



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 06:32 PM UTC

PDB ID : 8DH2 / pdb_00008dh2
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:

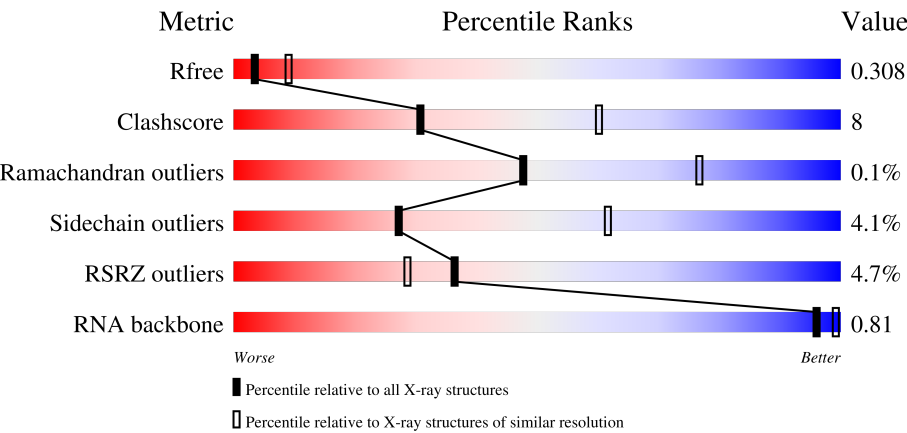
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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.



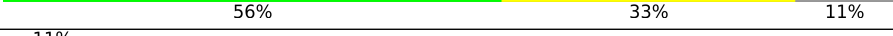
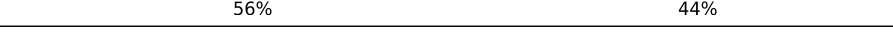
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 $\leq 5\%$. 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	4% 77% 19% • •
1	E	883	3% 79% 16% • 5%
1	I	883	7% 68% 25% • 6%
1	L	883	4% 63% 20% • 16%

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Mol	Chain	Length	Quality of chain
2	A	18	 72%22%6%
2	F	18	 78%17%6%
2	J	18	 61%6%33%
2	M	18	 56%22%22%
3	C	12	 58%8%33%
3	G	12	 67%33%
3	K	12	 58%8%33%
3	N	12	 67%33%
4	D	9	 56%33%11%
4	H	9	 11%89%11%
4	O	9	 56%44%

2 Entry composition

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
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
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.

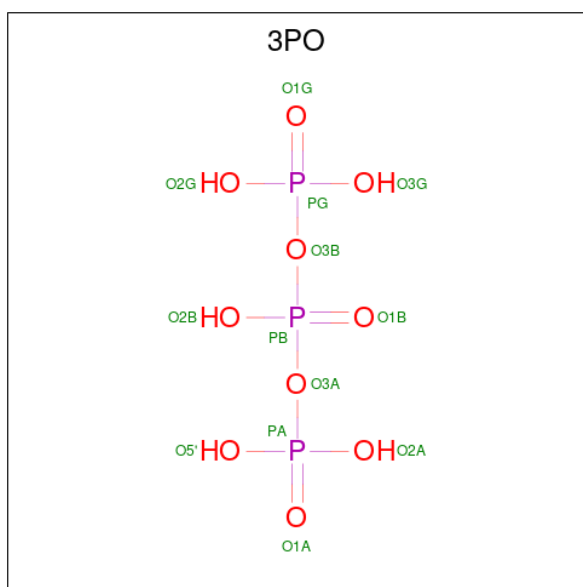
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	H	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	O	5	Total	C	N	O	P	0	0	0
			102	49	17	31	5			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

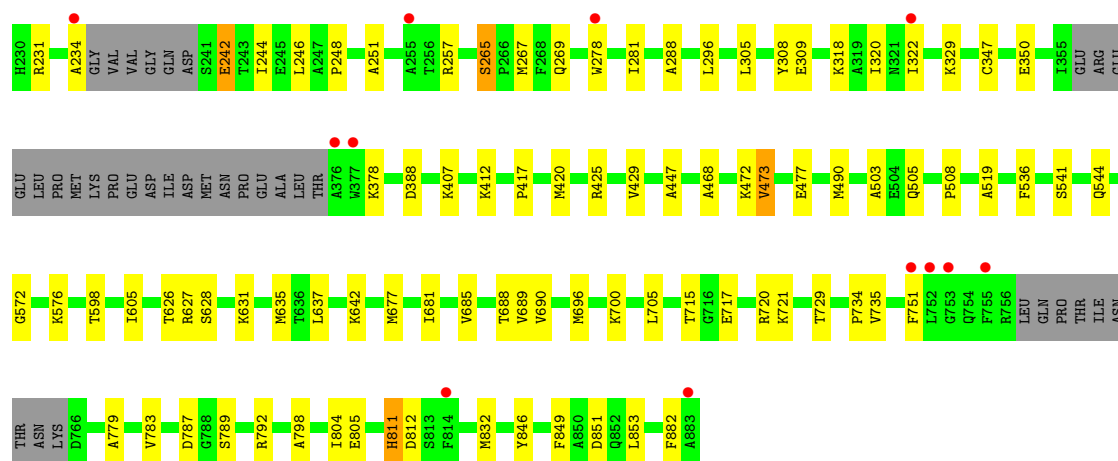
- Molecule 6 is TRIPHOSPHATE (CCD ID: 3PO) (formula: $H_5O_{10}P_3$) (labeled as "Ligand of Interest" by depositor).



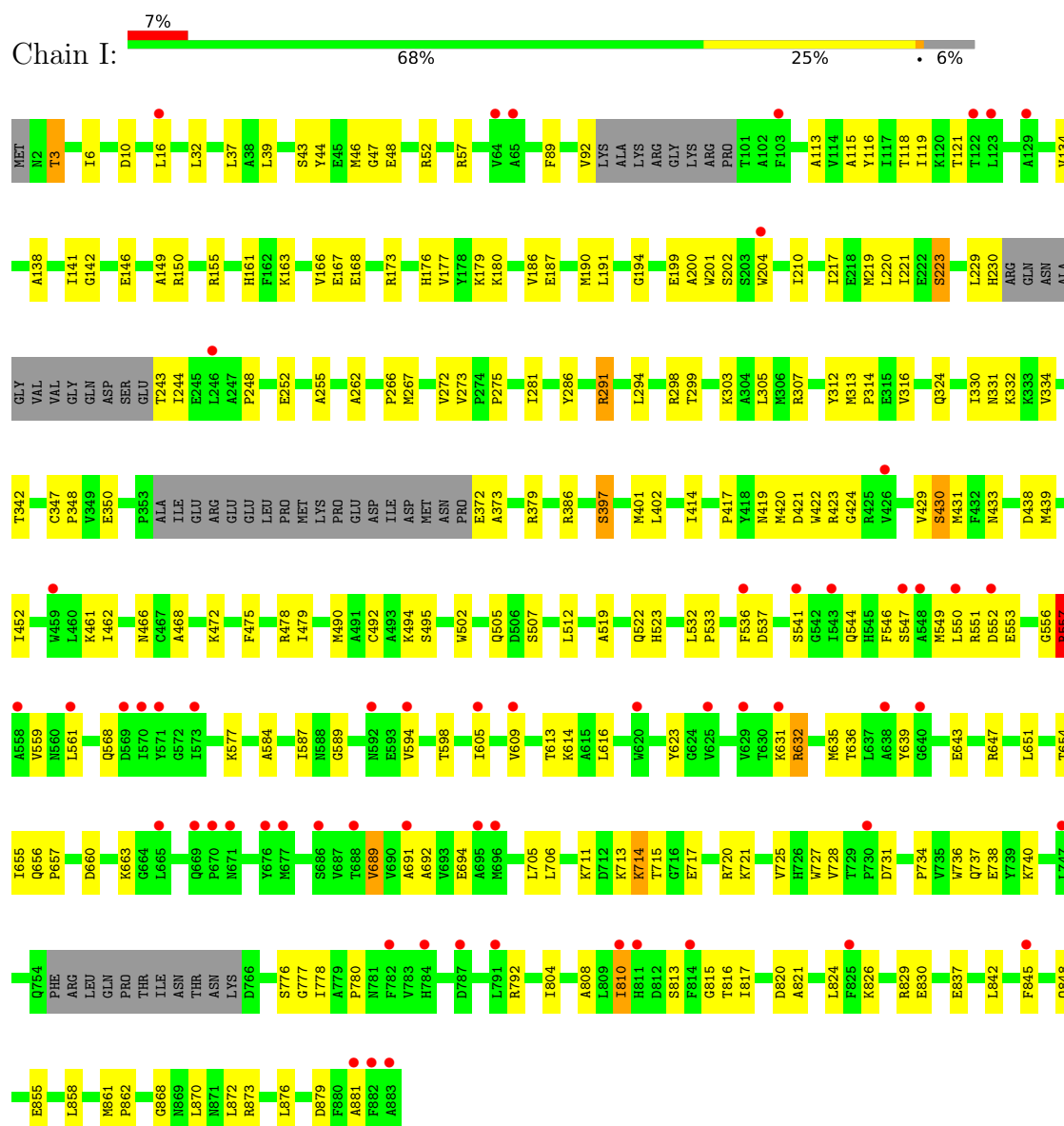
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			13	10	3		
6	E	1	Total	O	P	0	0
			13	10	3		
6	I	1	Total	O	P	0	0
			13	10	3		
6	L	1	Total	O	P	0	0
			13	10	3		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

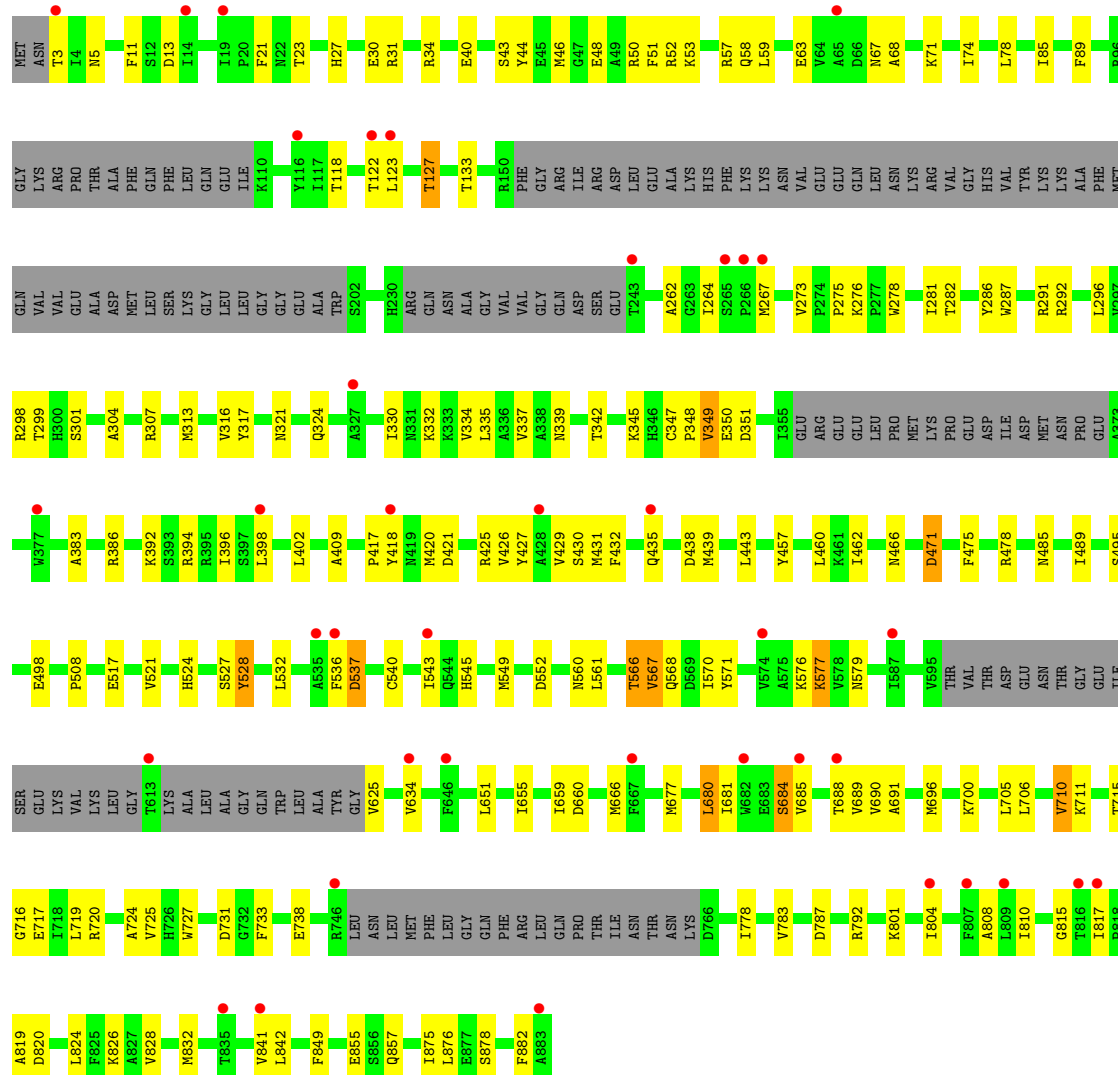
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		
7	I	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		



• Molecule 1: T7 RNA polymerase



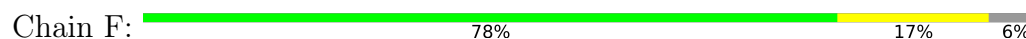
• Molecule 1: T7 RNA polymerase



• Molecule 2: Template strand DNA

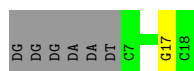


• Molecule 2: Template strand DNA



• Molecule 2: Template strand DNA

Chain J:  61% 6% 33%



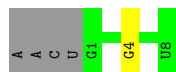
- Molecule 2: Template strand DNA

Chain M:  56% 22% 22%



- Molecule 3: RNA

Chain C:  58% 8% 33%



- Molecule 3: RNA

Chain G:  67% 33%



- Molecule 3: RNA

Chain K:  58% 8% 33%



- Molecule 3: RNA

Chain N:  67% 33%



- Molecule 4: Non-template strand DNA

Chain D:  56% 33% 11%



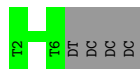
- Molecule 4: Non-template strand DNA

Chain H:  11% 89% 11%



- Molecule 4: Non-template strand DNA

Chain O:  56% 44%



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) 97.9 (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)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.260 , 0.307 0.261 , 0.308	Depositor DCC
R_{free} test set	2005 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 91N, 3PO, 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	0.18	0/6856	0.42	2/9277 (0.0%)
1	E	0.19	0/6770	0.44	4/9153 (0.0%)
1	I	0.22	0/6664	0.51	1/9020 (0.0%)
1	L	0.20	0/5653	0.48	1/7668 (0.0%)
2	A	0.18	0/365	0.31	0/559
2	F	0.18	0/365	0.32	0/559
2	J	0.19	0/248	0.34	0/377
2	M	0.18	0/294	0.36	0/448
3	C	0.11	0/193	0.28	0/299
3	G	0.10	0/193	0.23	0/299
3	K	0.08	0/193	0.21	0/299
3	N	0.10	0/190	0.22	0/295
4	D	0.21	0/177	0.48	0/270
4	H	0.19	0/177	0.39	0/270
4	O	0.20	0/113	0.44	0/172
All	All	0.20	0/28451	0.45	8/38965 (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 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	714	LYS	CD-CE-NZ	-6.47	91.21	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	811	HIS	CA-C-N	6.01	133.03	121.54
1	E	811	HIS	C-N-CA	6.01	133.03	121.54
1	L	577	LYS	CB-CG-CD	5.95	124.98	111.30
1	E	219	MET	CA-CB-CG	5.37	124.83	114.10

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 ⓘ

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	95	0
1	E	6622	0	6583	85	0
1	I	6518	0	6414	141	0
1	L	5536	0	5251	118	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	3	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	444	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 444 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%)	43	72
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%)	48	77

All (2) Ramachandran outliers are listed below:

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

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	B	695/729 (95%)	663 (95%)	32 (5%)	24	57
1	E	688/729 (94%)	670 (97%)	18 (3%)	40	73
1	I	674/729 (92%)	646 (96%)	28 (4%)	26	60
1	L	530/729 (73%)	502 (95%)	28 (5%)	20	52
All	All	2587/2916 (89%)	2481 (96%)	106 (4%)	27	61

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	230	HIS
1	I	643	GLU
1	L	680	LEU
1	I	291	ARG
1	I	492	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	41	HIS
1	L	486	HIS
1	L	786	GLN
1	E	86	ASN
1	E	67	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
5	GOL	I	901	-	5,5,5	0.94	0	5,5,5	1.04	0
6	3PO	B	902	7	10,12,12	2.41	2 (20%)	17,20,20	0.83	0
5	GOL	B	901	-	5,5,5	0.96	0	5,5,5	1.07	0
6	3PO	L	901	7	10,12,12	2.47	2 (20%)	17,20,20	0.80	0
6	3PO	I	902	7	10,12,12	2.50	2 (20%)	17,20,20	0.83	0
5	GOL	C	101	-	5,5,5	0.95	0	5,5,5	1.07	0
6	3PO	E	901	7	10,12,12	2.45	2 (20%)	17,20,20	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	I	901	-	-	3/4/4/4	-
6	3PO	B	902	7	-	1/12/12/12	-
5	GOL	B	901	-	-	0/4/4/4	-
6	3PO	L	901	7	-	3/12/12/12	-
6	3PO	I	902	7	-	2/12/12/12	-
5	GOL	C	101	-	-	2/4/4/4	-
6	3PO	E	901	7	-	0/12/12/12	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	901	3PO	PB-O3B	5.45	1.65	1.59
6	I	902	3PO	PB-O3A	5.41	1.65	1.59
6	I	902	3PO	PB-O3B	5.40	1.65	1.59
6	E	901	3PO	PB-O3B	5.29	1.65	1.59
6	E	901	3PO	PB-O3A	5.28	1.65	1.59

There are no bond angle outliers.

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	C	101	GOL	O1-C1-C2-O2

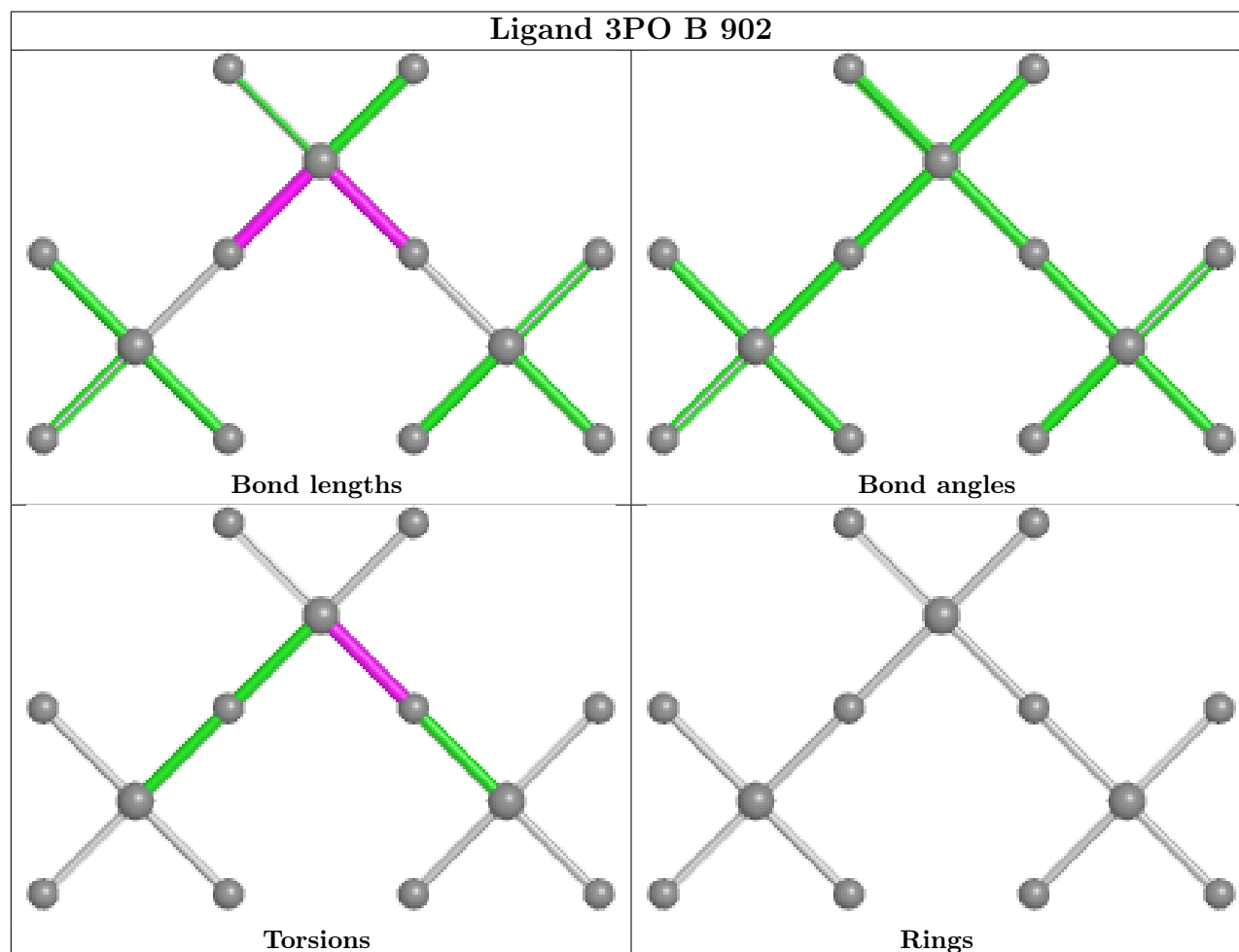
There are no ring outliers.

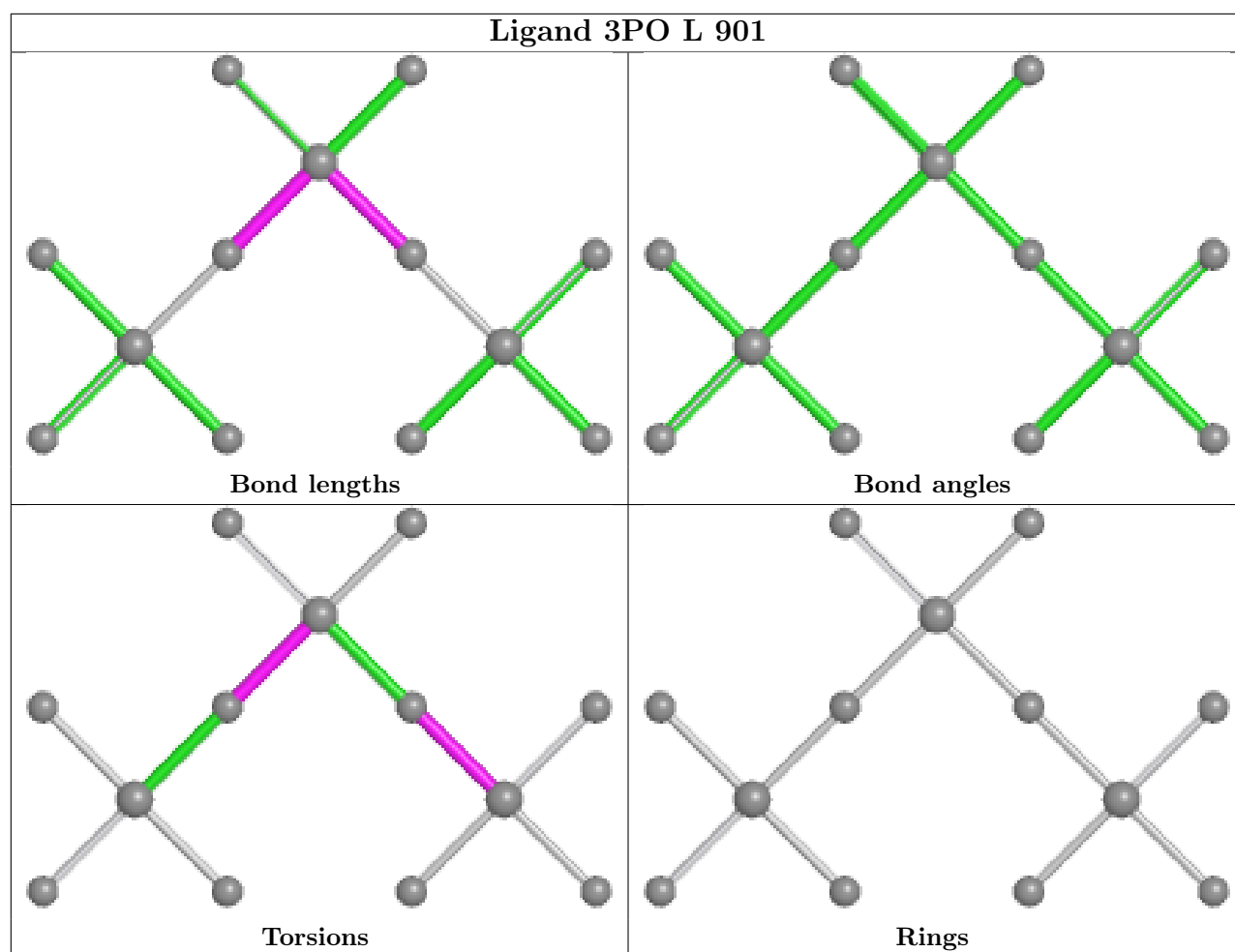
1 monomer is involved in 2 short contacts:

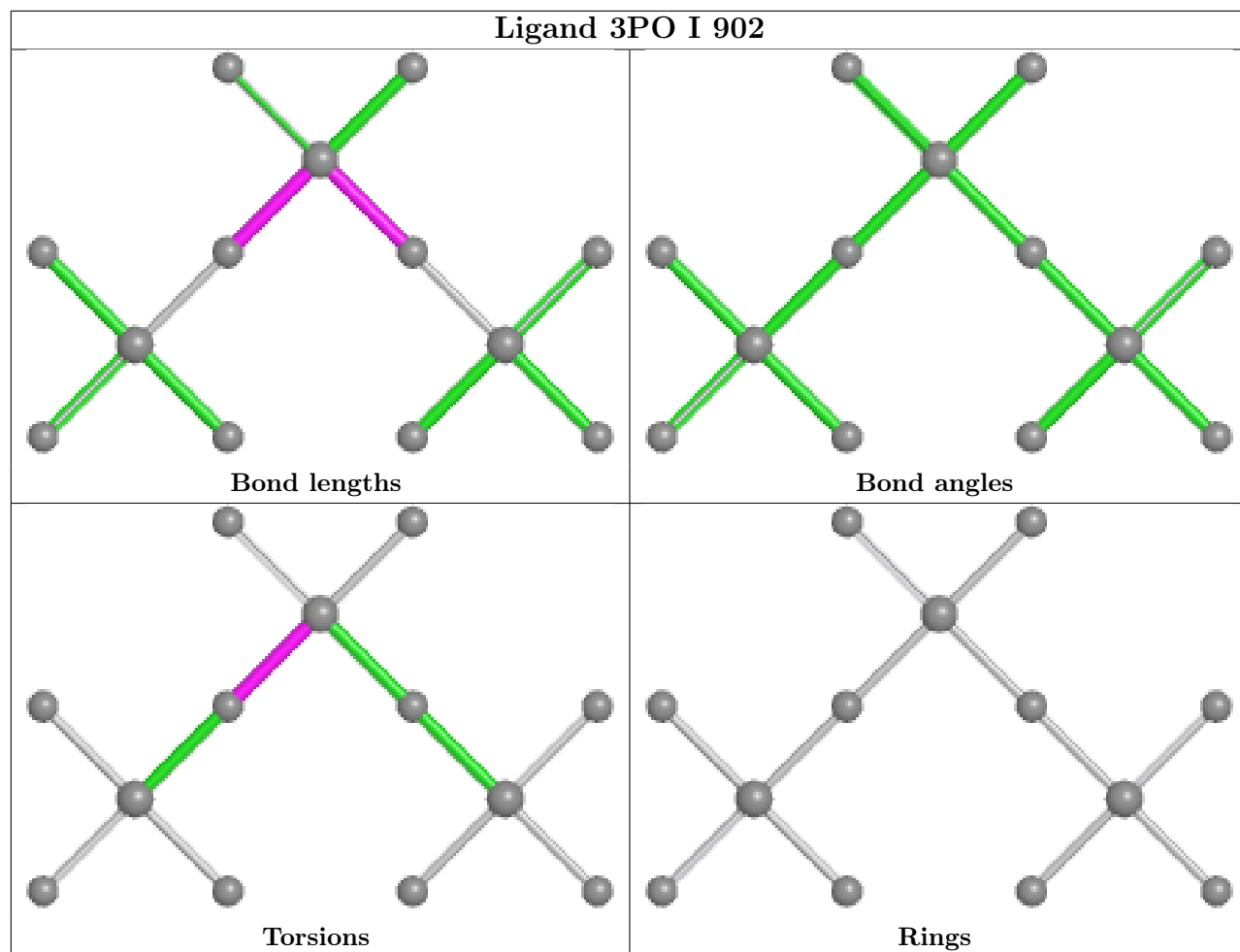
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	901	3PO	2	0

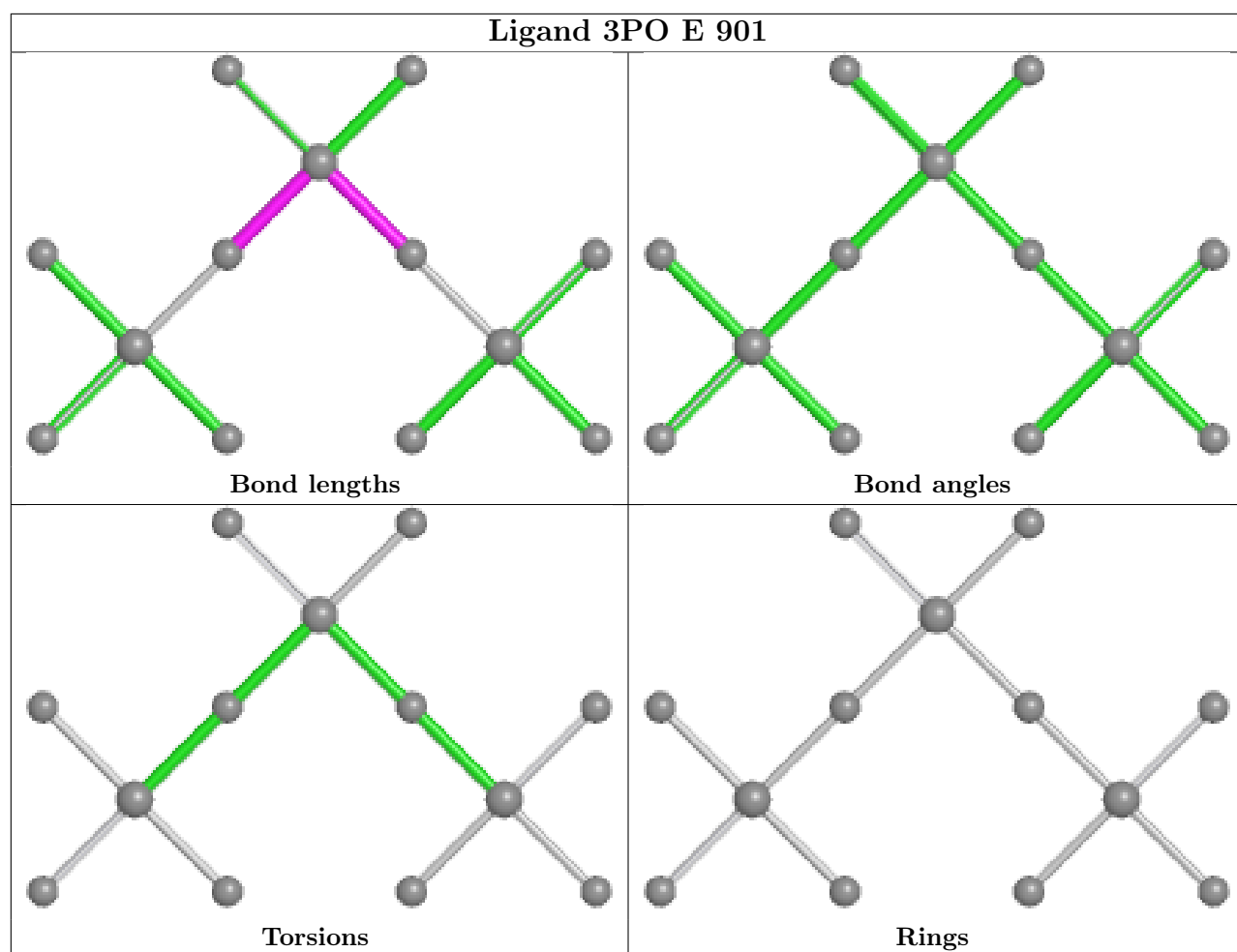
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.32	36 (4%)	40	32	39, 81, 191, 296	0
1	E	841/883 (95%)	0.30	24 (2%)	53	45	46, 81, 202, 308	0
1	I	833/883 (94%)	0.68	59 (7%)	22	17	86, 153, 225, 304	0
1	L	741/883 (83%)	0.50	38 (5%)	33	26	84, 128, 189, 245	0
2	A	16/18 (88%)	-0.00	0	100	100	68, 109, 266, 271	0
2	F	16/18 (88%)	0.30	0	100	100	63, 119, 255, 275	0
2	J	11/18 (61%)	-0.06	0	100	100	105, 111, 194, 228	0
2	M	13/18 (72%)	0.09	0	100	100	104, 127, 200, 238	0
3	C	8/12 (66%)	-0.51	0	100	100	63, 80, 96, 113	0
3	G	8/12 (66%)	-0.21	0	100	100	65, 90, 148, 176	0
3	K	8/12 (66%)	-0.12	0	100	100	119, 121, 163, 193	0
3	N	8/12 (66%)	-0.03	0	100	100	110, 137, 190, 191	0
4	D	8/9 (88%)	0.50	0	100	100	205, 222, 229, 271	0
4	H	8/9 (88%)	0.85	1 (12%)	8	7	189, 207, 227, 255	0
4	O	5/9 (55%)	0.18	0	100	100	200, 215, 229, 246	0
All	All	3380/3679 (91%)	0.44	158 (4%)	36	28	39, 121, 209, 308	0

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	883	ALA	8.7
1	I	558	ALA	5.8
1	L	816	THR	4.9
1	L	122	THR	4.4
1	E	883	ALA	4.4

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

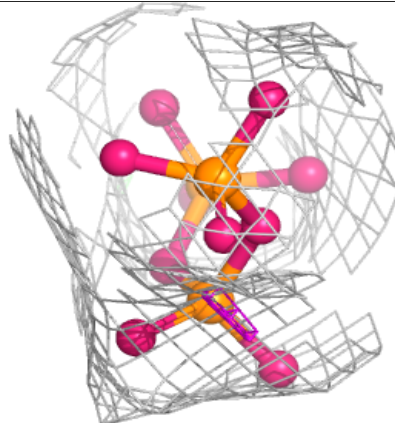
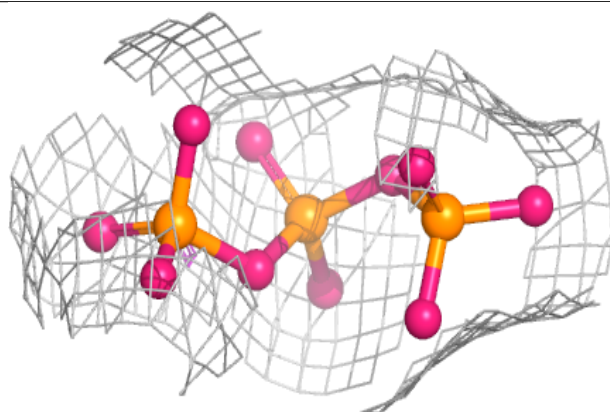
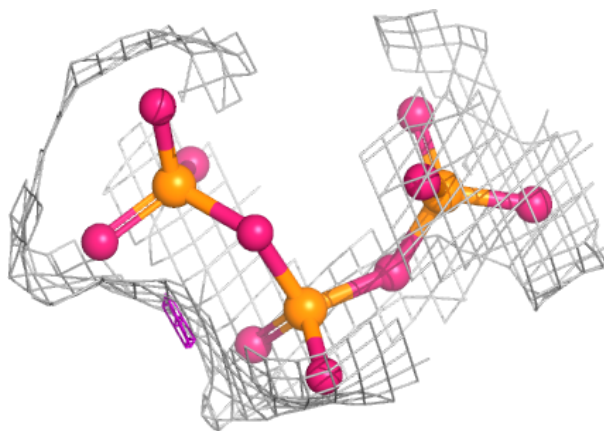
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.54	0.19	135,140,144,150	0
6	3PO	I	902	13/13	0.60	0.09	148,166,176,176	0
5	GOL	C	101	6/6	0.72	0.14	77,88,95,101	0
6	3PO	L	901	13/13	0.73	0.08	141,154,163,168	0
6	3PO	B	902	13/13	0.79	0.10	72,103,111,126	0
7	MG	L	902	1/1	0.81	0.13	124,124,124,124	0
6	3PO	E	901	13/13	0.83	0.07	77,108,138,139	0
7	MG	I	903	1/1	0.88	0.09	125,125,125,125	0
7	MG	E	902	1/1	0.90	0.06	74,74,74,74	0
5	GOL	B	901	6/6	0.92	0.10	69,70,90,90	0
7	MG	B	903	1/1	0.93	0.15	66,66,66,66	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.

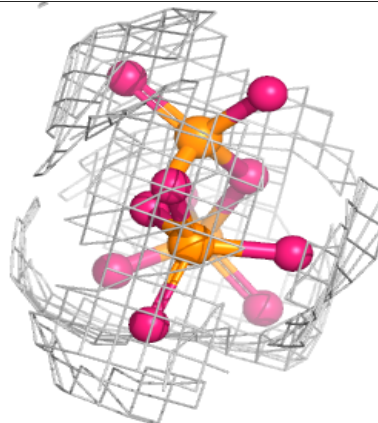
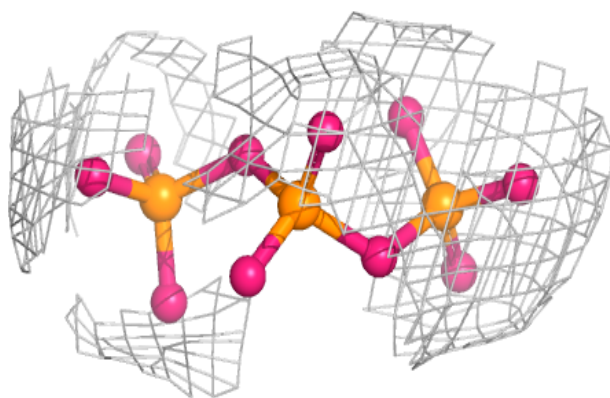
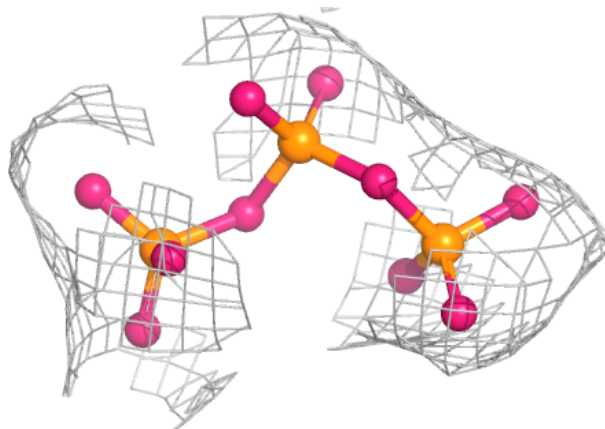
Electron density around 3PO I 902:

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



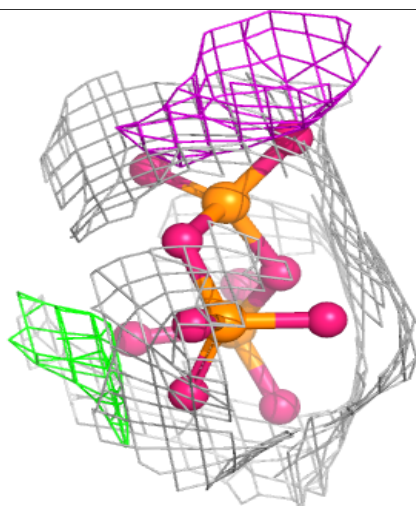
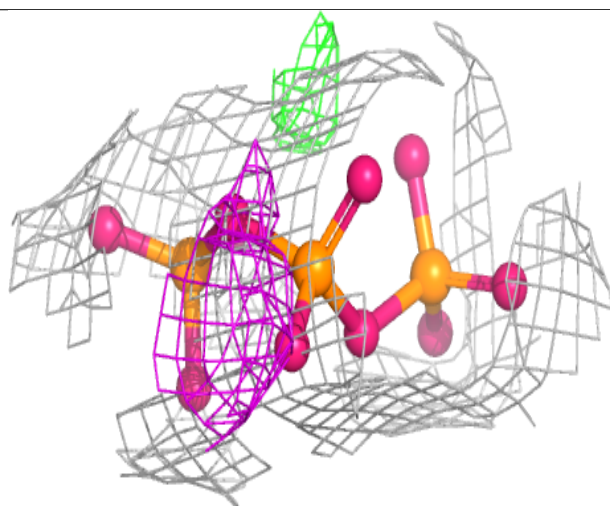
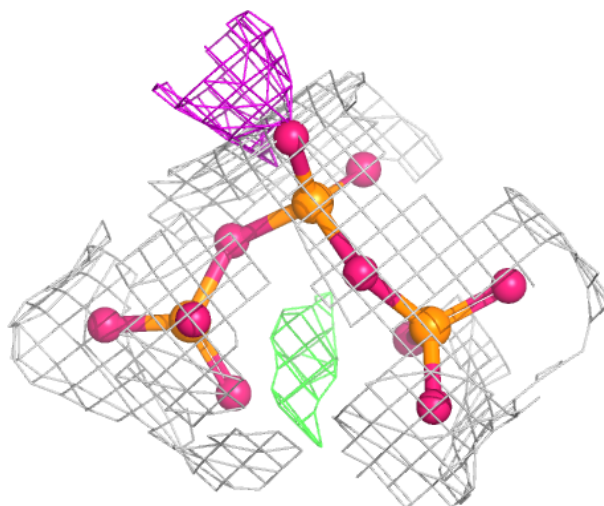
Electron density around 3PO L 901:

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



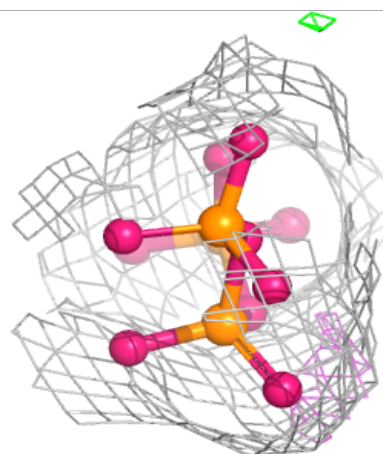
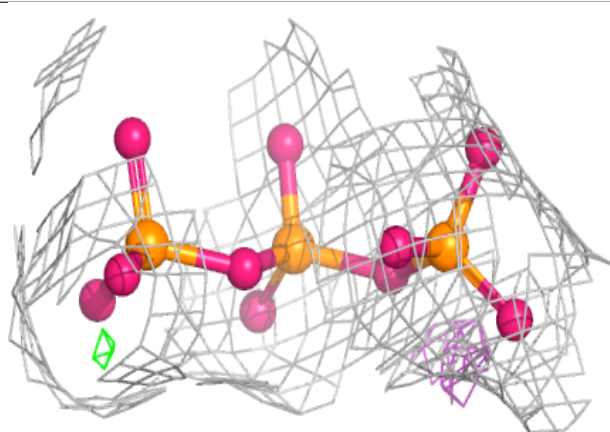
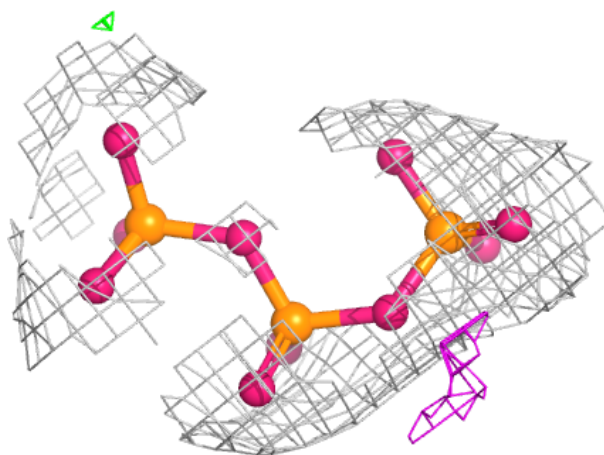
Electron density around 3PO B 902:

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



Electron density around 3PO E 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.