Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 10:10 AM JST

PDB ID	:	8HUH
Title	:	Crystal structure of T2R-TTL-3a complex
Authors	:	Wang, Y.X.; Chen, J.J.
Deposited on	:	2022-12-23
Resolution	:	2.80 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:

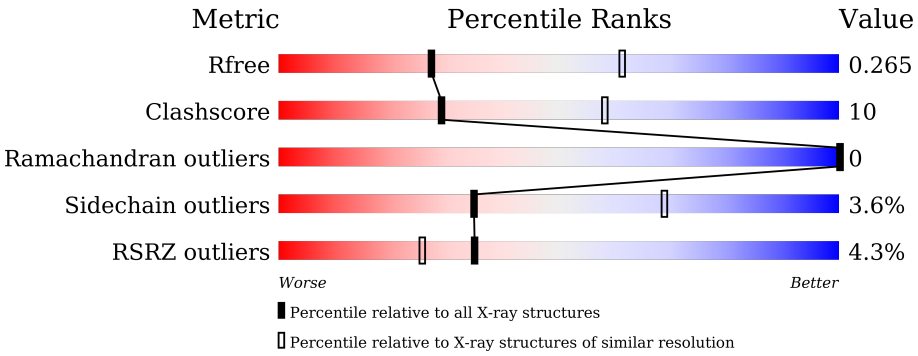
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	72% 24% • •
1	C	450	81% 16% •
2	B	445	4% 74% 21% •
2	D	445	5% 68% 26% • 5%
3	E	143	6% 66% 18% • 15%
4	F	384	11% 63% 18% • 18%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16899 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3403	2156	579	646	22			
1	C	440	Total	C	N	O	S	0	0	0
			3427	2169	581	655	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3336	2098	570	642	26			
2	D	421	Total	C	N	O	S	0	0	0
			3156	1975	534	622	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			983	605	178	195	5			

There are 2 discrepancies between the modelled and reference sequences:

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

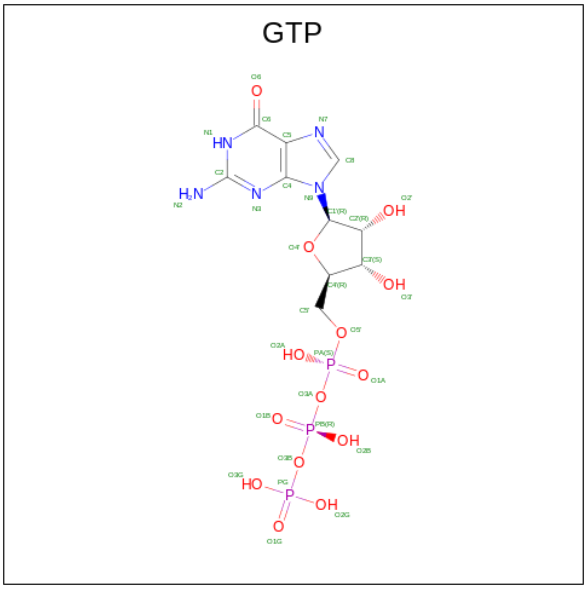
- Molecule 4 is a protein called TTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	316	Total	C	N	O	S	0	0	0
			2383	1531	404	437	11			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

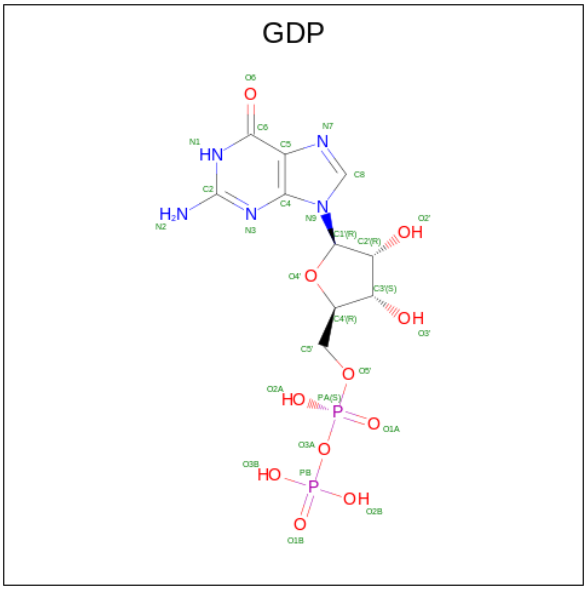
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

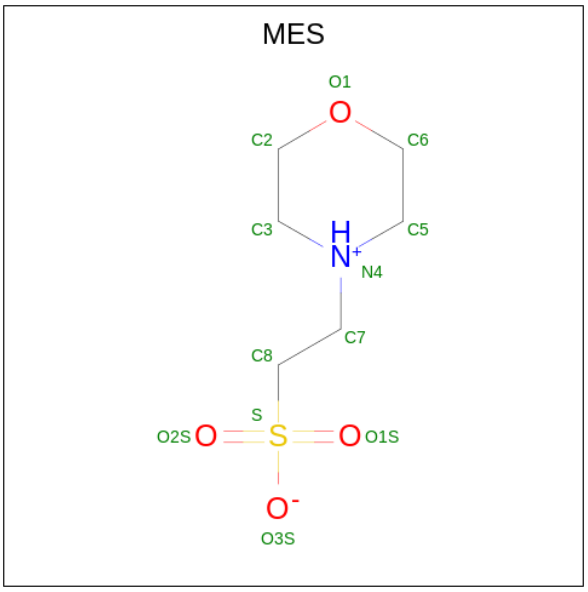
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



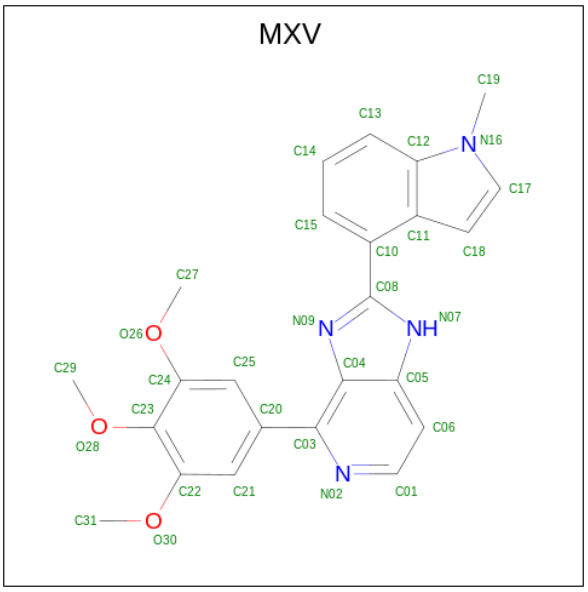
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

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



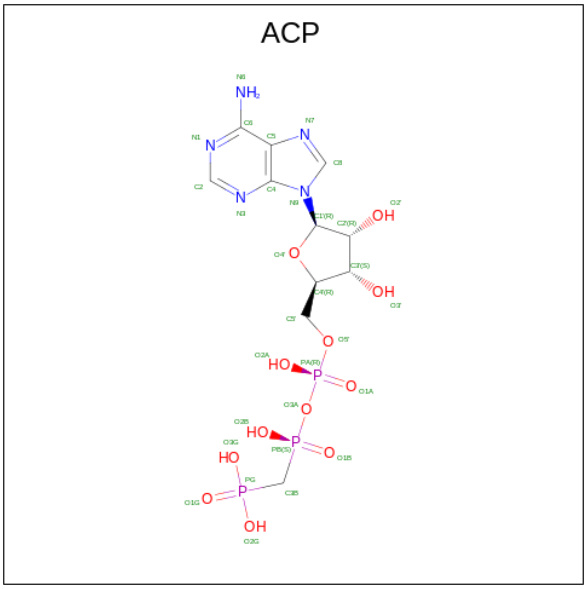
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 2-(1-methylindol-4-yl)-4-(3,4,5-trimethoxyphenyl)-1 {H}-imidazo[4,5-c]pyridine (three-letter code: MXV) (formula: $C_{24}H_{22}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			31	24	4	3		

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

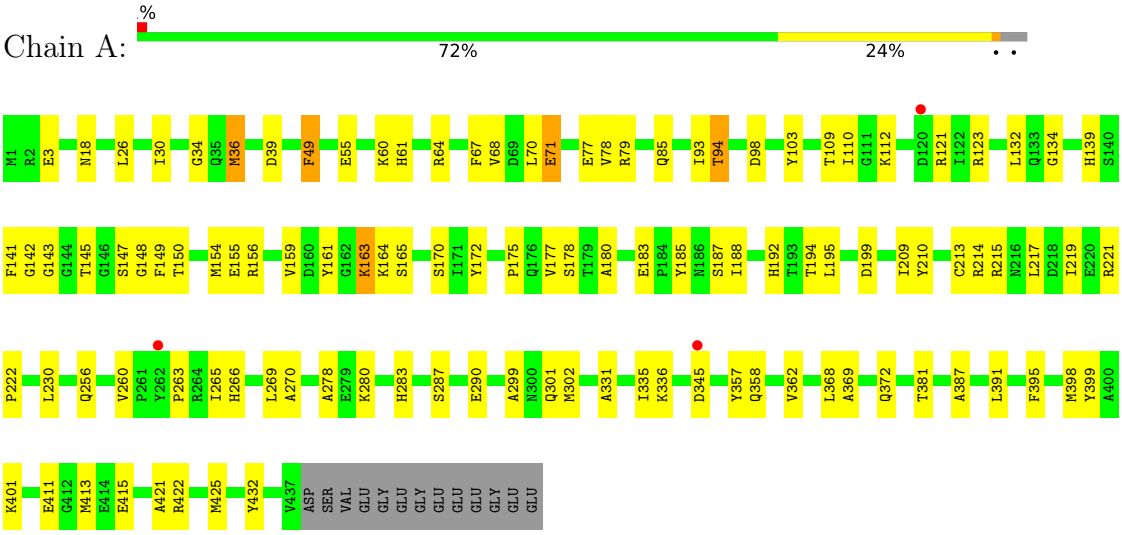


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	F	1	31	11	5	12	3	0	0

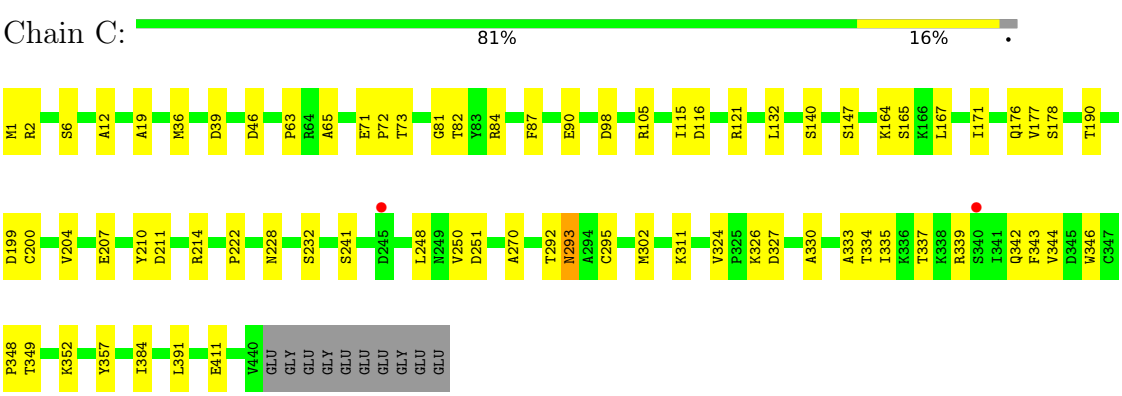
3 Residue-property plots (i)

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.

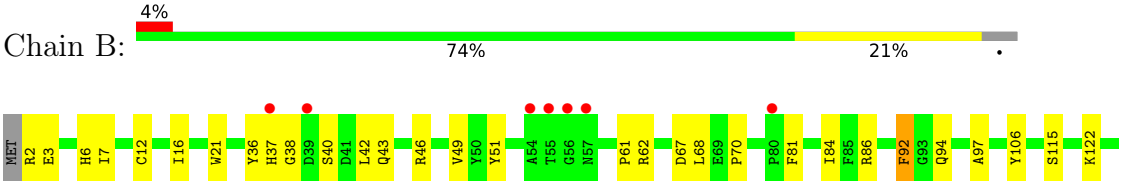
• Molecule 1: Tubulin alpha-1B chain

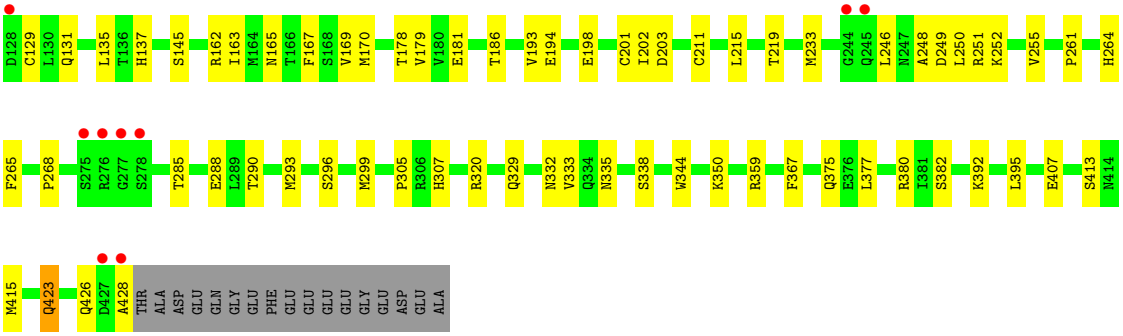


• Molecule 1: Tubulin alpha-1B chain



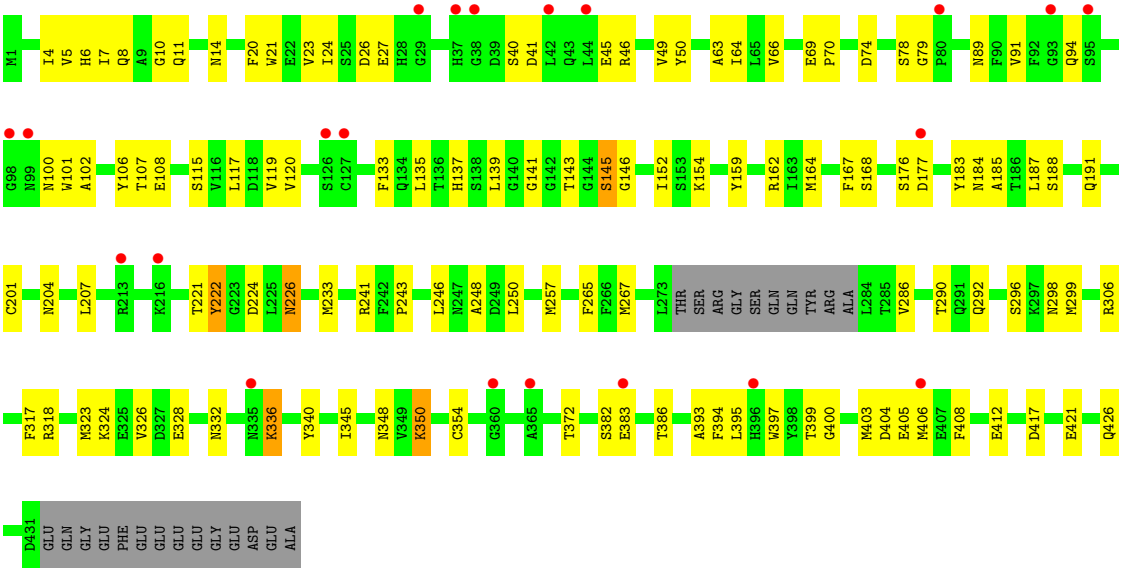
• Molecule 2: Tubulin beta-2B chain





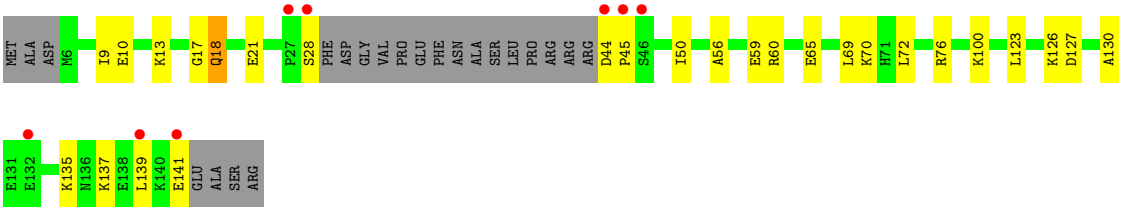
• Molecule 2: Tubulin beta-2B chain

Chain D:



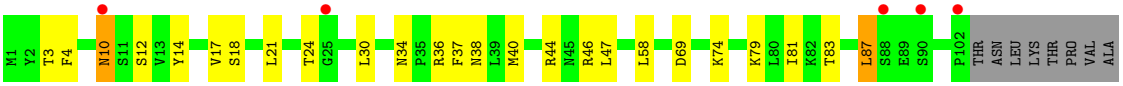
• Molecule 3: Stathmin-4

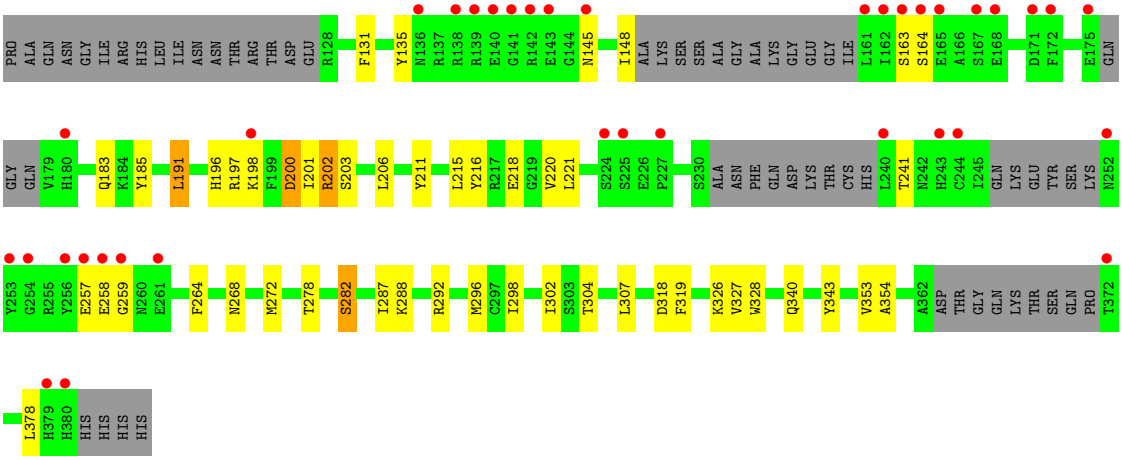
Chain E:



• Molecule 4: TTL

Chain F:




PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG THR ASP GLU R128 F131 Y135 N136 R137 R138 R139 E140 G141 R142 E143 G144 N145 I148 ALA LYS SER SER ALA GLY ALA LYS GLY GLU GLY ILE L161 I162 S163 S164 E165 A166 S167 E168 D171 F172 E175 GLN
GLY GLN V179 H180 Q183 K184 Y185 L191 H196 R197 K198 F199 D200 I201 R202 S203 L206 Y211 L215 Y216 R217 E218 G219 V220 L221 S224 S225 E226 P227 S230 ALA ASN PHE GLN ASP LYS THR CYS HIS L240 T241 N242 H243 C244 I245 GLN LYS GLU TYR SER LYS N252
Y253 G254 R255 Y256 E257 E258 G259 N260 E261 F264 N268 M272 T278 S282 I287 K288 R292 M296 C297 I298 I302 S303 T304 L307 D318 F319 K326 V327 W328 Q340 Y343 V353 A354 A362 ASP THR GLY GLN LYS THR SER GLN PRO T372
L378 H379 H380 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	105.19Å 157.88Å 182.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.80 19.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.89-2.80) 99.3 (19.89-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.79Å)	Xtriage
Refinement program	PHENIX v1.2	Depositor
R, R_{free}	0.214 , 0.266 0.215 , 0.265	Depositor DCC
R_{free} test set	1999 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16899	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.48	0/3480	0.67	0/4725
1	C	0.53	0/3505	0.70	0/4759
2	B	0.50	0/3411	0.68	0/4622
2	D	0.47	1/3224 (0.0%)	0.68	3/4389 (0.1%)
3	E	0.50	0/995	0.67	0/1327
4	F	0.42	0/2434	0.62	1/3311 (0.0%)
All	All	0.49	1/17049 (0.0%)	0.67	4/23133 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	226	ASN	CB-CG	6.26	1.65	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	393	ALA	N-CA-C	6.54	128.66	111.00
4	F	200	ASP	CB-CG-OD2	5.54	123.28	118.30
2	D	145	SER	N-CA-C	5.34	125.42	111.00
2	D	246	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3318	80	0
1	C	3427	0	3325	46	0
2	B	3336	0	3197	65	0
2	D	3156	0	2893	70	0
3	E	983	0	966	20	0
4	F	2383	0	2181	49	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	5	0
9	B	24	0	24	2	0
10	B	31	0	0	2	0
11	F	31	0	14	2	0
All	All	16899	0	15966	316	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 10.

All (316) 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)
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.62	0.79
1:A:175:PRO:HA	1:A:178:SER:HB2	1.64	0.79
4:F:79:LYS:O	4:F:83:THR:HG22	1.83	0.77
2:D:292:GLN:HE21	2:D:298:ASN:HD21	1.31	0.77
4:F:292:ARG:HG2	4:F:296:MET:HE1	1.67	0.76
1:A:36:MET:HE1	1:A:49:PHE:CZ	2.21	0.75
2:D:324:LYS:O	2:D:328:GLU:HG3	1.89	0.72
2:D:226:ASN:OD1	8:D:501:GDP:N1	2.19	0.72
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.70	0.72
1:A:79:ARG:HH22	1:A:94:THR:HG22	1.56	0.71
2:D:204:ASN:HA	2:D:207:LEU:HD12	1.72	0.70
4:F:197:ARG:NH2	4:F:257:GLU:OE1	2.23	0.70
2:D:143:THR:N	8:D:501:GDP:O1B	2.26	0.69
4:F:135:TYR:O	4:F:145:ASN:ND2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:H	1:A:163:LYS:HD3	1.57	0.69
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.73	0.68
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.75	0.68
2:D:100:ASN:HD22	2:D:397:TRP:HE3	1.40	0.66
11:F:401:ACP:H5'2	11:F:401:ACP:O1B	1.97	0.65
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.26	0.65
2:B:94:GLN:HB3	1:C:1:MET:HE1	1.79	0.64
2:B:81:PHE:O	2:B:84:ILE:HG22	1.97	0.64
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.64
2:B:375:GLN:HE22	2:B:423:GLN:NE2	1.95	0.64
2:B:211:CYS:HA	2:B:215:LEU:HD12	1.79	0.63
2:D:4:ILE:HG12	2:D:250:LEU:HD11	1.80	0.63
4:F:197:ARG:HH22	4:F:257:GLU:CD	2.01	0.63
2:D:107:THR:OG1	2:D:108:GLU:N	2.31	0.63
2:D:102:ALA:HB2	2:D:403:MET:HE3	1.81	0.63
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.80	0.62
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.35	0.62
1:C:178:SER:OG	2:D:350:LYS:NZ	2.31	0.62
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.66	0.61
1:A:331:ALA:O	1:A:335:ILE:HG13	2.01	0.60
2:B:3:GLU:HB3	2:B:62:ARG:NH1	2.16	0.60
2:B:307:HIS:O	2:B:426:GLN:NE2	2.35	0.60
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.37	0.59
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.83	0.59
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.21	0.59
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.84	0.59
1:C:211:ASP:OD1	1:C:214:ARG:NH2	2.36	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.59
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.85	0.59
2:D:70:PRO:HG3	2:D:94:GLN:HA	1.85	0.58
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.68	0.58
1:C:132:LEU:O	1:C:164:LYS:NZ	2.37	0.58
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.69	0.58
2:B:46:ARG:HH11	2:B:46:ARG:HG2	1.68	0.58
1:A:143:GLY:O	1:A:147:SER:HB3	2.03	0.58
2:D:221:THR:HG23	2:D:224:ASP:H	1.68	0.58
4:F:148:ILE:N	4:F:183:GLN:O	2.30	0.57
2:D:152:ILE:HD12	2:D:164:MET:SD	2.45	0.57
4:F:4:PHE:CZ	4:F:18:SER:HB2	2.40	0.57
4:F:3:THR:OG1	4:F:37:PHE:HA	2.05	0.57
2:D:11:GLN:N	8:D:501:GDP:O2B	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG21	1:A:411:GLU:OE1	2.06	0.56
2:B:165:ASN:OD1	2:B:198:GLU:HB2	2.05	0.56
1:C:204:VAL:HG22	1:C:302:MET:HE3	1.86	0.56
4:F:191:LEU:H	4:F:191:LEU:HD12	1.71	0.56
2:B:203:ASP:OD2	2:B:380:ARG:NH1	2.35	0.56
2:D:183:TYR:CD1	2:D:408:PHE:HE2	2.23	0.56
2:B:40:SER:OG	2:B:42:LEU:HB2	2.06	0.56
3:E:44:ASP:OD1	3:E:44:ASP:N	2.37	0.56
1:A:401:LYS:HE2	2:B:428:ALA:HB1	1.88	0.56
2:D:404:ASP:OD1	2:D:405:GLU:N	2.39	0.56
1:A:103:TYR:HD1	1:A:147:SER:OG	1.88	0.56
1:C:81:GLY:O	1:C:84:ARG:HG2	2.05	0.56
2:B:350:LYS:HB2	10:B:505:MXV:C12	2.36	0.55
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.89	0.55
4:F:81:ILE:HA	4:F:87:LEU:HD23	1.87	0.55
2:B:296:SER:N	9:B:504:MES:O3S	2.35	0.55
3:E:135:LYS:O	3:E:139:LEU:HB2	2.07	0.55
4:F:268:ASN:O	4:F:272:MET:HG3	2.07	0.55
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.42	0.55
1:A:34:GLY:O	1:A:61:HIS:N	2.32	0.54
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.71	0.54
2:B:86:ARG:HE	2:B:122:LYS:HZ3	1.56	0.54
1:A:177:VAL:O	1:A:177:VAL:HG22	2.07	0.54
2:D:23:VAL:O	2:D:27:GLU:HG3	2.07	0.54
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.37	0.54
2:B:38:GLY:HA3	2:B:43:GLN:HE22	1.72	0.54
2:B:392:LYS:HB3	2:B:395:LEU:HD12	1.89	0.54
2:D:50:TYR:CE2	2:D:241:ARG:HG2	2.43	0.54
2:B:178:THR:O	2:B:181:GLU:HG3	2.07	0.54
1:A:180:ALA:O	1:A:183:GLU:HG3	2.08	0.54
2:D:101:TRP:HD1	2:D:145:SER:OG	1.91	0.54
4:F:278:THR:O	4:F:282:SER:OG	2.25	0.54
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.90	0.53
2:D:78:SER:OG	2:D:79:GLY:N	2.40	0.53
4:F:201:ILE:HG12	4:F:221:LEU:HD11	1.90	0.53
1:A:213:CYS:O	1:A:217:LEU:HB2	2.09	0.53
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.40	0.53
1:A:185:TYR:OH	1:A:398:MET:HB3	2.08	0.53
2:B:12:CYS:O	2:B:16:ILE:HG12	2.09	0.53
2:D:394:PHE:O	2:D:397:TRP:HB2	2.09	0.53
1:A:134:GLY:HA2	1:A:164:LYS:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.44	0.52
1:A:132:LEU:HD23	1:A:164:LYS:HG3	1.92	0.52
2:D:139:LEU:HG	2:D:188:SER:CB	2.40	0.52
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.45	0.51
4:F:202:ARG:HH21	4:F:318:ASP:CG	2.13	0.51
2:D:139:LEU:HG	2:D:188:SER:HB3	1.93	0.51
1:A:163:LYS:HE2	1:A:164:LYS:HZ2	1.75	0.51
2:B:338:SER:OG	4:F:34:ASN:ND2	2.37	0.51
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.46	0.51
2:D:141:GLY:O	2:D:184:ASN:ND2	2.43	0.51
4:F:326:LYS:HD3	4:F:328:TRP:CE2	2.46	0.51
2:B:249:ASP:OD1	2:B:252:LYS:HB2	2.10	0.51
4:F:340:GLN:HA	4:F:343:TYR:HD1	1.76	0.50
4:F:203:SER:HB3	4:F:215:LEU:HD11	1.92	0.50
2:B:329:GLN:O	2:B:332:ASN:HB3	2.12	0.50
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.94	0.50
2:B:86:ARG:HE	2:B:122:LYS:NZ	2.09	0.50
2:B:68:LEU:CD1	2:B:97:ALA:HB2	2.42	0.50
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.94	0.50
4:F:21:LEU:O	4:F:24:THR:OG1	2.29	0.50
4:F:10:ASN:HD22	4:F:10:ASN:C	2.12	0.50
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.95	0.50
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.38	0.50
2:D:141:GLY:HA3	8:D:501:GDP:O5'	2.12	0.50
2:B:7:ILE:O	2:B:135:LEU:HD12	2.12	0.49
4:F:4:PHE:HZ	4:F:18:SER:HB2	1.75	0.49
2:D:417:ASP:O	2:D:421:GLU:HG3	2.12	0.49
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.95	0.48
1:A:60:LYS:NZ	1:A:85:GLN:O	2.46	0.48
1:A:134:GLY:HA3	1:A:165:SER:O	2.13	0.48
2:B:2:ARG:O	2:B:49:VAL:HG13	2.13	0.48
2:D:159:TYR:HB3	2:D:162:ARG:HG3	1.95	0.48
2:B:169:VAL:HA	2:B:202:ILE:O	2.14	0.48
1:C:19:ALA:HB1	1:C:232:SER:OG	2.13	0.48
4:F:258:GLU:OE1	4:F:259:GLY:N	2.47	0.48
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.49	0.48
2:D:46:ARG:NH2	2:D:248:ALA:O	2.46	0.48
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48
2:D:383:GLU:HA	2:D:386:THR:HG22	1.96	0.48
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.96	0.48
4:F:288:LYS:HG2	4:F:378:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HG3	1:A:194:THR:HG23	1.94	0.47
1:C:330:ALA:O	1:C:334:THR:HG23	2.14	0.47
2:D:290:THR:HG22	2:D:317:PHE:CZ	2.49	0.47
1:A:163:LYS:HG2	1:A:164:LYS:HD3	1.96	0.47
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.96	0.47
1:A:362:VAL:HG21	1:A:368:LEU:O	2.13	0.47
2:D:117:LEU:HA	2:D:120:VAL:HG22	1.95	0.47
2:D:286:VAL:O	2:D:290:THR:HG23	2.14	0.47
1:A:30:ILE:HG12	1:A:36:MET:HB2	1.95	0.47
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.32	0.47
1:A:155:GLU:HB3	3:E:50:ILE:HD11	1.97	0.47
2:B:293:MET:CG	2:B:367:PHE:HB2	2.44	0.47
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.49	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.47
2:B:122:LYS:HE3	2:B:122:LYS:HB3	1.75	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.47
1:C:147:SER:HB2	1:C:190:THR:OG1	2.15	0.47
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.50	0.47
2:B:335:ASN:OD1	4:F:36:ARG:NH1	2.47	0.47
2:D:191:GLN:OE1	3:E:126:LYS:NZ	2.48	0.47
1:A:70:LEU:HG	1:A:145:THR:HG23	1.96	0.46
1:A:132:LEU:O	1:A:164:LYS:HE2	2.15	0.46
2:D:183:TYR:O	2:D:187:LEU:HD12	2.15	0.46
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.97	0.46
2:D:50:TYR:HE2	2:D:241:ARG:HG2	1.80	0.46
1:A:163:LYS:H	1:A:163:LYS:CD	2.27	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HG2	2.50	0.46
2:D:400:GLY:O	3:E:137:LYS:HG3	2.15	0.46
1:A:36:MET:HE3	1:A:39:ASP:HB2	1.97	0.46
1:A:123:ARG:HG3	1:A:123:ARG:NH1	2.31	0.46
1:A:345:ASP:O	3:E:28:SER:N	2.47	0.46
2:D:332:ASN:HD21	2:D:336:LYS:HE3	1.81	0.46
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.98	0.46
1:A:399:TYR:OH	1:A:415:GLU:HG2	2.17	0.45
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.51	0.45
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.98	0.45
1:A:192:HIS:CG	1:A:421:ALA:HA	2.52	0.45
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.16	0.45
2:D:45:GLU:OE1	2:D:243:PRO:HB3	2.15	0.45
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.50	0.45
2:B:2:ARG:HA	2:B:129:CYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:PRO:HG3	2:B:94:GLN:HE22	1.81	0.45
2:D:139:LEU:HB3	2:D:185:ALA:HA	1.96	0.45
2:D:267:MET:SD	2:D:299:MET:HG3	2.56	0.45
1:A:109:THR:OG1	1:A:110:ILE:N	2.50	0.45
2:D:290:THR:HG22	2:D:317:PHE:HZ	1.81	0.45
4:F:87:LEU:HD13	4:F:87:LEU:N	2.30	0.45
1:A:55:GLU:HG2	1:A:61:HIS:CE1	2.52	0.45
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.45
1:C:171:ILE:HD12	1:C:171:ILE:N	2.31	0.45
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.98	0.45
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.52	0.45
2:B:193:VAL:HG12	2:B:194:GLU:HG3	1.99	0.45
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.56	0.45
1:C:292:THR:O	1:C:295:CYS:HB2	2.17	0.45
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.45
4:F:3:THR:O	4:F:38:ASN:HB2	2.17	0.45
1:C:140:SER:HA	1:C:171:ILE:HB	1.99	0.45
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.67	0.45
2:D:323:MET:HA	2:D:326:VAL:HG12	1.99	0.45
1:A:156:ARG:O	1:A:159:VAL:HG22	2.17	0.45
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.52	0.44
1:A:287:SER:OG	1:A:290:GLU:HG3	2.17	0.44
4:F:87:LEU:N	4:F:87:LEU:CD1	2.80	0.44
1:A:36:MET:HE3	1:A:36:MET:HB3	1.62	0.44
2:B:329:GLN:O	2:B:333:VAL:HG23	2.16	0.44
2:D:10:GLY:O	2:D:14:ASN:ND2	2.27	0.44
2:D:306:ARG:HG3	2:D:340:TYR:CZ	2.52	0.44
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.53	0.44
2:D:7:ILE:HG12	2:D:64:ILE:HB	2.00	0.44
4:F:287:ILE:HG12	4:F:319:PHE:CE2	2.51	0.44
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.32	0.44
1:C:293:ASN:OD1	1:C:339:ARG:NH1	2.51	0.44
2:D:318:ARG:HG2	2:D:354:CYS:HB3	1.99	0.44
2:B:186:THR:HG23	2:B:415:MET:HE2	2.00	0.44
1:C:176:GLN:NE2	1:C:207:GLU:HG3	2.33	0.44
2:D:7:ILE:O	2:D:135:LEU:HD12	2.17	0.44
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.99	0.44
1:A:280:LYS:HD3	1:A:283:HIS:HB2	2.00	0.44
2:B:261:PRO:O	2:B:264:HIS:ND1	2.50	0.44
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.18	0.44
4:F:14:TYR:HA	4:F:17:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.53	0.43
2:B:67:ASP:O	2:B:92:PHE:HA	2.17	0.43
1:C:270:ALA:HB3	1:C:302:MET:HE2	2.00	0.43
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.53	0.43
2:B:296:SER:HA	2:B:299:MET:HG2	1.99	0.43
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.43
9:B:504:MES:H81	9:B:504:MES:H51	1.64	0.43
1:C:46:ASP:OD1	1:C:46:ASP:N	2.49	0.43
2:D:66:VAL:HA	2:D:91:VAL:O	2.18	0.43
3:E:10:GLU:O	3:E:10:GLU:HG2	2.17	0.43
4:F:3:THR:HB	4:F:30:LEU:HD11	2.00	0.43
2:B:106:TYR:OH	2:B:407:GLU:OE2	2.24	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.43
2:D:89:ASN:HA	2:D:119:VAL:HG11	2.01	0.43
2:D:221:THR:OG1	2:D:222:TYR:N	2.51	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.43
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.53	0.43
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.00	0.43
2:D:106:TYR:HE2	3:E:130:ALA:HA	1.83	0.43
4:F:163:SER:OG	4:F:164:SER:N	2.50	0.43
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.82	0.43
2:B:320:ARG:HH11	2:B:320:ARG:HG2	1.84	0.43
4:F:298:ILE:HD12	4:F:302:ILE:HD13	2.00	0.43
1:A:221:ARG:HA	1:A:221:ARG:HD2	1.63	0.43
1:A:401:LYS:HD3	2:B:344:TRP:CD2	2.54	0.43
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.01	0.43
2:D:395:LEU:O	2:D:399:THR:HG22	2.19	0.43
1:A:269:LEU:HD11	1:A:301:GLN:HB3	2.01	0.43
2:B:246:LEU:HD12	2:B:246:LEU:HA	1.81	0.43
2:B:251:ARG:O	2:B:255:VAL:HG23	2.18	0.43
3:E:69:LEU:HD23	3:E:69:LEU:HA	1.82	0.43
4:F:288:LYS:HG2	4:F:378:LEU:CD2	2.49	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.19	0.42
2:D:63:ALA:C	2:D:64:ILE:HD13	2.40	0.42
4:F:221:LEU:HD12	4:F:221:LEU:HA	1.45	0.42
1:A:68:VAL:HG22	1:A:93:ILE:HB	2.01	0.42
2:D:372:THR:OG1	2:D:426:GLN:HG3	2.19	0.42
2:B:36:TYR:C	2:B:37:HIS:HD1	2.21	0.42
2:B:46:ARG:O	2:B:49:VAL:HG23	2.18	0.42
2:B:285:THR:HG23	2:B:288:GLU:OE1	2.19	0.42
2:B:219:THR:HG21	1:C:326:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CE2	1:A:387:ALA:HB1	2.54	0.42
2:B:51:TYR:O	2:B:62:ARG:NH2	2.53	0.42
1:C:1:MET:HB2	1:C:2:ARG:H	1.48	0.42
2:D:4:ILE:HD12	2:D:49:VAL:CG1	2.50	0.42
3:E:13:LYS:HZ2	3:E:13:LYS:HB3	1.84	0.42
3:E:44:ASP:HA	3:E:45:PRO:HD3	1.80	0.42
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.02	0.42
1:A:263:PRO:O	1:A:266:HIS:ND1	2.41	0.42
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.46	0.42
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.35	0.42
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.44	0.42
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.88	0.42
1:A:199:ASP:HB3	1:A:256:GLN:HG2	2.02	0.42
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.20	0.42
4:F:287:ILE:HG12	4:F:319:PHE:CD2	2.55	0.42
1:C:228:ASN:O	1:C:232:SER:OG	2.35	0.41
3:E:56:ALA:O	3:E:59:GLU:HG3	2.20	0.41
4:F:197:ARG:CZ	4:F:257:GLU:OE1	2.68	0.41
1:C:6:SER:O	1:C:65:ALA:HA	2.20	0.41
1:C:105:ARG:NH1	1:C:411:GLU:OE2	2.51	0.41
1:C:204:VAL:HG22	1:C:302:MET:CE	2.47	0.41
2:D:106:TYR:CE2	3:E:130:ALA:HA	2.54	0.41
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.60	0.41
1:A:163:LYS:HE2	1:A:164:LYS:NZ	2.35	0.41
2:B:293:MET:HG3	2:B:367:PHE:HB2	2.02	0.41
1:C:71:GLU:OE2	1:C:73:THR:N	2.49	0.41
1:C:90:GLU:HB3	1:C:121:ARG:HD2	2.01	0.41
3:E:123:LEU:O	3:E:126:LYS:HB3	2.19	0.41
4:F:191:LEU:HD23	4:F:196:HIS:HE1	1.84	0.41
1:C:84:ARG:HG2	1:C:84:ARG:HH11	1.85	0.41
1:A:67:PHE:N	1:A:67:PHE:CD2	2.89	0.41
2:D:139:LEU:HD13	2:D:168:SER:HB3	2.02	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.83	0.41
1:A:49:PHE:CD1	1:A:49:PHE:C	2.93	0.41
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.21	0.41
1:C:36:MET:HG2	1:C:39:ASP:H	1.85	0.41
1:C:204:VAL:HG22	1:C:302:MET:SD	2.61	0.41
4:F:74:LYS:HE2	11:F:401:ACP:O2A	2.21	0.41
2:B:290:THR:HG22	2:B:333:VAL:HG21	2.03	0.41
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.02	0.41
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.56	0.41
2:D:257:MET:HE3	2:D:257:MET:HB3	1.92	0.41
2:D:332:ASN:ND2	2:D:336:LYS:HE3	2.36	0.41
4:F:40:MET:HE2	4:F:47:LEU:HG	2.03	0.41
2:B:36:TYR:HE1	2:B:43:GLN:NE2	2.19	0.40
2:D:69:GLU:HA	2:D:70:PRO:HD3	1.92	0.40
4:F:200:ASP:O	4:F:221:LEU:HD12	2.19	0.40
2:B:299:MET:CE	2:B:305:PRO:HG3	2.51	0.40
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.02	0.40
1:A:214:ARG:HG2	1:A:219:ILE:O	2.22	0.40
2:B:248:ALA:HA	10:B:505:MXV:N02	2.36	0.40
1:C:115:ILE:HG23	1:C:116:ASP:N	2.36	0.40
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.56	0.40
2:D:141:GLY:CA	8:D:501:GDP:H5'	2.51	0.40
4:F:287:ILE:HG13	4:F:327:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	409 (94%)	26 (6%)	0	100	100
1	C	438/450 (97%)	421 (96%)	17 (4%)	0	100	100
2	B	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	395 (95%)	22 (5%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	302/384 (79%)	290 (96%)	12 (4%)	0	100	100
All	All	2135/2317 (92%)	2045 (96%)	90 (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	365/378 (97%)	354 (97%)	11 (3%)	41	75
1	C	368/378 (97%)	360 (98%)	8 (2%)	52	83
2	B	362/383 (94%)	352 (97%)	10 (3%)	43	77
2	D	326/383 (85%)	311 (95%)	15 (5%)	27	60
3	E	104/127 (82%)	98 (94%)	6 (6%)	20	50
4	F	233/342 (68%)	219 (94%)	14 (6%)	19	48
All	All	1758/1991 (88%)	1694 (96%)	64 (4%)	35	69

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	MET
1	A	49	PHE
1	A	71	GLU
1	A	77	GLU
1	A	94	THR
1	A	112	LYS
1	A	163	LYS
1	A	336	LYS
1	A	358	GLN
1	A	381	THR
1	A	413	MET
2	B	92	PHE
2	B	115	SER
2	B	137	HIS
2	B	145	SER
2	B	162	ARG
2	B	268	PRO
2	B	359	ARG
2	B	382	SER
2	B	413	SER
2	B	423	GLN
1	C	82	THR

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Mol	Chain	Res	Type
1	C	177	VAL
1	C	241	SER
1	C	251	ASP
1	C	293	ASN
1	C	311	LYS
1	C	342	GLN
1	C	384	ILE
2	D	26	ASP
2	D	40	SER
2	D	41	ASP
2	D	74	ASP
2	D	115	SER
2	D	137	HIS
2	D	176	SER
2	D	177	ASP
2	D	222	TYR
2	D	296	SER
2	D	336	LYS
2	D	350	LYS
2	D	382	SER
2	D	406	MET
2	D	412	GLU
3	E	18	GLN
3	E	65	GLU
3	E	70	LYS
3	E	100	LYS
3	E	127	ASP
3	E	141	GLU
4	F	10	ASN
4	F	12	SER
4	F	44	ARG
4	F	46	ARG
4	F	69	ASP
4	F	87	LEU
4	F	131	PHE
4	F	191	LEU
4	F	202	ARG
4	F	211	TYR
4	F	220	VAL
4	F	264	PHE
4	F	282	SER
4	F	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	128	GLN
2	B	11	GLN
2	B	43	GLN
2	B	423	GLN
1	C	107	HIS
1	C	356	ASN
2	D	134	GLN
2	D	292	GLN
2	D	335	ASN
3	E	108	ASN
3	E	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MES	B	503	-	12,12,12	2.25	1 (8%)	14,16,16	2.11	5 (35%)
11	ACP	F	401	-	27,33,33	1.15	1 (3%)	32,52,52	1.25	4 (12%)
5	GTP	C	501	6	26,34,34	1.15	1 (3%)	32,54,54	1.61	9 (28%)
9	MES	B	504	-	12,12,12	2.48	1 (8%)	14,16,16	1.92	4 (28%)
8	GDP	B	501	6	24,30,30	0.91	1 (4%)	30,47,47	1.30	3 (10%)
5	GTP	A	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.53	6 (18%)
8	GDP	D	501	-	24,30,30	1.63	3 (12%)	30,47,47	1.56	7 (23%)
10	MXV	B	505	-	30,35,35	1.82	4 (13%)	36,51,51	1.54	5 (13%)

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
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
11	ACP	F	401	-	-	4/15/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
8	GDP	D	501	-	-	4/12/32/32	0/3/3/3
10	MXV	B	505	-	-	0/14/14/14	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-8.25	1.65	1.77
9	B	503	MES	C8-S	-7.40	1.67	1.77
10	B	505	MXV	C20-C03	-6.74	1.39	1.49
11	F	401	ACP	PB-O3A	5.26	1.64	1.58
8	D	501	GDP	C6-N1	-4.91	1.30	1.37
5	A	501	GTP	C5-C6	-4.17	1.38	1.47
5	C	501	GTP	C5-C6	-4.10	1.39	1.47
10	B	505	MXV	C10-C08	-3.98	1.38	1.48
8	D	501	GDP	C2'-C1'	-2.90	1.49	1.53
10	B	505	MXV	O30-C22	2.81	1.41	1.37
8	B	501	GDP	C6-N1	-2.56	1.34	1.37
5	A	501	GTP	C2-N3	2.44	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MXV	C17-N16	-2.35	1.33	1.37
8	D	501	GDP	C2-N1	-2.28	1.32	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	504	MES	C5-N4-C3	5.53	121.27	108.83
11	F	401	ACP	PB-O3A-PA	-4.67	117.74	132.56
10	B	505	MXV	C31-O30-C22	-4.22	111.16	117.53
9	B	503	MES	C5-N4-C3	4.07	117.99	108.83
8	D	501	GDP	C3'-C2'-C1'	3.70	106.55	100.98
9	B	503	MES	C6-C5-N4	-3.65	104.56	110.10
5	C	501	GTP	C8-N7-C5	3.53	109.72	102.99
10	B	505	MXV	C01-N02-C03	3.44	120.47	117.99
9	B	503	MES	O3S-S-C8	3.43	111.31	105.77
10	B	505	MXV	C08-C10-C11	-3.40	119.48	123.46
5	C	501	GTP	PB-O3B-PG	-3.36	121.30	132.83
5	A	501	GTP	C2-N1-C6	-3.30	119.02	125.10
5	A	501	GTP	C5-C6-N1	3.07	119.37	113.95
5	A	501	GTP	C8-N7-C5	3.01	108.72	102.99
11	F	401	ACP	O2B-PB-O1B	-2.99	100.10	110.07
5	A	501	GTP	PA-O3A-PB	-2.98	122.58	132.83
5	C	501	GTP	O4'-C1'-C2'	-2.96	102.59	106.93
8	B	501	GDP	C8-N7-C5	2.89	108.50	102.99
5	C	501	GTP	C5-C6-N1	2.84	118.97	113.95
5	A	501	GTP	O6-C6-C5	-2.78	118.95	124.37
8	B	501	GDP	C5-C6-N1	2.75	118.81	113.95
9	B	503	MES	C7-N4-C5	2.70	118.14	111.23
8	D	501	GDP	C8-N7-C5	2.62	107.98	102.99
5	A	501	GTP	O2G-PG-O3B	2.62	113.41	104.64
5	C	501	GTP	C2-N1-C6	-2.57	120.36	125.10
9	B	503	MES	O1S-S-C8	2.52	109.95	106.92
8	D	501	GDP	C2-N1-C6	-2.51	120.47	125.10
5	C	501	GTP	N2-C2-N1	2.47	121.98	116.71
8	D	501	GDP	C5-C6-N1	2.43	118.25	113.95
9	B	504	MES	O2S-S-C8	2.40	109.81	106.92
9	B	504	MES	C6-C5-N4	-2.36	106.52	110.10
8	D	501	GDP	PA-O3A-PB	-2.34	124.78	132.83
10	B	505	MXV	O30-C22-C23	2.34	119.28	115.16
8	D	501	GDP	O3B-PB-O2B	2.24	116.21	107.64
9	B	504	MES	O3S-S-C8	2.22	109.36	105.77
11	F	401	ACP	C5-C6-N6	2.21	123.72	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	505	MXV	C10-C08-N09	2.13	126.39	123.67
5	C	501	GTP	PA-O3A-PB	-2.12	125.54	132.83
5	C	501	GTP	O3'-C3'-C4'	-2.10	104.97	111.05
5	C	501	GTP	O6-C6-C5	-2.08	120.31	124.37
8	B	501	GDP	C2-N1-C6	-2.07	121.28	125.10
8	D	501	GDP	C5'-C4'-C3'	-2.07	107.44	115.18
11	F	401	ACP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (32) 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-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O3S
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O3S
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
9	B	503	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	PG-O3B-PB-O1B
5	C	501	GTP	PG-O3B-PB-O1B
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C3'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'

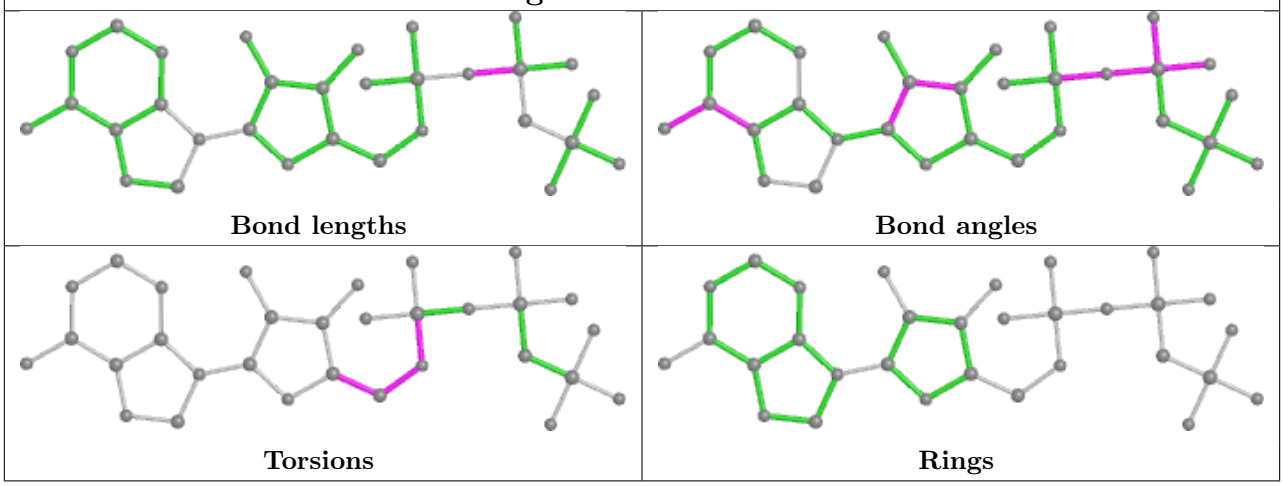
There are no ring outliers.

5 monomers are involved in 12 short contacts:

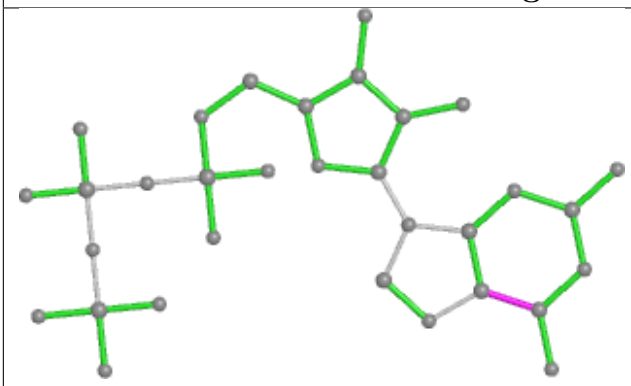
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	2	0
9	B	504	MES	2	0
8	B	501	GDP	1	0
8	D	501	GDP	5	0
10	B	505	MXV	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

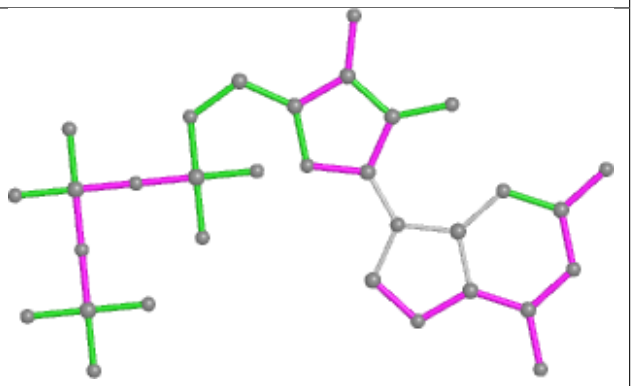
Ligand ACP F 401



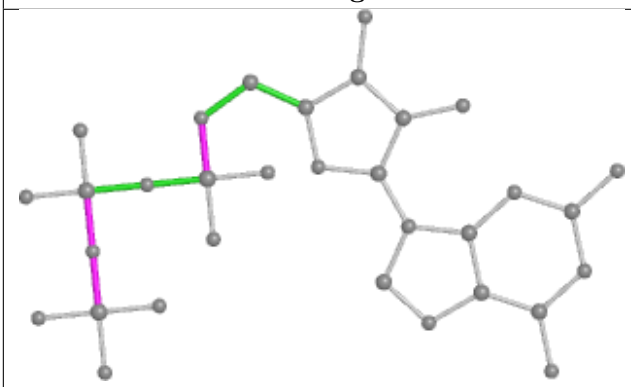
Ligand GTP C 501



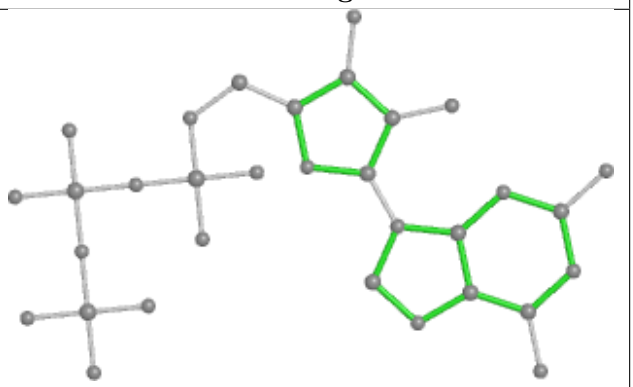
Bond lengths



Bond angles

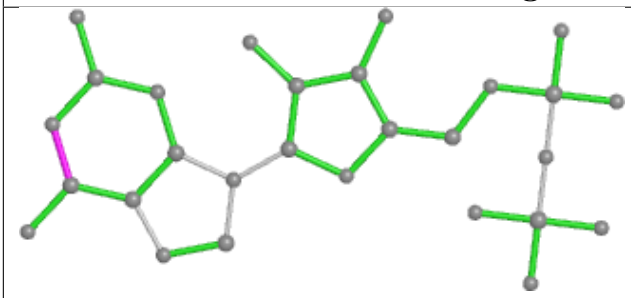


Torsions

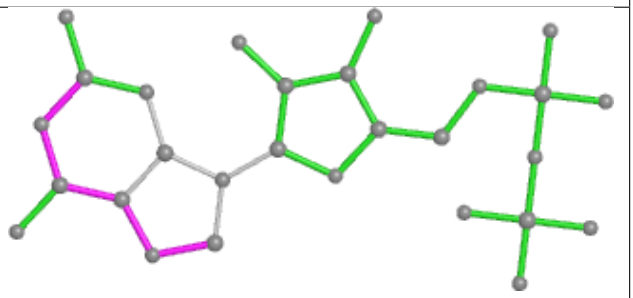


Rings

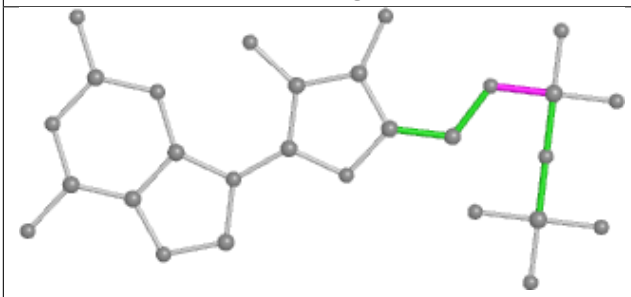
Ligand GDP B 501



Bond lengths



Bond angles



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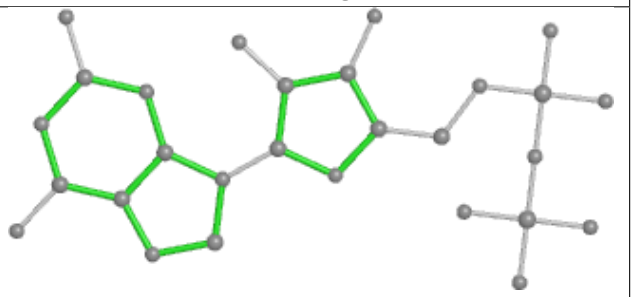
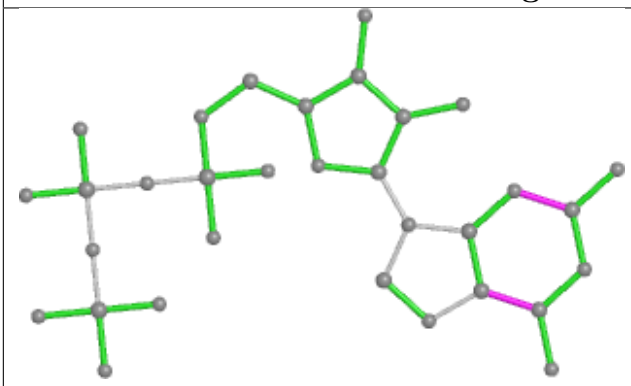


Rings

Ligand GTP A 501



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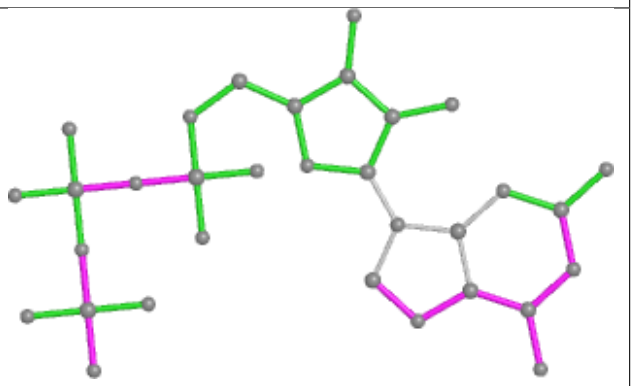
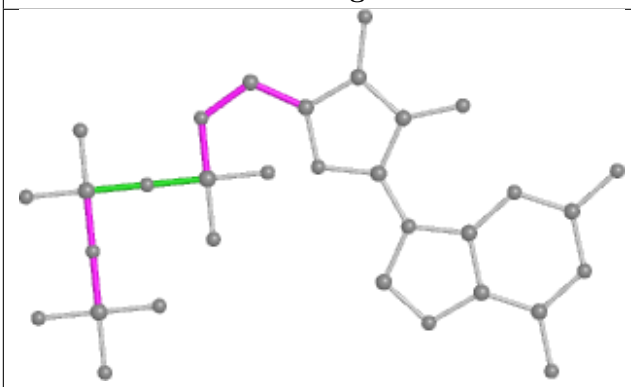
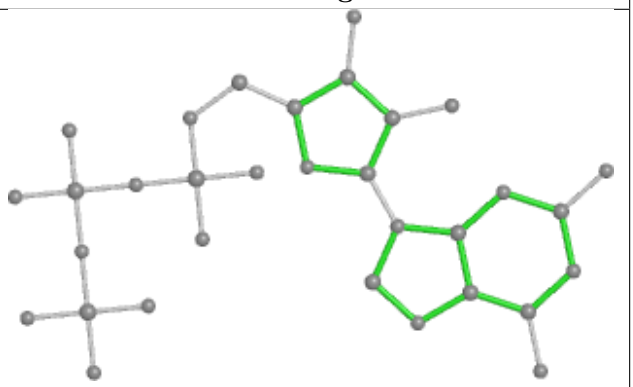


Bond angles

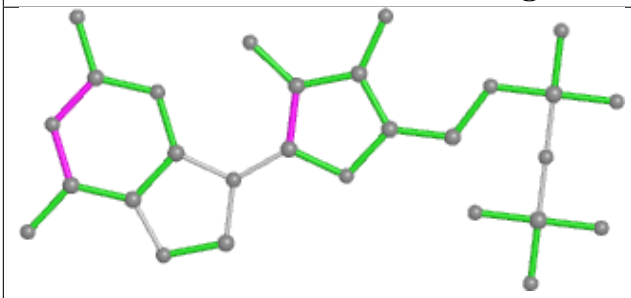


Torsions

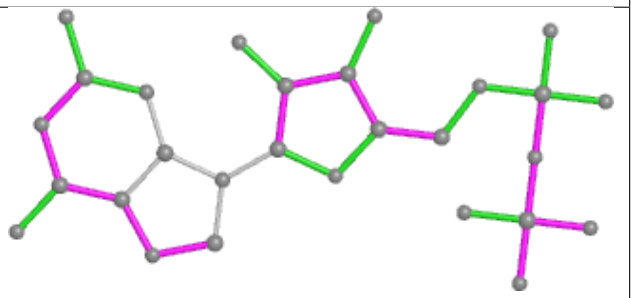


Rings

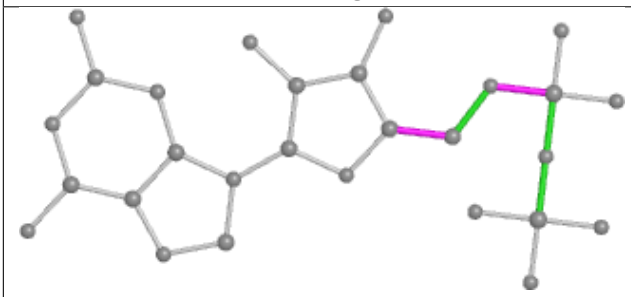
Ligand GDP D 501



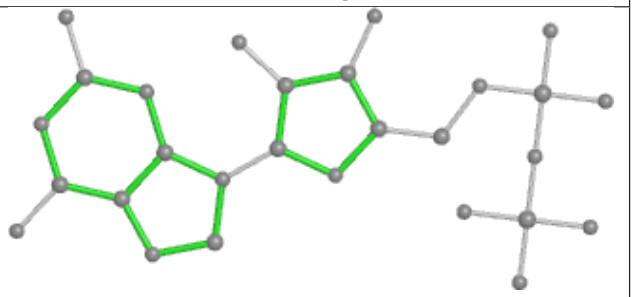
Bond lengths



Bond angles

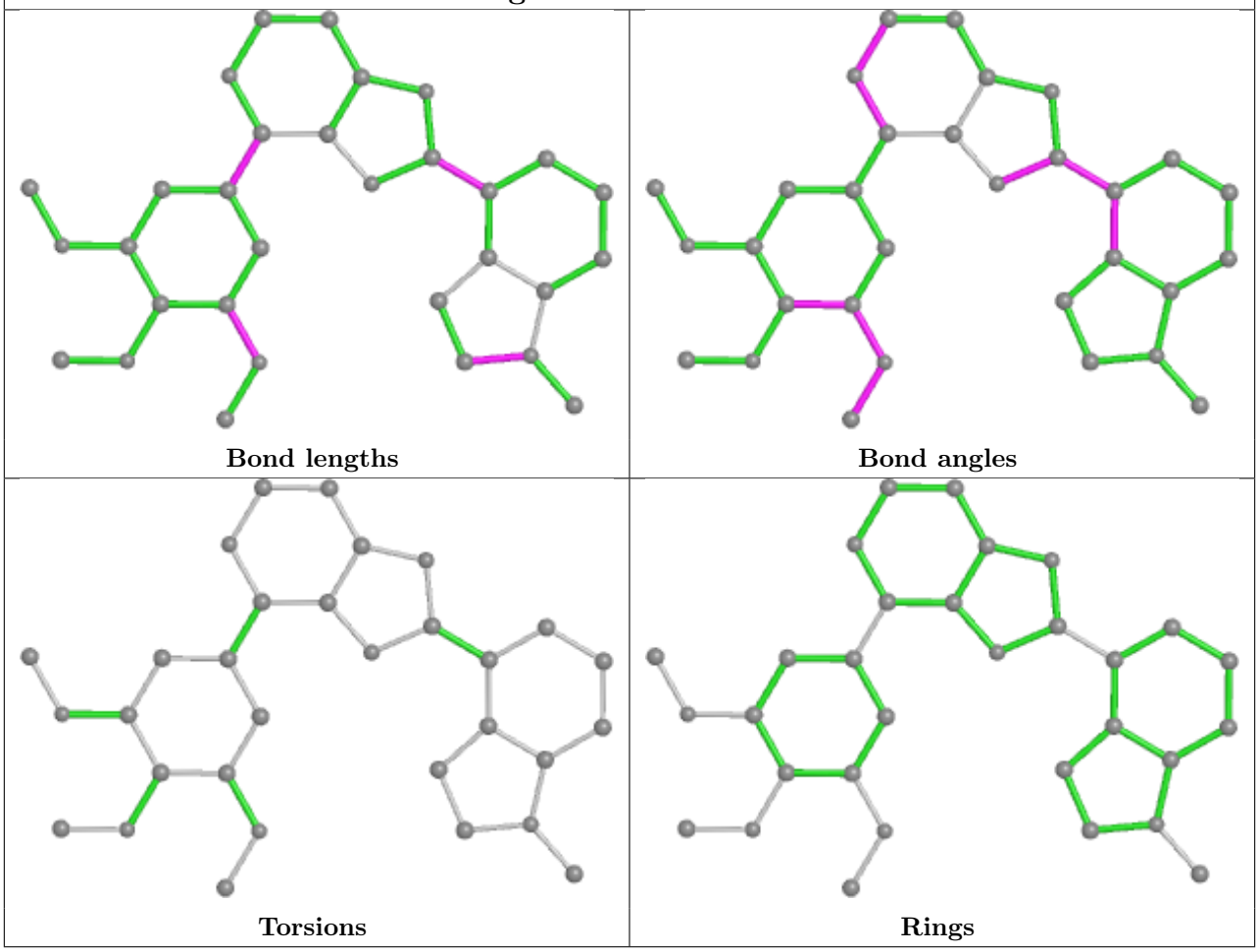


Torsions



Rings

Ligand MXV B 505



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	437/450 (97%)	-0.31	3 (0%) 87 84	30, 51, 78, 90	0
1	C	440/450 (97%)	-0.51	2 (0%) 91 88	23, 38, 64, 82	0
2	B	427/445 (95%)	-0.20	16 (3%) 41 31	25, 48, 85, 128	0
2	D	421/445 (94%)	0.16	21 (4%) 28 19	35, 74, 109, 130	0
3	E	121/143 (84%)	0.30	8 (6%) 18 11	36, 67, 108, 122	0
4	F	316/384 (82%)	0.48	42 (13%) 3 2	40, 79, 134, 150	0
All	All	2162/2317 (93%)	-0.09	92 (4%) 35 25	23, 56, 107, 150	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	225	SER	6.7
4	F	244	CYS	5.6
4	F	163	SER	4.9
2	D	98	GLY	4.8
2	D	216	LYS	4.6
4	F	167	SER	4.6
4	F	171	ASP	4.4
2	D	360	GLY	4.4
4	F	140	GLU	4.3
4	F	372	THR	4.2
4	F	142	ARG	4.1
2	B	56	GLY	3.8
4	F	143	GLU	3.8
2	B	245	GLN	3.6
4	F	141	GLY	3.6
4	F	136	ASN	3.6
4	F	139	ARG	3.6
2	B	55	THR	3.5
3	E	27	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	277	GLY	3.5
2	B	57	ASN	3.4
2	B	128	ASP	3.4
4	F	175	GLU	3.4
2	B	80	PRO	3.4
2	D	80	PRO	3.4
2	D	37	HIS	3.3
2	D	95	SER	3.3
4	F	102	PRO	3.3
4	F	243	HIS	3.3
3	E	139	LEU	3.2
2	B	39	ASP	3.1
2	D	383	GLU	3.1
4	F	259	GLY	3.0
2	B	54	ALA	3.0
2	B	244	GLY	3.0
4	F	198	LYS	2.8
4	F	168	GLU	2.8
2	D	126	SER	2.8
4	F	380	HIS	2.8
2	D	99	ASN	2.8
1	C	340	SER	2.7
2	B	278	SER	2.7
3	E	132	GLU	2.7
4	F	172	PHE	2.7
4	F	161	LEU	2.7
3	E	44	ASP	2.6
2	D	177	ASP	2.6
2	D	29	GLY	2.6
3	E	45	PRO	2.6
2	D	42	LEU	2.6
4	F	10	ASN	2.6
4	F	138	ARG	2.6
4	F	224	SER	2.6
4	F	164	SER	2.5
2	D	335	ASN	2.5
4	F	254	GLY	2.5
4	F	227	PRO	2.5
2	D	396	HIS	2.5
3	E	141	GLU	2.5
4	F	256	TYR	2.5
4	F	261	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	275	SER	2.4
3	E	46	SER	2.4
1	A	120	ASP	2.4
4	F	25	GLY	2.4
2	B	37	HIS	2.4
2	B	427	ASP	2.4
4	F	180	HIS	2.4
1	A	262	TYR	2.4
2	B	428	ALA	2.4
2	D	213	ARG	2.4
4	F	165	GLU	2.3
3	E	28	SER	2.3
2	B	276	ARG	2.3
2	D	365	ALA	2.3
4	F	257	GLU	2.3
4	F	145	ASN	2.3
2	D	38	GLY	2.3
1	C	245	ASP	2.2
4	F	90	SER	2.2
4	F	162	ILE	2.2
4	F	88	SER	2.2
4	F	379	HIS	2.2
4	F	258	GLU	2.1
1	A	345	ASP	2.1
4	F	253	TYR	2.1
2	D	44	LEU	2.1
2	D	406	MET	2.1
4	F	240	LEU	2.1
2	D	93	GLY	2.1
2	D	127	CYS	2.1
4	F	252	ASN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

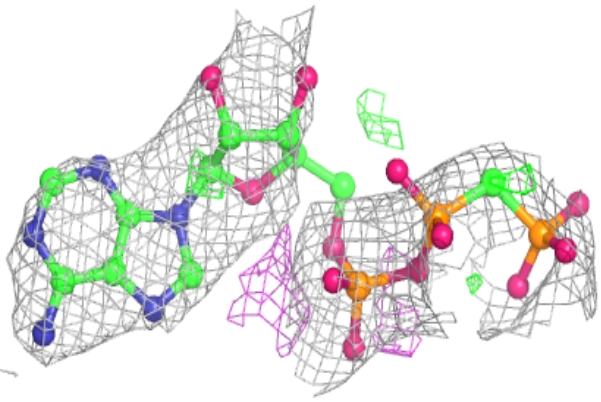
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

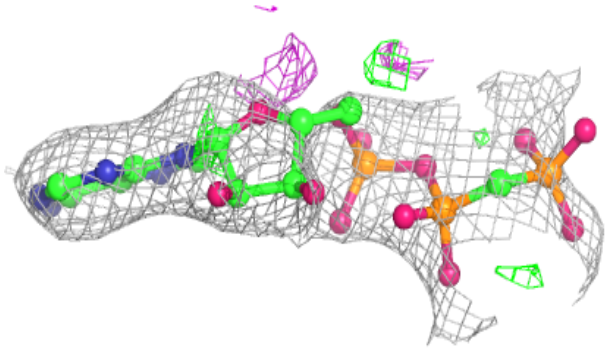
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	ACP	F	401	31/31	0.78	0.29	93,117,154,164	0
8	GDP	D	501	28/28	0.88	0.20	65,77,89,96	0
9	MES	B	504	12/12	0.90	0.27	74,78,87,92	0
7	CA	C	503	1/1	0.93	0.06	57,57,57,57	0
10	MXV	B	505	31/31	0.93	0.15	41,51,57,61	0
6	MG	B	502	1/1	0.93	0.26	40,40,40,40	0
9	MES	B	503	12/12	0.95	0.16	47,59,80,84	0
6	MG	C	502	1/1	0.95	0.31	37,37,37,37	0
5	GTP	C	501	32/32	0.98	0.12	29,34,37,39	0
6	MG	A	502	1/1	0.98	0.40	39,39,39,39	0
8	GDP	B	501	28/28	0.98	0.13	22,37,46,68	0
5	GTP	A	501	32/32	0.98	0.11	34,40,45,45	0
7	CA	A	503	1/1	0.99	0.07	82,82,82,82	0

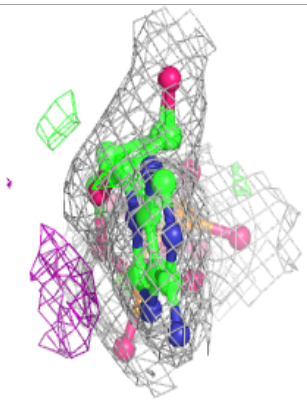
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

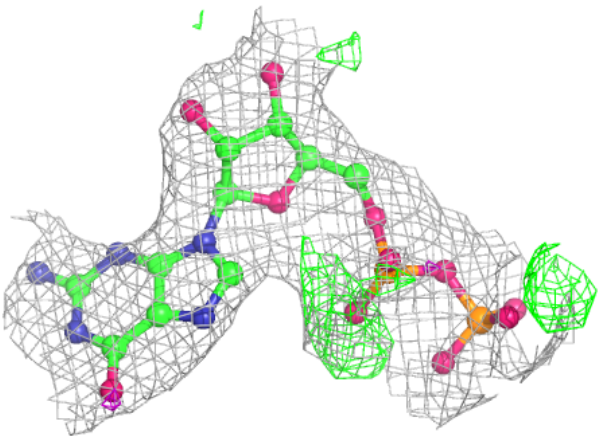


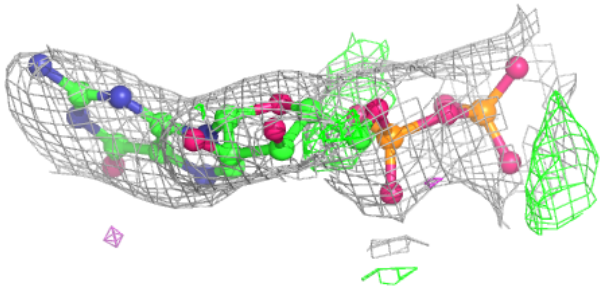


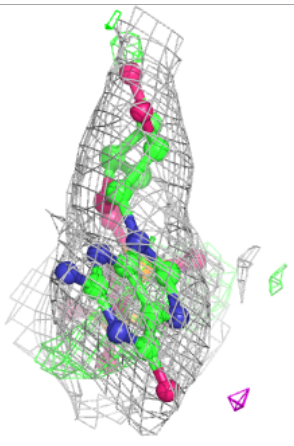


Electron density around GDP D 501:

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

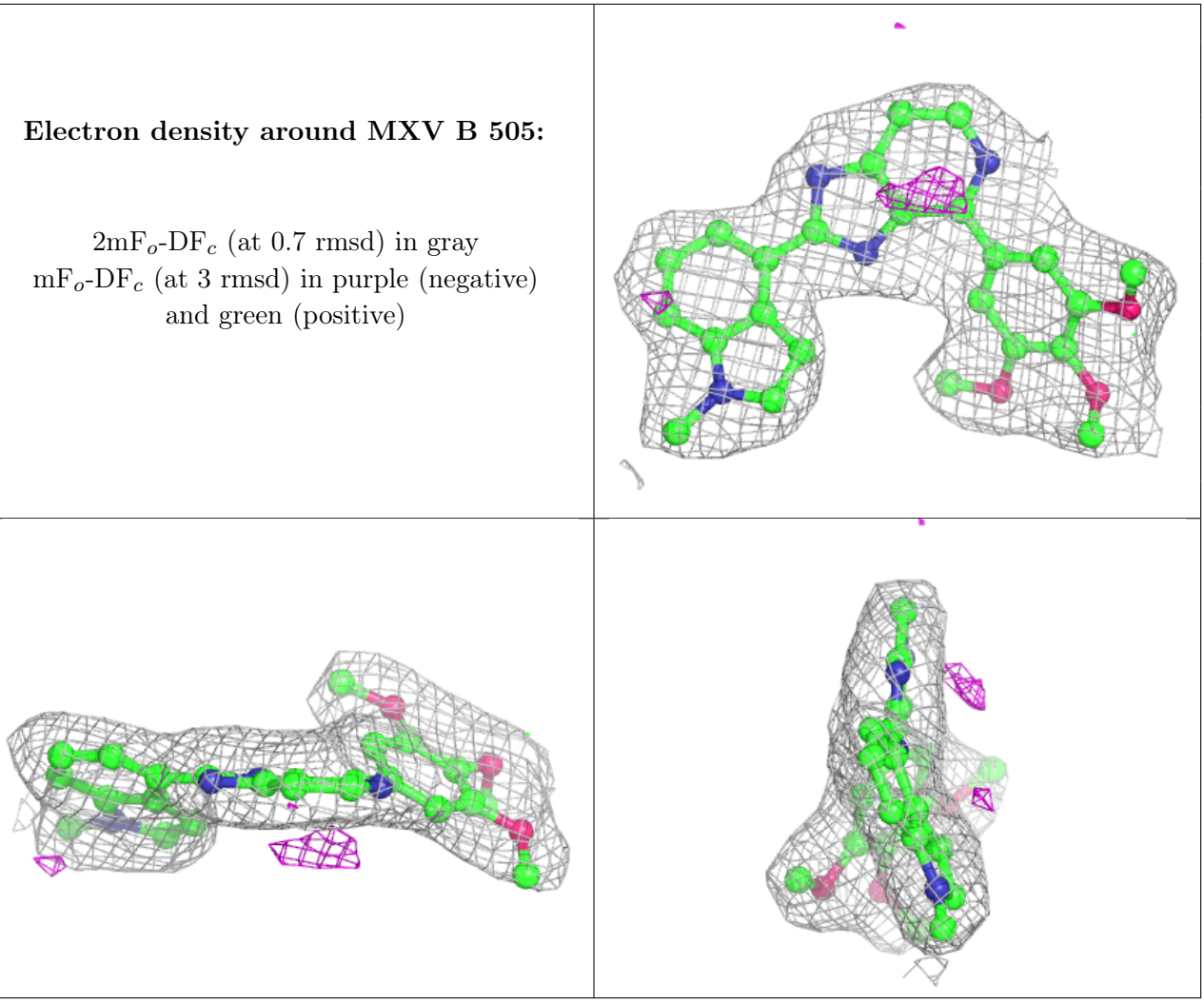






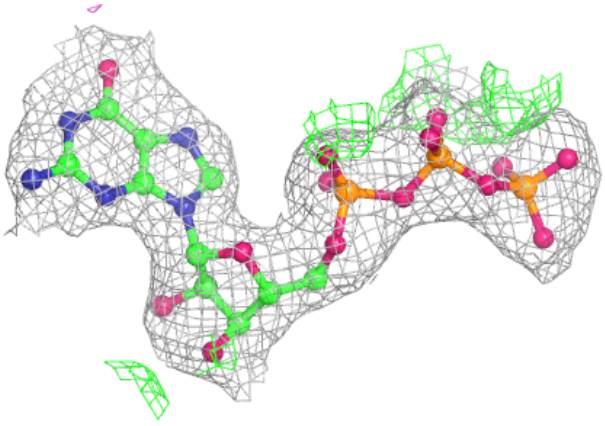
Electron density around MXV B 505:

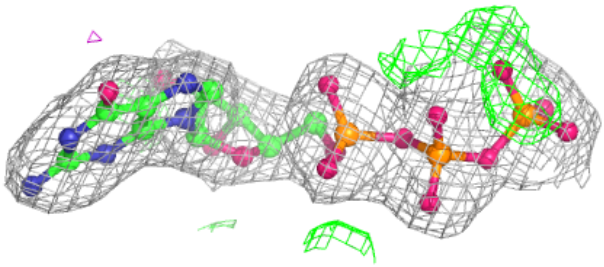
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

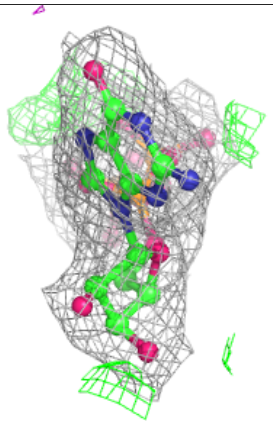


Electron density around GTP C 501:

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

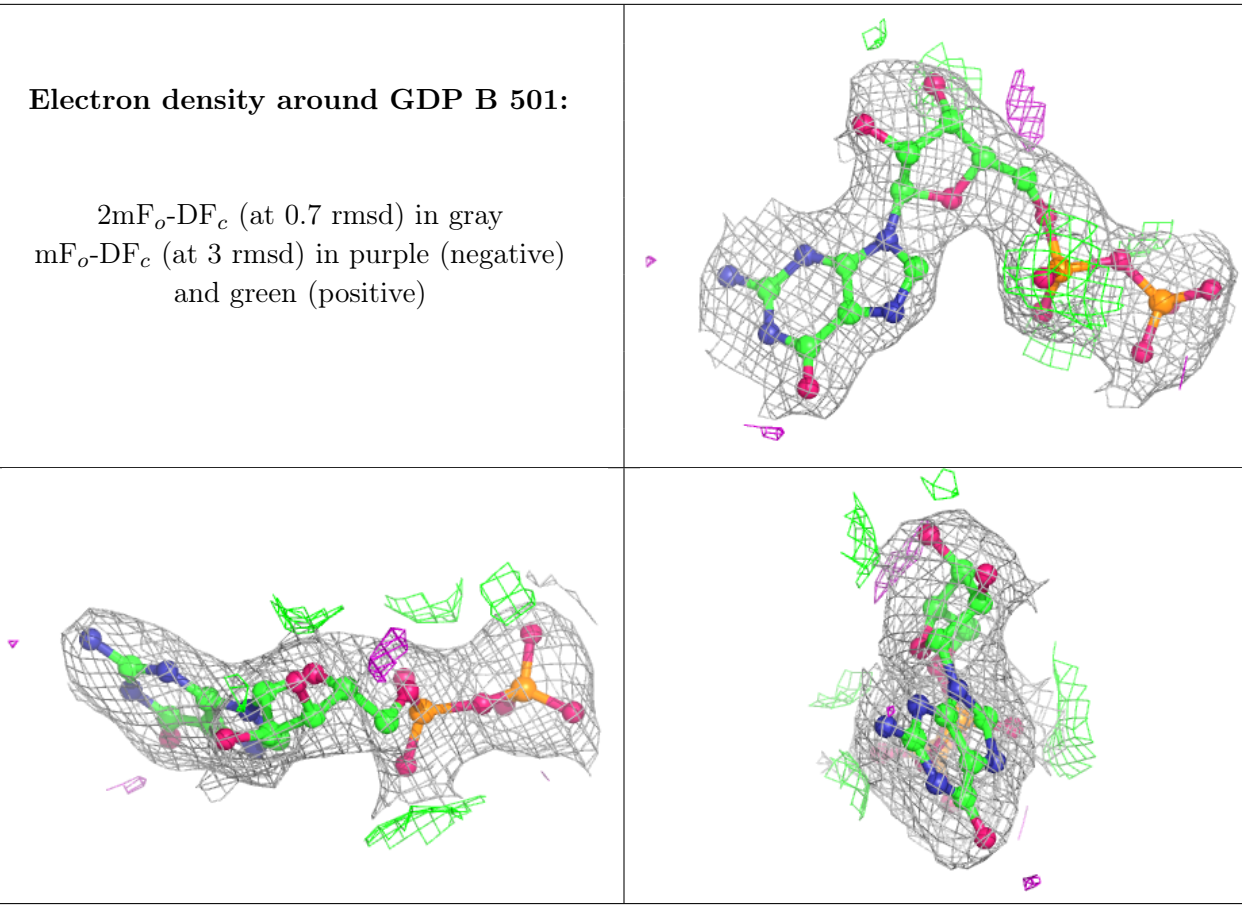






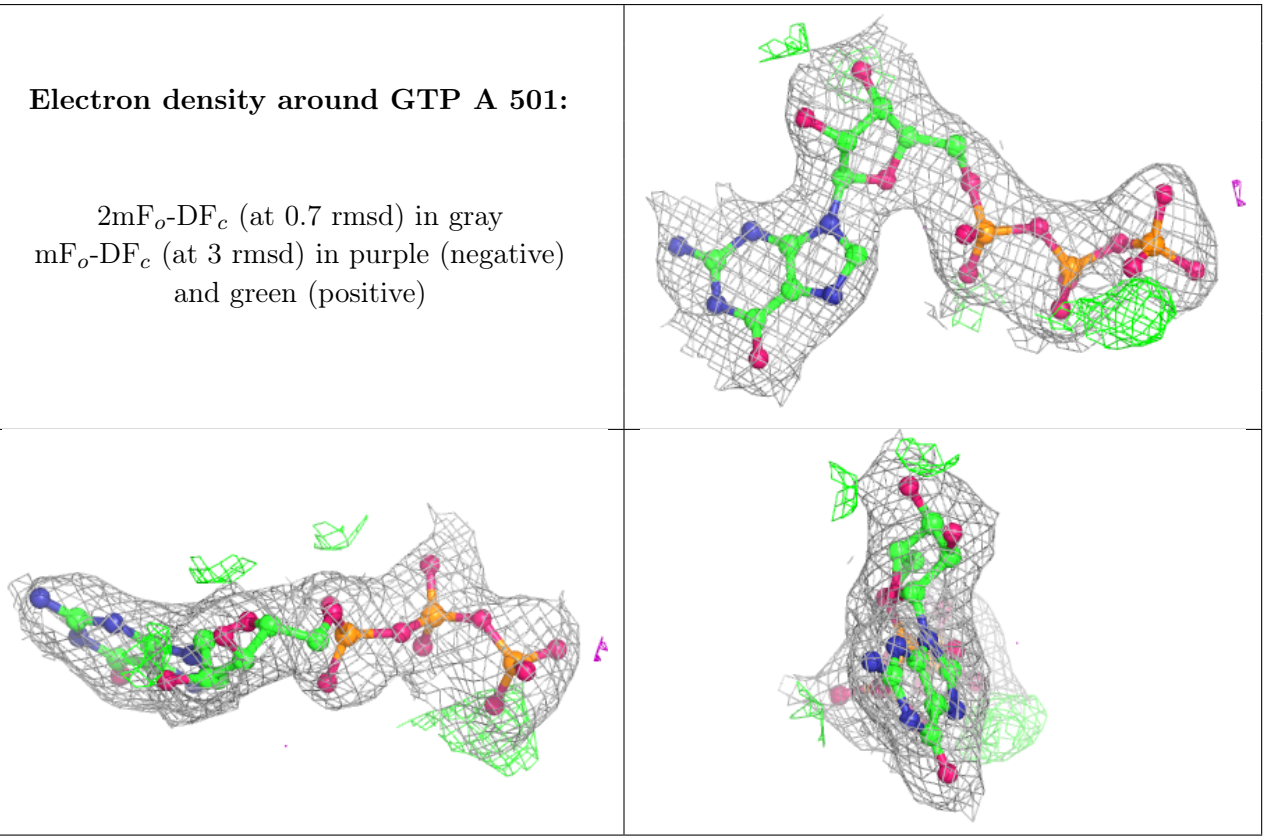
Electron density around GDP B 501:

$2mF_o$-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.