

wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 12:11 PM EDT

:	8SCR
:	Bst DNA polymerase I Large Fragment wildtype D598A with 3'-amino primer,
	dGTP, and calcium time-resolved 4h
:	Fang, Z.; Lelyveld, V.S.; Szostak, J.W.
:	2023-04-05
:	2.00 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 (1)) were used in the production of this report:

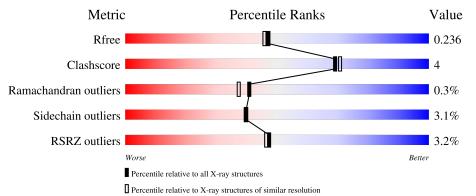
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	А	579	% 93%		7% •					
1	D	579	<u>6%</u> 86%		13% •					
2	В	10	60%	40%						
2	Е	10	70%	20%	10%					
3	С	13	77%	2	23%					



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Mol	Chain	Length		Quality of chain
			8%	
3	F	13	38%	62%

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
7	SO4	А	908	-	-	-	Х
7	SO4	А	909	-	-	-	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10712 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 I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	579	Total	С	Ν	0	S	0	3	0
-		010	4659	2966	808	867	18	0	9	Ŭ
1	Л	579	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	D	515	4645	2955	807	866	17	0	0	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	713	VAL	PRO	variant	UNP D9N168
D	713	VAL	PRO	variant	UNP D9N168

• Molecule 2 is a DNA chain called DNA primer/product.

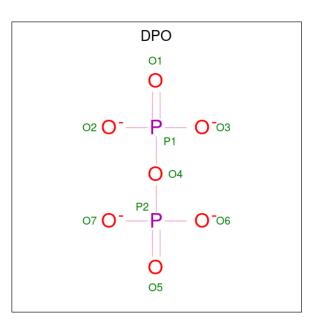
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	В	10	Total	С	Ν	Ο	Р	0	2	0
	D	10	223	106	46	61	10	0		
0	F	10	Total	С	Ν	Ο	Р	0	2	0
	Ľ	10	223	106	46	61	10		2	

• Molecule 3 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	13	Total	С	Ν	Ο	Р	0	0	1
5	3 U		246	116	46	72	12	0	0	
2	Б	13	Total	С	Ν	Ο	Р	0	0	1
5	Г	10	246	116	46	72	12	0	U	

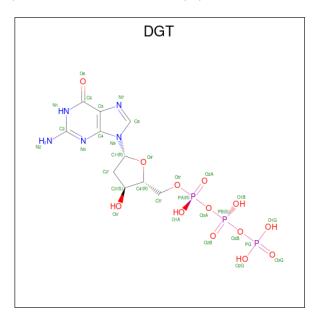
• Molecule 4 is DIPHOSPHATE (three-letter code: DPO) (formula: O₇P₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	TotalOP972	0	1
4	D	1	TotalOP972	0	1

• Molecule 5 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	Δ	1	Total	С	Ν	0	Р	0	1
5	A	1	31	10	5	13	3	0	1



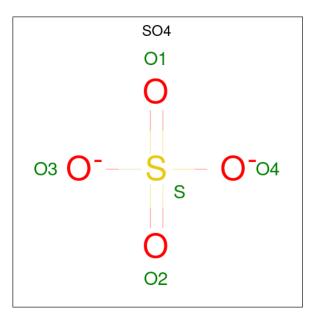
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Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	D	1	Total	С	Ν	0	Р	0	1
	D	1	31	10	5	13	3	Ŭ	1

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mo	bl	Chain	Residues	Atoms	ZeroOcc	AltConf
6		А	1	Total Ca 1 1	0	0
6		D	1	Total Ca 1 1	0	0

• Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	С	1	$\begin{array}{c c} \hline Total & O & S \\ \hline 5 & 4 & 1 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

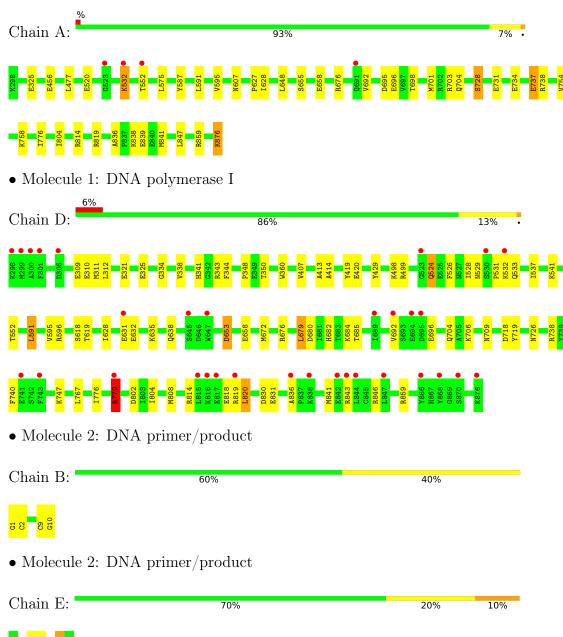
• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	190	Total O 190 190	0	0
8	В	16	Total O 16 16	0	0
8	С	25	TotalO2525	0	0
8	D	74	Total O 74 74	0	0
8	Е	11	Total O 11 11	0	0
8	F	17	Total O 17 17	0	0



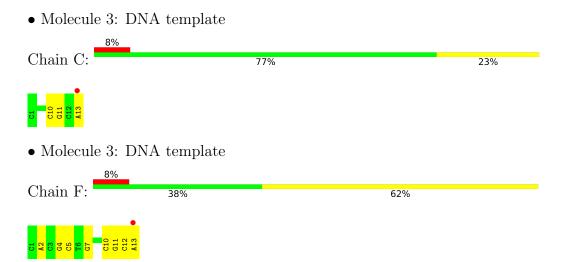
3 Residue-property plots (i)

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 I







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	93.77Å 109.08Å 151.19Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.39 – 2.00	Depositor
Resolution (A)	44.39 - 2.00	EDS
% Data completeness	95.2 (44.39-2.00)	Depositor
(in resolution range)	95.2 (44.39-2.00)	EDS
R _{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.14 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
B B.	0.194 , 0.236	Depositor
R, R_{free}	0.194 , 0.236	DCC
R_{free} test set	5145 reflections (5.13%)	wwPDB-VP
Wilson B-factor $(Å^2)$	23.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 49.2	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10712	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: CA, DPO, DGT, SO4, C42

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).

Mal	Mol Chain		lengths	Bond angles		
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/4752	0.58	0/6420	
1	D	0.35	0/4729	0.51	0/6391	
2	В	0.90	0/207	1.02	0/316	
2	Е	0.88	0/207	1.00	2/316~(0.6%)	
3	С	1.08	0/275	0.98	0/423	
3	F	1.01	0/275	0.94	0/423	
All	All	0.48	0/10445	0.60	2/14289~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	Е	5	DT	C1'-O4'-C4'	-5.09	105.01	110.10
2	Е	6	DC	O4'-C1'-N1	5.05	111.53	108.00

There are no chirality outliers.

There are no planarity outliers.

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	А	4659	0	4732	21	1
1	D	4645	0	4705	44	1
2	В	223	0	123	2	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
2	Ε	223	0	123	2	0		
3	С	246	0	135	4	0		
3	F	246	0	135	7	0		
4	А	9	0	0	0	0		
4	D	9	0	0	0	0		
5	А	31	0	8	0	0		
5	D	31	0	9	1	0		
6	А	1	0	0	0	0		
6	D	1	0	0	0	0		
7	А	35	0	0	0	0		
7	С	5	0	0	1	0		
7	D	10	0	0	0	0		
7	Ε	5	0	0	0	0		
8	А	190	0	0	4	0		
8	В	16	0	0	0	0		
8	С	25	0	0	0	0		
8	D	74	0	0	1	0		
8	Е	11	0	0	1	0		
8	F	17	0	0	0	0		
All	All	10712	0	9970	74	1		

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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 4.

The worst 5 of 74 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:814:ARG:HG2	1:A:847:LEU:HD11	1.50	0.93
1:D:653:ASP:HB2	1:D:831:GLU:HG2	1.52	0.89
1:A:876:LYS:NZ	8:A:1001:HOH:O	2.07	0.86
1:D:596:ARG:NH2	8:D:1001:HOH:O	2.05	0.79
1:D:779:ARG:HA	1:D:779:ARG:NH1	2.09	0.67

All (1) 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:859:ARG:O	1:D:779:ARG:NH2[4_445]	2.12	0.08



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	Perce	Percentiles	
1	А	580/579~(100%)	569~(98%)	10 (2%)	1 (0%)	47	44	
1	D	577/579~(100%)	558~(97%)	16 (3%)	3~(0%)	29	23	
All	All	1157/1158~(100%)	1127~(97%)	26~(2%)	4 (0%)	41	37	

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	628	ILE
1	D	779	ARG
1	D	819	ARG
1	А	628	ILE

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	А	498/495~(101%)	483~(97%)	15 (3%)	41 41		
1	D	495/495~(100%)	479 (97%)	16 (3%)	39 38		
All	All	993/990~(100%)	962~(97%)	31 (3%)	40 40		

5 of 31 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	876	LYS
1	D	776	ILE



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Mol	Chain	Res	Type
1	D	420	GLU
1	D	814	ARG
1	D	704	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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).

Mal	Mol Type	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
INIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C42	Е	9[A]	2,3	18,20,21	3.40	8 (44%)	18,28,31	1.06	1 (5%)
2	C42	В	9[A]	2,3	18,20,21	<mark>3.36</mark>	8 (44%)	18,28,31	1.03	1 (5%)
2	C42	В	9[B]	2,3	18,20,21	<mark>3.24</mark>	9 (50%)	18,28,31	0.87	1 (5%)
2	C42	Е	9[B]	2,3	18,20,21	<mark>3.29</mark>	9 (50%)	18,28,31	1.12	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C42	Ε	9[A]	2,3	-	0/7/21/22	0/2/2/2
2	C42	В	9[A]	2,3	-	0/7/21/22	0/2/2/2
2	C42	В	9[B]	2,3	-	0/7/21/22	0/2/2/2
2	C42	Е	9[B]	2,3	-	0/7/21/22	0/2/2/2



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	Е	9[B]	C42	O4'-C1'	7.15	1.58	1.42
2	Е	9[A]	C42	O4'-C1'	7.10	1.58	1.42
2	В	9[A]	C42	O4'-C1'	7.09	1.58	1.42
2	В	9[B]	C42	O4'-C1'	6.98	1.58	1.42
2	Е	9[A]	C42	O4'-C4'	-6.57	1.30	1.45

The worst 5 of 34 bond length outliers are listed below:

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	Е	9[B]	C42	O4'-C1'-N1	2.52	112.36	107.86
2	Е	9[B]	C42	O2-C2-N3	-2.35	118.51	122.33
2	В	9[B]	C42	O2-C2-N3	-2.20	118.76	122.33
2	Е	9[A]	C42	C2'-C1'-N1	-2.17	108.77	113.77
2	В	9[A]	C42	O2-C2-N3	-2.07	118.97	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Ε	9[B]	C42	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	Trune	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DGT	А	902[B]	6	26,33,33	<mark>3.19</mark>	7 (26%)	$32,\!52,\!52$	1.53	6 (18%)
5	DGT	D	902[B]	6	26,33,33	<mark>3.35</mark>	9 (34%)	$32,\!52,\!52$	1.56	6 (18%)
7	SO4	А	910	-	4,4,4	0.19	0	$6,\!6,\!6$	0.12	0
4	DPO	D	901[A]	6	6,8,8	0.74	0	13,13,13	1.16	1 (7%)
7	SO4	А	907	-	4,4,4	0.15	0	$6,\!6,\!6$	0.09	0
7	SO4	А	909	-	4,4,4	0.19	0	6,6,6	0.12	0
7	SO4	Е	101	-	4,4,4	0.19	0	$6,\!6,\!6$	0.22	0
4	DPO	А	901[A]	6	$6,\!8,\!8$	0.75	0	$13,\!13,\!13$	1.01	1 (7%)
7	SO4	А	908	-	4,4,4	0.19	0	$6,\!6,\!6$	0.12	0
7	SO4	С	101	-	$4,\!4,\!4$	0.19	0	$6,\!6,\!6$	0.14	0
7	SO4	D	904	-	4,4,4	0.21	0	$6,\!6,\!6$	0.23	0
7	SO4	А	906	-	4,4,4	0.18	0	$6,\!6,\!6$	0.13	0
7	SO4	А	904	-	4,4,4	0.19	0	$6,\!6,\!6$	0.27	0
7	SO4	А	905	-	4,4,4	0.12	0	$6,\!6,\!6$	0.56	0
7	SO4	D	905	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.12	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	DGT	А	902[B]	6	-	4/18/34/34	0/3/3/3
4	DPO	А	901[A]	6	-	3/6/6/6	-
4	DPO	D	901[A]	6	-	0/6/6/6	-
5	DGT	D	902[B]	6	-	4/18/34/34	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
5	А	902[B]	DGT	O6-C6	8.52	1.40	1.23
5	D	902[B]	DGT	O6-C6	8.04	1.39	1.23
5	D	902[B]	DGT	O4'-C1'	7.83	1.59	1.42
5	D	902[B]	DGT	O4'-C4'	-7.30	1.28	1.45
5	А	902[B]	DGT	O4'-C1'	7.22	1.58	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	D	902[B]	DGT	C2'-C1'-N9	-4.39	104.16	114.27



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	D	902[B]	DGT	C5-C6-N1	3.49	120.12	113.95
5	А	902[B]	DGT	C2'-C1'-N9	-3.28	106.70	114.27
4	D	901[A]	DPO	P2-O4-P1	-3.01	122.49	132.83
5	А	902[B]	DGT	C5-C6-N1	2.95	119.15	113.95

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There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	901[A]	DPO	P2-O4-P1-O2
5	А	902[B]	DGT	PB-O3B-PG-O2G
5	D	902[B]	DGT	PB-O3B-PG-O2G
4	А	901[A]	DPO	P2-O4-P1-O3
5	А	902[B]	DGT	PB-O3B-PG-O3G

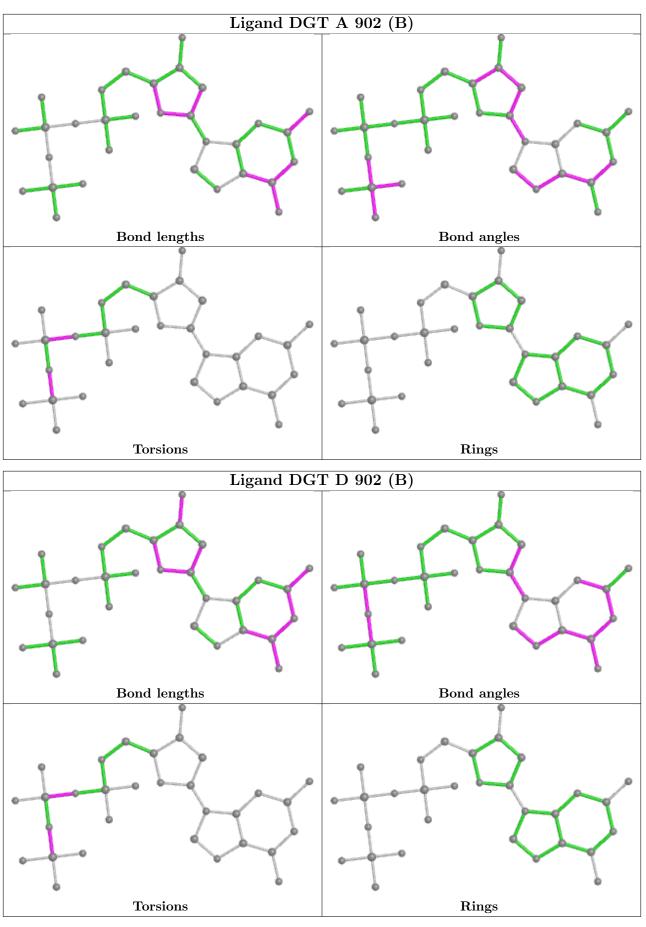
There are no ring outliers.

2 monomers are involved in 2 short contacts:

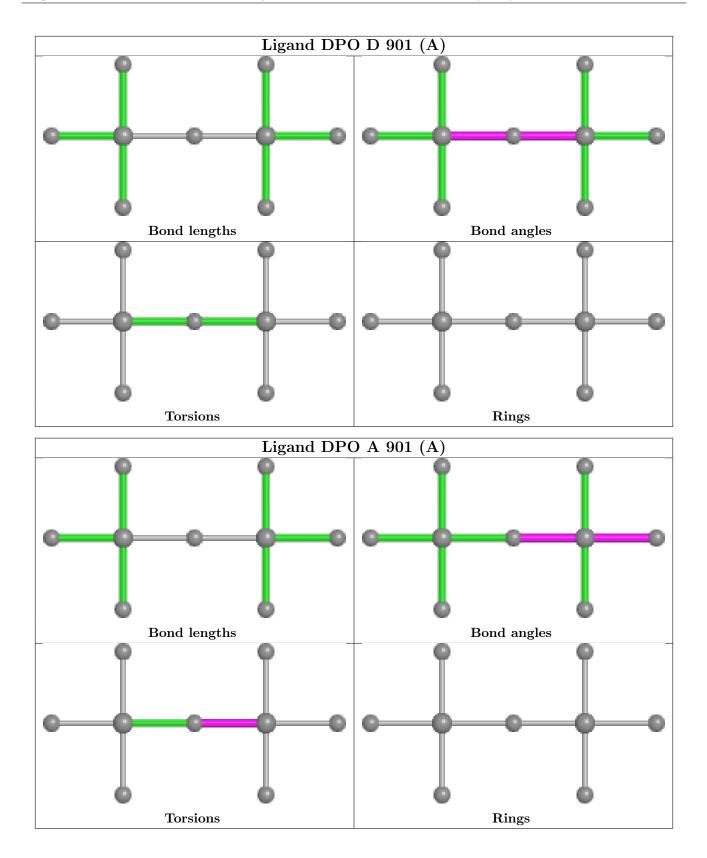
	Mol	Chain	Res	Type	Clashes	Symm-Clashes
Γ	5	D	902[B]	DGT	1	0
	7	С	101	SO4	1	0

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









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, 95^{th} 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	$OWAB(A^2)$	Q<0.9
1	А	579/579~(100%)	-0.03	4 (0%) 87 87	8, 21, 46, 60	0
1	D	579/579~(100%)	0.28	32 (5%) 25 24	18, 38, 61, 74	0
2	В	9/10~(90%)	-0.37	0 100 100	14, 21, 38, 42	1 (11%)
2	Е	9/10 (90%)	-0.40	0 100 100	23, 26, 40, 42	1 (11%)
3	С	13/13~(100%)	-0.17	1 (7%) 13 12	12, 19, 51, 75	0
3	F	13/13~(100%)	-0.09	1 (7%) 13 12	18, 26, 67, 70	0
All	All	1202/1204~(99%)	0.11	38 (3%) 47 46	8, 30, 57, 75	2 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	819	ARG	4.4
1	D	299	MET	3.8
1	D	779	ARG	3.8
1	D	876	LYS	3.7
1	D	300	ALA	3.5

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	C42	Е	9[A]	19/20	0.93	0.14	23,26,32,33	19
2	C42	Е	9[B]	19/20	0.93	0.14	21,26,32,33	0
2	C42	В	9[A]	19/20	0.97	0.15	12,14,22,22	19
2	C42	В	9[B]	19/20	0.97	0.15	12,14,23,23	19



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

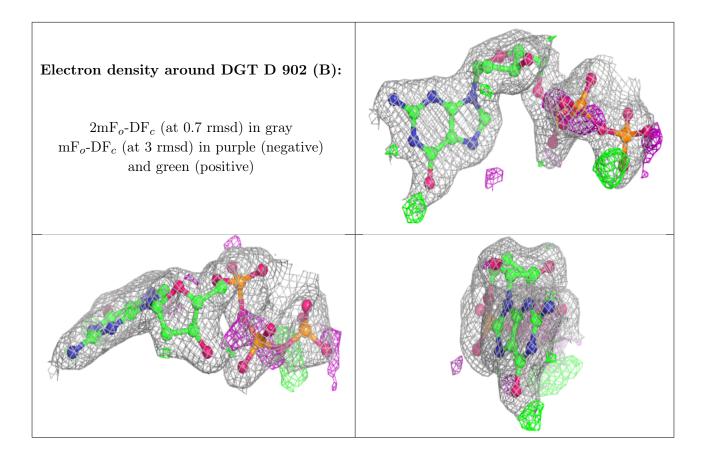
6.4 Ligands (i)

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^{th} 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.

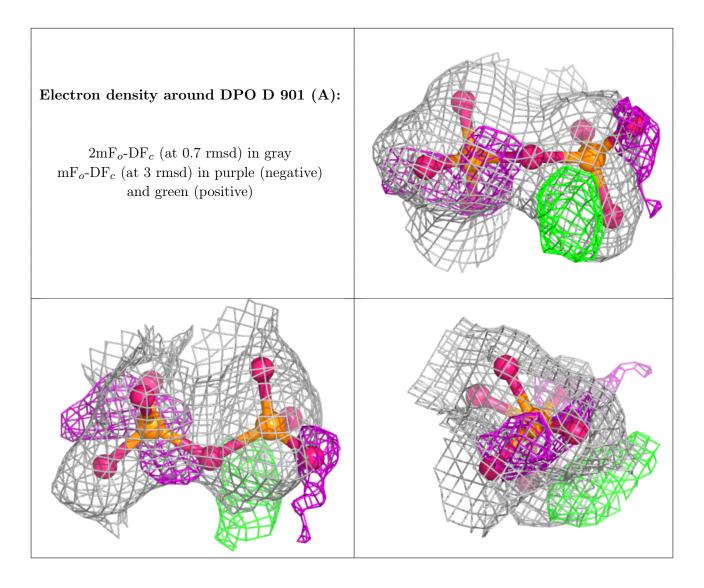
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	С	101	5/5	0.42	0.36	$56,\!57,\!68,\!92$	0
7	SO4	D	904	5/5	0.66	0.28	54,57,68,89	0
7	SO4	А	907	5/5	0.70	0.37	69,70,80,97	0
7	SO4	А	908	5/5	0.72	0.41	34,48,80,85	0
7	SO4	А	904	5/5	0.78	0.21	39,43,52,77	0
7	SO4	А	909	5/5	0.78	0.42	57,65,70,87	0
7	SO4	Е	101	5/5	0.82	0.27	53,55,70,81	0
7	SO4	А	910	5/5	0.84	0.19	47,48,72,75	0
7	SO4	D	905	5/5	0.92	0.24	54,59,66,79	0
7	SO4	А	906	5/5	0.93	0.34	53,57,64,74	0
5	DGT	D	902[B]	31/31	0.95	0.12	20,27,35,39	0
4	DPO	D	901[A]	9/9	0.96	0.14	$28,\!32,\!36,\!37$	9
7	SO4	А	905	5/5	0.97	0.13	$28,\!33,\!50,\!52$	0
5	DGT	А	902[B]	31/31	0.98	0.13	11,14,20,21	31
6	CA	D	903	1/1	0.99	0.06	32,32,32,32	0
4	DPO	А	901[A]	9/9	0.99	0.12	$16,\!18,\!20,\!20$	9
6	CA	А	903	1/1	0.99	0.09	$19,\!19,\!19,\!19$	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.

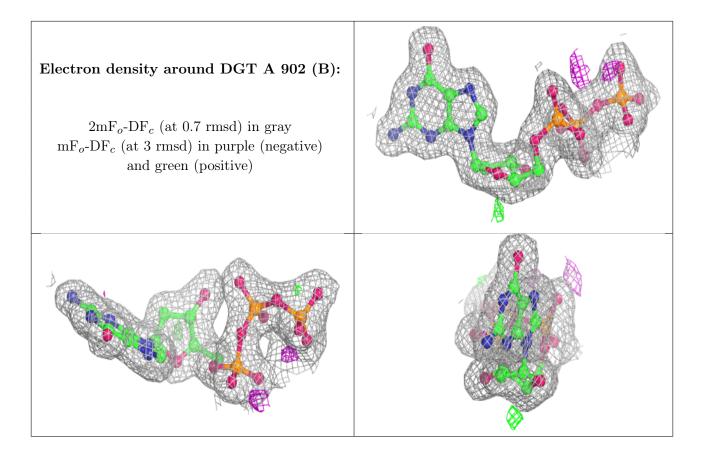




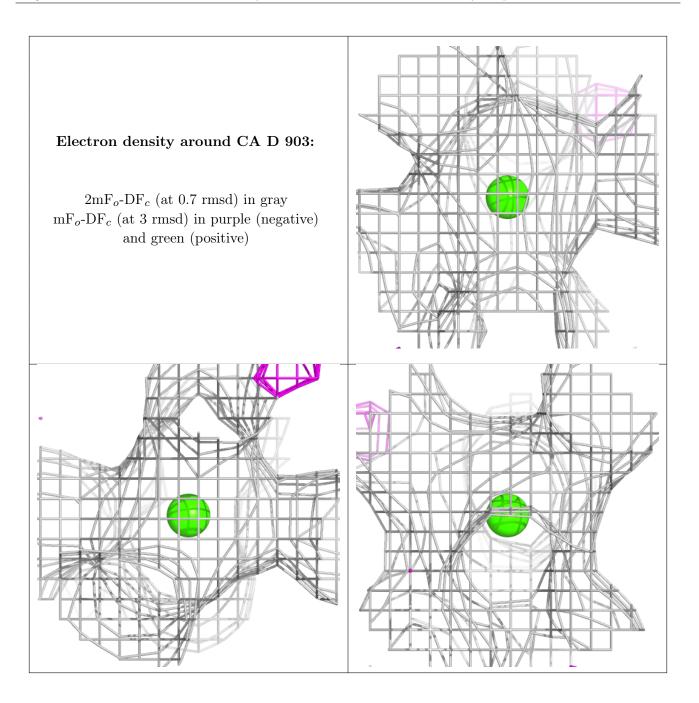




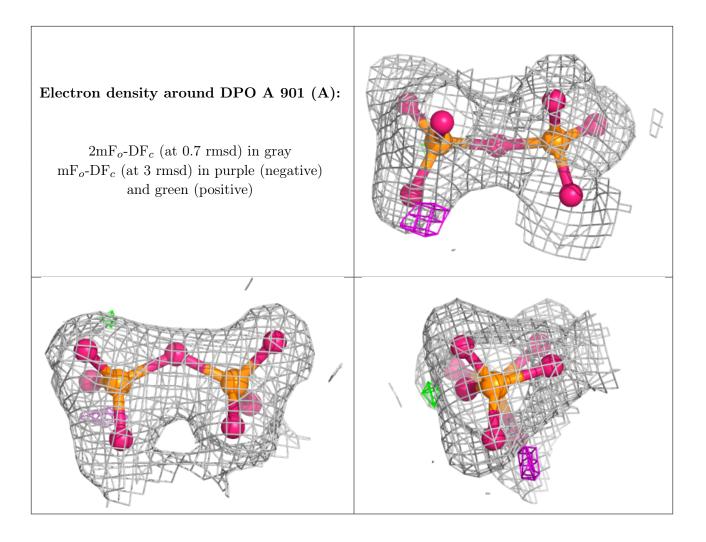




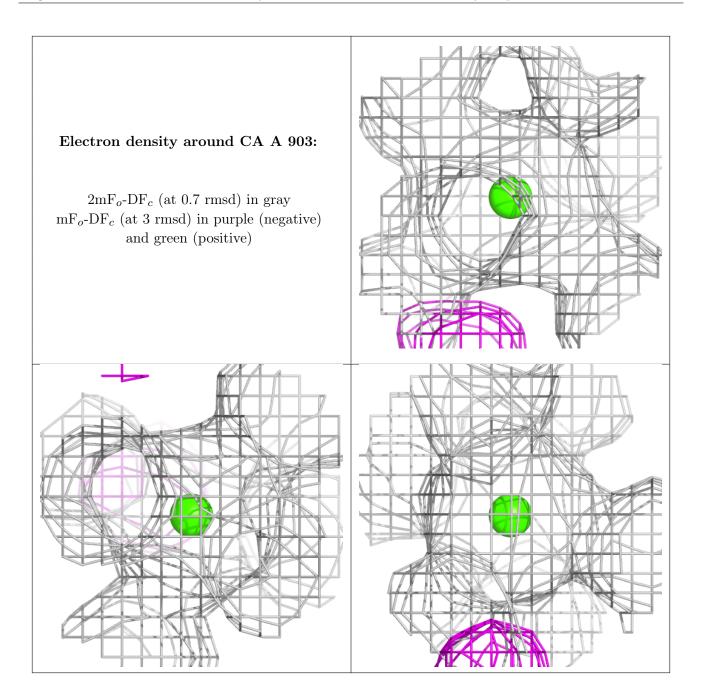












6.5 Other polymers (i)

There are no such residues in this entry.

