



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:22 pm BST

PDB ID : 5OES  
Title : The structure of a glutathione synthetase (StGSS1) from *Solanum tuberosum* in ADP and  $\gamma$ -EC bound closed conformation.  
Authors : Lilley, C.J.; Maqbool, A.; Wu, D.; Yusup, H.B.; Jones, L.M.; Birch, P.R.J.; Banfield, M.J.; Urwin, P.E.; Eves-van den Akker, S.  
Deposited on : 2017-07-10  
Resolution : 2.48 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

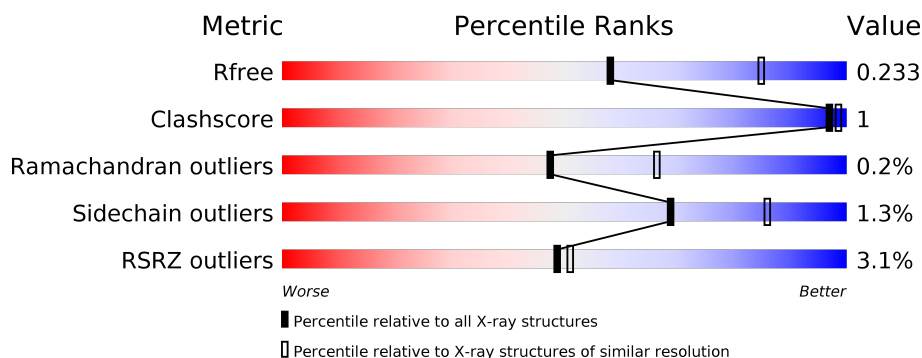
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 on 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	483	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>89%</span> <span>• 8%</span> </div> </div>
1	B	483	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>88%</span> <span>• 8%</span> </div> </div>
1	C	483	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 90%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>5%</span> <span>90%</span> <span>• 7%</span> </div> </div>
1	D	483	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 89%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>4%</span> <span>89%</span> <span>• 8%</span> </div> </div>
1	E	483	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 88%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>2%</span> <span>88%</span> <span>• • 7%</span> </div> </div>
1	F	483	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 89%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>4%</span> <span>89%</span> <span>• 7%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22152 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 Glutathione synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3563	2252	623	672	16			
1	B	446	Total	C	N	O	S	0	0	0
			3572	2257	625	674	16			
1	C	447	Total	C	N	O	S	0	0	0
			3578	2263	625	674	16			
1	D	446	Total	C	N	O	S	0	1	0
			3579	2262	626	675	16			
1	E	448	Total	C	N	O	S	0	0	0
			3592	2268	630	678	16			
1	F	448	Total	C	N	O	S	0	1	0
			3599	2273	630	680	16			

There are 30 discrepancies between the modelled and reference sequences:

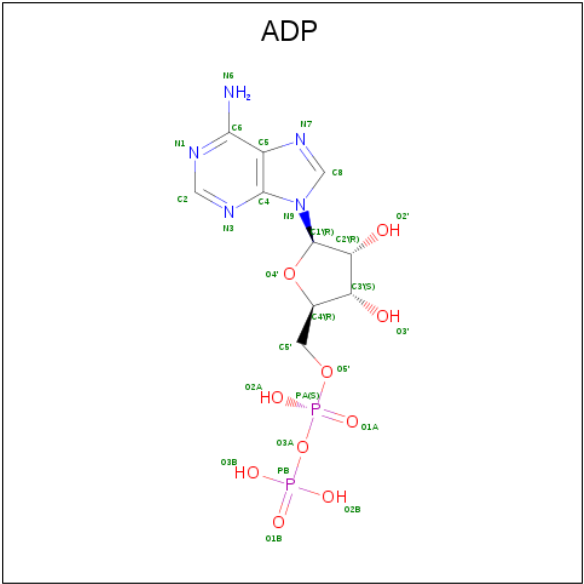
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	PRO	ALA	conflict	UNP M1CSC4
A	127	LYS	THR	conflict	UNP M1CSC4
A	220	ALA	VAL	conflict	UNP M1CSC4
A	288	ASN	HIS	conflict	UNP M1CSC4
A	449	VAL	LEU	conflict	UNP M1CSC4
B	20	PRO	ALA	conflict	UNP M1CSC4
B	127	LYS	THR	conflict	UNP M1CSC4
B	220	ALA	VAL	conflict	UNP M1CSC4
B	288	ASN	HIS	conflict	UNP M1CSC4
B	449	VAL	LEU	conflict	UNP M1CSC4
C	20	PRO	ALA	conflict	UNP M1CSC4
C	127	LYS	THR	conflict	UNP M1CSC4
C	220	ALA	VAL	conflict	UNP M1CSC4
C	288	ASN	HIS	conflict	UNP M1CSC4
C	449	VAL	LEU	conflict	UNP M1CSC4
D	20	PRO	ALA	conflict	UNP M1CSC4
D	127	LYS	THR	conflict	UNP M1CSC4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	220	ALA	VAL	conflict	UNP M1CSC4
D	288	ASN	HIS	conflict	UNP M1CSC4
D	449	VAL	LEU	conflict	UNP M1CSC4
E	20	PRO	ALA	conflict	UNP M1CSC4
E	127	LYS	THR	conflict	UNP M1CSC4
E	220	ALA	VAL	conflict	UNP M1CSC4
E	288	ASN	HIS	conflict	UNP M1CSC4
E	449	VAL	LEU	conflict	UNP M1CSC4
F	20	PRO	ALA	conflict	UNP M1CSC4
F	127	LYS	THR	conflict	UNP M1CSC4
F	220	ALA	VAL	conflict	UNP M1CSC4
F	288	ASN	HIS	conflict	UNP M1CSC4
F	449	VAL	LEU	conflict	UNP M1CSC4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



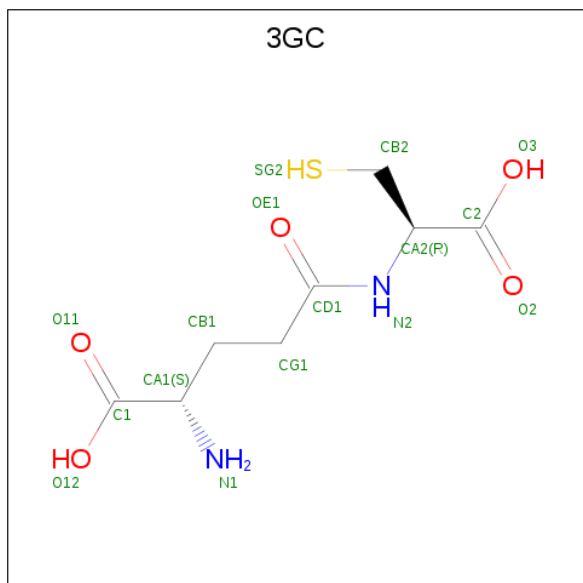
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is GAMMA-GLUTAMYLCYSTEINE (three-letter code: 3GC) (formula:  $C_8H_{14}N_2O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	S	0	0
			16	8	2	5	1		
3	C	1	Total	C	N	O	S	0	0
			16	8	2	5	1		
3	D	1	Total	C	N	O	S	0	0
			16	8	2	5	1		
3	E	1	Total	C	N	O	S	0	0
			16	8	2	5	1		
3	F	1	Total	C	N	O	S	0	0
			16	8	2	5	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total 2	Mg 2	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	2	Total 2	Mg 2	0	0
4	A	2	Total 2	Mg 2	0	0
4	F	1	Total 1	Mg 1	0	0

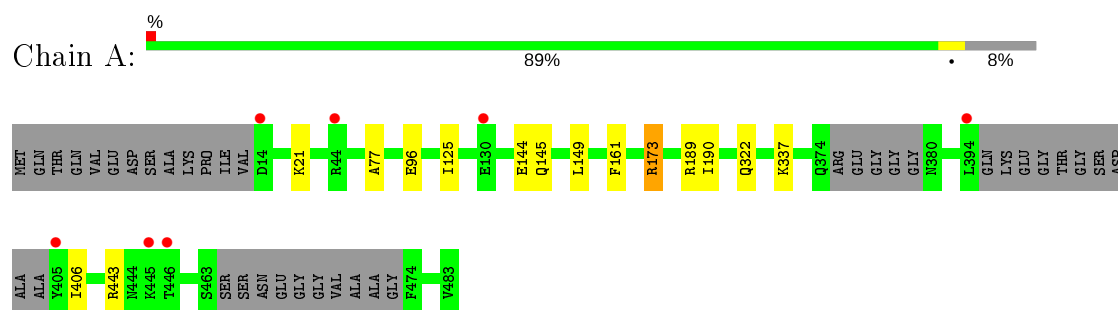
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total 78	O 78	0	0
5	B	85	Total 85	O 85	0	0
5	C	60	Total 60	O 60	0	0
5	D	49	Total 49	O 49	0	0
5	E	67	Total 67	O 67	0	0
5	F	62	Total 62	O 62	0	0

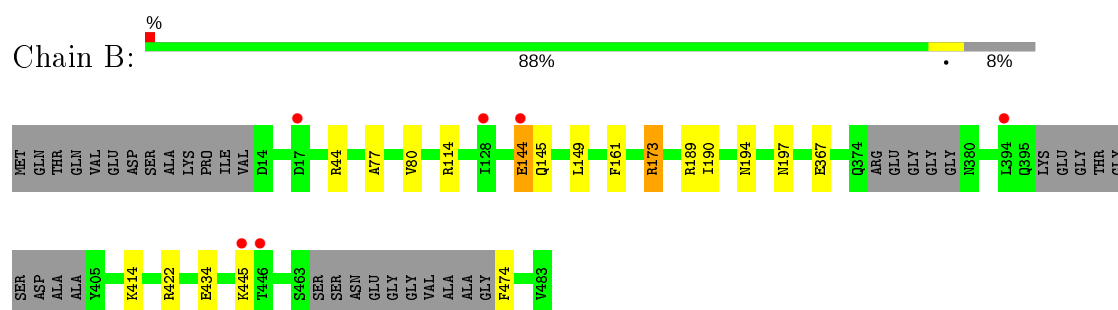
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

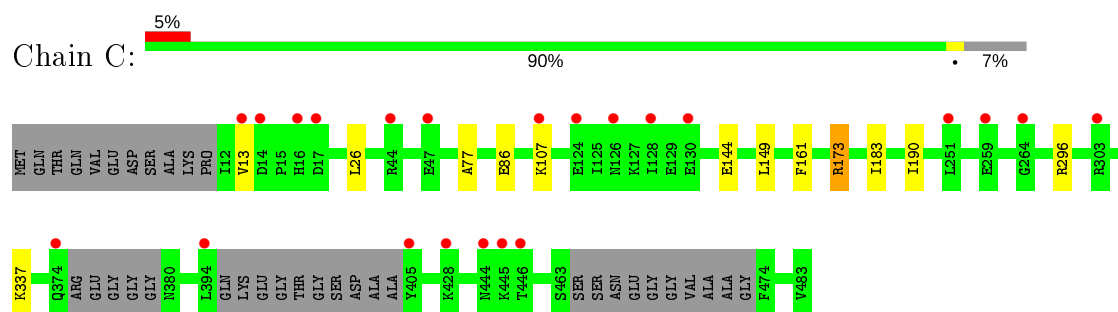
#### • Molecule 1: Glutathione synthetase



#### • Molecule 1: Glutathione synthetase

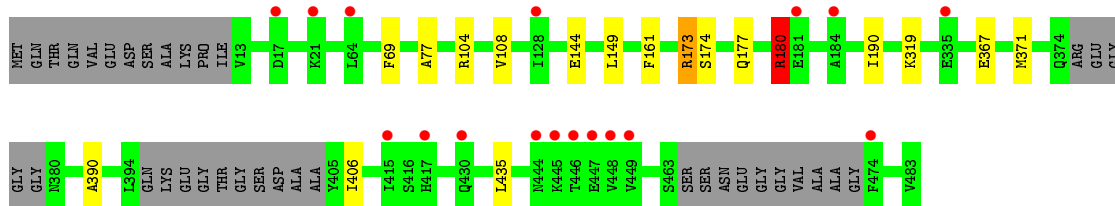


#### • Molecule 1: Glutathione synthetase

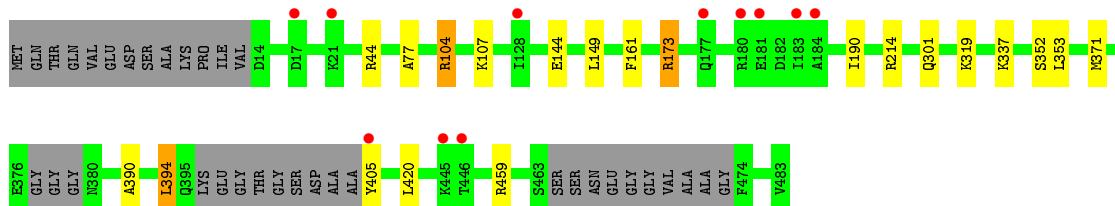
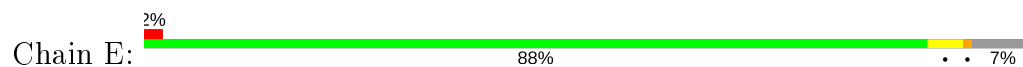


#### • Molecule 1: Glutathione synthetase

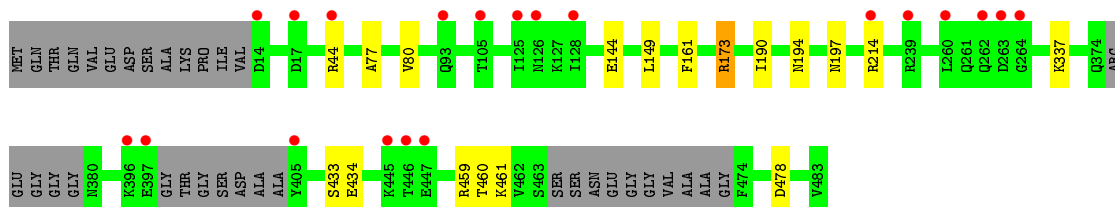
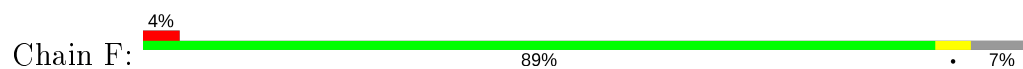




• Molecule 1: Glutathione synthetase



• Molecule 1: Glutathione synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.39Å 154.39Å 344.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.48 49.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.48) 99.8 (49.31-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.224 , 0.241 0.218 , 0.233	Depositor DCC
$R_{free}$ test set	6994 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4574e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 3GC, MG, ADP

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	0.44	0/3627	0.76	4/4903 (0.1%)
1	B	0.43	0/3636	0.69	2/4915 (0.0%)
1	C	0.47	0/3642	0.74	4/4924 (0.1%)
1	D	0.47	0/3643	0.73	2/4925 (0.0%)
1	E	0.45	0/3656	0.75	6/4941 (0.1%)
1	F	0.45	0/3663	0.70	3/4950 (0.1%)
All	All	0.45	0/21867	0.73	21/29558 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	NE-CZ-NH1	-16.61	111.99	120.30
1	A	173	ARG	NE-CZ-NH2	14.50	127.55	120.30
1	E	173	ARG	NE-CZ-NH1	-11.59	114.51	120.30
1	E	173	ARG	NE-CZ-NH2	10.35	125.47	120.30
1	B	173	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	F	173	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	C	173	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	C	173	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	173	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	C	296	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	C	296	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	F	173	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	173	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	F	459	ARG	NE-CZ-NH1	-6.15	117.23	120.30
1	E	394	LEU	CB-CG-CD2	6.08	121.34	111.00
1	D	180	ARG	CA-CB-CG	6.00	126.60	113.40
1	E	104	ARG	CA-CB-CG	5.88	126.33	113.40
1	E	301	GLN	CA-CB-CG	5.73	126.00	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	459	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	443	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	189	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3563	0	3572	4	0
1	B	3572	0	3580	8	0
1	C	3578	0	3592	4	0
1	D	3579	0	3588	6	0
1	E	3592	0	3599	9	0
1	F	3599	0	3606	9	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	2	0
3	A	16	0	12	0	0
3	B	16	0	12	0	0
3	C	16	0	12	0	0
3	D	16	0	12	0	0
3	E	16	0	12	0	0
3	F	16	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
5	A	78	0	0	0	0
5	B	85	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	60	0	0	1	0
5	D	49	0	0	0	0
5	E	67	0	0	0	0
5	F	62	0	0	1	0
All	All	22152	0	21681	39	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 1.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:SER:OG	1:F:460:THR:HG22	1.71	0.91
1:E:319:LYS:NZ	1:E:352:SER:HB3	2.14	0.63
1:A:173:ARG:NH2	1:A:190:ILE:O	2.34	0.60
1:F:173:ARG:NH2	1:F:190:ILE:O	2.35	0.60
1:B:173:ARG:NH2	1:B:190:ILE:O	2.35	0.60
1:C:173:ARG:NH2	1:C:190:ILE:O	2.35	0.59
1:D:319:LYS:HA	1:D:406:ILE:HD11	1.84	0.59
1:E:173:ARG:NH1	1:E:190:ILE:O	2.36	0.58
1:B:144:GLU:HG3	1:B:414:LYS:HA	1.87	0.56
1:D:173:ARG:NH1	1:D:190:ILE:O	2.38	0.56
1:E:390:ALA:O	1:E:394:LEU:HD23	2.10	0.52
1:D:69:PHE:CZ	1:D:435:LEU:HD22	2.46	0.51
1:B:422:ARG:HD3	1:B:474:PHE:CE1	2.48	0.48
1:A:322:GLN:HG3	1:A:406:ILE:HD12	1.95	0.48
1:F:194:ASN:HD21	1:F:197:ASN:HD22	1.63	0.47
1:B:434:GLU:OE1	2:B:501:ADP:O3'	2.24	0.47
1:F:460:THR:HG21	1:F:478:ASP:OD2	2.15	0.47
1:C:13:VAL:HG13	5:C:603:HOH:O	2.14	0.47
1:B:194:ASN:HD21	1:B:197:ASN:HD22	1.63	0.46
1:B:189:ARG:HA	1:E:214:ARG:HD3	1.97	0.46
1:B:77:ALA:HB2	1:B:149:LEU:HD21	1.97	0.46
1:D:177:GLN:O	1:D:180:ARG:HG3	2.16	0.46
1:F:433:SER:HG	1:F:460:THR:HG22	1.77	0.46
1:D:77:ALA:HB2	1:D:149:LEU:HD21	1.99	0.45
1:F:77:ALA:HB2	1:F:149:LEU:HD21	1.99	0.45
1:C:77:ALA:HB2	1:C:149:LEU:HD21	1.99	0.45
1:F:434:GLU:OE1	2:F:501:ADP:O3'	2.30	0.45
1:A:77:ALA:HB2	1:A:149:LEU:HD21	1.99	0.45
1:E:319:LYS:NZ	1:E:352:SER:CB	2.80	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:LEU:HD13	1:E:405:TYR:O	2.18	0.44
1:E:77:ALA:HB2	1:E:149:LEU:HD21	1.99	0.44
1:A:125:ILE:O	1:A:125:ILE:HG22	2.16	0.44
1:E:420:LEU:HD12	1:E:420:LEU:N	2.33	0.43
1:F:461:LYS:NZ	2:F:501:ADP:O3'	2.49	0.42
1:E:371:MET:HE1	1:E:390:ALA:HB3	2.01	0.42
1:B:80:VAL:HG13	5:B:654:HOH:O	2.18	0.42
1:F:80:VAL:HG13	5:F:643:HOH:O	2.19	0.41
1:D:371:MET:HE1	1:D:390:ALA:HB3	2.03	0.40
1:C:26:LEU:HD11	1:C:183:ILE:HD11	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	437/483 (90%)	430 (98%)	6 (1%)	1 (0%)	47	66
1	B	438/483 (91%)	432 (99%)	5 (1%)	1 (0%)	47	66
1	C	439/483 (91%)	431 (98%)	7 (2%)	1 (0%)	47	66
1	D	439/483 (91%)	432 (98%)	6 (1%)	1 (0%)	47	66
1	E	440/483 (91%)	433 (98%)	6 (1%)	1 (0%)	47	66
1	F	441/483 (91%)	434 (98%)	6 (1%)	1 (0%)	47	66
All	All	2634/2898 (91%)	2592 (98%)	36 (1%)	6 (0%)	47	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PHE
1	B	161	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	161	PHE
1	D	161	PHE
1	E	161	PHE
1	F	161	PHE

### 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	393/418 (94%)	388 (99%)	5 (1%)	69	86
1	B	394/418 (94%)	388 (98%)	6 (2%)	65	83
1	C	395/418 (94%)	391 (99%)	4 (1%)	76	89
1	D	395/418 (94%)	389 (98%)	6 (2%)	65	83
1	E	396/418 (95%)	391 (99%)	5 (1%)	69	86
1	F	397/418 (95%)	393 (99%)	4 (1%)	76	89
All	All	2370/2508 (94%)	2340 (99%)	30 (1%)	69	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	96	GLU
1	A	144	GLU
1	A	145	GLN
1	A	337	LYS
1	B	44	ARG
1	B	114	ARG
1	B	144	GLU
1	B	145	GLN
1	B	367	GLU
1	B	445	LYS
1	C	86	GLU
1	C	107	LYS
1	C	144	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	337	LYS
1	D	104	ARG
1	D	108	VAL
1	D	144	GLU
1	D	174	SER
1	D	180	ARG
1	D	367	GLU
1	E	44	ARG
1	E	104	ARG
1	E	107	LYS
1	E	144	GLU
1	E	337	LYS
1	F	44	ARG
1	F	144	GLU
1	F	214	ARG
1	F	337	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	B	99	GLN
1	B	194	ASN
1	B	198	GLN
1	D	178	GLN
1	E	76	GLN
1	E	395	GLN
1	E	452	GLN
1	F	188	ASN
1	F	194	ASN
1	F	452	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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
2	ADP	D	501	-	24,29,29	0.99	1 (4%)	29,45,45	1.27	3 (10%)
2	ADP	F	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.33	3 (10%)
2	ADP	C	501	-	24,29,29	0.95	2 (8%)	29,45,45	1.26	3 (10%)
3	3GC	A	502	-	8,15,15	0.33	0	8,19,19	0.96	0
2	ADP	A	501	4	24,29,29	1.00	2 (8%)	29,45,45	1.27	4 (13%)
3	3GC	D	502	-	8,15,15	0.25	0	8,19,19	1.36	1 (12%)
3	3GC	B	502	-	8,15,15	0.60	0	8,19,19	2.13	3 (37%)
3	3GC	E	502	-	8,15,15	0.39	0	8,19,19	1.16	1 (12%)
3	3GC	C	502	-	8,15,15	0.41	0	8,19,19	0.60	0
3	3GC	F	502	-	8,15,15	0.23	0	8,19,19	1.00	0
2	ADP	B	501	-	24,29,29	0.98	2 (8%)	29,45,45	1.31	4 (13%)
2	ADP	E	501	-	24,29,29	1.05	2 (8%)	29,45,45	1.28	3 (10%)

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
2	ADP	D	501	-	-	8/12/32/32	0/3/3/3
2	ADP	F	501	-	-	2/12/32/32	0/3/3/3
2	ADP	C	501	-	-	3/12/32/32	0/3/3/3
3	3GC	A	502	-	-	0/11/19/19	-
2	ADP	A	501	4	-	0/12/32/32	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3GC	D	502	-	-	0/11/19/19	-
3	3GC	B	502	-	-	4/11/19/19	-
3	3GC	E	502	-	-	0/11/19/19	-
3	3GC	C	502	-	-	0/11/19/19	-
3	3GC	F	502	-	-	1/11/19/19	-
2	ADP	B	501	-	-	0/12/32/32	0/3/3/3
2	ADP	E	501	-	-	3/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ADP	C5-C4	2.82	1.48	1.40
2	E	501	ADP	C5-C4	2.60	1.47	1.40
2	A	501	ADP	C5-C4	2.53	1.47	1.40
2	B	501	ADP	C5-C4	2.52	1.47	1.40
2	C	501	ADP	C5-C4	2.49	1.47	1.40
2	F	501	ADP	C5-C4	2.45	1.47	1.40
2	C	501	ADP	O4'-C1'	2.29	1.44	1.41
2	E	501	ADP	O4'-C1'	2.29	1.44	1.41
2	A	501	ADP	O4'-C1'	2.20	1.44	1.41
2	B	501	ADP	O4'-C1'	2.10	1.44	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ADP	N3-C2-N1	-4.22	122.08	128.68
3	B	502	3GC	OE1-CD1-CG1	-3.94	114.81	122.02
2	E	501	ADP	N3-C2-N1	-3.82	122.70	128.68
3	B	502	3GC	CG1-CD1-N2	3.74	122.31	115.83
2	F	501	ADP	N3-C2-N1	-3.73	122.84	128.68
2	A	501	ADP	N3-C2-N1	-3.70	122.89	128.68
2	C	501	ADP	N3-C2-N1	-3.69	122.92	128.68
2	D	501	ADP	N3-C2-N1	-3.66	122.96	128.68
2	B	501	ADP	C2-N1-C6	2.80	123.55	118.75
2	D	501	ADP	C2-N1-C6	2.61	123.23	118.75
2	F	501	ADP	C4-C5-N7	-2.58	106.70	109.40
2	C	501	ADP	C2-N1-C6	2.51	123.05	118.75
2	A	501	ADP	C2-N1-C6	2.51	123.05	118.75
2	F	501	ADP	C2-N1-C6	2.50	123.02	118.75
2	C	501	ADP	N6-C6-N1	2.48	123.73	118.57
3	E	502	3GC	CB2-CA2-N2	-2.48	107.75	111.28
2	E	501	ADP	C2-N1-C6	2.35	122.77	118.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	ADP	C4-C5-N7	-2.28	107.02	109.40
2	D	501	ADP	N6-C6-N1	2.23	123.20	118.57
2	A	501	ADP	N6-C6-N1	2.21	123.15	118.57
3	B	502	3GC	CB2-CA2-N2	2.16	114.36	111.28
2	B	501	ADP	C1'-N9-C4	-2.10	122.95	126.64
2	A	501	ADP	C4-C5-N7	-2.04	107.28	109.40
3	D	502	3GC	CA2-N2-CD1	2.01	126.52	123.33
2	B	501	ADP	N6-C6-N1	2.01	122.74	118.57

There are no chirality outliers.

All (21) torsion outliers are listed below:

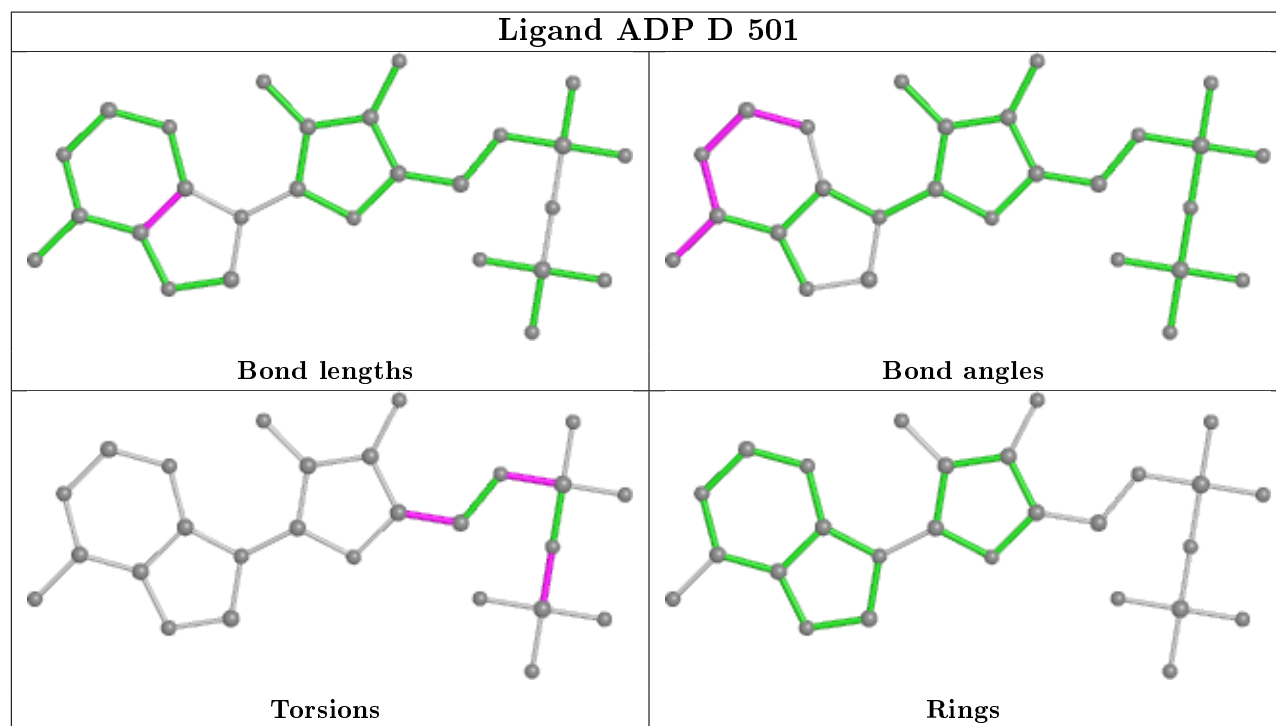
Mol	Chain	Res	Type	Atoms
2	F	501	ADP	PA-O3A-PB-O2B
2	C	501	ADP	C5'-O5'-PA-O1A
2	C	501	ADP	C5'-O5'-PA-O3A
3	B	502	3GC	N1-CA1-CB1-CG1
3	B	502	3GC	C1-CA1-CB1-CG1
2	D	501	ADP	PA-O3A-PB-O2B
2	D	501	ADP	PA-O3A-PB-O3B
2	D	501	ADP	C5'-O5'-PA-O1A
2	D	501	ADP	C5'-O5'-PA-O2A
2	D	501	ADP	C5'-O5'-PA-O3A
2	E	501	ADP	PA-O3A-PB-O3B
3	B	502	3GC	N2-CD1-CG1-CB1
3	B	502	3GC	OE1-CD1-CG1-CB1
2	D	501	ADP	O4'-C4'-C5'-O5'
2	D	501	ADP	C3'-C4'-C5'-O5'
2	C	501	ADP	C5'-O5'-PA-O2A
2	F	501	ADP	PA-O3A-PB-O1B
2	E	501	ADP	O4'-C4'-C5'-O5'
2	E	501	ADP	PA-O3A-PB-O2B
3	F	502	3GC	N2-CA2-CB2-SG2
2	D	501	ADP	PA-O3A-PB-O1B

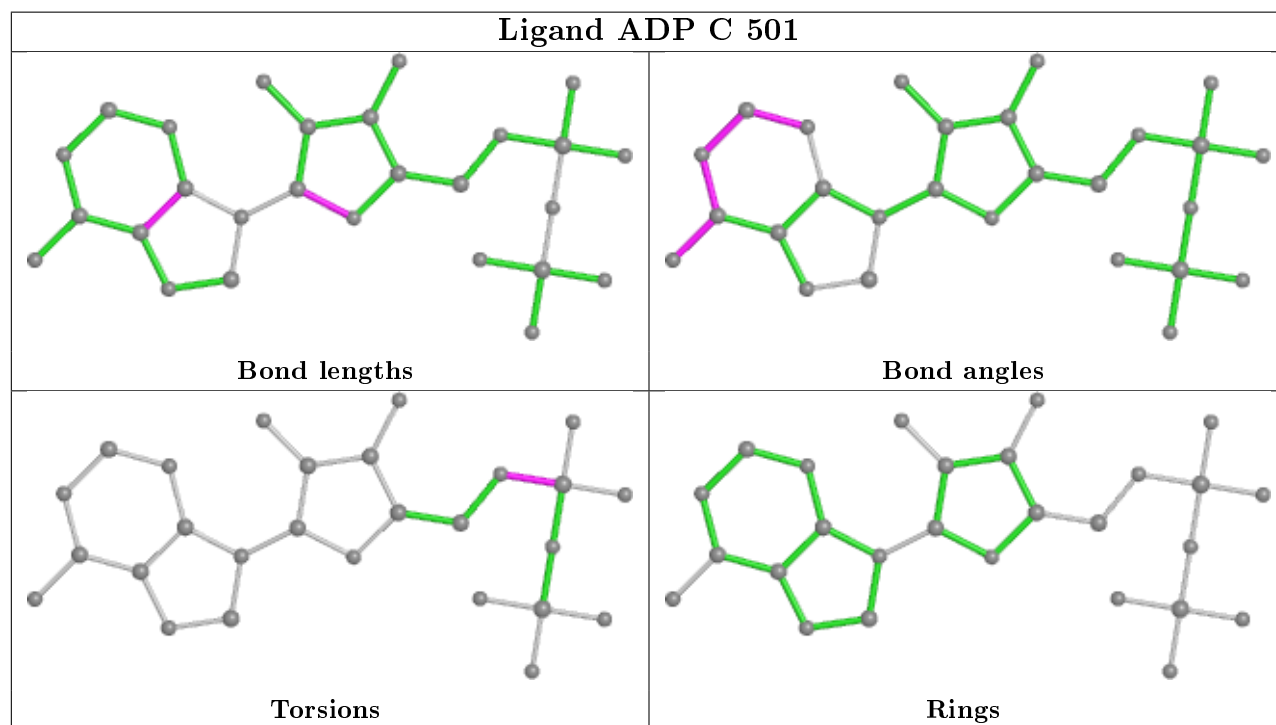
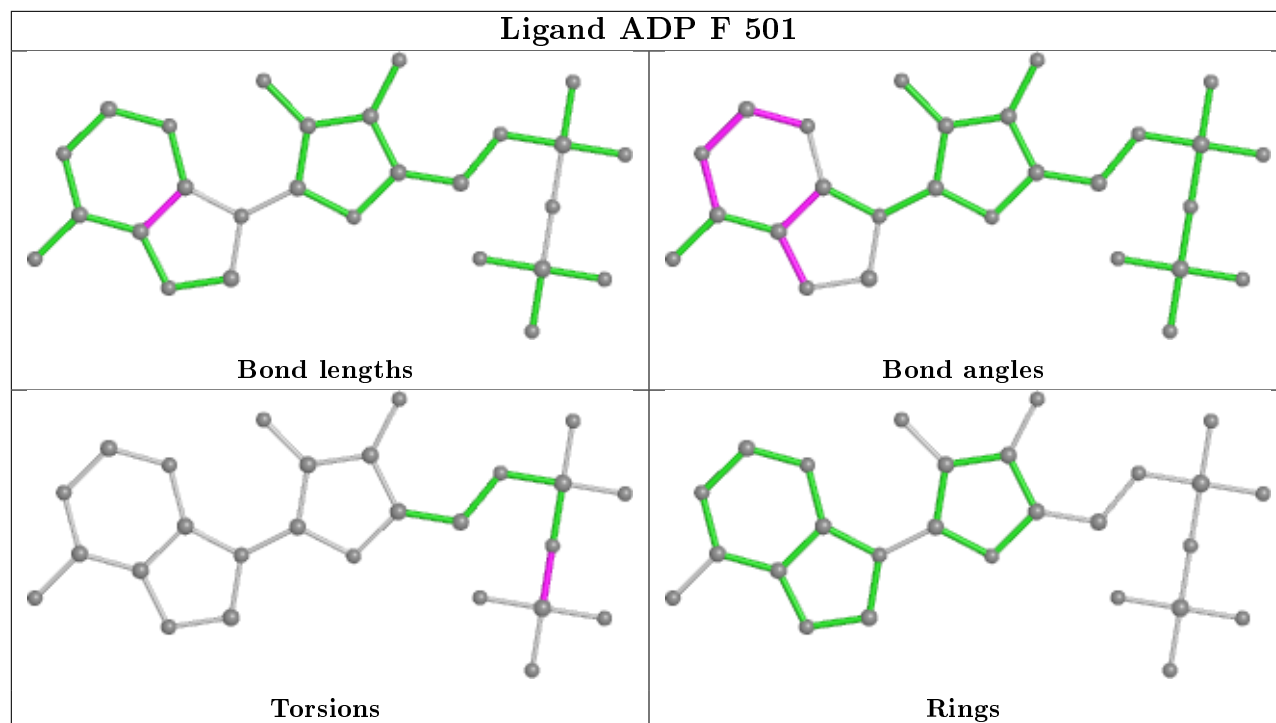
There are no ring outliers.

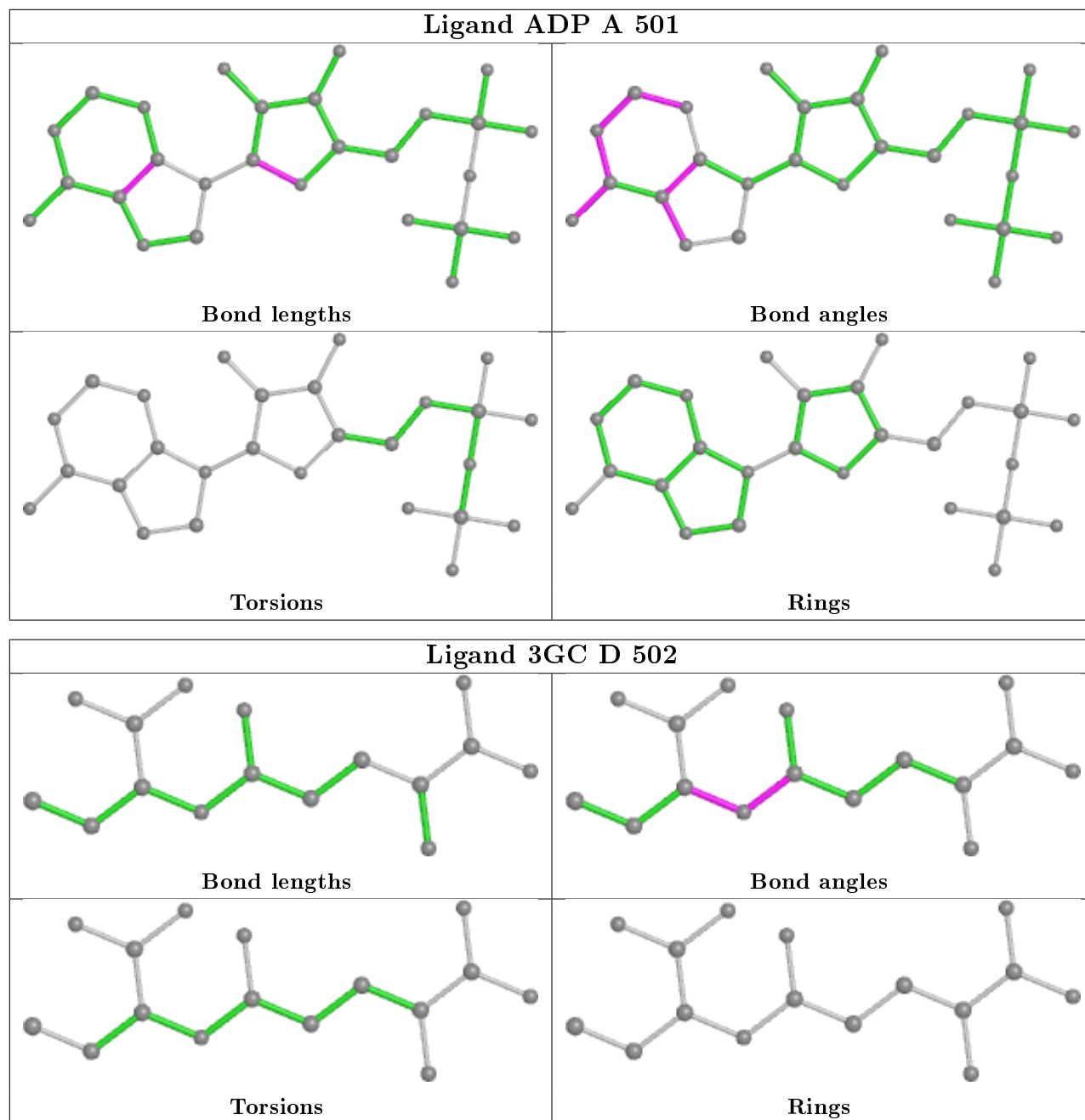
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	ADP	2	0
2	B	501	ADP	1	0

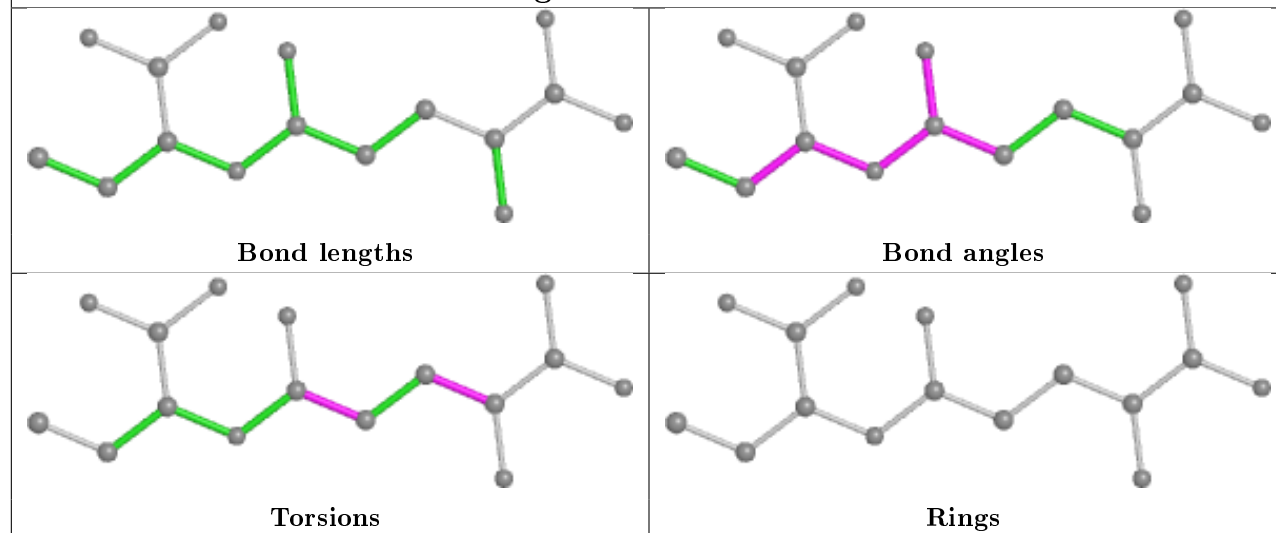
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



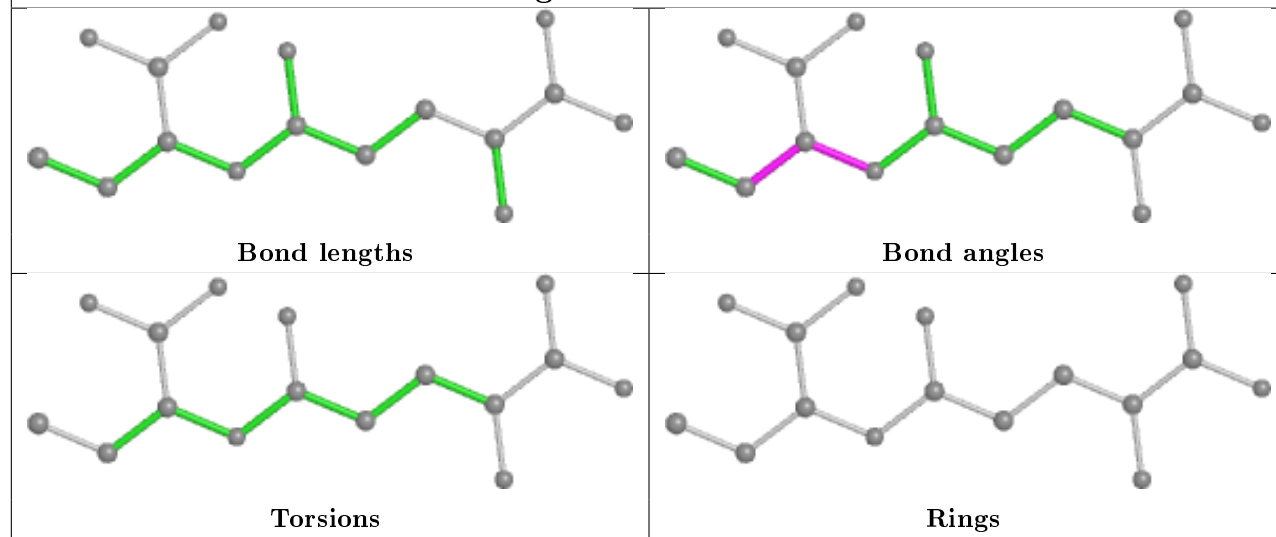




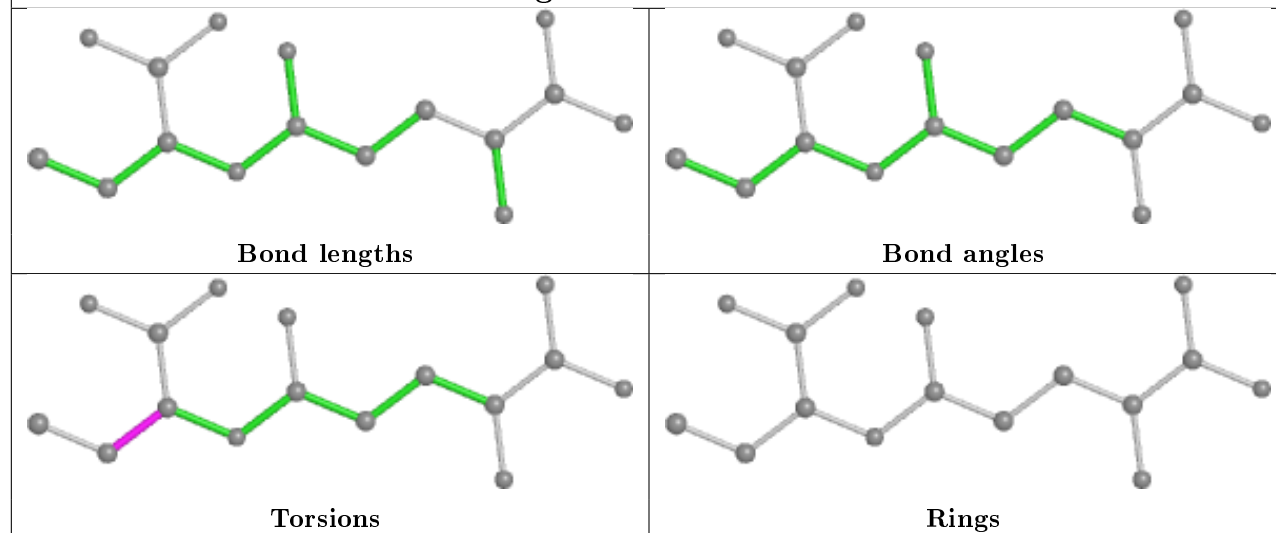
## Ligand 3GC B 502

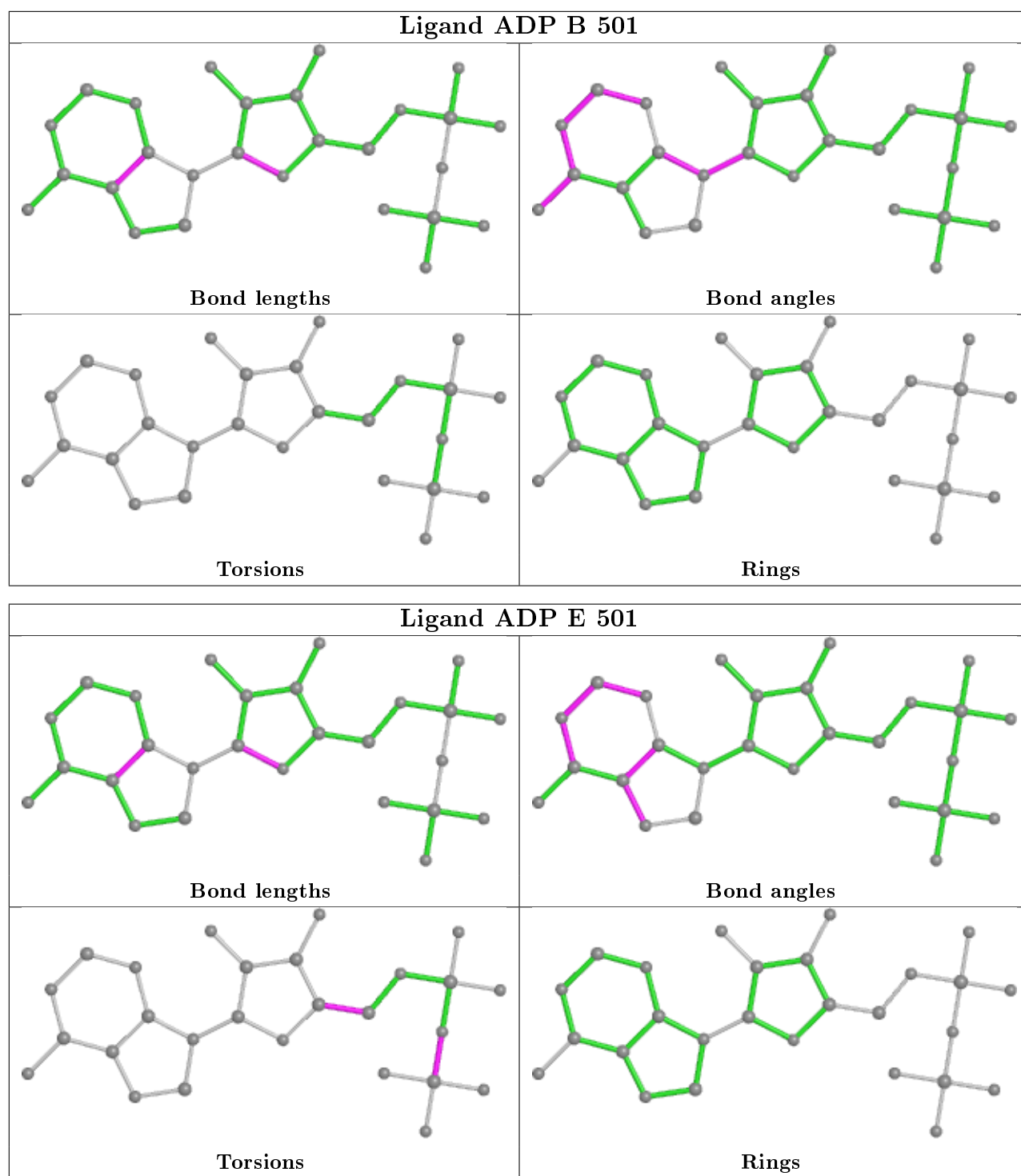


## Ligand 3GC E 502



## Ligand 3GC F 502





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	445/483 (92%)	0.08	7 (1%) 72 73	30, 46, 69, 85	0
1	B	446/483 (92%)	0.09	6 (1%) 77 78	31, 45, 67, 85	0
1	C	447/483 (92%)	0.24	22 (4%) 29 31	35, 49, 72, 93	0
1	D	446/483 (92%)	0.25	17 (3%) 40 42	35, 51, 75, 89	0
1	E	448/483 (92%)	0.19	11 (2%) 57 59	33, 50, 76, 93	0
1	F	448/483 (92%)	0.27	20 (4%) 33 35	34, 50, 77, 92	0
All	All	2680/2898 (92%)	0.19	83 (3%) 49 51	30, 48, 74, 93	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	446	THR	5.3
1	F	446	THR	5.0
1	D	446	THR	4.9
1	A	446	THR	4.7
1	E	446	THR	4.6
1	E	181	GLU	4.2
1	C	128	ILE	4.1
1	B	445	LYS	4.0
1	A	445	LYS	4.0
1	F	128	ILE	3.9
1	F	262	GLN	3.9
1	F	445	LYS	3.8
1	E	445	LYS	3.7
1	F	17	ASP	3.7
1	C	44	ARG	3.3
1	B	446	THR	3.3
1	D	21	LYS	3.3
1	E	184	ALA	3.3
1	C	126	ASN	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	21	LYS	3.2
1	C	13	VAL	3.2
1	B	17	ASP	3.2
1	E	17	ASP	3.2
1	D	445	LYS	3.1
1	C	394	LEU	3.1
1	B	128	ILE	3.1
1	F	125	ILE	3.0
1	D	184	ALA	3.0
1	C	17	ASP	3.0
1	E	183	ILE	2.9
1	F	126	ASN	2.9
1	D	417	HIS	2.9
1	F	105	THR	2.9
1	C	445	LYS	2.8
1	D	128	ILE	2.8
1	A	405	TYR	2.8
1	F	214	ARG	2.8
1	C	405	TYR	2.8
1	F	397	GLU	2.7
1	F	264	GLY	2.6
1	C	130	GLU	2.6
1	F	263	ASP	2.6
1	F	14	ASP	2.6
1	A	394	LEU	2.5
1	D	430	GLN	2.5
1	D	449	VAL	2.4
1	C	14	ASP	2.4
1	C	251	LEU	2.4
1	A	44	ARG	2.4
1	C	374	GLN	2.4
1	C	124	GLU	2.4
1	D	415	ILE	2.4
1	A	14	ASP	2.3
1	F	396	LYS	2.3
1	E	180	ARG	2.3
1	C	107	LYS	2.3
1	E	405	TYR	2.3
1	C	47	GLU	2.3
1	D	335	GLU	2.3
1	D	444	ASN	2.3
1	F	239	ARG	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	16	HIS	2.3
1	F	260	LEU	2.3
1	E	128	ILE	2.2
1	D	474	PHE	2.2
1	C	259	GLU	2.2
1	D	181	GLU	2.2
1	D	17	ASP	2.2
1	C	303	ARG	2.2
1	F	405	TYR	2.2
1	F	447	GLU	2.2
1	F	44	ARG	2.2
1	C	428	LYS	2.2
1	C	264	GLY	2.1
1	D	64	LEU	2.1
1	D	448	VAL	2.0
1	B	394	LEU	2.0
1	C	444	ASN	2.0
1	D	447	GLU	2.0
1	B	144	GLU	2.0
1	E	177	GLN	2.0
1	A	130	GLU	2.0
1	F	93	GLN	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 carbohydrates 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
4	MG	D	503	1/1	0.76	0.15	68,68,68,68	0

*Continued on next page...*

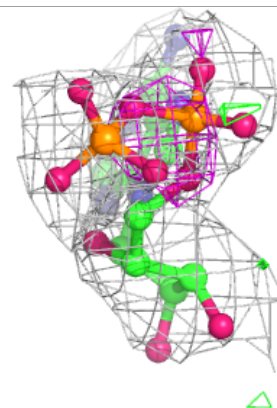
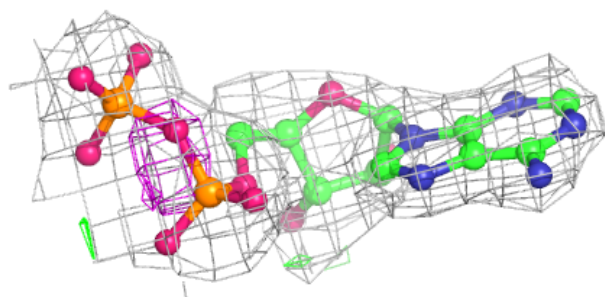
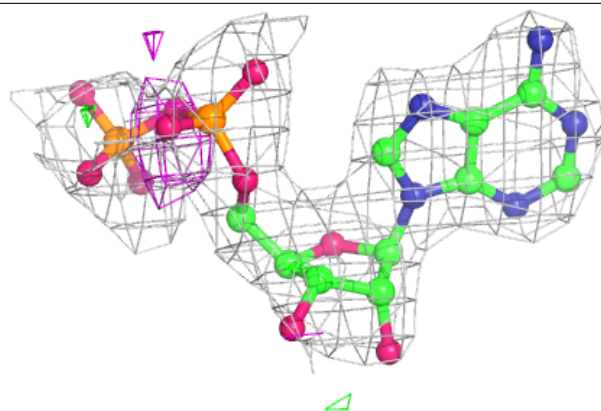
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	F	503	1/1	0.80	0.19	61,61,61,61	0
2	ADP	D	501	27/27	0.81	0.20	69,81,112,114	0
4	MG	E	504	1/1	0.81	0.18	67,67,67,67	0
2	ADP	B	501	27/27	0.81	0.21	54,66,108,109	0
4	MG	D	504	1/1	0.83	0.22	55,55,55,55	0
2	ADP	A	501	27/27	0.85	0.20	51,61,100,104	0
2	ADP	F	501	27/27	0.85	0.23	57,69,112,113	0
4	MG	C	504	1/1	0.86	0.12	60,60,60,60	0
2	ADP	C	501	27/27	0.87	0.21	57,68,115,118	0
4	MG	E	503	1/1	0.87	0.19	67,67,67,67	0
2	ADP	E	501	27/27	0.89	0.17	59,70,99,103	0
4	MG	C	503	1/1	0.90	0.18	64,64,64,64	0
4	MG	A	504	1/1	0.90	0.17	64,64,64,64	0
4	MG	A	503	1/1	0.91	0.11	45,45,45,45	0
4	MG	B	503	1/1	0.91	0.18	46,46,46,46	0
3	3GC	F	502	16/16	0.92	0.17	55,59,61,61	0
3	3GC	C	502	16/16	0.93	0.14	50,52,54,54	0
3	3GC	B	502	16/16	0.94	0.15	45,48,51,54	0
3	3GC	A	502	16/16	0.94	0.15	47,49,51,53	0
3	3GC	E	502	16/16	0.95	0.15	51,53,55,55	0
3	3GC	D	502	16/16	0.95	0.13	46,48,50,51	0

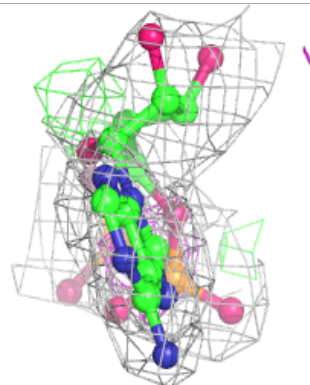
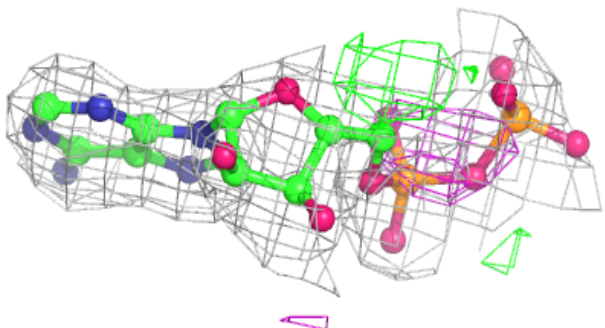
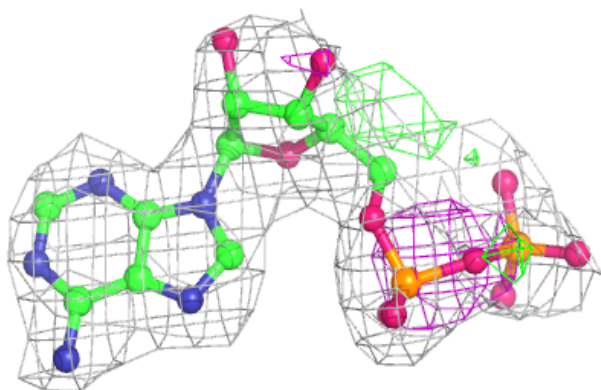
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP 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)

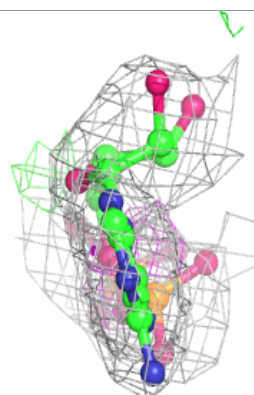
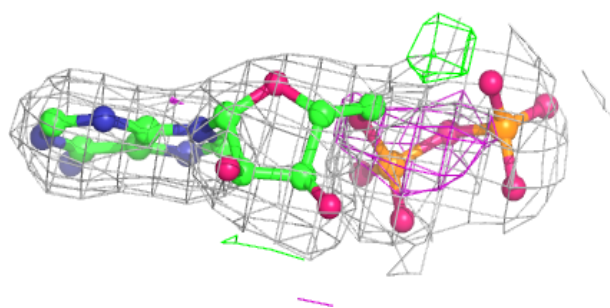
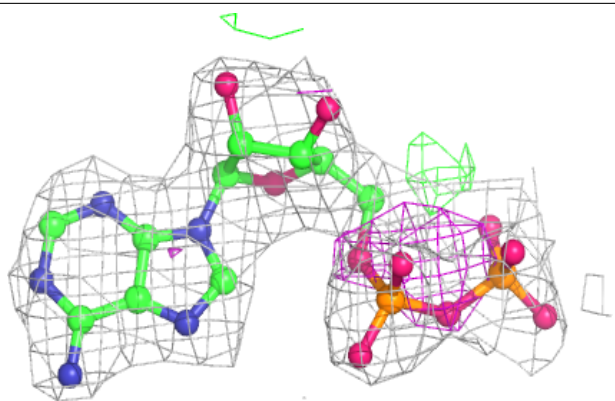
**Electron density around ADP B 501:**

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

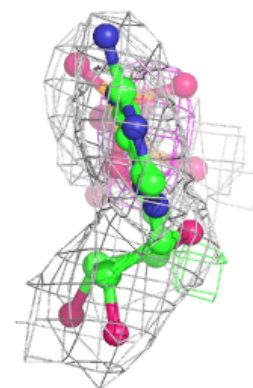
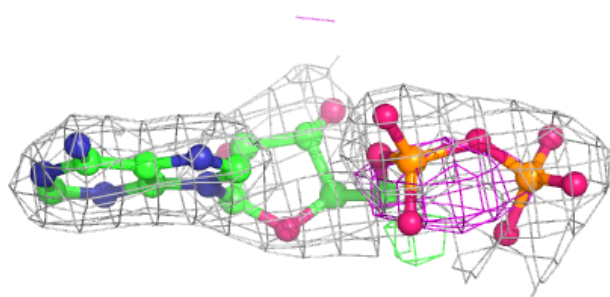
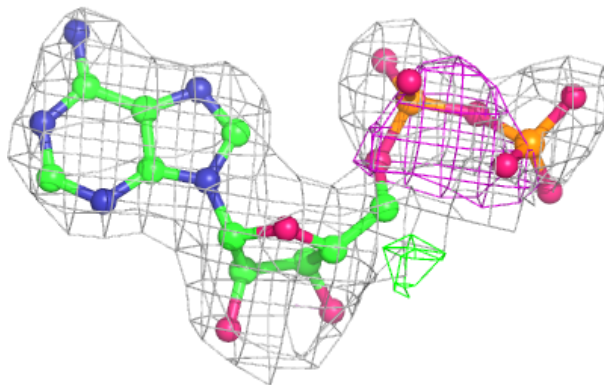


**Electron density around ADP A 501:**

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

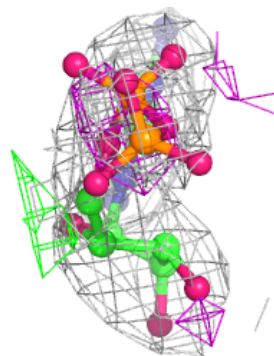
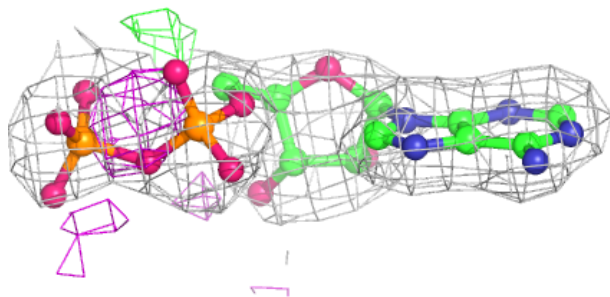
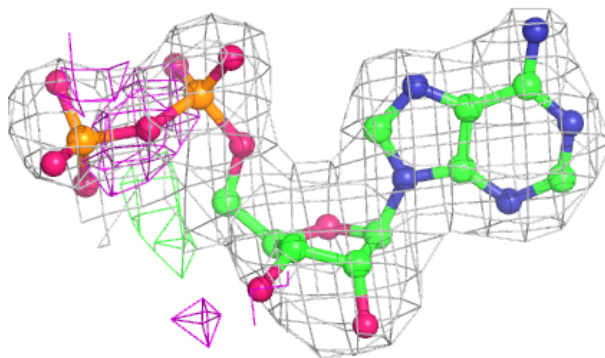
**Electron density around ADP F 501:**

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

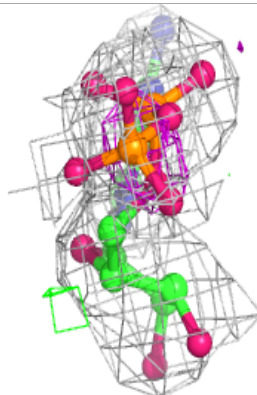
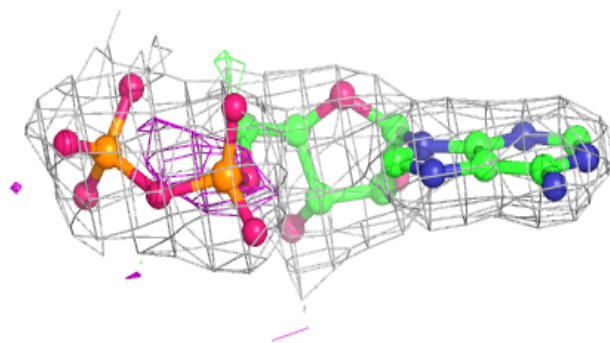
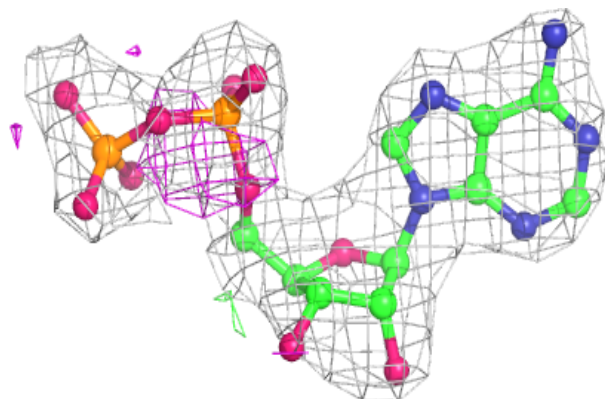


**Electron density around ADP C 501:**

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

**Electron density around ADP E 501:**

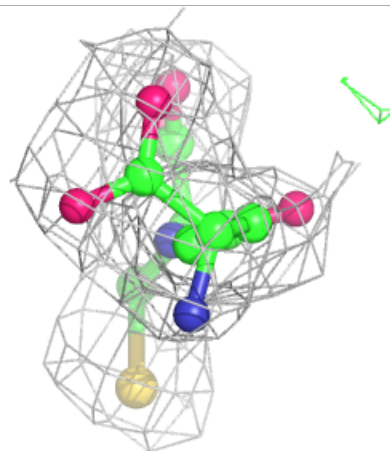
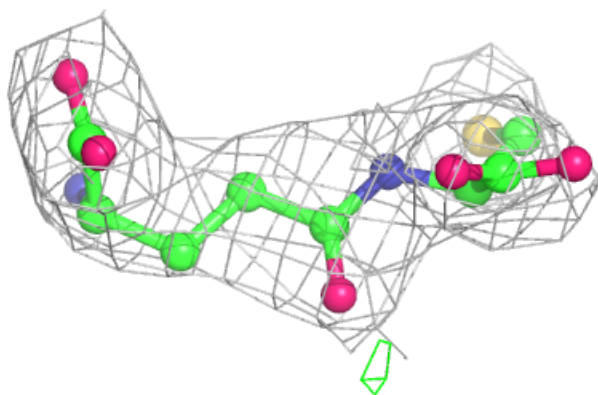
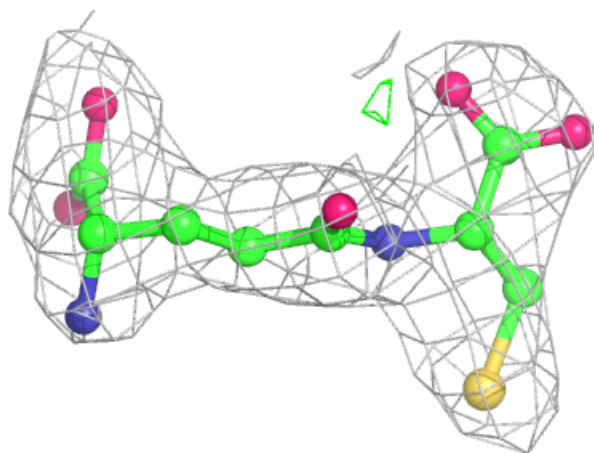
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 3GC F 502:**

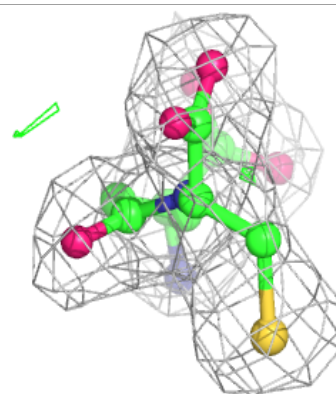
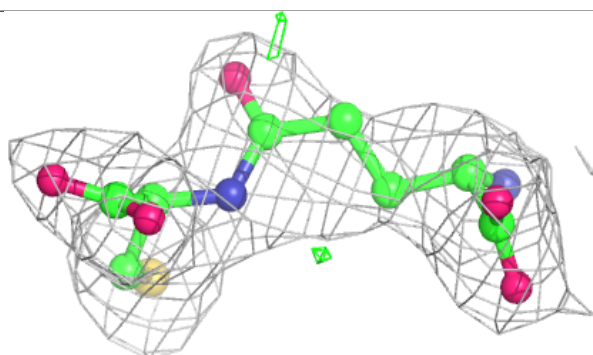
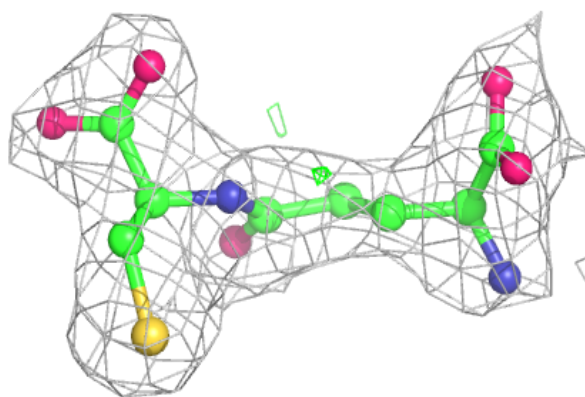
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



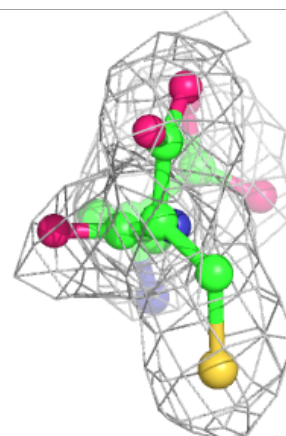
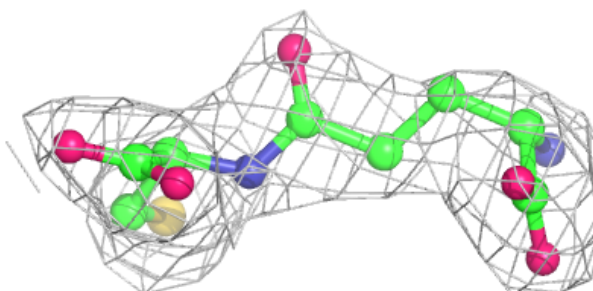
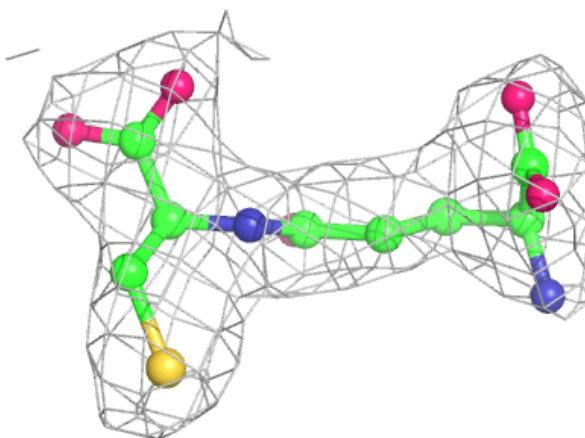


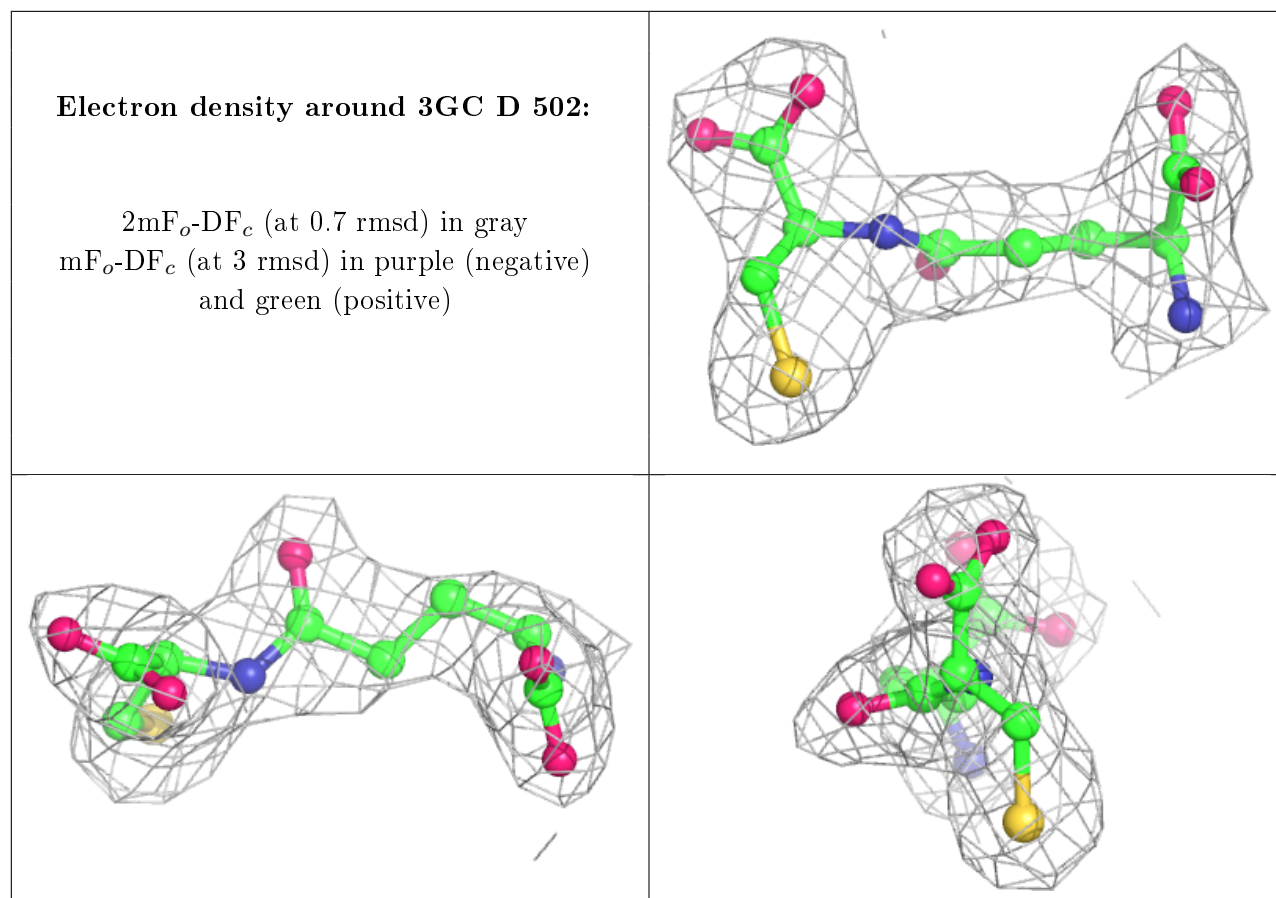
**Electron density around 3GC B 502:**

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

**Electron density around 3GC E 502:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.