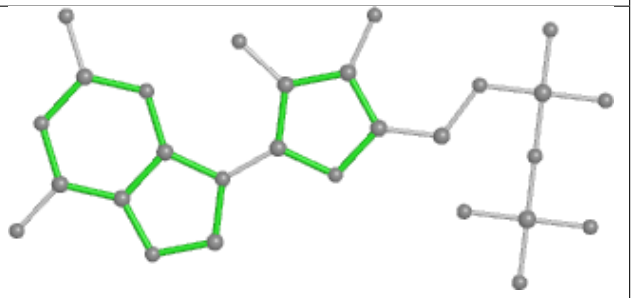
Bond lengths



Bond angles

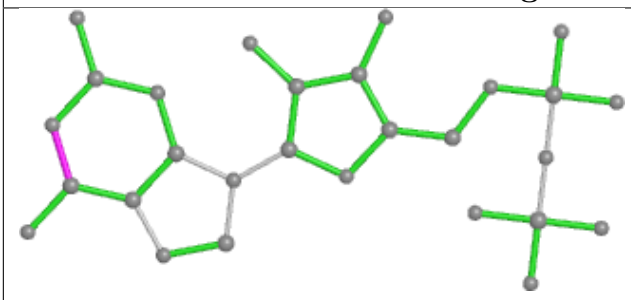


Torsions

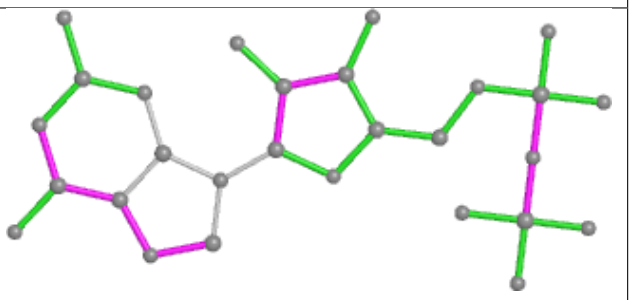


Rings

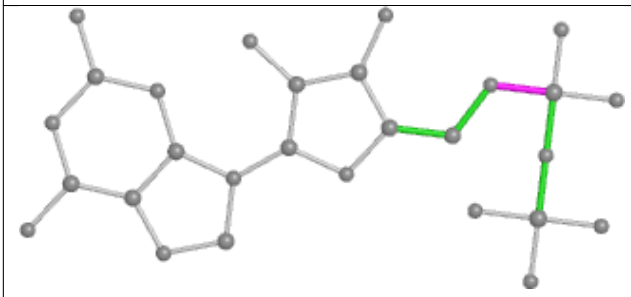
Ligand GDP D 501



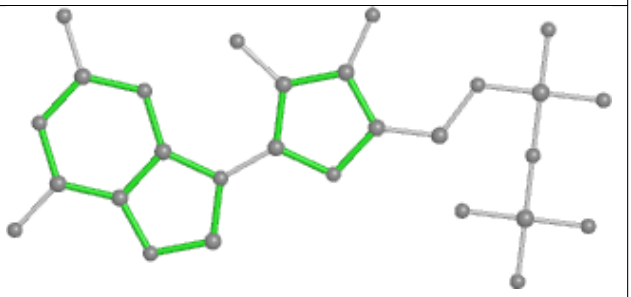
Bond lengths



Bond angles

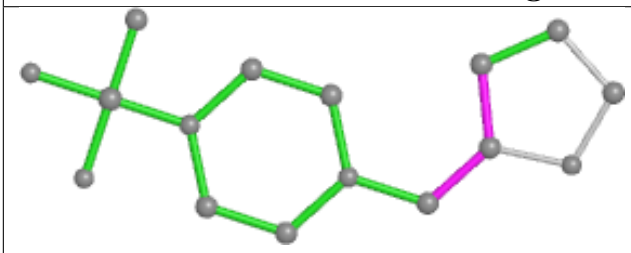


Torsions

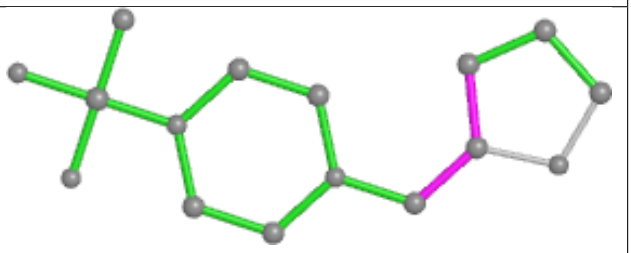


Rings

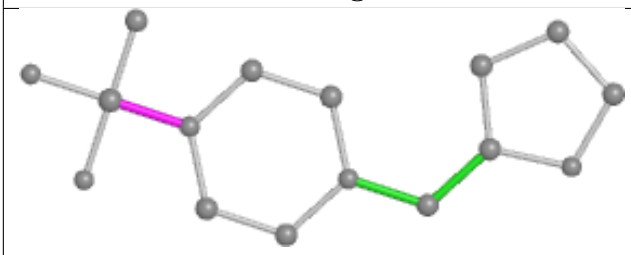
Ligand NV7 C 601



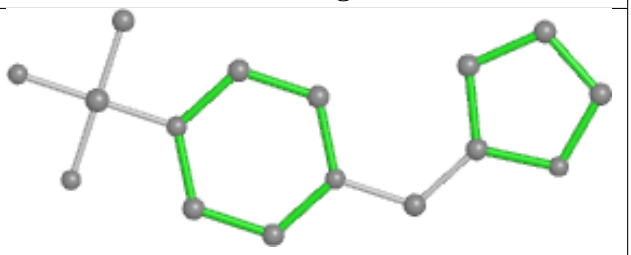
Bond lengths



Bond angles

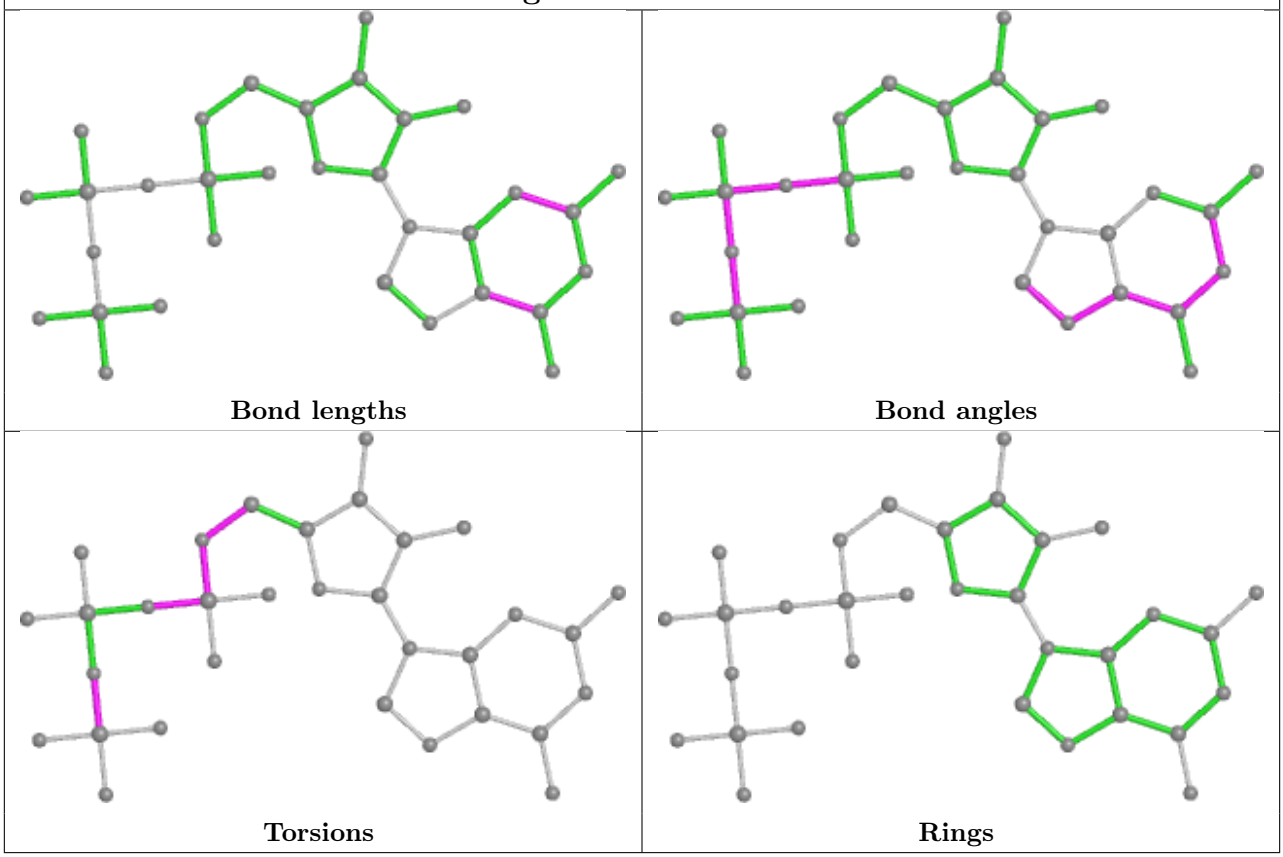


Torsions



Rings

Ligand GTP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	438/451 (97%)	0.15	3 (0%)	87	86	55, 70, 106, 190	0
1	C	440/451 (97%)	0.17	9 (2%)	65	60	46, 59, 86, 125	0
2	B	425/445 (95%)	0.26	11 (2%)	56	50	47, 70, 112, 162	3 (0%)
2	D	427/445 (95%)	0.25	21 (4%)	29	23	55, 81, 116, 164	4 (0%)
3	E	123/143 (86%)	0.56	11 (8%)	9	6	64, 88, 132, 177	0
4	F	349/384 (90%)	0.09	10 (2%)	51	45	65, 100, 169, 208	0
All	All	2202/2319 (94%)	0.21	65 (2%)	50	43	46, 74, 132, 208	7 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	281	GLN	6.4
2	B	281	GLN	6.1
2	D	277	SER	5.4
2	D	276	THR	5.0
2	D	280	SER	4.9
2	D	401	ARG	4.3
4	F	169	LEU	4.2
2	B	284	ARG	4.1
2	D	371	LEU	4.1
2	B	286	LEU	3.6
3	E	6	MET	3.6
2	D	217	LEU	3.6
3	E	123	LEU	3.4
2	D	279	GLY	3.3
2	D	275	LEU	3.2
3	E	54	LEU	3.1
4	F	105	LEU	3.0
4	F	142	ARG	3.0
1	C	302	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	339	ARG	2.9
1	C	357	TYR	2.8
1	A	88	HIS	2.8
2	D	372	LYS	2.8
2	D	278	ARG	2.8
2	D	215	ARG	2.8
4	F	131	PHE	2.7
1	C	341	ILE	2.7
3	E	7	GLU	2.7
2	D	272	PHE	2.7
3	E	26	PRO	2.7
2	B	124	LYS	2.6
2	D	218	LYS	2.5
4	F	240	LEU	2.5
4	F	141	GLY	2.5
3	E	115	HIS	2.4
3	E	25	LYS	2.4
2	D	415	GLU	2.4
3	E	27	PRO	2.4
2	B	59	ASN	2.4
1	C	245	ASP	2.3
2	B	229	HIS	2.3
2	B	285	ALA	2.3
2	D	299	LYS	2.3
1	C	368	LEU	2.3
1	A	282	TYR	2.3
2	D	370	GLY	2.3
4	F	90	SER	2.3
2	D	248	LEU	2.2
2	D	291	LEU	2.2
3	E	24	LEU	2.2
2	B	62	VAL	2.2
4	F	173	ILE	2.2
2	D	195	VAL	2.1
1	C	230	LEU	2.1
1	C	282	TYR	2.1
2	B	373	MET	2.1
2	D	229	HIS	2.1
2	B	437	ASP	2.1
4	F	89	GLU	2.1
3	E	80	ARG	2.1
3	E	22	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	278	ARG	2.1
1	A	179	THR	2.0
4	F	147	TRP	2.0
1	C	281	ALA	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.

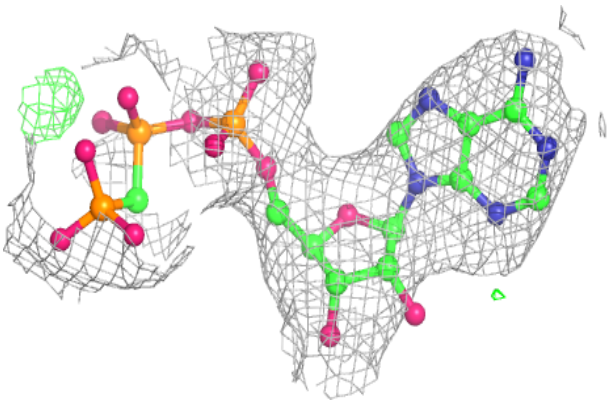
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	E	201	1/1	0.75	0.14	97,97,97,97	0
6	MG	D	502	1/1	0.80	0.19	79,79,79,79	0
9	MES	B	504	12/12	0.85	0.23	114,123,140,141	0
11	ACP	F	401	31/31	0.86	0.14	99,112,124,127	0
7	CA	B	503	1/1	0.88	0.08	105,105,105,105	0
6	MG	B	502	1/1	0.93	0.16	46,46,46,46	0
7	CA	A	503	1/1	0.93	0.13	92,92,92,92	0
8	GDP	D	501	28/28	0.95	0.18	72,76,83,88	0
10	NV7	C	601	16/16	0.97	0.19	66,72,85,87	0
6	MG	F	402	1/1	0.97	0.19	99,99,99,99	0
5	GTP	C	602	32/32	0.98	0.17	42,51,55,58	0
6	MG	A	502	1/1	0.98	0.16	58,58,58,58	0
5	GTP	A	501	32/32	0.98	0.17	51,57,61,63	0
6	MG	C	603	1/1	0.98	0.17	55,55,55,55	0
7	CA	C	604	1/1	0.98	0.10	78,78,78,78	0
8	GDP	B	501	28/28	0.99	0.15	39,50,55,56	0

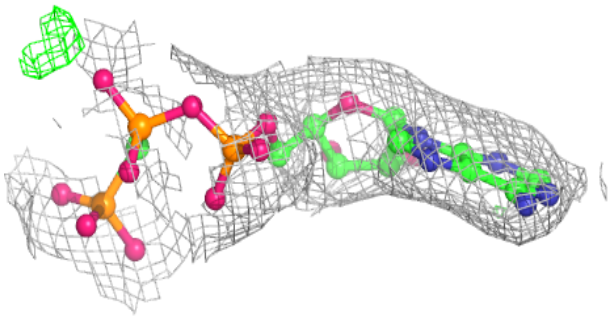
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

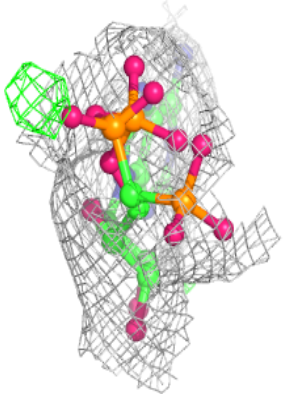
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

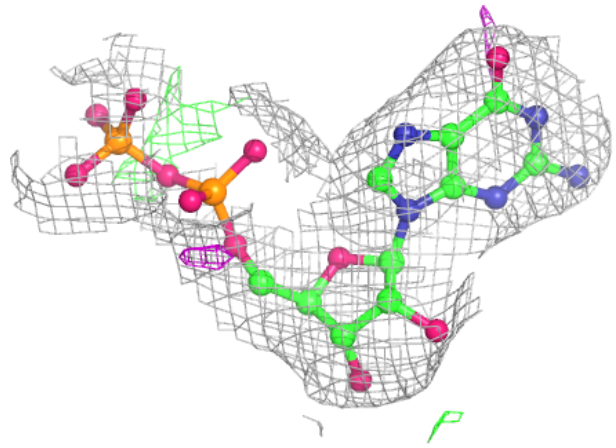


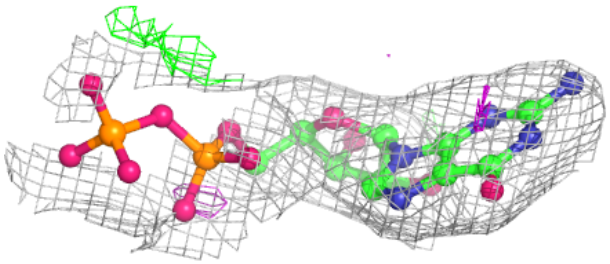


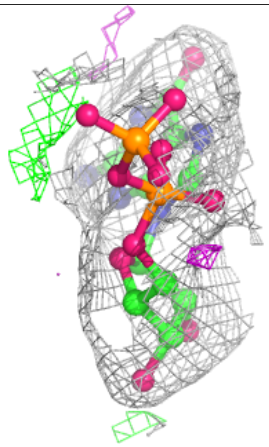


Electron density around GDP D 501:

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

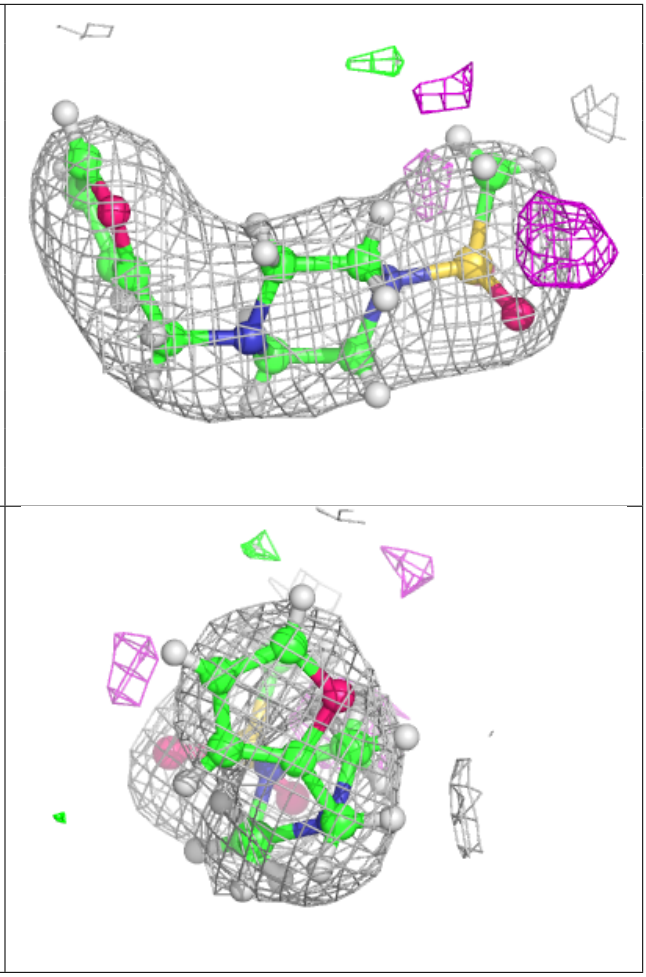






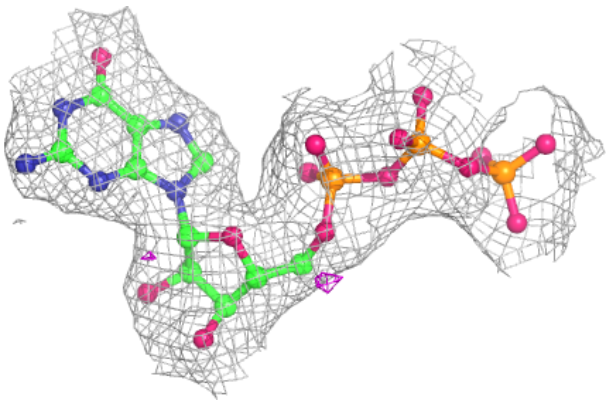
Electron density around NV7 C 601:

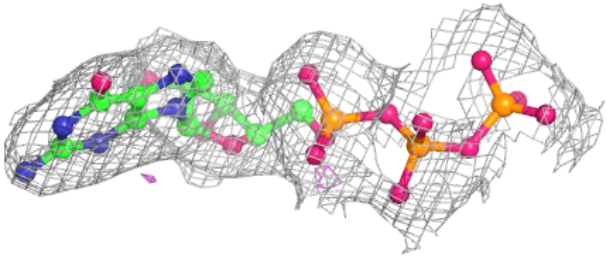
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

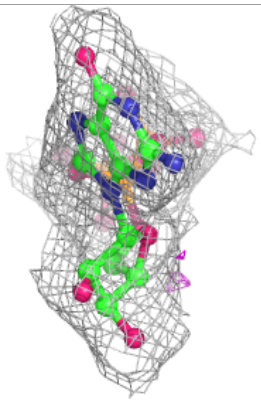


Electron density around GTP C 602:

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

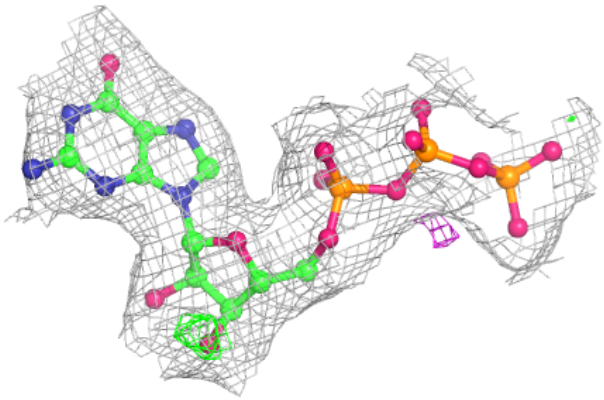


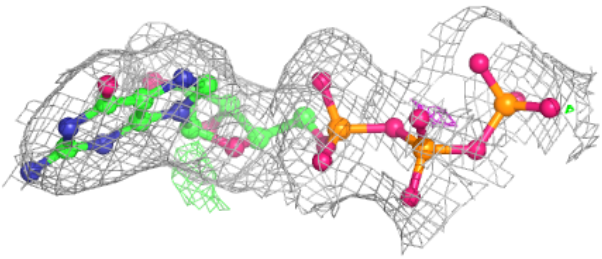


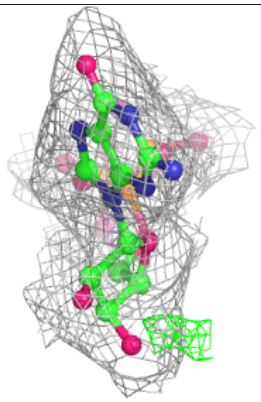


Electron density around GTP A 501:

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

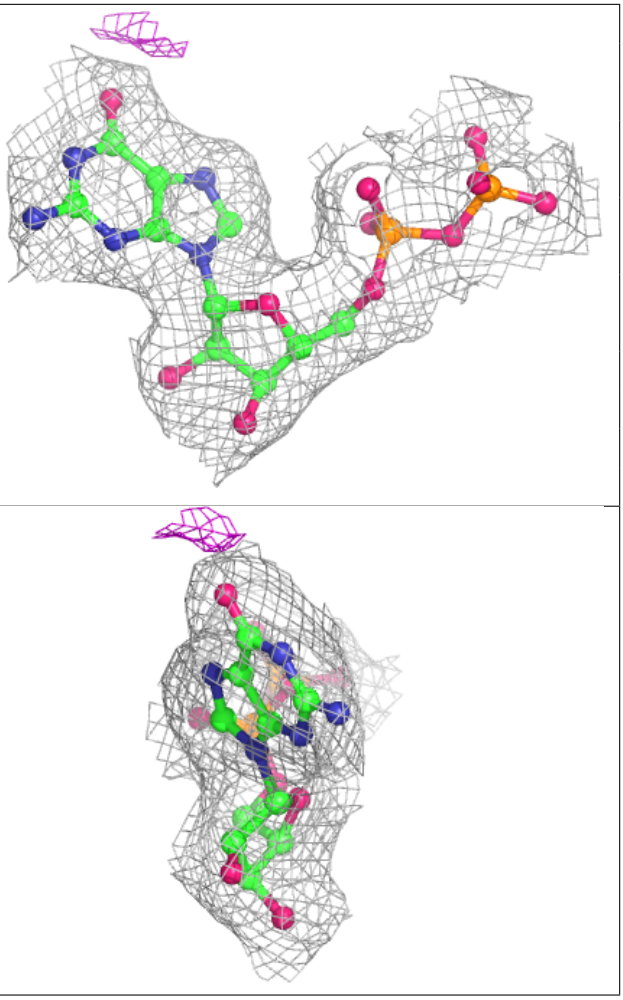






Electron density around GDP B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.