



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:27 PM UTC

PDB ID : 4UOR / pdb_00004uor
Title : Structure of lipoteichoic acid synthase LtaS from *Listeria monocytogenes* in complex with glycerol phosphate
Authors : Campeotto, I.; Freemont, P.; Grundling, A.
Deposited on : 2014-06-09
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

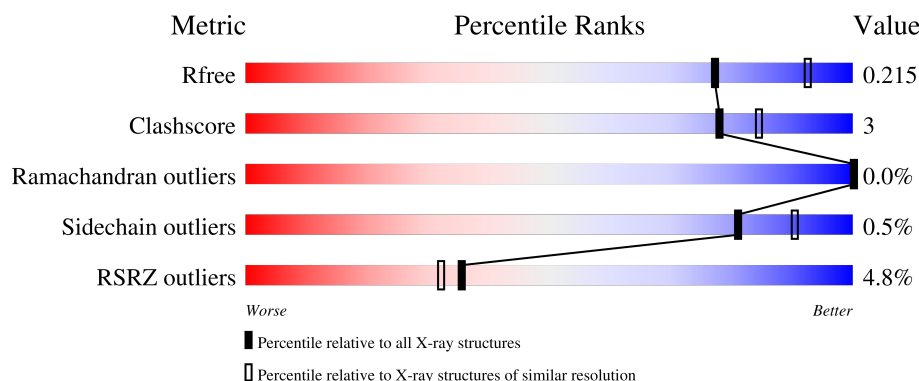
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	A	459	0% 86% 5% 9%
1	B	459	2% 85% 6% 9%
1	C	459	0% 86% 5% 9%
1	D	459	2% 86% • 9%
1	E	459	2% 84% 6% 9%

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Mol	Chain	Length	Quality of chain
1	F	459	2% 82% 9% 9%
1	G	459	2% 86% 5% 9%
1	H	459	3% 87% • 9%
1	I	459	2% 86% 5% 9%
1	J	459	4% 83% 8% 9%
1	K	459	28% 73% 15% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40238 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 LIPOTEICHOIC ACID SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	P	S	0	2	0
			3380	2158	537	676	1	8			
1	B	418	Total	C	N	O	P	S	0	2	0
			3380	2158	537	676	1	8			
1	C	417	Total	C	N	O	P	S	0	2	0
			3374	2155	536	674	1	8			
1	D	417	Total	C	N	O	P	S	0	2	0
			3374	2155	536	674	1	8			
1	E	418	Total	C	N	O	P	S	0	2	0
			3380	2158	537	676	1	8			
1	F	417	Total	C	N	O	P	S	0	2	0
			3374	2155	536	674	1	8			
1	G	418	Total	C	N	O	P	S	0	3	0
			3386	2161	538	678	1	8			
1	H	418	Total	C	N	O	P	S	0	2	0
			3380	2158	537	676	1	8			
1	I	418	Total	C	N	O	P	S	0	2	0
			3380	2158	537	676	1	8			
1	J	417	Total	C	N	O	P	S	0	0	0
			3359	2146	533	671	1	8			
1	K	415	Total	C	N	O	P	S	0	1	0
			3353	2143	532	669	1	8			

There are 341 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	MET	-	expression tag	UNP Q8Y8H6
A	196	SER	-	expression tag	UNP Q8Y8H6
A	197	TYR	-	expression tag	UNP Q8Y8H6
A	198	TYR	-	expression tag	UNP Q8Y8H6
A	199	HIS	-	expression tag	UNP Q8Y8H6
A	200	HIS	-	expression tag	UNP Q8Y8H6
A	201	HIS	-	expression tag	UNP Q8Y8H6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	202	HIS	-	expression tag	UNP Q8Y8H6
A	203	HIS	-	expression tag	UNP Q8Y8H6
A	204	HIS	-	expression tag	UNP Q8Y8H6
A	205	ASP	-	expression tag	UNP Q8Y8H6
A	206	TYR	-	expression tag	UNP Q8Y8H6
A	207	ASP	-	expression tag	UNP Q8Y8H6
A	208	ILE	-	expression tag	UNP Q8Y8H6
A	209	PRO	-	expression tag	UNP Q8Y8H6
A	210	THR	-	expression tag	UNP Q8Y8H6
A	211	THR	-	expression tag	UNP Q8Y8H6
A	212	GLU	-	expression tag	UNP Q8Y8H6
A	213	ASN	-	expression tag	UNP Q8Y8H6
A	214	LEU	-	expression tag	UNP Q8Y8H6
A	215	TYR	-	expression tag	UNP Q8Y8H6
A	216	PHE	-	expression tag	UNP Q8Y8H6
A	217	GLN	-	expression tag	UNP Q8Y8H6
A	218	GLY	-	expression tag	UNP Q8Y8H6
A	219	ALA	-	expression tag	UNP Q8Y8H6
A	220	MET	-	expression tag	UNP Q8Y8H6
A	221	GLY	-	expression tag	UNP Q8Y8H6
A	222	SER	-	expression tag	UNP Q8Y8H6
A	223	GLY	-	expression tag	UNP Q8Y8H6
A	224	ILE	-	expression tag	UNP Q8Y8H6
A	225	GLN	-	expression tag	UNP Q8Y8H6
B	195	MET	-	expression tag	UNP Q8Y8H6
B	196	SER	-	expression tag	UNP Q8Y8H6
B	197	TYR	-	expression tag	UNP Q8Y8H6
B	198	TYR	-	expression tag	UNP Q8Y8H6
B	199	HIS	-	expression tag	UNP Q8Y8H6
B	200	HIS	-	expression tag	UNP Q8Y8H6
B	201	HIS	-	expression tag	UNP Q8Y8H6
B	202	HIS	-	expression tag	UNP Q8Y8H6
B	203	HIS	-	expression tag	UNP Q8Y8H6
B	204	HIS	-	expression tag	UNP Q8Y8H6
B	205	ASP	-	expression tag	UNP Q8Y8H6
B	206	TYR	-	expression tag	UNP Q8Y8H6
B	207	ASP	-	expression tag	UNP Q8Y8H6
B	208	ILE	-	expression tag	UNP Q8Y8H6
B	209	PRO	-	expression tag	UNP Q8Y8H6
B	210	THR	-	expression tag	UNP Q8Y8H6
B	211	THR	-	expression tag	UNP Q8Y8H6
B	212	GLU	-	expression tag	UNP Q8Y8H6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	213	ASN	-	expression tag	UNP Q8Y8H6
B	214	LEU	-	expression tag	UNP Q8Y8H6
B	215	TYR	-	expression tag	UNP Q8Y8H6
B	216	PHE	-	expression tag	UNP Q8Y8H6
B	217	GLN	-	expression tag	UNP Q8Y8H6
B	218	GLY	-	expression tag	UNP Q8Y8H6
B	219	ALA	-	expression tag	UNP Q8Y8H6
B	220	MET	-	expression tag	UNP Q8Y8H6
B	221	GLY	-	expression tag	UNP Q8Y8H6
B	222	SER	-	expression tag	UNP Q8Y8H6
B	223	GLY	-	expression tag	UNP Q8Y8H6
B	224	ILE	-	expression tag	UNP Q8Y8H6
B	225	GLN	-	expression tag	UNP Q8Y8H6
C	195	MET	-	expression tag	UNP Q8Y8H6
C	196	SER	-	expression tag	UNP Q8Y8H6
C	197	TYR	-	expression tag	UNP Q8Y8H6
C	198	TYR	-	expression tag	UNP Q8Y8H6
C	199	HIS	-	expression tag	UNP Q8Y8H6
C	200	HIS	-	expression tag	UNP Q8Y8H6
C	201	HIS	-	expression tag	UNP Q8Y8H6
C	202	HIS	-	expression tag	UNP Q8Y8H6
C	203	HIS	-	expression tag	UNP Q8Y8H6
C	204	HIS	-	expression tag	UNP Q8Y8H6
C	205	ASP	-	expression tag	UNP Q8Y8H6
C	206	TYR	-	expression tag	UNP Q8Y8H6
C	207	ASP	-	expression tag	UNP Q8Y8H6
C	208	ILE	-	expression tag	UNP Q8Y8H6
C	209	PRO	-	expression tag	UNP Q8Y8H6
C	210	THR	-	expression tag	UNP Q8Y8H6
C	211	THR	-	expression tag	UNP Q8Y8H6
C	212	GLU	-	expression tag	UNP Q8Y8H6
C	213	ASN	-	expression tag	UNP Q8Y8H6
C	214	LEU	-	expression tag	UNP Q8Y8H6
C	215	TYR	-	expression tag	UNP Q8Y8H6
C	216	PHE	-	expression tag	UNP Q8Y8H6
C	217	GLN	-	expression tag	UNP Q8Y8H6
C	218	GLY	-	expression tag	UNP Q8Y8H6
C	219	ALA	-	expression tag	UNP Q8Y8H6
C	220	MET	-	expression tag	UNP Q8Y8H6
C	221	GLY	-	expression tag	UNP Q8Y8H6
C	222	SER	-	expression tag	UNP Q8Y8H6
C	223	GLY	-	expression tag	UNP Q8Y8H6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	224	ILE	-	expression tag	UNP Q8Y8H6
C	225	GLN	-	expression tag	UNP Q8Y8H6
D	195	MET	-	expression tag	UNP Q8Y8H6
D	196	SER	-	expression tag	UNP Q8Y8H6
D	197	TYR	-	expression tag	UNP Q8Y8H6
D	198	TYR	-	expression tag	UNP Q8Y8H6
D	199	HIS	-	expression tag	UNP Q8Y8H6
D	200	HIS	-	expression tag	UNP Q8Y8H6
D	201	HIS	-	expression tag	UNP Q8Y8H6
D	202	HIS	-	expression tag	UNP Q8Y8H6
D	203	HIS	-	expression tag	UNP Q8Y8H6
D	204	HIS	-	expression tag	UNP Q8Y8H6
D	205	ASP	-	expression tag	UNP Q8Y8H6
D	206	TYR	-	expression tag	UNP Q8Y8H6
D	207	ASP	-	expression tag	UNP Q8Y8H6
D	208	ILE	-	expression tag	UNP Q8Y8H6
D	209	PRO	-	expression tag	UNP Q8Y8H6
D	210	THR	-	expression tag	UNP Q8Y8H6
D	211	THR	-	expression tag	UNP Q8Y8H6
D	212	GLU	-	expression tag	UNP Q8Y8H6
D	213	ASN	-	expression tag	UNP Q8Y8H6
D	214	LEU	-	expression tag	UNP Q8Y8H6
D	215	TYR	-	expression tag	UNP Q8Y8H6
D	216	PHE	-	expression tag	UNP Q8Y8H6
D	217	GLN	-	expression tag	UNP Q8Y8H6
D	218	GLY	-	expression tag	UNP Q8Y8H6
D	219	ALA	-	expression tag	UNP Q8Y8H6
D	220	MET	-	expression tag	UNP Q8Y8H6
D	221	GLY	-	expression tag	UNP Q8Y8H6
D	222	SER	-	expression tag	UNP Q8Y8H6
D	223	GLY	-	expression tag	UNP Q8Y8H6
D	224	ILE	-	expression tag	UNP Q8Y8H6
D	225	GLN	-	expression tag	UNP Q8Y8H6
E	195	MET	-	expression tag	UNP Q8Y8H6
E	196	SER	-	expression tag	UNP Q8Y8H6
E	197	TYR	-	expression tag	UNP Q8Y8H6
E	198	TYR	-	expression tag	UNP Q8Y8H6
E	199	HIS	-	expression tag	UNP Q8Y8H6
E	200	HIS	-	expression tag	UNP Q8Y8H6
E	201	HIS	-	expression tag	UNP Q8Y8H6
E	202	HIS	-	expression tag	UNP Q8Y8H6
E	203	HIS	-	expression tag	UNP Q8Y8H6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	204	HIS	-	expression tag	UNP Q8Y8H6
E	205	ASP	-	expression tag	UNP Q8Y8H6
E	206	TYR	-	expression tag	UNP Q8Y8H6
E	207	ASP	-	expression tag	UNP Q8Y8H6
E	208	ILE	-	expression tag	UNP Q8Y8H6
E	209	PRO	-	expression tag	UNP Q8Y8H6
E	210	THR	-	expression tag	UNP Q8Y8H6
E	211	THR	-	expression tag	UNP Q8Y8H6
E	212	GLU	-	expression tag	UNP Q8Y8H6
E	213	ASN	-	expression tag	UNP Q8Y8H6
E	214	LEU	-	expression tag	UNP Q8Y8H6
E	215	TYR	-	expression tag	UNP Q8Y8H6
E	216	PHE	-	expression tag	UNP Q8Y8H6
E	217	GLN	-	expression tag	UNP Q8Y8H6
E	218	GLY	-	expression tag	UNP Q8Y8H6
E	219	ALA	-	expression tag	UNP Q8Y8H6
E	220	MET	-	expression tag	UNP Q8Y8H6
E	221	GLY	-	expression tag	UNP Q8Y8H6
E	222	SER	-	expression tag	UNP Q8Y8H6
E	223	GLY	-	expression tag	UNP Q8Y8H6
E	224	ILE	-	expression tag	UNP Q8Y8H6
E	225	GLN	-	expression tag	UNP Q8Y8H6
F	195	MET	-	expression tag	UNP Q8Y8H6
F	196	SER	-	expression tag	UNP Q8Y8H6
F	197	TYR	-	expression tag	UNP Q8Y8H6
F	198	TYR	-	expression tag	UNP Q8Y8H6
F	199	HIS	-	expression tag	UNP Q8Y8H6
F	200	HIS	-	expression tag	UNP Q8Y8H6
F	201	HIS	-	expression tag	UNP Q8Y8H6
F	202	HIS	-	expression tag	UNP Q8Y8H6
F	203	HIS	-	expression tag	UNP Q8Y8H6
F	204	HIS	-	expression tag	UNP Q8Y8H6
F	205	ASP	-	expression tag	UNP Q8Y8H6
F	206	TYR	-	expression tag	UNP Q8Y8H6
F	207	ASP	-	expression tag	UNP Q8Y8H6
F	208	ILE	-	expression tag	UNP Q8Y8H6
F	209	PRO	-	expression tag	UNP Q8Y8H6
F	210	THR	-	expression tag	UNP Q8Y8H6
F	211	THR	-	expression tag	UNP Q8Y8H6
F	212	GLU	-	expression tag	UNP Q8Y8H6
F	213	ASN	-	expression tag	UNP Q8Y8H6
F	214	LEU	-	expression tag	UNP Q8Y8H6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	215	TYR	-	expression tag	UNP Q8Y8H6
F	216	PHE	-	expression tag	UNP Q8Y8H6
F	217	GLN	-	expression tag	UNP Q8Y8H6
F	218	GLY	-	expression tag	UNP Q8Y8H6
F	219	ALA	-	expression tag	UNP Q8Y8H6
F	220	MET	-	expression tag	UNP Q8Y8H6
F	221	GLY	-	expression tag	UNP Q8Y8H6
F	222	SER	-	expression tag	UNP Q8Y8H6
F	223	GLY	-	expression tag	UNP Q8Y8H6
F	224	ILE	-	expression tag	UNP Q8Y8H6
F	225	GLN	-	expression tag	UNP Q8Y8H6
G	195	MET	-	expression tag	UNP Q8Y8H6
G	196	SER	-	expression tag	UNP Q8Y8H6
G	197	TYR	-	expression tag	UNP Q8Y8H6
G	198	TYR	-	expression tag	UNP Q8Y8H6
G	199	HIS	-	expression tag	UNP Q8Y8H6
G	200	HIS	-	expression tag	UNP Q8Y8H6
G	201	HIS	-	expression tag	UNP Q8Y8H6
G	202	HIS	-	expression tag	UNP Q8Y8H6
G	203	HIS	-	expression tag	UNP Q8Y8H6
G	204	HIS	-	expression tag	UNP Q8Y8H6
G	205	ASP	-	expression tag	UNP Q8Y8H6
G	206	TYR	-	expression tag	UNP Q8Y8H6
G	207	ASP	-	expression tag	UNP Q8Y8H6
G	208	ILE	-	expression tag	UNP Q8Y8H6
G	209	PRO	-	expression tag	UNP Q8Y8H6
G	210	THR	-	expression tag	UNP Q8Y8H6
G	211	THR	-	expression tag	UNP Q8Y8H6
G	212	GLU	-	expression tag	UNP Q8Y8H6
G	213	ASN	-	expression tag	UNP Q8Y8H6
G	214	LEU	-	expression tag	UNP Q8Y8H6
G	215	TYR	-	expression tag	UNP Q8Y8H6
G	216	PHE	-	expression tag	UNP Q8Y8H6
G	217	GLN	-	expression tag	UNP Q8Y8H6
G	218	GLY	-	expression tag	UNP Q8Y8H6
G	219	ALA	-	expression tag	UNP Q8Y8H6
G	220	MET	-	expression tag	UNP Q8Y8H6
G	221	GLY	-	expression tag	UNP Q8Y8H6
G	222	SER	-	expression tag	UNP Q8Y8H6
G	223	GLY	-	expression tag	UNP Q8Y8H6
G	224	ILE	-	expression tag	UNP Q8Y8H6
G	225	GLN	-	expression tag	UNP Q8Y8H6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	195	MET	-	expression tag	UNP Q8Y8H6
H	196	SER	-	expression tag	UNP Q8Y8H6
H	197	TYR	-	expression tag	UNP Q8Y8H6
H	198	TYR	-	expression tag	UNP Q8Y8H6
H	199	HIS	-	expression tag	UNP Q8Y8H6
H	200	HIS	-	expression tag	UNP Q8Y8H6
H	201	HIS	-	expression tag	UNP Q8Y8H6
H	202	HIS	-	expression tag	UNP Q8Y8H6
H	203	HIS	-	expression tag	UNP Q8Y8H6
H	204	HIS	-	expression tag	UNP Q8Y8H6
H	205	ASP	-	expression tag	UNP Q8Y8H6
H	206	TYR	-	expression tag	UNP Q8Y8H6
H	207	ASP	-	expression tag	UNP Q8Y8H6
H	208	ILE	-	expression tag	UNP Q8Y8H6
H	209	PRO	-	expression tag	UNP Q8Y8H6
H	210	THR	-	expression tag	UNP Q8Y8H6
H	211	THR	-	expression tag	UNP Q8Y8H6
H	212	GLU	-	expression tag	UNP Q8Y8H6
H	213	ASN	-	expression tag	UNP Q8Y8H6
H	214	LEU	-	expression tag	UNP Q8Y8H6
H	215	TYR	-	expression tag	UNP Q8Y8H6
H	216	PHE	-	expression tag	UNP Q8Y8H6
H	217	GLN	-	expression tag	UNP Q8Y8H6
H	218	GLY	-	expression tag	UNP Q8Y8H6
H	219	ALA	-	expression tag	UNP Q8Y8H6
H	220	MET	-	expression tag	UNP Q8Y8H6
H	221	GLY	-	expression tag	UNP Q8Y8H6
H	222	SER	-	expression tag	UNP Q8Y8H6
H	223	GLY	-	expression tag	UNP Q8Y8H6
H	224	ILE	-	expression tag	UNP Q8Y8H6
H	225	GLN	-	expression tag	UNP Q8Y8H6
I	195	MET	-	expression tag	UNP Q8Y8H6
I	196	SER	-	expression tag	UNP Q8Y8H6
I	197	TYR	-	expression tag	UNP Q8Y8H6
I	198	TYR	-	expression tag	UNP Q8Y8H6
I	199	HIS	-	expression tag	UNP Q8Y8H6
I	200	HIS	-	expression tag	UNP Q8Y8H6
I	201	HIS	-	expression tag	UNP Q8Y8H6
I	202	HIS	-	expression tag	UNP Q8Y8H6
I	203	HIS	-	expression tag	UNP Q8Y8H6
I	204	HIS	-	expression tag	UNP Q8Y8H6
I	205	ASP	-	expression tag	UNP Q8Y8H6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	206	TYR	-	expression tag	UNP Q8Y8H6
I	207	ASP	-	expression tag	UNP Q8Y8H6
I	208	ILE	-	expression tag	UNP Q8Y8H6
I	209	PRO	-	expression tag	UNP Q8Y8H6
I	210	THR	-	expression tag	UNP Q8Y8H6
I	211	THR	-	expression tag	UNP Q8Y8H6
I	212	GLU	-	expression tag	UNP Q8Y8H6
I	213	ASN	-	expression tag	UNP Q8Y8H6
I	214	LEU	-	expression tag	UNP Q8Y8H6
I	215	TYR	-	expression tag	UNP Q8Y8H6
I	216	PHE	-	expression tag	UNP Q8Y8H6
I	217	GLN	-	expression tag	UNP Q8Y8H6
I	218	GLY	-	expression tag	UNP Q8Y8H6
I	219	ALA	-	expression tag	UNP Q8Y8H6
I	220	MET	-	expression tag	UNP Q8Y8H6
I	221	GLY	-	expression tag	UNP Q8Y8H6
I	222	SER	-	expression tag	UNP Q8Y8H6
I	223	GLY	-	expression tag	UNP Q8Y8H6
I	224	ILE	-	expression tag	UNP Q8Y8H6
I	225	GLN	-	expression tag	UNP Q8Y8H6
J	195	MET	-	expression tag	UNP Q8Y8H6
J	196	SER	-	expression tag	UNP Q8Y8H6
J	197	TYR	-	expression tag	UNP Q8Y8H6
J	198	TYR	-	expression tag	UNP Q8Y8H6
J	199	HIS	-	expression tag	UNP Q8Y8H6
J	200	HIS	-	expression tag	UNP Q8Y8H6
J	201	HIS	-	expression tag	UNP Q8Y8H6
J	202	HIS	-	expression tag	UNP Q8Y8H6
J	203	HIS	-	expression tag	UNP Q8Y8H6
J	204	HIS	-	expression tag	UNP Q8Y8H6
J	205	ASP	-	expression tag	UNP Q8Y8H6
J	206	TYR	-	expression tag	UNP Q8Y8H6
J	207	ASP	-	expression tag	UNP Q8Y8H6
J	208	ILE	-	expression tag	UNP Q8Y8H6
J	209	PRO	-	expression tag	UNP Q8Y8H6
J	210	THR	-	expression tag	UNP Q8Y8H6
J	211	THR	-	expression tag	UNP Q8Y8H6
J	212	GLU	-	expression tag	UNP Q8Y8H6
J	213	ASN	-	expression tag	UNP Q8Y8H6
J	214	LEU	-	expression tag	UNP Q8Y8H6
J	215	TYR	-	expression tag	UNP Q8Y8H6
J	216	PHE	-	expression tag	UNP Q8Y8H6

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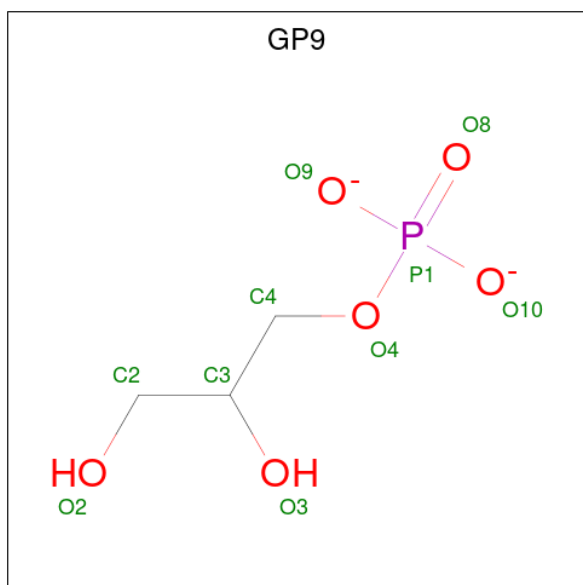
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Chain	Residue	Modelled	Actual	Comment	Reference
J	217	GLN	-	expression tag	UNP Q8Y8H6
J	218	GLY	-	expression tag	UNP Q8Y8H6
J	219	ALA	-	expression tag	UNP Q8Y8H6
J	220	MET	-	expression tag	UNP Q8Y8H6
J	221	GLY	-	expression tag	UNP Q8Y8H6
J	222	SER	-	expression tag	UNP Q8Y8H6
J	223	GLY	-	expression tag	UNP Q8Y8H6
J	224	ILE	-	expression tag	UNP Q8Y8H6
J	225	GLN	-	expression tag	UNP Q8Y8H6
K	195	MET	-	expression tag	UNP Q8Y8H6
K	196	SER	-	expression tag	UNP Q8Y8H6
K	197	TYR	-	expression tag	UNP Q8Y8H6
K	198	TYR	-	expression tag	UNP Q8Y8H6
K	199	HIS	-	expression tag	UNP Q8Y8H6
K	200	HIS	-	expression tag	UNP Q8Y8H6
K	201	HIS	-	expression tag	UNP Q8Y8H6
K	202	HIS	-	expression tag	UNP Q8Y8H6
K	203	HIS	-	expression tag	UNP Q8Y8H6
K	204	HIS	-	expression tag	UNP Q8Y8H6
K	205	ASP	-	expression tag	UNP Q8Y8H6
K	206	TYR	-	expression tag	UNP Q8Y8H6
K	207	ASP	-	expression tag	UNP Q8Y8H6
K	208	ILE	-	expression tag	UNP Q8Y8H6
K	209	PRO	-	expression tag	UNP Q8Y8H6
K	210	THR	-	expression tag	UNP Q8Y8H6
K	211	THR	-	expression tag	UNP Q8Y8H6
K	212	GLU	-	expression tag	UNP Q8Y8H6
K	213	ASN	-	expression tag	UNP Q8Y8H6
K	214	LEU	-	expression tag	UNP Q8Y8H6
K	215	TYR	-	expression tag	UNP Q8Y8H6
K	216	PHE	-	expression tag	UNP Q8Y8H6
K	217	GLN	-	expression tag	UNP Q8Y8H6
K	218	GLY	-	expression tag	UNP Q8Y8H6
K	219	ALA	-	expression tag	UNP Q8Y8H6
K	220	MET	-	expression tag	UNP Q8Y8H6
K	221	GLY	-	expression tag	UNP Q8Y8H6
K	222	SER	-	expression tag	UNP Q8Y8H6
K	223	GLY	-	expression tag	UNP Q8Y8H6
K	224	ILE	-	expression tag	UNP Q8Y8H6
K	225	GLN	-	expression tag	UNP Q8Y8H6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0

- Molecule 3 is (2R)-2,3-dihydroxypropyl phosphate (CCD ID: GP9) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 10 3 6 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		
3	E	1	Total	C	O	P	0	0
			10	3	6	1		
3	F	1	Total	C	O	P	0	0
			10	3	6	1		
3	G	1	Total	C	O	P	0	0
			10	3	6	1		
3	H	1	Total	C	O	P	0	0
			10	3	6	1		
3	I	1	Total	C	O	P	0	0
			10	3	6	1		
3	J	1	Total	C	O	P	0	0
			10	3	6	1		
3	K	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	370	Total	O	0	0
			370	370		
4	B	277	Total	O	0	0
			277	277		
4	C	368	Total	O	0	0
			368	368		
4	D	300	Total	O	0	0
			300	300		
4	E	310	Total	O	0	0
			310	310		
4	F	308	Total	O	0	0
			308	308		
4	G	281	Total	O	0	0
			281	281		
4	H	264	Total	O	0	0
			264	264		
4	I	234	Total	O	0	0
			234	234		

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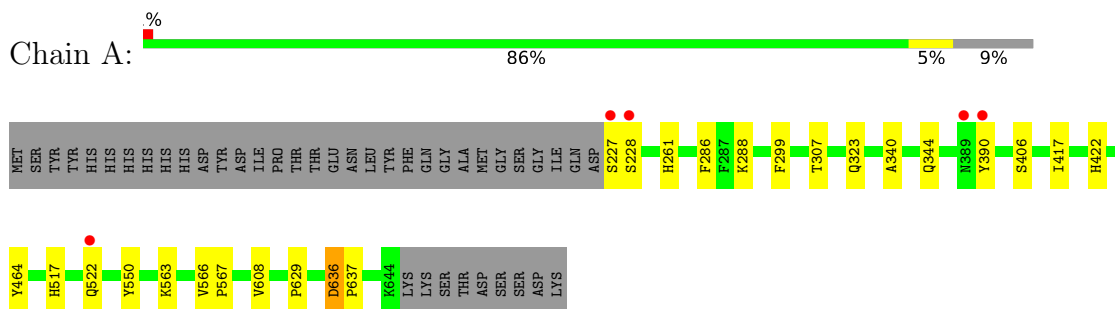
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	202	Total 202	O 202	0	0
4	K	83	Total 83	O 83	0	0

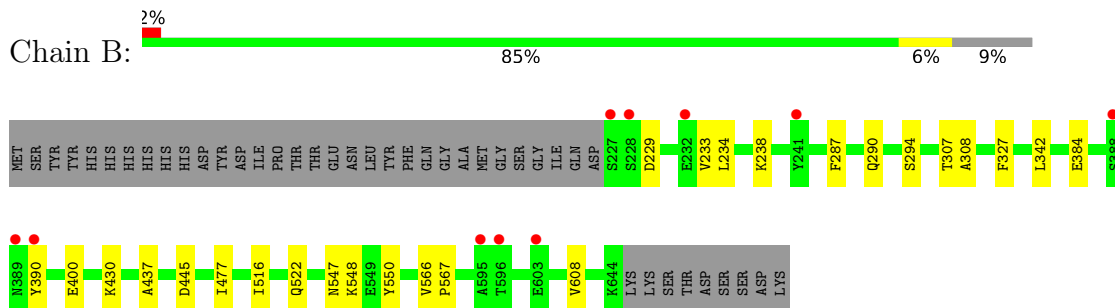
3 Residue-property plots

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.

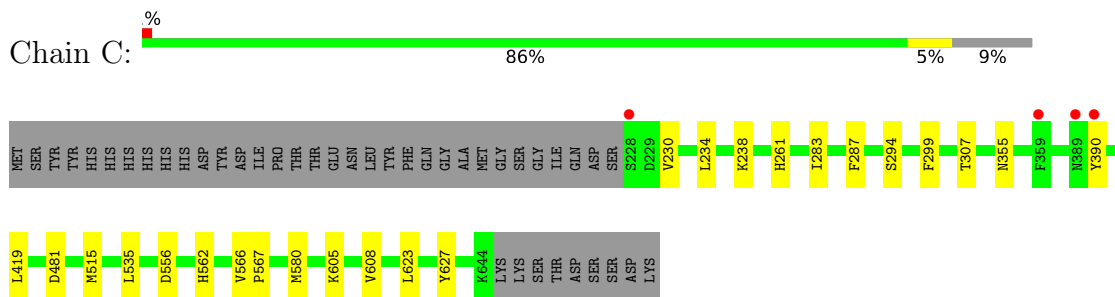
● Molecule 1: LIPOTEICHOIC ACID SYNTHASE



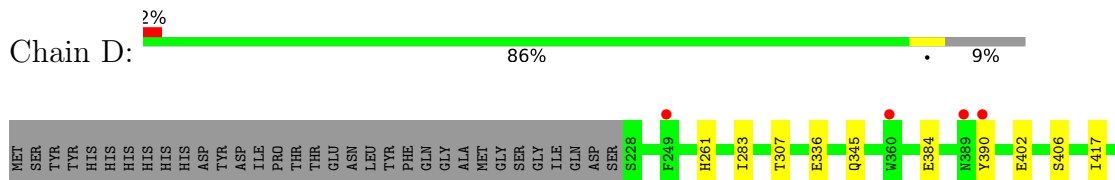
- Molecule 1: LIPOTEICHOIC ACID SYNTHASE



● Molecule 1: LIPOTEICHOIC ACID SYNTHASE

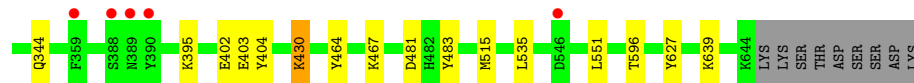
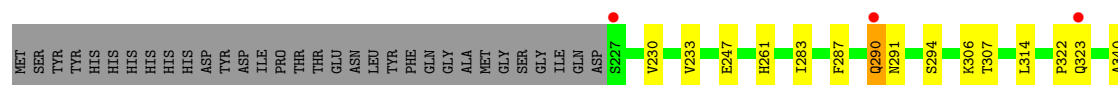
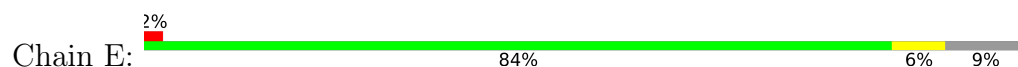


- Molecule 1: LIPOTEICHOIC ACID SYNTHASE

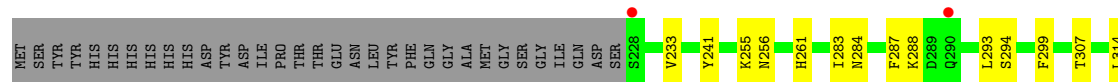
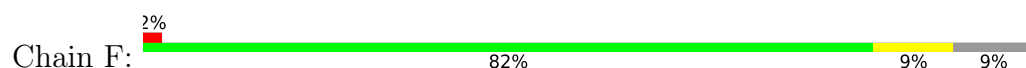




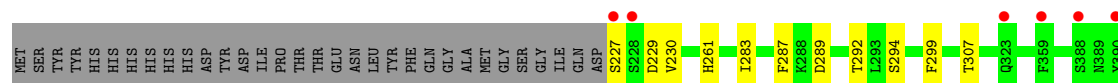
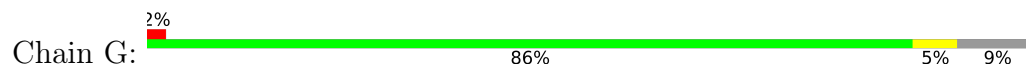
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



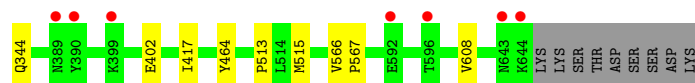
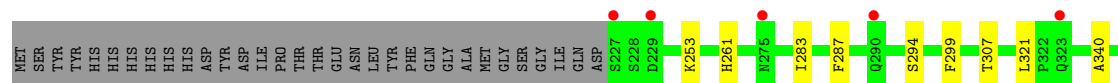
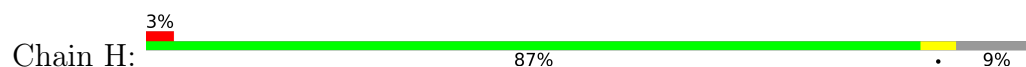
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



• Molecule 1: LIPOTEICHOIC ACID SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.25Å 119.62Å 472.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 2.19 48.71 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.71-2.19) 99.0 (48.71-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.178 , 0.214 0.180 , 0.215	Depositor DCC
R_{free} test set	17158 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
Reported twinning fraction	0.000 for K,H,-L	Depositor
Outliers	0 of 341744 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40238	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.66% 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, TPO, GP9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/3454	0.77	2/4672 (0.0%)
1	B	0.48	0/3454	0.75	1/4672 (0.0%)
1	C	0.49	0/3448	0.76	0/4664
1	D	0.50	0/3448	0.76	1/4664 (0.0%)
1	E	0.47	0/3454	0.75	2/4672 (0.0%)
1	F	0.49	0/3448	0.76	0/4664
1	G	0.46	0/3460	0.75	1/4680 (0.0%)
1	H	0.47	0/3454	0.77	2/4672 (0.0%)
1	I	0.45	0/3454	0.75	1/4672 (0.0%)
1	J	0.44	0/3433	0.76	0/4645
1	K	0.52	0/3427	0.91	7/4637 (0.2%)
All	All	0.48	0/37934	0.77	17/51314 (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	K	0	3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	431	ASP	N-CA-C	-11.87	98.82	113.18
1	G	229	ASP	N-CA-C	-8.41	101.64	112.23
1	K	428	ASP	N-CA-C	7.45	121.30	110.28
1	E	395	LYS	CA-C-N	-6.29	112.53	119.19
1	E	395	LYS	C-N-CA	-6.29	112.53	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	402	GLU	N-CA-C	6.15	118.07	111.36
1	K	450	THR	N-CA-C	-5.93	104.94	111.82
1	A	636	ASP	CA-C-N	5.77	125.45	119.56
1	A	636	ASP	C-N-CA	5.77	125.45	119.56
1	K	434	ILE	N-CA-C	5.63	115.40	108.53
1	K	445	ASP	N-CA-C	5.56	117.42	111.36
1	K	464	TYR	N-CA-C	5.52	117.38	111.36
1	H	321	LEU	CA-C-N	-5.22	113.65	119.19
1	H	321	LEU	C-N-CA	-5.22	113.65	119.19
1	I	229	ASP	N-CA-C	-5.17	105.10	111.40
1	B	566	VAL	N-CA-C	5.15	113.25	108.15
1	D	345	GLN	N-CA-C	-5.02	106.40	112.88

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	428	ASP	Peptide
1	K	429	GLU	Peptide
1	K	430	LYS	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	A	3380	0	3200	12	0
1	B	3380	0	3200	15	0
1	C	3374	0	3195	12	0
1	D	3374	0	3195	12	0
1	E	3380	0	3200	16	0
1	F	3374	0	3195	23	0
1	G	3386	0	3204	11	1
1	H	3380	0	3200	9	0
1	I	3380	0	3200	13	0
1	J	3359	0	3179	21	0
1	K	3353	0	3173	59	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	10	0	7	0	0
3	B	10	0	7	1	0
3	C	10	0	7	0	0
3	D	10	0	7	0	0
3	E	10	0	7	0	0
3	F	10	0	7	1	0
3	G	10	0	7	0	0
3	H	10	0	7	0	0
3	I	10	0	7	0	0
3	J	10	0	7	2	0
3	K	10	0	7	0	0
4	A	370	0	0	2	0
4	B	277	0	0	3	0
4	C	368	0	0	1	0
4	D	300	0	0	2	0
4	E	310	0	0	2	0
4	F	308	0	0	4	0
4	G	281	0	0	0	1
4	H	264	0	0	0	0
4	I	234	0	0	2	0
4	J	202	0	0	4	2
4	K	83	0	0	0	0
All	All	40238	0	35218	204	2

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 3.

All (204) 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:K:434:ILE:HG13	1:K:452:ARG:HD2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:MET:HE1	1:C:605:LYS:HD2	1.59	0.82
1:K:290:GLN:HE21	1:K:291:ASN:ND2	1.78	0.81
1:J:580:MET:HE1	1:J:605:LYS:HD2	1.65	0.79
1:K:429:GLU:HG3	1:K:430:LYS:N	2.01	0.76
1:K:290:GLN:HE21	1:K:291:ASN:HD22	1.32	0.74
1:K:229:ASP:OD1	1:K:230:VAL:N	2.20	0.74
1:I:253:LYS:NZ	4:I:2013:HOH:O	2.22	0.73
1:K:283:ILE:HG12	1:K:478:MET:HE1	1.72	0.72
1:K:282:PHE:HE2	1:K:456:GLU:HG3	1.56	0.70
1:E:596:THR:O	4:E:2286:HOH:O	2.10	0.69
1:K:580:MET:HE1	1:K:605:LYS:HD2	1.75	0.68
1:K:462:VAL:HG12	1:K:466:LYS:HE2	1.76	0.66
1:C:234:LEU:HG	1:C:238:LYS:HE2	1.77	0.66
1:K:399:LYS:NZ	1:K:402:GLU:OE1	2.22	0.64
1:F:255:LYS:NZ	4:F:2023:HOH:O	2.30	0.63
1:K:462:VAL:O	1:K:466:LYS:HG3	2.00	0.62
1:G:567:PRO:HB3	1:G:608:VAL:HG13	1.81	0.61
1:A:227:SER:OG	1:A:228:SER:N	2.35	0.59
1:D:406:SER:OG	1:D:464:TYR:OH	2.14	0.59
1:I:567:PRO:HB3	1:I:608:VAL:HG13	1.85	0.59
1:C:567:PRO:HB3	1:C:608:VAL:HG13	1.85	0.58
1:K:261:HIS:HB3	1:K:417:ILE:HA	1.84	0.58
1:F:406:SER:OG	1:F:464:TYR:OH	2.22	0.58
4:A:2333:HOH:O	1:K:500:ASP:OD1	2.17	0.57
3:J:700:GP9:H22	4:J:2123:HOH:O	2.04	0.57
1:I:261:HIS:HB3	1:I:417:ILE:HA	1.87	0.57
1:B:234:LEU:HG	1:B:238:LYS:HE2	1.88	0.56
1:J:299:PHE:HB2	1:J:566:VAL:HG11	1.87	0.56
1:D:521:VAL:HA	1:F:429:GLU:HG3	1.87	0.56
1:K:282:PHE:CE2	1:K:456:GLU:HG3	2.40	0.56
1:F:241:TYR:OH	4:F:2015:HOH:O	2.18	0.56
1:K:229:ASP:CG	1:K:230:VAL:H	2.12	0.56
1:C:355:ASN:HB2	1:C:419:LEU:HD11	1.88	0.56
1:K:465:LEU:HD21	1:K:476:ILE:HD11	1.88	0.56
1:G:261:HIS:HB3	1:G:417:ILE:HA	1.88	0.55
1:B:390:TYR:HB2	4:B:2138:HOH:O	2.04	0.55
1:K:429:GLU:CG	1:K:430:LYS:N	2.69	0.55
1:K:290:GLN:NE2	1:K:291:ASN:ND2	2.53	0.55
1:H:261:HIS:HB3	1:H:417:ILE:HA	1.90	0.54
1:J:261:HIS:HB3	1:J:417:ILE:HA	1.89	0.54
1:K:399:LYS:HZ3	1:K:464:TYR:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:PHE:CE1	1:C:294:SER:HB3	2.43	0.53
1:K:282:PHE:HB3	1:K:459:LYS:CG	2.39	0.53
1:B:567:PRO:HB3	1:B:608:VAL:HG13	1.90	0.53
1:F:355:ASN:HB2	1:F:419:LEU:HD11	1.91	0.53
1:K:427:ILE:HG21	1:K:449:GLN:HG3	1.91	0.53
1:G:287:PHE:CE1	1:G:294:SER:HB3	2.44	0.52
4:C:2342:HOH:O	1:E:639:LYS:HG3	2.09	0.52
1:H:340:ALA:O	1:H:344:GLN:HG2	2.09	0.52
1:I:234:LEU:HD11	1:I:627:TYR:CZ	2.45	0.52
1:C:390:TYR:HB3	1:C:419:LEU:HD22	1.93	0.51
1:F:355:ASN:ND2	1:F:359:PHE:HD2	2.09	0.51
1:G:230:VAL:HG22	1:G:623:LEU:HB3	1.93	0.51
1:J:406:SER:OG	1:J:464:TYR:OH	2.16	0.51
1:D:495:LYS:NZ	4:D:2214:HOH:O	2.44	0.51
1:K:336:GLU:HG2	1:K:632:PHE:CE2	2.46	0.51
1:B:290:GLN:HE22	1:B:522:GLN:HE22	1.60	0.50
1:D:567:PRO:HB3	1:D:608:VAL:HG13	1.93	0.50
1:J:344:GLN:NE2	1:J:633:LYS:H	2.10	0.50
1:K:464:TYR:HA	1:K:467:LYS:HB2	1.94	0.49
1:A:261:HIS:HB3	1:A:417:ILE:HA	1.95	0.49
1:F:293:LEU:HD13	1:F:523:GLY:HA2	1.95	0.49
1:F:567:PRO:HB3	1:F:608:VAL:HG13	1.95	0.48
1:J:495:LYS:NZ	4:J:2134:HOH:O	2.45	0.48
1:K:434:ILE:HD12	1:K:449:GLN:HB3	1.96	0.48
1:E:283:ILE:HG23	1:E:515:MET:HE1	1.95	0.48
1:F:261:HIS:HB3	1:F:417:ILE:HA	1.95	0.48
1:K:597:GLU:HG2	1:K:602:LYS:HG3	1.94	0.48
1:G:550:TYR:CE1	1:G:629:PRO:HG2	2.49	0.47
1:J:567:PRO:HB3	1:J:608:VAL:HG13	1.95	0.47
1:A:286:PHE:CZ	1:A:517:HIS:HB2	2.49	0.47
1:C:556:ASP:O	1:C:562:HIS:HB2	2.14	0.47
1:D:639:LYS:HE3	1:D:639:LYS:HA	1.97	0.47
1:H:299:PHE:HB2	1:H:566:VAL:HG11	1.95	0.47
1:K:567:PRO:HB3	1:K:608:VAL:HG13	1.96	0.47
1:A:406:SER:OG	1:A:464:TYR:OH	2.07	0.47
1:K:274:LEU:O	1:K:277:GLU:HB2	2.15	0.47
1:C:283:ILE:HG23	1:C:515:MET:HE1	1.97	0.47
1:I:287:PHE:CE1	1:I:294:SER:HB3	2.50	0.46
1:K:314:LEU:HD11	1:K:535:LEU:HD23	1.97	0.46
1:H:287:PHE:CE1	1:H:294:SER:HB3	2.51	0.46
1:I:314:LEU:HD11	1:I:535:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:336:GLU:HG2	1:J:632:PHE:CE2	2.50	0.46
1:D:283:ILE:HG23	1:D:515:MET:HE1	1.97	0.46
1:F:283:ILE:HG23	1:F:515:MET:HE1	1.96	0.46
1:B:477:ILE:HG12	1:B:516:ILE:HG23	1.98	0.46
1:F:314:LEU:HD11	1:F:535:LEU:HD23	1.98	0.46
1:E:230:VAL:HG11	1:E:627:TYR:HB2	1.97	0.46
1:K:299:PHE:HB2	1:K:566:VAL:HG11	1.98	0.46
1:F:233:VAL:HG11	1:F:551:LEU:HD21	1.97	0.46
1:K:279:VAL:HA	1:K:452:ARG:NH1	2.31	0.45
1:F:399:LYS:HG3	4:F:2157:HOH:O	2.15	0.45
1:C:230:VAL:HG11	1:C:627:TYR:HB2	1.98	0.45
3:F:700:GP9:H22	4:F:2204:HOH:O	2.15	0.45
1:J:513:PRO:HB3	1:J:515:MET:HE2	1.98	0.45
1:K:460:SER:O	1:K:463:ASP:HB2	2.16	0.45
1:E:290:GLN:N	1:E:290:GLN:CD	2.74	0.45
1:D:336:GLU:HG2	1:D:632:PHE:CE2	2.51	0.45
1:H:283:ILE:HG23	1:H:515:MET:HE1	1.98	0.45
1:K:386:ASP:O	1:K:393:LYS:HG3	2.17	0.45
1:E:233:VAL:HG12	1:E:551:LEU:HD22	1.98	0.45
1:B:437:ALA:HB3	1:B:445:ASP:HA	1.99	0.45
1:E:306:LYS:NZ	1:E:483:TYR:OH	2.50	0.45
1:H:402:GLU:HG2	1:H:464:TYR:CD2	2.52	0.45
1:I:299:PHE:HB2	1:I:566:VAL:HG11	1.99	0.45
1:K:467:LYS:HA	1:K:467:LYS:HD2	1.76	0.45
1:A:299:PHE:HB2	1:A:566:VAL:HG11	1.99	0.45
1:A:522:GLN:NE2	1:B:430:LYS:HE2	2.31	0.44
1:C:299:PHE:HB2	1:C:566:VAL:HG11	1.98	0.44
1:G:610:LYS:HD2	1:G:613:GLU:OE1	2.17	0.44
1:K:269:LEU:HD11	1:K:447:TYR:CE2	2.53	0.44
1:D:390:TYR:HB2	4:D:2133:HOH:O	2.16	0.44
1:G:299:PHE:HB2	1:G:566:VAL:HG11	1.98	0.44
1:I:251:LYS:HD2	1:I:251:LYS:HA	1.77	0.44
1:K:290:GLN:HG2	1:K:291:ASN:ND2	2.32	0.44
1:K:495:LYS:HB2	1:K:495:LYS:HE2	1.81	0.44
1:D:643:ASN:O	1:D:644:LYS:HB3	2.16	0.44
1:F:299:PHE:HB2	1:F:566:VAL:HG11	2.00	0.44
1:B:238:LYS:HE3	1:B:238:LYS:HB2	1.58	0.44
1:D:261:HIS:HB3	1:D:417:ILE:HA	2.00	0.44
1:E:340:ALA:O	1:E:344:GLN:HG2	2.17	0.44
1:K:315:GLU:OE2	1:K:415:LYS:NZ	2.37	0.44
1:J:287:PHE:CE1	1:J:294:SER:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:344:GLN:HE22	1:J:633:LYS:H	1.65	0.44
1:H:567:PRO:HB3	1:H:608:VAL:HG13	2.00	0.43
1:J:349:SER:O	1:J:372:ASP:HB2	2.18	0.43
1:G:227:SER:O	1:G:230:VAL:HB	2.18	0.43
1:B:400:GLU:OE2	4:B:2134:HOH:O	2.20	0.43
1:I:550:TYR:CE1	1:I:629:PRO:HG2	2.54	0.43
1:E:287:PHE:CE1	1:E:294:SER:HB3	2.53	0.43
1:F:550:TYR:CE1	1:F:629:PRO:HG2	2.54	0.43
1:A:563:LYS:NZ	4:A:2305:HOH:O	2.35	0.43
1:C:261:HIS:CE1	1:C:481:ASP:HB3	2.54	0.43
1:E:261:HIS:CE1	1:E:481:ASP:HB3	2.53	0.43
1:J:238:LYS:HD3	4:J:2008:HOH:O	2.18	0.43
1:A:567:PRO:HB3	1:A:608:VAL:HG13	2.01	0.43
1:E:291:ASN:ND2	4:E:2056:HOH:O	2.52	0.43
1:A:550:TYR:CE1	1:A:629:PRO:HG2	2.54	0.43
1:B:308:ALA:HB1	1:B:327:PHE:CG	2.54	0.43
1:F:287:PHE:CE1	1:F:294:SER:HB3	2.54	0.43
1:I:233:VAL:HG12	1:I:551:LEU:HD22	2.00	0.43
1:J:306:LYS:NZ	3:J:700:GP9:H21	2.34	0.43
1:K:282:PHE:CD2	1:K:459:LYS:HG2	2.54	0.42
1:K:356:TYR:CD1	1:K:377:ALA:HB3	2.54	0.42
1:K:360:TRP:HA	1:K:360:TRP:CE3	2.53	0.42
1:F:256:ASN:OD1	1:F:411:PRO:HA	2.19	0.42
1:K:536:LEU:HB3	1:K:537:PRO:HD3	2.01	0.42
1:K:262:LEU:HD11	1:K:478:MET:HE2	2.00	0.42
1:K:290:GLN:HG3	1:K:522:GLN:NE2	2.35	0.42
1:G:289:ASP:HB3	1:G:292:THR:OG1	2.20	0.42
1:K:279:VAL:HG12	1:K:280:THR:HG23	2.01	0.42
1:C:230:VAL:HG22	1:C:623:LEU:HB3	2.02	0.42
1:D:402:GLU:HG2	1:D:464:TYR:CD2	2.54	0.42
1:J:573:TYR:C	1:J:574:ILE:HD12	2.45	0.42
1:K:529:TYR:HB2	1:K:564:GLN:HB3	2.01	0.42
1:A:390:TYR:CE2	1:A:422:HIS:CD2	3.07	0.42
1:K:308:ALA:HB1	1:K:327:PHE:CG	2.55	0.42
1:K:459:LYS:HD2	1:K:459:LYS:HA	1.44	0.42
1:I:234:LEU:HG	1:I:551:LEU:HD21	2.02	0.42
1:J:229:ASP:HB2	4:J:2005:HOH:O	2.19	0.42
1:K:243:ALA:HA	1:K:244:PRO:HD3	1.94	0.42
1:K:429:GLU:C	1:K:430:LYS:CG	2.93	0.42
1:D:384:GLU:O	1:D:384:GLU:HG2	2.20	0.41
1:G:283:ILE:HG23	1:G:515:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:ALA:HB3	1:F:445:ASP:HA	2.02	0.41
1:J:402:GLU:HG2	1:J:464:TYR:CD2	2.55	0.41
1:B:287:PHE:CE1	1:B:294:SER:HB3	2.55	0.41
1:E:402:GLU:HG2	1:E:464:TYR:CD2	2.55	0.41
1:E:430:LYS:H	1:E:430:LYS:HG2	1.51	0.41
1:F:284:ASN:O	1:F:288:LYS:HE3	2.21	0.41
1:K:238:LYS:HB2	1:K:238:LYS:HE3	1.90	0.41
1:F:353:HIS:CE1	1:F:419:LEU:HG	2.56	0.41
1:J:467:LYS:HE3	1:J:467:LYS:HB2	1.86	0.41
1:K:284:ASN:O	1:K:288:LYS:HG2	2.21	0.41
1:K:464:TYR:CD1	1:K:464:TYR:C	2.98	0.41
1:A:340:ALA:O	1:A:344:GLN:HG2	2.21	0.41
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.91	0.41
1:E:314:LEU:HD11	1:E:535:LEU:HD23	2.01	0.41
1:J:504:PHE:O	1:J:508:GLN:HG2	2.21	0.41
1:J:536:LEU:HB3	1:J:537:PRO:HD3	2.01	0.41
1:K:278:GLU:O	1:K:452:ARG:NH2	2.54	0.41
1:K:287:PHE:CE1	1:K:294:SER:HB3	2.56	0.41
1:K:459:LYS:O	1:K:463:ASP:N	2.51	0.41
1:B:229:ASP:O	1:B:233:VAL:HG23	2.20	0.41
1:E:322:PRO:HG2	1:E:323:GLN:NE2	2.36	0.41
1:F:536:LEU:HB3	1:F:537:PRO:HD3	2.02	0.41
1:I:356:TYR:O	1:I:359:PHE:HD2	2.04	0.41
1:J:477:ILE:HD11	1:J:539:LEU:HD13	2.02	0.41
1:B:547:ASN:HA	1:B:550:TYR:HD2	1.86	0.41
3:B:700:GP9:H22	4:B:2208:HOH:O	2.20	0.41
1:G:402:GLU:HG2	1:G:464:TYR:CD2	2.56	0.41
1:K:281:PRO:HD2	1:K:455:ASP:OD2	2.21	0.41
1:K:282:PHE:CB	1:K:459:LYS:HG2	2.51	0.41
1:K:283:ILE:HG23	1:K:515:MET:HE1	2.02	0.41
1:A:636:ASP:HA	1:A:637:PRO:HD2	1.95	0.40
1:B:548:LYS:HB2	1:B:548:LYS:HE2	1.94	0.40
1:H:253:LYS:HB3	1:H:253:LYS:HE2	1.67	0.40
1:F:550:TYR:CD1	1:F:629:PRO:HG2	2.56	0.40
1:H:513:PRO:HB3	1:H:515:MET:HE2	2.03	0.40
1:I:362:ARG:HD2	4:I:2095:HOH:O	2.21	0.40
1:K:425:TYR:CZ	1:K:447:TYR:HD1	2.38	0.40
1:F:573:TYR:C	1:F:574:ILE:HD12	2.46	0.40
1:E:403:GLU:HG3	1:E:404:TYR:N	2.36	0.40

All (2) 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)
4:G:2150:HOH:O	4:J:2012:HOH:O[4_445]	1.95	0.25
1:G:407:SER:O	4:J:2012:HOH:O[4_445]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/459 (91%)	410 (98%)	7 (2%)	0	100	100
1	B	417/459 (91%)	410 (98%)	7 (2%)	0	100	100
1	C	416/459 (91%)	409 (98%)	7 (2%)	0	100	100
1	D	416/459 (91%)	408 (98%)	8 (2%)	0	100	100
1	E	417/459 (91%)	409 (98%)	8 (2%)	0	100	100
1	F	416/459 (91%)	409 (98%)	7 (2%)	0	100	100
1	G	418/459 (91%)	412 (99%)	6 (1%)	0	100	100
1	H	417/459 (91%)	408 (98%)	9 (2%)	0	100	100
1	I	417/459 (91%)	409 (98%)	8 (2%)	0	100	100
1	J	414/459 (90%)	406 (98%)	8 (2%)	0	100	100
1	K	413/459 (90%)	401 (97%)	10 (2%)	2 (0%)	24	27
All	All	4578/5049 (91%)	4491 (98%)	85 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	429	GLU
1	K	430	LYS

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/403 (91%)	366 (100%)	2 (0%)	81	90
1	B	368/403 (91%)	367 (100%)	1 (0%)	86	93
1	C	367/403 (91%)	366 (100%)	1 (0%)	86	93
1	D	367/403 (91%)	367 (100%)	0	100	100
1	E	368/403 (91%)	364 (99%)	4 (1%)	65	79
1	F	367/403 (91%)	366 (100%)	1 (0%)	86	93
1	G	369/403 (92%)	368 (100%)	1 (0%)	86	93
1	H	368/403 (91%)	368 (100%)	0	100	100
1	I	368/403 (91%)	367 (100%)	1 (0%)	86	93
1	J	365/403 (91%)	363 (100%)	2 (0%)	81	90
1	K	364/403 (90%)	356 (98%)	8 (2%)	45	61
All	All	4039/4433 (91%)	4018 (100%)	21 (0%)	81	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	A	323	GLN
1	B	384	GLU
1	C	535	LEU
1	E	247	GLU
1	E	290	GLN
1	E	430	LYS
1	E	467	LYS
1	F	389	ASN
1	G	644	LYS
1	I	613	GLU
1	J	467	LYS
1	J	625	ARG
1	K	290	GLN
1	K	399	LYS
1	K	430	LYS
1	K	452	ARG
1	K	459	LYS
1	K	465	LEU

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Mol	Chain	Res	Type
1	K	467	LYS
1	K	490	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	506	ASN
1	B	290	GLN
1	B	449	GLN
1	B	506	ASN
1	C	449	GLN
1	C	643	ASN
1	D	383	ASN
1	D	409	GLN
1	D	449	GLN
1	D	506	ASN
1	D	643	ASN
1	E	267	GLN
1	E	291	ASN
1	E	323	GLN
1	E	383	ASN
1	E	506	ASN
1	F	589	GLN
1	G	449	GLN
1	G	506	ASN
1	H	271	ASN
1	H	449	GLN
1	H	506	ASN
1	I	449	GLN
1	I	506	ASN
1	I	641	ASN
1	I	643	ASN
1	J	449	GLN
1	J	506	ASN
1	K	291	ASN
1	K	389	ASN
1	K	506	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	K	307	2,1	8,10,11	1.21	0	10,14,16	1.80	1 (10%)
1	TPO	G	307	2,1	8,10,11	1.18	0	10,14,16	1.69	2 (20%)
1	TPO	F	307	2,1	8,10,11	1.16	0	10,14,16	1.72	2 (20%)
1	TPO	E	307	2,1	8,10,11	1.07	0	10,14,16	1.71	2 (20%)
1	TPO	C	307	2,1	8,10,11	1.19	0	10,14,16	1.46	2 (20%)
1	TPO	D	307	2,1	8,10,11	1.15	0	10,14,16	1.77	1 (10%)
1	TPO	J	307	2,1	8,10,11	1.10	0	10,14,16	1.65	1 (10%)
1	TPO	I	307	2,1	8,10,11	1.21	0	10,14,16	1.52	1 (10%)
1	TPO	H	307	2,1	8,10,11	1.18	0	10,14,16	1.67	1 (10%)
1	TPO	B	307	2,1	8,10,11	1.21	0	10,14,16	1.55	1 (10%)
1	TPO	A	307	2,1	8,10,11	1.24	1 (12%)	10,14,16	1.48	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	K	307	2,1	-	1/9/11/13	-
1	TPO	G	307	2,1	-	2/9/11/13	-
1	TPO	F	307	2,1	-	1/9/11/13	-
1	TPO	E	307	2,1	-	3/9/11/13	-
1	TPO	C	307	2,1	-	3/9/11/13	-
1	TPO	D	307	2,1	-	2/9/11/13	-
1	TPO	J	307	2,1	-	1/9/11/13	-
1	TPO	I	307	2,1	-	2/9/11/13	-
1	TPO	H	307	2,1	-	1/9/11/13	-
1	TPO	B	307	2,1	-	1/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	307	2,1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	TPO	P-OG1	2.03	1.63	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	307	TPO	P-OG1-CB	-5.01	109.72	123.33
1	K	307	TPO	P-OG1-CB	-4.91	110.00	123.33
1	F	307	TPO	P-OG1-CB	-4.57	110.91	123.33
1	H	307	TPO	P-OG1-CB	-4.46	111.22	123.33
1	J	307	TPO	P-OG1-CB	-4.43	111.30	123.33
1	E	307	TPO	P-OG1-CB	-4.27	111.71	123.33
1	B	307	TPO	P-OG1-CB	-4.23	111.83	123.33
1	G	307	TPO	P-OG1-CB	-4.17	111.99	123.33
1	A	307	TPO	P-OG1-CB	-3.90	112.73	123.33
1	I	307	TPO	P-OG1-CB	-3.87	112.81	123.33
1	C	307	TPO	P-OG1-CB	-3.24	114.53	123.33
1	E	307	TPO	CG2-CB-CA	-2.45	108.49	113.26
1	C	307	TPO	CG2-CB-CA	-2.24	108.89	113.26
1	G	307	TPO	CG2-CB-CA	-2.07	109.23	113.26
1	F	307	TPO	CG2-CB-CA	-2.07	109.24	113.26

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	307	TPO	O-C-CA-CB
1	E	307	TPO	O-C-CA-CB
1	J	307	TPO	O-C-CA-CB
1	I	307	TPO	CB-OG1-P-O1P
1	C	307	TPO	CB-OG1-P-O1P
1	D	307	TPO	CB-OG1-P-O1P
1	C	307	TPO	CB-OG1-P-O2P
1	E	307	TPO	CB-OG1-P-O2P
1	G	307	TPO	CB-OG1-P-O2P
1	B	307	TPO	O-C-CA-CB
1	C	307	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	D	307	TPO	O-C-CA-CB
1	F	307	TPO	O-C-CA-CB
1	G	307	TPO	O-C-CA-CB
1	H	307	TPO	O-C-CA-CB
1	I	307	TPO	O-C-CA-CB
1	K	307	TPO	O-C-CA-CB
1	E	307	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 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	$\# Z > 2$
3	GP9	G	700	-	9,9,9	0.48	0	10,12,12	0.92	0
3	GP9	B	700	-	9,9,9	0.49	0	10,12,12	0.94	0
3	GP9	A	700	-	9,9,9	0.53	0	10,12,12	0.82	0
3	GP9	H	700	-	9,9,9	0.60	0	10,12,12	0.77	0
3	GP9	K	700	-	9,9,9	0.54	0	10,12,12	0.83	0
3	GP9	E	700	-	9,9,9	0.60	0	10,12,12	0.87	0
3	GP9	I	700	-	9,9,9	0.60	0	10,12,12	0.89	0
3	GP9	J	700	-	9,9,9	0.56	0	10,12,12	1.08	1 (10%)
3	GP9	D	700	-	9,9,9	0.64	0	10,12,12	0.95	0
3	GP9	C	700	-	9,9,9	0.60	0	10,12,12	0.98	1 (10%)
3	GP9	F	700	-	9,9,9	0.48	0	10,12,12	1.10	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GP9	G	700	-	-	4/8/8/8	-
3	GP9	B	700	-	-	2/8/8/8	-
3	GP9	A	700	-	-	7/8/8/8	-
3	GP9	H	700	-	-	2/8/8/8	-
3	GP9	K	700	-	-	4/8/8/8	-
3	GP9	E	700	-	-	4/8/8/8	-
3	GP9	I	700	-	-	2/8/8/8	-
3	GP9	J	700	-	-	2/8/8/8	-
3	GP9	D	700	-	-	2/8/8/8	-
3	GP9	C	700	-	-	2/8/8/8	-
3	GP9	F	700	-	-	2/8/8/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	700	GP9	O10-P1-O9	2.34	116.58	107.80
3	C	700	GP9	O9-P1-O4	-2.12	101.15	106.67
3	F	700	GP9	O10-P1-O9	2.04	115.44	107.80

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	GP9	O2-C2-C3-C4
3	A	700	GP9	O3-C3-C4-O4
3	A	700	GP9	C4-O4-P1-O8
3	A	700	GP9	C4-O4-P1-O9
3	C	700	GP9	O2-C2-C3-O3
3	E	700	GP9	O2-C2-C3-C4
3	G	700	GP9	C4-O4-P1-O9
3	G	700	GP9	C4-O4-P1-O10
3	E	700	GP9	O3-C3-C4-O4
3	G	700	GP9	O3-C3-C4-O4
3	D	700	GP9	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	H	700	GP9	O2-C2-C3-O3
3	E	700	GP9	C2-C3-C4-O4
3	B	700	GP9	O2-C2-C3-C4
3	C	700	GP9	O2-C2-C3-C4
3	D	700	GP9	O2-C2-C3-C4
3	F	700	GP9	O2-C2-C3-C4
3	H	700	GP9	O2-C2-C3-C4
3	I	700	GP9	O2-C2-C3-C4
3	J	700	GP9	O2-C2-C3-C4
3	K	700	GP9	O2-C2-C3-C4
3	A	700	GP9	O2-C2-C3-O3
3	E	700	GP9	O2-C2-C3-O3
3	I	700	GP9	O2-C2-C3-O3
3	A	700	GP9	C2-C3-C4-O4
3	K	700	GP9	O3-C3-C4-O4
3	F	700	GP9	O2-C2-C3-O3
3	K	700	GP9	O2-C2-C3-O3
3	B	700	GP9	O2-C2-C3-O3
3	K	700	GP9	C2-C3-C4-O4
3	J	700	GP9	O2-C2-C3-O3
3	G	700	GP9	C2-C3-C4-O4
3	A	700	GP9	C4-O4-P1-O10

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	GP9	1	0
3	J	700	GP9	2	0
3	F	700	GP9	1	0

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 ⓘ

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(Å ²)	Q<0.9
1	A	417/459 (90%)	-0.30	5 (1%) 76 74	9, 24, 41, 65	2 (0%)
1	B	417/459 (90%)	-0.14	10 (2%) 59 56	11, 28, 49, 67	2 (0%)
1	C	416/459 (90%)	-0.31	4 (0%) 79 77	11, 25, 42, 69	2 (0%)
1	D	416/459 (90%)	-0.07	7 (1%) 69 66	14, 28, 47, 69	2 (0%)
1	E	417/459 (90%)	-0.22	8 (1%) 66 63	11, 26, 43, 73	2 (0%)
1	F	416/459 (90%)	-0.24	8 (1%) 66 63	11, 26, 43, 76	2 (0%)
1	G	417/459 (90%)	-0.12	7 (1%) 69 66	12, 28, 47, 70	3 (0%)
1	H	417/459 (90%)	-0.09	12 (2%) 53 50	13, 30, 49, 76	2 (0%)
1	I	417/459 (90%)	0.11	11 (2%) 57 54	14, 33, 51, 88	2 (0%)
1	J	416/459 (90%)	0.31	18 (4%) 40 36	22, 37, 58, 88	0
1	K	414/459 (90%)	1.57	128 (30%) 1 1	20, 53, 84, 115	2 (0%)
All	All	4580/5049 (90%)	0.05	218 (4%) 35 32	9, 29, 60, 115	21 (0%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	465	LEU	7.7
1	K	401	SER	6.4
1	K	282	PHE	6.3
1	J	390	TYR	6.3
1	K	274	LEU	5.7
1	K	434	ILE	5.3
1	E	390	TYR	5.2
1	K	390	TYR	5.1
1	G	359	PHE	4.8
1	K	459	LYS	4.8
1	F	390	TYR	4.8
1	K	399	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	K	464	TYR	4.7
1	K	419	LEU	4.7
1	K	432	ALA	4.7
1	K	420	THR	4.6
1	A	390	TYR	4.6
1	K	424	PRO	4.4
1	K	398	PHE	4.3
1	I	227	SER	4.1
1	K	359	PHE	4.1
1	K	439	THR	4.1
1	I	390	TYR	4.0
1	K	462	VAL	4.0
1	K	497	LEU	4.0
1	K	241	TYR	3.9
1	K	458	VAL	3.8
1	H	227	SER	3.8
1	K	453	TYR	3.8
1	K	273	LYS	3.8
1	B	389	ASN	3.7
1	I	389	ASN	3.7
1	K	427	ILE	3.7
1	K	444	VAL	3.7
1	F	359	PHE	3.7
1	K	272	TYR	3.6
1	K	276	GLY	3.6
1	F	389	ASN	3.5
1	K	397	PHE	3.5
1	K	287	PHE	3.5
1	K	423	PHE	3.4
1	K	435	ALA	3.4
1	K	279	VAL	3.4
1	K	229	ASP	3.4
1	K	461	PHE	3.4
1	K	385	ALA	3.4
1	H	389	ASN	3.4
1	K	452	ARG	3.4
1	C	228	SER	3.4
1	K	392	LEU	3.4
1	G	644	LYS	3.3
1	K	232	GLU	3.3
1	I	644	LYS	3.3
1	K	463	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	356	TYR	3.3
1	K	468	SER	3.2
1	K	440	GLY	3.2
1	B	390	TYR	3.2
1	K	492	ALA	3.2
1	K	281	PRO	3.2
1	H	644	LYS	3.2
1	K	275	ASN	3.2
1	K	380	TYR	3.2
1	K	396	PRO	3.2
1	C	389	ASN	3.2
1	K	387	VAL	3.1
1	B	228	SER	3.1
1	E	389	ASN	3.1
1	K	471	TYR	3.1
1	J	389	ASN	3.1
1	K	426	PRO	3.1
1	K	430	LYS	3.1
1	K	454	LEU	3.1
1	F	388	SER	3.1
1	K	436	PRO	3.0
1	K	271	ASN	3.0
1	B	241	TYR	3.0
1	G	390	TYR	3.0
1	K	603	GLU	3.0
1	K	499	LYS	3.0
1	B	227	SER	3.0
1	K	404	TYR	3.0
1	K	443	SER	3.0
1	G	323	GLN	2.9
1	K	360	TRP	3.0
1	K	456	GLU	2.9
1	K	283	ILE	2.9
1	K	438	THR	2.9
1	K	286	PHE	2.9
1	G	227	SER	2.9
1	K	260	ILE	2.9
1	J	359	PHE	2.9
1	K	291	ASN	2.9
1	K	395	LYS	2.9
1	K	448	PHE	2.9
1	K	437	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	249	PHE	2.8
1	H	390	TYR	2.8
1	K	391	GLY	2.8
1	K	431	ASP	2.8
1	K	485	ILE	2.8
1	K	354	GLY	2.8
1	I	359	PHE	2.8
1	E	323	GLN	2.7
1	E	388	SER	2.7
1	K	375	PHE	2.7
1	F	228	SER	2.7
1	K	394	ASP	2.7
1	C	390	TYR	2.7
1	K	451	ALA	2.7
1	K	277	GLU	2.7
1	K	379	TYR	2.7
1	H	596	THR	2.6
1	J	378	SER	2.6
1	K	457	SER	2.6
1	D	390	TYR	2.6
1	K	447	TYR	2.6
1	J	631	GLY	2.6
1	K	473	ASN	2.6
1	B	595	ALA	2.6
1	I	595	ALA	2.6
1	K	429	GLU	2.6
1	K	280	THR	2.6
1	K	545	VAL	2.5
1	K	446	THR	2.5
1	J	388	SER	2.5
1	E	290	GLN	2.5
1	H	323	GLN	2.5
1	I	323	GLN	2.5
1	K	455	ASP	2.5
1	K	400	GLU	2.5
1	I	469	GLY	2.5
1	K	270	VAL	2.5
1	K	365	ILE	2.5
1	H	229	ASP	2.5
1	K	402	GLU	2.5
1	K	393	LYS	2.5
1	J	331	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	476	ILE	2.5
1	K	487	ASP	2.4
1	K	248	TYR	2.4
1	K	425	TYR	2.4
1	K	288	LYS	2.4
1	K	460	SER	2.4
1	J	467	LYS	2.4
1	K	306	LYS	2.4
1	K	314	LEU	2.4
1	K	352	PHE	2.4
1	K	495	LYS	2.4
1	H	275	ASN	2.4
1	A	227	SER	2.4
1	B	603	GLU	2.3
1	A	522	GLN	2.3
1	D	389	ASN	2.3
1	K	262	LEU	2.3
1	K	470	LEU	2.3
1	E	546	ASP	2.3
1	E	359	PHE	2.3
1	D	596	THR	2.3
1	K	491	GLU	2.3
1	K	595	ALA	2.3
1	K	293	LEU	2.3
1	K	378	SER	2.3
1	K	442	SER	2.3
1	F	630	ASP	2.3
1	J	419	LEU	2.3
1	K	498	GLY	2.3
1	G	388	SER	2.3
1	K	518	VAL	2.3
1	K	377	ALA	2.3
1	J	323	GLN	2.2
1	J	409	GLN	2.2
1	K	418	THR	2.2
1	K	521	VAL	2.2
1	K	599	LYS	2.2
1	J	346	GLY	2.2
1	K	388	SER	2.2
1	K	626	PHE	2.2
1	B	596	THR	2.2
1	H	399	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	596	THR	2.2
1	H	592	GLU	2.2
1	F	290	GLN	2.2
1	J	290	GLN	2.2
1	K	323	GLN	2.2
1	J	407	SER	2.2
1	D	360	TRP	2.2
1	F	626	PHE	2.2
1	K	417	ILE	2.2
1	K	247	GLU	2.2
1	K	449	GLN	2.2
1	J	643	ASN	2.2
1	K	231	THR	2.2
1	I	230	VAL	2.1
1	K	422	HIS	2.1
1	K	269	LEU	2.1
1	A	228	SER	2.1
1	D	644	LYS	2.1
1	B	232	GLU	2.1
1	K	445	ASP	2.1
1	H	290	GLN	2.1
1	I	388	SER	2.1
1	H	643	ASN	2.1
1	J	344	GLN	2.1
1	J	596	THR	2.1
1	J	387	VAL	2.1
1	K	635	VAL	2.1
1	K	278	GLU	2.1
1	A	389	ASN	2.1
1	C	359	PHE	2.1
1	B	388	SER	2.1
1	E	227	SER	2.1
1	G	228	SER	2.1
1	K	245	ASN	2.0
1	D	546	ASP	2.0
1	K	353	HIS	2.0
1	K	408	LEU	2.0
1	K	517	HIS	2.0

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, 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
1	TPO	K	307	11/12	0.90	0.11	47,60,71,72	0
1	TPO	J	307	11/12	0.97	0.07	26,32,39,40	0
1	TPO	B	307	11/12	0.97	0.06	20,24,28,32	0
1	TPO	D	307	11/12	0.98	0.06	20,22,26,26	0
1	TPO	E	307	11/12	0.98	0.05	22,24,28,29	0
1	TPO	F	307	11/12	0.98	0.05	18,23,31,31	0
1	TPO	G	307	11/12	0.98	0.05	22,24,32,40	0
1	TPO	H	307	11/12	0.98	0.05	22,26,31,32	0
1	TPO	I	307	11/12	0.98	0.06	26,30,32,35	0
1	TPO	A	307	11/12	0.98	0.06	20,23,27,32	0
1	TPO	C	307	11/12	0.98	0.05	19,21,25,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
2	MG	J	699	1/1	0.70	0.27	54,54,54,54	0
3	GP9	K	700	10/10	0.77	0.14	72,79,88,89	0
2	MG	E	699	1/1	0.85	0.25	41,41,41,41	0
2	MG	B	699	1/1	0.86	0.18	46,46,46,46	0
2	MG	G	699	1/1	0.88	0.15	40,40,40,40	0
2	MG	F	699	1/1	0.89	0.14	43,43,43,43	0
2	MG	C	699	1/1	0.89	0.19	40,40,40,40	0
2	MG	H	699	1/1	0.91	0.10	40,40,40,40	0
2	MG	K	699	1/1	0.92	0.09	69,69,69,69	0
2	MG	I	699	1/1	0.93	0.15	47,47,47,47	0
3	GP9	B	700	10/10	0.94	0.11	24,35,39,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GP9	I	700	10/10	0.95	0.10	29,34,47,48	0
3	GP9	H	700	10/10	0.95	0.09	29,33,43,47	0
2	MG	A	699	1/1	0.96	0.15	40,40,40,40	0
3	GP9	C	700	10/10	0.96	0.09	26,29,41,44	0
3	GP9	J	700	10/10	0.96	0.09	28,32,40,46	0
3	GP9	D	700	10/10	0.96	0.10	20,24,33,44	0
3	GP9	F	700	10/10	0.97	0.08	22,29,38,42	0
3	GP9	G	700	10/10	0.97	0.08	27,33,47,55	0
2	MG	D	699	1/1	0.97	0.09	36,36,36,36	0
3	GP9	A	700	10/10	0.98	0.06	19,25,38,39	0
3	GP9	E	700	10/10	0.98	0.07	23,29,39,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.