



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 02:55 PM EDT

PDB ID : 4O4H / pdb\_00004o4h  
Title : Tubulin-Laulimalide complex  
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Deposited on : 2013-12-18  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

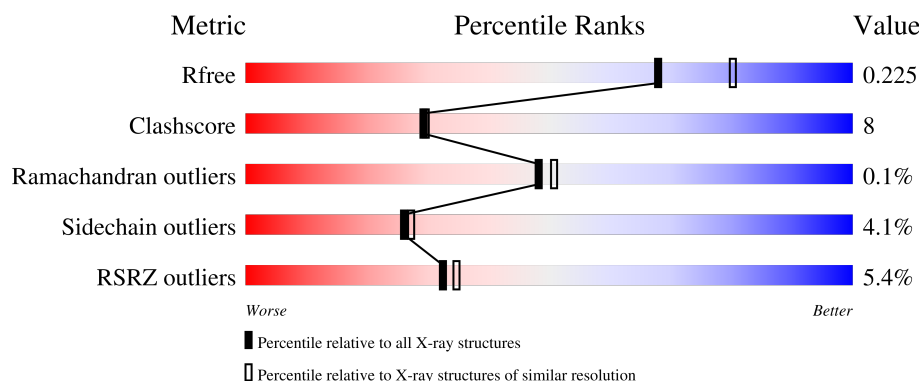
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	B	504	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18548 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	439	Total	C	N	O	S	0	12	0
			3481	2214	584	658	25			
1	C	440	Total	C	N	O	S	0	19	0
			3519	2235	586	672	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	10	0
			3397	2137	573	660	27			
2	D	427	Total	C	N	O	S	0	6	0
			3370	2117	571	653	29			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	5	0
			1039	642	187	205	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

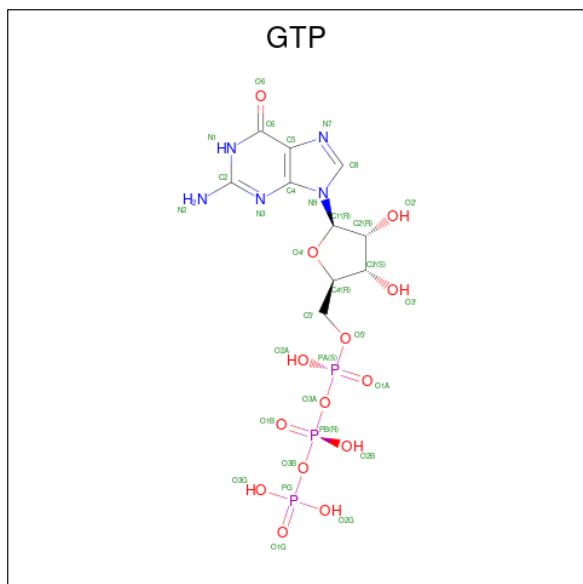
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	348	Total	C	N	O	S	0	6	0
			2878	1852	487	525	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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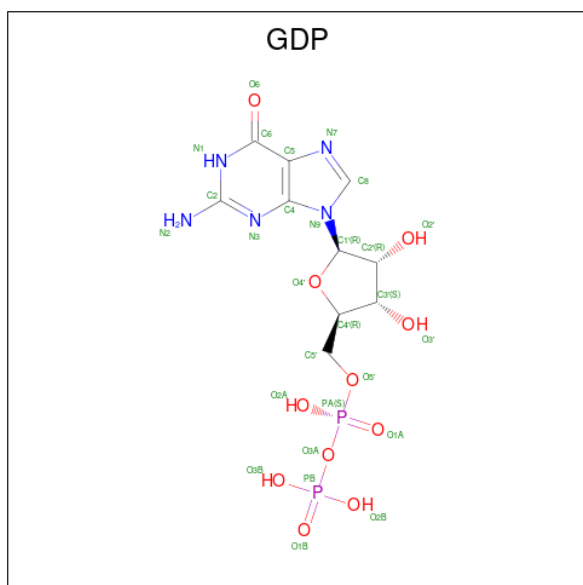
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

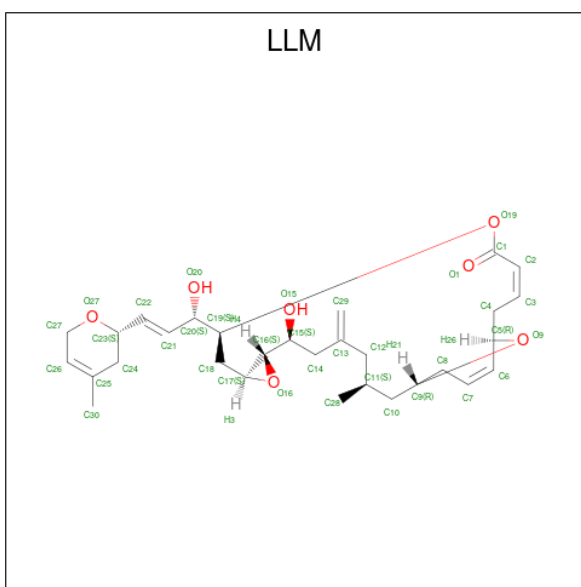
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	2	Total	Ca	0	0
			2	2		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



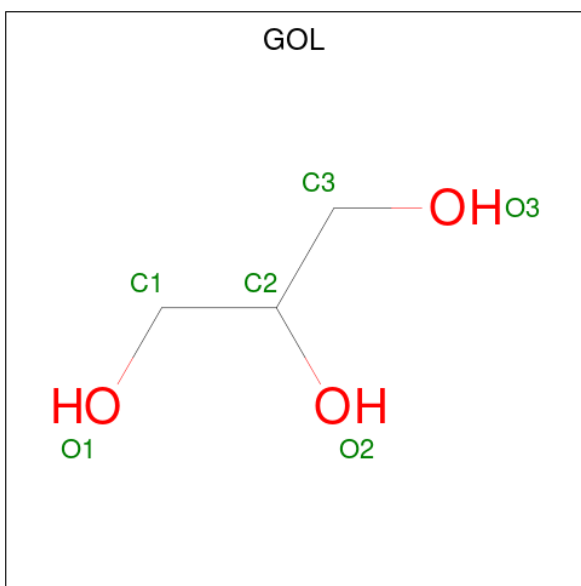
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is Laulimalide (CCD ID: LLM) (formula: C<sub>30</sub>H<sub>42</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			37	30	7		

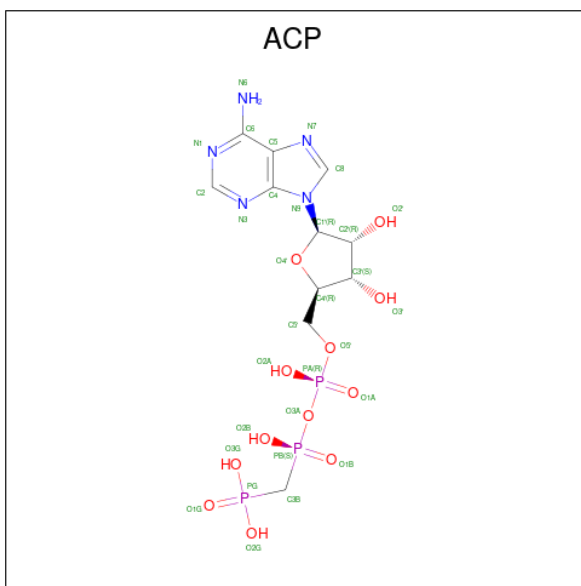
- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 6 3 3	0	0
10	D	1	Total C O 6 3 3	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD

ID: ACP) (formula:  $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$ ).



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

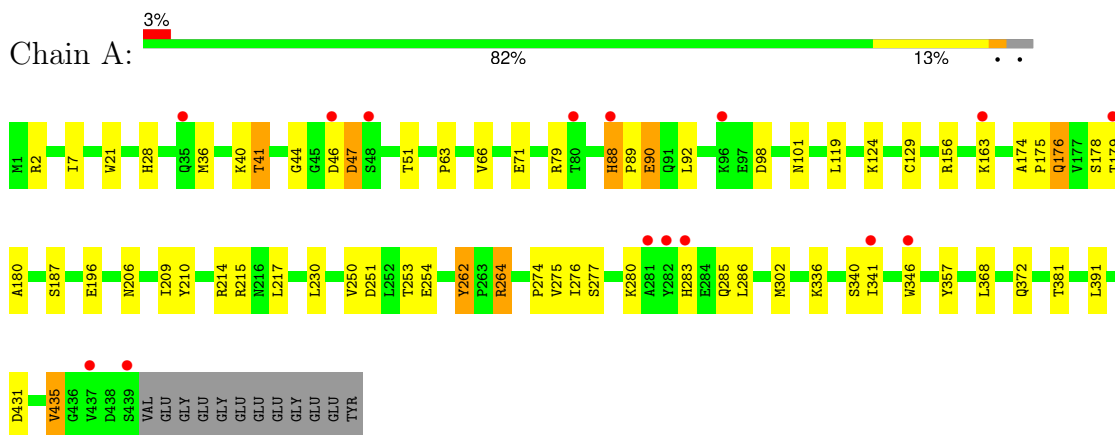
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	110	Total O 110 110	0	0
12	B	142	Total O 142 142	0	0
12	C	231	Total O 231 231	0	0
12	D	102	Total O 102 102	0	0
12	E	31	Total O 31 31	0	0
12	F	40	Total O 40 40	0	0

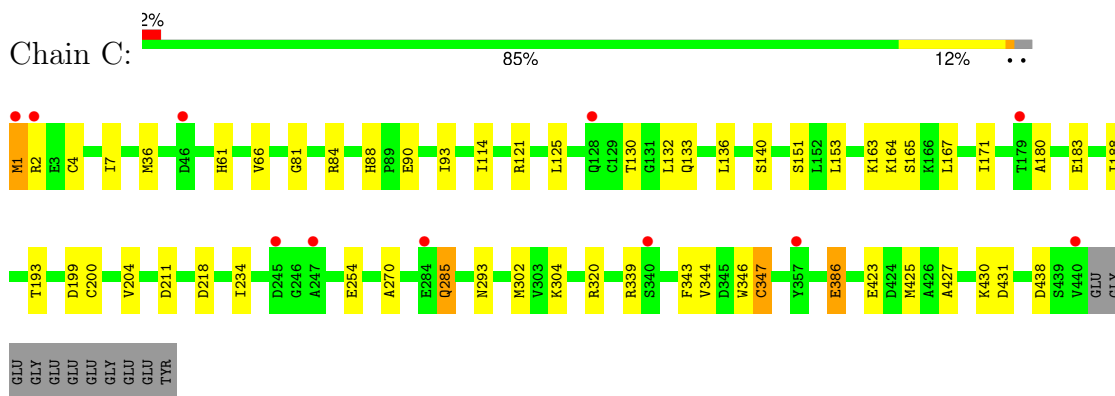
### 3 Residue-property plots

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.

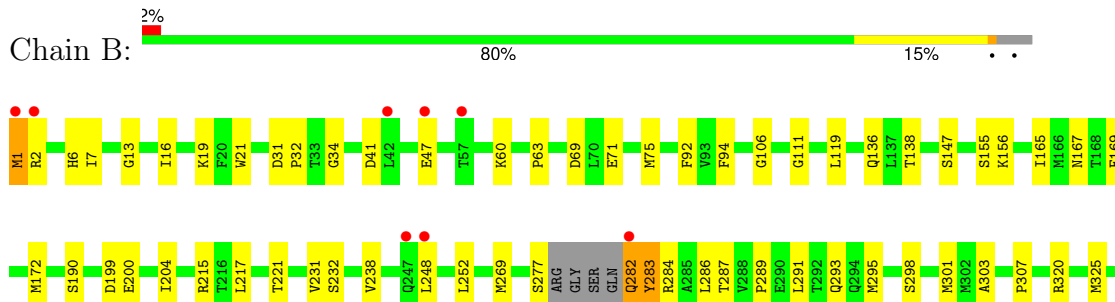
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.69Å 156.87Å 180.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.90 – 2.10 71.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.90-2.10) 99.8 (71.90-2.10)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.192 , 0.224 0.194 , 0.225	Depositor DCC
$R_{free}$ test set	8659 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: ACP, GOL, MG, GDP, GTP, CA, LLM

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	0.41	2/3596 (0.1%)	0.77	4/4883 (0.1%)
1	C	0.40	0/3655	0.74	0/4965
2	B	0.39	0/3498	0.75	0/4738
2	D	0.38	0/3461	0.78	2/4689 (0.0%)
3	E	0.36	0/1063	0.69	0/1412
4	F	0.41	1/2961 (0.0%)	0.75	0/4002
All	All	0.40	3/18234 (0.0%)	0.75	6/24689 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	90	SER	CB-OG	-8.32	1.25	1.42
1	A	89	PRO	N-CD	5.35	1.55	1.47
1	A	88	HIS	C-N	5.34	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	338	LYS	CD-CE-NZ	-8.77	83.83	111.90
1	A	88	HIS	CA-C-N	-5.37	113.37	119.28
1	A	88	HIS	C-N-CA	-5.37	113.37	119.28
2	D	358	ILE	N-CA-C	5.14	112.95	107.76
1	A	262	TYR	CA-C-N	5.03	124.47	119.24
1	A	262	TYR	C-N-CA	5.03	124.47	119.24

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	3481	0	3437	53	2
1	C	3519	0	3469	43	0
2	B	3397	0	3291	52	0
2	D	3370	0	3265	51	1
3	E	1039	0	1062	11	0
4	F	2878	0	2872	88	3
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
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	37	0	42	7	0
10	B	6	0	8	5	0
10	D	6	0	8	0	0
11	F	31	0	14	6	0
12	A	110	0	0	6	0
12	B	142	0	0	6	0
12	C	231	0	0	5	0
12	D	102	0	0	6	0
12	E	31	0	0	0	0
12	F	40	0	0	3	0
All	All	18548	0	17516	300	3

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 8.

All (300) 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)
9:B:503:LLM:H18	9:B:503:LLM:H11	1.29	1.14
1:A:88:HIS:CD2	1:A:90:GLU:HB2	1.99	0.96
4:F:19:ARG:HA	4:F:22:LEU:HD12	1.53	0.90
1:A:88:HIS:CD2	1:A:90:GLU:H	1.90	0.88
2:B:282:GLN:HG2	2:B:283:TYR:H	1.43	0.84
2:B:320:ARG:NH1	10:B:504:GOL:O3	2.09	0.84
1:A:88:HIS:HD2	1:A:90:GLU:HB2	1.40	0.82
2:D:164:ARG:NH1	12:D:616:HOH:O	2.11	0.82
4:F:146:VAL:O	4:F:184:LYS:NZ	2.10	0.82
1:C:293[A]:ASN:OD1	1:C:339:ARG:NH1	2.13	0.81
2:B:71:GLU:O	12:B:724:HOH:O	1.99	0.81
4:F:21:LEU:O	4:F:24:THR:OG1	1.99	0.81
1:C:163:LYS:NZ	12:C:770:HOH:O	2.09	0.78
4:F:241:THR:HG22	11:F:401:ACP:O2'	1.84	0.77
4:F:81:ILE:O	4:F:88:SER:HA	1.85	0.77
2:B:282:GLN:HG2	2:B:283:TYR:N	1.99	0.76
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.19	0.76
11:F:401:ACP:H3'	11:F:401:ACP:C8	2.17	0.75
9:B:503:LLM:H11	9:B:503:LLM:C28	2.13	0.74
4:F:128:ARG:HH11	4:F:170:LEU:HD13	1.52	0.74
2:D:180:THR:O	12:D:653:HOH:O	2.06	0.72
1:A:88:HIS:HD2	1:A:90:GLU:H	1.36	0.72
2:B:217:LEU:HD13	2:B:277:SER:HB3	1.70	0.72
2:B:269:MET:SD	2:B:301:MET:HE3	2.29	0.71
2:D:229:HIS:ND1	12:D:701:HOH:O	2.22	0.71
1:C:132:LEU:O	1:C:164:LYS:HE2	1.89	0.71
2:D:181:VAL:O	2:D:398:MET:HE1	1.91	0.71
9:B:503:LLM:H18	9:B:503:LLM:C29	2.17	0.70
2:D:175:PRO:HA	2:D:178:SER:HB2	1.74	0.69
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.24	0.69
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.33	0.69
2:B:215:ARG:NH1	12:B:740:HOH:O	2.26	0.68
2:B:289:PRO:O	2:B:293:GLN:HG3	1.95	0.67
2:B:301:MET:HE2	2:B:307:PRO:HG3	1.77	0.66
4:F:88:SER:OG	4:F:89:GLU:N	2.17	0.66
1:A:285:GLN:NE2	12:A:681:HOH:O	2.28	0.66
1:A:196:GLU:OE1	12:A:680:HOH:O	2.14	0.65
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.11	0.65
2:B:335:VAL:HG23	9:B:503:LLM:C6	2.27	0.65
4:F:222:ARG:O	4:F:241:THR:OG1	2.14	0.64
2:B:338:LYS:NZ	12:B:671:HOH:O	2.30	0.64
9:B:503:LLM:O1	9:B:503:LLM:H27	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.61	0.64
4:F:56:PRO:O	12:F:521:HOH:O	2.15	0.64
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.32	0.64
2:D:269[B]:MET:HG2	2:D:384:ILE:HD13	1.80	0.63
4:F:128:ARG:HH12	4:F:170:LEU:HB3	1.62	0.63
4:F:288:LYS:NZ	12:F:527:HOH:O	2.32	0.63
2:B:282:GLN:CG	2:B:283:TYR:H	2.08	0.63
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.80	0.62
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.81	0.62
1:A:179:THR:HA	2:B:248:LEU:HD21	1.81	0.62
2:B:19:LYS:HB3	2:B:232:SER:OG	2.00	0.62
4:F:129:GLU:HG2	4:F:130:VAL:N	2.14	0.62
4:F:101:TYR:CE2	4:F:126:ASP:HA	2.35	0.61
1:C:438:ASP:OD1	12:C:725:HOH:O	2.16	0.61
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.81	0.61
4:F:259:GLY:O	4:F:261:GLU:HG3	2.01	0.60
1:A:175:PRO:HA	1:A:178:SER:HB3	1.83	0.60
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.82	0.60
1:A:88:HIS:NE2	1:A:90:GLU:OE1	2.26	0.60
2:D:272:PHE:CE1	2:D:302:MET:HE3	2.36	0.60
4:F:242:ASN:ND2	11:F:401:ACP:O2B	2.33	0.60
2:D:180:THR:OG1	2:D:181:VAL:N	2.35	0.60
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.36	0.60
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.31	0.60
2:D:174:SER:OG	2:D:207:GLU:OE1	2.19	0.60
11:F:401:ACP:H5'1	11:F:401:ACP:H8	1.84	0.60
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.42	0.59
1:C:81:GLY:O	1:C:84:ARG:HD2	2.02	0.59
4:F:131:PHE:CD1	4:F:132:LEU:HD23	2.38	0.59
4:F:247:LYS:HD2	4:F:247:LYS:O	2.02	0.59
2:D:214:PHE:HD2	2:D:215:ARG:HG2	1.68	0.58
1:A:28:HIS:O	1:A:36:MET:HE3	2.04	0.57
2:B:282:GLN:N	2:B:282:GLN:HE21	2.02	0.57
2:D:147[A]:SER:HG	2:D:190:SER:HG	1.45	0.57
2:B:136:GLN:HA	2:B:167:ASN:O	2.04	0.57
4:F:90:SER:O	4:F:90:SER:OG	2.19	0.57
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.86	0.57
4:F:81:ILE:O	4:F:88:SER:CA	2.52	0.57
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.40	0.56
4:F:128:ARG:NH1	4:F:170:LEU:HB3	2.20	0.56
2:D:1:MET:HB2	2:D:133:GLN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:SER:C	1:A:341:ILE:HD13	2.31	0.56
1:A:88:HIS:HD2	1:A:90:GLU:CB	2.17	0.55
2:B:106:GLY:O	2:B:111:GLY:HA3	2.06	0.55
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.21	0.55
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.41	0.55
4:F:101:TYR:HE2	4:F:126:ASP:HA	1.71	0.55
2:D:106:GLY:O	2:D:111:GLY:HA3	2.06	0.55
1:A:217:LEU:HA	1:A:277:SER:HB3	1.89	0.54
1:C:234:ILE:HD13	1:C:302[B]:MET:SD	2.47	0.54
1:C:386[A]:GLU:HG2	12:C:691:HOH:O	2.08	0.54
4:F:16:GLU:HA	4:F:19:ARG:HG2	1.90	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.53
4:F:99:VAL:O	4:F:127:GLU:HB2	2.08	0.53
1:A:340:SER:O	1:A:341:ILE:HD13	2.08	0.53
4:F:209:HIS:CD2	4:F:210:LEU:HD13	2.43	0.53
1:A:41:THR:HB	1:A:44:GLY:O	2.08	0.53
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.90	0.53
1:C:270:ALA:HB3	1:C:302[B]:MET:HE2	1.90	0.53
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.89	0.53
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.53
2:B:1:MET:O	2:B:1:MET:HE2	2.10	0.52
4:F:1:MET:HE2	4:F:26:GLN:HA	1.90	0.52
1:C:430:LYS:NZ	1:C:431:ASP:OD1	2.40	0.52
4:F:16:GLU:OE2	4:F:19:ARG:HD3	2.09	0.52
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.44	0.52
4:F:19:ARG:HA	4:F:22:LEU:CD1	2.35	0.52
1:A:88:HIS:HD2	1:A:90:GLU:N	2.06	0.52
4:F:73:ARG:HB3	4:F:76[B]:SER:HB3	1.92	0.51
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.25	0.51
2:D:170:SER:O	2:D:172:MET:HE2	2.11	0.51
4:F:80:LEU:O	4:F:84:SER:OG	2.15	0.51
1:C:204:VAL:HG22	1:C:302[B]:MET:HE1	1.91	0.51
2:D:136:GLN:HA	2:D:167:ASN:O	2.11	0.51
4:F:19:ARG:CA	4:F:22:LEU:HD12	2.35	0.51
1:A:285:GLN:OE1	1:A:372[B]:GLN:HG2	2.11	0.50
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.92	0.50
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.36	0.50
4:F:16:GLU:OE1	4:F:19:ARG:NH1	2.43	0.50
1:A:262:TYR:CE2	1:A:346:TRP:CH2	2.99	0.50
2:B:320:ARG:HD3	10:B:504:GOL:H31	1.92	0.50
1:A:336:LYS:HG3	3:E:24:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:THR:HG22	2:D:335:VAL:HG11	1.93	0.50
4:F:200:ASP:HB3	4:F:241:THR:HG21	1.93	0.50
4:F:81:ILE:O	4:F:88:SER:N	2.44	0.49
1:C:254:GLU:OE2	12:C:831:HOH:O	2.20	0.49
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.94	0.49
4:F:170:LEU:N	4:F:170:LEU:HD23	2.26	0.49
2:B:2:ARG:HB2	2:B:2:ARG:HH11	1.76	0.49
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.78	0.49
1:A:372[B]:GLN:OE1	12:A:651:HOH:O	2.20	0.49
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.94	0.49
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.30	0.49
4:F:131:PHE:HD1	4:F:132:LEU:HD23	1.78	0.48
2:D:2:ARG:NH2	12:D:669:HOH:O	2.46	0.48
2:D:82:PRO:O	2:D:83:PHE:HB2	2.13	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.48
2:B:360:PRO:HB3	10:B:504:GOL:H32	1.95	0.48
1:A:346:TRP:H	1:A:346:TRP:CD1	2.30	0.48
4:F:319:PHE:CE1	4:F:329:LEU:HD23	2.49	0.48
2:B:400:ARG:NH1	12:B:702:HOH:O	2.39	0.48
2:D:396:THR:HG22	2:D:422:GLU:OE2	2.14	0.48
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	1.95	0.48
1:C:204:VAL:HG22	1:C:302[B]:MET:HE3	1.96	0.48
1:C:343:PHE:HD2	1:C:347[B]:CYS:SG	2.37	0.48
2:D:22:GLU:OE1	2:D:82:PRO:HG2	2.14	0.48
1:A:47:ASP:OD1	1:A:47:ASP:N	2.45	0.47
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.96	0.47
2:D:217:LEU:HD22	2:D:277:SER:HA	1.97	0.47
2:B:360:PRO:HG3	10:B:504:GOL:H32	1.96	0.47
2:D:296:PHE:HE2	2:D:332:MET:HE1	1.80	0.47
1:C:423:GLU:OE1	12:C:675:HOH:O	2.20	0.47
4:F:219:GLY:O	12:F:501:HOH:O	2.20	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.47
2:D:7:ILE:O	2:D:137:LEU:HA	2.14	0.47
4:F:200:ASP:OD2	4:F:241:THR:HG23	2.14	0.47
4:F:331:GLU:OE2	4:F:333:ASN:ND2	2.47	0.47
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.97	0.47
4:F:129:GLU:HG2	4:F:130:VAL:H	1.80	0.47
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.96	0.47
2:D:338:LYS:HB2	2:D:338:LYS:HE3	1.60	0.47
4:F:304:THR:HG21	4:F:311:SER:OG	2.15	0.47
4:F:320:MET:HE3	4:F:320:MET:HB3	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ALA:HA	1:C:430:LYS:HE3	1.97	0.47
2:B:69:ASP:O	2:B:94:PHE:HA	2.15	0.46
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.96	0.46
1:A:176:GLN:HB2	12:A:611:HOH:O	2.15	0.46
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	1.98	0.46
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.98	0.46
4:F:253:TYR:CD1	4:F:253:TYR:C	2.93	0.46
1:A:264:ARG:HD2	12:A:680:HOH:O	2.16	0.46
12:B:659:HOH:O	1:C:1:MET:HE2	2.16	0.46
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.16	0.46
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.80	0.46
4:F:131:PHE:CD1	4:F:131:PHE:C	2.93	0.46
2:B:320:ARG:HD3	10:B:504:GOL:C3	2.45	0.46
4:F:170:LEU:C	4:F:172:PHE:H	2.24	0.46
4:F:225:SER:HB2	4:F:250:SER:OG	2.16	0.46
4:F:131:PHE:CE1	4:F:132:LEU:HD23	2.50	0.46
1:A:40:LYS:HA	1:A:40:LYS:HD3	1.59	0.45
9:B:503:LLM:H26	9:B:503:LLM:H20	1.79	0.45
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.98	0.45
4:F:150:LYS:HB3	4:F:160:ILE:HG23	1.98	0.45
4:F:14:TYR:HA	4:F:17:VAL:HB	1.97	0.45
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.98	0.45
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.98	0.45
4:F:220[A]:VAL:HG12	4:F:263:PHE:CD1	2.51	0.45
3:E:136:ASN:O	3:E:140:LYS:HG2	2.17	0.45
4:F:371:PRO:HA	4:F:372:THR:HB	1.98	0.45
11:F:401:ACP:H3'	11:F:401:ACP:H8	1.94	0.45
2:B:34:GLY:O	2:B:60:LYS:HB2	2.16	0.45
4:F:251:LYS:H	4:F:251:LYS:HG3	1.50	0.45
2:D:176:LYS:HD3	2:D:210:TYR:CD2	2.52	0.45
1:C:1:MET:SD	1:C:130:THR:HG23	2.57	0.44
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	1.99	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.44
2:D:27:GLU:OE1	2:D:236:SER:OG	2.35	0.44
4:F:226:GLU:OE2	4:F:250:SER:OG	2.22	0.44
1:A:7:ILE:HG23	1:A:66[A]:VAL:HG23	1.98	0.44
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.44
4:F:78:VAL:O	4:F:81:ILE:HG22	2.18	0.44
1:C:165[A]:SER:HA	1:C:199:ASP:OD2	2.17	0.44
4:F:31:ARG:CZ	4:F:32:LYS:H	2.31	0.44
2:D:116:ASP:HB2	12:D:652:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:272:PHE:CD1	2:D:302:MET:HE3	2.52	0.44
2:D:19:LYS:HA	2:D:19:LYS:HD3	1.79	0.44
2:D:277:SER:O	2:D:278:ARG:HB3	2.17	0.44
4:F:135:TYR:OH	4:F:165:GLU:HA	2.18	0.44
1:A:276:ILE:HD12	1:A:283:HIS:CE1	2.53	0.44
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.53	0.44
2:D:414:ASP:N	2:D:414:ASP:OD1	2.51	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.54	0.43
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.43
1:A:277:SER:OG	1:A:280:LYS:HG3	2.18	0.43
2:B:199:ASP:C	2:B:200:GLU:HG3	2.43	0.43
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.34	0.43
4:F:1:MET:HB2	4:F:1:MET:HE3	1.73	0.43
4:F:10:ASN:OD1	4:F:10:ASN:N	2.51	0.43
1:A:250[B]:VAL:HG22	1:A:254:GLU:OE1	2.19	0.43
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.84	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.43
1:C:165[B]:SER:HA	1:C:199:ASP:OD2	2.19	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.43
2:D:385:GLN:O	2:D:389:LYS:HB2	2.19	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.54	0.43
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.00	0.43
1:C:285:GLN:H	1:C:285:GLN:HG2	1.68	0.43
3:E:100:LYS:HB3	3:E:100:LYS:HE3	1.68	0.43
4:F:70:LYS:HA	4:F:76[B]:SER:OG	2.18	0.43
2:D:323:MET:HB3	2:D:373:MET:HE1	2.01	0.42
2:B:136:GLN:NE2	12:B:742:HOH:O	2.51	0.42
2:B:156:LYS:HD3	3:E:76:ARG:CZ	2.49	0.42
2:B:402:LYS:HB3	2:B:405:LEU:HD12	2.01	0.42
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.50	0.42
2:D:402:LYS:C	2:D:405:LEU:HD23	2.45	0.42
2:D:153:LEU:HD13	2:D:153:LEU:HA	1.89	0.42
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.42
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.55	0.42
4:F:184:LYS:HD3	4:F:185:TYR:N	2.34	0.42
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.19	0.42
4:F:73:ARG:HB3	4:F:76[A]:SER:HB2	2.02	0.42
2:B:402:LYS:HD3	2:B:415:GLU:OE2	2.19	0.42
1:C:430:LYS:HE3	1:C:430:LYS:HB3	1.89	0.42
4:F:181:VAL:O	4:F:181:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:371:PRO:HA	4:F:372:THR:C	2.44	0.42
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.89	0.42
1:C:2:ARG:HB3	1:C:133:GLN:HB2	2.00	0.42
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.55	0.42
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG23	2.02	0.42
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.91	0.42
1:A:251:ASP:OD1	1:A:253:THR:HB	2.20	0.42
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.02	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.20	0.42
2:D:406:HIS:NE2	2:D:407:TRP:CD1	2.88	0.42
4:F:209:HIS:NE2	4:F:210:LEU:HD13	2.35	0.42
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.02	0.42
1:C:302[B]:MET:HE3	1:C:302[B]:MET:HB3	1.83	0.42
2:D:47:GLU:HG2	2:D:245:PRO:HG3	2.01	0.42
2:D:56:ALA:HB3	2:D:60:LYS:HB2	2.02	0.42
2:B:293:GLN:O	9:B:503:LLM:H30	2.20	0.41
4:F:178:GLN:HG2	4:F:179:VAL:N	2.35	0.41
1:A:129:CYS:O	12:A:684:HOH:O	2.22	0.41
4:F:102:PRO:HG3	4:F:173:ILE:HG22	2.00	0.41
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.03	0.41
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.56	0.41
2:D:287:THR:OG1	2:D:290:GLU:HG3	2.20	0.41
4:F:288:LYS:HG2	4:F:378:LEU:HD11	2.02	0.41
4:F:380:HIS:ND1	4:F:380:HIS:C	2.78	0.41
1:A:79:ARG:HG2	1:A:92:LEU:HD12	2.02	0.41
1:A:174:ALA:HA	1:A:175:PRO:HD2	1.87	0.41
2:B:284:ARG:HE	2:B:284:ARG:HB3	1.65	0.41
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.51	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.03	0.41
1:A:336:LYS:HD3	1:A:336:LYS:O	2.20	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.41
2:D:251:ASP:OD2	12:D:601:HOH:O	2.21	0.41
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.41
1:C:163:LYS:HG3	3:E:90:ASN:OD1	2.19	0.41
4:F:47:LEU:HA	4:F:48:PRO:HD3	1.82	0.41
4:F:101:TYR:HE2	4:F:125:THR:O	2.04	0.41
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.03	0.41
4:F:331:GLU:HG2	11:F:401:ACP:O3G	2.20	0.41
1:A:250[A]:VAL:HG22	1:A:254:GLU:OE1	2.20	0.40
1:A:431:ASP:O	1:A:435:VAL:HG13	2.20	0.40
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:HIS:NE2	2:D:407:TRP:HD1	2.19	0.40
2:B:41:ASP:O	2:B:47:GLU:HG3	2.21	0.40
2:D:109:THR:HB	2:D:110:GLU:H	1.71	0.40
2:B:287:THR:HB	2:B:289:PRO:HD2	2.03	0.40
3:E:72:LEU:HD12	3:E:72:LEU:HA	1.92	0.40
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.86	0.40
1:A:163:LYS:HE3	1:A:163:LYS:HB2	1.86	0.40
1:C:140:SER:HA	1:C:171:ILE:HB	2.03	0.40
4:F:3:THR:HB	4:F:30:LEU:HD11	2.03	0.40
4:F:238:CYS:HG	4:F:239:HIS:CE1	2.40	0.40
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CE1	4:F:142:ARG:NH2[2_564]	1.14	1.06
1:A:88:HIS:ND1	4:F:142:ARG:NH2[2_564]	1.95	0.25
2:D:338:LYS:NZ	4:F:90:SER:OG[3_545]	2.05	0.15

## 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	449/451 (100%)	440 (98%)	9 (2%)	0	100	100
1	C	457/451 (101%)	447 (98%)	10 (2%)	0	100	100
2	B	432/445 (97%)	417 (96%)	14 (3%)	1 (0%)	44	45
2	D	429/445 (96%)	410 (96%)	18 (4%)	1 (0%)	44	45
3	E	124/143 (87%)	123 (99%)	1 (1%)	0	100	100
4	F	346/384 (90%)	327 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2237/2319 (96%)	2164 (97%)	71 (3%)	2 (0%)	48	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	TYR
2	D	181	VAL

### 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	382/379 (101%)	373 (98%)	9 (2%)	44	49
1	C	390/379 (103%)	383 (98%)	7 (2%)	54	61
2	B	378/383 (99%)	366 (97%)	12 (3%)	34	37
2	D	374/383 (98%)	360 (96%)	14 (4%)	29	31
3	E	115/127 (91%)	110 (96%)	5 (4%)	25	25
4	F	320/342 (94%)	287 (90%)	33 (10%)	6	3
All	All	1959/1993 (98%)	1879 (96%)	80 (4%)	26	27

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	46	ASP
1	A	47	ASP
1	A	90	GLU
1	A	176	GLN
1	A	215	ARG
1	A	264	ARG
1	A	381	THR
1	A	435	VAL
2	B	1	MET

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Mol	Chain	Res	Type
2	B	7	ILE
2	B	119	LEU
2	B	204	ILE
2	B	221	THR
2	B	282	GLN
2	B	286	LEU
2	B	298	SER
2	B	325	MET
2	B	335	VAL
2	B	372	LYS
2	B	414	ASP
1	C	1	MET
1	C	218	ASP
1	C	285	GLN
1	C	347[A]	CYS
1	C	347[B]	CYS
1	C	386[A]	GLU
1	C	386[B]	GLU
2	D	1	MET
2	D	39	ASP
2	D	77	SER
2	D	116	ASP
2	D	153	LEU
2	D	247	GLN
2	D	248	LEU
2	D	276	THR
2	D	278	ARG
2	D	280	SER
2	D	298	SER
2	D	322	ARG
2	D	389	LYS
2	D	415	GLU
3	E	9	ILE
3	E	22	VAL
3	E	72	LEU
3	E	100	LYS
3	E	141	GLU
4	F	1	MET
4	F	10	ASN
4	F	12	SER
4	F	22	LEU
4	F	24	THR

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Mol	Chain	Res	Type
4	F	30	LEU
4	F	73	ARG
4	F	81	ILE
4	F	89	GLU
4	F	127	GLU
4	F	129	GLU
4	F	130	VAL
4	F	131	PHE
4	F	152	SER
4	F	160	ILE
4	F	170	LEU
4	F	183	GLN
4	F	184	LYS
4	F	186	LEU
4	F	210	LEU
4	F	229	ASN
4	F	244	CYS
4	F	247	LYS
4	F	251	LYS
4	F	257	GLU
4	F	258	GLU
4	F	307	LEU
4	F	311	SER
4	F	320	MET
4	F	326	LYS
4	F	331	GLU
4	F	378	LEU
4	F	380	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	101	ASN
1	A	256	GLN
2	B	136	GLN
2	B	167	ASN
2	B	300	ASN
2	B	331	GLN
2	B	334	ASN
2	B	385	GLN
1	C	11	GLN

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Mol	Chain	Res	Type
1	C	15	GLN
2	D	15	GLN
2	D	193	GLN
4	F	178	GLN
4	F	229	ASN
4	F	260	ASN
4	F	269	GLN
4	F	333	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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	$\# Z  > 2$
10	GOL	D	503	-	5,5,5	0.42	0	5,5,5	0.45	0
11	ACP	F	401	-	27,33,33	2.53	11 (40%)	33,52,52	4.64	14 (42%)
8	GDP	D	501	6	25,30,30	0.96	2 (8%)	30,47,47	1.16	2 (6%)
9	LLM	B	503	-	39,40,40	2.55	14 (35%)	41,55,55	1.95	8 (19%)
8	GDP	B	501	6	25,30,30	0.97	2 (8%)	30,47,47	1.29	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	A	501	6	29,34,34	1.17	1 (3%)	35,54,54	1.22	4 (11%)
5	GTP	C	501	6	29,34,34	1.23	2 (6%)	35,54,54	1.35	8 (22%)
10	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.50	0

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
10	GOL	D	503	-	-	2/4/4/4	-
11	ACP	F	401	-	-	5/15/38/38	0/3/3/3
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3
9	LLM	B	503	-	-	9/39/64/64	0/3/4/4
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
10	GOL	B	504	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	LLM	C22-C21	6.85	1.52	1.32
11	F	401	ACP	PG-O1G	5.68	1.61	1.50
9	B	503	LLM	C5-C6	-5.49	1.40	1.50
11	F	401	ACP	C2-N3	5.07	1.39	1.32
9	B	503	LLM	C30-C25	-5.04	1.38	1.50
11	F	401	ACP	PB-O1B	4.46	1.62	1.51
9	B	503	LLM	C27-C26	-4.19	1.40	1.48
9	B	503	LLM	C8-C7	-4.07	1.41	1.49
5	A	501	GTP	C5-C6	-4.01	1.39	1.47
5	C	501	GTP	C5-C6	-3.99	1.39	1.47
9	B	503	LLM	C2-C1	-3.91	1.39	1.48
9	B	503	LLM	C4-C3	-3.84	1.39	1.50
9	B	503	LLM	C14-C13	-3.75	1.39	1.50
11	F	401	ACP	PA-O3A	3.64	1.63	1.59
9	B	503	LLM	C24-C25	-3.61	1.41	1.50
11	F	401	ACP	C2-N1	3.60	1.40	1.33
9	B	503	LLM	C12-C13	-3.45	1.40	1.50
11	F	401	ACP	PB-O2B	-3.28	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	LLM	C6-C7	3.23	1.40	1.32
9	B	503	LLM	C29-C13	2.93	1.39	1.32
11	F	401	ACP	C6-C5	-2.78	1.33	1.43
11	F	401	ACP	C3'-C4'	2.77	1.60	1.53
11	F	401	ACP	PG-O2G	-2.76	1.48	1.55
11	F	401	ACP	C2'-C3'	-2.74	1.46	1.53
11	F	401	ACP	PA-O1A	2.73	1.60	1.50
9	B	503	LLM	C16-C17	2.71	1.50	1.46
9	B	503	LLM	C2-C3	2.69	1.39	1.32
5	C	501	GTP	PA-O3A	2.38	1.62	1.59
8	B	501	GDP	O4'-C1'	2.21	1.43	1.40
8	B	501	GDP	C6-N1	-2.14	1.34	1.37
8	D	501	GDP	C6-N1	-2.09	1.34	1.37
8	D	501	GDP	O4'-C1'	2.00	1.43	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	O4'-C4'-C5'	12.84	150.47	109.33
11	F	401	ACP	O4'-C4'-C3'	-10.42	84.48	105.15
11	F	401	ACP	C4'-O4'-C1'	9.26	118.41	109.92
11	F	401	ACP	C1'-N9-C4	-8.71	111.34	126.64
11	F	401	ACP	N3-C2-N1	-7.91	117.93	128.67
11	F	401	ACP	O4'-C1'-N9	7.67	118.91	108.75
11	F	401	ACP	C5'-C4'-C3'	-6.38	92.23	115.21
9	B	503	LLM	C20-C21-C22	-5.81	116.11	124.94
9	B	503	LLM	C23-C22-C21	-5.54	113.00	125.02
11	F	401	ACP	PB-O3A-PA	-4.31	118.30	132.37
11	F	401	ACP	O2G-PG-C3B	4.26	116.73	106.40
11	F	401	ACP	O3'-C3'-C2'	-4.06	98.81	111.82
9	B	503	LLM	C18-C17-C16	-4.02	114.42	123.98
11	F	401	ACP	C2'-C3'-C4'	3.67	109.71	102.61
5	C	501	GTP	C8-N7-C5	3.64	108.74	102.55
5	A	501	GTP	C8-N7-C5	3.57	108.62	102.55
9	B	503	LLM	C16-O16-C17	3.26	62.67	60.62
11	F	401	ACP	C5-C6-N6	-2.87	115.94	120.31
8	D	501	GDP	C8-N7-C5	2.80	107.32	102.55
11	F	401	ACP	O5'-C5'-C4'	2.75	118.36	108.99
9	B	503	LLM	C11-C10-C9	-2.74	110.27	115.35
11	F	401	ACP	O3G-PG-O1G	-2.69	105.44	112.39
5	C	501	GTP	C5-C6-N1	2.66	119.14	114.07
9	B	503	LLM	C9-C8-C7	2.65	114.73	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C8-N7-C5	2.64	107.04	102.55
8	B	501	GDP	O4'-C1'-N9	-2.63	105.25	108.75
8	B	501	GDP	C5-C6-N1	2.52	118.87	114.07
5	A	501	GTP	C5-C6-N1	2.45	118.74	114.07
5	C	501	GTP	C2-N1-C6	-2.42	120.68	125.11
5	C	501	GTP	O2A-PA-O3A	2.37	113.67	107.27
9	B	503	LLM	O19-C1-C2	2.32	116.43	111.39
5	A	501	GTP	C2-N1-C6	-2.26	120.97	125.11
8	B	501	GDP	O6-C6-C5	-2.20	119.96	124.32
9	B	503	LLM	C4-C5-C6	-2.18	109.16	113.00
5	C	501	GTP	O6-C6-C5	-2.15	120.06	124.32
8	B	501	GDP	O2A-PA-O3A	2.15	113.07	107.27
5	A	501	GTP	O2A-PA-O3A	2.14	113.07	107.27
8	D	501	GDP	C5-C6-N1	2.13	118.13	114.07
5	C	501	GTP	N1-C2-N3	-2.04	119.58	123.32
5	C	501	GTP	N2-C2-N1	2.03	121.05	116.76
5	C	501	GTP	O2B-PB-O3A	2.02	112.73	107.27

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	LLM	C11-C12-C13-C14
9	B	503	LLM	C11-C12-C13-C29
9	B	503	LLM	C9-C10-C11-C12
9	B	503	LLM	C9-C10-C11-C28
10	B	504	GOL	O1-C1-C2-C3
10	D	503	GOL	O1-C1-C2-C3
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	503	LLM	C11-C10-C9-O9

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Mol	Chain	Res	Type	Atoms
10	B	504	GOL	O1-C1-C2-O2
10	D	503	GOL	O1-C1-C2-O2
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PB-O3A-PA-O2A
9	B	503	LLM	O19-C19-C20-C21
9	B	503	LLM	C12-C13-C14-C15
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	C5'-O5'-PA-O1A
9	B	503	LLM	C29-C13-C14-C15
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
9	B	503	LLM	C11-C10-C9-C8
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-C3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O1A

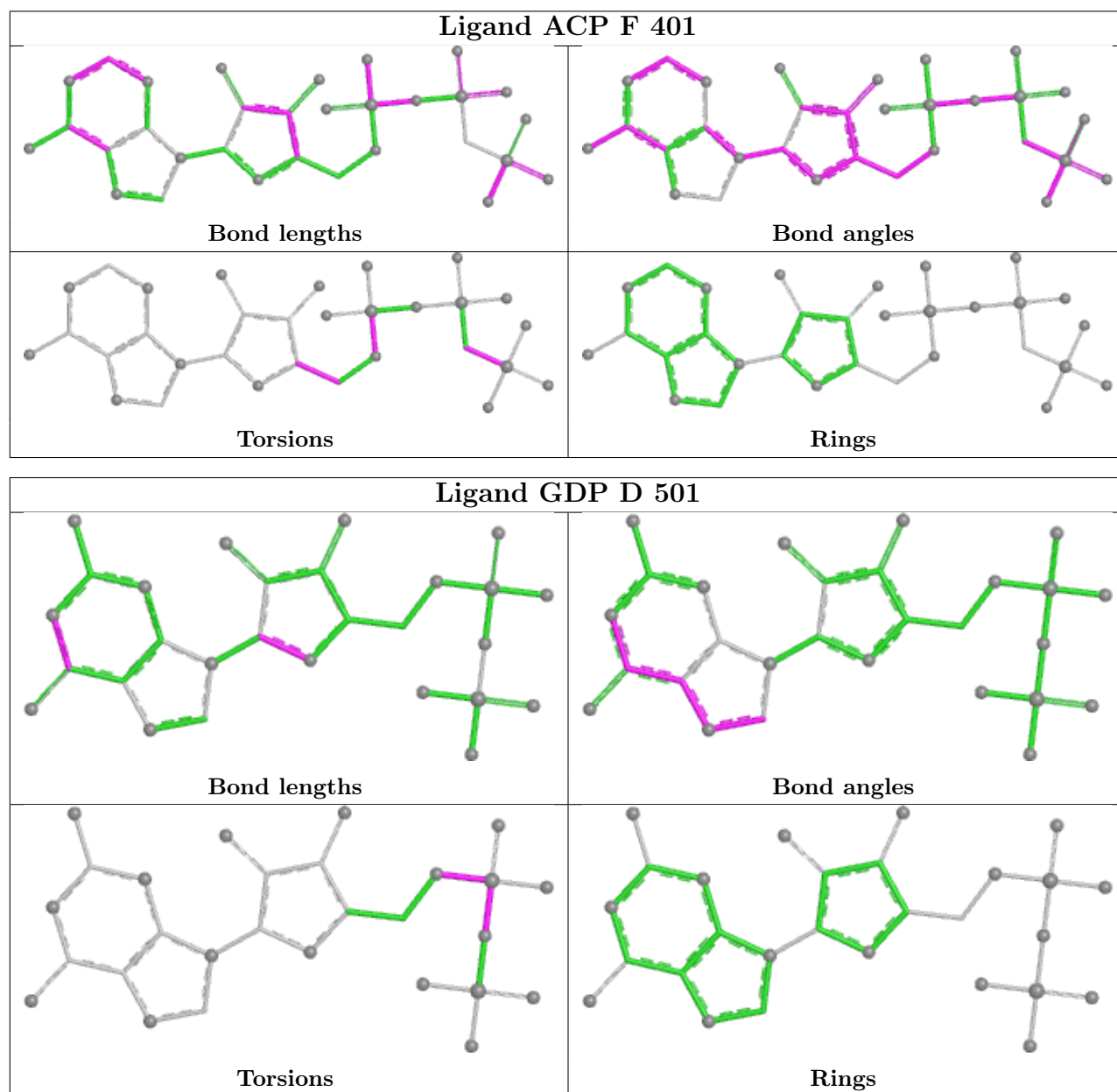
There are no ring outliers.

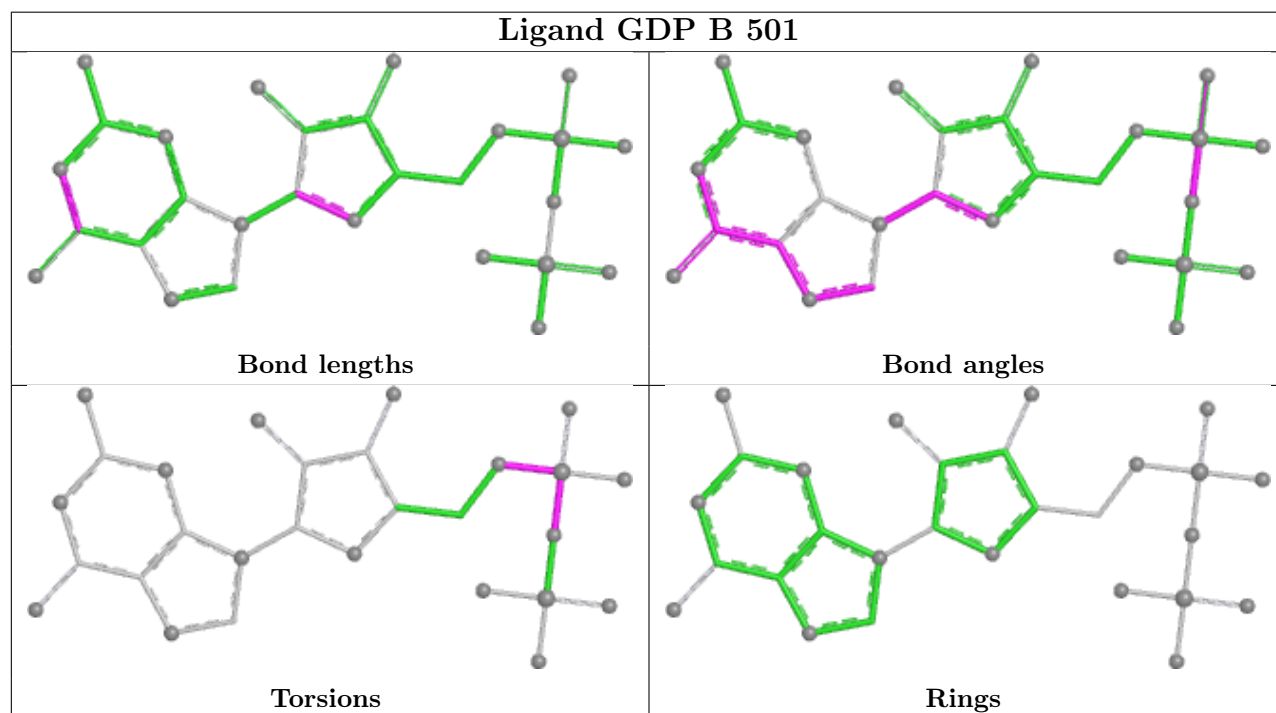
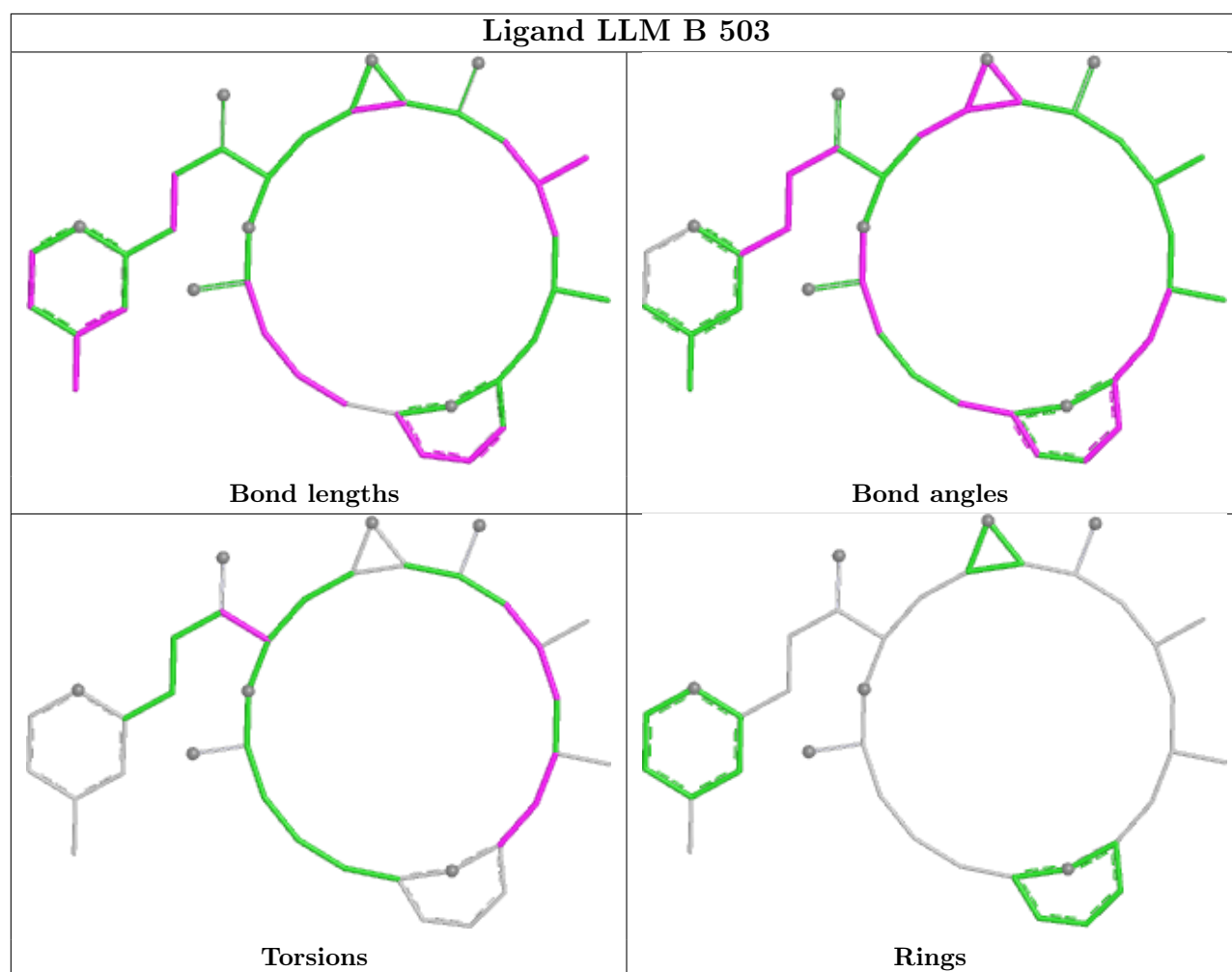
3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	6	0
9	B	503	LLM	7	0
10	B	504	GOL	5	0

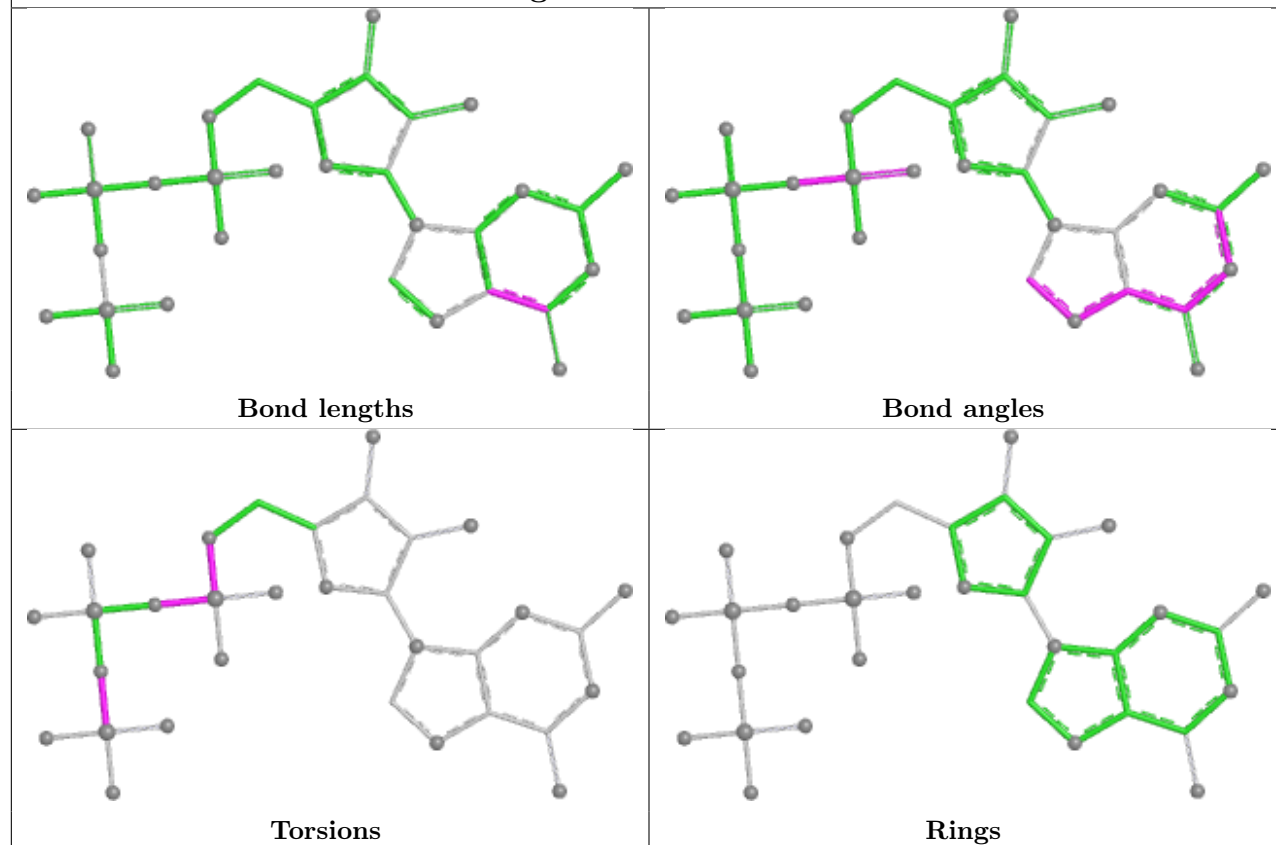
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

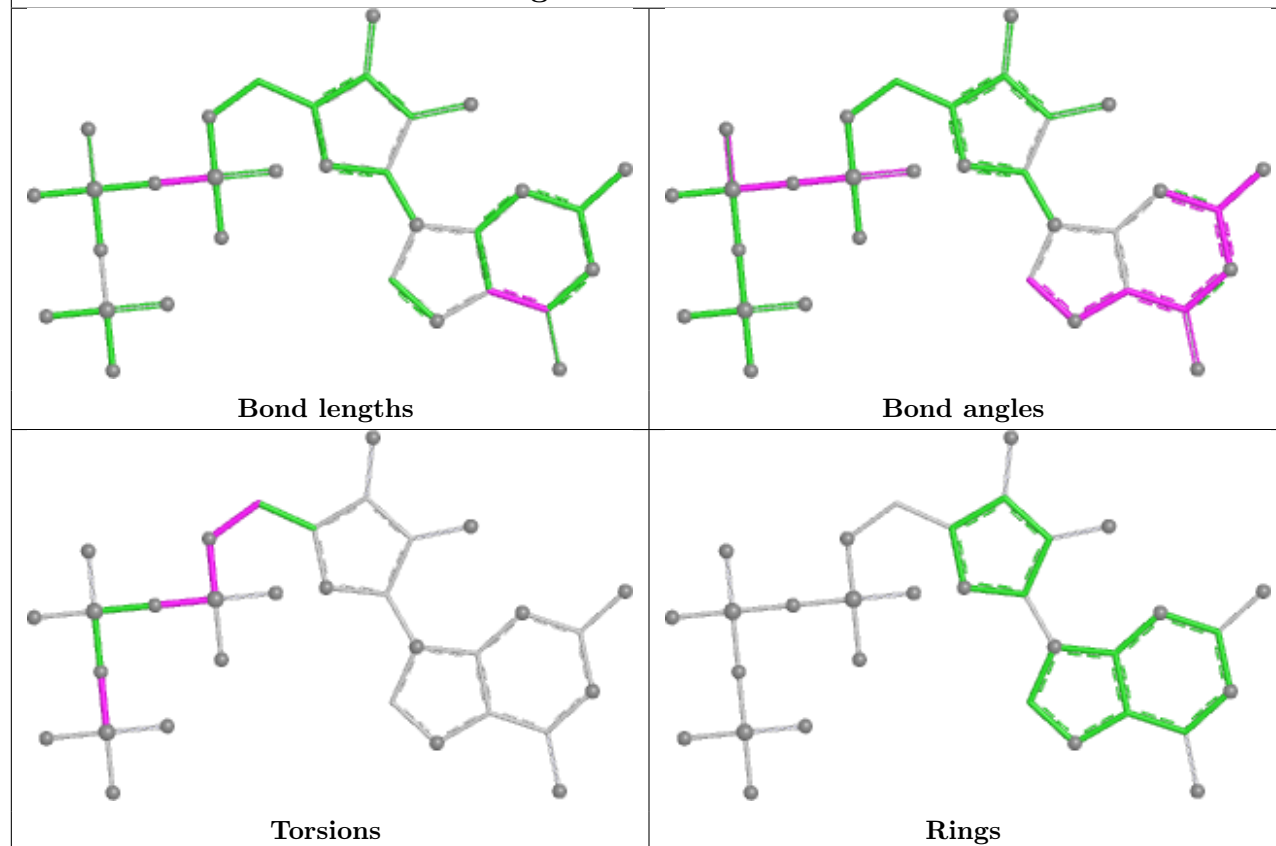




## Ligand GTP A 501



## Ligand GTP C 501



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	439/451 (97%)	0.01	15 (3%)	48	50	20, 44, 80, 131	12 (2%)
1	C	440/451 (97%)	-0.27	11 (2%)	58	60	17, 33, 58, 99	19 (4%)
2	B	426/445 (95%)	0.02	9 (2%)	63	65	18, 41, 71, 126	12 (2%)
2	D	427/445 (95%)	0.19	22 (5%)	34	36	23, 47, 78, 123	12 (2%)
3	E	123/143 (86%)	0.53	9 (7%)	22	24	23, 56, 93, 139	5 (4%)
4	F	348/384 (90%)	0.88	53 (15%)	6	7	30, 69, 131, 174	6 (1%)
All	All	2203/2319 (94%)	0.16	119 (5%)	32	35	17, 45, 96, 174	66 (2%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	7.0
2	D	285	ALA	5.8
2	D	1	MET	5.6
4	F	105	LEU	5.0
3	E	143	ALA	5.0
2	D	277	SER	4.1
1	A	282	TYR	4.0
2	D	179	ASP	4.0
4	F	130	VAL	3.9
1	C	1	MET	3.8
4	F	182	ILE	3.8
4	F	177	GLY	3.8
4	F	249	TYR	3.8
4	F	380	HIS	3.7
1	A	439	SER	3.7
4	F	371	PRO	3.6
2	D	280	SER	3.6
2	D	276	THR	3.6
4	F	179	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	3.6
2	D	407	TRP	3.5
1	C	340	SER	3.4
2	B	57	THR	3.4
4	F	372	THR	3.4
4	F	181	VAL	3.2
4	F	233	PHE	3.2
4	F	90	SER	3.2
4	F	152	SER	3.2
1	C	46	ASP	3.2
4	F	81	ILE	3.1
2	B	247	GLN	3.1
2	D	279	GLY	3.1
1	C	440	VAL	3.1
2	D	82	PRO	3.1
1	A	179	THR	3.1
4	F	36	ARG	3.1
4	F	237	THR	3.0
4	F	379	HIS	3.0
2	D	404	PHE	3.0
4	F	125	THR	3.0
2	B	47	GLU	3.0
2	D	405	LEU	2.9
4	F	161	LEU	2.9
3	E	28	SER	2.9
2	D	2	ARG	2.9
2	D	247	GLN	2.9
4	F	24	THR	2.9
1	A	283	HIS	2.8
4	F	31	ARG	2.8
2	B	248	LEU	2.8
4	F	169	LEU	2.8
1	A	281	ALA	2.8
4	F	173	ILE	2.8
4	F	244	CYS	2.8
4	F	103	THR	2.7
1	A	88	HIS	2.7
4	F	101	TYR	2.7
4	F	236	LYS	2.7
4	F	178	GLN	2.7
3	E	45	PRO	2.7
1	A	48	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	362	ALA	2.6
4	F	172	PHE	2.6
4	F	241	THR	2.6
4	F	6	VAL	2.6
4	F	259	GLY	2.6
1	A	346	TRP	2.6
2	D	278	ARG	2.6
2	B	282	GLN	2.6
4	F	162	ILE	2.5
4	F	88	SER	2.5
4	F	170	LEU	2.5
2	D	304	ALA	2.5
1	C	179	THR	2.5
1	A	437	VAL	2.5
3	E	27	PRO	2.4
2	D	83	PHE	2.4
4	F	160	ILE	2.4
2	D	286	LEU	2.4
4	F	32	LYS	2.4
4	F	128	ARG	2.4
4	F	132	LEU	2.4
1	C	357	TYR	2.4
2	D	81	GLY	2.4
2	B	42	LEU	2.4
4	F	247	LYS	2.4
1	A	163	LYS	2.3
1	A	46	ASP	2.3
1	C	2	ARG	2.3
1	A	80[A]	THR	2.3
3	E	51	GLN	2.3
4	F	159	GLY	2.2
1	C	247	ALA	2.2
3	E	138	GLU	2.2
4	F	230	SER	2.2
1	A	96	LYS	2.2
1	C	245	ASP	2.2
2	B	2	ARG	2.2
2	D	37	HIS	2.2
4	F	126	ASP	2.1
4	F	135	TYR	2.1
3	E	139	LEU	2.1
2	B	439	THR	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	33	ASP	2.1
4	F	242	ASN	2.1
1	A	35	GLN	2.1
1	C	284	GLU	2.1
4	F	91	CYS	2.1
2	D	400	ARG	2.1
2	D	57	THR	2.1
4	F	167	SER	2.1
4	F	28	LYS	2.1
4	F	305	LYS	2.1
4	F	231	ALA	2.0
3	E	106	GLU	2.0
1	C	128	GLN	2.0
2	D	220	THR	2.0
1	A	341	ILE	2.0
3	E	140	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	Q<0.9
7	CA	B	505	1/1	0.66	0.17	109,109,109,109	0
10	GOL	D	503	6/6	0.75	0.26	63,74,92,100	0
7	CA	B	506	1/1	0.80	0.11	93,93,93,93	0
10	GOL	B	504	6/6	0.85	0.18	55,62,66,75	0
11	ACP	F	401	31/31	0.85	0.13	49,73,130,140	0
9	LLM	B	503	37/37	0.87	0.17	91,93,102,104	0
7	CA	A	503	1/1	0.90	0.13	80,80,80,80	0

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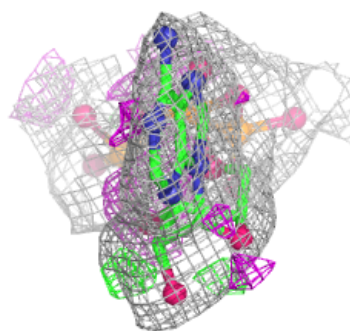
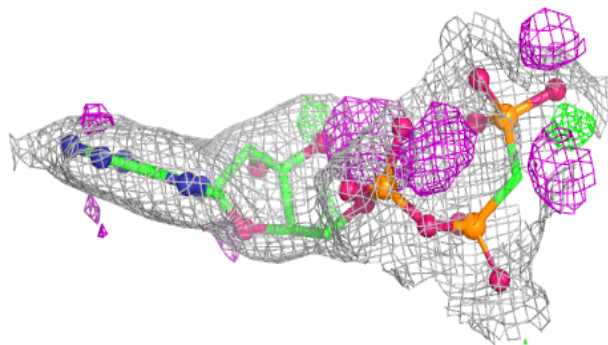
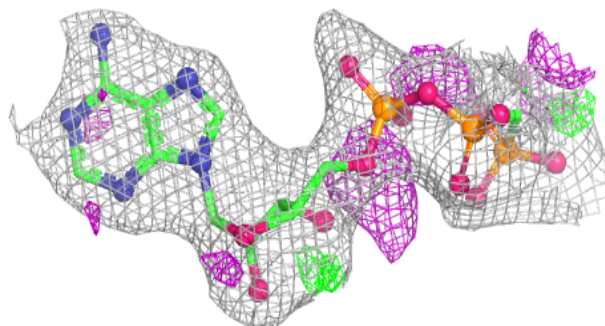
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	F	402	1/1	0.92	0.24	30,30,30,30	0
8	GDP	D	501	28/28	0.95	0.09	34,44,53,59	0
6	MG	B	502	1/1	0.98	0.07	22,22,22,22	0
6	MG	C	502	1/1	0.98	0.14	34,34,34,34	0
6	MG	D	502	1/1	0.98	0.05	44,44,44,44	0
6	MG	A	502	1/1	0.98	0.12	38,38,38,38	0
8	GDP	B	501	28/28	0.99	0.04	21,27,33,37	0
5	GTP	A	501	32/32	0.99	0.04	25,30,34,43	0
5	GTP	C	501	32/32	0.99	0.04	21,26,32,36	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.

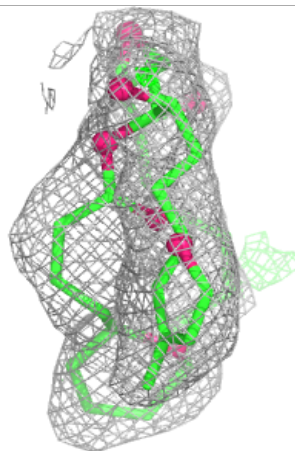
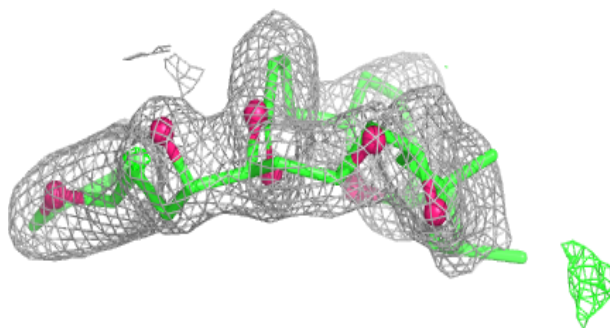
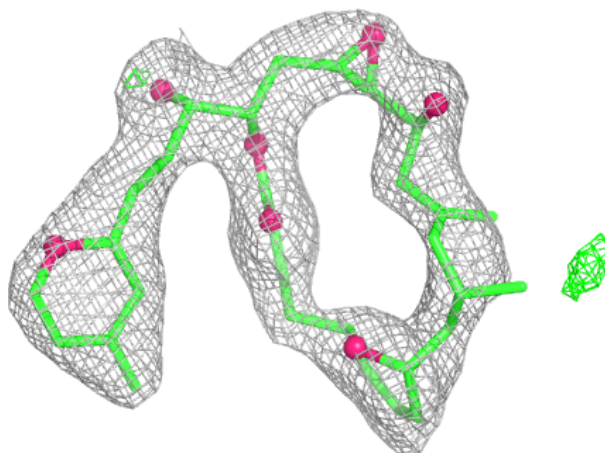
**Electron density around ACP F 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



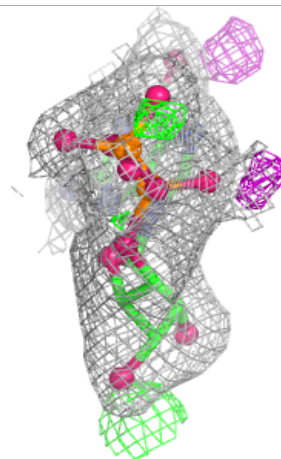
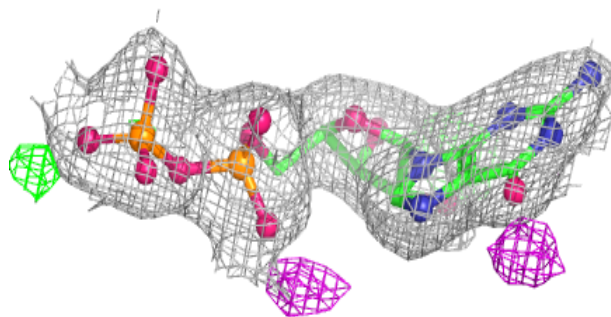
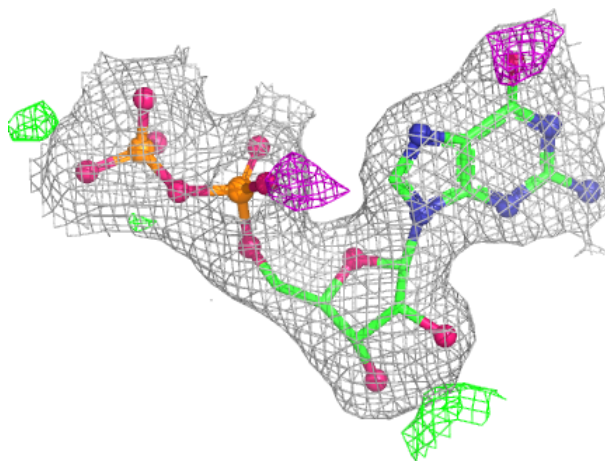
**Electron density around LLM B 503:**

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



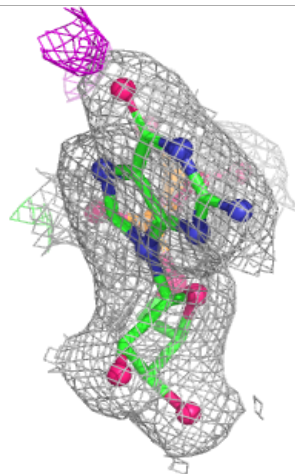
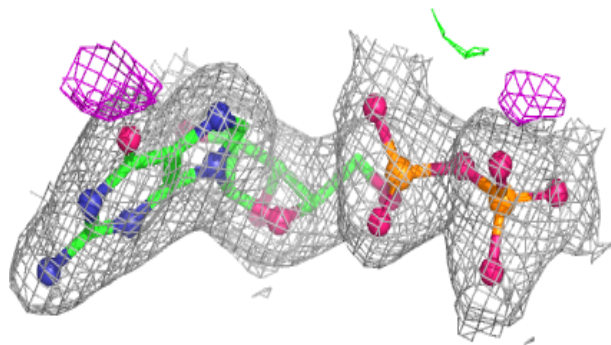
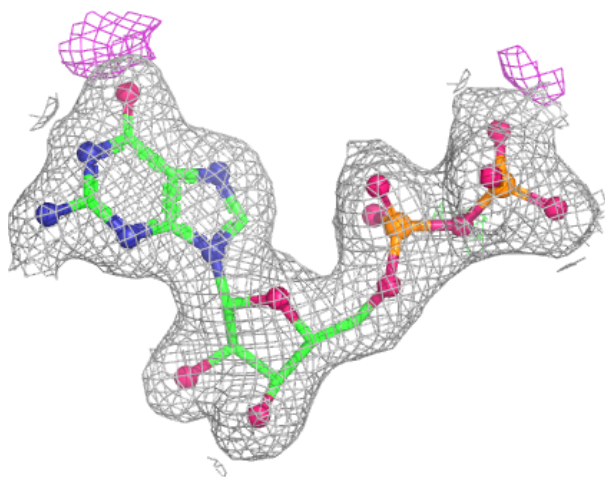
**Electron density around GDP D 501:**

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



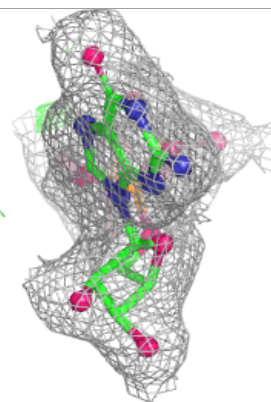
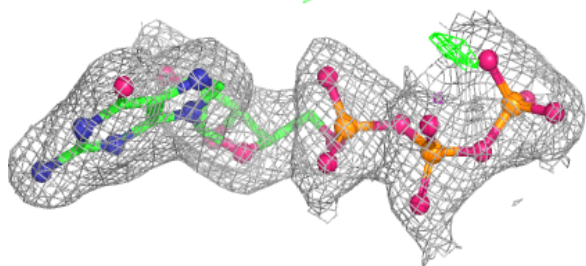
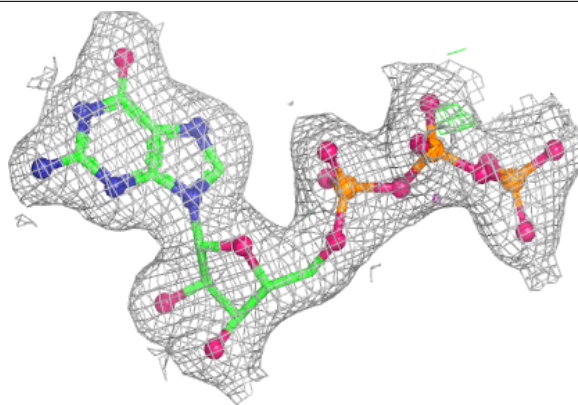
**Electron density around GDP B 501:**

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

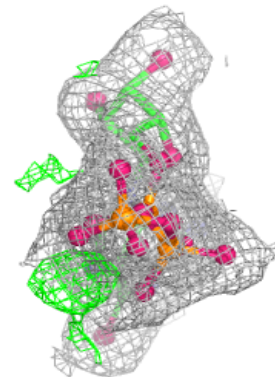
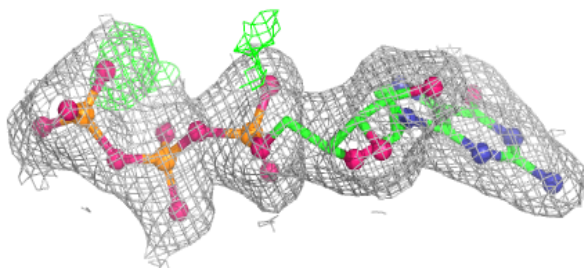
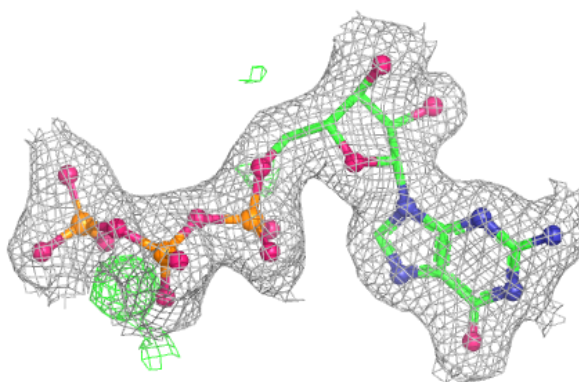


**Electron density around GTP A 501:**

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

**Electron density around GTP C 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.