



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 12:08 AM EDT

PDB ID : 8DH2
Title : T7 RNA polymerase elongation complex with unnatural base dDs-ATP mismatch
Authors : Oh, J.; Wang, D.
Deposited on : 2022-06-24
Resolution : 2.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

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

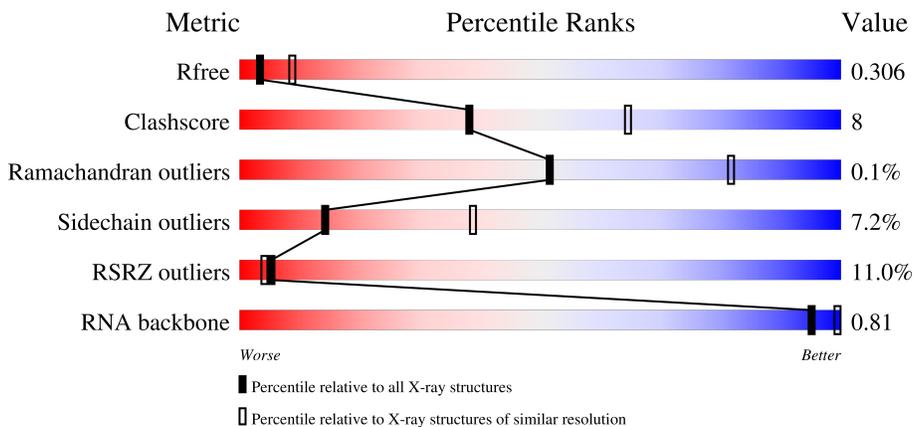
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 $\leq 5\%$. 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	B	883	 5% 76% 20% ••
1	E	883	 7% 78% 16% • 5%
1	I	883	 19% 68% 24% • 6%
1	L	883	 10% 62% 20% • 16%

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Mol	Chain	Length	Quality of chain
2	A	18	
2	F	18	
2	J	18	
2	M	18	
3	C	12	
3	G	12	
3	K	12	
3	N	12	
4	D	9	
4	H	9	
4	O	9	

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	GOL	I	901	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 27806 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 T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	856	Total 6706	C 4270	N 1165	O 1236	S 35	0	0	0
1	E	841	Total 6622	C 4222	N 1151	O 1214	S 35	0	0	0
1	I	833	Total 6518	C 4151	N 1124	O 1209	S 34	0	0	0
1	L	741	Total 5536	C 3517	N 967	O 1022	S 30	0	0	0

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	A	17	Total 351	C 170	N 67	O 97	P 16	S 1	0	0	0
2	F	17	Total 351	C 170	N 67	O 97	P 16	S 1	0	0	0
2	J	12	Total 248	C 120	N 45	O 70	P 12	S 1	0	0	0
2	M	14	Total 289	C 140	N 52	O 82	P 14	S 1	0	0	0

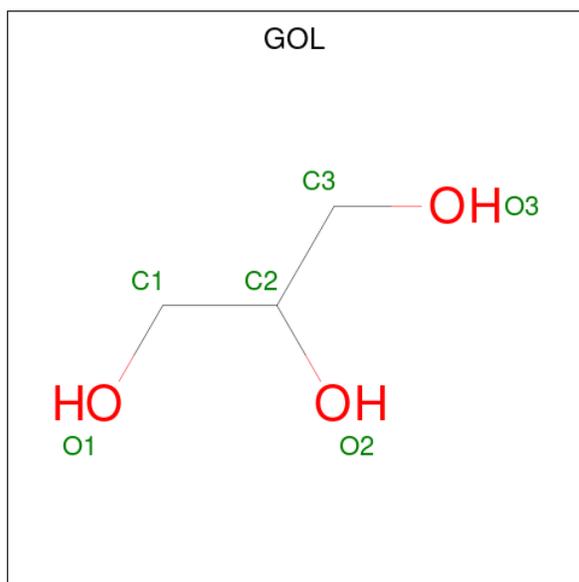
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	8	Total 173	C 77	N 33	O 55	P 8	0	0	0
3	G	8	Total 173	C 77	N 33	O 55	P 8	0	0	0
3	K	8	Total 173	C 77	N 33	O 55	P 8	0	0	0
3	N	8	Total 170	C 77	N 33	O 53	P 7	0	0	0

- Molecule 4 is a DNA chain called Non-template strand DNA.

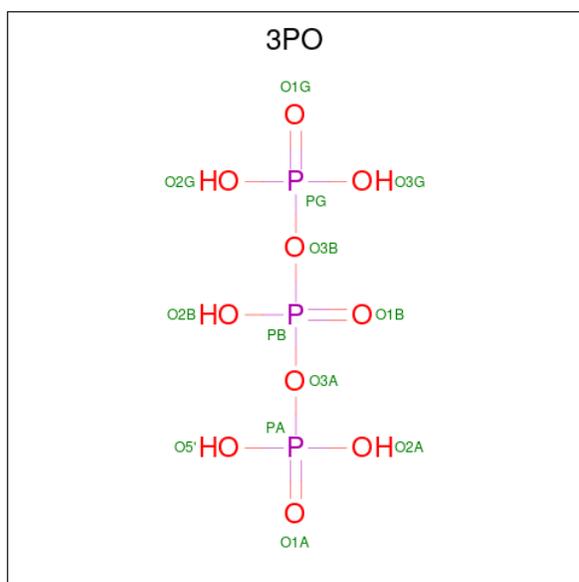
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	8	Total 160	C 77	N 25	O 50	P 8	0	0	0
4	H	8	Total 160	C 77	N 25	O 50	P 8	0	0	0
4	O	5	Total 102	C 49	N 17	O 31	P 5	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
5	B	1	Total 6	C O 3 3	0	0
5	C	1	Total 6	C O 3 3	0	0
5	I	1	Total 6	C O 3 3	0	0

- Molecule 6 is TRIPHOSPHATE (three-letter code: 3PO) (formula: $H_5O_{10}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			13	10	3		
6	E	1	Total	O	P	0	0
			13	10	3		
6	I	1	Total	O	P	0	0
			13	10	3		
6	L	1	Total	O	P	0	0
			13	10	3		

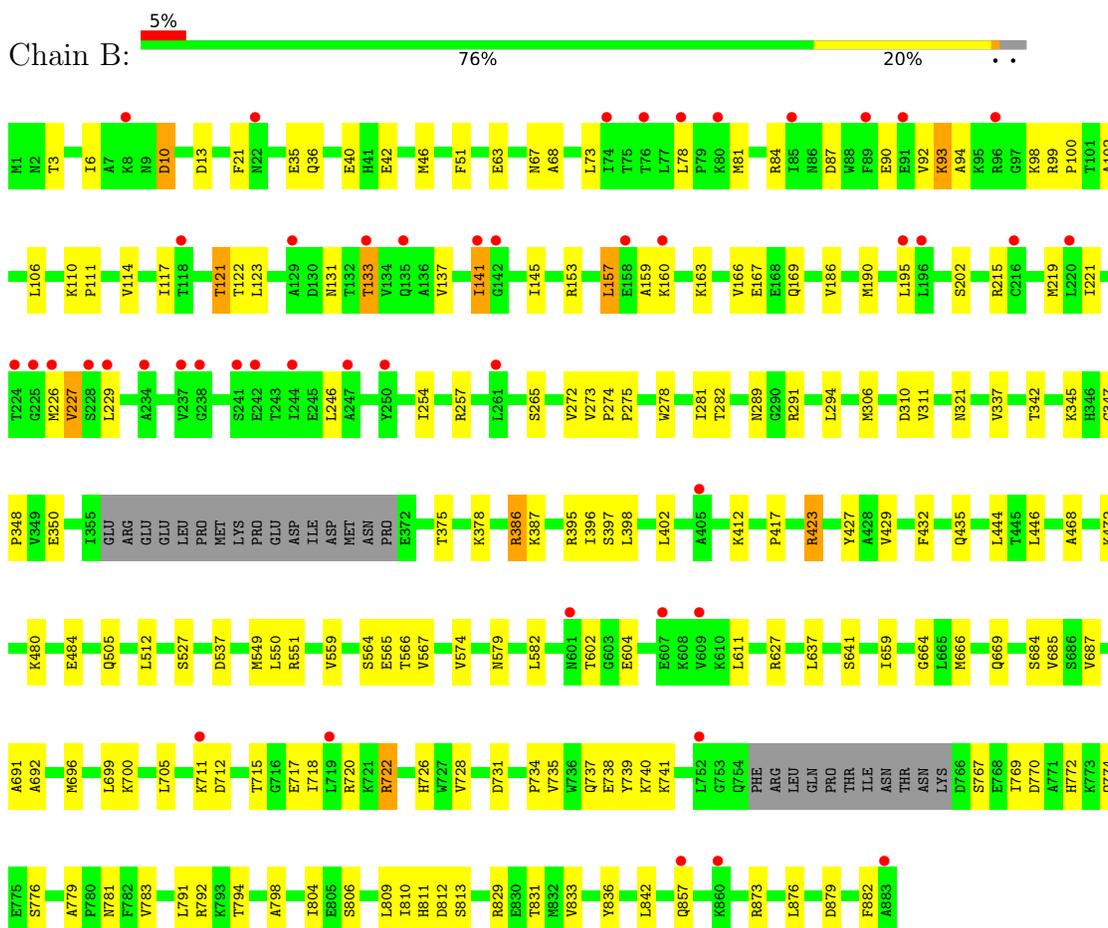
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		
7	I	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		

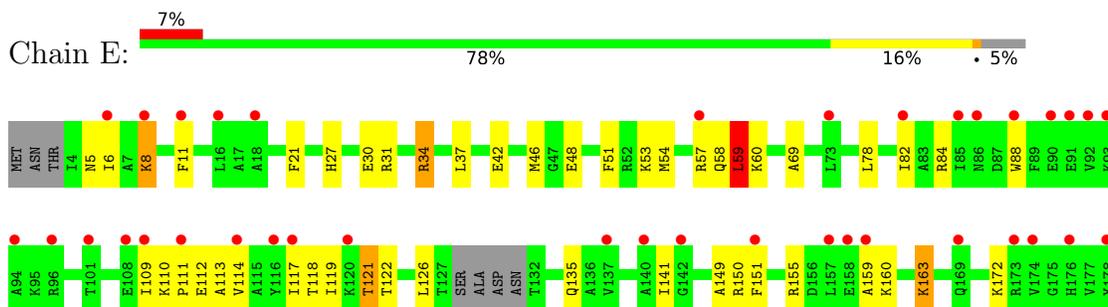
3 Residue-property plots [i](#)

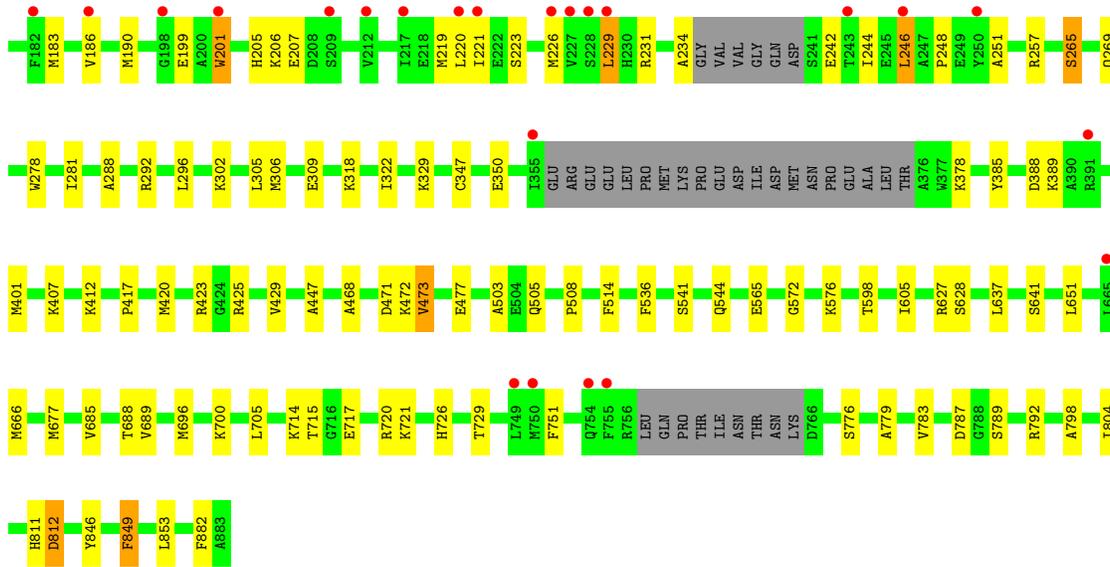
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: T7 RNA polymerase

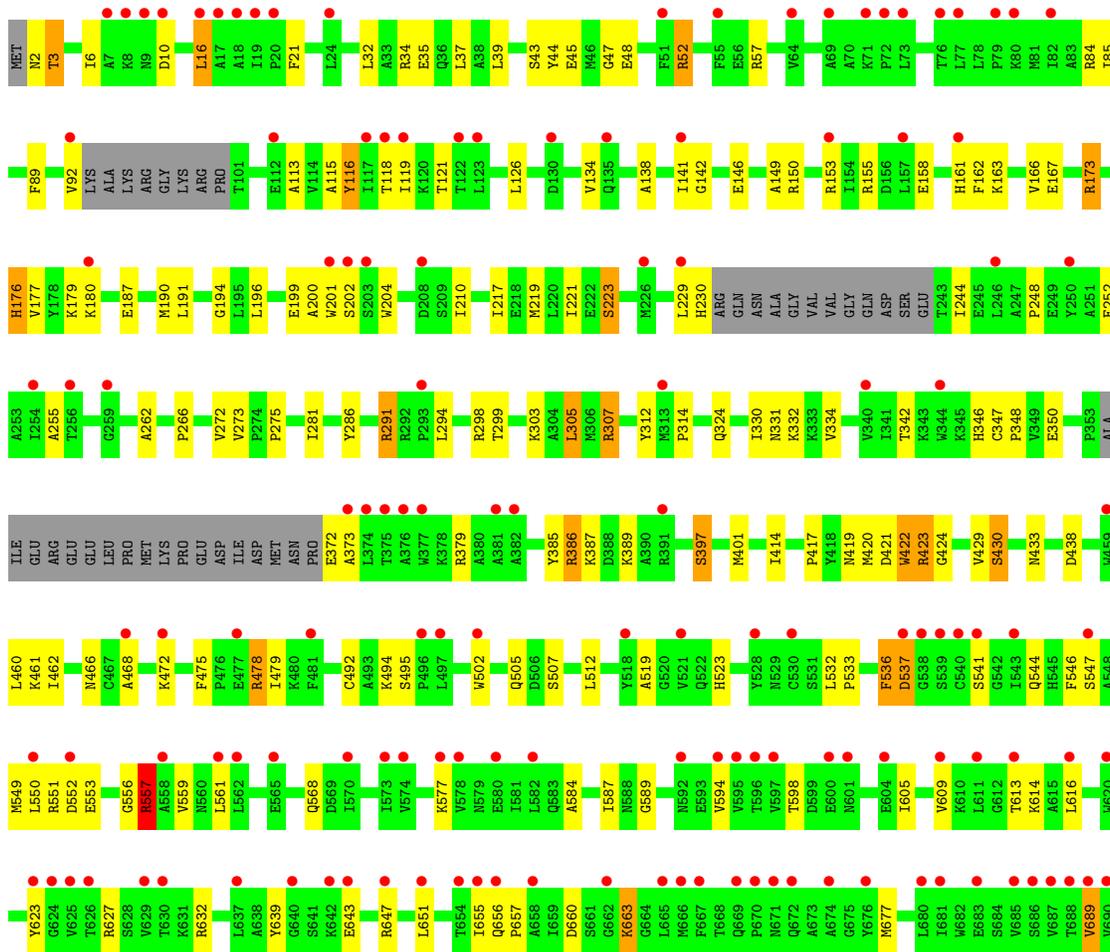


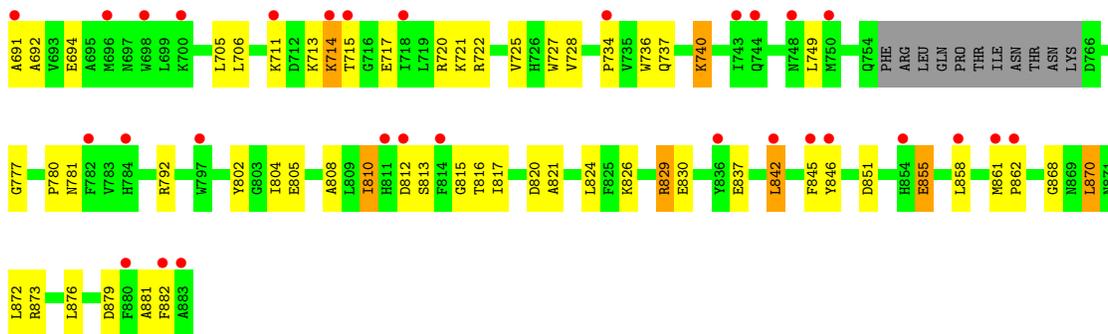
- Molecule 1: T7 RNA polymerase



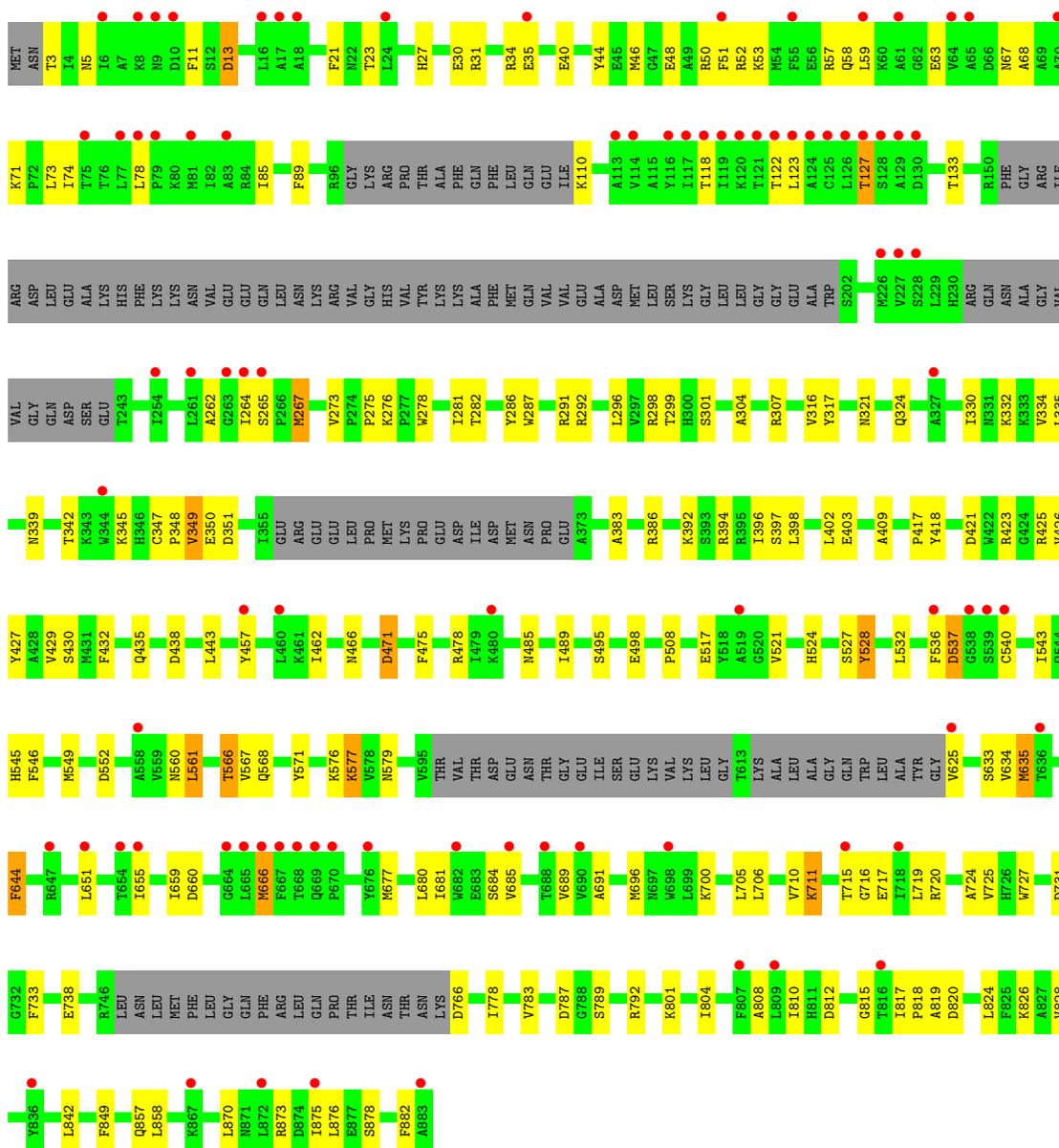


• Molecule 1: T7 RNA polymerase





● Molecule 1: T7 RNA polymerase



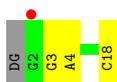
● Molecule 2: Template strand DNA

Chain A:  72% 22% 6%



- Molecule 2: Template strand DNA

Chain F:  6% 78% 17% 6%



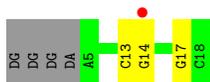
- Molecule 2: Template strand DNA

Chain J:  61% 6% 33%



- Molecule 2: Template strand DNA

Chain M:  6% 61% 17% 22%



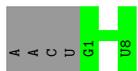
- Molecule 3: RNA

Chain C:  8% 58% 8% 33%



- Molecule 3: RNA

Chain G:  67% 33%

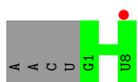


- Molecule 3: RNA

Chain K:  8% 58% 8% 33%



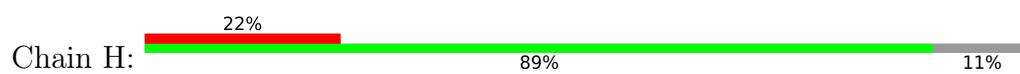
- Molecule 3: RNA



- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.70Å 85.05Å 200.48Å 89.87° 85.38° 69.51°	Depositor
Resolution (Å)	47.37 – 2.90 47.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.37-2.90) 98.0 (47.37-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.260 , 0.307 0.259 , 0.306	Depositor DCC
R_{free} test set	1978 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtrriage
Anisotropy	0.342	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27806	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PO, MG, 91N, GOL

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	B	0.28	0/6856	0.54	3/9277 (0.0%)
1	E	0.28	0/6770	0.56	4/9153 (0.0%)
1	I	0.31	0/6664	0.61	4/9020 (0.0%)
1	L	0.29	0/5653	0.57	7/7668 (0.1%)
2	A	0.53	0/365	0.83	0/559
2	F	0.51	0/365	0.84	0/559
2	J	0.53	0/248	0.85	0/377
2	M	0.50	0/294	0.89	0/448
3	C	0.20	0/193	0.80	0/299
3	G	0.19	0/193	0.74	0/299
3	K	0.16	0/193	0.71	0/299
3	N	0.21	0/190	0.78	0/295
4	D	0.55	0/177	1.07	0/270
4	H	0.52	0/177	0.98	0/270
4	O	0.56	0/113	1.03	0/172
All	All	0.31	0/28451	0.61	18/38965 (0.0%)

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	I	0	3

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	714	LYS	CD-CE-NZ	-8.91	91.21	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	16	LEU	CA-CB-CG	7.96	133.60	115.30
1	I	870	LEU	CA-CB-CG	7.48	132.51	115.30
1	E	219	MET	CA-CB-CG	6.79	124.83	113.30
1	E	59	LEU	CA-CB-CG	6.77	130.87	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	557	ARG	Sidechain
1	I	777	GLY	Peptide
1	I	810	ILE	Peptide

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	B	6706	0	6650	89	0
1	E	6622	0	6583	75	0
1	I	6518	0	6414	132	0
1	L	5536	0	5251	110	0
2	A	351	0	180	3	0
2	F	351	0	180	2	0
2	J	248	0	123	1	0
2	M	289	0	146	2	0
3	C	173	0	86	1	0
3	G	173	0	86	0	0
3	K	173	0	86	1	0
3	N	170	0	87	0	0
4	D	160	0	92	2	0
4	H	160	0	92	0	0
4	O	102	0	58	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	I	6	0	8	0	0
6	B	13	0	0	0	0
6	E	13	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	13	0	0	0	0
6	L	13	0	0	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
7	L	1	0	0	0	0
All	All	27806	0	26138	411	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 8.

The worst 5 of 411 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:B:278:TRP:H	1:B:321:ASN:HD21	1.19	0.87
1:I:155:ARG:HA	1:I:163:LYS:HD3	1.67	0.77
1:B:6:ILE:HB	1:B:291:ARG:HH22	1.51	0.75
1:I:468:ALA:HA	1:I:505:GLN:HG3	1.69	0.75
1:B:602:THR:HG23	1:B:604:GLU:H	1.53	0.74

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	B	850/883 (96%)	824 (97%)	24 (3%)	2 (0%)	47	78
1	E	831/883 (94%)	813 (98%)	18 (2%)	0	100	100
1	I	823/883 (93%)	800 (97%)	23 (3%)	0	100	100
1	L	726/883 (82%)	711 (98%)	15 (2%)	0	100	100
All	All	3230/3532 (91%)	3148 (98%)	80 (2%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	811	HIS
1	B	227	VAL

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	B	695/729 (95%)	649 (93%)	46 (7%)	16	44
1	E	688/729 (94%)	648 (94%)	40 (6%)	20	50
1	I	674/729 (92%)	611 (91%)	63 (9%)	9	27
1	L	530/729 (73%)	493 (93%)	37 (7%)	15	41
All	All	2587/2916 (89%)	2401 (93%)	186 (7%)	14	39

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	422	TRP
1	I	829	ARG
1	I	460	LEU
1	I	632	ARG
1	L	13	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	857	GLN
1	L	672	GLN
1	L	560	ASN
1	L	545	HIS
1	L	568	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	6/12 (50%)	0	0
3	G	6/12 (50%)	0	0
3	K	6/12 (50%)	0	0
3	N	6/12 (50%)	0	0
All	All	24/48 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	3PO	B	902	7	8,12,12	0.69	0	15,20,20	1.31	2 (13%)
5	GOL	B	901	-	5,5,5	0.93	0	5,5,5	0.99	0
6	3PO	E	901	7	8,12,12	0.69	0	15,20,20	1.17	2 (13%)
5	GOL	I	901	-	5,5,5	0.91	0	5,5,5	0.97	0
6	3PO	L	901	7	8,12,12	0.72	0	15,20,20	1.22	2 (13%)
5	GOL	C	101	-	5,5,5	0.92	0	5,5,5	0.99	0
6	3PO	I	902	7	8,12,12	0.69	0	15,20,20	1.23	2 (13%)

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
6	3PO	B	902	7	-	1/12/12/12	-
5	GOL	B	901	-	-	0/4/4/4	-
6	3PO	E	901	7	-	0/12/12/12	-
5	GOL	I	901	-	-	3/4/4/4	-
6	3PO	L	901	7	-	3/12/12/12	-
5	GOL	C	101	-	-	2/4/4/4	-
6	3PO	I	902	7	-	2/12/12/12	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	3PO	PB-O3A-PA	-2.92	122.80	132.83
6	B	902	3PO	PB-O3B-PG	-2.73	123.46	132.83
6	L	901	3PO	PB-O3A-PA	-2.69	123.61	132.83
6	E	901	3PO	PB-O3A-PA	-2.66	123.70	132.83
6	I	902	3PO	PB-O3B-PG	-2.59	123.94	132.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	901	3PO	PB-O3B-PG-O2G
6	L	901	3PO	PB-O3B-PG-O3G
5	C	101	GOL	O1-C1-C2-C3
5	I	901	GOL	O1-C1-C2-C3
5	I	901	GOL	C1-C2-C3-O3

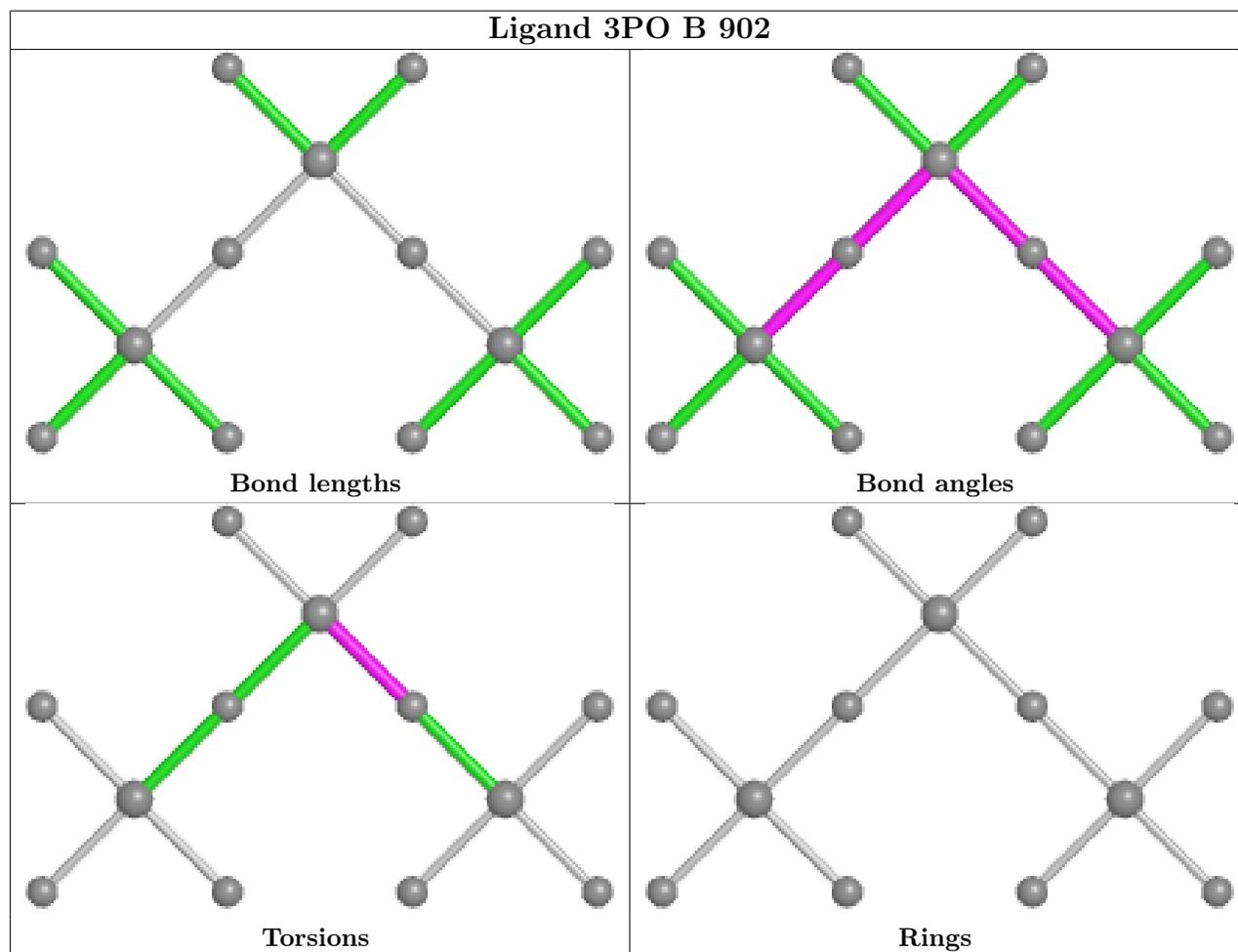
There are no ring outliers.

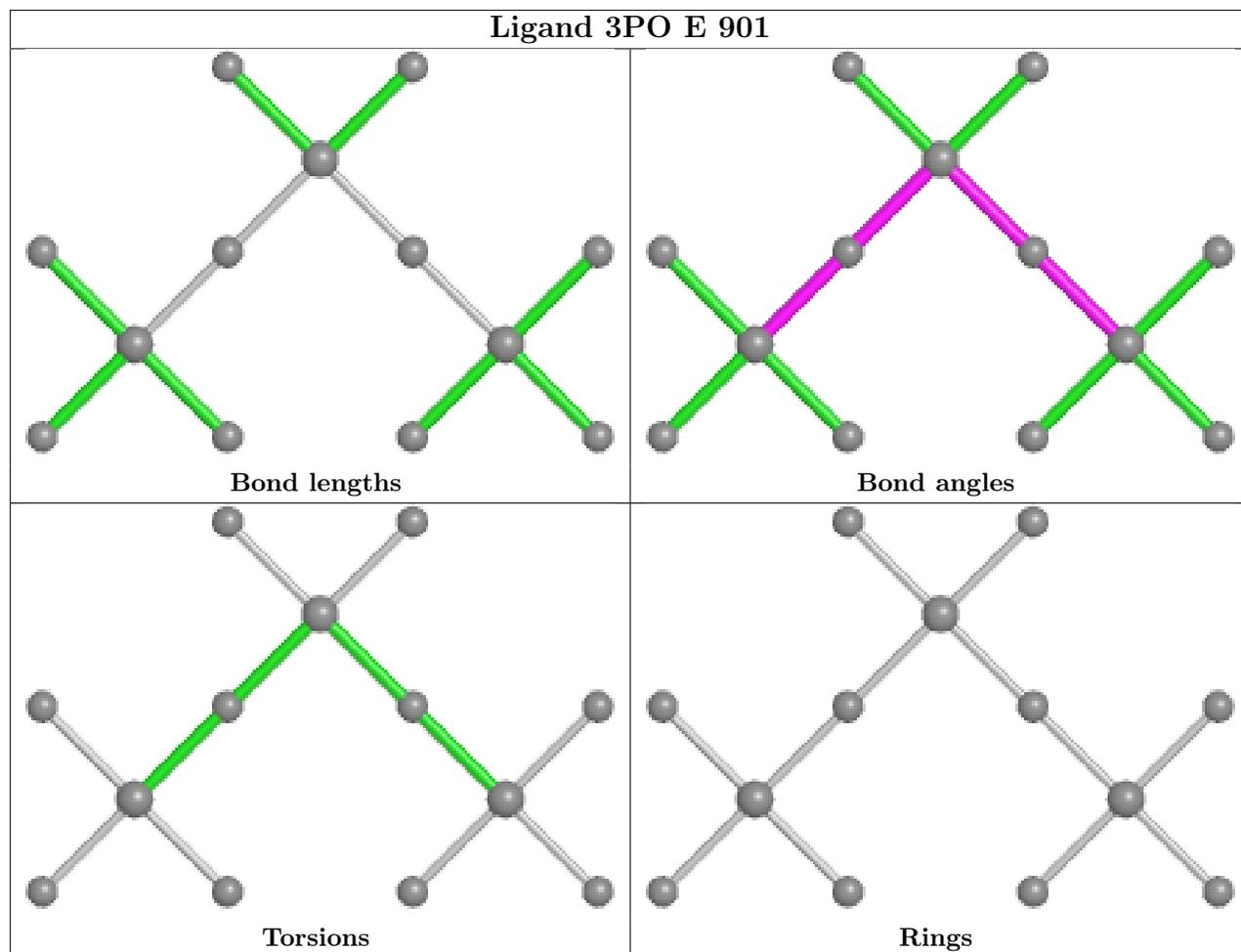
1 monomer is involved in 2 short contacts:

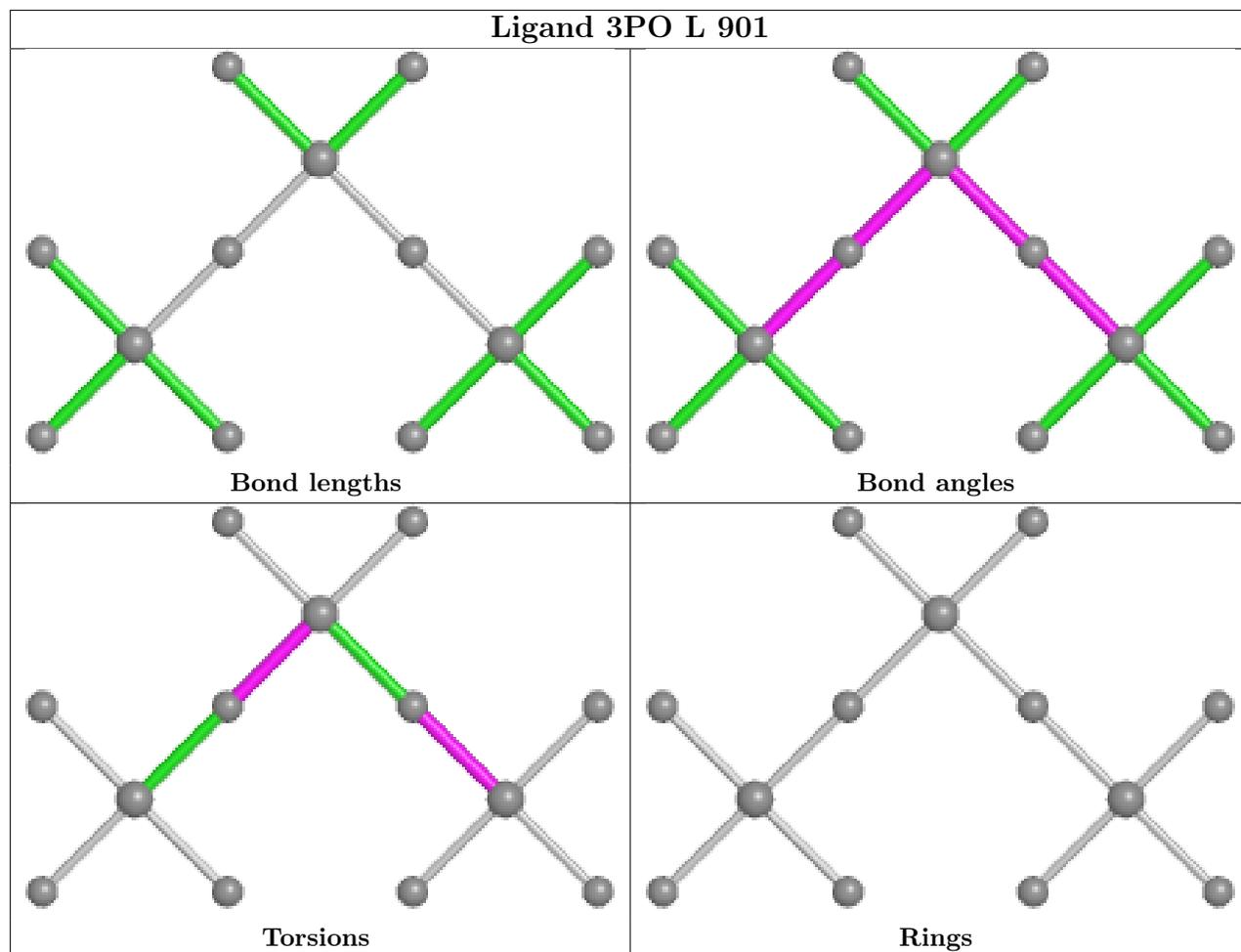
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	901	3PO	2	0

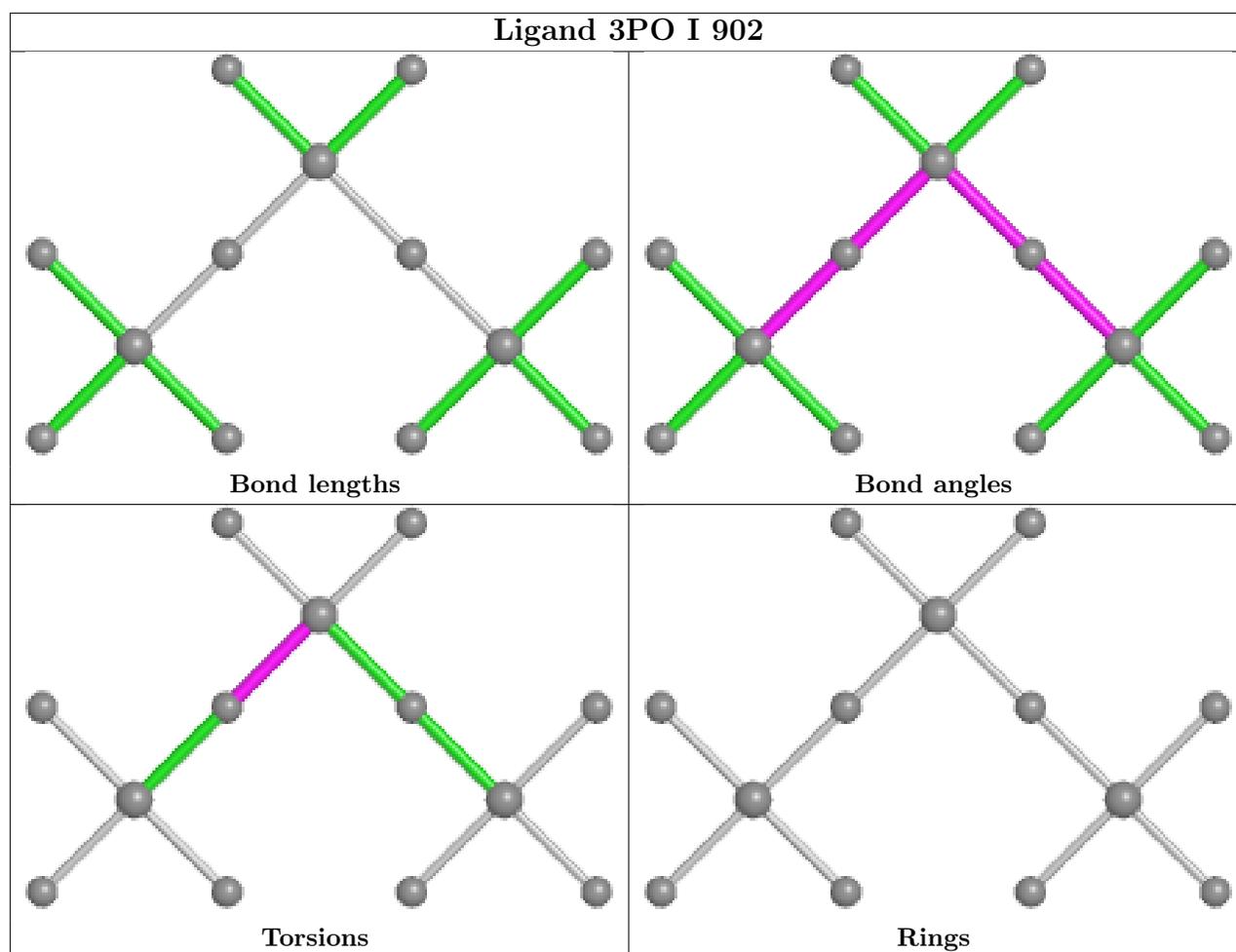
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	B	856/883 (96%)	0.36	46 (5%) 25 22	39, 81, 191, 296	0
1	E	841/883 (95%)	0.43	60 (7%) 16 12	46, 81, 202, 308	0
1	I	833/883 (94%)	1.02	169 (20%) 1 0	86, 153, 225, 304	0
1	L	741/883 (83%)	0.69	87 (11%) 4 3	84, 128, 189, 245	0
2	A	16/18 (88%)	0.52	0 100 100	68, 109, 266, 271	0
2	F	16/18 (88%)	0.39	1 (6%) 20 16	63, 119, 255, 275	0
2	J	11/18 (61%)	0.40	0 100 100	105, 111, 194, 228	0
2	M	13/18 (72%)	0.59	1 (7%) 13 10	104, 127, 200, 238	0
3	C	8/12 (66%)	0.80	1 (12%) 3 3	63, 80, 96, 113	0
3	G	8/12 (66%)	1.16	0 100 100	65, 90, 148, 176	0
3	K	8/12 (66%)	0.87	1 (12%) 3 3	119, 121, 163, 193	0
3	N	8/12 (66%)	0.81	1 (12%) 3 3	110, 137, 190, 191	0
4	D	8/9 (88%)	1.17	1 (12%) 3 3	205, 222, 229, 271	0
4	H	8/9 (88%)	0.69	2 (25%) 0 0	189, 207, 227, 255	0
4	O	5/9 (55%)	0.54	1 (20%) 1 0	200, 215, 229, 246	0
All	All	3380/3679 (91%)	0.62	371 (10%) 5 4	39, 121, 209, 308	0

The worst 5 of 371 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	625	VAL	8.3
1	L	129	ALA	7.4
1	I	472	LYS	6.9
1	L	816	THR	6.8
1	B	237	VAL	6.6

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](#)

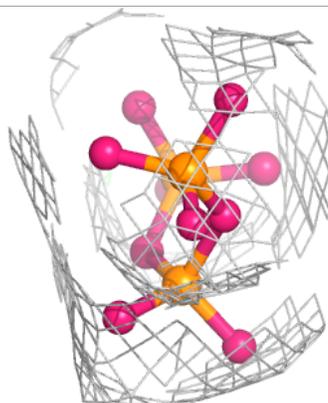
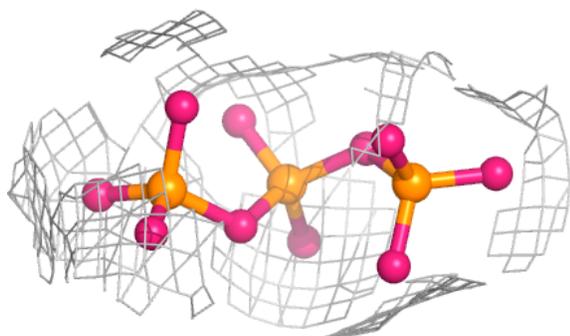
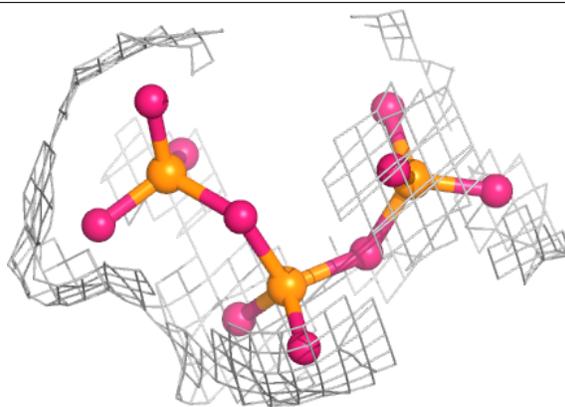
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	I	901	6/6	0.75	0.56	135,140,144,150	0
5	GOL	C	101	6/6	0.81	0.34	77,88,95,101	0
7	MG	L	902	1/1	0.83	0.96	124,124,124,124	0
7	MG	B	903	1/1	0.84	0.42	66,66,66,66	0
6	3PO	I	902	13/13	0.88	0.19	148,166,176,176	0
7	MG	E	902	1/1	0.92	0.28	74,74,74,74	0
6	3PO	B	902	13/13	0.92	0.26	72,103,111,126	0
7	MG	I	903	1/1	0.94	0.33	125,125,125,125	0
6	3PO	L	901	13/13	0.94	0.36	141,154,163,168	0
5	GOL	B	901	6/6	0.96	0.24	69,70,90,90	0
6	3PO	E	901	13/13	0.97	0.20	77,108,138,139	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.

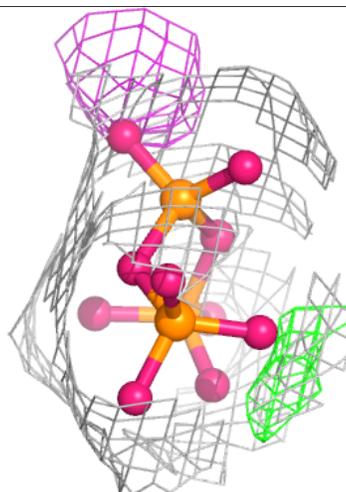
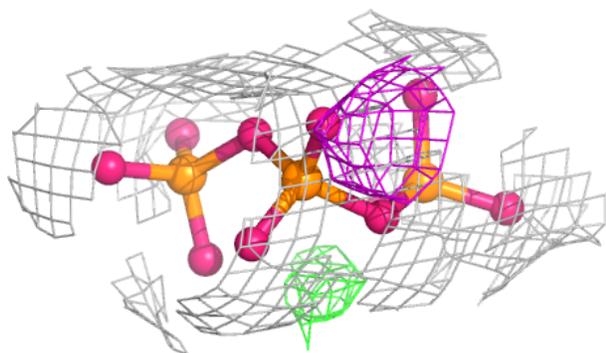
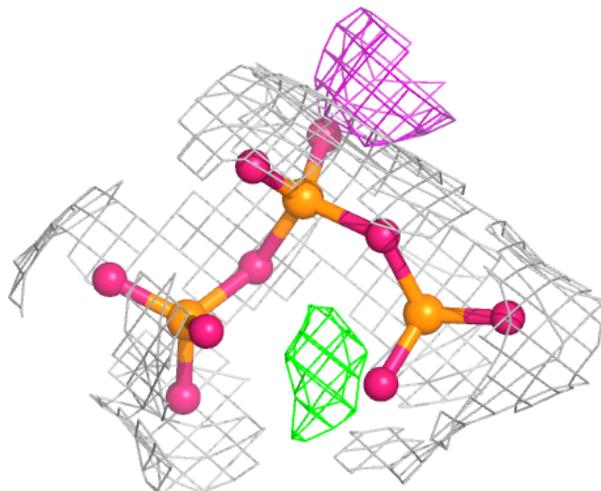
Electron density around 3PO I 902:

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



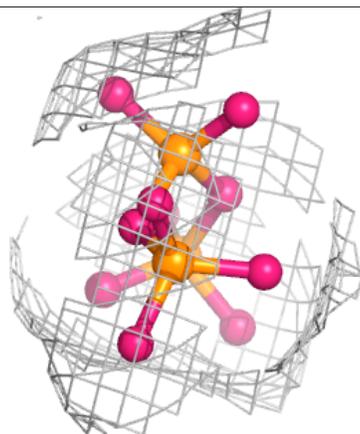
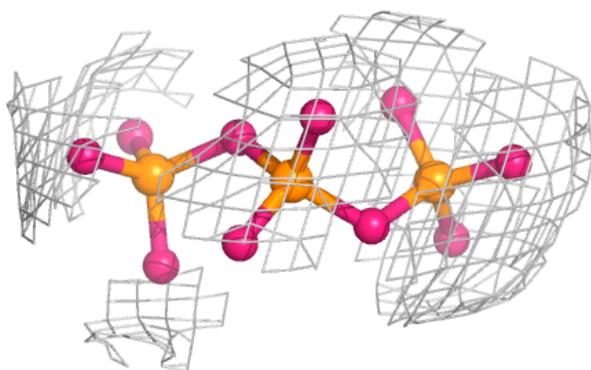
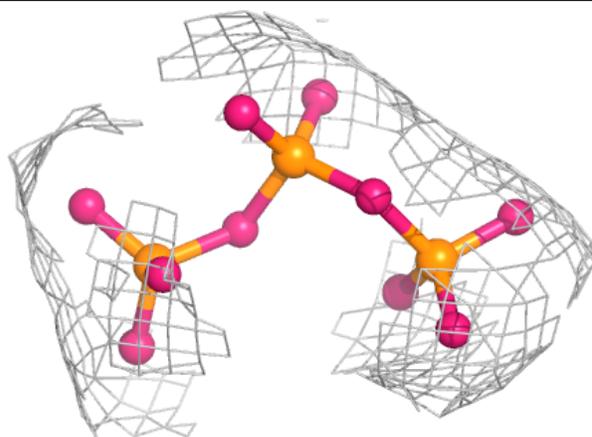
Electron density around 3PO B 902:

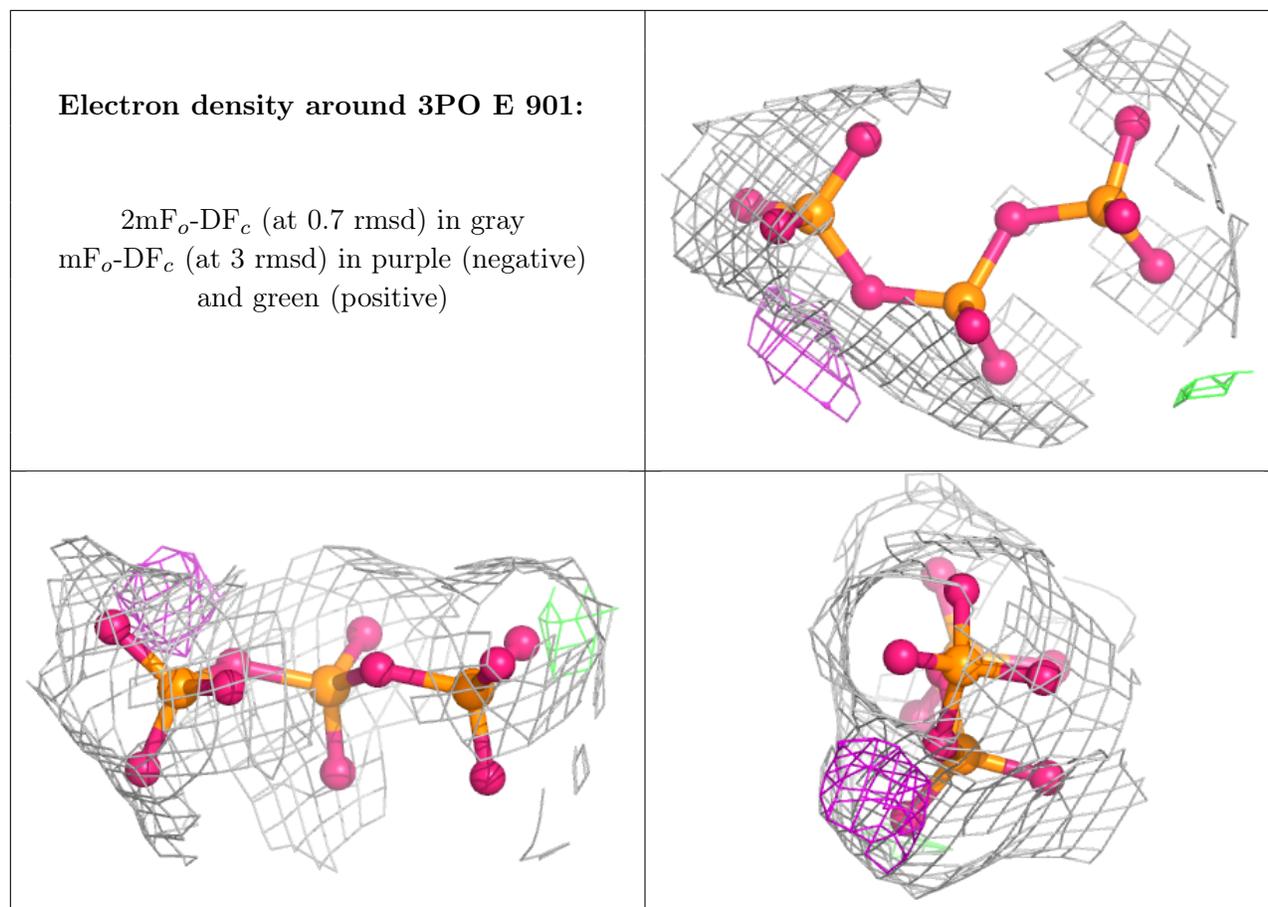
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3PO L 901:

$2mF_o-DF_c$ (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.