Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 09:27 PM EST

PDB ID	:	3UT5
Title	:	Tubulin-Colchicine-Ustiloxin: Stathmin-like domain complex
Authors	:	Ranaivoson, F.M.; Gigant, B.; Knossow, M.
Deposited on	:	2011-11-25
Resolution	:	2.73 Å(reported)

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

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

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

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

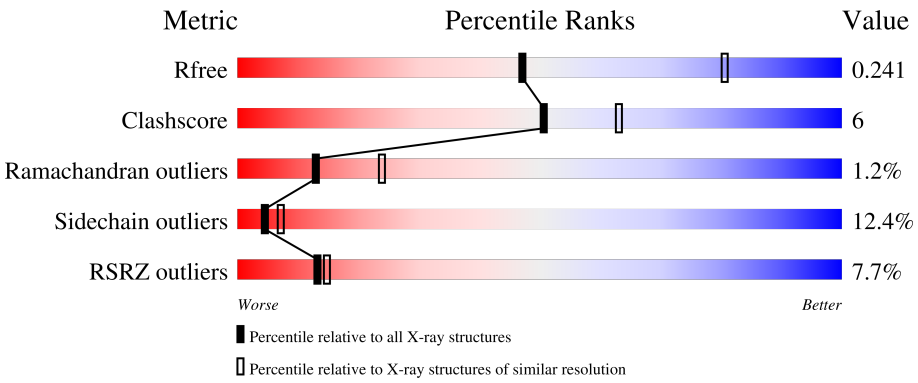
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	451	7% 77% 16% • •
1	C	451	4% 74% 20% • •
2	B	445	11% 76% 18% • •
2	D	445	5% 76% 16% • •
3	E	142	13% 73% 18% • 7%

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Mol	Chain	Length	Quality of chain
4	F	4	25% 50% 25% 25%

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
4	0E5	F	3	X	X	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15107 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3399	2153	577	647	22	0	1	0
1	C	432	3404	2158	575	648	23	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	432	3417	2141	584	665	27	0	3	0
2	D	432	3433	2153	584	670	26	0	5	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	132	1077	666	195	212	4	0	1	0

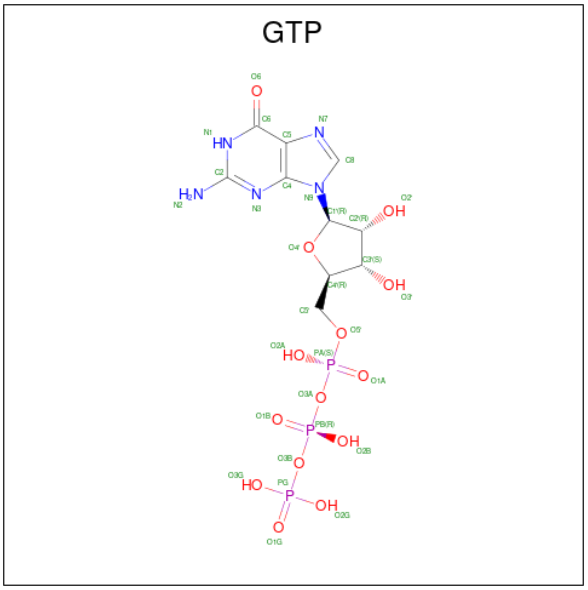
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is a protein called Vinca tetrapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	4	35	23	4	8	0	0	0

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

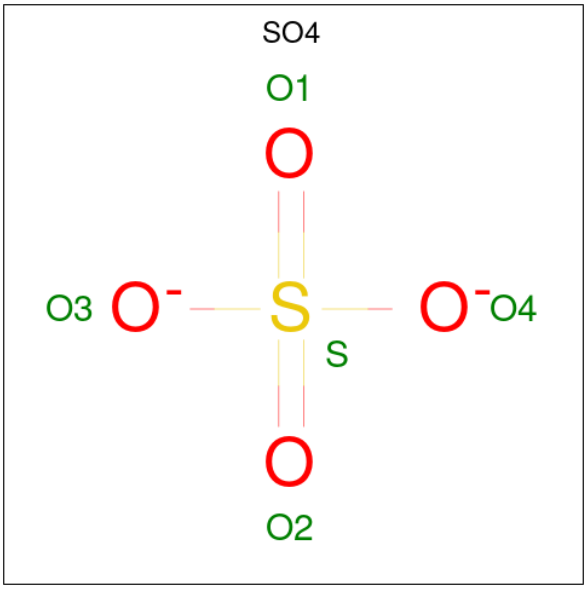


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
5	C	1	32	10	5	14	3	0	0

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

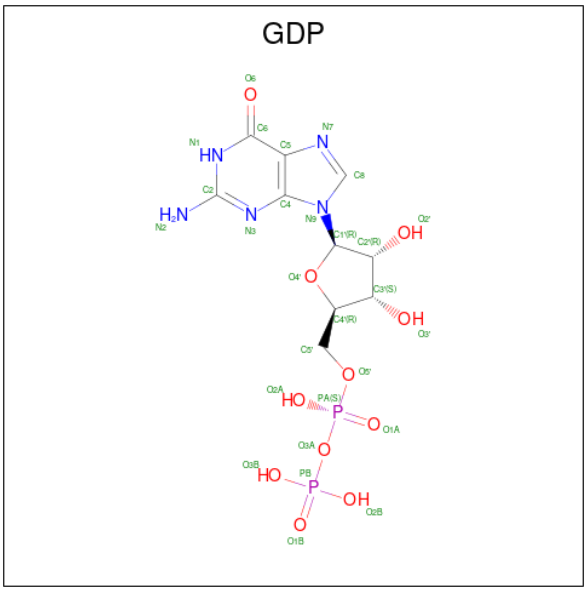
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



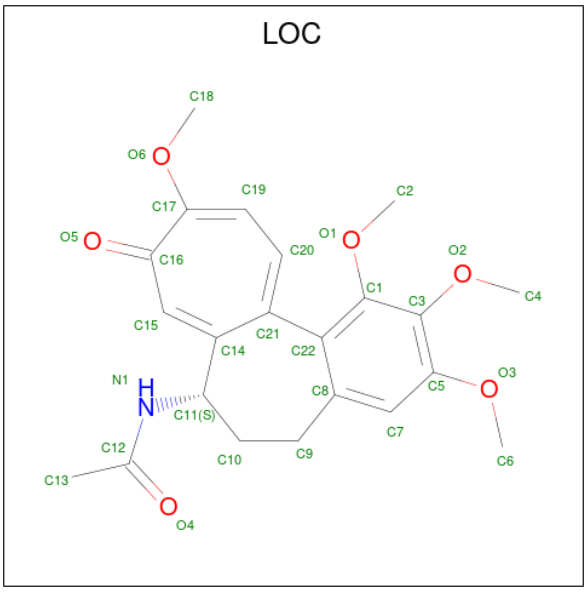
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0

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



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

- Molecule 9 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]eth anamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	B	1	29	22	1	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	D	1	29	22	1	6	0	0

- Molecule 10 is water.

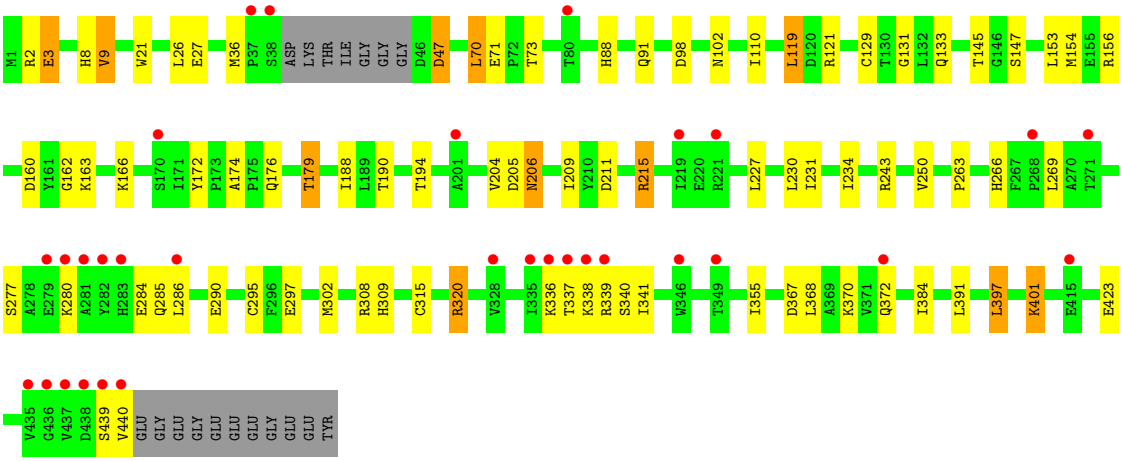
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	27	27	27	0	0
			Total	O		
10	B	28	28	28	0	0
			Total	O		
10	C	43	43	43	0	0
			Total	O		
10	D	36	36	36	0	0
			Total	O		
10	E	3	3	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

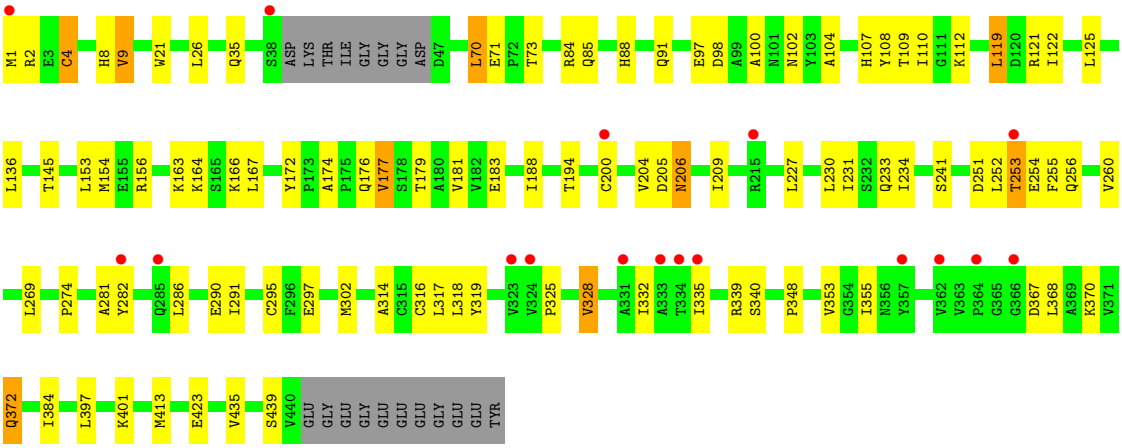
• Molecule 1: Tubulin alpha chain

Chain A:



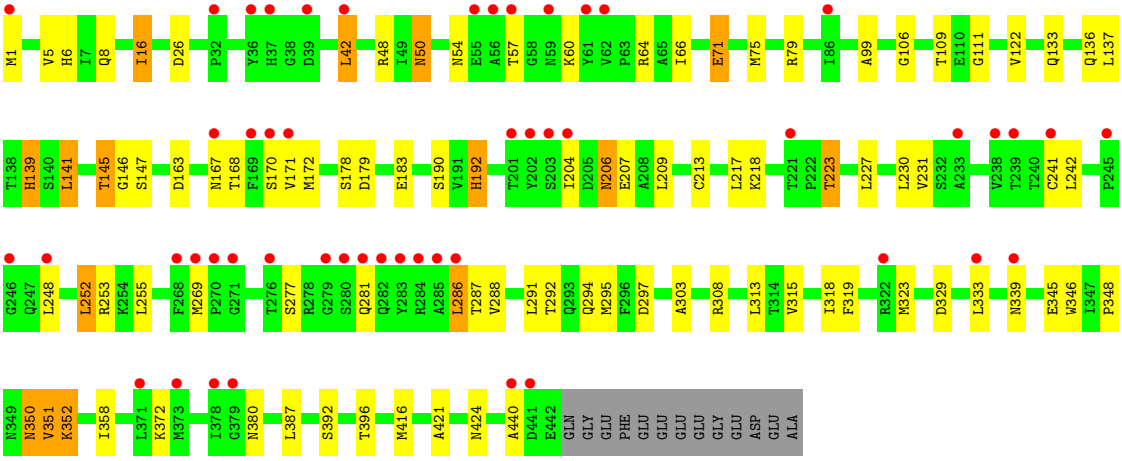
• Molecule 1: Tubulin alpha chain

Chain C:



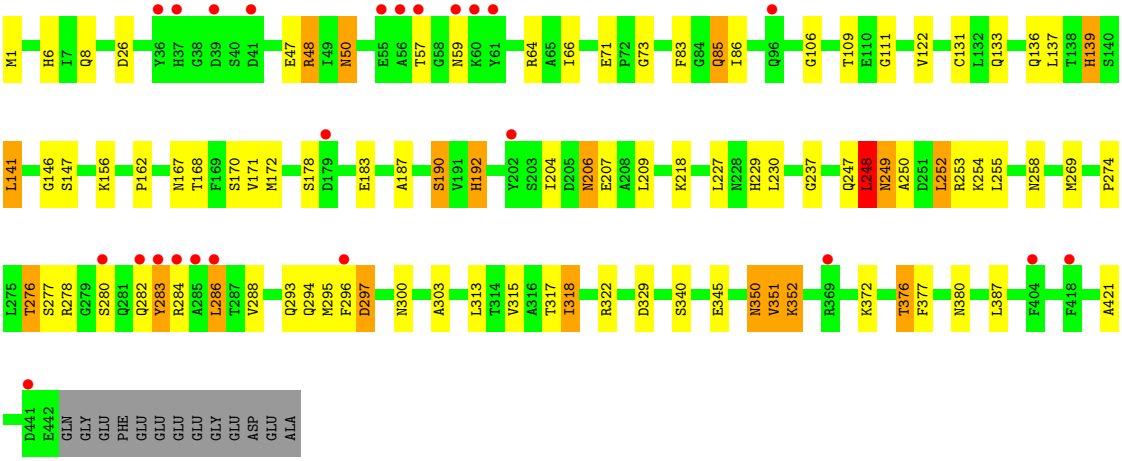
• Molecule 2: Tubulin beta chain

Chain B:



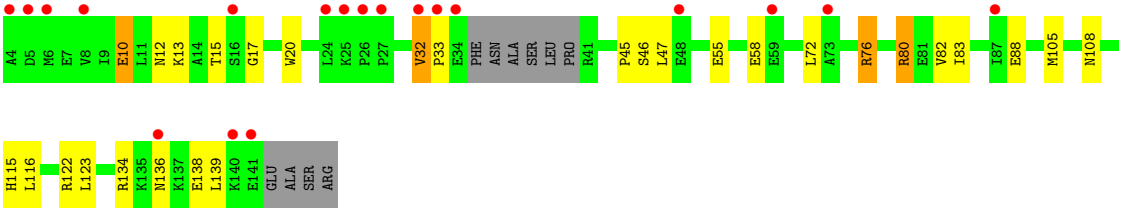
- Molecule 2: Tubulin beta chain

Chain D:



- Molecule 3: Stathmin-4

Chain E:



- Molecule 4: Vinca tetrapeptide

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.81Å 128.87Å 254.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.26 – 2.73 38.26 – 2.73	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.26-2.73) 97.6 (38.26-2.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.72Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.184 , 0.222 0.201 , 0.241	Depositor DCC
R_{free} test set	2872 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15107	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 0EA, GTP, MG, SO4, 0E5, LOC

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	0.43	0/3479	0.68	0/4723
1	C	0.45	0/3491	0.70	0/4741
2	B	0.42	0/3503	0.69	0/4744
2	D	0.43	0/3516	0.68	0/4762
3	E	0.46	0/1092	0.68	0/1455
4	F	1.32	0/10	0.38	0/9
All	All	0.44	0/15091	0.69	0/20434

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	0E5	C3

There are no planarity outliers.

5.2 Too-close contacts (i)

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	0	3312	31	0
1	C	3404	0	3311	39	0
2	B	3417	0	3283	47	0
2	D	3433	0	3301	53	0
3	E	1077	0	1068	7	0
4	F	35	0	24	1	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	D	10	0	0	0	0
8	B	28	0	12	3	0
8	D	28	0	12	2	0
9	B	29	0	25	4	0
9	D	29	0	25	3	0
10	A	27	0	0	0	0
10	B	28	0	0	1	0
10	C	43	0	0	0	0
10	D	36	0	0	1	0
10	E	3	0	0	0	0
All	All	15107	0	14397	168	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 6.

All (168) 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:B:206:ASN:HD21	8:B:501:GDP:HN22	1.24	0.86
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.59	0.85
1:C:206:ASN:HD21	5:C:600:GTP:HN22	1.24	0.83
1:A:206:ASN:HD21	5:A:501:GTP:HN22	1.26	0.82
2:D:206:ASN:HD21	8:D:501:GDP:HN22	1.25	0.82
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.51	0.76
2:D:237:GLY:CA	2:D:376:THR:HG21	2.17	0.74
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.37	0.72
2:D:318:ILE:HG23	2:D:376:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ASN:HD22	2:B:350:ASN:H	1.40	0.68
2:D:317:THR:HG22	2:D:377[B]:PHE:HD1	1.58	0.68
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.28	0.68
2:D:350:ASN:H	2:D:350:ASN:HD22	1.40	0.68
2:B:318:ILE:HD11	9:B:502:LOC:H4	1.76	0.68
2:D:172:MET:HG3	2:D:387:LEU:HD21	1.75	0.68
2:D:50:ASN:O	2:D:64:ARG:NH2	2.27	0.68
2:B:50:ASN:O	2:B:64:ARG:NH2	2.21	0.68
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.76	0.68
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.77	0.66
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.78	0.66
1:C:84:ARG:O	1:C:85:GLN:HB2	1.96	0.66
2:B:141:LEU:HD21	2:B:170:SER:HB3	1.78	0.65
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.79	0.64
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.79	0.64
2:B:71[B]:GLU:HG2	1:C:2:ARG:HH22	1.61	0.63
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.80	0.63
2:D:133:GLN:HE21	2:D:252:LEU:H	1.45	0.62
2:D:209:LEU:HB3	2:D:227:LEU:HG	1.83	0.60
2:D:352:LYS:HB2	9:D:502:LOC:H18B	1.84	0.59
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.83	0.59
2:D:66:ILE:HD13	2:D:122:VAL:HG12	1.84	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.03	0.59
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.86	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.87	0.57
1:C:70:LEU:HG	1:C:110:ILE:HG22	1.87	0.57
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.86	0.57
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.24	0.56
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.71	0.56
1:A:3:GLU:HG3	1:A:129:CYS:SG	2.46	0.56
1:A:70:LEU:HG	1:A:110:ILE:HG22	1.88	0.56
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.88	0.55
2:D:229:HIS:NE2	2:D:276:THR:HG22	2.21	0.55
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.53	0.55
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.88	0.55
3:E:10:GLU:HA	3:E:20:TRP:HB2	1.89	0.55
2:B:133:GLN:HE21	2:B:252:LEU:H	1.55	0.55
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.71	0.55
2:B:136:GLN:HA	2:B:167:ASN:O	2.08	0.54
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.89	0.54
1:A:285:GLN:HE22	1:A:372:GLN:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD23	2:B:348:PRO:HG3	1.90	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.08	0.53
2:B:315:VAL:HB	2:B:351:VAL:HB	1.92	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.58	0.52
2:B:392:SER:O	2:B:396:THR:HG23	2.09	0.52
2:D:133:GLN:NE2	2:D:252:LEU:H	2.08	0.52
1:A:308:ARG:HH21	1:A:309:HIS:HD2	1.57	0.52
2:B:424:ASN:HB2	10:B:619:HOH:O	2.08	0.52
1:C:97:GLU:HB2	2:D:1:MET:HG2	1.91	0.52
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.92	0.51
2:D:248:LEU:HD13	2:D:249:ASN:H	1.75	0.51
2:D:278:ARG:C	2:D:280:SER:H	2.14	0.51
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.24	0.51
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.57	0.51
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.43	0.51
1:C:241:SER:HB2	1:C:251:ASP:HA	1.93	0.50
1:A:211:ASP:O	1:A:215:ARG:HD2	2.11	0.50
2:B:99:ALA:HB2	2:B:145:THR:HG22	1.93	0.50
2:B:286:LEU:HD21	2:B:291:LEU:HD13	1.94	0.50
2:D:315:VAL:HB	2:D:351:VAL:HB	1.92	0.50
1:A:263:PRO:O	1:A:266:HIS:HD2	1.94	0.50
2:B:171:VAL:HA	2:B:204:ILE:O	2.11	0.50
2:B:42:LEU:HD12	2:B:358:ILE:HD11	1.94	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
1:C:325:PRO:HA	1:C:328:VAL:CG2	2.42	0.49
1:C:100:ALA:HA	2:D:254:LYS:HG2	1.93	0.49
3:E:115:HIS:HD2	3:E:116:LEU:HD22	1.77	0.49
2:D:350:ASN:H	2:D:350:ASN:ND2	2.09	0.49
2:B:223:THR:HA	4:F:3:0E5:H5	1.95	0.49
1:A:154:MET:HG3	1:A:194:THR:HG23	1.96	0.48
2:D:106:GLY:O	2:D:111:GLY:HA3	2.14	0.48
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.95	0.48
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.95	0.47
2:D:147[A]:SER:HB2	2:D:190:SER:HG	1.78	0.47
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.96	0.47
1:A:174:ALA:HB1	1:A:176:GLN:HE21	1.80	0.47
2:B:318:ILE:HD11	9:B:502:LOC:C4	2.45	0.47
1:C:174:ALA:HB1	1:C:176:GLN:HE21	1.79	0.47
1:A:2:ARG:HB3	1:A:133[A]:GLN:NE2	2.30	0.47
1:C:154:MET:HG3	1:C:194:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD23	2:B:172:MET:SD	2.56	0.46
1:A:355:ILE:O	3:E:17:GLY:HA2	2.15	0.46
2:B:183:GLU:OE2	8:B:501:GDP:H3'	2.16	0.46
2:D:183:GLU:OE2	8:D:501:GDP:H3'	2.16	0.46
1:C:179:THR:HG22	1:C:183:GLU:OE2	2.15	0.46
2:B:163:ASP:O	2:B:253[B]:ARG:NH2	2.48	0.45
1:A:9:VAL:HG23	1:A:145:THR:HG22	1.98	0.45
2:D:85:GLN:H	2:D:85:GLN:CD	2.19	0.45
1:C:181:VAL:HG22	2:D:258:ASN:HD22	1.80	0.45
2:B:16:ILE:HG12	2:B:231:VAL:HG11	1.98	0.45
2:D:141:LEU:HD23	2:D:172:MET:SD	2.56	0.45
2:B:346:TRP:HB3	2:B:440:ALA:HB2	1.99	0.45
2:D:253:ARG:NH2	10:D:633:HOH:O	2.49	0.45
2:B:99:ALA:CB	2:B:145:THR:HG22	2.46	0.45
2:D:139:HIS:HD2	2:D:146:GLY:O	2.00	0.45
2:D:350:ASN:HD22	2:D:350:ASN:N	2.10	0.45
2:B:350:ASN:H	2:B:350:ASN:ND2	2.09	0.44
1:C:9:VAL:HG23	1:C:145:THR:HG22	1.99	0.44
1:C:286:LEU:HD21	1:C:291:ILE:HG23	1.99	0.44
2:B:352:LYS:HE3	9:B:502:LOC:O5	2.18	0.44
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.35	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.44
1:A:230:LEU:O	1:A:234:ILE:HD12	2.17	0.44
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.44
2:D:294:GLN:HA	2:D:297:ASP:HB2	2.00	0.44
1:C:84:ARG:O	1:C:85:GLN:CB	2.66	0.44
2:D:162:PRO:HB2	3:E:116:LEU:HD12	2.00	0.43
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.58	0.43
1:A:2:ARG:HB3	1:A:133[A]:GLN:HE21	1.83	0.43
2:D:133:GLN:HE21	2:D:252:LEU:HB2	1.83	0.43
3:E:76:ARG:HG3	3:E:80:ARG:HH21	1.83	0.43
2:B:139:HIS:HD2	2:B:146:GLY:O	2.01	0.43
1:A:401:LYS:HD3	2:B:346:TRP:CG	2.53	0.43
1:C:251:ASP:OD2	1:C:253:THR:OG1	2.37	0.43
2:B:1:MET:HE3	2:B:133:GLN:HG3	2.01	0.43
2:D:1:MET:HE3	2:D:133:GLN:HG3	2.00	0.43
1:C:119:LEU:HD21	1:C:156:ARG:HB3	2.01	0.42
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.00	0.42
1:C:255:PHE:CD2	1:C:316:CYS:HB3	2.54	0.42
1:C:255:PHE:CE1	1:C:318:LEU:HD21	2.54	0.42
2:D:1:MET:N	2:D:131:CYS:SG	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.01	0.42
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.84	0.42
2:D:352:LYS:HE3	9:D:502:LOC:O5	2.20	0.42
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.55	0.42
2:B:241[A]:CYS:SG	9:B:502:LOC:O3	2.77	0.42
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.37	0.42
2:D:141:LEU:HB3	2:D:187:ALA:HA	2.02	0.42
1:A:206:ASN:HD22	1:A:206:ASN:HA	1.67	0.41
2:B:206:ASN:HD22	2:B:206:ASN:HA	1.72	0.41
2:B:133:GLN:NE2	2:B:252:LEU:H	2.18	0.41
1:A:286:LEU:HD23	1:A:290:GLU:HG2	2.03	0.41
1:A:27:GLU:OE2	1:A:320:ARG:NH2	2.53	0.41
1:A:71:GLU:OE2	1:A:73:THR:HB	2.20	0.41
2:B:192:HIS:CD2	2:B:421:ALA:HA	2.55	0.41
2:D:229:HIS:HB2	2:D:278:ARG:HB3	2.02	0.41
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.84	0.41
2:D:297:ASP:HB3	2:D:300:ASN:HD22	1.85	0.41
2:B:213:CYS:HA	2:B:217:LEU:HD12	2.03	0.41
1:C:286:LEU:HD11	1:C:291:ILE:CG2	2.51	0.41
1:C:317:LEU:HB2	1:C:353:VAL:HG22	2.03	0.41
1:A:440:VAL:CG2	3:E:33:PRO:HD2	2.51	0.41
2:D:250:ALA:HB1	9:D:502:LOC:H6B	2.02	0.41
2:D:274:PRO:HB3	2:D:286:LEU:HG	2.03	0.41
1:A:119:LEU:HD21	1:A:156:ARG:HB3	2.03	0.41
2:B:133:GLN:HE22	2:B:242:LEU:HD22	1.86	0.41
1:C:177:VAL:HG22	1:C:177:VAL:O	2.22	0.41
1:C:107:HIS:HD2	1:C:108[A]:TYR:CE2	2.39	0.40
1:C:274:PRO:HG3	1:C:286:LEU:HG	2.03	0.40
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.40
2:D:48:ARG:HE	2:D:248:LEU:HD11	1.87	0.40
1:C:372:GLN:H	1:C:372:GLN:HG3	1.73	0.40
2:B:206:ASN:HD21	8:B:501:GDP:N2	2.05	0.40
2:D:139:HIS:HE1	2:D:170:SER:OG	2.05	0.40
2:B:350:ASN:HD22	2:B:350:ASN:N	2.10	0.40
1:C:71:GLU:OE2	1:C:73:THR:HB	2.21	0.40
1:C:122:ILE:HA	1:C:125:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	430/451 (95%)	404 (94%)	21 (5%)	5 (1%)	13 24
1	C	432/451 (96%)	406 (94%)	23 (5%)	3 (1%)	22 40
2	B	433/445 (97%)	411 (95%)	18 (4%)	4 (1%)	17 32
2	D	435/445 (98%)	411 (94%)	17 (4%)	7 (2%)	9 17
3	E	129/142 (91%)	118 (92%)	7 (5%)	4 (3%)	4 6
4	F	1/4 (25%)	0	1 (100%)	0	100 100
All	All	1860/1938 (96%)	1750 (94%)	87 (5%)	23 (1%)	13 24

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	178[A]	SER
2	D	178[B]	SER
2	D	248	LEU
2	B	178	SER
2	B	248	LEU
1	C	281	ALA
2	D	249	ASN
1	A	179	THR
1	A	340	SER
2	B	109	THR
2	D	109	THR
2	D	283	TYR
1	A	162	GLY
1	C	109	THR
3	E	45	PRO
2	B	286	LEU
1	C	314	ALA
3	E	10	GLU
3	E	32	VAL
3	E	46	SER

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Mol	Chain	Res	Type
1	A	47	ASP
2	D	73	GLY
1	A	131	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	368/379 (97%)	326 (89%)	42 (11%)	5 9
1	C	369/379 (97%)	322 (87%)	47 (13%)	4 6
2	B	378/385 (98%)	331 (88%)	47 (12%)	4 7
2	D	380/385 (99%)	336 (88%)	44 (12%)	5 9
3	E	113/125 (90%)	93 (82%)	20 (18%)	2 2
4	F	1/1 (100%)	1 (100%)	0	100 100
All	All	1609/1654 (97%)	1409 (88%)	200 (12%)	4 7

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	9	VAL
1	A	26	LEU
1	A	36	MET
1	A	47	ASP
1	A	70	LEU
1	A	102	ASN
1	A	119	LEU
1	A	121	ARG
1	A	153	LEU
1	A	160	ASP
1	A	163	LYS
1	A	166	LYS
1	A	179	THR
1	A	188	ILE

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	215	ARG
1	A	227	LEU
1	A	250	VAL
1	A	269	LEU
1	A	277	SER
1	A	280	LYS
1	A	284	GLU
1	A	295	CYS
1	A	297	GLU
1	A	302	MET
1	A	315	CYS
1	A	320	ARG
1	A	336	LYS
1	A	337	THR
1	A	338	LYS
1	A	339	ARG
1	A	341	ILE
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	384	ILE
1	A	391	LEU
1	A	397	LEU
1	A	401	LYS
1	A	423	GLU
1	A	439	SER
2	B	5	VAL
2	B	16	ILE
2	B	26	ASP
2	B	42	LEU
2	B	48	ARG
2	B	50	ASN
2	B	54	ASN
2	B	57	THR
2	B	60	LYS
2	B	71[A]	GLU
2	B	71[B]	GLU
2	B	75	MET
2	B	79	ARG
2	B	139	HIS
2	B	141	LEU

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Mol	Chain	Res	Type
2	B	145	THR
2	B	147	SER
2	B	179	ASP
2	B	190	SER
2	B	192	HIS
2	B	206	ASN
2	B	207	GLU
2	B	218	LYS
2	B	223	THR
2	B	230	LEU
2	B	252	LEU
2	B	255	LEU
2	B	277	SER
2	B	281	GLN
2	B	287	THR
2	B	288	VAL
2	B	294	GLN
2	B	295	MET
2	B	297	ASP
2	B	308	ARG
2	B	313	LEU
2	B	323	MET
2	B	329	ASP
2	B	333	LEU
2	B	339	ASN
2	B	345	GLU
2	B	350	ASN
2	B	351	VAL
2	B	352	LYS
2	B	372	LYS
2	B	380	ASN
2	B	416	MET
1	C	1	MET
1	C	4[A]	CYS
1	C	4[B]	CYS
1	C	9	VAL
1	C	26	LEU
1	C	35	GLN
1	C	70	LEU
1	C	102	ASN
1	C	112	LYS
1	C	119	LEU

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Mol	Chain	Res	Type
1	C	121	ARG
1	C	153	LEU
1	C	163	LYS
1	C	164	LYS
1	C	166	LYS
1	C	177	VAL
1	C	188	ILE
1	C	206	ASN
1	C	227	LEU
1	C	233	GLN
1	C	252	LEU
1	C	253	THR
1	C	254	GLU
1	C	256	GLN
1	C	260	VAL
1	C	269	LEU
1	C	282	TYR
1	C	290	GLU
1	C	295	CYS
1	C	297	GLU
1	C	302	MET
1	C	328	VAL
1	C	332	ILE
1	C	335	ILE
1	C	339	ARG
1	C	340	SER
1	C	348	PRO
1	C	367	ASP
1	C	368	LEU
1	C	370	LYS
1	C	372	GLN
1	C	384	ILE
1	C	397	LEU
1	C	401	LYS
1	C	423	GLU
1	C	435	VAL
1	C	439	SER
2	D	26	ASP
2	D	47	GLU
2	D	48	ARG
2	D	50	ASN
2	D	57	THR

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Mol	Chain	Res	Type
2	D	59	ASN
2	D	71	GLU
2	D	85	GLN
2	D	139	HIS
2	D	141	LEU
2	D	156	LYS
2	D	190	SER
2	D	192	HIS
2	D	206	ASN
2	D	207	GLU
2	D	218	LYS
2	D	230	LEU
2	D	247	GLN
2	D	248	LEU
2	D	252	LEU
2	D	255	LEU
2	D	276	THR
2	D	277	SER
2	D	282	GLN
2	D	283	TYR
2	D	284	ARG
2	D	286	LEU
2	D	288	VAL
2	D	293	GLN
2	D	295	MET
2	D	296	PHE
2	D	297	ASP
2	D	313	LEU
2	D	318	ILE
2	D	322	ARG
2	D	329	ASP
2	D	340	SER
2	D	345	GLU
2	D	350	ASN
2	D	351	VAL
2	D	352	LYS
2	D	372	LYS
2	D	376	THR
2	D	380	ASN
3	E	12	ASN
3	E	13	LYS
3	E	15	THR

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Mol	Chain	Res	Type
3	E	47	LEU
3	E	55	GLU
3	E	58	GLU
3	E	72	LEU
3	E	76	ARG
3	E	80	ARG
3	E	82	VAL
3	E	83	ILE
3	E	88	GLU
3	E	105	MET
3	E	108	ASN
3	E	122	ARG
3	E	123	LEU
3	E	134	ARG
3	E	136	ASN
3	E	138	GLU
3	E	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	91	GLN
1	A	102	ASN
1	A	139	HIS
1	A	176	GLN
1	A	197	HIS
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	309	HIS
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	85	GLN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS

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Mol	Chain	Res	Type
2	B	206	ASN
2	B	229	HIS
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	15	GLN
1	C	91	GLN
1	C	101	ASN
1	C	102	ASN
1	C	107	HIS
1	C	139	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	300	ASN
1	C	301	GLN
1	C	380	ASN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	85	GLN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	197	ASN
2	D	206	ASN
2	D	247	GLN
2	D	258	ASN
2	D	300	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	433	GLN
2	D	436	GLN
3	E	91	ASN
3	E	108	ASN
3	E	111	ASN
3	E	115	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
4	0E5	F	3	4	6,7,9	1.26	0	5,8,13	4.69	4 (80%)
4	0EA	F	1	4	13,15,16	2.71	8 (61%)	17,20,22	2.90	3 (17%)

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
4	0E5	F	3	4	1/1/2/3	6/7/8/13	-
4	0EA	F	1	4	-	0/9/12/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	0EA	O5-C7	-4.89	1.26	1.36
4	F	1	0EA	C6-C5	3.98	1.44	1.38
4	F	1	0EA	O1-C5	3.92	1.44	1.36
4	F	1	0EA	C6-C10	3.64	1.44	1.39
4	F	1	0EA	O8-C11	2.72	1.48	1.42
4	F	1	0EA	C9-C10	2.42	1.43	1.39
4	F	1	0EA	O-C	2.27	1.29	1.19
4	F	1	0EA	C10-C11	2.13	1.55	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	3	0E5	C3-CA-C	9.21	126.91	112.83
4	F	1	0EA	C10-C11-CA	-7.28	102.82	112.16
4	F	1	0EA	C6-C5-C7	-6.11	114.46	119.86
4	F	1	0EA	C8-C7-C5	5.56	125.77	119.67
4	F	3	0E5	O-C-CA	-3.52	115.54	124.78
4	F	3	0E5	C2-C3-CA	-2.90	103.90	111.19
4	F	3	0E5	C4-C3-C2	-2.09	106.50	111.78

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	0E5	C3

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	0E5	C2-C3-CA-C
4	F	3	0E5	C4-C3-CA-C
4	F	3	0E5	C4-C3-CA-N
4	F	3	0E5	C1-C2-C3-CA
4	F	3	0E5	C1-C2-C3-C4
4	F	3	0E5	O-C-CA-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	0E5	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	LOC	D	502	-	31,31,31	2.60	8 (25%)	44,44,44	3.21	20 (45%)
7	SO4	B	503	-	4,4,4	0.17	0	6,6,6	0.09	0
5	GTP	C	600	6	26,34,34	1.27	2 (7%)	32,54,54	1.57	7 (21%)
7	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.12	0
9	LOC	B	502	-	31,31,31	2.41	8 (25%)	44,44,44	2.74	20 (45%)
7	SO4	D	503	-	4,4,4	0.30	0	6,6,6	0.08	0
8	GDP	D	501	-	24,30,30	0.98	2 (8%)	30,47,47	1.12	3 (10%)
7	SO4	A	503	-	4,4,4	0.29	0	6,6,6	0.10	0
8	GDP	B	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.30	4 (13%)
5	GTP	A	501	6	26,34,34	1.19	2 (7%)	32,54,54	1.55	7 (21%)
7	SO4	D	504	-	4,4,4	0.17	0	6,6,6	0.13	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
9	LOC	D	502	-	-	2/12/25/25	0/3/3/3
5	GTP	C	600	6	-	5/18/38/38	0/3/3/3
9	LOC	B	502	-	-	2/12/25/25	0/3/3/3
8	GDP	D	501	-	-	4/12/32/32	0/3/3/3
8	GDP	B	501	-	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	502	LOC	C11-C14	-9.13	1.38	1.53
9	B	502	LOC	C22-C21	-6.77	1.41	1.50
9	B	502	LOC	C11-C14	-6.43	1.42	1.53
9	D	502	LOC	C9-C8	-5.30	1.39	1.51
9	B	502	LOC	C9-C8	-5.28	1.39	1.51
9	D	502	LOC	O6-C18	-5.15	1.33	1.45
9	D	502	LOC	C22-C21	-5.09	1.43	1.50
9	B	502	LOC	C20-C21	3.65	1.42	1.37
5	A	501	GTP	O4'-C1'	3.60	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	600	GTP	C8-N7	-3.43	1.29	1.35
5	C	600	GTP	O4'-C1'	3.16	1.45	1.41
9	B	502	LOC	O6-C18	-3.14	1.37	1.45
9	D	502	LOC	C15-C14	2.94	1.41	1.36
9	B	502	LOC	O2-C3	-2.72	1.33	1.38
9	D	502	LOC	C22-C8	2.55	1.46	1.41
9	D	502	LOC	O2-C3	-2.54	1.33	1.38
5	A	501	GTP	C8-N7	-2.45	1.30	1.35
9	B	502	LOC	C15-C14	2.35	1.40	1.36
8	D	501	GDP	PB-O2B	2.25	1.63	1.54
9	B	502	LOC	C22-C8	2.19	1.45	1.41
8	B	501	GDP	PB-O3B	2.16	1.63	1.54
9	D	502	LOC	C20-C21	2.15	1.40	1.37
8	D	501	GDP	C8-N7	-2.05	1.31	1.35

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	502	LOC	C1-C22-C21	7.19	128.59	121.09
9	D	502	LOC	C22-C21-C14	6.61	123.83	118.51
9	D	502	LOC	O6-C17-C16	6.61	116.01	109.56
9	D	502	LOC	C11-C14-C15	-6.60	110.88	117.12
9	B	502	LOC	C9-C8-C22	6.28	129.77	119.97
9	B	502	LOC	C14-C11-N1	6.08	119.13	114.34
9	D	502	LOC	C10-C11-N1	5.84	120.65	110.11
9	B	502	LOC	C9-C8-C7	-5.31	107.70	119.42
9	D	502	LOC	C15-C16-C17	5.25	129.68	121.91
9	D	502	LOC	C8-C22-C21	-4.93	114.47	120.25
9	D	502	LOC	C22-C21-C20	-4.92	108.11	117.12
9	B	502	LOC	O6-C17-C16	4.84	114.28	109.56
9	D	502	LOC	C9-C8-C22	4.54	127.05	119.97
9	B	502	LOC	C20-C21-C14	4.52	130.04	124.83
9	B	502	LOC	C22-C21-C20	-4.41	109.05	117.12
9	D	502	LOC	C11-C14-C21	4.39	119.73	115.27
9	B	502	LOC	C15-C16-C17	4.38	128.38	121.91
5	C	600	GTP	PA-O3A-PB	-4.25	118.25	132.83
5	A	501	GTP	PA-O3A-PB	-4.22	118.34	132.83
9	D	502	LOC	C9-C10-C11	4.16	117.54	112.21
9	D	502	LOC	C9-C8-C7	-4.16	110.24	119.42
9	B	502	LOC	C10-C11-N1	3.84	117.05	110.11
9	B	502	LOC	C11-C14-C21	3.79	119.11	115.27
9	B	502	LOC	C4-O2-C3	-3.77	104.44	114.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	GDP	PA-O3A-PB	-3.68	120.19	132.83
8	D	501	GDP	PA-O3A-PB	-3.48	120.88	132.83
9	B	502	LOC	C1-C22-C21	3.42	124.66	121.09
8	B	501	GDP	C8-N7-C5	3.34	109.35	102.99
5	C	600	GTP	C5-C6-N1	3.30	119.78	113.95
9	D	502	LOC	C14-C15-C16	-3.28	127.31	133.89
9	D	502	LOC	O6-C17-C19	-3.21	117.24	122.30
5	A	501	GTP	C8-N7-C5	3.19	109.07	102.99
9	B	502	LOC	C11-C14-C15	-3.05	114.24	117.12
5	C	600	GTP	PB-O3B-PG	-3.03	122.41	132.83
8	B	501	GDP	O2B-PB-O3A	3.02	114.75	104.64
9	D	502	LOC	O5-C16-C15	-3.01	110.30	118.68
5	A	501	GTP	PB-O3B-PG	-2.99	122.57	132.83
9	B	502	LOC	C22-C21-C14	2.96	120.89	118.51
9	B	502	LOC	C8-C22-C21	-2.95	116.79	120.25
5	C	600	GTP	C8-N7-C5	2.94	108.59	102.99
9	D	502	LOC	C6-O3-C5	-2.85	113.23	117.53
5	A	501	GTP	C5-C6-N1	2.79	118.88	113.95
9	D	502	LOC	C20-C21-C14	2.77	128.03	124.83
9	B	502	LOC	O3-C5-C3	2.74	119.97	115.16
9	D	502	LOC	C7-C8-C22	2.69	122.70	119.47
8	D	501	GDP	C8-N7-C5	2.68	108.10	102.99
9	B	502	LOC	O5-C16-C15	-2.67	111.25	118.68
9	D	502	LOC	C4-O2-C3	-2.56	107.77	114.78
9	B	502	LOC	C7-C8-C22	2.54	122.52	119.47
5	C	600	GTP	C2-N1-C6	-2.53	120.44	125.10
8	D	501	GDP	O2B-PB-O3A	2.47	112.91	104.64
5	A	501	GTP	O3G-PG-O3B	2.31	112.38	104.64
5	A	501	GTP	C2-N1-C6	-2.24	120.97	125.10
8	B	501	GDP	O6-C6-N1	-2.23	118.01	120.65
9	D	502	LOC	C5-C3-C1	2.21	122.31	119.56
9	B	502	LOC	C14-C15-C16	-2.18	129.52	133.89
9	B	502	LOC	O6-C17-C19	-2.14	118.93	122.30
5	A	501	GTP	O4'-C4'-C5'	-2.07	102.58	109.37
5	C	600	GTP	O3G-PG-O3B	2.04	111.49	104.64
5	C	600	GTP	O4'-C4'-C5'	-2.00	102.78	109.37
9	B	502	LOC	O4-C12-N1	2.00	125.63	121.95

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	600	GTP	PB-O3B-PG-O2G
5	C	600	GTP	C5'-O5'-PA-O1A
5	C	600	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	502	LOC	C19-C17-O6-C18
9	B	502	LOC	C16-C17-O6-C18
9	D	502	LOC	C19-C17-O6-C18
9	D	502	LOC	C16-C17-O6-C18
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	600	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	600	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

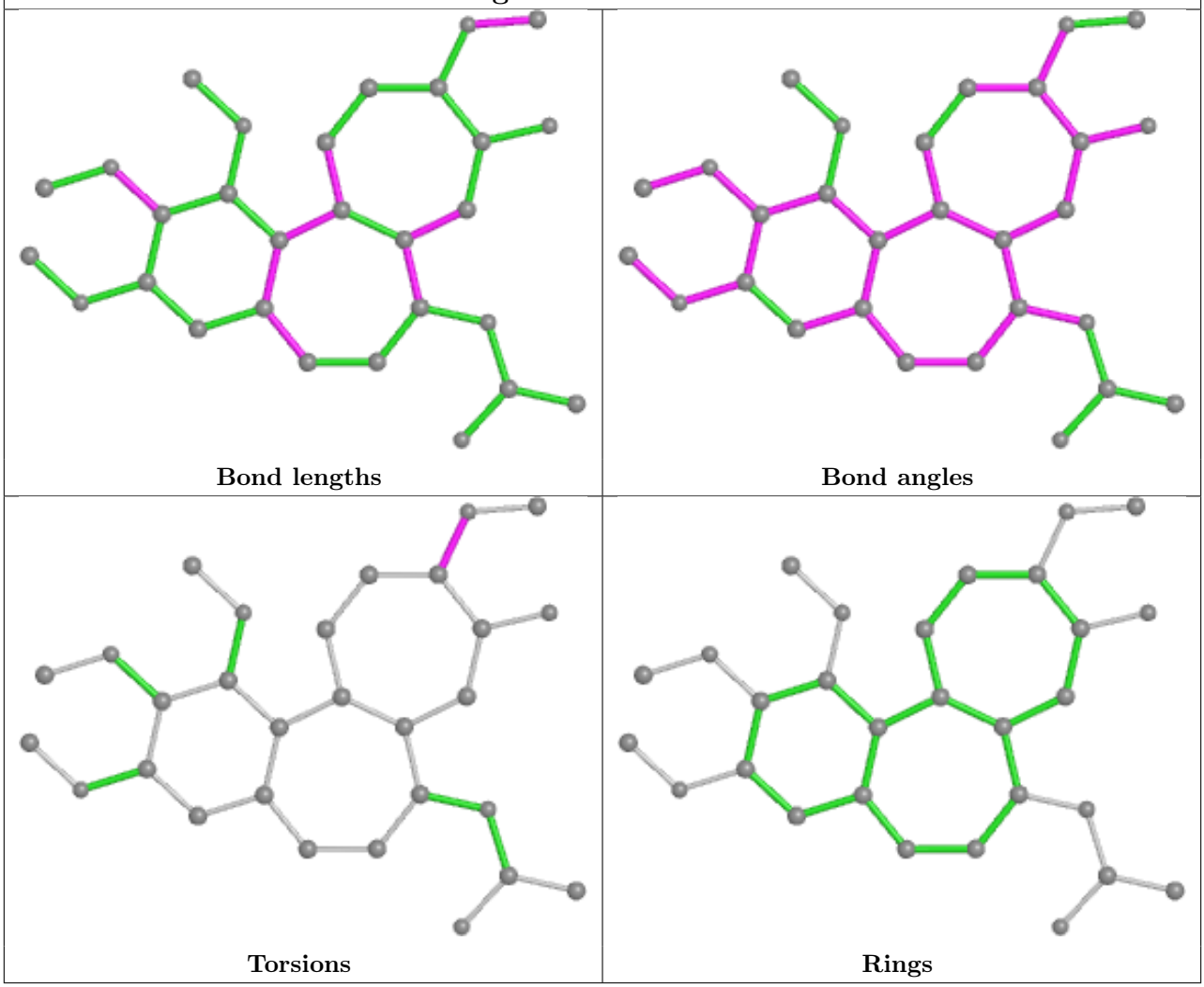
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	502	LOC	3	0
5	C	600	GTP	1	0
9	B	502	LOC	4	0
8	D	501	GDP	2	0
8	B	501	GDP	3	0
5	A	501	GTP	1	0

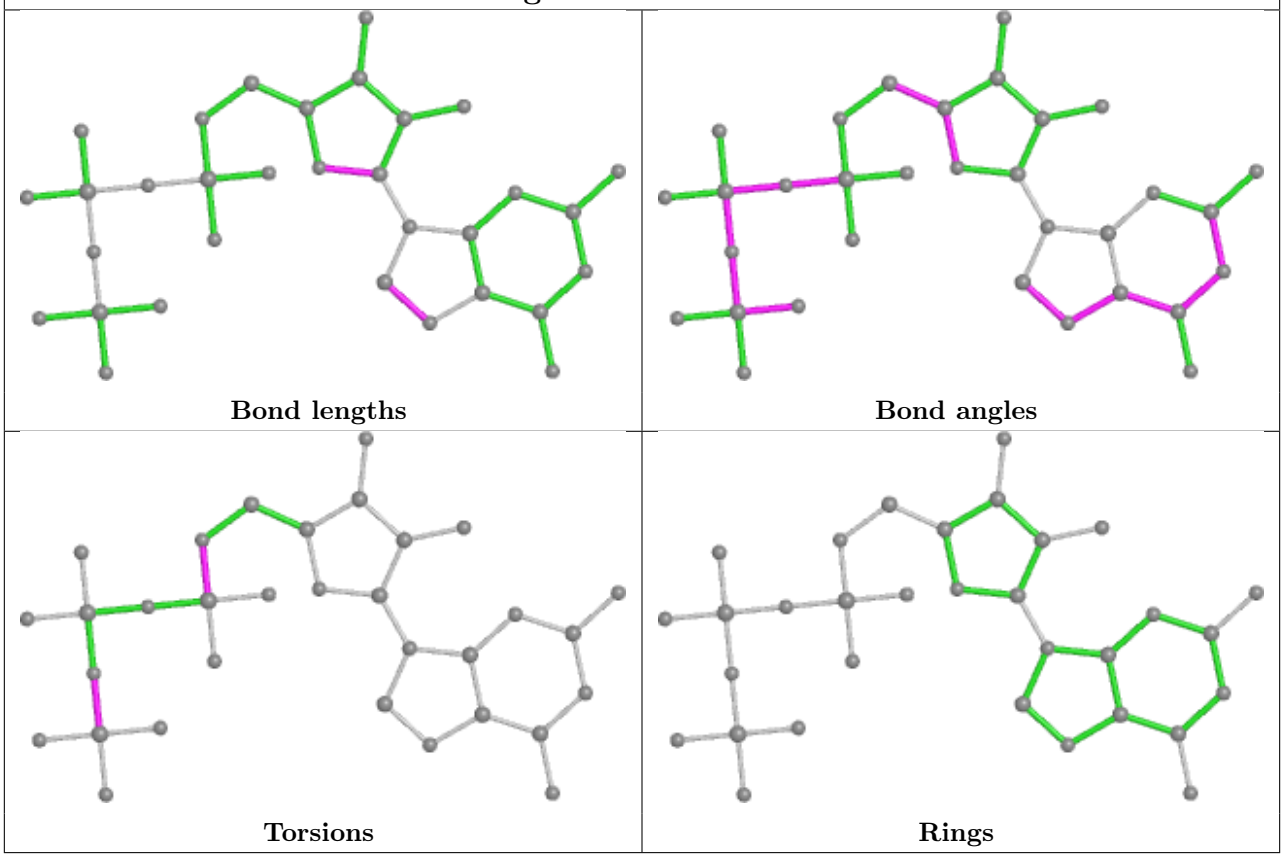
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

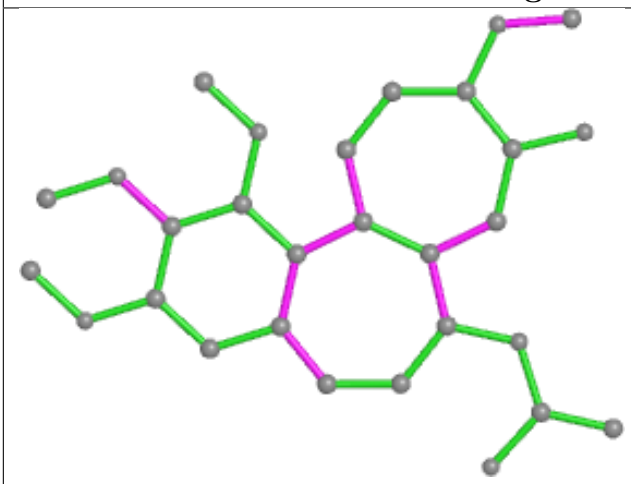
Ligand LOC D 502



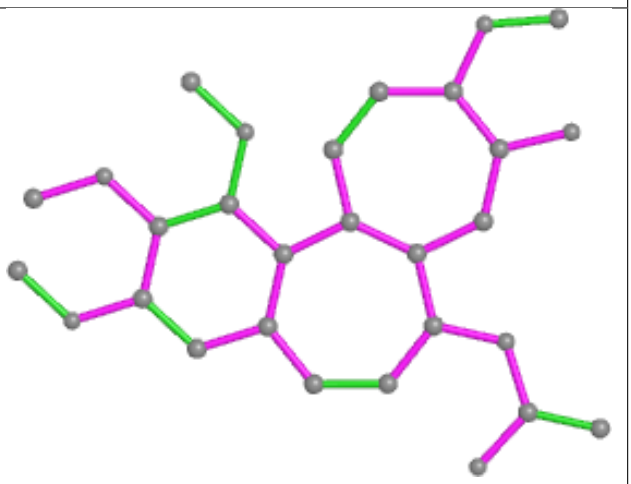
Ligand GTP C 600



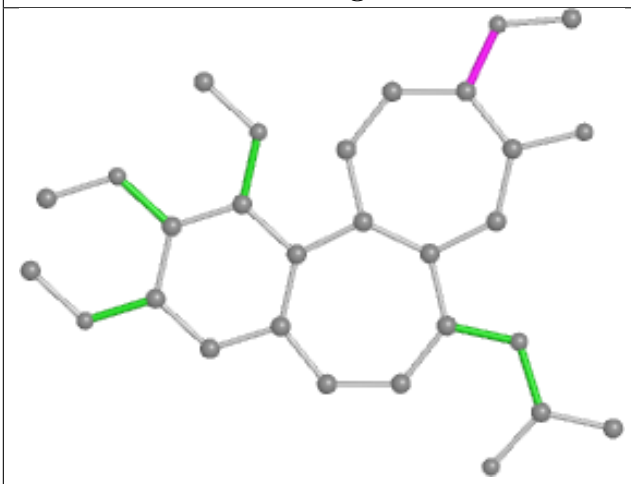
Ligand LOC B 502



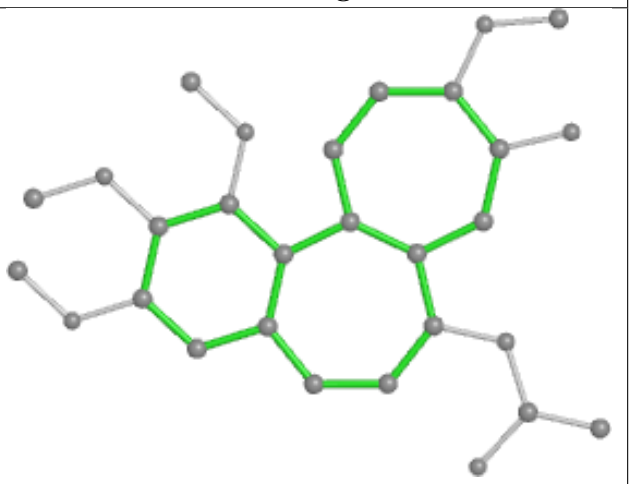
Bond lengths



Bond angles

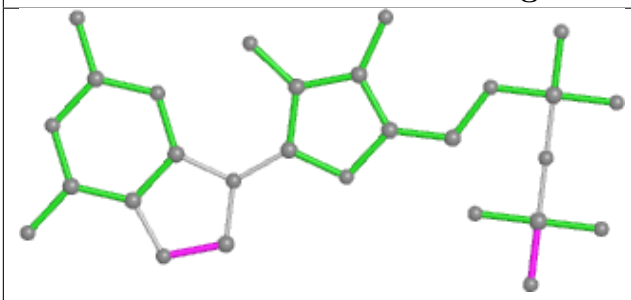


Torsions

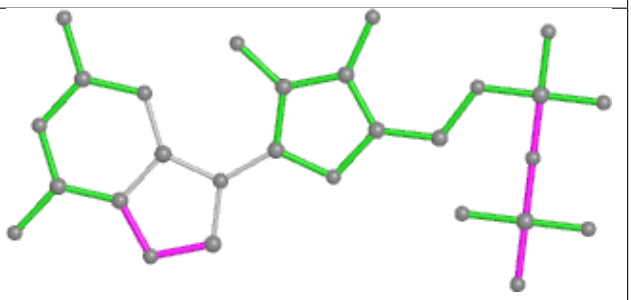


Rings

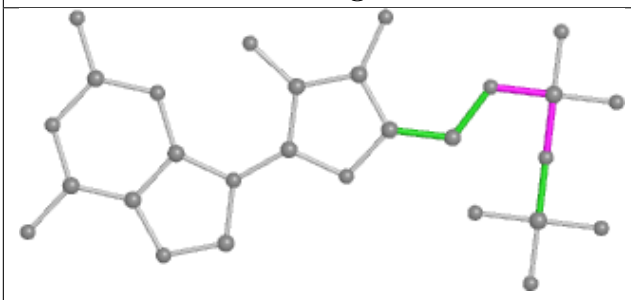
Ligand GDP D 501



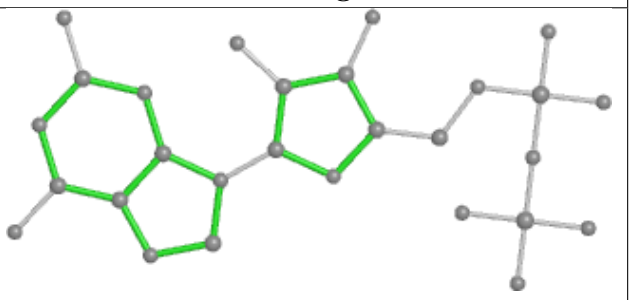
Bond lengths



Bond angles

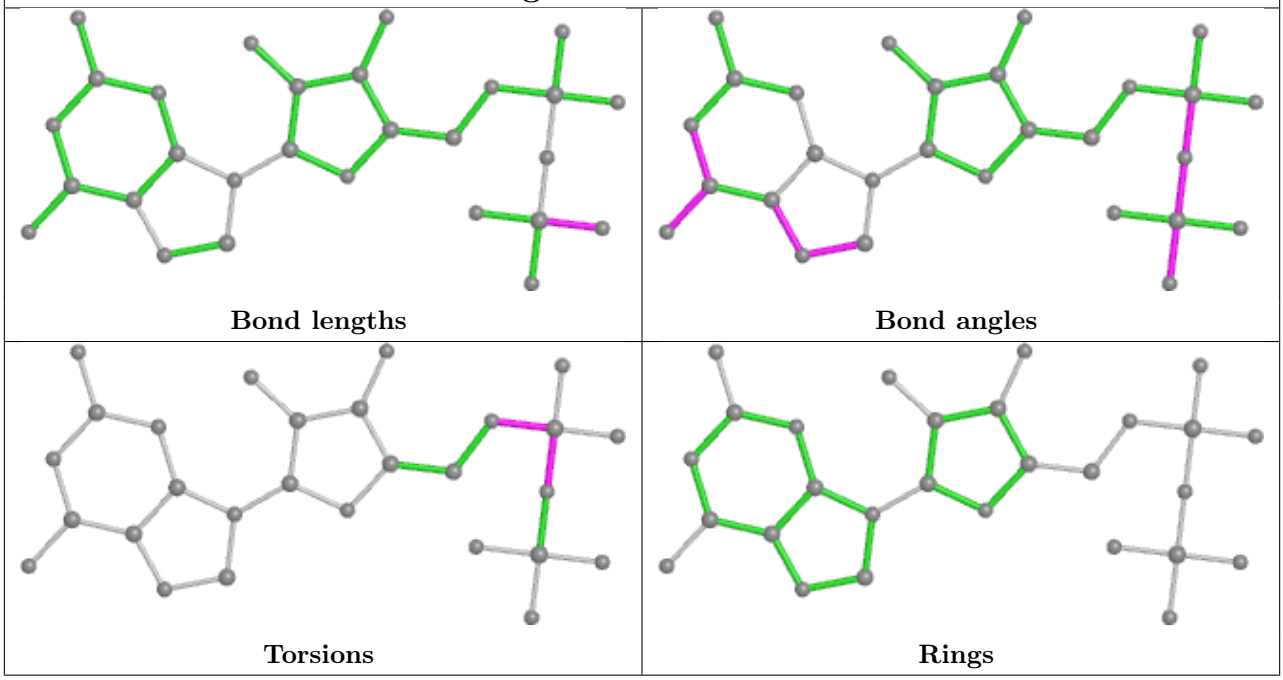


Torsions

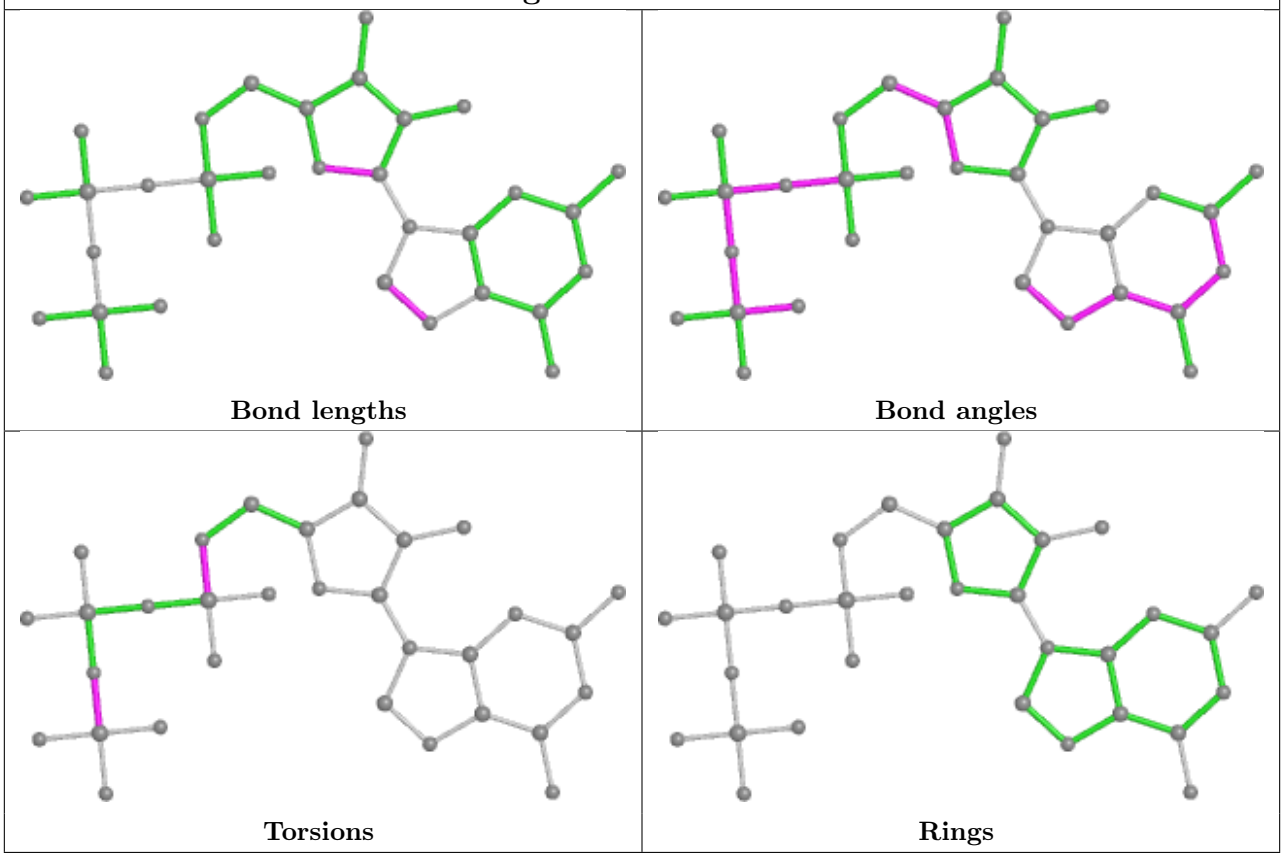


Rings

Ligand GDP B 501



Ligand GTP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	433/451 (96%)	0.39	31 (7%)	15	17	60, 97, 153, 198	0
1	C	432/451 (95%)	0.25	17 (3%)	39	43	42, 81, 133, 180	0
2	B	432/445 (97%)	0.54	51 (11%)	4	4	59, 90, 155, 215	2 (0%)
2	D	432/445 (97%)	0.24	24 (5%)	24	27	44, 77, 122, 162	2 (0%)
3	E	132/142 (92%)	0.98	19 (14%)	2	2	62, 107, 176, 214	0
4	F	2/4 (50%)	1.33	1 (50%)	0	0	117, 117, 117, 129	0
All	All	1863/1938 (96%)	0.40	143 (7%)	13	15	42, 89, 145, 215	4 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	34	GLU	8.4
3	E	141	GLU	7.8
2	B	283	TYR	7.5
3	E	140	LYS	7.4
3	E	32	VAL	7.3
2	D	283	TYR	6.8
1	A	337	THR	6.5
3	E	6	MET	5.9
3	E	4	ALA	5.6
3	E	33	PRO	5.3
2	B	279	GLY	5.1
2	D	56	ALA	4.9
3	E	5	ASP	4.8
2	D	284	ARG	4.7
1	C	335	ILE	4.6
2	D	39	ASP	4.4
1	A	338	LYS	4.4
1	C	366	GLY	4.3
1	C	323	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	276	THR	4.2
2	D	36	TYR	4.2
1	A	280	LYS	4.1
1	C	364	PRO	4.0
2	D	282	GLN	4.0
2	B	246	GLY	3.8
1	A	38	SER	3.7
1	A	437	VAL	3.7
2	B	440	ALA	3.6
3	E	16	SER	3.6
1	A	37	PRO	3.6
1	C	1	MET	3.6
1	A	221	ARG	3.6
1	A	282	TYR	3.5
1	A	346	TRP	3.5
2	B	61	TYR	3.5
1	A	440	VAL	3.5
2	B	281	GLN	3.4
2	D	57	THR	3.4
2	B	441	ASP	3.4
2	B	86	ILE	3.4
2	B	55	GLU	3.4
2	B	282	GLN	3.4
2	B	284	ARG	3.4
1	A	279	GLU	3.3
3	E	27	PRO	3.3
1	A	170	SER	3.3
2	D	285	ALA	3.3
2	D	60	LYS	3.3
2	B	37	HIS	3.3
2	B	59	ASN	3.3
1	A	281	ALA	3.3
2	D	37	HIS	3.2
1	C	334	THR	3.2
1	A	219	ILE	3.2
2	B	379	GLY	3.1
1	C	38	SER	3.1
1	C	357	TYR	3.1
1	A	335	ILE	3.0
2	D	418	PHE	3.0
2	B	241[A]	CYS	3.0
2	B	270	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	87	ILE	2.9
1	A	80	THR	2.9
3	E	24	LEU	2.9
2	D	296	PHE	2.8
2	B	56	ALA	2.8
1	A	349	THR	2.8
2	B	285	ALA	2.7
1	C	282	TYR	2.7
2	B	203	SER	2.7
2	B	238	VAL	2.7
4	F	4	GLY	2.7
1	A	286	LEU	2.7
3	E	26	PRO	2.6
2	B	42	LEU	2.6
2	B	286	LEU	2.6
2	B	245	PRO	2.6
2	D	179[A]	ASP	2.5
1	A	439	SER	2.5
1	A	435	VAL	2.5
2	B	62	VAL	2.5
2	B	202	TYR	2.5
2	B	373	MET	2.5
1	A	201	ALA	2.5
2	B	36	TYR	2.5
2	B	269	MET	2.5
1	C	253	THR	2.4
3	E	8	VAL	2.4
1	A	339	ARG	2.4
2	B	322	ARG	2.4
3	E	136	ASN	2.4
3	E	73	ALA	2.4
2	D	59	ASN	2.4
2	B	201	THR	2.4
2	B	271	GLY	2.4
2	B	371	LEU	2.3
1	A	283	HIS	2.3
3	E	48	GLU	2.3
1	A	268	PRO	2.3
2	B	1	MET	2.3
2	B	280	SER	2.3
2	B	268	PHE	2.3
1	C	331	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	59	GLU	2.3
2	B	32	PRO	2.2
1	C	200	CYS	2.2
2	B	339	ASN	2.2
2	D	55	GLU	2.2
1	C	362	VAL	2.2
2	D	280	SER	2.2
3	E	25	LYS	2.2
2	B	204	ILE	2.2
2	B	333	LEU	2.2
1	A	336	LYS	2.2
1	A	328	VAL	2.2
2	B	378	ILE	2.2
2	B	248	LEU	2.2
2	D	61	TYR	2.2
2	B	170	SER	2.2
2	B	39	ASP	2.1
2	D	41	ASP	2.1
2	B	233	ALA	2.1
2	B	239	THR	2.1
2	D	96	GLN	2.1
2	B	169	PHE	2.1
1	C	324	VAL	2.1
1	A	438	ASP	2.1
1	C	215	ARG	2.1
1	A	372	GLN	2.1
1	C	285	GLN	2.1
2	B	57	THR	2.1
2	D	286	LEU	2.1
1	A	271	THR	2.1
2	D	441	ASP	2.1
1	C	333	ALA	2.0
1	A	436	GLY	2.0
2	B	167	ASN	2.0
2	B	221	THR	2.0
2	D	404	PHE	2.0
2	D	369	ARG	2.0
2	D	202	TYR	2.0
1	A	415	GLU	2.0
2	B	171	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	0EA	F	1	15/16	0.93	0.26	113,115,118,119	0
4	0E5	F	3	8/10	0.93	0.27	110,113,121,122	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

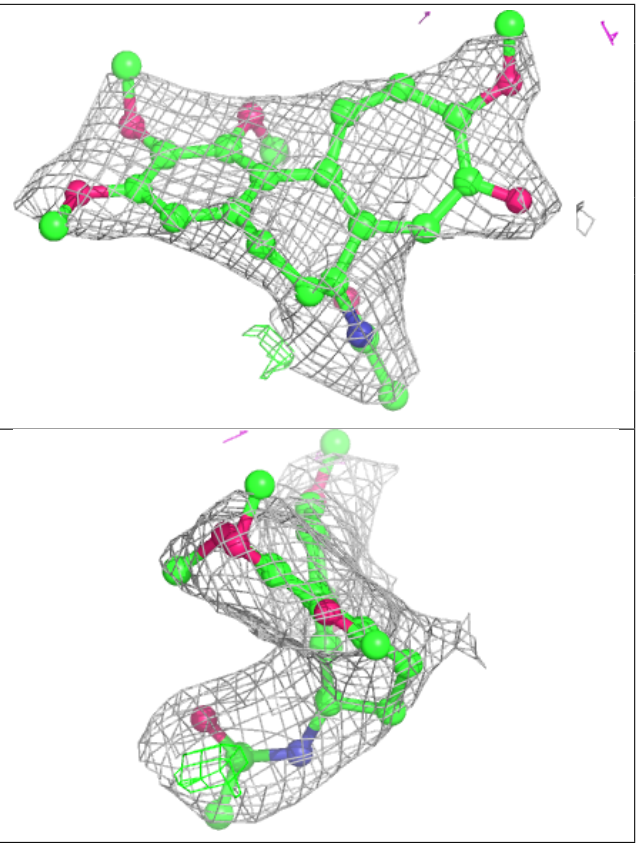
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	D	504	5/5	0.88	0.18	141,143,147,149	0
7	SO4	A	504	5/5	0.90	0.21	140,143,147,147	0
7	SO4	A	503	5/5	0.91	0.16	127,130,133,134	0
7	SO4	B	503	5/5	0.92	0.09	157,160,165,165	0
9	LOC	B	502	29/29	0.94	0.18	75,79,83,85	0
6	MG	A	502	1/1	0.95	0.16	74,74,74,74	0
7	SO4	D	503	5/5	0.95	0.30	142,143,148,149	0
6	MG	C	601	1/1	0.96	0.13	56,56,56,56	0
9	LOC	D	502	29/29	0.97	0.18	51,63,67,67	0
8	GDP	B	501	28/28	0.98	0.18	69,71,76,76	0
8	GDP	D	501	28/28	0.98	0.17	62,66,70,73	0
5	GTP	C	600	32/32	0.98	0.17	57,59,66,68	0
5	GTP	A	501	32/32	0.98	0.20	63,70,76,76	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.

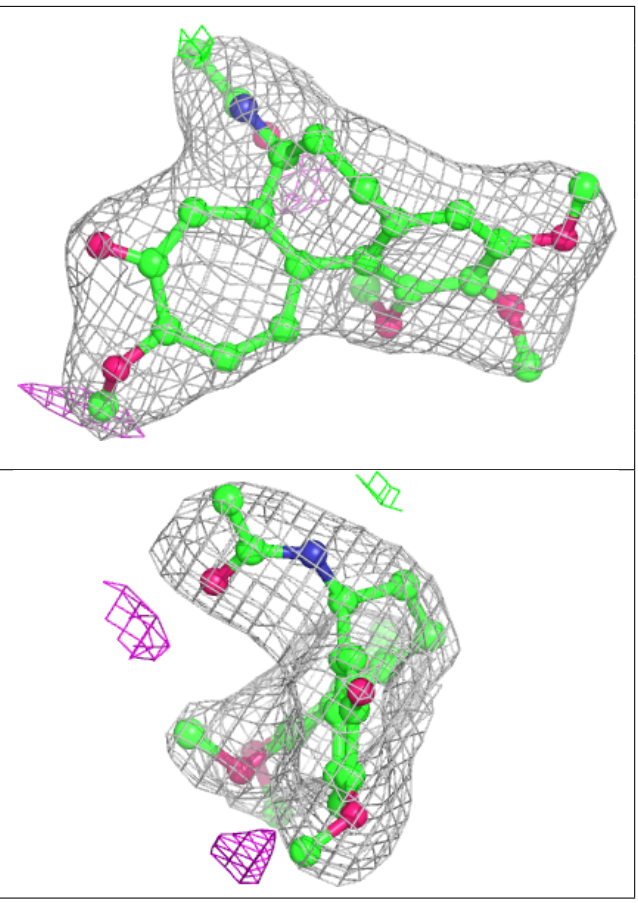
Electron density around LOC B 502:

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



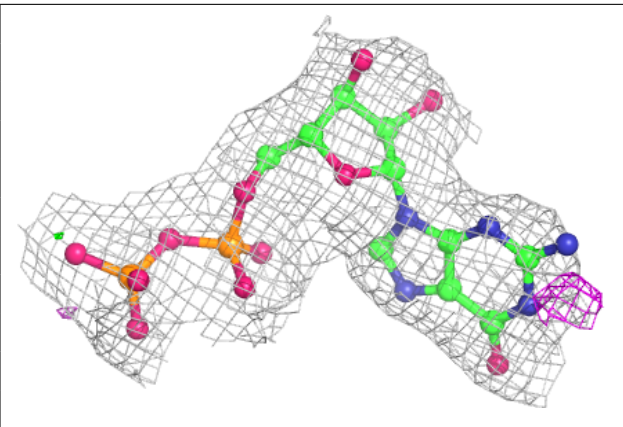
Electron density around LOC D 502:

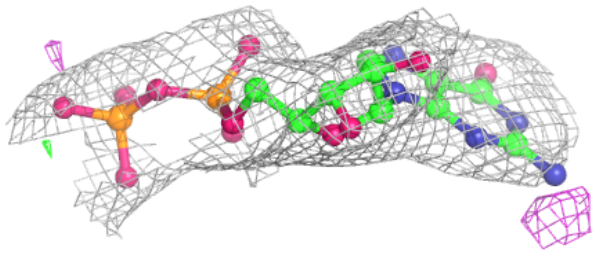
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

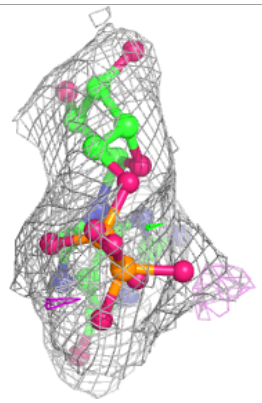


Electron density around GDP B 501:

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

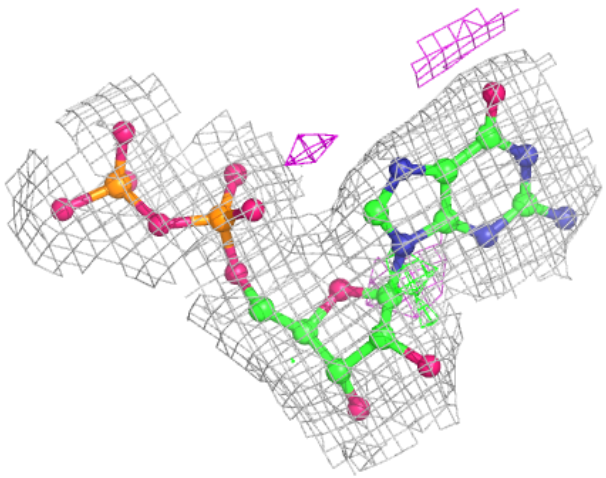


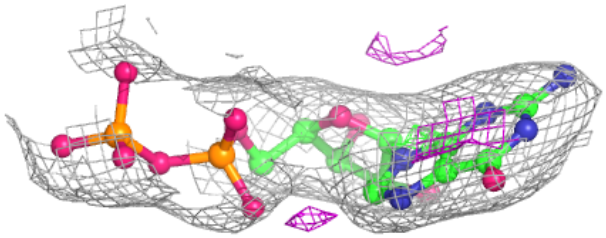


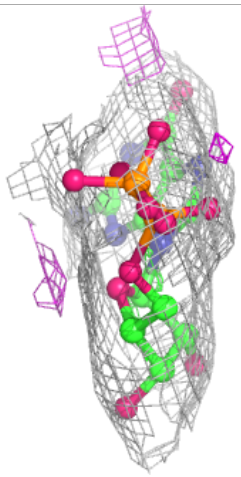


Electron density around GDP D 501:

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

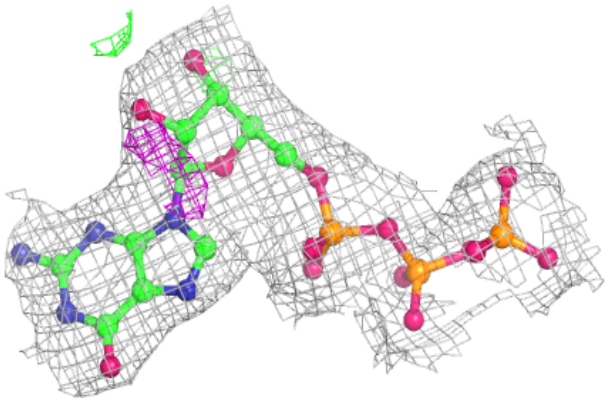


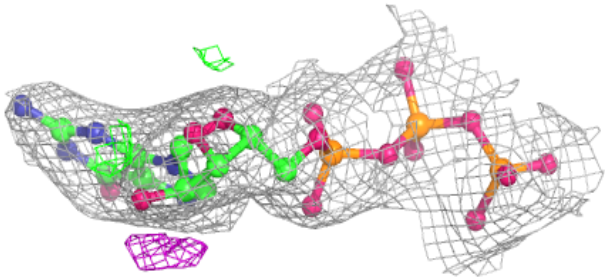


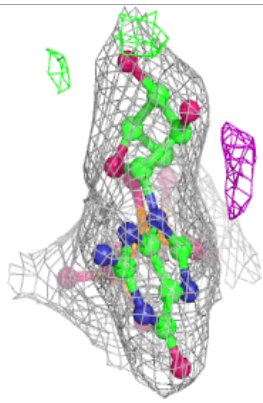


Electron density around GTP C 600:

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

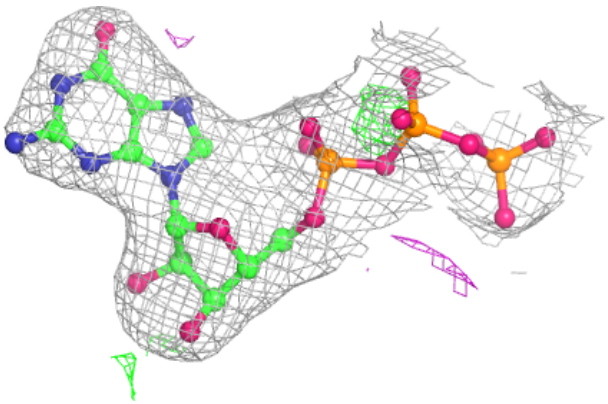


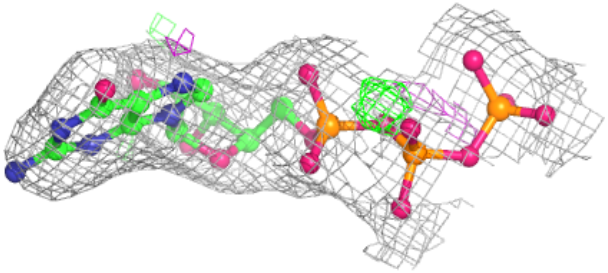


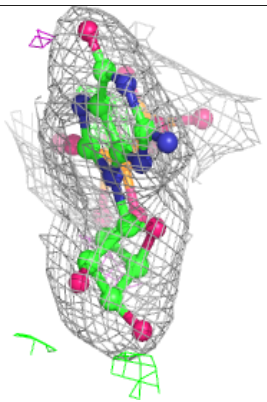


Electron density around GTP A 501:

$2mF_o$-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.