WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 27, 2022 – 10:24 pm BST

PDB ID	:	7A9G
Title	:	Truncated 1-deoxy-D-xylulose 5-phosphate synthase (DXS) from Mycobacterium tuberculosis with intermediate 2-acetyl-thiamine diphosphate
Authors	:	Gierse, R.M.; Reddem, E.; Grooves, M.R.
Deposited on	:	2020-09-02
Resolution	:	1.90 Å(reported)

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

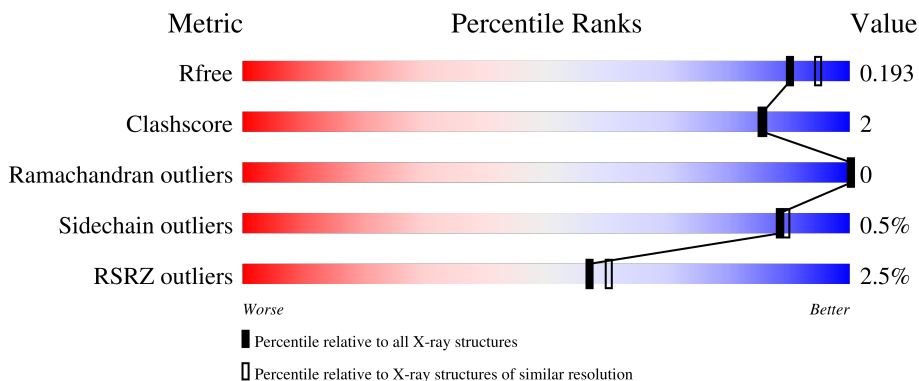|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.90 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	Percentile Ranks	Value
Rfree		0.193
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		2.5%

Worse   *Better*

∎ Percentile relative to all X-ray structures
⊓ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	AAA	666	2% — 77% / 5% / 18%
1	BBB	666	2% — 76% / • / 19%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 17181 atoms, of which 8414 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 1-deoxy-D-xylulose-5-phosphate synthase,1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	549	Total	C	H	N	O	S	163	1	0
			8197	2574	4097	748	761	17			
1	BBB	537	Total	C	H	N	O	S	159	3	0
			8110	2543	4063	746	743	15			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP P9WNS3
AAA	2	LYS	-	expression tag	UNP P9WNS3
AAA	3	HIS	-	expression tag	UNP P9WNS3
AAA	4	HIS	-	expression tag	UNP P9WNS3
AAA	5	HIS	-	expression tag	UNP P9WNS3
AAA	6	HIS	-	expression tag	UNP P9WNS3
AAA	7	HIS	-	expression tag	UNP P9WNS3
AAA	8	HIS	-	expression tag	UNP P9WNS3
AAA	9	PRO	-	expression tag	UNP P9WNS3
AAA	10	MET	-	expression tag	UNP P9WNS3
AAA	11	SER	-	expression tag	UNP P9WNS3
AAA	12	ASP	-	expression tag	UNP P9WNS3
AAA	13	TYR	-	expression tag	UNP P9WNS3
AAA	14	ASP	-	expression tag	UNP P9WNS3
AAA	15	ILE	-	expression tag	UNP P9WNS3
AAA	16	PRO	-	expression tag	UNP P9WNS3
AAA	17	THR	-	expression tag	UNP P9WNS3
AAA	18	THR	-	expression tag	UNP P9WNS3
AAA	19	GLU	-	expression tag	UNP P9WNS3
AAA	20	ASN	-	expression tag	UNP P9WNS3
AAA	21	LEU	-	expression tag	UNP P9WNS3
AAA	22	TYR	-	expression tag	UNP P9WNS3
AAA	23	PHE	-	expression tag	UNP P9WNS3
AAA	24	GLN	-	expression tag	UNP P9WNS3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	25	GLY	-	expression tag	UNP P9WNS3
AAA	26	ALA	-	expression tag	UNP P9WNS3
AAA	27	MET	-	expression tag	UNP P9WNS3
AAA	28	GLY	-	expression tag	UNP P9WNS3
AAA	204C	GLY	-	linker	UNP P9WNS3
AAA	204D	GLY	-	linker	UNP P9WNS3
AAA	204E	GLY	-	linker	UNP P9WNS3
AAA	204F	GLY	-	linker	UNP P9WNS3
AAA	223	GLY	-	linker	UNP P9WNS3
AAA	224	GLY	-	linker	UNP P9WNS3
BBB	1	MET	-	initiating methionine	UNP P9WNS3
BBB	2	LYS	-	expression tag	UNP P9WNS3
BBB	3	HIS	-	expression tag	UNP P9WNS3
BBB	4	HIS	-	expression tag	UNP P9WNS3
BBB	5	HIS	-	expression tag	UNP P9WNS3
BBB	6	HIS	-	expression tag	UNP P9WNS3
BBB	7	HIS	-	expression tag	UNP P9WNS3
BBB	8	HIS	-	expression tag	UNP P9WNS3
BBB	9	PRO	-	expression tag	UNP P9WNS3
BBB	10	MET	-	expression tag	UNP P9WNS3
BBB	11	SER	-	expression tag	UNP P9WNS3
BBB	12	ASP	-	expression tag	UNP P9WNS3
BBB	13	TYR	-	expression tag	UNP P9WNS3
BBB	14	ASP	-	expression tag	UNP P9WNS3
BBB	15	ILE	-	expression tag	UNP P9WNS3
BBB	16	PRO	-	expression tag	UNP P9WNS3
BBB	17	THR	-	expression tag	UNP P9WNS3
BBB	18	THR	-	expression tag	UNP P9WNS3
BBB	19	GLU	-	expression tag	UNP P9WNS3
BBB	20	ASN	-	expression tag	UNP P9WNS3
BBB	21	LEU	-	expression tag	UNP P9WNS3
BBB	22	TYR	-	expression tag	UNP P9WNS3
BBB	23	PHE	-	expression tag	UNP P9WNS3
BBB	24	GLN	-	expression tag	UNP P9WNS3
BBB	25	GLY	-	expression tag	UNP P9WNS3
BBB	26	ALA	-	expression tag	UNP P9WNS3
BBB	27	MET	-	expression tag	UNP P9WNS3
BBB	28	GLY	-	expression tag	UNP P9WNS3
BBB	205B	GLY	-	linker	UNP P9WNS3
BBB	205C	GLY	-	linker	UNP P9WNS3
BBB	205D	GLY	-	linker	UNP P9WNS3
BBB	205E	GLY	-	linker	UNP P9WNS3

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	223	GLY	-	linker	UNP P9WNS3
BBB	224	GLY	-	linker	UNP P9WNS3

- Molecule 2 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$) (labeled as "Ligand of Interest" by depositor).
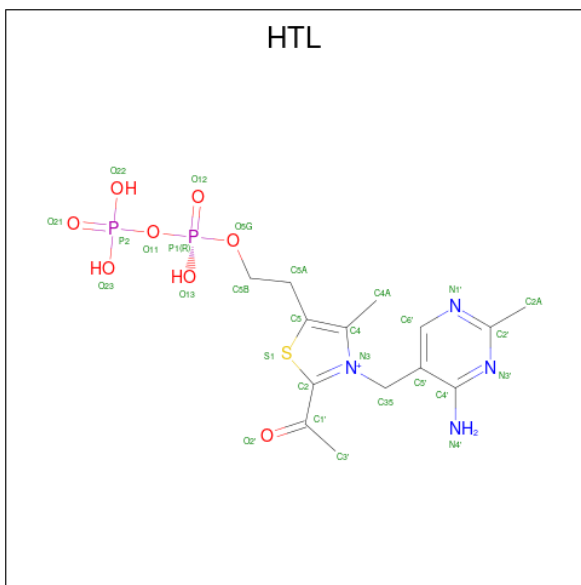
HTL

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	P	S	2	0
			47	14	18	4	8	2	1		
2	BBB	1	Total	C	H	N	O	P	S	2	0
			47	14	18	4	8	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Mg	0	0
			1	1		
3	BBB	1	Total	Mg	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

C4

OH O4

O2

O

C3

C1

HO

C2

O1

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
4	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
4	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
4	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
4	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
4	BBB	1	Total	C	H	O	1	0
			17	4	10	3		
4	BBB	1	Total	C	H	O	1	0
			17	4	10	3		
4	BBB	1	Total	C	H	O	1	0
			17	4	10	3		
4	BBB	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE

O4
OH

C5

C6

C4

O2

O

O3

C1

C3

C2

HO

O1

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			24	6	14	4		
5	AAA	1	Total	C	H	O	1	0
			24	6	14	4		
5	AAA	1	Total	C	H	O	1	0
			24	6	14	4		
5	BBB	1	Total	C	H	O	1	0
			24	6	14	4		
5	BBB	1	Total	C	H	O	1	0
			24	6	14	4		
5	BBB	1	Total	C	H	O	1	0
			24	6	14	4		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4

```
                              C8   OH O5
                         O4
                         O    C7
                    C5
                         C6
              C4
         O2   O    O3
         O    C3
    C1
    HO   C2
    O1
```

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total 31	C 8	H 18	O 5	1	0
6	BBB	1	Total 31	C 8	H 18	O 5	1	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

```
              C3
              OH O3

    C1   C2

    HO   OH
    O1   O2
```
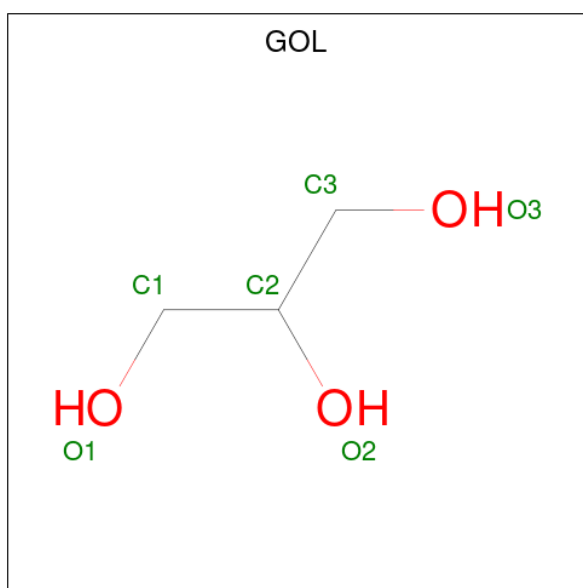
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	AAA	1	Total 14	C 3	H 8	O 3	2	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O^-

$O2$ O^- — P $=$ O O1

P

O^-

O4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	BBB	1	Total 5	O 4	P 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	211	Total 211	O 211	0	0
9	BBB	189	Total 189	O 189	0	0

W O R L D W I D E

PDB

PROTEIN DATA BANK

3 Residue-property plots ⓘ

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

• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase,1-deoxy-D-xylulose-5-phosphate synthase
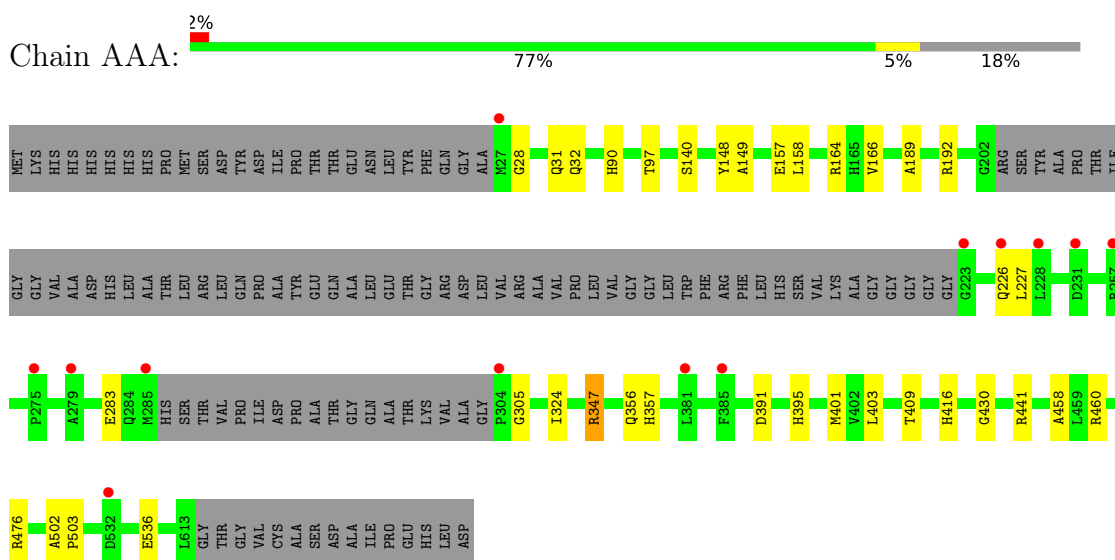
• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase,1-deoxy-D-xylulose-5-phosphate synthase
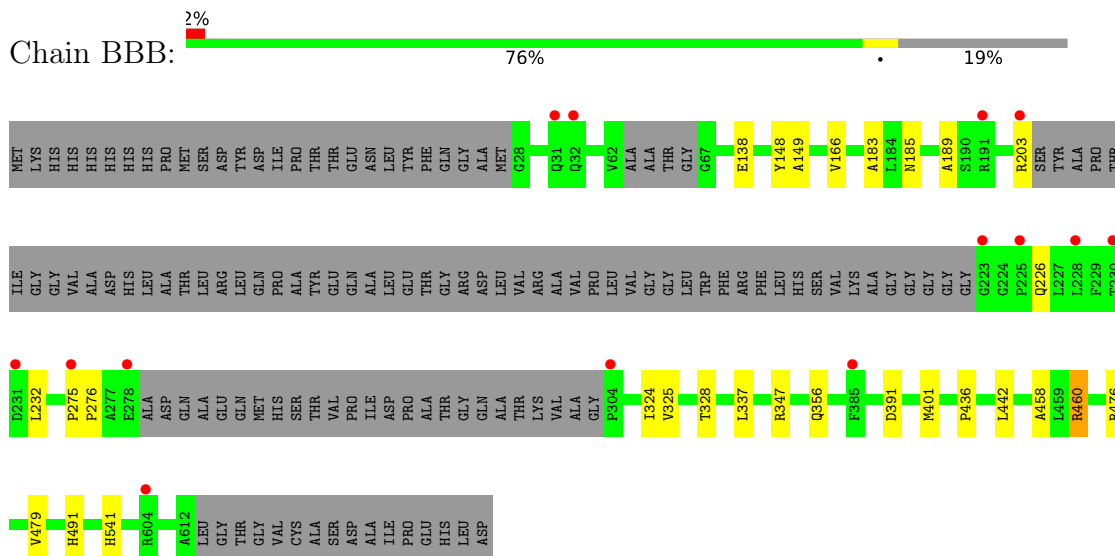
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.87Å 126.17Å 79.03Å 90.00° 106.28° 90.00°	Depositor
Resolution (Å)	48.55 – 1.90 48.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.55-1.90) 99.4 (48.50-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.154 , 0.190 0.166 , 0.193	Depositor DCC
R_{free} test set	971 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17181	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PGE, PO4, PEG, PG4, HTL, GOL, MG

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	AAA	0.69	0/4184	0.81	1/5682 (0.0%)
1	BBB	0.70	0/4136	0.81	0/5615
All	All	0.70	0/8320	0.81	1/11297 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	347	ARG	NE-CZ-NH1	5.38	122.99	120.30

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	AAA	4100	4097	4064	27	0
1	BBB	4047	4063	4035	20	0
2	AAA	29	18	18	1	0
2	BBB	29	18	18	1	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	35	50	50	0	0
4	BBB	28	40	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	30	42	42	0	0
5	BBB	30	42	42	0	0
6	AAA	13	18	18	0	0
6	BBB	13	18	18	0	0
7	AAA	6	8	8	1	0
8	BBB	5	0	0	0	0
9	AAA	211	0	0	1	0
9	BBB	189	0	0	0	0
All	All	8767	8414	8353	37	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 2.

The worst 5 of 37 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:AAA:395:HIS:HE1	1:BBB:138:GLU:H	1.22	0.85
1:AAA:189:ALA:HB2	1:BBB:226:GLN:HG3	1.77	0.64
1:AAA:395:HIS:CE1	1:BBB:138:GLU:H	2.10	0.63
1:AAA:226:GLN:HG3	1:BBB:189:ALA:HB2	1.81	0.62
1:AAA:430:GLY:HA3	7:AAA:712:GOL:H2	1.85	0.57

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	544/666 (82%)	533 (98%)	11 (2%)	0	100	100
1	BBB	532/666 (80%)	520 (98%)	12 (2%)	0	100	100
All	All	1076/1332 (81%)	1053 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	415/508 (82%)	413 (100%)	2 (0%)	88	89
1	BBB	412/508 (81%)	410 (100%)	2 (0%)	88	89
All	All	827/1016 (81%)	823 (100%)	4 (0%)	88	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	441	ARG
1	AAA	460	ARG
1	BBB	203	ARG
1	BBB	460	ARG

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

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	#$|Z| > 2$
4	PEG	BBB	705	-	6,6,6	0.19	0	5,5,5	0.09	0
6	PG4	BBB	706	-	12,12,12	0.21	0	11,11,11	0.18	0
6	PG4	AAA	711	-	12,12,12	0.24	0	11,11,11	0.23	0
5	PGE	AAA	707	-	9,9,9	0.21	0	8,8,8	0.12	0
5	PGE	AAA	709	-	9,9,9	0.27	0	8,8,8	0.15	0
4	PEG	AAA	703	-	6,6,6	0.12	0	5,5,5	0.12	0
4	PEG	BBB	711	-	6,6,6	0.18	0	5,5,5	0.27	0
4	PEG	AAA	704	-	6,6,6	0.21	0	5,5,5	0.15	0
5	PGE	BBB	710	-	9,9,9	0.20	0	8,8,8	0.16	0
2	HTL	BBB	701	3	23,30,30	0.81	1 (4%)	31,45,45	2.00	3 (9%)
4	PEG	BBB	708	-	6,6,6	0.30	0	5,5,5	0.17	0
5	PGE	BBB	704	-	9,9,9	0.11	0	8,8,8	0.21	0
7	GOL	AAA	712	-	5,5,5	0.14	0	5,5,5	0.62	0
5	PGE	AAA	710	-	9,9,9	0.17	0	8,8,8	0.37	0
5	PGE	BBB	709	-	9,9,9	0.17	0	8,8,8	0.11	0
2	HTL	AAA	701	3	23,30,30	0.78	0	31,45,45	1.76	2 (6%)
4	PEG	AAA	708	-	6,6,6	0.15	0	5,5,5	0.11	0
4	PEG	AAA	705	-	6,6,6	0.25	0	5,5,5	0.19	0
8	PO4	BBB	703	-	4,4,4	0.68	0	6,6,6	0.45	0
4	PEG	AAA	706	-	6,6,6	0.21	0	5,5,5	0.19	0
4	PEG	BBB	707	-	6,6,6	0.17	0	5,5,5	0.27	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
4	PEG	BBB	705	-	-	3/4/4/4	-
6	PG4	BBB	706	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	AAA	711	-	-	5/10/10/10	-
5	PGE	AAA	707	-	-	2/7/7/7	-
5	PGE	AAA	709	-	-	2/7/7/7	-
4	PEG	AAA	703	-	-	3/4/4/4	-
4	PEG	BBB	711	-	-	3/4/4/4	-
4	PEG	AAA	704	-	-	2/4/4/4	-
5	PGE	BBB	710	-	-	4/7/7/7	-
2	HTL	BBB	701	3	-	3/16/21/21	0/2/2/2
4	PEG	BBB	708	-	-	2/4/4/4	-
5	PGE	BBB	704	-	-	2/7/7/7	-
7	GOL	AAA	712	-	-	3/4/4/4	-
5	PGE	AAA	710	-	-	2/7/7/7	-
5	PGE	BBB	709	-	-	6/7/7/7	-
2	HTL	AAA	701	3	-	2/16/21/21	0/2/2/2
4	PEG	AAA	708	-	-	3/4/4/4	-
4	PEG	AAA	705	-	-	4/4/4/4	-
4	PEG	AAA	706	-	-	3/4/4/4	-
4	PEG	BBB	707	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	701	HTL	C5A-C5	-2.81	1.49	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	701	HTL	C4-N3-C2	9.51	113.93	108.64
2	AAA	701	HTL	C4-N3-C2	8.05	113.11	108.64
2	BBB	701	HTL	O2'-C1'-C3'	-3.22	112.93	120.17
2	AAA	701	HTL	C5-C4-N3	2.10	112.05	107.66
2	BBB	701	HTL	C5-C4-N3	2.06	111.97	107.66

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	701	HTL	P1-O11-P2-O23

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Mol	Chain	Res	Type	Atoms
2	BBB	701	HTL	C4-C5-C5A-C5B
2	BBB	701	HTL	P1-O11-P2-O22
6	AAA	711	PG4	O4-C7-C8-O5
5	BBB	710	PGE	O2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	701	HTL	1	0
7	AAA	712	GOL	1	0
2	AAA	701	HTL	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.

Ligand HTL BBB 701

Bond lengths

Bond angles

Torsions

Rings

Ligand HTL AAA 701

Bond lengths

Bond angles

Torsions

Rings
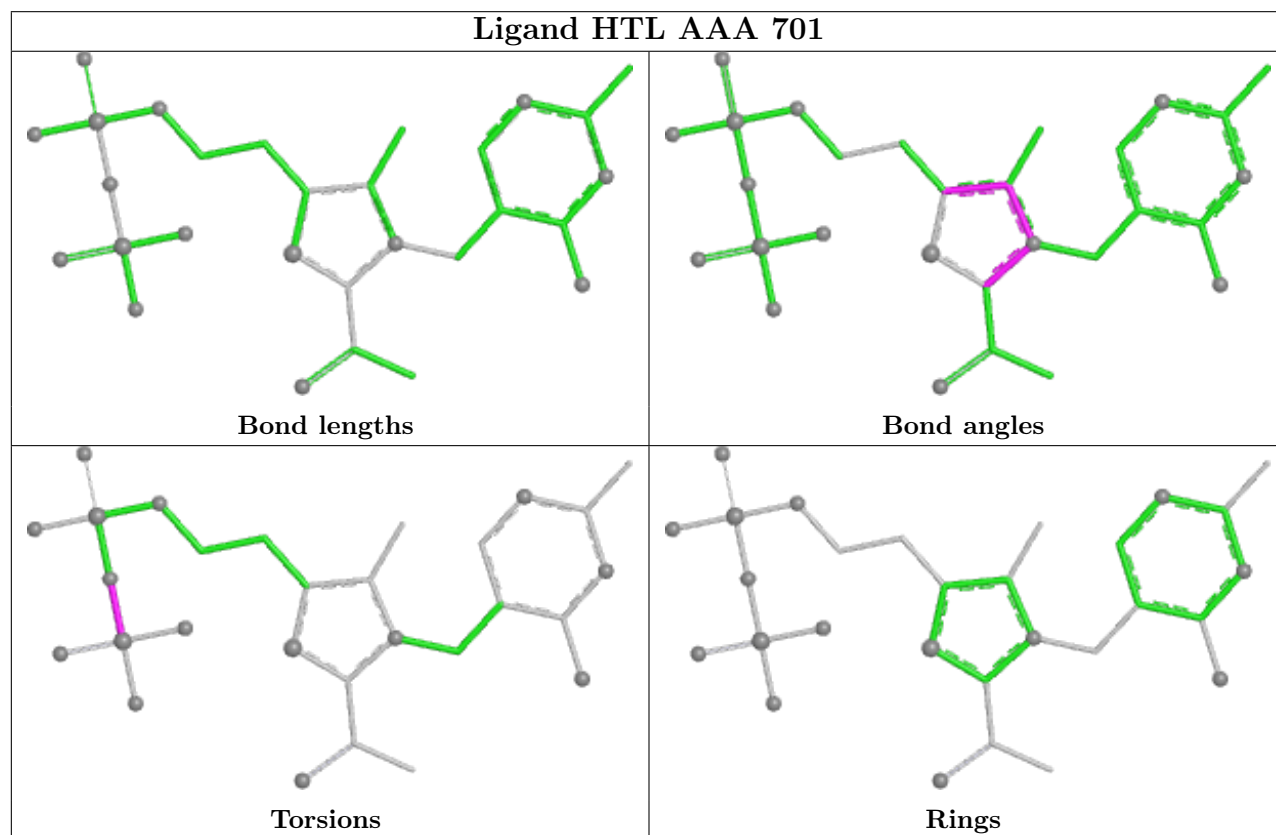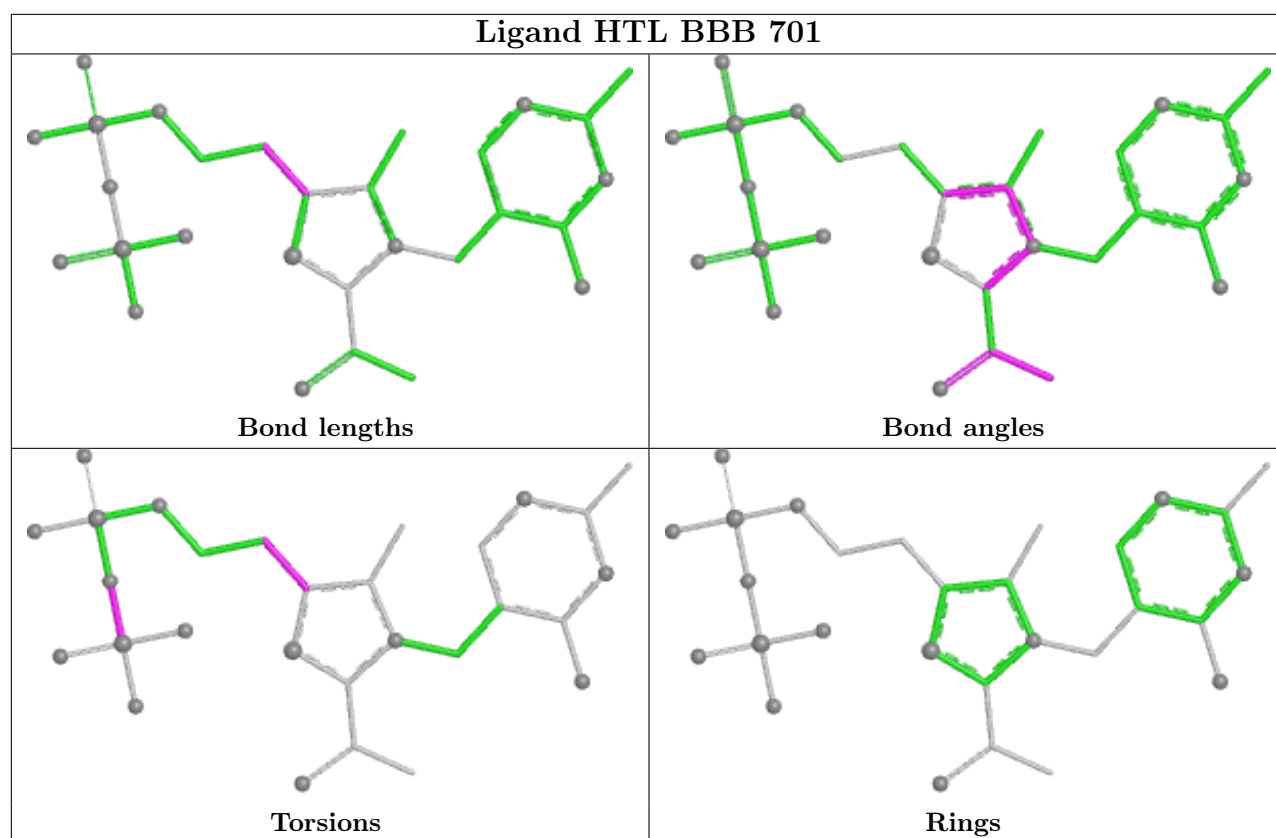
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	AAA	549/666 (82%)	-0.22	13 (2%)	59	62	14, 20, 40, 56	0
1	BBB	537/666 (80%)	-0.16	14 (2%)	56	58	15, 21, 39, 63	0
All	All	1086/1332 (81%)	-0.19	27 (2%)	57	60	14, 21, 40, 63	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	228	LEU	4.7
1	BBB	223	GLY	4.2
1	BBB	231	ASP	4.1
1	BBB	203	ARG	4.0
1	AAA	279	ALA	3.6

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 monosaccharides 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.

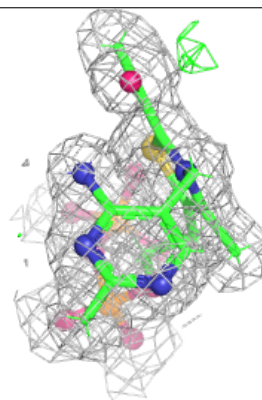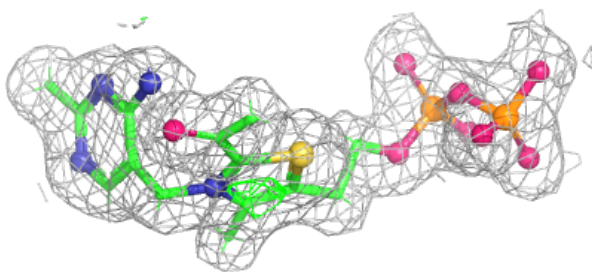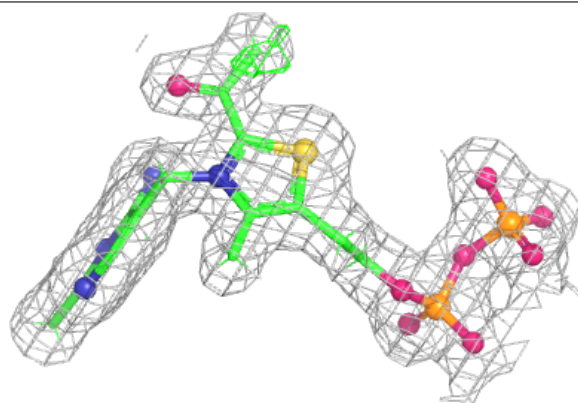| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	BBB	710	10/10	0.75	0.21	51,63,63,65	1
6	PG4	AAA	711	13/13	0.75	0.24	50,57,61,63	1
5	PGE	AAA	709	10/10	0.77	0.17	38,46,52,52	1
4	PEG	BBB	705	7/7	0.80	0.18	47,54,60,60	1
4	PEG	AAA	708	7/7	0.80	0.21	51,55,64,64	1
4	PEG	AAA	705	7/7	0.82	0.11	47,48,51,51	1
7	GOL	AAA	712	6/6	0.82	0.23	37,39,41,41	2
4	PEG	AAA	704	7/7	0.83	0.13	41,44,46,46	1
4	PEG	AAA	703	7/7	0.85	0.12	48,53,61,61	1
4	PEG	BBB	707	7/7	0.85	0.20	34,41,52,52	1
5	PGE	AAA	707	10/10	0.90	0.14	37,40,45,46	1
4	PEG	BBB	711	7/7	0.90	0.13	39,41,46,46	1
6	PG4	BBB	706	13/13	0.90	0.15	27,31,44,51	1
5	PGE	BBB	709	10/10	0.90	0.14	41,44,51,51	1
5	PGE	BBB	704	10/10	0.92	0.15	43,49,56,62	1
4	PEG	AAA	706	7/7	0.92	0.11	35,38,47,47	1
8	PO4	BBB	703	5/5	0.92	0.12	38,44,49,54	0
4	PEG	BBB	708	7/7	0.95	0.12	46,49,57,57	1
5	PGE	AAA	710	10/10	0.96	0.09	26,28,36,44	1
2	HTL	BBB	701	29/29	0.97	0.11	16,20,37,37	2
2	HTL	AAA	701	29/29	0.98	0.09	14,17,25,26	2
3	MG	BBB	702	1/1	0.99	0.07	18,18,18,18	0
3	MG	AAA	702	1/1	0.99	0.09	17,17,17,17	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 HTL BBB 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
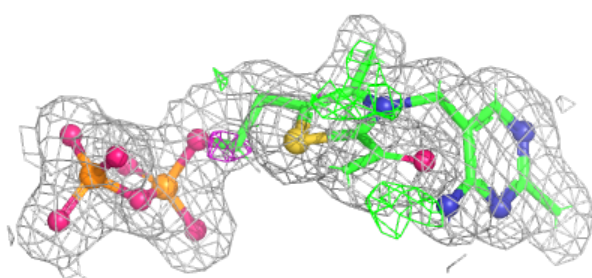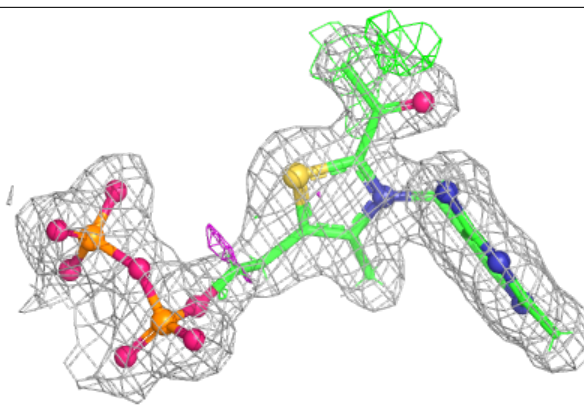
Electron density around HTL AAA 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.