



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:10 PM JST

PDB ID : 7DBB  
Title : SSE in complex with tubulin  
Authors : Wu, C.Y.; Wang, Y.X.  
Deposited on : 2020-10-19  
Resolution : 2.81 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

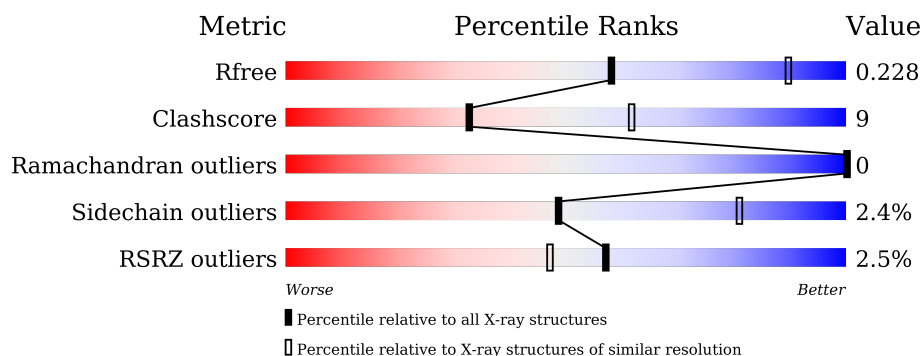
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div style="width: 81%;"></div> <div style="width: 16%;"></div> <div style="width: 3%;"></div> </div> <div>81% 16% .</div>
1	C	451	<div> <div style="width: 82%;"></div> <div style="width: 15%;"></div> <div style="width: 3%;"></div> </div> <div>82% 15% ..</div>
2	B	445	<div> <div style="width: 74%;"></div> <div style="width: 20%;"></div> <div style="width: 6%;"></div> </div> <div>74% 20% . .</div>
2	D	445	<div> <div style="width: 73%;"></div> <div style="width: 21%;"></div> <div style="width: 6%;"></div> </div> <div>73% 21% 5%</div>
3	E	143	<div> <div style="width: 78%;"></div> <div style="width: 7%;"></div> <div style="width: 14%;"></div> </div> <div>78% 7% . 14%</div>
4	F	384	<div> <div style="width: 68%;"></div> <div style="width: 22%;"></div> <div style="width: 10%;"></div> </div> <div>68% 22% . 8%</div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	5	0
			3447	2182	586	655	24			
1	C	440	Total	C	N	O	S	0	10	0
			3476	2201	586	663	26			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	6	0
			3381	2126	577	651	27			
2	D	421	Total	C	N	O	S	0	3	0
			3310	2080	561	644	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	3	0
			1011	622	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	3	0
			2894	1857	495	527	15			

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		
5	D	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	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		

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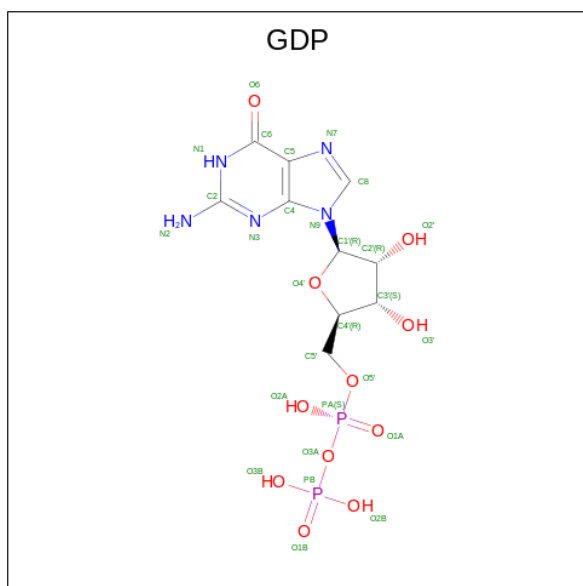
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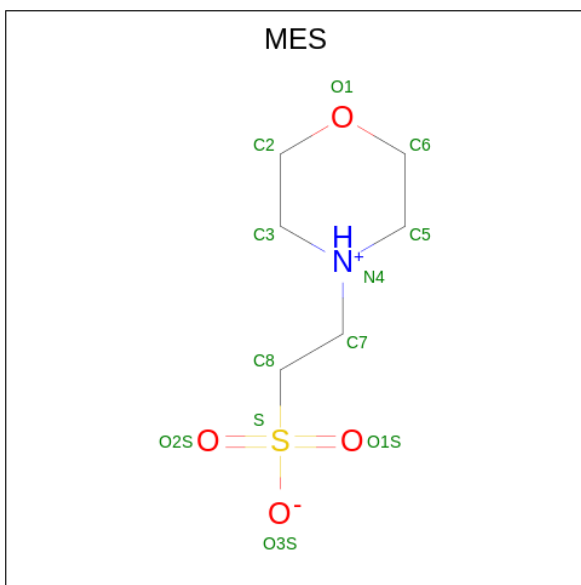
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

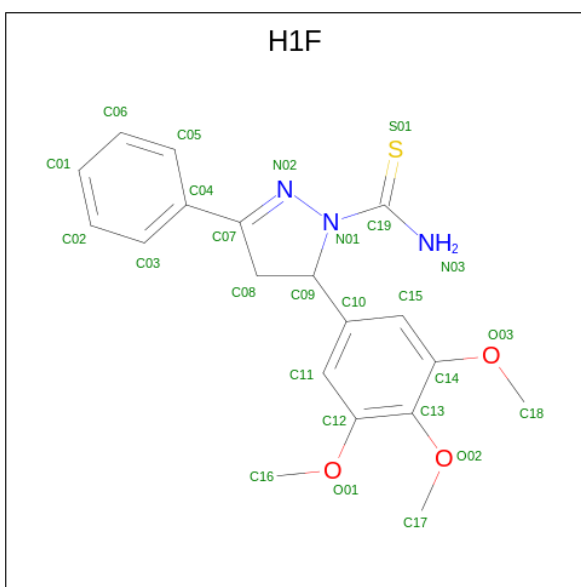
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





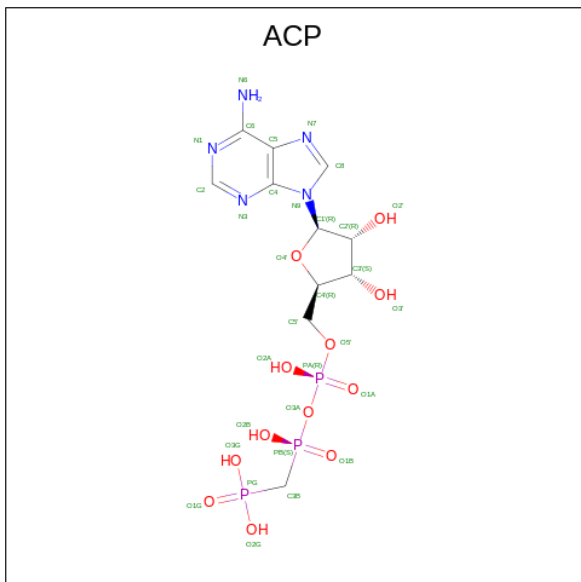
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 5-phenyl-3-(3,4,5-trimethoxyphenyl)-3,4-dihydropyrazole-2-carbothioamide (three-letter code: H1F) (formula: C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			26	19	3	3	1		

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

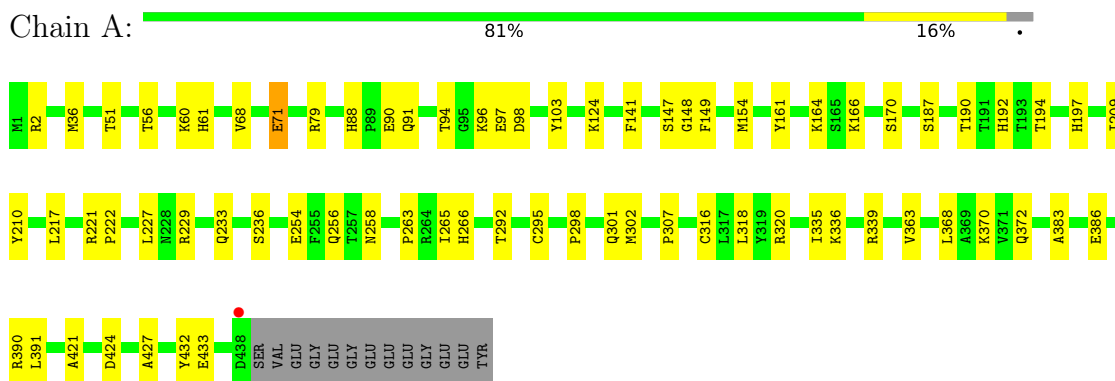


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

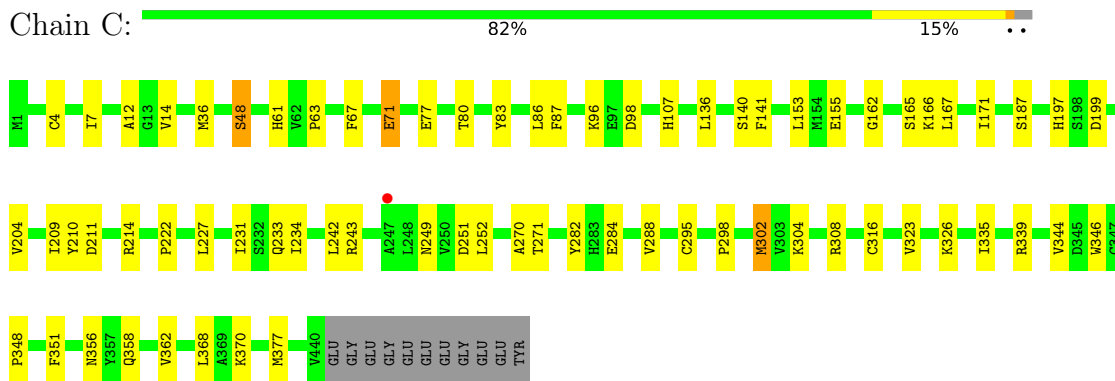
### 3 Residue-property plots

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.

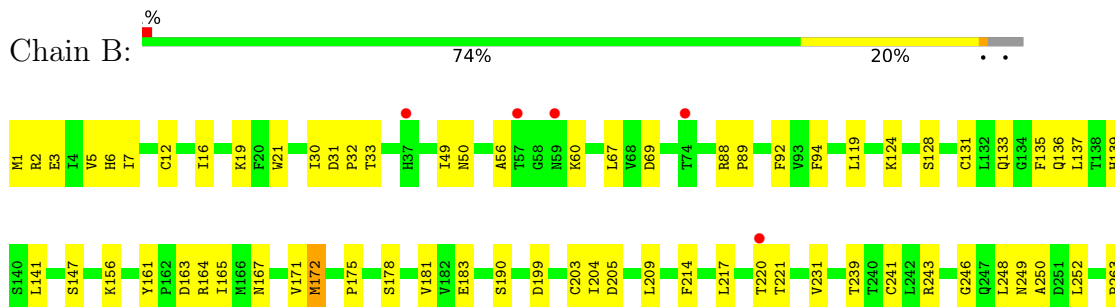
- Molecule 1: Tubulin alpha-1B chain



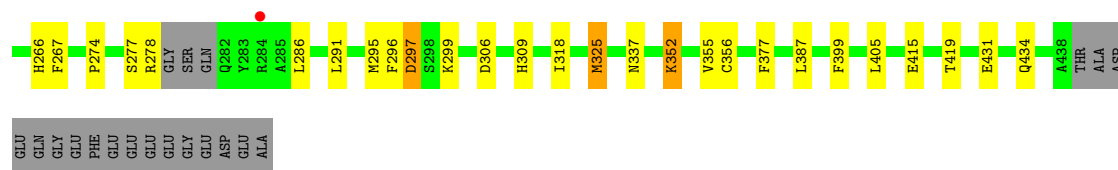
- Molecule 1: Tubulin alpha-1B chain



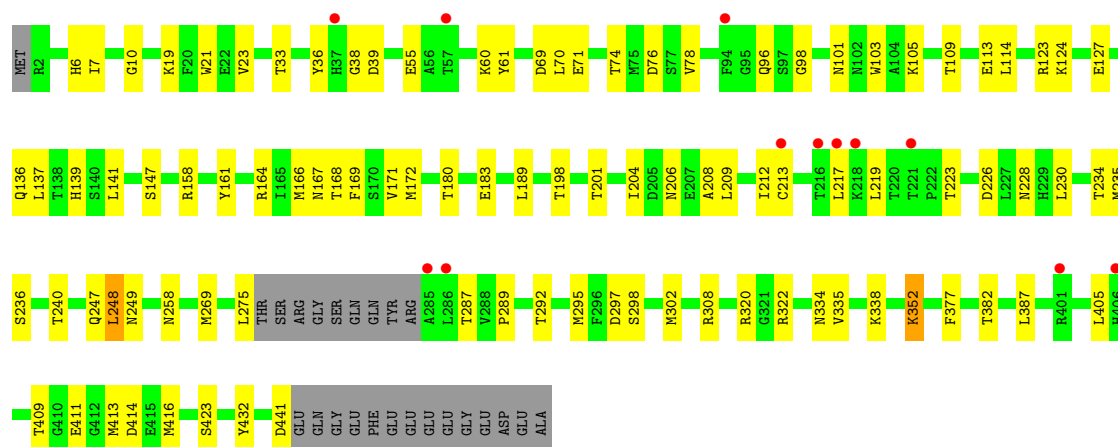
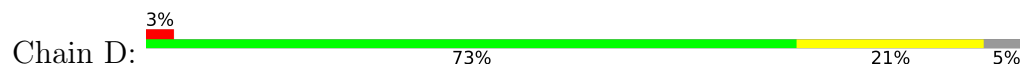
- Molecule 2: Tubulin beta chain



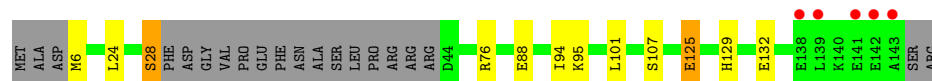
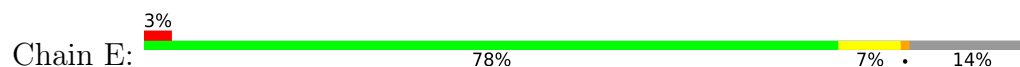




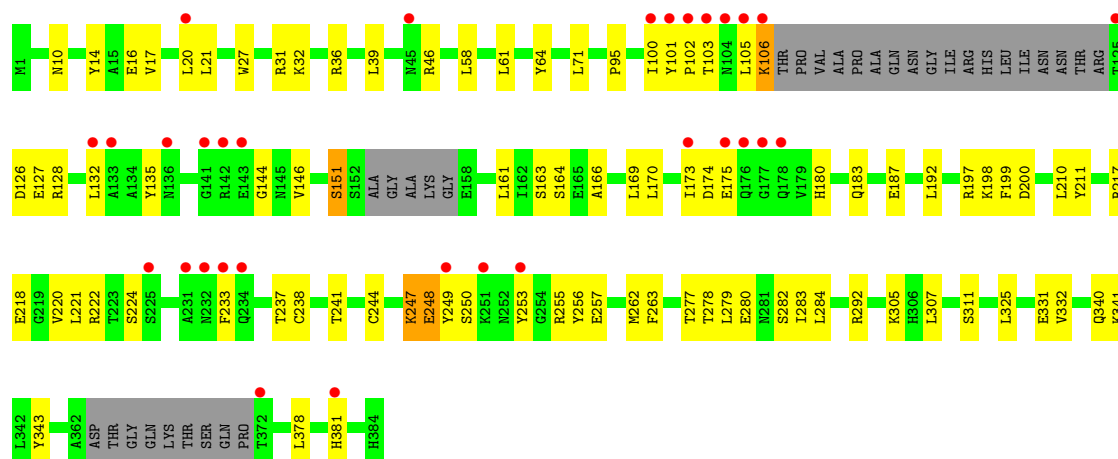
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.00Å 157.57Å 181.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.81 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.88-2.81) 99.3 (29.88-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.172 , 0.230 0.173 , 0.228	Depositor DCC
$R_{free}$ test set	1994 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MES, GTP, GDP, CA, ACP, H1F, MG

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	0.54	0/3540	0.68	0/4805
1	C	0.60	0/3581	0.69	0/4862
2	B	0.53	0/3470	0.67	1/4698 (0.0%)
2	D	0.46	0/3394	0.62	0/4601
3	E	0.55	0/1029	0.65	0/1372
4	F	0.43	0/2971	0.63	0/4017
All	All	0.52	0/17985	0.66	1/24355 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	MET	CG-SD-CE	5.52	109.03	100.20

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	3447	0	3370	50	0
1	C	3476	0	3400	54	0
2	B	3381	0	3271	67	0
2	D	3310	0	3178	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1011	0	1000	10	0
4	F	2894	0	2847	61	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	11	2	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	10	1	0
9	B	24	0	26	3	0
10	B	26	0	0	8	0
11	F	31	0	13	2	0
All	All	17733	0	17150	302	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 9.

All (302) 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:71:GLU:OE2	2:D:98:GLY:HA3	1.38	1.23
2:B:248:LEU:HD11	10:B:507:H1F:N03	1.62	1.11
2:D:71:GLU:CD	2:D:98:GLY:HA3	1.77	1.03
3:E:125:GLU:O	3:E:125:GLU:OE1	1.81	0.97
1:A:141:PHE:HB3	1:A:187:SER:HB3	1.50	0.90
1:C:298:PRO:HG2	1:C:308:ARG:NH2	1.86	0.90
2:D:287:THR:HB	2:D:289:PRO:HD2	1.62	0.81
4:F:102:PRO:HA	4:F:174:ASP:OD1	1.80	0.80
4:F:31:ARG:HH21	4:F:32:LYS:HG3	1.45	0.80
1:A:79:ARG:HH22	1:A:94:THR:HG23	1.47	0.79
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.65	0.78
2:D:71:GLU:OE2	2:D:98:GLY:CA	2.29	0.76
2:B:199:ASP:OD1	9:B:504:MES:H32	1.85	0.75
2:D:101:ASN:HD22	2:D:180:THR:HG21	1.50	0.75
2:B:250:ALA:CB	10:B:507:H1F:S01	2.76	0.74
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.68	0.73
1:C:298:PRO:CD	1:C:308:ARG:HH21	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.70	0.73
2:D:69:ASP:OD2	2:D:74:THR:HG21	1.89	0.73
4:F:237:THR:HG21	4:F:250:SER:HB2	1.71	0.71
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.31	0.70
2:B:325:MET:HG3	2:B:355:VAL:HG21	1.73	0.70
2:D:96:GLN:N	2:D:96:GLN:OE1	2.24	0.70
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.75	0.69
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.23	0.69
1:C:298:PRO:HD2	1:C:308:ARG:HH21	1.58	0.68
2:D:168:THR:OG1	2:D:201:THR:HG22	1.94	0.67
4:F:16:GLU:O	4:F:20:LEU:HD12	1.94	0.67
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.77	0.67
2:B:250:ALA:HB1	10:B:507:H1F:S01	2.35	0.66
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.60	0.66
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.35	0.66
2:D:71:GLU:CG	2:D:98:GLY:HA3	2.24	0.66
2:D:71:GLU:HG2	2:D:98:GLY:CA	2.25	0.66
1:A:263:PRO:O	1:A:266:HIS:HD2	1.79	0.66
1:C:298:PRO:CG	1:C:308:ARG:NH2	2.58	0.66
2:D:249:ASN:HD21	2:D:352:LYS:HZ1	1.43	0.64
3:E:129:HIS:HA	3:E:132:GLU:OE2	1.98	0.64
2:D:136:GLN:HA	2:D:167:ASN:O	1.98	0.64
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.80	0.63
2:D:71:GLU:HG2	2:D:98:GLY:HA2	1.79	0.63
2:B:1:MET:N	2:B:131:CYS:SG	2.69	0.63
2:B:239:THR:O	2:B:243:ARG:HG3	1.98	0.63
2:B:217:LEU:HD13	2:B:277:SER:HB3	1.80	0.63
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.80	0.62
2:B:141:LEU:HA	2:B:147:SER:HB3	1.81	0.62
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.82	0.62
2:B:2:ARG:HD2	2:B:3:GLU:CD	2.20	0.62
2:B:248:LEU:HD23	10:B:507:H1F:C16	2.30	0.61
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.82	0.61
2:B:248:LEU:CD2	10:B:507:H1F:C16	2.79	0.61
2:B:221:THR:HG21	1:C:326:LYS:HA	1.83	0.60
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.30	0.60
1:A:154:MET:HG3	1:A:194:THR:HG23	1.82	0.60
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.34	0.60
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.84	0.60
1:A:229:ARG:HD3	1:A:363:VAL:HG21	1.83	0.60
2:D:74:THR:O	2:D:78:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:103:THR:H	4:F:174:ASP:HB3	1.66	0.60
2:B:88:ARG:HH22	2:B:124:LYS:HE2	1.67	0.60
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.83	0.59
4:F:146:VAL:HG21	4:F:233:PHE:CE2	2.37	0.59
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.67	0.58
3:E:88:GLU:OE2	3:E:88:GLU:HA	2.03	0.58
1:A:88:HIS:HB3	1:A:91:GLN:NE2	2.18	0.58
1:C:288:VAL:HG22	1:C:323:VAL:HG22	1.86	0.58
4:F:166:ALA:O	4:F:170:LEU:HD12	2.03	0.58
4:F:255:ARG:HD3	4:F:256:TYR:CZ	2.38	0.58
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.43	0.58
2:B:250:ALA:HB2	10:B:507:H1F:S01	2.44	0.57
2:B:50:ASN:H	2:B:50:ASN:ND2	2.02	0.57
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.86	0.57
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.87	0.57
2:B:136:GLN:HA	2:B:167:ASN:O	2.05	0.57
1:C:4[B]:CYS:SG	1:C:242:LEU:HD23	2.44	0.57
1:C:298:PRO:HG2	1:C:308:ARG:CZ	2.33	0.57
4:F:126:ASP:OD1	4:F:127:GLU:N	2.38	0.57
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.37	0.57
1:A:433:GLU:OE2	4:F:46:ARG:NH2	2.36	0.56
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.41	0.56
4:F:166:ALA:O	4:F:169:LEU:HB2	2.05	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.56
4:F:31:ARG:NE	4:F:32:LYS:H	2.04	0.56
2:D:161:TYR:HB3	2:D:164:ARG:HG3	1.88	0.55
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.55
1:A:2:ARG:O	1:A:51:THR:HG23	2.06	0.55
1:A:79:ARG:NH2	1:A:94:THR:HG23	2.19	0.55
1:A:292:THR:O	1:A:295:CYS:HB2	2.07	0.55
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.42	0.55
4:F:277:THR:HG22	4:F:278:THR:H	1.72	0.54
2:B:337:ASN:OD1	4:F:36:ARG:NH1	2.39	0.54
2:D:123:ARG:O	2:D:127:GLU:HG2	2.08	0.54
2:D:206:ASN:HA	2:D:209:LEU:HD12	1.88	0.54
2:D:249:ASN:HD21	2:D:352:LYS:NZ	2.06	0.54
1:C:362:VAL:HG22	1:C:370:LYS:HD3	1.91	0.53
2:D:297:ASP:HA	2:D:308:ARG:NH2	2.24	0.53
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.40	0.53
1:C:298:PRO:CD	1:C:308:ARG:NH2	2.70	0.53
2:D:230:LEU:O	2:D:234:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.43	0.53
1:C:204:VAL:HG22	1:C:302[B]:MET:HE3	1.90	0.53
2:D:168:THR:OG1	2:D:201:THR:CG2	2.56	0.53
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.39	0.53
4:F:151:SER:HB2	4:F:180:HIS:NE2	2.24	0.53
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.90	0.53
2:D:297:ASP:HA	2:D:308:ARG:HH22	1.73	0.52
2:D:171:VAL:HA	2:D:204:ILE:O	2.09	0.52
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.91	0.52
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.91	0.52
2:D:10:GLY:HA3	5:D:602:GTP:O1B	2.09	0.52
4:F:247:LYS:HD3	4:F:253:TYR:CZ	2.45	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
3:E:125:GLU:O	3:E:125:GLU:CD	2.46	0.52
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.28	0.52
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.44	0.52
1:A:56:THR:OG1	1:A:60:LYS:HB3	2.10	0.51
1:A:166:LYS:HE2	1:A:197:HIS:O	2.10	0.51
10:B:507:H1F:C11	10:B:507:H1F:N02	2.73	0.51
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.51	0.51
2:B:30:ILE:HD11	2:B:49:ILE:CD1	2.41	0.51
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.20	0.51
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.46	0.50
1:A:147:SER:HB2	1:A:190:THR:HB	1.94	0.50
1:C:282:TYR:O	1:C:284:GLU:OE2	2.28	0.50
2:D:212:ILE:HG21	2:D:275:LEU:HD13	1.94	0.50
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.47	0.49
4:F:14:TYR:HA	4:F:17:VAL:HB	1.93	0.49
4:F:71:LEU:HG	4:F:332:VAL:HG21	1.93	0.49
4:F:247:LYS:O	4:F:247:LYS:HG3	2.11	0.49
1:A:164:LYS:N	1:A:164:LYS:HD3	2.27	0.49
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.94	0.49
4:F:21:LEU:HD22	4:F:27:TRP:CG	2.47	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.49
2:D:234:THR:HG21	2:D:302:MET:HG3	1.95	0.49
4:F:135:TYR:CE1	4:F:166:ALA:HB2	2.48	0.49
2:B:431[B]:GLU:O	2:B:434:GLN:HB3	2.13	0.49
2:B:156:LYS:HD3	3:E:76:ARG:CZ	2.42	0.49
4:F:101:TYR:N	4:F:126:ASP:OD2	2.29	0.49
2:B:147:SER:HB2	2:B:190:SER:OG	2.13	0.48
3:E:129:HIS:HA	3:E:132:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.95	0.48
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.94	0.48
1:A:88:HIS:HD2	1:A:90:GLU:HB2	1.77	0.48
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.95	0.48
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.96	0.48
2:B:246:GLY:N	2:B:249:ASN:OD1	2.37	0.48
4:F:166:ALA:HA	4:F:169:LEU:HD12	1.96	0.48
4:F:210:LEU:O	4:F:305:LYS:HE3	2.14	0.48
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.48	0.48
2:D:103:TRP:HD1	2:D:147:SER:HB2	1.77	0.48
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.49	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.49	0.47
2:D:33:THR:O	2:D:60:LYS:HD3	2.14	0.47
2:D:105:LYS:HE3	2:D:411:GLU:OE2	2.14	0.47
2:D:141:LEU:HA	2:D:147:SER:HB3	1.94	0.47
2:D:334:ASN:OD1	2:D:338:LYS:HE2	2.14	0.47
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.49	0.47
2:D:109:THR:O	2:D:113:GLU:HG3	2.14	0.47
1:A:236:SER:OG	1:A:320:ARG:NH2	2.45	0.47
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.47
2:B:1:MET:SD	2:B:133:GLN:HB3	2.55	0.47
2:B:306:ASP:OD2	2:B:309:HIS:NE2	2.48	0.47
1:A:88:HIS:CD2	1:A:90:GLU:H	2.33	0.47
2:B:296:PHE:O	9:B:505:MES:H81	2.15	0.47
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.55	0.47
2:B:297:ASP:OD2	2:B:299:LYS:HD3	2.15	0.47
1:A:263:PRO:O	1:A:266:HIS:CD2	2.64	0.47
1:C:298:PRO:HD2	1:C:308:ARG:NH2	2.28	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.46
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.97	0.46
1:C:107:HIS:HE1	1:C:155:GLU:OE1	1.98	0.46
11:F:401:ACP:O1A	11:F:401:ACP:H3B2	2.15	0.46
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.15	0.46
4:F:173:ILE:HG22	4:F:174:ASP:OD1	2.15	0.46
4:F:217:ARG:HG3	4:F:218:GLU:N	2.30	0.46
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.97	0.46
2:D:298:SER:OG	2:D:308:ARG:NH1	2.48	0.46
2:B:161:TYR:HB3	2:B:164[B]:ARG:HG2	1.98	0.46
2:B:205:ASP:O	2:B:209:LEU:HG	2.16	0.46
2:B:241:CYS:SG	2:B:318:ILE:HD13	2.55	0.46
2:D:101:ASN:ND2	2:D:180:THR:HG21	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:409:THR:HG22	2:D:413:MET:O	2.16	0.46
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.30	0.46
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.98	0.46
4:F:16:GLU:HG3	4:F:20:LEU:HD11	1.97	0.46
4:F:198:LYS:HG2	4:F:199:PHE:H	1.81	0.46
4:F:263:PHE:CZ	4:F:341:LYS:HD3	2.51	0.46
1:C:242:LEU:HD11	1:C:252:LEU:CB	2.46	0.46
4:F:105:LEU:O	4:F:106:LYS:HB2	2.15	0.46
1:C:166:LYS:HE2	1:C:197:HIS:O	2.16	0.45
4:F:331:GLU:OE2	11:F:401:ACP:H3B2	2.16	0.45
2:B:405:LEU:CD1	2:B:415:GLU:HG2	2.47	0.45
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.81	0.45
2:D:180:THR:O	2:D:183:GLU:HG3	2.17	0.45
2:B:5:VAL:O	2:B:135:PHE:HA	2.17	0.45
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.81	0.45
2:D:7:ILE:O	2:D:137:LEU:HD12	2.16	0.45
4:F:255:ARG:HG2	4:F:255:ARG:HH11	1.81	0.45
2:D:223:THR:HG23	2:D:226:ASP:H	1.82	0.45
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.45
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.99	0.45
2:D:71:GLU:CG	2:D:98:GLY:CA	2.88	0.44
2:D:208:ALA:O	2:D:212:ILE:HG13	2.17	0.44
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.52	0.44
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.44
4:F:292:ARG:HG3	4:F:378:LEU:HB3	1.98	0.44
2:B:119:LEU:HD11	2:B:156:LYS:CB	2.46	0.44
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.44
1:C:358[B]:GLN:CD	1:C:358[B]:GLN:H	2.21	0.44
4:F:146:VAL:HG21	4:F:233:PHE:HE2	1.83	0.44
4:F:151:SER:HB2	4:F:180:HIS:CD2	2.53	0.44
4:F:255:ARG:HD3	4:F:256:TYR:CE2	2.53	0.44
1:A:209:ILE:HD11	1:A:302:MET:SD	2.58	0.44
3:E:28:SER:O	3:E:28:SER:OG	2.27	0.44
4:F:248:GLU:HB3	4:F:249:TYR:CD1	2.53	0.44
2:D:166:MET:HG3	2:D:198:THR:HG22	1.99	0.44
4:F:198:LYS:HG2	4:F:199:PHE:N	2.33	0.44
2:B:175:PRO:HA	2:B:178:SER:HB3	2.00	0.43
2:D:19:LYS:O	2:D:23:VAL:HG23	2.18	0.43
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.54	0.43
1:A:68:VAL:HG11	1:A:149:PHE:HE2	1.84	0.43
1:C:271:THR:HG21	1:C:295:CYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ASP:O	2:B:164[A]:ARG:NE	2.51	0.43
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.83	0.43
1:A:97:GLU:HB3	2:B:131:CYS:SG	2.58	0.43
4:F:10:ASN:OD1	4:F:10:ASN:N	2.52	0.43
1:C:288:VAL:CG2	1:C:323:VAL:HG22	2.47	0.43
1:C:210:TYR:HE1	1:C:214:ARG:HE	1.66	0.43
1:A:88:HIS:NE2	1:A:90:GLU:HG3	2.33	0.43
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.01	0.43
1:C:63:PRO:HD3	1:C:86:LEU:HG	1.99	0.43
1:A:370:LYS:NZ	1:A:372:GLN:OE1	2.51	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.42
2:B:199:ASP:OD2	9:B:504:MES:H52	2.19	0.42
1:C:242:LEU:HD11	1:C:252:LEU:HB3	2.01	0.42
2:D:228:ASN:OD1	5:D:602:GTP:N1	2.36	0.42
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.77	0.42
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.49	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.42
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.54	0.42
1:C:141:PHE:HB3	1:C:187:SER:OG	2.18	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.42
2:B:306:ASP:OD2	2:B:309:HIS:CD2	2.72	0.42
2:B:431[A]:GLU:O	2:B:434:GLN:HB3	2.18	0.42
1:C:48:SER:HB3	1:C:243:ARG:O	2.19	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
2:D:258:ASN:HD22	2:D:352:LYS:HZ2	1.68	0.42
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE2	2.55	0.42
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.79	0.42
2:B:178:SER:HB2	2:B:183:GLU:OE1	2.19	0.42
2:B:352:LYS:HB2	10:B:507:H1F:C06	2.49	0.42
1:C:77:GLU:HA	1:C:80:THR:HG22	2.00	0.42
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.02	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.42
1:A:386:GLU:O	1:A:390[A]:ARG:HD3	2.19	0.42
4:F:161:LEU:HD23	4:F:169:LEU:HA	2.01	0.42
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.55	0.42
2:D:236:SER:O	2:D:240[B]:THR:HG23	2.19	0.42
2:D:269:MET:HE2	2:D:269:MET:HB2	1.85	0.42
2:D:382:THR:HA	2:D:432:TYR:CD1	2.55	0.42
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.01	0.42
1:A:424:ASP:O	1:A:427:ALA:HB3	2.20	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:HA	2:B:89:PRO:HD3	1.94	0.42
2:B:164[B]:ARG:HA	2:B:164[B]:ARG:HD2	1.91	0.42
4:F:39:LEU:HD23	4:F:61:LEU:HD23	2.01	0.42
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.55	0.41
2:D:70:LEU:HD23	2:D:114:LEU:HD22	2.02	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.72	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.41
1:A:265:ILE:H	1:A:265:ILE:HG12	1.66	0.41
2:B:399:PHE:CE2	2:B:419:THR:HG22	2.55	0.41
1:C:107:HIS:CE1	1:C:155:GLU:OE1	2.74	0.41
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.41
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.51	0.41
2:B:214:PHE:HE1	2:B:220:THR:HG23	1.86	0.41
1:C:83:TYR:CD2	1:C:86:LEU:HD22	2.56	0.41
1:A:229:ARG:HD3	1:A:229:ARG:HH11	1.72	0.41
2:B:181:VAL:HG12	1:C:348:PRO:HG2	2.01	0.41
2:D:19:LYS:HB3	2:D:19:LYS:HE3	1.88	0.41
2:D:295:MET:CG	2:D:377:PHE:HB2	2.51	0.41
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.03	0.41
1:A:307:PRO:HA	1:A:383:ALA:HB2	2.01	0.41
1:C:316:CYS:O	1:C:377:MET:HG3	2.21	0.41
2:D:55:GLU:HG3	2:D:61:TYR:CE1	2.56	0.41
2:B:19:LYS:HB3	2:B:19:LYS:NZ	2.35	0.41
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.03	0.41
1:C:351:PHE:N	1:C:351:PHE:CD1	2.88	0.41
2:D:275:LEU:HA	2:D:275:LEU:HD23	1.81	0.41
4:F:282:SER:HB2	4:F:325:LEU:HD22	2.02	0.41
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.02	0.41
4:F:64:TYR:O	4:F:311:SER:HB3	2.20	0.41
1:A:96:LYS:HB2	1:A:96:LYS:HE2	1.87	0.40
2:D:247:GLN:N	2:D:247:GLN:CD	2.74	0.40
2:B:263:PRO:O	2:B:266:HIS:ND1	2.47	0.40
3:E:101:LEU:HD12	3:E:101:LEU:HA	1.72	0.40
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.56	0.40
2:D:213:CYS:HB3	2:D:219:LEU:HD12	2.04	0.40
3:E:6:MET:HG3	3:E:24:LEU:CD2	2.52	0.40
4:F:192:LEU:HD22	4:F:262:MET:CE	2.52	0.40
2:B:387:LEU:HD23	2:B:387:LEU:C	2.41	0.40
1:C:227:LEU:O	1:C:231:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	441/451 (98%)	419 (95%)	22 (5%)	0	100	100
1	C	447/451 (99%)	434 (97%)	13 (3%)	0	100	100
2	B	427/445 (96%)	417 (98%)	10 (2%)	0	100	100
2	D	420/445 (94%)	403 (96%)	17 (4%)	0	100	100
3	E	122/143 (85%)	121 (99%)	1 (1%)	0	100	100
4	F	347/384 (90%)	335 (96%)	12 (4%)	0	100	100
All	All	2204/2319 (95%)	2129 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/379 (99%)	369 (99%)	5 (1%)	69	91
1	C	380/379 (100%)	374 (98%)	6 (2%)	62	88
2	B	373/383 (97%)	366 (98%)	7 (2%)	57	85
2	D	364/383 (95%)	352 (97%)	12 (3%)	38	72
3	E	108/127 (85%)	104 (96%)	4 (4%)	34	68
4	F	318/342 (93%)	305 (96%)	13 (4%)	30	64
All	All	1917/1993 (96%)	1870 (98%)	47 (2%)	49	80

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	124	LYS
1	A	221	ARG
1	A	256	GLN
1	A	336	LYS
2	B	128	SER
2	B	139	HIS
2	B	278	ARG
2	B	297	ASP
2	B	325	MET
2	B	352	LYS
2	B	356	CYS
1	C	48	SER
1	C	71	GLU
1	C	96	LYS
1	C	251	ASP
1	C	302[A]	MET
1	C	302[B]	MET
2	D	39	ASP
2	D	76	ASP
2	D	124	LYS
2	D	139	HIS
2	D	158	ARG
2	D	248	LEU
2	D	322	ARG
2	D	352	LYS
2	D	414	ASP
2	D	416	MET
2	D	423	SER
2	D	441	ASP
3	E	28	SER
3	E	95	LYS
3	E	107	SER
3	E	125	GLU
4	F	106	LYS
4	F	151	SER
4	F	163	SER
4	F	164	SER
4	F	175	GLU
4	F	211	TYR
4	F	222	ARG
4	F	224	SER

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Mol	Chain	Res	Type
4	F	238	CYS
4	F	244	CYS
4	F	247	LYS
4	F	248	GLU
4	F	381	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	266	HIS
2	D	15	GLN
2	D	37	HIS
2	D	101	ASN
2	D	258	ASN
4	F	252	ASN
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 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GTP	C	501	6	26,34,34	5.30	12 (46%)	33,54,54	2.21	10 (30%)
9	MES	B	505	-	12,12,12	1.64	2 (16%)	14,16,16	1.97	4 (28%)
8	GDP	B	501	6	24,30,30	4.57	15 (62%)	31,47,47	2.14	9 (29%)
9	MES	B	504	-	12,12,12	1.62	3 (25%)	14,16,16	2.19	6 (42%)
5	GTP	A	501	6	26,34,34	5.28	12 (46%)	33,54,54	1.85	10 (30%)
10	H1F	B	507	-	28,28,28	5.47	10 (35%)	39,39,39	5.25	16 (41%)
11	ACP	F	401	-	27,33,33	4.71	10 (37%)	32,52,52	2.09	4 (12%)
5	GTP	D	602	6	26,34,34	5.46	12 (46%)	33,54,54	1.99	9 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
9	MES	B	505	-	-	0/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	H1F	B	507	-	-	5/18/30/30	0/3/3/3
11	ACP	F	401	-	-	3/15/38/38	0/3/3/3
5	GTP	D	602	6	-	7/18/38/38	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	507	H1F	C19-N01	18.56	1.45	1.35
5	C	501	GTP	C2'-C1'	-16.20	1.29	1.53
5	D	602	GTP	C2'-C1'	-15.72	1.29	1.53
5	A	501	GTP	C2'-C1'	-15.71	1.29	1.53
11	F	401	ACP	C2'-C1'	-15.04	1.30	1.53
11	F	401	ACP	O4'-C1'	14.96	1.62	1.41
5	D	602	GTP	O4'-C1'	13.66	1.60	1.41
5	C	501	GTP	O4'-C1'	13.37	1.59	1.41
5	A	501	GTP	O4'-C1'	13.16	1.59	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	507	H1F	C07-N02	12.45	1.48	1.29
10	B	507	H1F	C19-N03	11.13	1.45	1.33
8	B	501	GDP	C4-N3	9.29	1.50	1.35
8	B	501	GDP	C3'-C4'	-8.80	1.30	1.53
5	D	602	GTP	C4-N3	8.56	1.49	1.35
10	B	507	H1F	C19-S01	-8.43	1.55	1.68
8	B	501	GDP	C2-N2	8.31	1.50	1.33
5	D	602	GTP	C6-C5	8.23	1.55	1.41
8	B	501	GDP	O4'-C4'	8.14	1.63	1.45
5	A	501	GTP	C4-N3	8.12	1.48	1.35
5	C	501	GTP	C6-C5	7.85	1.54	1.41
10	B	507	H1F	C10-C09	7.75	1.63	1.51
5	A	501	GTP	C6-C5	7.37	1.54	1.41
5	C	501	GTP	C4-N3	7.22	1.47	1.35
5	D	602	GTP	C6-N1	7.00	1.45	1.33
8	B	501	GDP	C6-N1	6.94	1.45	1.33
11	F	401	ACP	PB-O3A	6.87	1.66	1.58
5	A	501	GTP	C6-N1	6.69	1.44	1.33
5	C	501	GTP	C6-N1	6.36	1.44	1.33
8	B	501	GDP	C6-C5	6.35	1.52	1.41
11	F	401	ACP	O4'-C4'	-6.31	1.30	1.45
5	D	602	GTP	O4'-C4'	-6.25	1.31	1.45
5	C	501	GTP	C2-N2	6.02	1.45	1.33
8	B	501	GDP	O4'-C1'	-6.02	1.32	1.41
5	D	602	GTP	C2-N2	5.78	1.45	1.33
5	D	602	GTP	C2-N1	5.70	1.45	1.35
5	A	501	GTP	O4'-C4'	-5.66	1.32	1.45
10	B	507	H1F	C08-C07	-5.64	1.42	1.50
5	A	501	GTP	C2-N2	5.48	1.44	1.33
5	A	501	GTP	C2-N1	5.48	1.45	1.35
5	C	501	GTP	O4'-C4'	-5.25	1.33	1.45
5	C	501	GTP	C2-N1	5.03	1.44	1.35
8	B	501	GDP	C2-N1	4.67	1.43	1.35
10	B	507	H1F	C04-C07	3.68	1.55	1.47
9	B	505	MES	C8-S	3.56	1.82	1.77
9	B	504	MES	C8-S	3.46	1.82	1.77
8	B	501	GDP	O2'-C2'	-3.40	1.35	1.43
11	F	401	ACP	C6-N6	3.35	1.46	1.34
5	D	602	GTP	C2-N3	3.24	1.49	1.34
5	D	602	GTP	O2'-C2'	3.18	1.50	1.43
5	A	501	GTP	O2'-C2'	3.05	1.50	1.43
11	F	401	ACP	O3'-C3'	-2.98	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	602	GTP	O3'-C3'	-2.98	1.36	1.43
11	F	401	ACP	O2'-C2'	2.71	1.49	1.43
11	F	401	ACP	C5-C4	-2.70	1.33	1.40
10	B	507	H1F	C11-C10	2.66	1.43	1.39
5	C	501	GTP	O3'-C3'	-2.59	1.36	1.43
10	B	507	H1F	O03-C14	2.53	1.41	1.37
5	C	501	GTP	C2-N3	2.51	1.46	1.34
5	C	501	GTP	O2'-C2'	2.51	1.48	1.43
5	A	501	GTP	C2-N3	2.49	1.46	1.34
8	B	501	GDP	C5-C4	-2.48	1.34	1.40
5	C	501	GTP	PG-O1G	2.48	1.58	1.50
8	B	501	GDP	O3'-C3'	2.45	1.48	1.43
8	B	501	GDP	O6-C6	-2.44	1.18	1.24
5	A	501	GTP	PG-O1G	2.39	1.58	1.50
8	B	501	GDP	C2'-C1'	-2.37	1.50	1.53
9	B	504	MES	O1S-S	2.34	1.51	1.45
11	F	401	ACP	C2-N3	2.30	1.35	1.32
9	B	505	MES	O1S-S	2.25	1.51	1.45
8	B	501	GDP	PA-O5'	2.17	1.68	1.59
5	A	501	GTP	O3'-C3'	-2.15	1.37	1.43
9	B	504	MES	C7-N4	2.12	1.52	1.47
8	B	501	GDP	PA-O1A	2.12	1.58	1.50
10	B	507	H1F	O01-C12	2.10	1.40	1.37
11	F	401	ACP	PB-O2B	-2.08	1.51	1.56
5	D	602	GTP	O5'-C5'	-2.07	1.36	1.44

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	507	H1F	C10-C09-N01	-26.30	79.38	112.25
10	B	507	H1F	C08-C09-C10	-10.64	94.38	113.86
11	F	401	ACP	C5-C6-N6	7.54	131.81	120.35
10	B	507	H1F	C08-C07-N02	-7.22	104.92	113.69
10	B	507	H1F	N03-C19-N01	7.12	120.16	115.81
8	B	501	GDP	N3-C2-N1	-6.25	118.89	127.22
5	C	501	GTP	N3-C2-N1	-5.85	119.41	127.22
10	B	507	H1F	C11-C10-C09	5.73	131.39	120.42
11	F	401	ACP	N3-C2-N1	-5.43	120.19	128.68
10	B	507	H1F	C09-C08-C07	5.07	107.44	102.73
5	D	602	GTP	N3-C2-N1	-5.01	120.54	127.22
5	A	501	GTP	N3-C2-N1	-4.93	120.65	127.22
10	B	507	H1F	C16-O01-C12	-4.86	110.19	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N6-C6-N1	-4.61	109.00	118.57
5	C	501	GTP	PB-O3B-PG	-4.49	117.43	132.83
5	C	501	GTP	C5-C6-N1	-4.46	117.33	123.43
8	B	501	GDP	N2-C2-N1	4.08	123.59	117.25
9	B	504	MES	O3S-S-C8	4.06	112.34	105.77
5	D	602	GTP	PB-O3B-PG	-4.04	118.96	132.83
5	C	501	GTP	C2-N3-C4	3.99	119.91	115.36
9	B	504	MES	O3S-S-O2S	-3.99	101.54	111.27
5	D	602	GTP	C2-N3-C4	3.90	119.81	115.36
8	B	501	GDP	C6-C5-C4	-3.84	117.13	120.80
9	B	505	MES	O3S-S-O2S	-3.66	102.33	111.27
8	B	501	GDP	C6-N1-C2	3.58	121.61	115.93
8	B	501	GDP	C1'-N9-C4	3.54	132.85	126.64
5	C	501	GTP	C6-N1-C2	3.53	121.54	115.93
11	F	401	ACP	C3'-C2'-C1'	3.50	106.25	100.98
9	B	504	MES	C6-C5-N4	3.50	115.41	110.10
5	A	501	GTP	PB-O3B-PG	-3.39	121.20	132.83
9	B	505	MES	O2S-S-C8	3.38	110.99	106.92
5	D	602	GTP	O4'-C1'-C2'	-3.35	102.04	106.93
10	B	507	H1F	C15-C10-C09	-3.34	114.02	120.42
5	A	501	GTP	O3G-PG-O1G	3.32	123.67	110.68
5	A	501	GTP	C5-C6-N1	-3.29	118.94	123.43
10	B	507	H1F	C09-N01-N02	-3.28	109.85	112.98
10	B	507	H1F	C07-N02-N01	-3.25	105.66	107.97
8	B	501	GDP	C2-N3-C4	3.17	118.97	115.36
5	A	501	GTP	N2-C2-N1	3.17	122.17	117.25
10	B	507	H1F	C15-C10-C11	-3.13	113.63	118.08
8	B	501	GDP	C5-C6-N1	-3.11	119.18	123.43
5	D	602	GTP	C5-C6-N1	-3.08	119.22	123.43
5	C	501	GTP	O4'-C1'-C2'	-2.98	102.57	106.93
5	C	501	GTP	N2-C2-N1	2.97	121.87	117.25
5	D	602	GTP	C1'-N9-C4	2.90	131.73	126.64
5	D	602	GTP	O3G-PG-O3B	2.83	114.12	104.64
5	A	501	GTP	C6-N1-C2	2.73	120.27	115.93
5	C	501	GTP	C4-C5-N7	-2.71	106.57	109.40
5	A	501	GTP	C2-N3-C4	2.70	118.44	115.36
5	D	602	GTP	PA-O3A-PB	-2.55	124.08	132.83
10	B	507	H1F	C14-C15-C10	2.53	123.87	119.83
10	B	507	H1F	S01-C19-N03	-2.45	118.44	122.56
9	B	504	MES	O1S-S-C8	2.40	109.80	106.92
9	B	505	MES	C6-C5-N4	2.38	113.71	110.10
9	B	504	MES	C5-N4-C3	2.36	114.14	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	602	GTP	C6-N1-C2	2.32	119.61	115.93
5	A	501	GTP	O3G-PG-O3B	-2.29	96.96	104.64
8	B	501	GDP	O4'-C4'-C3'	2.25	109.56	105.11
5	A	501	GTP	O5'-C5'-C4'	-2.24	101.29	108.99
5	C	501	GTP	O3G-PG-O1G	2.21	119.31	110.68
10	B	507	H1F	C19-N01-N02	2.19	121.37	119.83
9	B	504	MES	C2-C3-N4	2.16	113.38	110.10
5	C	501	GTP	O5'-C5'-C4'	-2.14	101.64	108.99
8	B	501	GDP	C4-C5-N7	-2.11	107.20	109.40
10	B	507	H1F	O01-C12-C13	2.07	118.80	115.16
9	B	505	MES	C6-O1-C2	2.05	116.75	109.89
5	A	501	GTP	C4-C5-N7	-2.02	107.29	109.40
10	B	507	H1F	O01-C12-C11	-2.02	120.65	124.12

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	602	GTP	PB-O3B-PG-O3G
5	D	602	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
9	B	504	MES	C8-C7-N4-C5
10	B	507	H1F	C13-C12-O01-C16
11	F	401	ACP	O4'-C4'-C5'-O5'
10	B	507	H1F	C11-C12-O01-C16
10	B	507	H1F	C03-C04-C07-N02
10	B	507	H1F	C05-C04-C07-N02
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	602	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	C3'-C4'-C5'-O5'
10	B	507	H1F	C08-C09-C10-C11
5	D	602	GTP	PG-O3B-PB-O1B
5	C	501	GTP	C3'-C4'-C5'-O5'
5	D	602	GTP	PB-O3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O1G

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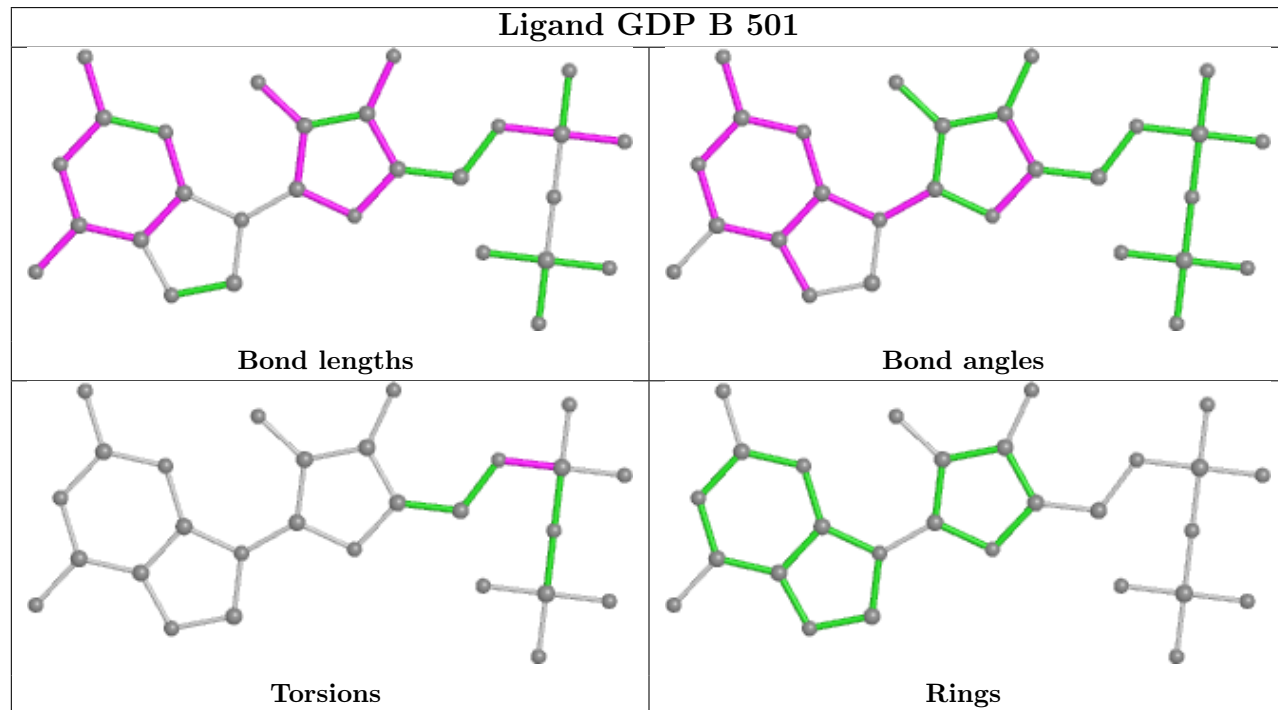
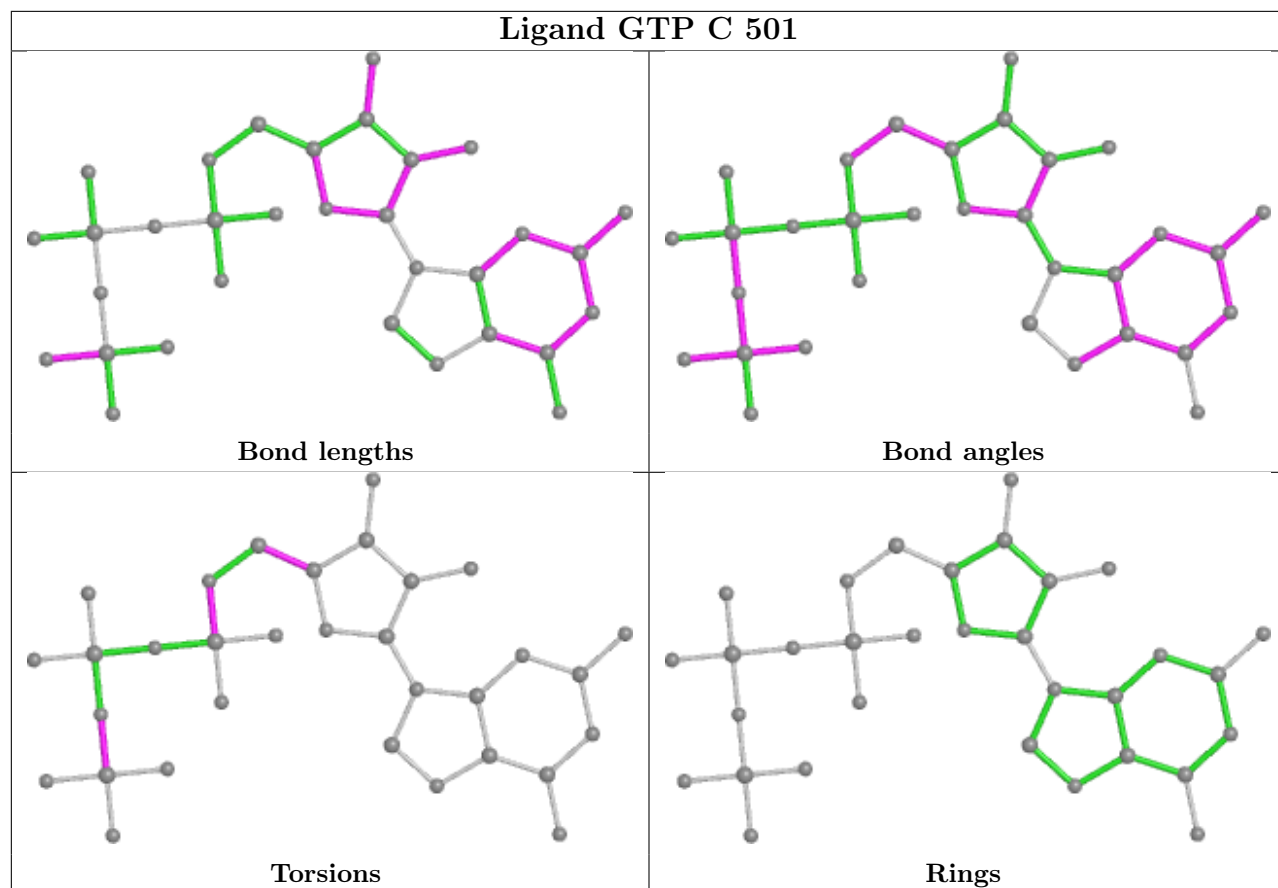
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	602	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	D	602	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

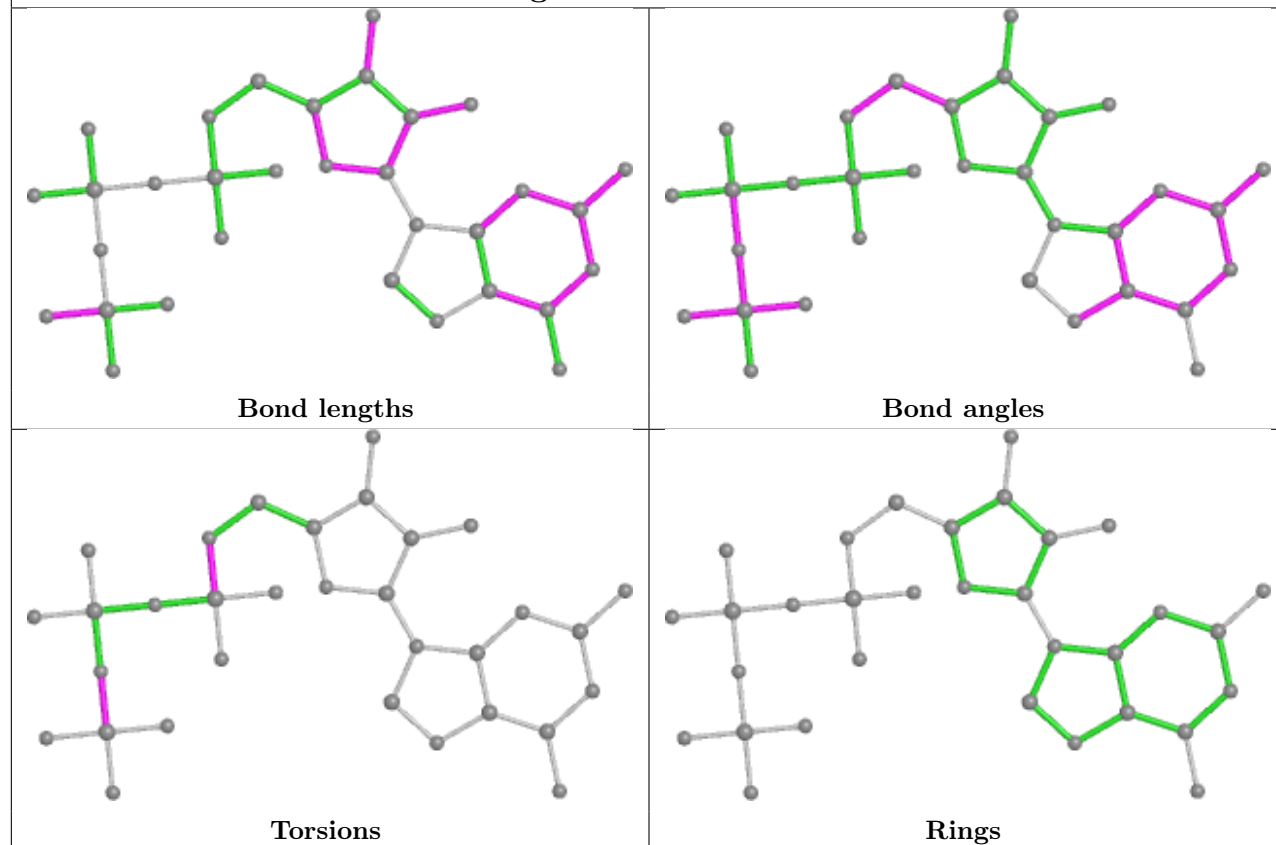
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	505	MES	1	0
8	B	501	GDP	1	0
9	B	504	MES	2	0
10	B	507	H1F	8	0
11	F	401	ACP	2	0
5	D	602	GTP	2	0

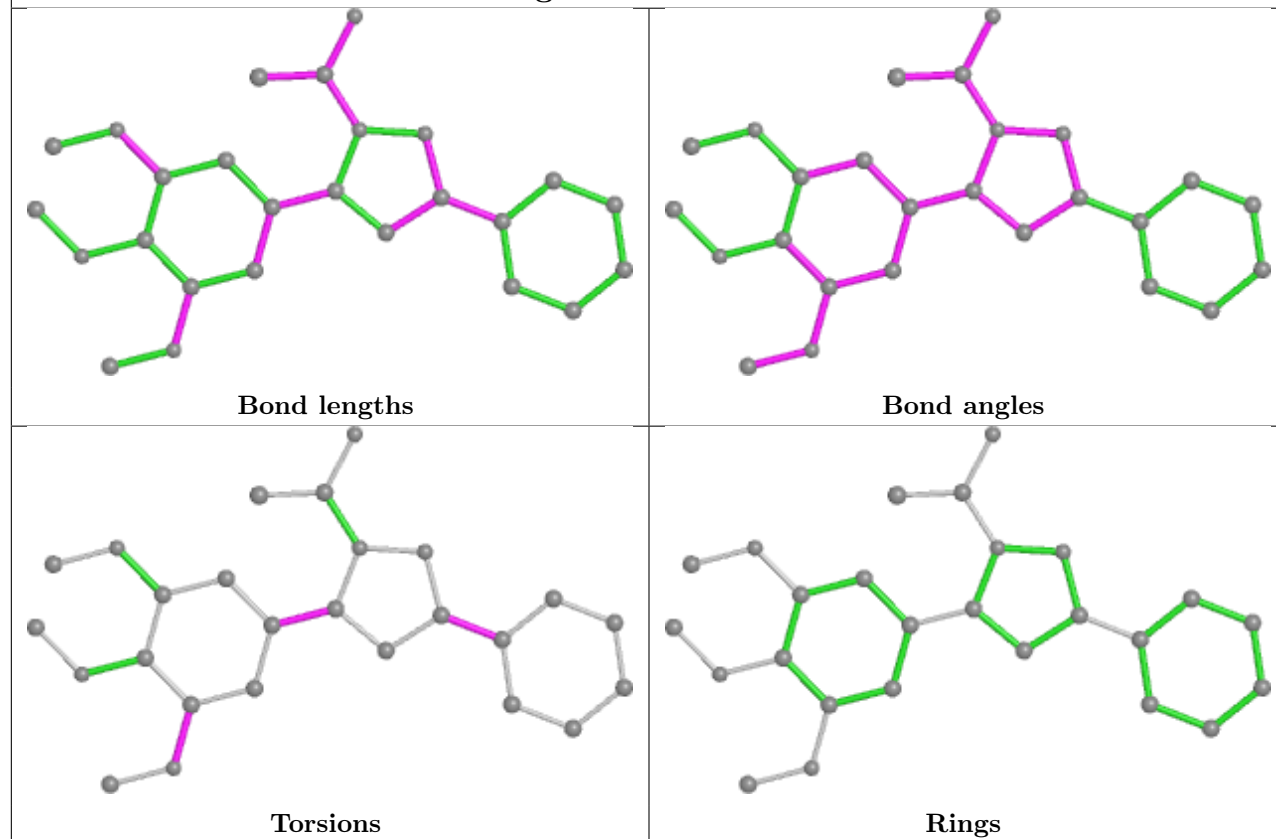
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

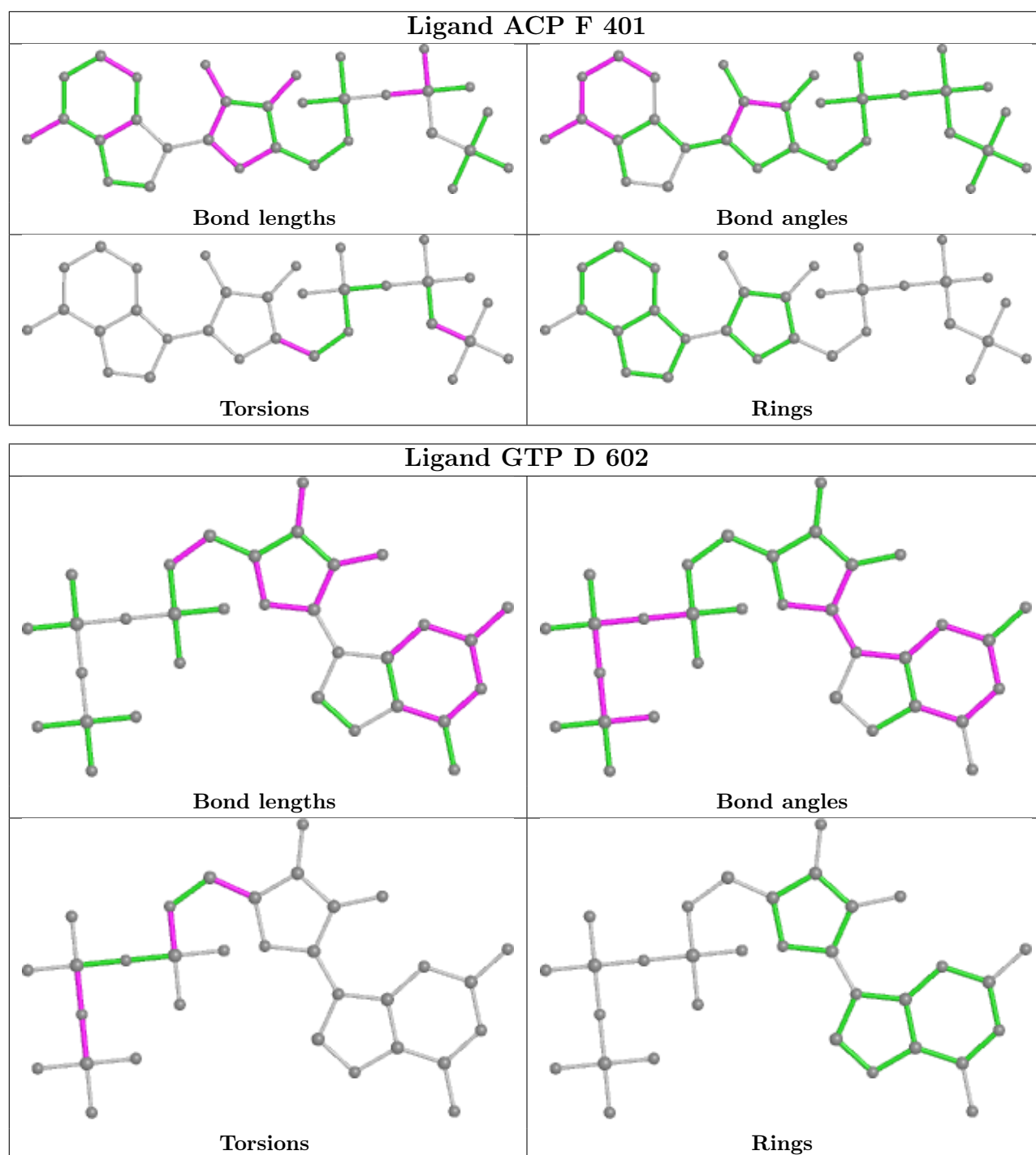


## Ligand GTP A 501



## Ligand H1F B 507





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	438/451 (97%)	-0.46	1 (0%)	95 94	25, 43, 73, 107	0
1	C	440/451 (97%)	-0.61	1 (0%)	95 94	18, 34, 61, 95	0
2	B	425/445 (95%)	-0.36	6 (1%)	75 70	23, 42, 78, 125	1 (0%)
2	D	421/445 (94%)	-0.14	12 (2%)	51 41	25, 60, 95, 134	1 (0%)
3	E	123/143 (86%)	0.04	5 (4%)	37 27	27, 57, 95, 136	0
4	F	352/384 (91%)	0.13	31 (8%)	10 5	34, 71, 141, 166	0
All	All	2199/2319 (94%)	-0.29	56 (2%)	57 47	18, 49, 100, 166	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	285	ALA	7.6
4	F	105	LEU	5.7
4	F	177	GLY	5.0
4	F	249	TYR	4.6
3	E	143	ALA	4.4
4	F	103	THR	4.3
2	B	57	THR	3.9
4	F	104	ASN	3.9
4	F	102	PRO	3.8
4	F	232	ASN	3.7
4	F	178	GLN	3.6
4	F	142	ARG	3.6
4	F	106	LYS	3.5
4	F	251	LYS	3.2
4	F	133	ALA	3.2
4	F	231	ALA	3.1
4	F	125	THR	3.0
3	E	142	GLU	3.0
2	D	37	HIS	2.9

*Continued on next page...*



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Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	2.9
2	B	74	THR	2.9
2	D	221	THR	2.8
4	F	173	ILE	2.8
2	D	286	LEU	2.7
4	F	176	GLN	2.6
4	F	141	GLY	2.6
4	F	101	TYR	2.6
2	D	401	ARG	2.5
2	B	284	ARG	2.4
4	F	143	GLU	2.4
4	F	372	THR	2.4
2	D	218	LYS	2.4
4	F	136	ASN	2.4
4	F	20	LEU	2.4
4	F	234	GLN	2.4
4	F	253	TYR	2.3
1	A	438	ASP	2.3
2	D	94	PHE	2.3
3	E	138	GLU	2.2
2	B	37	HIS	2.2
2	D	217	LEU	2.2
2	D	57	THR	2.2
4	F	225	SER	2.2
2	B	220	THR	2.2
2	B	59	ASN	2.2
2	D	406	HIS	2.2
2	D	216	THR	2.1
4	F	175	GLU	2.1
1	C	247	ALA	2.1
3	E	139	LEU	2.1
4	F	45	ASN	2.1
4	F	381	HIS	2.1
3	E	141	GLU	2.1
2	D	213	CYS	2.1
4	F	132	LEU	2.0
4	F	100	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

## 6.3 Carbohydrates

There are no monosaccharides in this entry.

## 6.4 Ligands

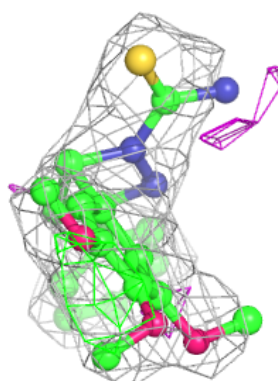
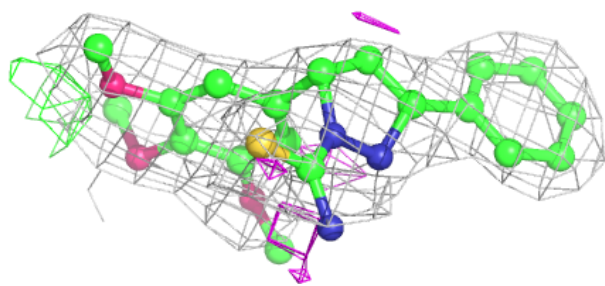
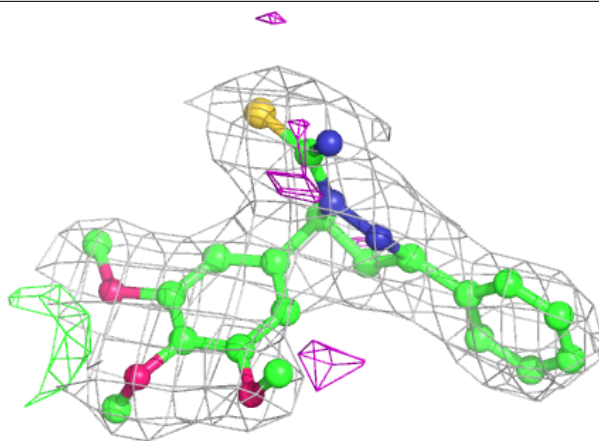
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	506	1/1	0.71	0.18	60,60,60,60	0
7	CA	B	503	1/1	0.83	0.21	81,81,81,81	0
6	MG	B	502	1/1	0.85	0.20	38,38,38,38	0
7	CA	A	504	1/1	0.90	0.12	76,76,76,76	0
6	MG	C	502	1/1	0.91	0.20	32,32,32,32	0
10	H1F	B	507	26/26	0.93	0.23	30,57,72,93	0
11	ACP	F	401	31/31	0.93	0.20	69,91,122,138	0
6	MG	D	601	1/1	0.94	0.12	68,68,68,68	0
7	CA	C	503	1/1	0.95	0.12	50,50,50,50	0
9	MES	B	505	12/12	0.96	0.16	59,70,94,97	0
7	CA	A	503	1/1	0.96	0.08	68,68,68,68	0
5	GTP	D	602	32/32	0.96	0.14	42,54,75,122	0
8	GDP	B	501	28/28	0.98	0.13	21,34,41,44	0
9	MES	B	504	12/12	0.98	0.11	36,55,82,86	0
6	MG	A	502	1/1	0.98	0.35	36,36,36,36	0
5	GTP	C	501	32/32	0.98	0.15	19,30,37,47	0
5	GTP	A	501	32/32	0.98	0.14	25,33,45,55	0

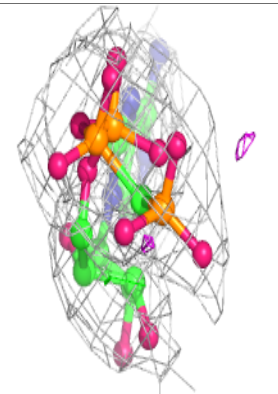
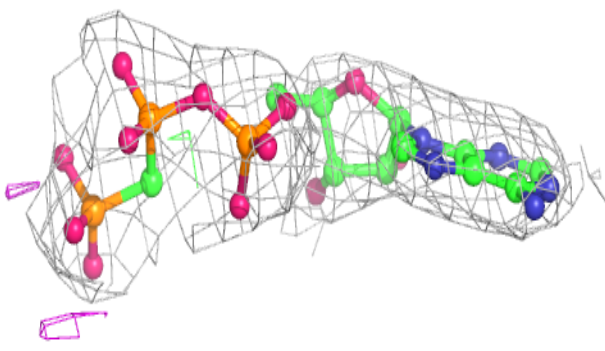
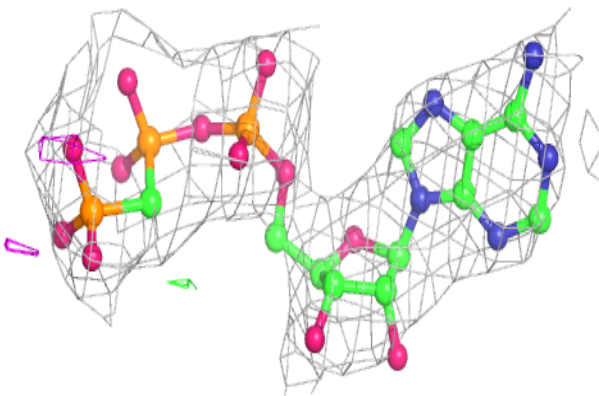
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around H1F B 507:**

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

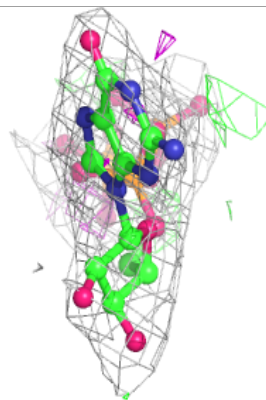
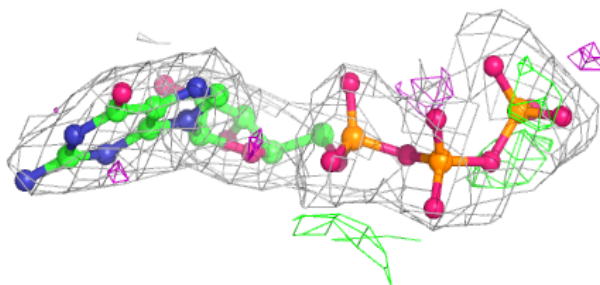
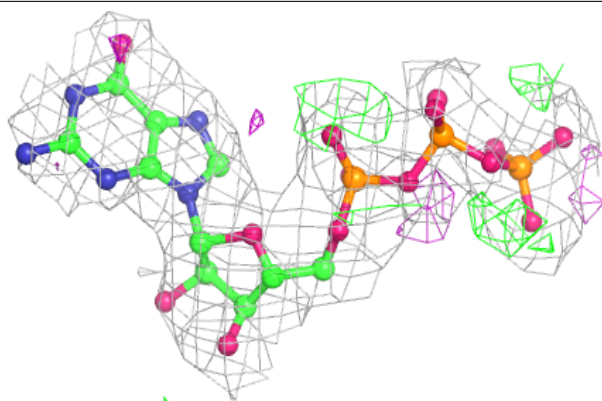
**Electron density around ACP F 401:**

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

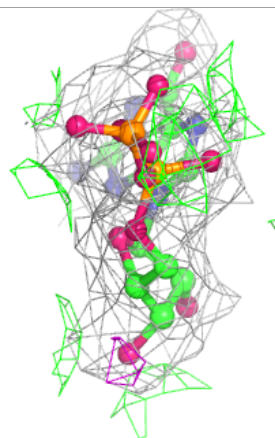
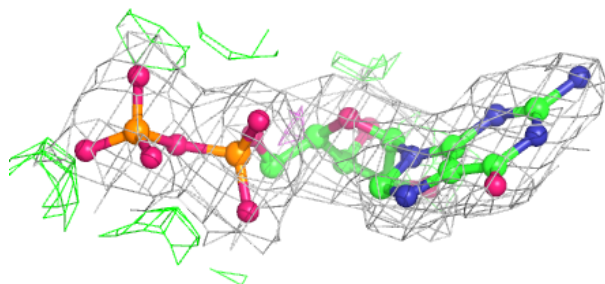
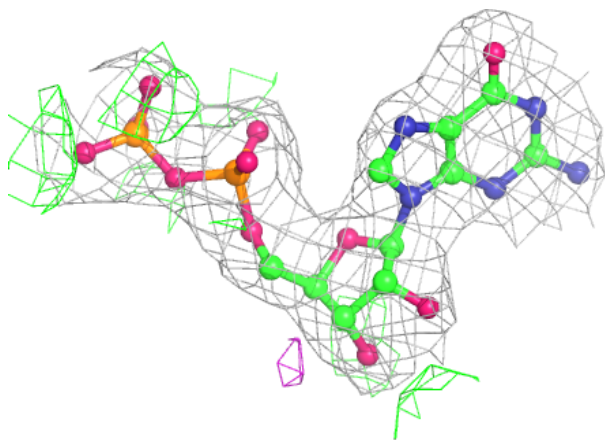


**Electron density around GTP D 602:**

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

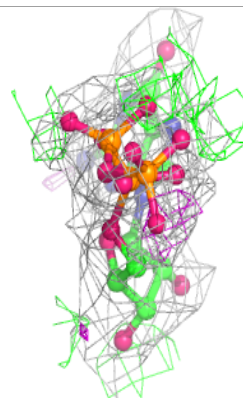
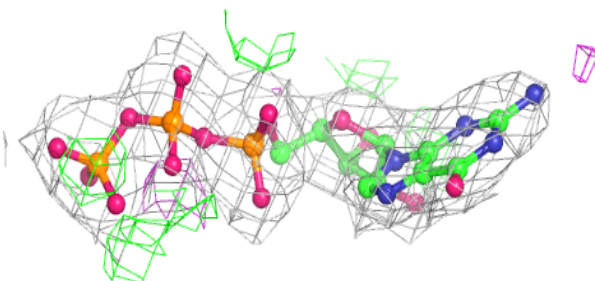
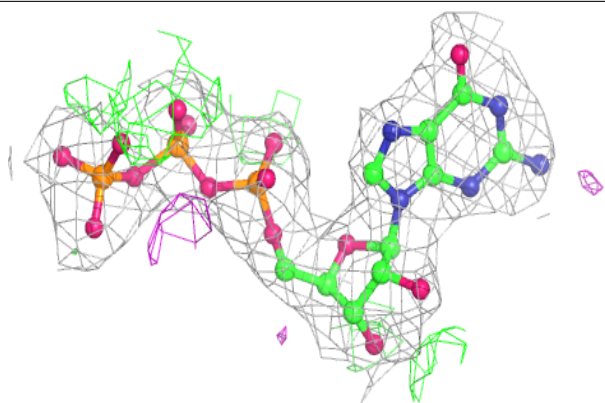
**Electron density around GDP B 501:**

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

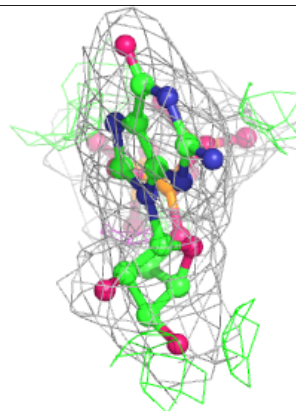
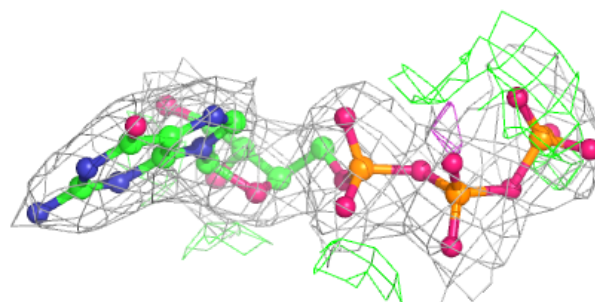
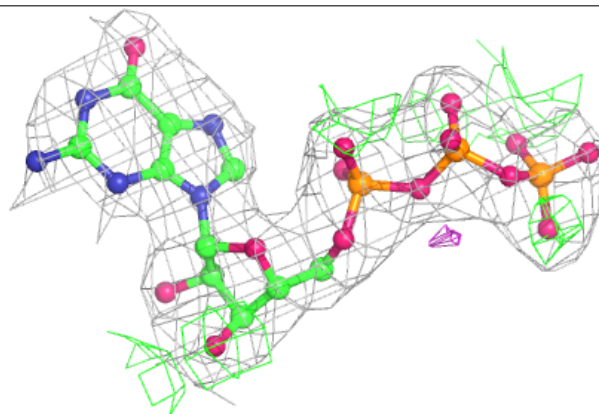


**Electron density around GTP C 501:**

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

**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.