



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 09:26 PM EDT

PDB ID : 1XXH  
Title : ATPgS Bound E. Coli Clamp Loader Complex  
Authors : Kazmirski, S.L.; Podobnik, M.; Weitze, T.F.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2004-11-05  
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

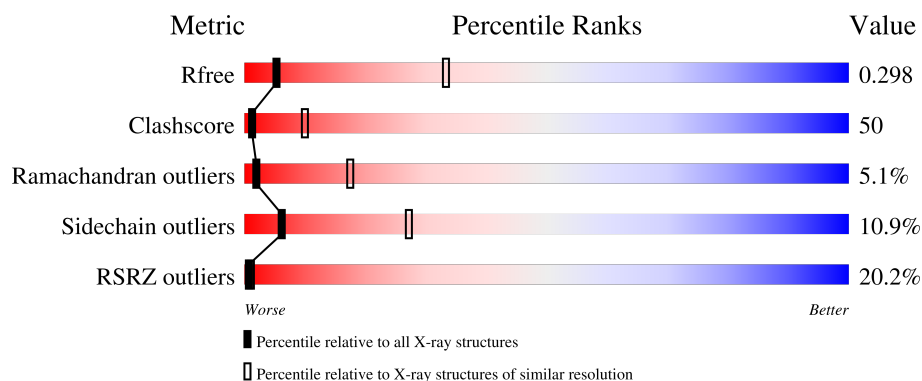
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	343	
1	F	343	
2	B	373	
2	C	373	
2	D	373	

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Mol	Chain	Length	Quality of chain
2	G	373	
2	H	373	
2	I	373	
3	E	334	
3	J	334	

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
5	AGS	I	803	-	-	X	-
6	PO4	C	1300	-	-	X	-
6	PO4	H	1400	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27736 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 DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	Se	0	0	0
			2687	1702	488	487	5	5			
1	F	338	Total	C	N	O	S	Se	0	0	0
			2687	1702	488	487	5	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	71	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	223	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	285	MSE	MET	MODIFIED RESIDUE	UNP P28630
A	286	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	1	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	71	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	223	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	285	MSE	MET	MODIFIED RESIDUE	UNP P28630
F	286	MSE	MET	MODIFIED RESIDUE	UNP P28630

- Molecule 2 is a protein called DNA polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
2	D	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	G	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	H	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			

- Molecule 3 is a protein called DNA polymerase III, delta prime subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	Se	0	0	0
			2602	1655	468	466	7	6			
3	J	334	Total	C	N	O	S	Se	0	0	0
			2602	1655	468	466	7	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	35	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	68	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	182	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	253	MSE	MET	MODIFIED RESIDUE	UNP P28631
E	301	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	1	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	35	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	68	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	182	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	253	MSE	MET	MODIFIED RESIDUE	UNP P28631
J	301	MSE	MET	MODIFIED RESIDUE	UNP P28631

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

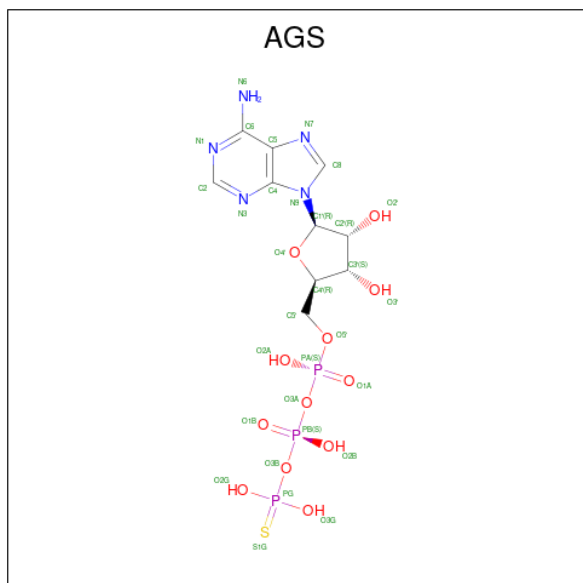
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	G	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		

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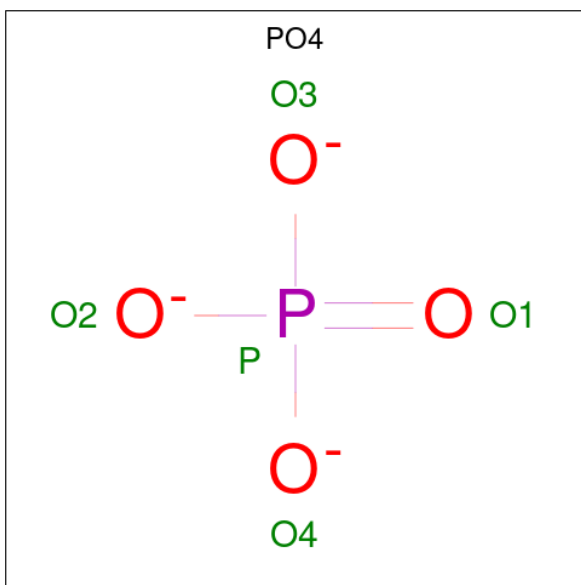
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	I	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

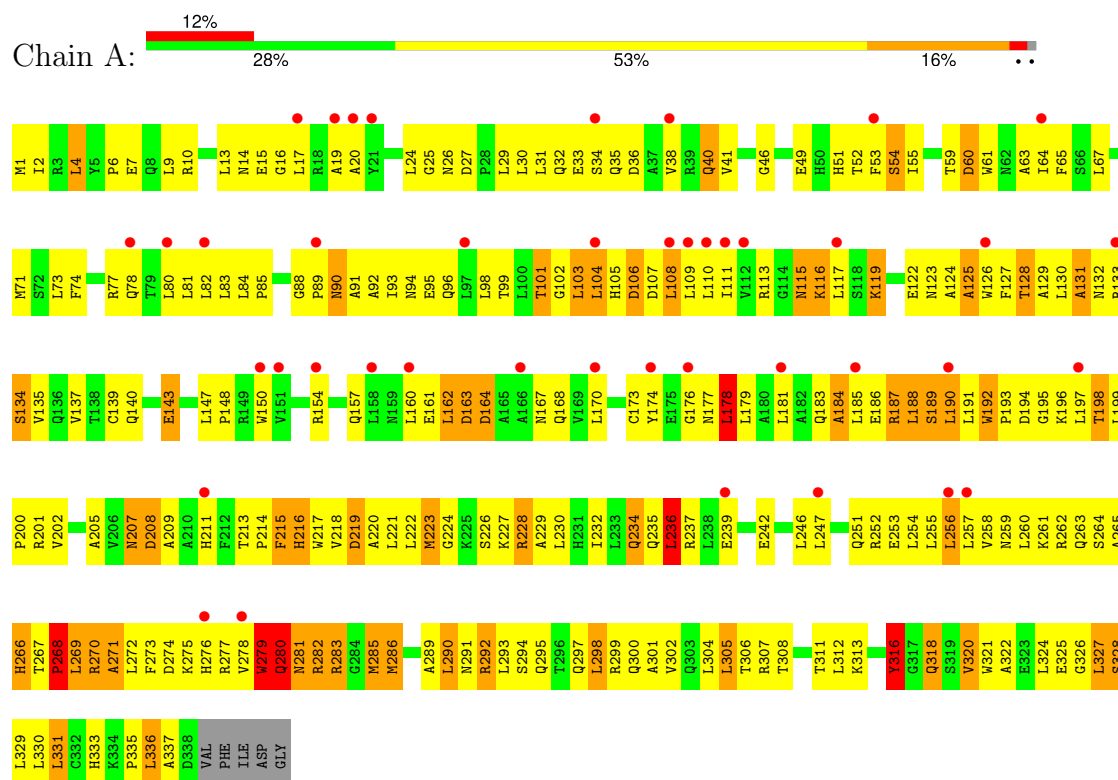


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		

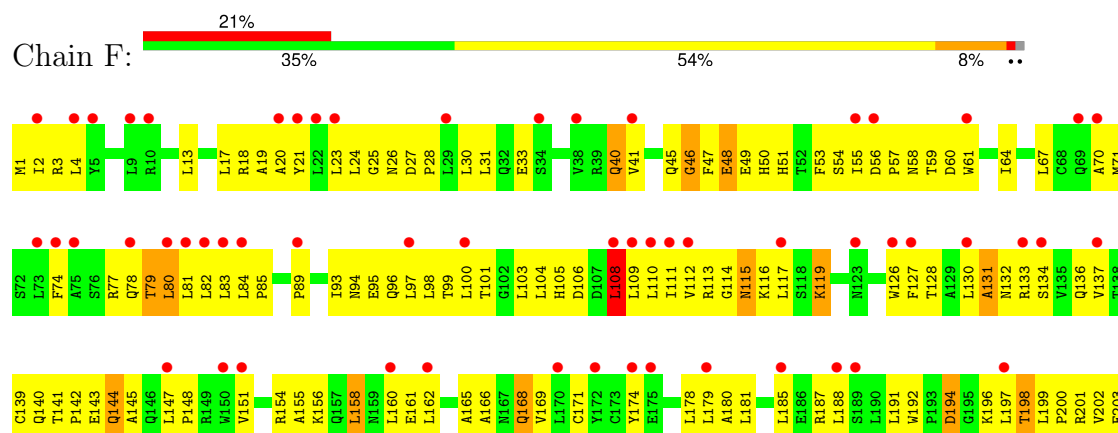
### 3 Residue-property plots

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

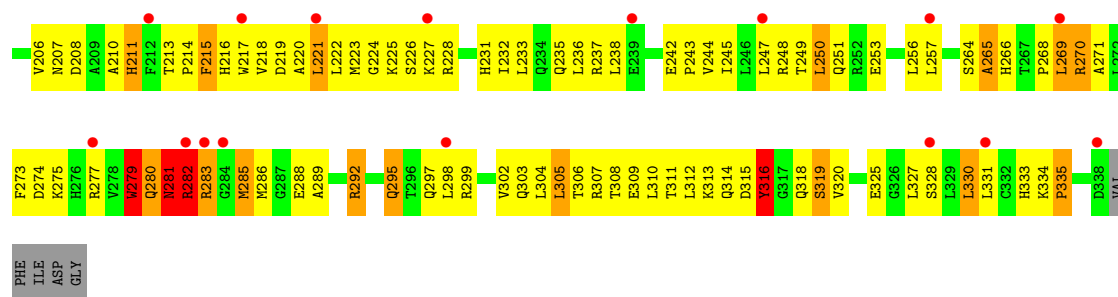
#### • Molecule 1: DNA polymerase III, delta subunit



#### • Molecule 1: DNA polymerase III, delta subunit



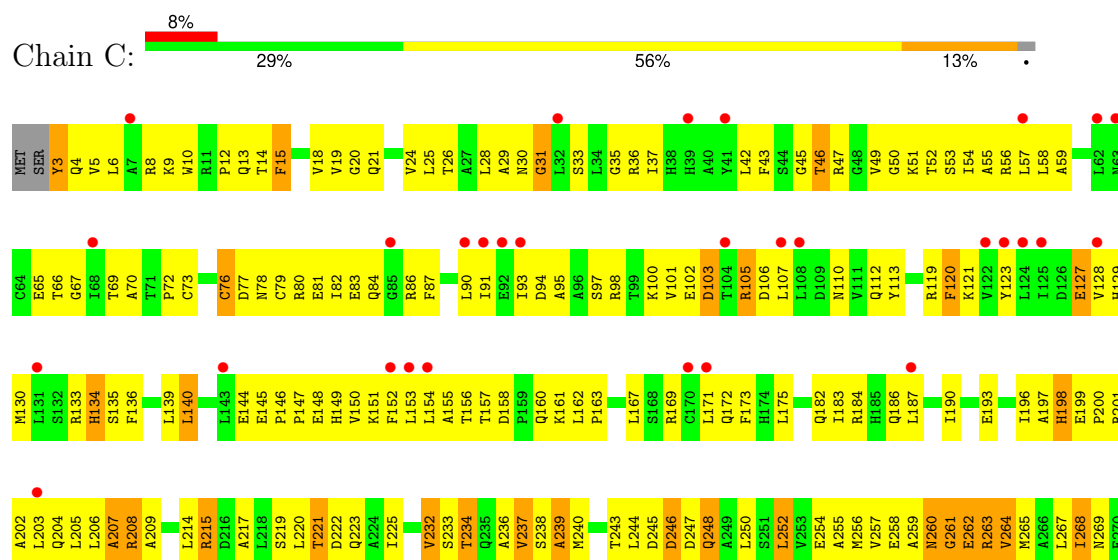




• Molecule 2: DNA polymerase III subunit gamma

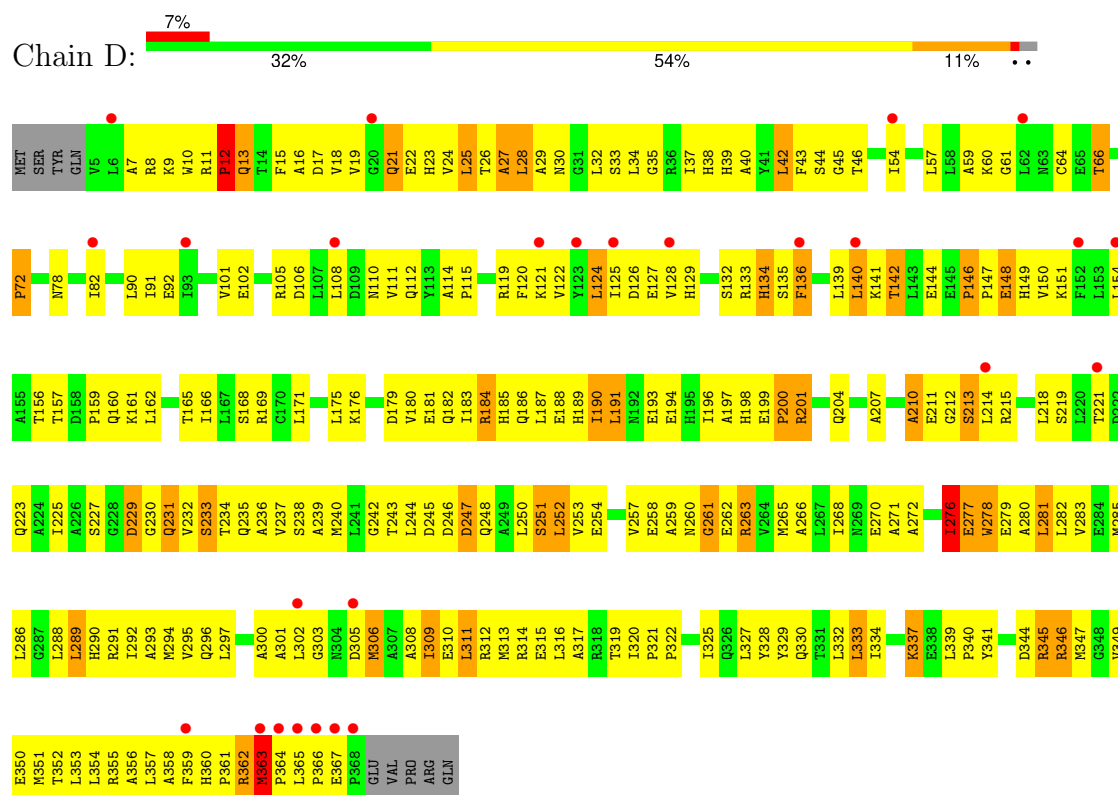


• Molecule 2: DNA polymerase III subunit gamma

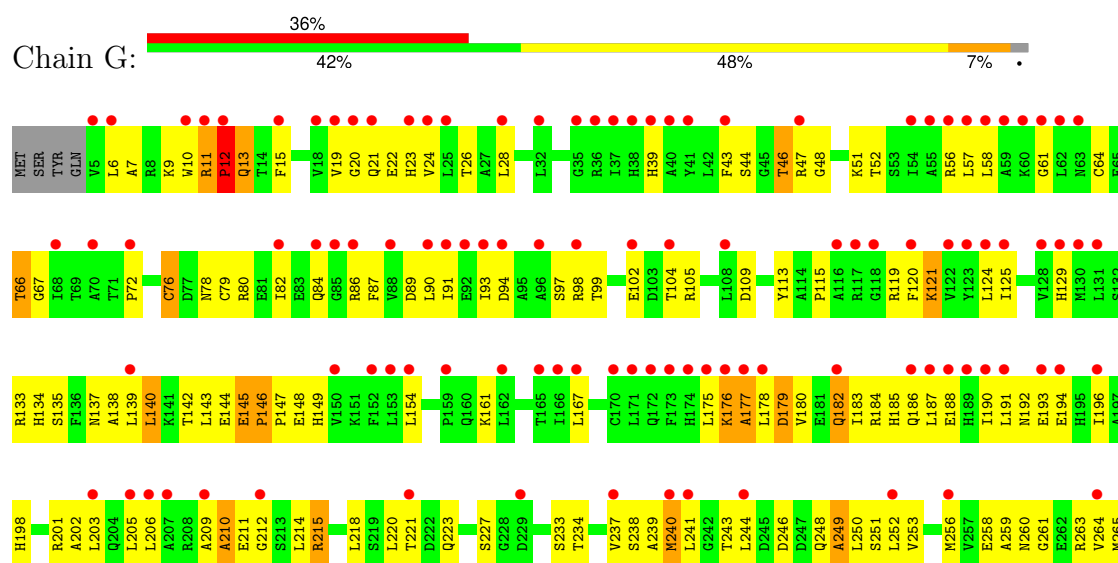




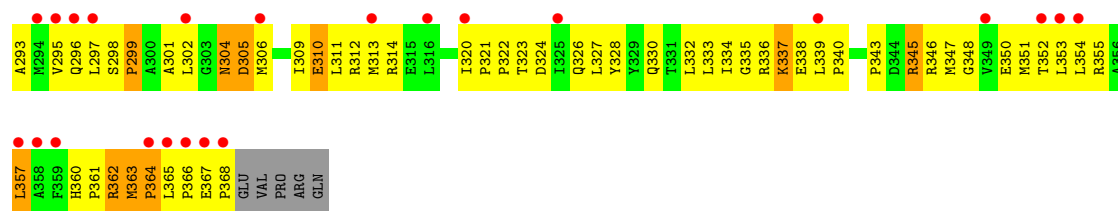
• Molecule 2: DNA polymerase III subunit gamma



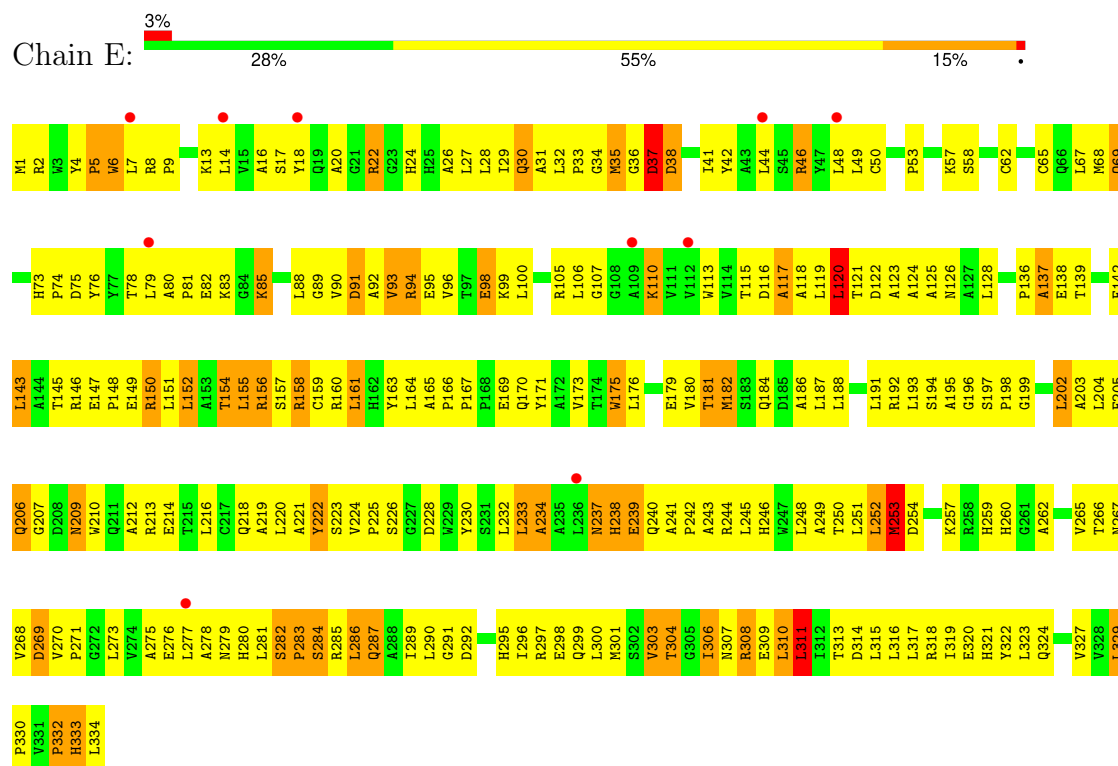
• Molecule 2: DNA polymerase III subunit gamma



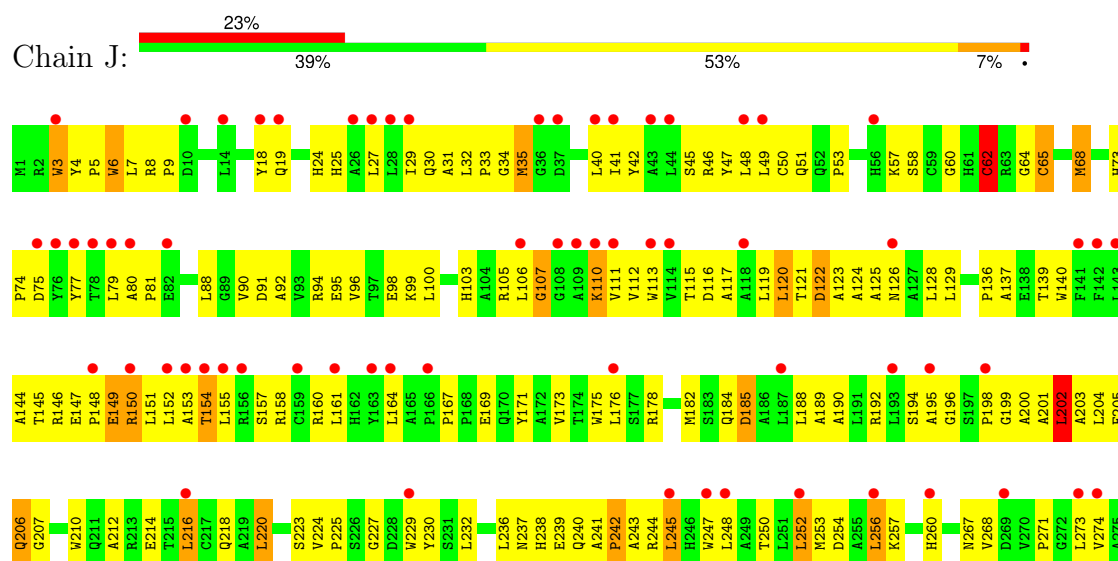




• Molecule 3: DNA polymerase III, delta prime subunit



• Molecule 3: DNA polymerase III, delta prime subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.45Å 106.46Å 535.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.45 98.93 – 3.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-3.45) 97.7 (98.93-3.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.315 , 0.350 0.256 , 0.298	Depositor DCC
$R_{free}$ test set	7449 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	106.7	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 116.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, ZN, PO4

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	0.60	3/2731 (0.1%)	0.88	6/3704 (0.2%)
1	F	0.55	2/2731 (0.1%)	0.73	4/3704 (0.1%)
2	B	0.52	1/2876 (0.0%)	0.81	1/3900 (0.0%)
2	C	0.61	0/2898	0.84	0/3930
2	D	0.63	0/2876	0.93	3/3900 (0.1%)
2	G	0.38	0/2876	0.66	1/3900 (0.0%)
2	H	0.29	0/2898	0.58	0/3930
2	I	0.34	0/2876	0.63	1/3900 (0.0%)
3	E	0.54	2/2662 (0.1%)	0.77	4/3624 (0.1%)
3	J	0.37	0/2662	0.56	1/3624 (0.0%)
All	All	0.50	8/28086 (0.0%)	0.75	21/38116 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	285	MSE	SE-CE	16.36	2.92	1.95
1	A	286	MSE	C-N	11.64	1.54	1.33
1	F	285	MSE	CG-SE	8.13	2.23	1.95
1	A	286	MSE	CG-SE	-8.08	1.68	1.95
3	E	253	MSE	CG-SE	-6.37	1.73	1.95

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	285	MSE	CG-SE-CE	-15.68	64.40	98.90
1	A	268	PRO	CA-N-CD	-13.61	92.44	111.50
1	F	283	ARG	CA-C-N	-8.30	99.59	116.20
2	D	12	PRO	CA-N-CD	-8.17	100.06	111.50
2	G	12	PRO	CA-N-CD	-7.64	100.81	111.50

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	2687	0	2743	371	0
1	F	2687	0	2737	337	6
2	B	2829	0	2881	302	0
2	C	2850	0	2897	334	0
2	D	2829	0	2879	361	0
2	G	2829	0	2881	274	0
2	H	2850	0	2898	276	0
2	I	2829	0	2877	267	6
3	E	2602	0	2605	304	0
3	J	2602	0	2605	238	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	4	0
5	D	31	0	12	4	0
5	G	31	0	12	2	0
5	I	31	0	12	27	0
6	C	5	0	0	3	0
6	H	5	0	0	4	0
All	All	27736	0	28051	2798	6

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 50.

The worst 5 of 2798 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MSE:SE	1:F:228:ARG:HA	1.53	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:LYS:NZ	2:I:133:ARG:CG	1.68	1.54
2:G:10:TRP:CZ2	2:G:193:GLU:HB3	1.47	1.48
1:A:74:PHE:CZ	1:F:206:VAL:HB	1.49	1.47
2:I:223:GLN:NE2	2:I:240:MET:HE1	1.29	1.46

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ASP:OD2	2:I:33:SER:O[1_455]	1.82	0.38
1:F:277:ARG:NH2	2:I:67:GLY:CA[1_455]	1.82	0.38
1:F:277:ARG:NE	2:I:66:THR:O[1_455]	1.87	0.33
1:F:277:ARG:CZ	2:I:67:GLY:CA[1_455]	2.03	0.17
1:F:277:ARG:NH2	2:I:67:GLY:C[1_455]	2.10	0.10

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/343 (98%)	244 (73%)	70 (21%)	22 (6%)	1	12
1	F	336/343 (98%)	270 (80%)	47 (14%)	19 (6%)	1	15
2	B	362/373 (97%)	278 (77%)	62 (17%)	22 (6%)	1	13
2	C	364/373 (98%)	283 (78%)	54 (15%)	27 (7%)	1	10
2	D	362/373 (97%)	261 (72%)	77 (21%)	24 (7%)	1	12
2	G	362/373 (97%)	312 (86%)	39 (11%)	11 (3%)	4	29
2	H	364/373 (98%)	312 (86%)	44 (12%)	8 (2%)	6	35
2	I	362/373 (97%)	335 (92%)	18 (5%)	9 (2%)	5	32
3	E	332/334 (99%)	237 (71%)	68 (20%)	27 (8%)	1	9
3	J	332/334 (99%)	271 (82%)	50 (15%)	11 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3512/3592 (98%)	2803 (80%)	529 (15%)	180 (5%)	2	17

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	116	LYS
1	A	125	ALA
1	A	131	ALA
1	A	223	MSE

### 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	287/286 (100%)	234 (82%)	53 (18%)	1	7
1	F	287/286 (100%)	260 (91%)	27 (9%)	8	33
2	B	301/310 (97%)	271 (90%)	30 (10%)	7	31
2	C	303/310 (98%)	263 (87%)	40 (13%)	4	19
2	D	301/310 (97%)	261 (87%)	40 (13%)	4	19
2	G	301/310 (97%)	274 (91%)	27 (9%)	9	35
2	H	303/310 (98%)	281 (93%)	22 (7%)	14	45
2	I	301/310 (97%)	283 (94%)	18 (6%)	19	51
3	E	270/264 (102%)	232 (86%)	38 (14%)	3	17
3	J	270/264 (102%)	245 (91%)	25 (9%)	9	34
All	All	2924/2960 (99%)	2604 (89%)	320 (11%)	6	27

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	39	HIS
2	I	201	ARG

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Mol	Chain	Res	Type
2	G	121	LYS
2	H	69	THR
3	J	91	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	216	HIS
2	G	326	GLN
1	F	235	GLN
2	G	172	GLN
2	H	174	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z  > 2$
6	PO4	C	1300	-	4,4,4	1.42	1 (25%)	6,6,6	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PO4	H	1400	-	4,4,4	0.40	0	6,6,6	0.38	0
5	AGS	I	803	-	28,33,33	2.02	4 (14%)	31,52,52	1.28	2 (6%)
5	AGS	D	801	-	28,33,33	2.01	4 (14%)	31,52,52	1.28	2 (6%)
5	AGS	G	804	-	28,33,33	2.02	4 (14%)	31,52,52	1.28	2 (6%)
5	AGS	B	802	-	28,33,33	2.01	4 (14%)	31,52,52	1.28	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	G	804	-	-	5/17/38/38	0/3/3/3
5	AGS	B	802	-	-	5/17/38/38	0/3/3/3
5	AGS	D	801	-	-	5/17/38/38	0/3/3/3
5	AGS	I	803	-	-	5/17/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	803	AGS	PG-S1G	-8.39	1.72	1.90
5	D	801	AGS	PG-S1G	-8.39	1.72	1.90
5	G	804	AGS	PG-S1G	-8.39	1.72	1.90
5	B	802	AGS	PG-S1G	-8.36	1.72	1.90
5	G	804	AGS	C2-N3	3.27	1.37	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	803	AGS	C1'-N9-C4	4.67	134.84	126.64
5	G	804	AGS	C1'-N9-C4	4.65	134.82	126.64
5	B	802	AGS	C1'-N9-C4	4.64	134.80	126.64
5	D	801	AGS	C1'-N9-C4	4.63	134.78	126.64
5	B	802	AGS	O3G-PG-O3B	2.34	112.46	104.64

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	802	AGS	C5'-O5'-PA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	802	AGS	C5'-O5'-PA-O3A
5	D	801	AGS	C5'-O5'-PA-O2A
5	D	801	AGS	C5'-O5'-PA-O3A
5	G	804	AGS	C5'-O5'-PA-O2A

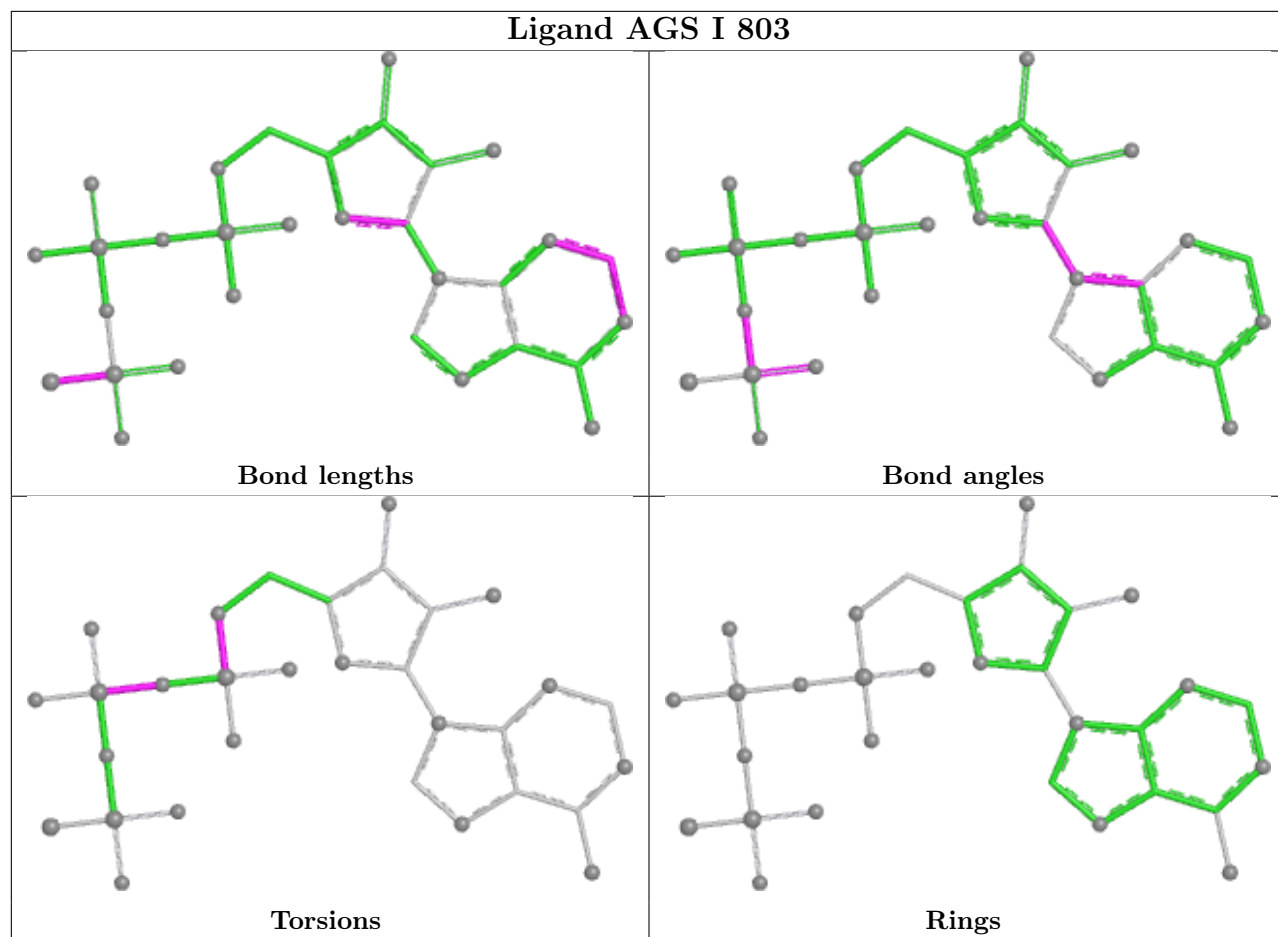
There are no ring outliers.

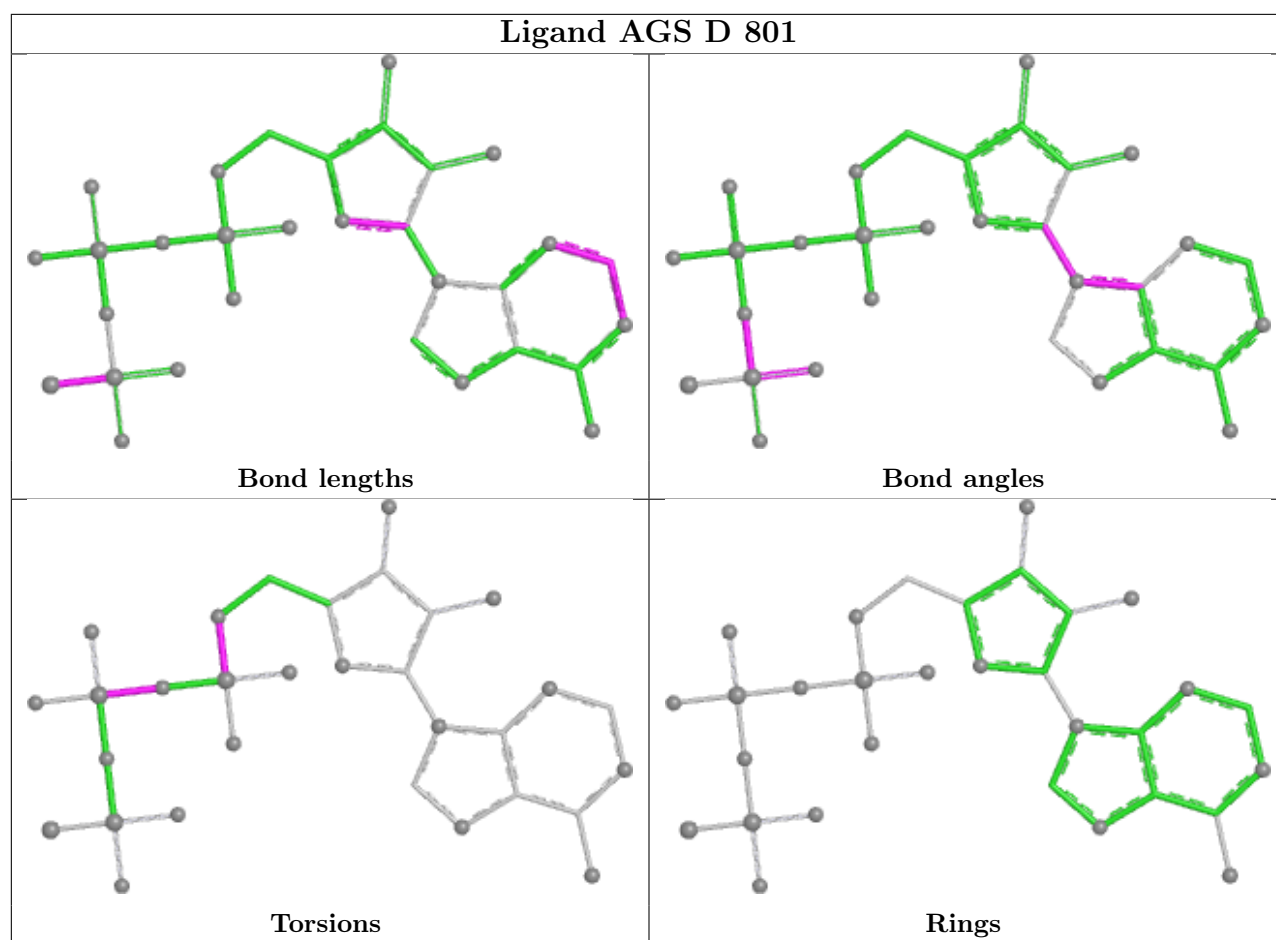
6 monomers are involved in 44 short contacts:

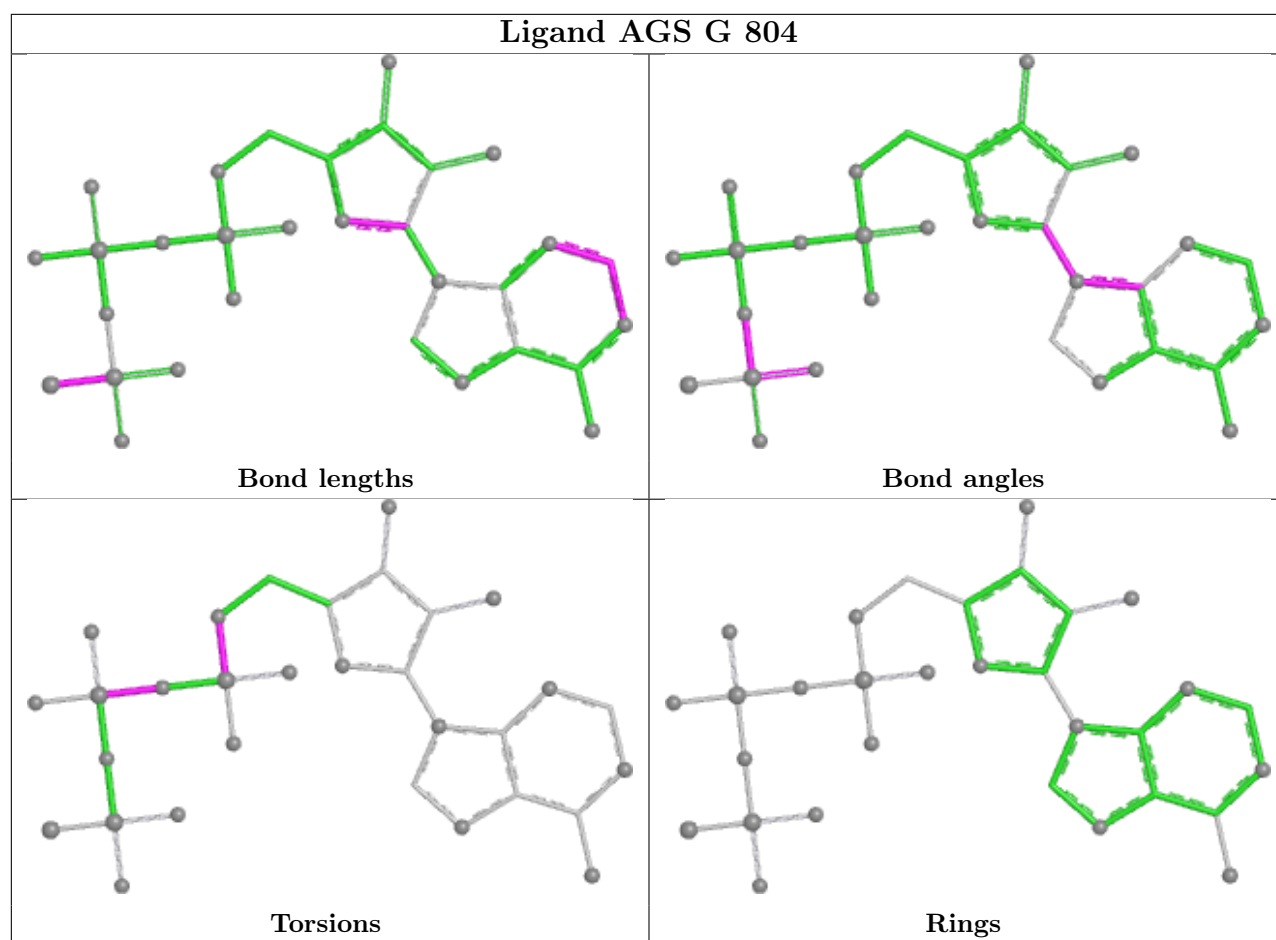
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1300	PO4	3	0
6	H	1400	PO4	4	0
5	I	803	AGS	27	0
5	D	801	AGS	4	0
5	G	804	AGS	2	0
5	B	802	AGS	4	0

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.

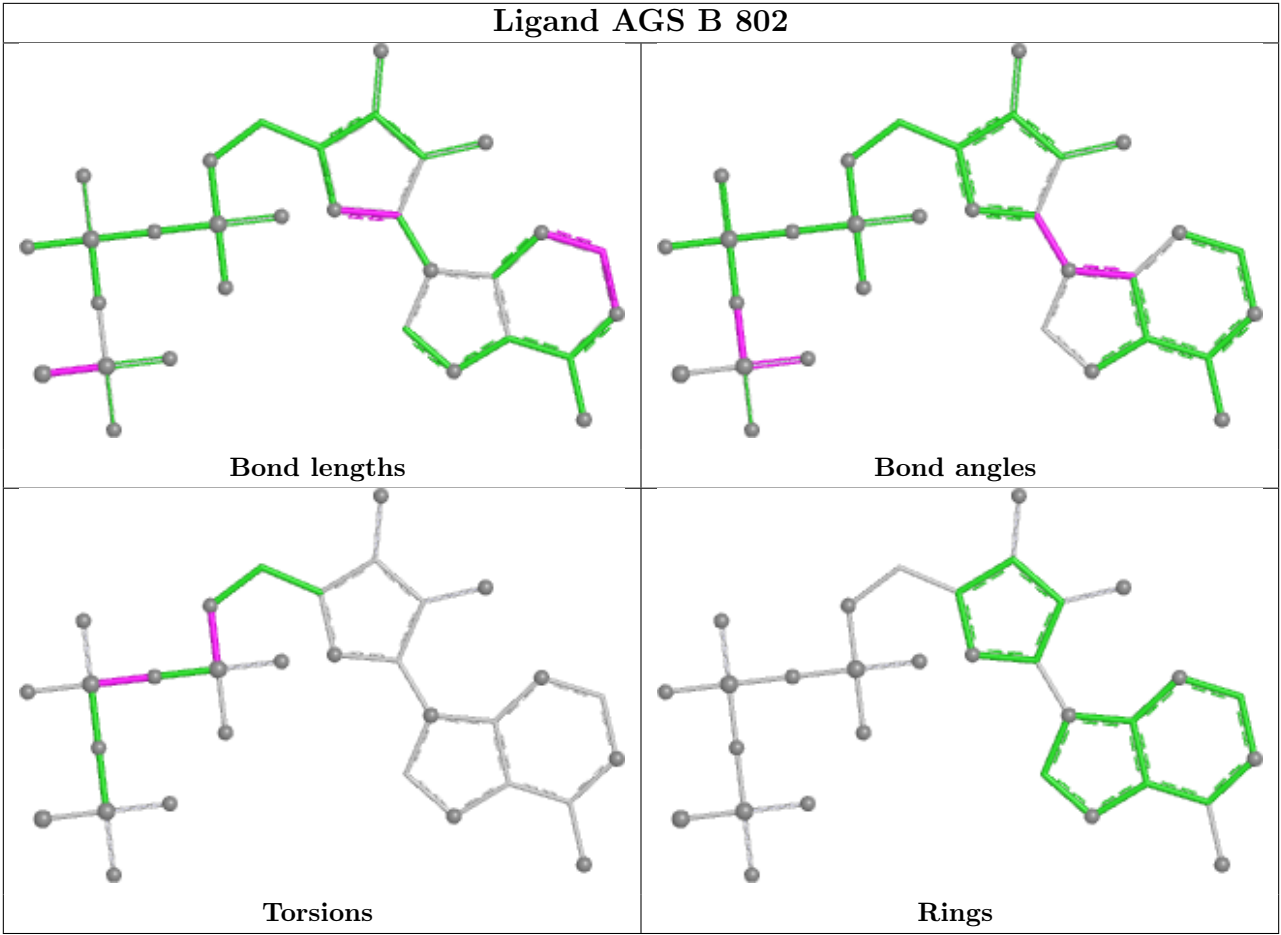
## Ligand AGS I 803











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	285:MSE	C	286:MSE	N	1.06

## 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(Å²)	Q<0.9
1	A	333/343 (97%)	0.73	42 (12%)	3	5	25, 164, 218, 268	0
1	F	333/343 (97%)	0.94	73 (21%)	0	1	107, 191, 234, 262	0
2	B	364/373 (97%)	0.78	48 (13%)	3	5	21, 146, 212, 262	0
2	C	366/373 (98%)	0.60	30 (8%)	11	14	15, 78, 194, 216	0
2	D	364/373 (97%)	0.74	26 (7%)	16	18	27, 71, 187, 248	0
2	G	364/373 (97%)	1.90	134 (36%)	0	0	131, 213, 247, 284	0
2	H	366/373 (98%)	1.67	134 (36%)	0	0	142, 205, 246, 278	0
2	I	364/373 (97%)	1.73	133 (36%)	0	0	121, 210, 286, 390	0
3	E	328/334 (98%)	0.45	10 (3%)	50	48	39, 90, 175, 206	0
3	J	328/334 (98%)	1.03	78 (23%)	0	0	121, 190, 229, 269	0
All	All	3510/3592 (97%)	1.07	708 (20%)	1	1	15, 174, 240, 390	0

The worst 5 of 708 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	366	PRO	22.0
2	H	152	PHE	18.7
2	D	368	PRO	16.9
2	H	41	TYR	13.4
2	D	366	PRO	12.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

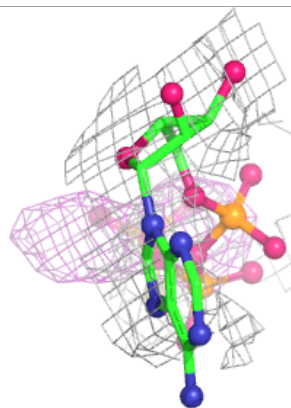
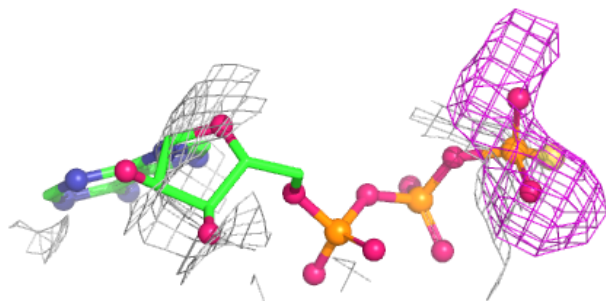
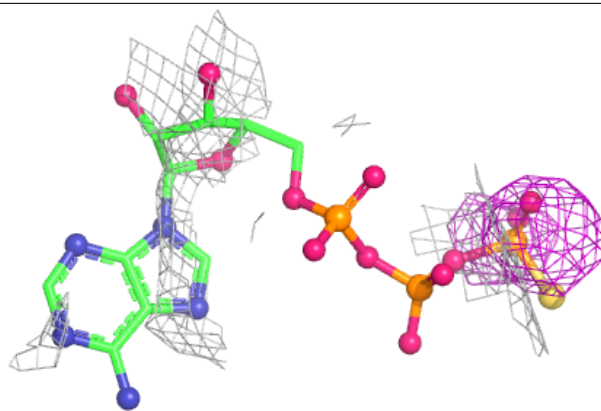
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	H	405	1/1	0.76	0.04	224,224,224,224	0
5	AGS	G	804	31/31	0.77	0.30	263,263,263,263	0
4	ZN	E	404	1/1	0.81	0.28	175,175,175,175	0
4	ZN	G	407	1/1	0.83	0.12	200,200,200,200	0
5	AGS	I	803	31/31	0.83	0.45	265,265,265,265	0
5	AGS	B	802	31/31	0.84	0.35	165,165,165,165	0
4	ZN	I	406	1/1	0.86	0.17	160,160,160,160	0
5	AGS	D	801	31/31	0.86	0.35	132,132,132,132	0
6	PO4	C	1300	5/5	0.88	0.25	116,116,116,116	0
6	PO4	H	1400	5/5	0.92	0.10	180,180,180,180	0
4	ZN	J	408	1/1	0.94	0.23	169,169,169,169	0
4	ZN	D	402	1/1	0.95	0.26	94,94,94,94	0
4	ZN	B	403	1/1	0.95	0.18	173,173,173,173	0
4	ZN	C	401	1/1	0.97	0.27	144,144,144,144	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.

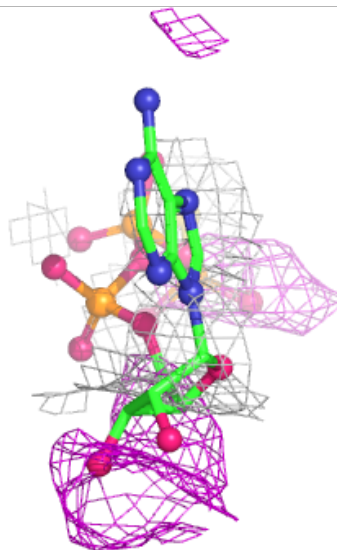
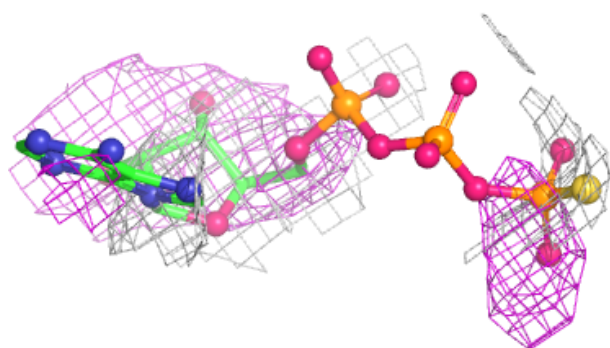
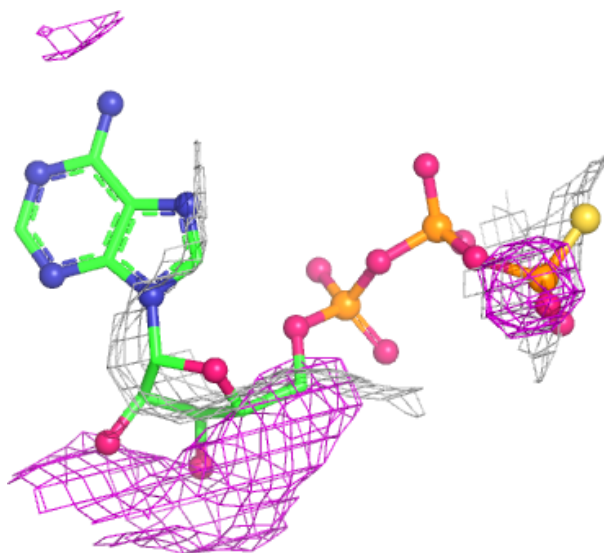
**Electron density around AGS G 804:**

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



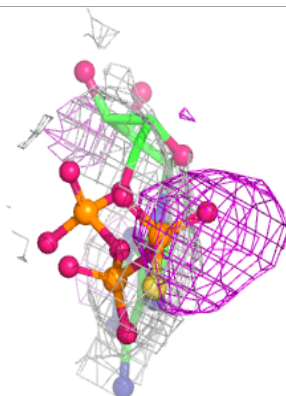
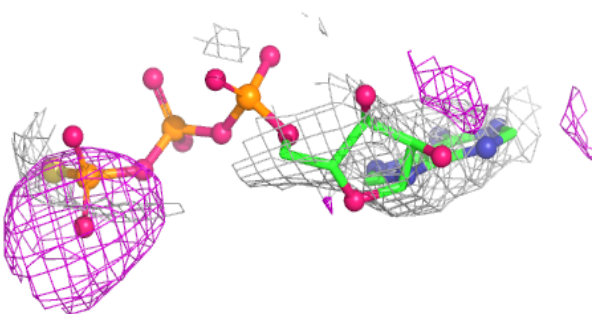
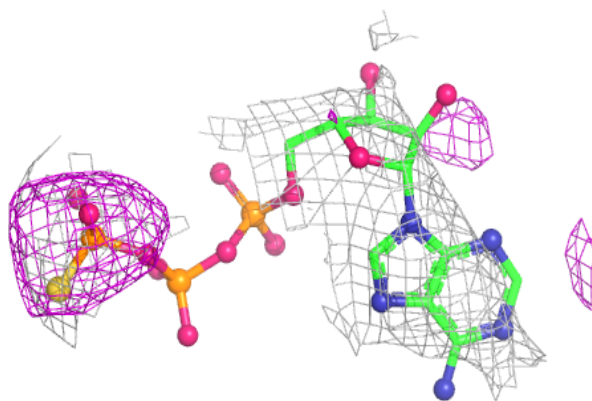
**Electron density around AGS I 803:**

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

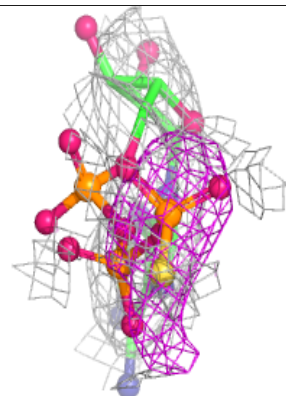
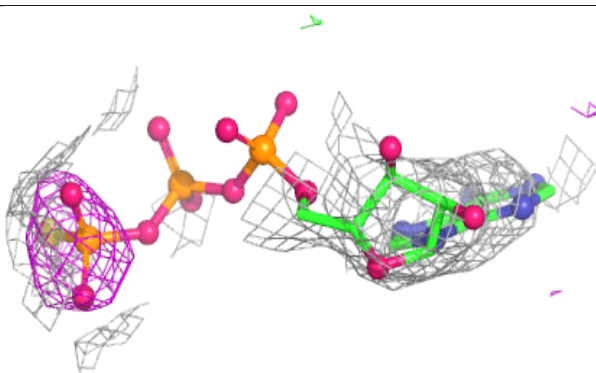
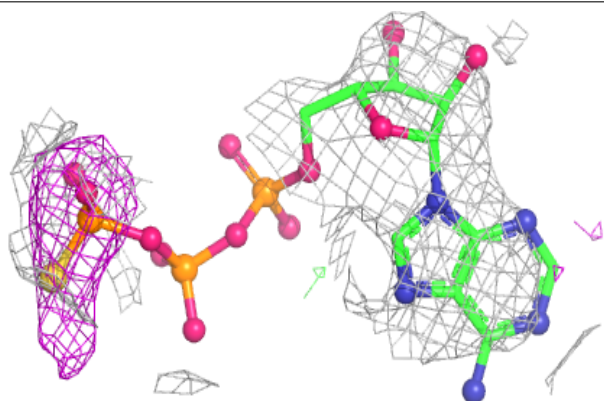


**Electron density around AGS B 802:**

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

**Electron density around AGS D 801:**

$2mF_o-DF_c$  (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.