wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 01:48 PM EDT

PDB ID	:	1XXI
Title	:	ADP 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	:	4.10 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*
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:

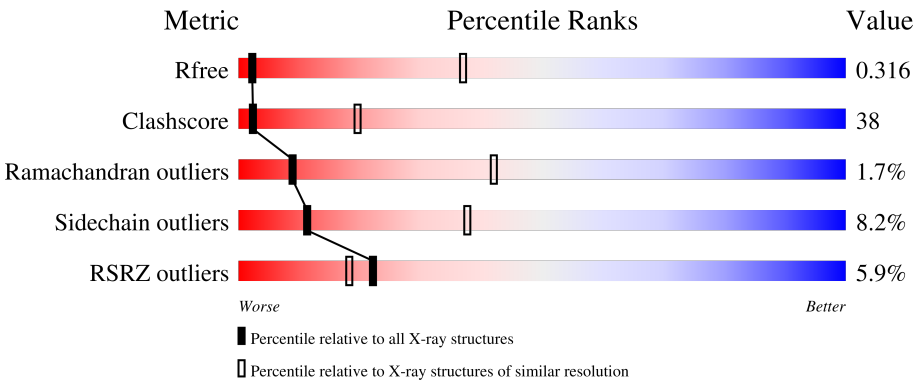
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	343	3% 50% 39% 8% • •
1	F	343	3% 45% 44% 8% • •
2	B	368	4% 60% 33% 5% • •
2	C	368	2% 57% 41% • •
2	D	368	2% 59% 35% 5% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	368	18% 57% 35% 5%
2	H	368	13% 54% 43%
2	I	368	5% 60% 35%
3	E	334	2% 57% 37% 5%
3	J	334	6% 58% 37% 5%

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	ZN	H	405	-	-	-	X
5	ADP	I	803	-	-	X	-
6	PO4	C	1300	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27688 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
			Total	C	N	O	S			
1	A	338	2687	1702	488	487	10	0	0	0
1	F	338	2687	1702	488	487	10	0	0	0

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

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

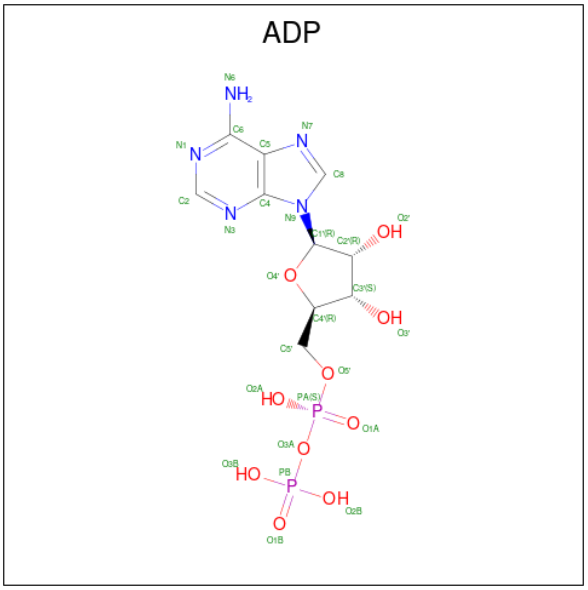
- Molecule 3 is a protein called DNA polymerase III, delta prime subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	334	2602	1655	468	466	13	0	0	0
3	J	334	2602	1655	468	466	13	0	0	0

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

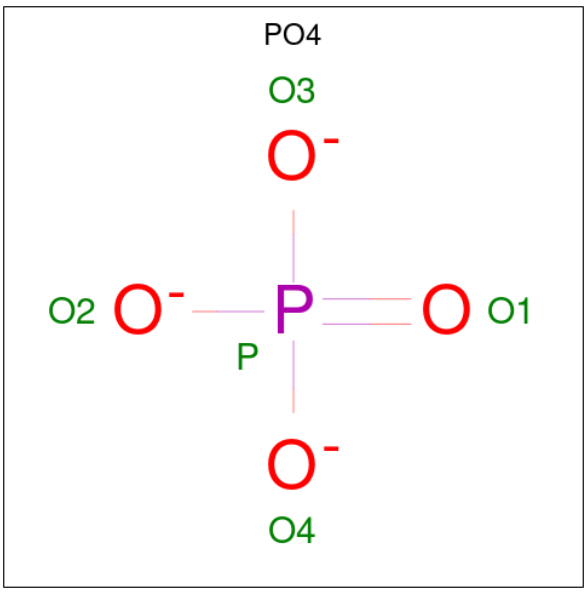
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0
4	E	1	1	1	0	0
4	G	1	1	1	0	0
4	H	1	1	1	0	0
4	I	1	1	1	0	0
4	J	1	1	1	0	0

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



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

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



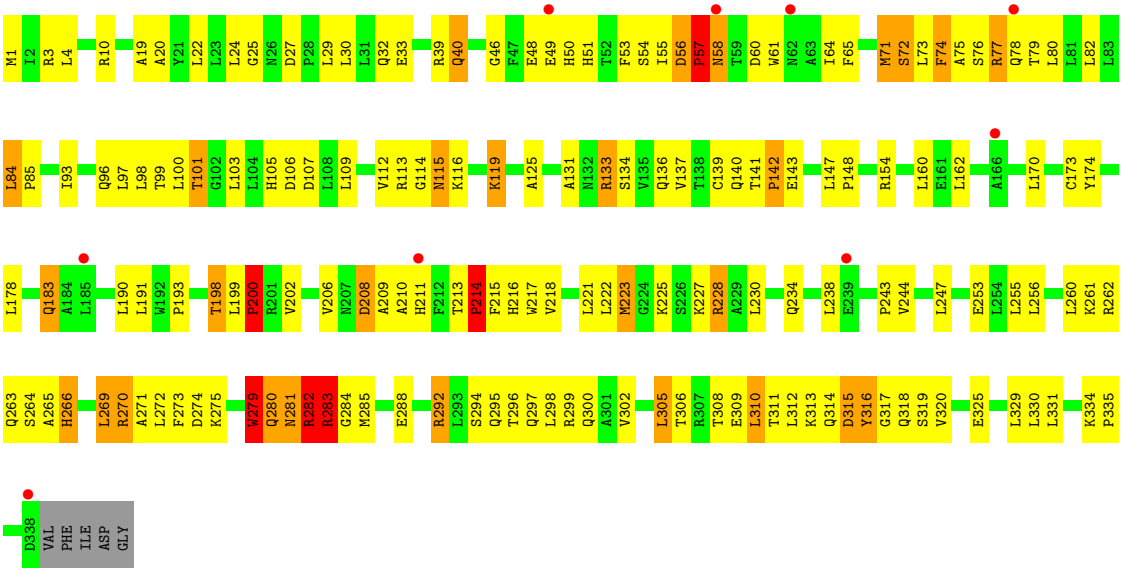
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 5 4 1	0	0

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.

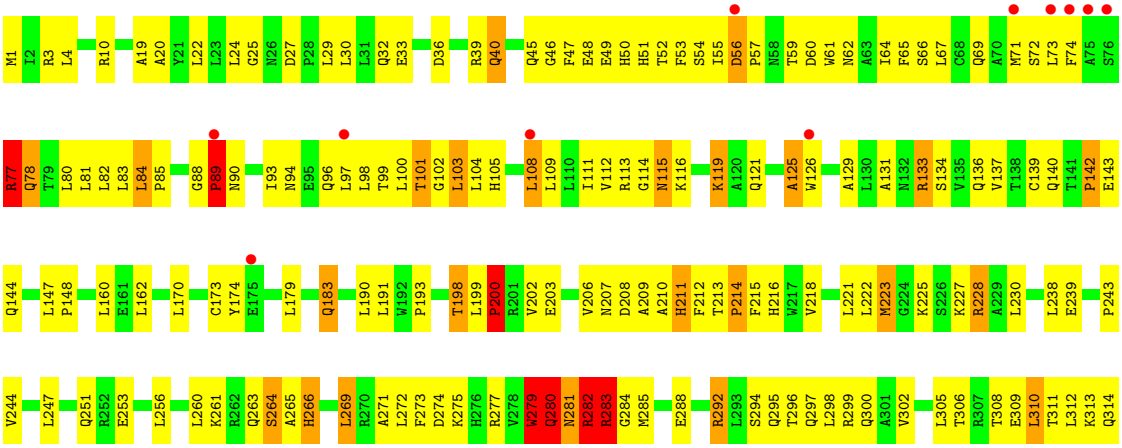
• Molecule 1: DNA polymerase III, delta subunit

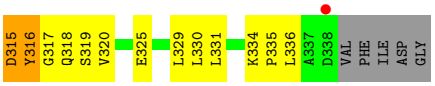
Chain A:



• Molecule 1: DNA polymerase III, delta subunit

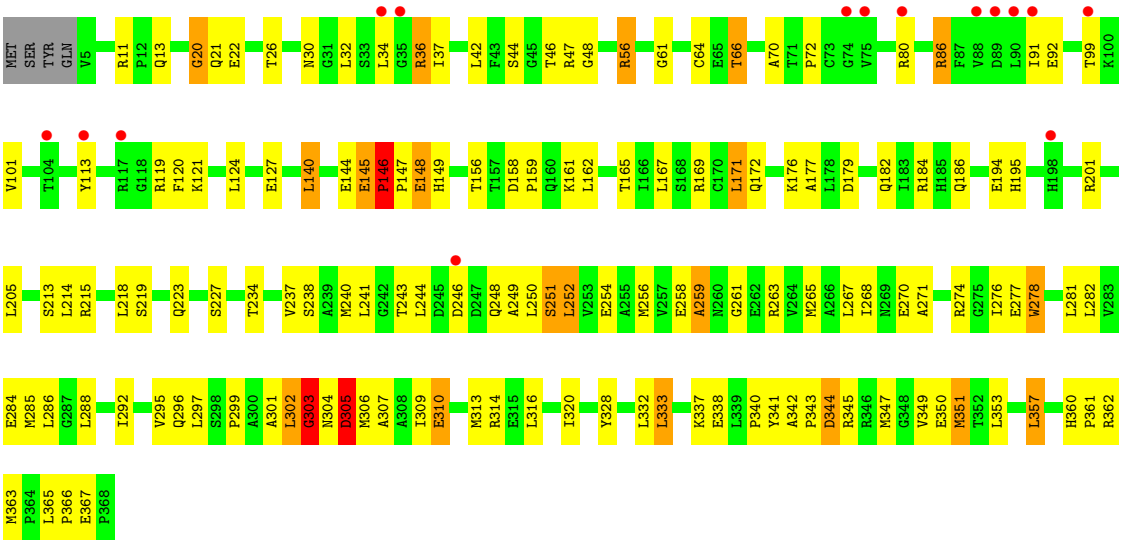
Chain F:





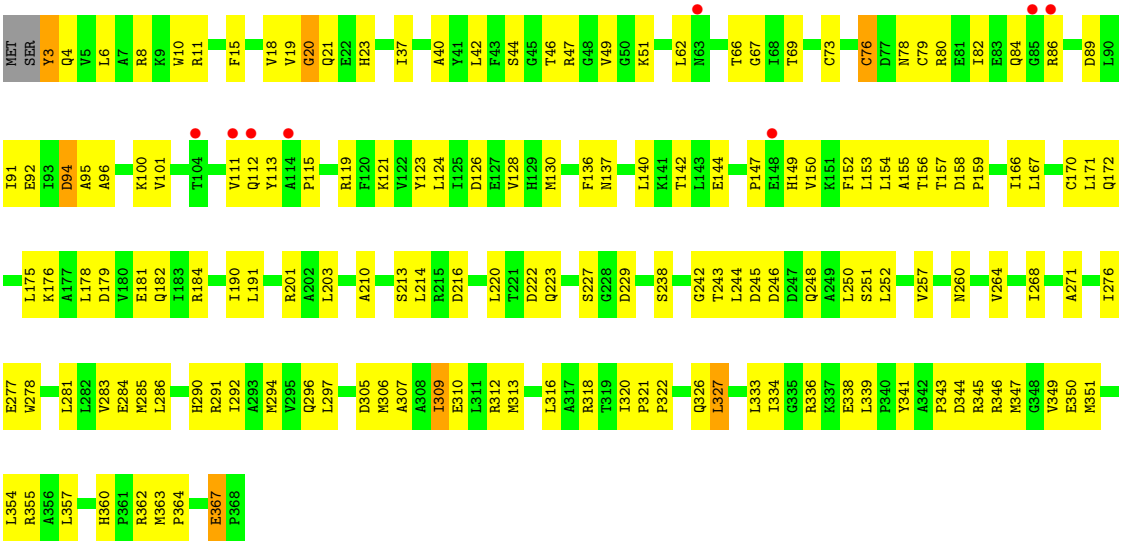
• Molecule 2: DNA polymerase III subunit gamma

Chain B:



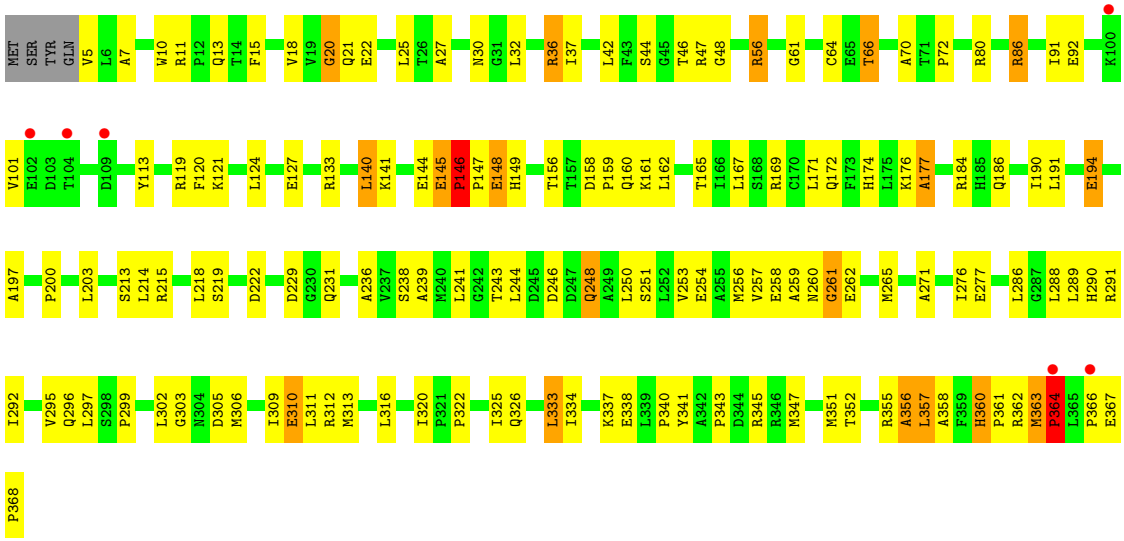
• Molecule 2: DNA polymerase III subunit gamma

Chain C:



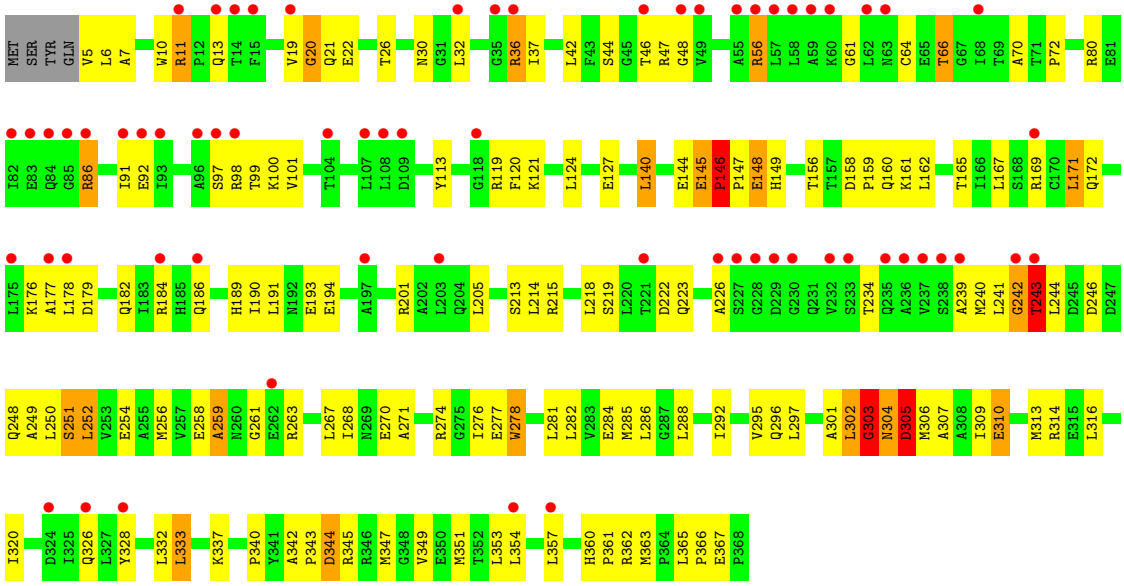
• Molecule 2: DNA polymerase III subunit gamma

Chain D:



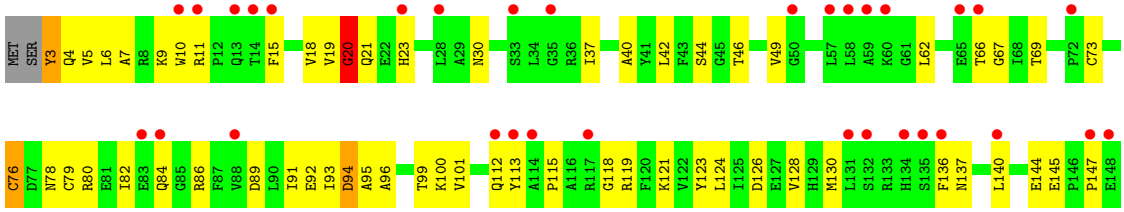
• Molecule 2: DNA polymerase III subunit gamma

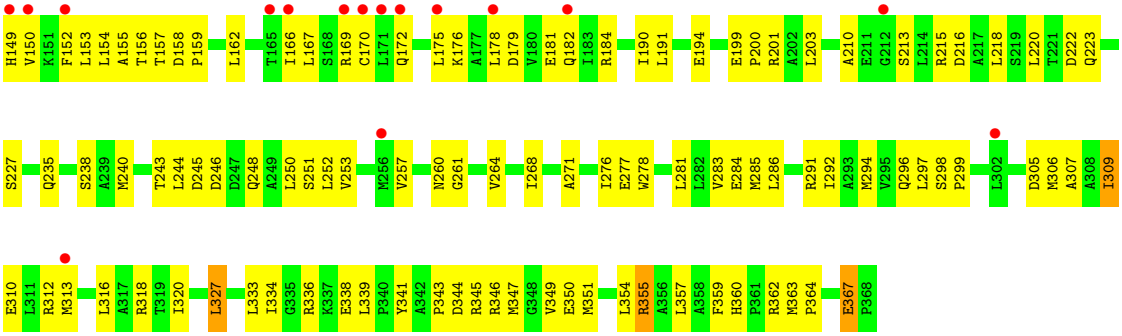
Chain G:



• Molecule 2: DNA polymerase III subunit gamma

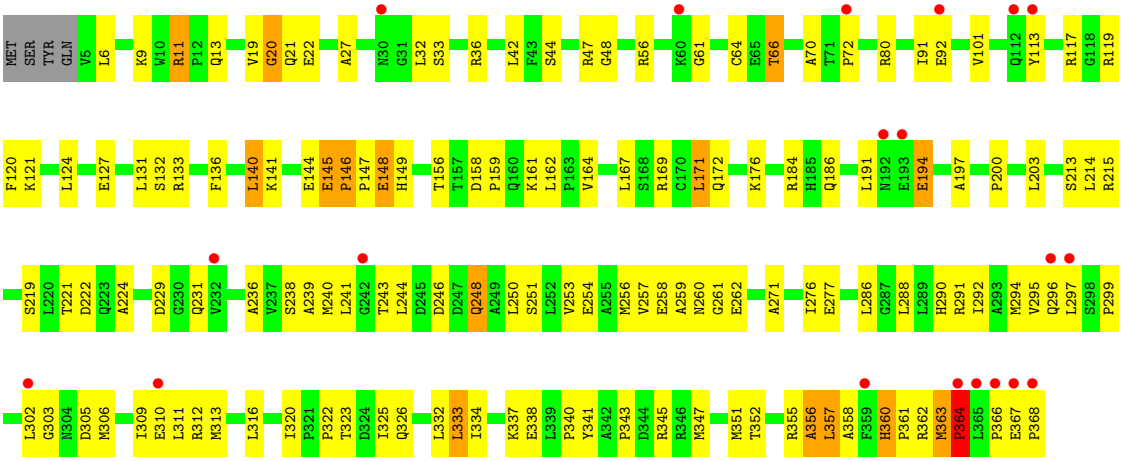
Chain H:





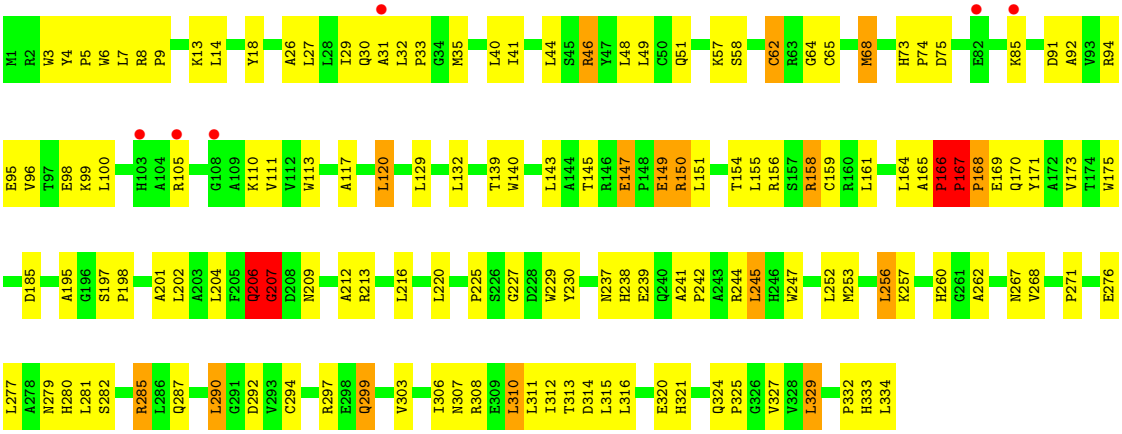
- Molecule 2: DNA polymerase III subunit gamma

Chain I:



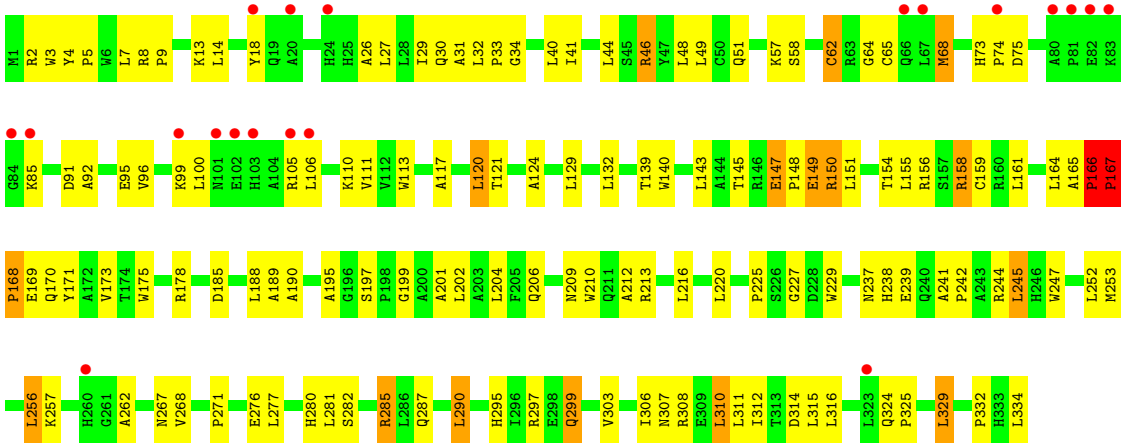
- Molecule 3: DNA polymerase III, delta prime subunit

Chain E:



- Molecule 3: DNA polymerase III, delta prime subunit

Chain J:


M1 R2 W3 Y4 P5 W6 L7 R8 P9 K13 L14 Y18 Q19 A20 H24 H25 A26 L27 L28 I29 Q30 A31 L32 P33 G34 L40 I41 L44 S45 R46 Y47 L48 L49 C50 Q51 K57 S58 C62 R63 G64 C65 Q66 L67 M68 H73 P74 D75 A80 P81 E82 K83
G84 K85 D91 A92 E95 V96 K99 L100 N101 E102 H103 A104 R105 L106 K110 V111 V112 W113 A117 L120 T121 A124 L129 L132 T139 W140 L143 A144 T145 R146 E147 P148 E149 R150 L151 T154 L155 R156 S157 R158 C159 R160 L161 L164 A165 P166 P167
P168 E169 Q170 Y171 A172 V173 T174 W175 R178 D185 L188 A189 A190 A195 G196 S197 P198 G199 A200 A201 L202 A203 L204 F205 Q206 N209 W210 Q211 A212 R213 L216 L220 P225 S226 G227 D228 W229 N237 H238 E239 Q240 A241 P242 A243 R244 L245 H246 W247 L252 M253
L256 K257 H260 G261 A262 N267 V268 P271 E276 L277 H280 L281 S282 R285 L286 Q287 L290 H295 I296 R297 E298 Q299 V303 I306 N307 R308 E309 L310 L311 I312 T313 D314 L315 L316 L323 Q324 P325 L329 P332 H333 L334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.21Å 106.57Å 535.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.10 49.11 – 4.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-4.10) 88.0 (49.11-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 4.14Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.366 , 0.369 0.322 , 0.316	Depositor DCC
R_{free} test set	4301 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	122.7	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 82.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	27688	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: PO4, ADP, ZN

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	0.90	9/2735 (0.3%)	1.07	14/3716 (0.4%)
1	F	0.96	11/2735 (0.4%)	1.06	13/3716 (0.3%)
2	B	0.49	0/2876	0.77	8/3900 (0.2%)
2	C	0.48	0/2898	0.75	2/3930 (0.1%)
2	D	0.63	5/2876 (0.2%)	0.88	9/3900 (0.2%)
2	G	0.49	1/2876 (0.0%)	0.86	12/3900 (0.3%)
2	H	0.47	0/2898	0.74	2/3930 (0.1%)
2	I	0.62	5/2876 (0.2%)	0.87	10/3900 (0.3%)
3	E	0.51	0/2667	0.82	5/3639 (0.1%)
3	J	0.50	0/2667	0.82	3/3639 (0.1%)
All	All	0.63	31/28104 (0.1%)	0.87	78/38170 (0.2%)

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
1	A	0	4
1	F	0	4
2	C	0	1
2	H	0	1
All	All	0	10

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	ASP	CB-CG	29.11	2.12	1.51
1	F	315	ASP	CB-CG	29.09	2.12	1.51
1	A	310	LEU	CG-CD2	-9.10	1.18	1.51
1	F	310	LEU	CG-CD2	-9.03	1.18	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	363	MET	SD-CE	8.94	2.27	1.77

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	363	MET	CG-SD-CE	17.09	127.54	100.20
2	I	363	MET	CG-SD-CE	17.05	127.49	100.20
2	G	242	GLY	C-N-CA	-16.32	80.90	121.70
1	A	214	PRO	CA-N-CD	-15.70	89.52	111.50
1	F	214	PRO	CA-N-CD	-15.29	90.09	111.50

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	GLN	Peptide
1	A	281	ASN	Mainchain
1	A	282	ARG	Mainchain
1	A	319	SER	Mainchain
2	C	94	ASP	Mainchain

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	2687	0	2741	337	4
1	F	2687	0	2733	391	10
2	B	2829	0	2877	190	6
2	C	2850	0	2896	198	0
2	D	2829	0	2878	270	4
2	G	2829	0	2871	268	0
2	H	2850	0	2894	256	0
2	I	2829	0	2878	327	6
3	E	2602	0	2603	155	6
3	J	2602	0	2603	170	4
4	B	1	0	0	0	0
4	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	27	0	12	8	0
5	D	27	0	12	5	0
5	I	27	0	12	28	0
6	C	5	0	0	3	0
All	All	27688	0	28010	2129	20

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 38.

The worst 5 of 2129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:GLU:HB3	3:E:149:GLU:CG	1.26	1.66
2:G:10:TRP:HZ2	2:G:193:GLU:CB	0.98	1.59
1:A:29:LEU:CD2	1:A:154:ARG:HH12	1.08	1.58
1:F:71:MET:HB3	1:F:108:LEU:CD1	1.23	1.58
1:A:65:PHE:CE1	1:A:99:THR:HG21	1.06	1.58

The worst 5 of 20 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:NZ	2:D:368:PRO:CG[4_455]	0.40	1.80
2:B:299:PRO:CG	3:E:279:ASN:ND2[4_455]	1.13	1.07
1:F:119:LYS:CB	2:I:117:ARG:NH2[1_455]	1.25	0.95
1:A:227:LYS:NZ	2:D:368:PRO:CD[4_455]	1.29	0.91
1:A:227:LYS:CE	2:D:368:PRO:CG[4_455]	1.51	0.69

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	336/343 (98%)	302 (90%)	24 (7%)	10 (3%)	4	31
1	F	336/343 (98%)	294 (88%)	32 (10%)	10 (3%)	4	31
2	B	362/368 (98%)	340 (94%)	16 (4%)	6 (2%)	9	42
2	C	364/368 (99%)	336 (92%)	24 (7%)	4 (1%)	14	50
2	D	362/368 (98%)	335 (92%)	19 (5%)	8 (2%)	6	37
2	G	362/368 (98%)	338 (93%)	18 (5%)	6 (2%)	9	42
2	H	364/368 (99%)	336 (92%)	24 (7%)	4 (1%)	14	50
2	I	362/368 (98%)	335 (92%)	22 (6%)	5 (1%)	11	45
3	E	332/334 (99%)	301 (91%)	28 (8%)	3 (1%)	17	54
3	J	332/334 (99%)	300 (90%)	30 (9%)	2 (1%)	25	63
All	All	3512/3562 (99%)	3217 (92%)	237 (7%)	58 (2%)	9	42

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	TRP
2	B	310	GLU
2	C	20	GLY
2	C	364	PRO
2	D	261	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	287/291 (99%)	255 (89%)	32 (11%)	6	25
1	F	287/291 (99%)	256 (89%)	31 (11%)	6	26
2	B	301/305 (99%)	281 (93%)	20 (7%)	16	44
2	C	303/305 (99%)	287 (95%)	16 (5%)	22	51
2	D	301/305 (99%)	283 (94%)	18 (6%)	19	47
2	G	301/305 (99%)	279 (93%)	22 (7%)	14	41
2	H	303/305 (99%)	286 (94%)	17 (6%)	21	49
2	I	301/305 (99%)	285 (95%)	16 (5%)	22	51
3	E	270/270 (100%)	236 (87%)	34 (13%)	4	22
3	J	270/270 (100%)	237 (88%)	33 (12%)	5	23
All	All	2924/2952 (99%)	2685 (92%)	239 (8%)	11	38

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	292	ASP
3	J	170	GLN
1	F	228	ARG
3	J	167	PRO
3	J	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	326	GLN
3	J	73	HIS
2	H	30	ASN
2	I	21	GLN
3	J	307	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	D	801	-	24,29,29	1.72	6 (25%)	29,45,45	1.44	3 (10%)
6	PO4	C	1300	-	4,4,4	1.36	1 (25%)	6,6,6	0.86	0
5	ADP	B	802	-	24,29,29	1.71	6 (25%)	29,45,45	1.44	3 (10%)
5	ADP	I	803	-	24,29,29	1.71	6 (25%)	29,45,45	1.44	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
5	ADP	D	801	-	-	3/12/32/32	0/3/3/3
5	ADP	B	802	-	-	3/12/32/32	0/3/3/3
5	ADP	I	803	-	-	3/12/32/32	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	801	ADP	C2'-C1'	-4.34	1.47	1.53
5	I	803	ADP	C2'-C1'	-4.31	1.47	1.53
5	B	802	ADP	C2'-C1'	-4.27	1.47	1.53
5	D	801	ADP	C2-N3	3.30	1.37	1.32
5	I	803	ADP	C2-N3	3.28	1.37	1.32

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	803	ADP	C1'-N9-C4	4.63	134.77	126.64
5	B	802	ADP	C1'-N9-C4	4.61	134.74	126.64
5	D	801	ADP	C1'-N9-C4	4.58	134.69	126.64
5	D	801	ADP	C3'-C2'-C1'	2.97	105.44	100.98
5	B	802	ADP	C3'-C2'-C1'	2.91	105.35	100.98

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	802	ADP	C5'-O5'-PA-O3A
5	D	801	ADP	C5'-O5'-PA-O1A
5	D	801	ADP	C5'-O5'-PA-O2A
5	D	801	ADP	C5'-O5'-PA-O3A
5	I	803	ADP	C5'-O5'-PA-O3A

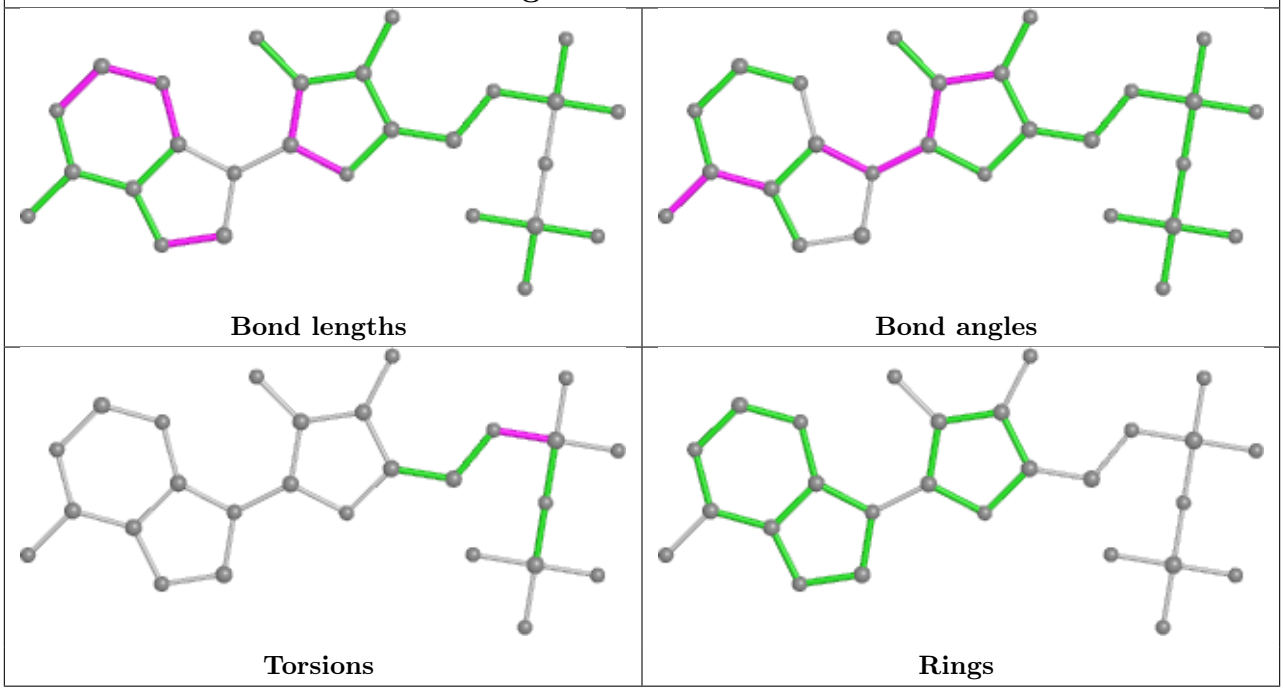
There are no ring outliers.

4 monomers are involved in 44 short contacts:

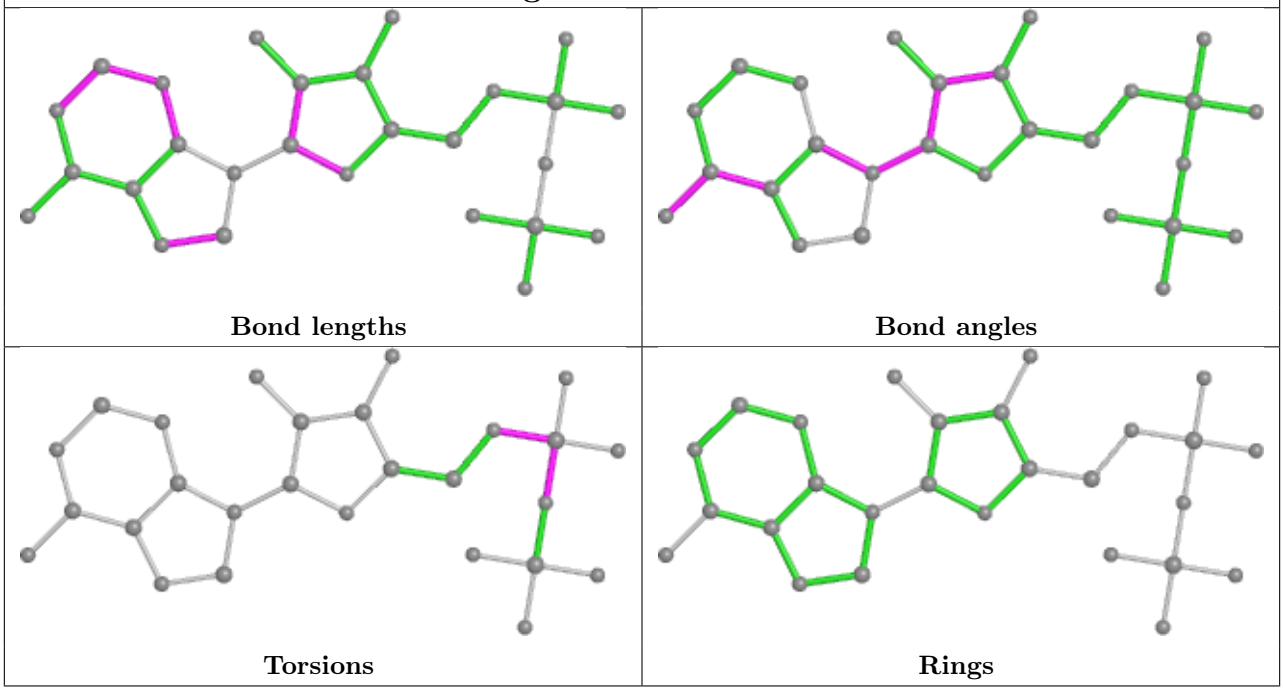
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	801	ADP	5	0
6	C	1300	PO4	3	0
5	B	802	ADP	8	0
5	I	803	ADP	28	0

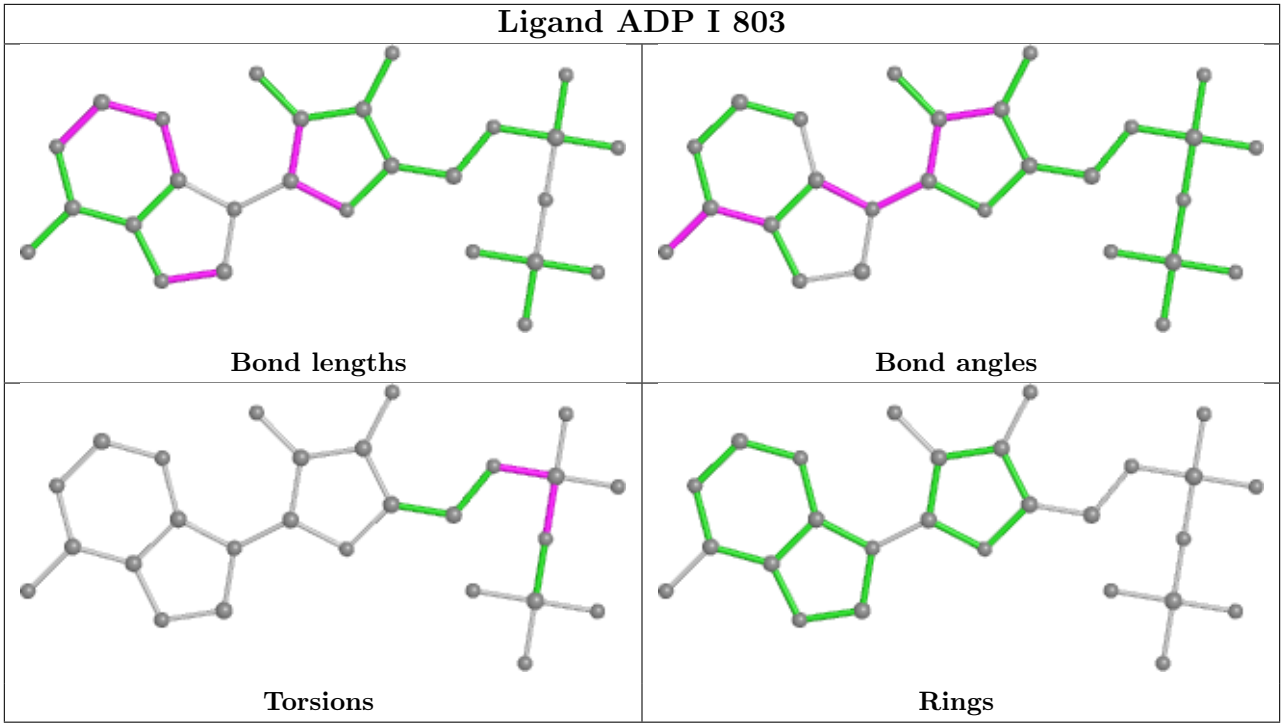
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADP D 801



Ligand ADP B 802





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	338/343 (98%)	0.15	9 (2%)	54	44	78, 150, 164, 164	0
1	F	338/343 (98%)	0.21	12 (3%)	42	34	149, 189, 201, 201	0
2	B	364/368 (98%)	0.19	15 (4%)	37	30	41, 130, 151, 151	0
2	C	366/368 (99%)	-0.00	8 (2%)	62	52	21, 41, 132, 132	0
2	D	364/368 (98%)	0.00	6 (1%)	72	62	36, 43, 73, 73	0
2	G	364/368 (98%)	0.89	65 (17%)	1	2	176, 263, 290, 290	0
2	H	366/368 (99%)	0.61	48 (13%)	3	4	180, 199, 272, 272	0
2	I	364/368 (98%)	0.40	20 (5%)	25	21	198, 201, 205, 205	0
3	E	334/334 (100%)	0.07	6 (1%)	68	59	37, 55, 98, 98	0
3	J	334/334 (100%)	0.38	20 (5%)	21	17	138, 169, 221, 221	0
All	All	3532/3562 (99%)	0.29	209 (5%)	22	18	21, 150, 272, 290	0

The worst 5 of 209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	60	LYS	7.9
2	H	170	CYS	6.7
2	G	59	ALA	6.4
2	I	366	PRO	6.3
3	J	82	GLU	6.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

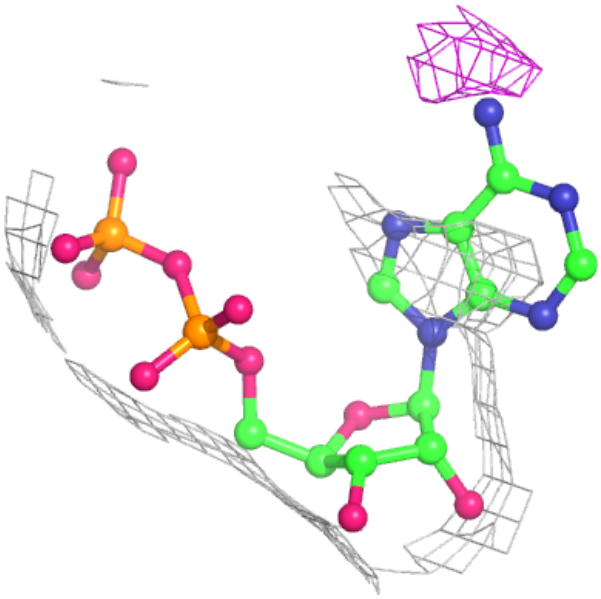
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

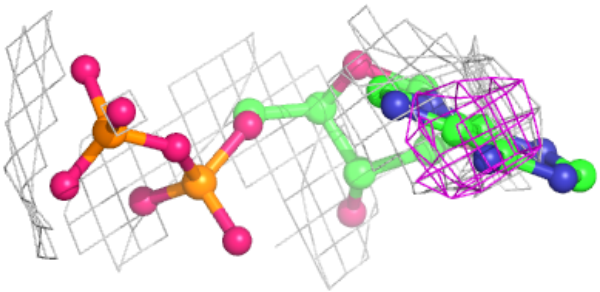
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	G	407	1/1	0.47	0.04	350,350,350,350	0
4	ZN	H	405	1/1	0.55	0.47	395,395,395,395	0
4	ZN	J	408	1/1	0.79	0.08	228,228,228,228	0
4	ZN	I	406	1/1	0.80	0.06	119,119,119,119	0
5	ADP	I	803	27/27	0.83	0.24	203,203,203,203	0
5	ADP	B	802	27/27	0.84	0.31	68,68,68,68	0
5	ADP	D	801	27/27	0.89	0.29	27,27,27,27	0
4	ZN	C	401	1/1	0.90	0.05	147,147,147,147	0
4	ZN	E	404	1/1	0.91	0.04	124,124,124,124	0
6	PO4	C	1300	5/5	0.91	0.15	58,58,58,58	0
4	ZN	B	403	1/1	0.93	0.06	138,138,138,138	0
4	ZN	D	402	1/1	0.96	0.10	43,43,43,43	0

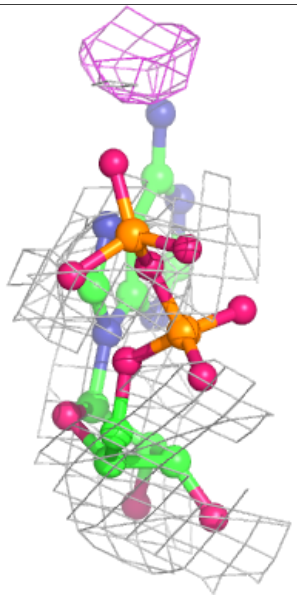
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP I 803:

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

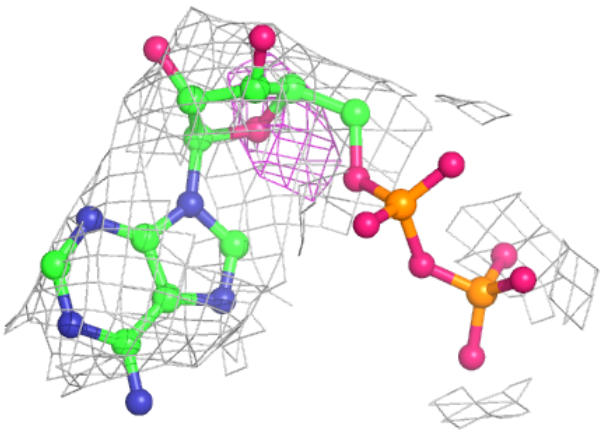


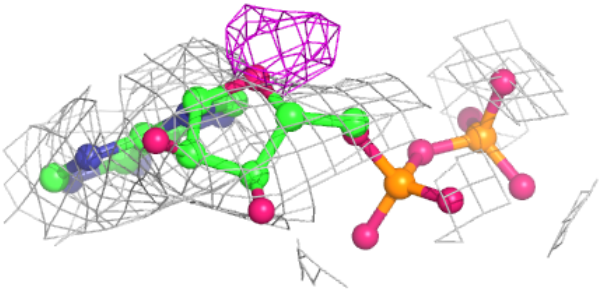


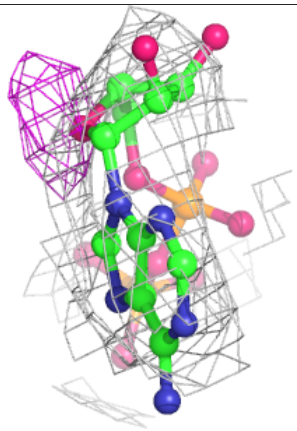


Electron density around ADP B 802:

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

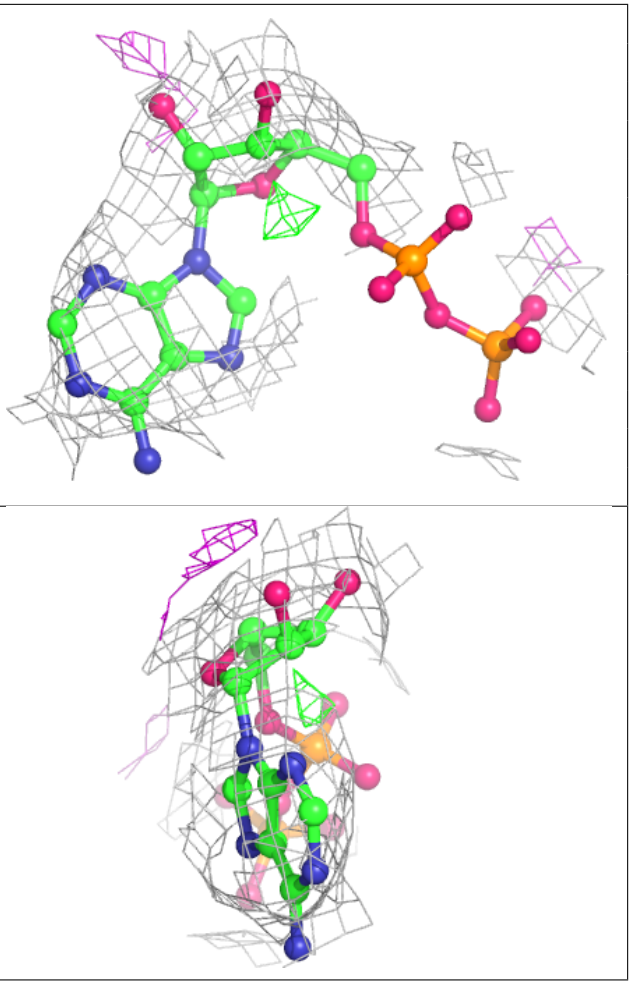






Electron density around ADP D 801:

$2mF_o$-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.