Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 07:35 am GMT

PDB ID	:	4UOR
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:

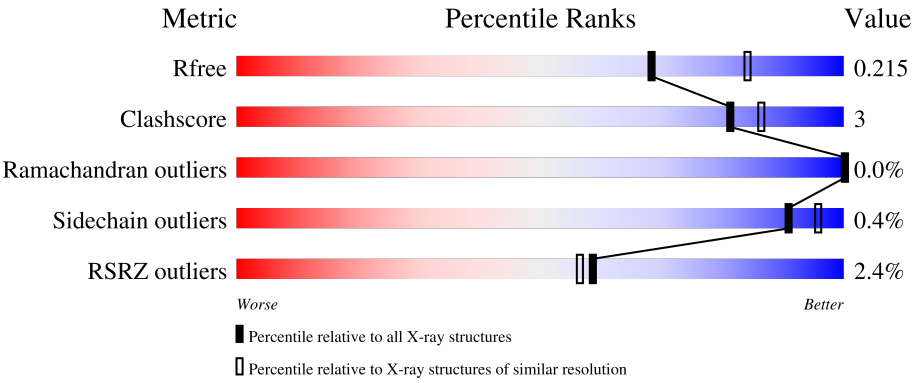
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	86% 5% 9%
1	B	459	86% 5% 9%
1	C	459	86% 5% 9%
1	D	459	87% . 9%
1	E	459	85% 6% 9%

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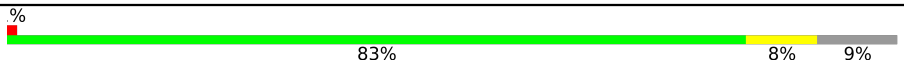
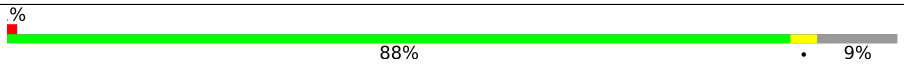
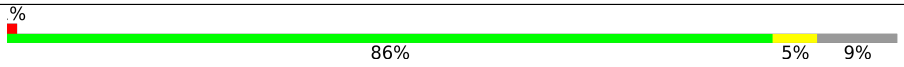
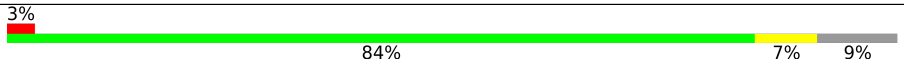
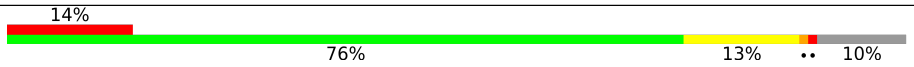
Mol	Chain	Length	Quality of chain
1	F	459	
1	G	459	
1	H	459	
1	I	459	
1	J	459	
1	K	459	

2 Entry composition (i)

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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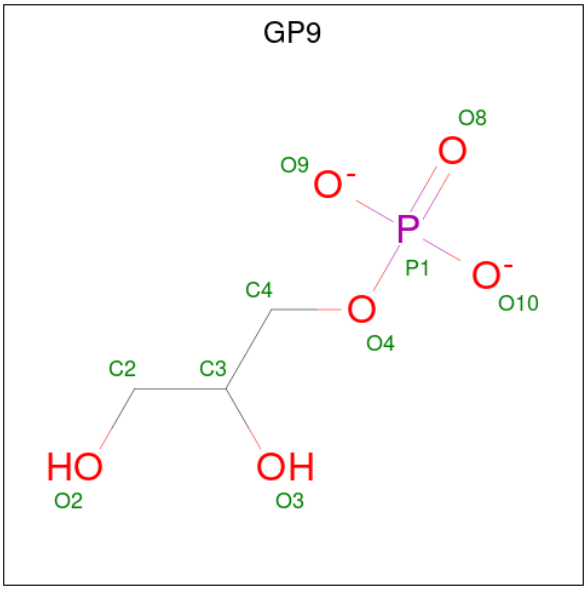
Chain	Residue	Modelled	Actual	Comment	Reference
J	217	GLN	-	expression tag	UNP Q8Y8H6
J	218	GLY	-	expression tag	UNP Q8Y8H6
J	219	ALA	-	expression tag	UNP Q8Y8H6
J	220	MET	-	expression tag	UNP Q8Y8H6
J	221	GLY	-	expression tag	UNP Q8Y8H6
J	222	SER	-	expression tag	UNP Q8Y8H6
J	223	GLY	-	expression tag	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 (three-letter code: 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 (three-letter code: GP9) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
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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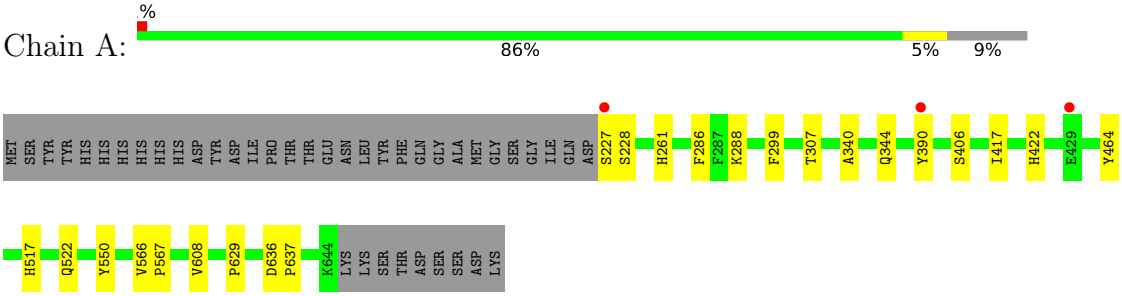
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	202	Total O 202 202	0	0
4	K	83	Total O 83 83	0	0

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.

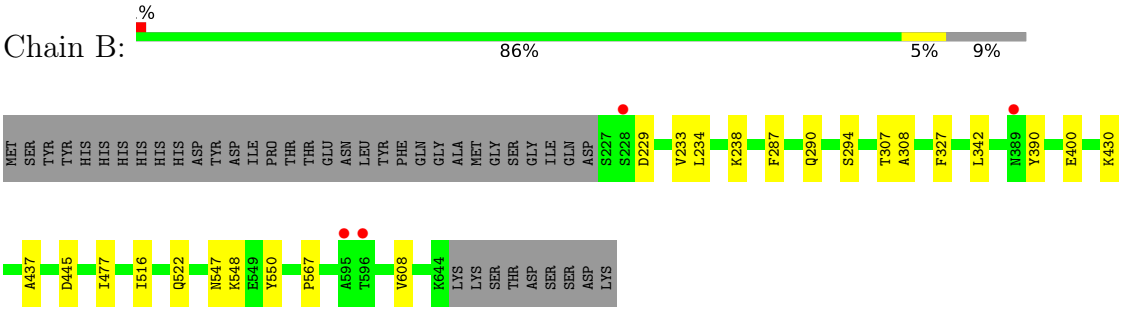
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain A:



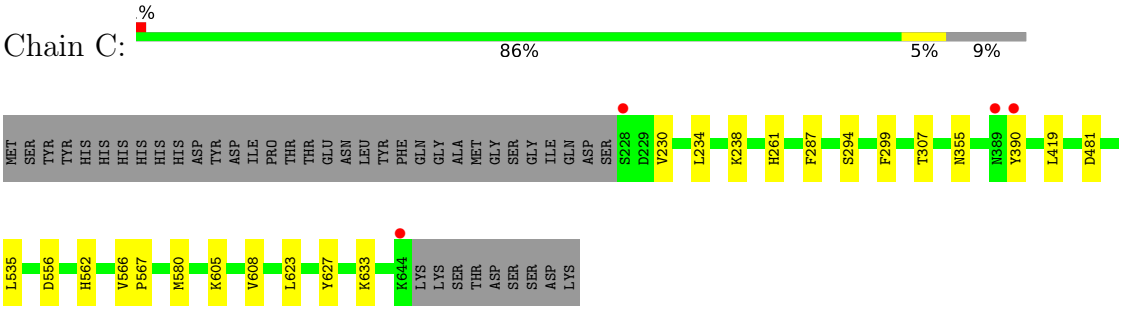
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain B:



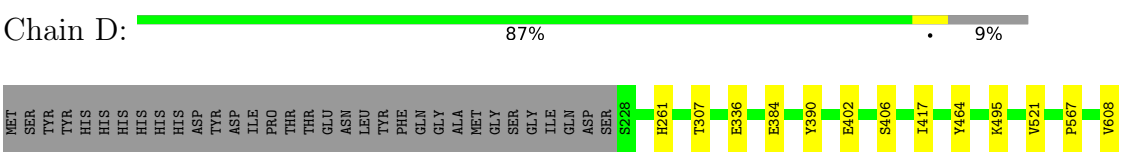
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

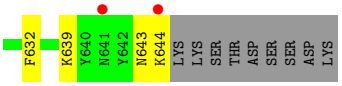
Chain C:



• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

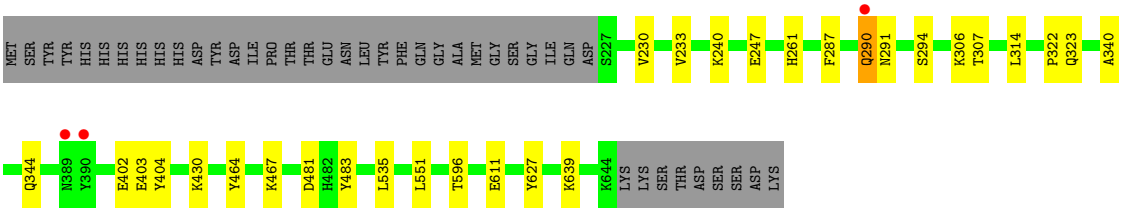
Chain D:





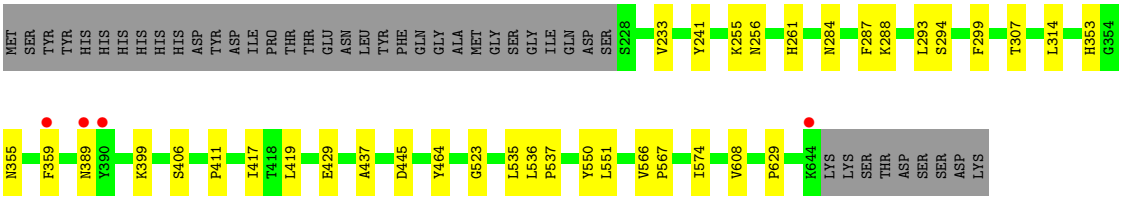
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain E:



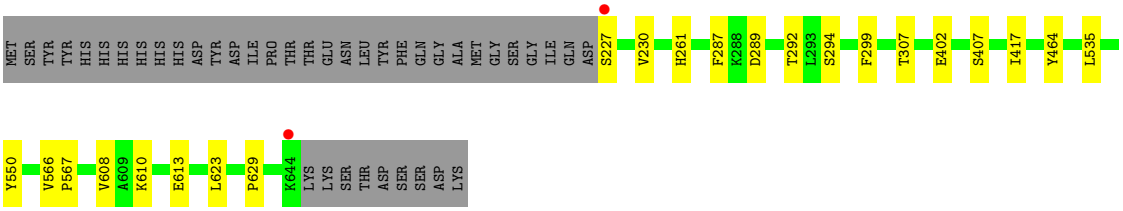
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain F:



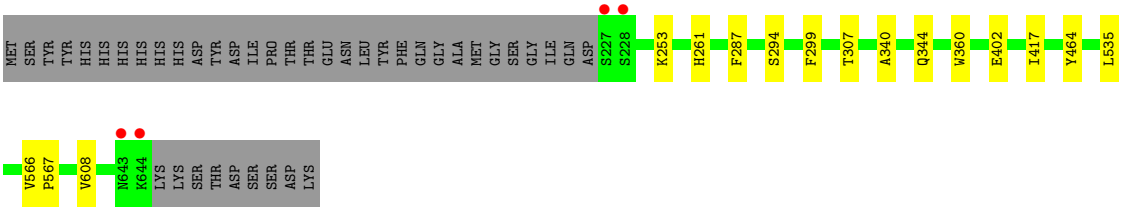
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain G:



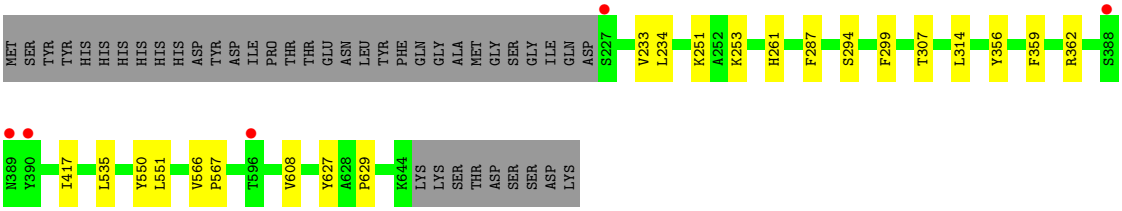
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain H:



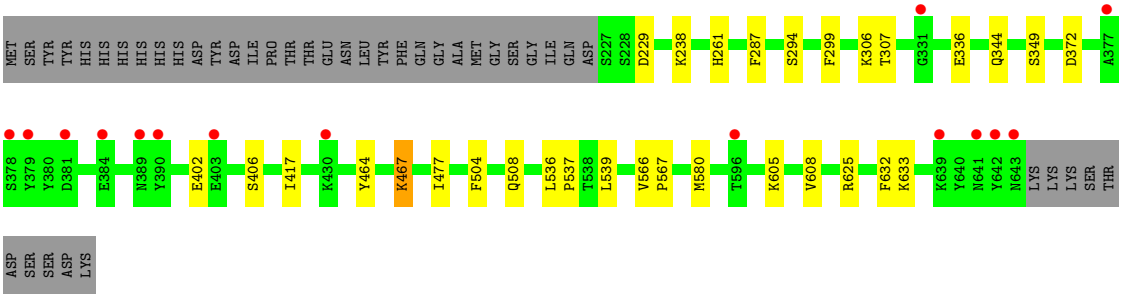
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain I:



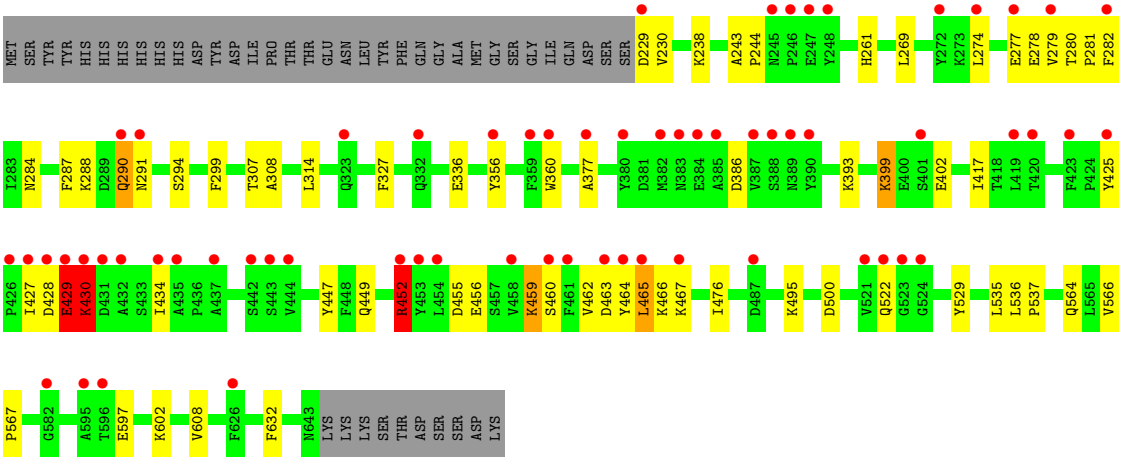
• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain J:



• Molecule 1: LIPOTEICHOIC ACID SYNTHASE

Chain K:



4 Data and refinement statistics (i)

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) 98.9 (48.71-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	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.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, GP9, 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	A	0.40	0/3454	0.52	0/4672
1	B	0.39	0/3454	0.51	0/4672
1	C	0.40	0/3448	0.53	0/4664
1	D	0.40	0/3448	0.52	0/4664
1	E	0.39	0/3454	0.51	0/4672
1	F	0.40	0/3448	0.53	1/4664 (0.0%)
1	G	0.38	0/3460	0.51	0/4680
1	H	0.37	0/3454	0.52	0/4672
1	I	0.36	0/3454	0.49	0/4672
1	J	0.36	0/3433	0.50	0/4645
1	K	0.44	0/3427	0.61	1/4637 (0.0%)
All	All	0.39	0/37934	0.52	2/51314 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	452	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	F	574	ILE	CG1-CB-CG2	-5.38	99.58	111.40

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	11	0
1	B	3380	0	3200	15	0
1	C	3374	0	3195	12	0
1	D	3374	0	3195	11	0
1	E	3380	0	3200	16	0
1	F	3374	0	3195	21	0
1	G	3386	0	3204	10	1
1	H	3380	0	3200	7	0
1	I	3380	0	3200	13	0
1	J	3359	0	3179	18	0
1	K	3353	0	3173	52	0
2	A	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	10	0	7	2	0
3	K	10	0	7	0	0
4	A	370	0	0	1	0
4	B	277	0	0	3	0
4	C	368	0	0	2	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	3	2
4	K	83	0	0	0	0
All	All	40238	0	35218	187	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 (187) 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
1:C:580:MET:HE1	1:C:605:LYS:HD2	1.58	0.84
1:K:290:GLN:HE21	1:K:291:ASN:ND2	1.78	0.81
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:K:399:LYS:NZ	1:K:402:GLU:OE1	2.22	0.73
1:I:253:LYS:NZ	4:I:2013:HOH:O	2.22	0.73
1:A:406:SER:HG	1:A:464:TYR:HH	1.31	0.71
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: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:F:255:LYS:NZ	4:F:2023:HOH:O	2.30	0.63
1:F:406:SER:HG	1:F:464:TYR:HH	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:229:ASP:CG	1:K:230:VAL:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:434:ILE:HD12	1:K:449:GLN:HB3	1.96	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:K:274:LEU:O	1:K:277:GLU:HB2	2.15	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
1:J:336:GLU:HG2	1:J:632:PHE:CE2	2.50	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:C:633:LYS:NZ	4:C:2362:HOH:O	2.48	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:K:460:SER:O	1:K:463:ASP:HB2	2.16	0.45
1:D:336:GLU:HG2	1:D:632:PHE:CE2	2.51	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:J:580:MET:HE1	1:J:605:LYS:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:287:PHE:CE1	1:J:294:SER:HB3	2.52	0.44
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:E:240:LYS:NZ	1:E:611:GLU:OE1	2.43	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: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: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:K:529:TYR:HB2	1:K:564:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:384:GLU:O	1:D:384:GLU:HG2	2.20	0.41
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: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:399:LYS:HZ3	1:K:464:TYR:HB2	1.86	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:E:403:GLU:HG3	1:E:404:TYR:N	2.36	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: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:E:290:GLN:N	1:E:290:GLN:CD	2.74	0.40
1:H:253:LYS:HB3	1:H:253:LYS:HE2	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:550:TYR:CD1	1:F:629:PRO:HG2	2.56	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

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%)	29	31
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%)	367 (100%)	1 (0%)	92 97
1	B	368/403 (91%)	368 (100%)	0	100 100
1	C	367/403 (91%)	366 (100%)	1 (0%)	92 97
1	D	367/403 (91%)	367 (100%)	0	100 100
1	E	368/403 (91%)	365 (99%)	3 (1%)	81 90
1	F	367/403 (91%)	366 (100%)	1 (0%)	92 97
1	G	369/403 (92%)	368 (100%)	1 (0%)	92 97
1	H	368/403 (91%)	366 (100%)	2 (0%)	88 94
1	I	368/403 (91%)	368 (100%)	0	100 100
1	J	365/403 (91%)	363 (100%)	2 (0%)	88 94
1	K	364/403 (90%)	358 (98%)	6 (2%)	62 76
All	All	4039/4433 (91%)	4022 (100%)	17 (0%)	91 96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	C	535	LEU
1	E	247	GLU
1	E	290	GLN
1	E	467	LYS
1	F	389	ASN
1	G	535	LEU
1	H	360	TRP

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Mol	Chain	Res	Type
1	H	535	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	GLN
1	B	290	GLN
1	K	291	ASN
1	K	389	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	F	307	1,2	8,10,11	1.13	0	10,14,16	1.56	1 (10%)
1	TPO	E	307	1,2	8,10,11	1.05	0	10,14,16	1.57	2 (20%)
1	TPO	B	307	1,2	8,10,11	1.18	0	10,14,16	1.40	1 (10%)
1	TPO	G	307	1,2	8,10,11	1.14	0	10,14,16	1.53	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TPO	I	307	1,2	8,10,11	1.17	0	10,14,16	1.39	1 (10%)
1	TPO	C	307	1,2	8,10,11	1.16	0	10,14,16	1.33	2 (20%)
1	TPO	J	307	1,2	8,10,11	1.07	0	10,14,16	1.49	1 (10%)
1	TPO	D	307	1,2	8,10,11	1.12	0	10,14,16	1.60	1 (10%)
1	TPO	H	307	1,2	8,10,11	1.15	0	10,14,16	1.52	1 (10%)
1	TPO	K	307	1,2	8,10,11	1.18	0	10,14,16	1.64	1 (10%)
1	TPO	A	307	1,2	8,10,11	1.21	0	10,14,16	1.34	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	F	307	1,2	-	1/9/11/13	-
1	TPO	E	307	1,2	-	2/9/11/13	-
1	TPO	B	307	1,2	-	1/9/11/13	-
1	TPO	G	307	1,2	-	2/9/11/13	-
1	TPO	I	307	1,2	-	3/9/11/13	-
1	TPO	C	307	1,2	-	2/9/11/13	-
1	TPO	J	307	1,2	-	1/9/11/13	-
1	TPO	D	307	1,2	-	2/9/11/13	-
1	TPO	H	307	1,2	-	1/9/11/13	-
1	TPO	K	307	1,2	-	1/9/11/13	-
1	TPO	A	307	1,2	-	1/9/11/13	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	307	TPO	P-OG1-CB	-4.46	109.72	123.21
1	K	307	TPO	P-OG1-CB	-4.37	110.00	123.21
1	F	307	TPO	P-OG1-CB	-4.07	110.91	123.21
1	H	307	TPO	P-OG1-CB	-3.97	111.22	123.21
1	J	307	TPO	P-OG1-CB	-3.94	111.30	123.21
1	E	307	TPO	P-OG1-CB	-3.81	111.71	123.21
1	B	307	TPO	P-OG1-CB	-3.77	111.83	123.21
1	G	307	TPO	P-OG1-CB	-3.71	111.99	123.21
1	A	307	TPO	P-OG1-CB	-3.47	112.73	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	307	TPO	P-OG1-CB	-3.44	112.81	123.21
1	C	307	TPO	P-OG1-CB	-2.87	114.53	123.21
1	E	307	TPO	CG2-CB-CA	-2.37	108.49	113.16
1	C	307	TPO	CG2-CB-CA	-2.17	108.89	113.16

There are no chirality outliers.

All (17) 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	C	307	TPO	CB-OG1-P-O2P
1	E	307	TPO	CB-OG1-P-O2P
1	G	307	TPO	CB-OG1-P-O2P
1	I	307	TPO	CB-OG1-P-O1P
1	D	307	TPO	CB-OG1-P-O2P
1	I	307	TPO	CB-OG1-P-O2P
1	B	307	TPO	O-C-CA-CB
1	C	307	TPO	O-C-CA-CB
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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	C	700	-	9,9,9	0.59	0	11,12,12	1.16	2 (18%)
3	GP9	I	700	-	9,9,9	0.59	0	11,12,12	1.17	1 (9%)
3	GP9	F	700	-	9,9,9	0.48	0	11,12,12	1.05	1 (9%)
3	GP9	K	700	-	9,9,9	0.53	0	11,12,12	0.94	0
3	GP9	A	700	-	9,9,9	0.52	0	11,12,12	0.84	0
3	GP9	E	700	-	9,9,9	0.59	0	11,12,12	0.84	0
3	GP9	J	700	-	9,9,9	0.55	0	11,12,12	1.10	1 (9%)
3	GP9	D	700	-	9,9,9	0.63	0	11,12,12	1.02	0
3	GP9	H	700	-	9,9,9	0.59	0	11,12,12	0.95	0
3	GP9	G	700	-	9,9,9	0.47	0	11,12,12	0.97	0
3	GP9	B	700	-	9,9,9	0.48	0	11,12,12	1.02	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
3	GP9	C	700	-	-	2/8/8/8	-
3	GP9	I	700	-	-	2/8/8/8	-
3	GP9	F	700	-	-	2/8/8/8	-
3	GP9	K	700	-	-	4/8/8/8	-
3	GP9	A	700	-	-	7/8/8/8	-
3	GP9	E	700	-	-	4/8/8/8	-
3	GP9	J	700	-	-	2/8/8/8	-
3	GP9	D	700	-	-	2/8/8/8	-
3	GP9	H	700	-	-	2/8/8/8	-
3	GP9	G	700	-	-	4/8/8/8	-
3	GP9	B	700	-	-	2/8/8/8	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	700	GP9	P1-O4-C4	2.68	125.67	118.30
3	J	700	GP9	O10-P1-O9	2.34	116.58	107.64
3	C	700	GP9	P1-O4-C4	2.24	124.47	118.30
3	C	700	GP9	O9-P1-O4	-2.10	101.15	106.73
3	F	700	GP9	O10-P1-O9	2.04	115.44	107.64

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
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	F	700	GP9	1	0
3	J	700	GP9	2	0
3	B	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, 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(Å^2)	Q<0.9
1	A	417/459 (90%)	-0.35	3 (0%) 87 86	16, 24, 41, 65	0
1	B	417/459 (90%)	-0.23	4 (0%) 82 81	20, 28, 49, 67	0
1	C	416/459 (90%)	-0.28	4 (0%) 82 81	16, 25, 42, 69	0
1	D	416/459 (90%)	-0.25	2 (0%) 91 90	16, 28, 47, 69	0
1	E	417/459 (90%)	-0.29	3 (0%) 87 86	18, 26, 43, 73	0
1	F	416/459 (90%)	-0.34	4 (0%) 82 81	18, 26, 43, 76	0
1	G	417/459 (90%)	-0.25	2 (0%) 91 90	20, 28, 47, 70	0
1	H	417/459 (90%)	-0.36	4 (0%) 82 81	21, 30, 49, 76	0
1	I	417/459 (90%)	-0.16	5 (1%) 79 77	24, 33, 51, 88	0
1	J	416/459 (90%)	-0.10	15 (3%) 42 41	22, 37, 58, 88	1 (0%)
1	K	414/459 (90%)	0.85	64 (15%) 2 1	34, 54, 84, 115	1 (0%)
All	All	4580/5049 (90%)	-0.16	110 (2%) 59 56	16, 29, 60, 115	2 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	420	THR	6.9
1	K	390	TYR	6.5
1	K	465	LEU	6.4
1	K	401	SER	5.8
1	K	282	PHE	5.7
1	K	464	TYR	5.6
1	K	434	ILE	5.2
1	G	644	LYS	5.1
1	K	453	TYR	5.0
1	B	595	ALA	4.8
1	K	383	ASN	4.7
1	K	387	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	K	435	ALA	4.5
1	K	595	ALA	4.3
1	I	390	TYR	4.1
1	J	390	TYR	4.1
1	K	385	ALA	4.0
1	K	419	LEU	4.0
1	K	384	GLU	4.0
1	K	359	PHE	3.9
1	K	596	THR	3.9
1	B	228	SER	3.8
1	H	227	SER	3.6
1	K	360	TRP	3.6
1	K	582	GLY	3.6
1	K	426	PRO	3.5
1	J	378	SER	3.5
1	K	277	GLU	3.5
1	K	432	ALA	3.5
1	G	227	SER	3.5
1	D	644	LYS	3.5
1	F	390	TYR	3.5
1	J	430	LYS	3.5
1	K	382	MET	3.4
1	I	227	SER	3.3
1	B	596	THR	3.3
1	K	247	GLU	3.2
1	B	389	ASN	3.2
1	K	389	ASN	3.2
1	K	423	PHE	3.2
1	K	443	SER	3.2
1	K	521	VAL	3.1
1	J	643	ASN	3.1
1	K	291	ASN	3.1
1	J	379	TYR	3.1
1	K	290	GLN	3.0
1	I	389	ASN	3.0
1	K	356	TYR	2.9
1	K	523	GLY	2.9
1	K	274	LEU	2.9
1	K	427	ILE	2.9
1	K	248	TYR	2.9
1	K	452	ARG	2.8
1	E	390	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	642	TYR	2.8
1	K	524	GLY	2.8
1	J	641	ASN	2.7
1	J	596	THR	2.7
1	K	229	ASP	2.7
1	K	467	LYS	2.7
1	K	323	GLN	2.7
1	K	332	GLN	2.7
1	K	388	SER	2.6
1	K	431	ASP	2.6
1	K	246	PRO	2.6
1	K	437	ALA	2.6
1	F	359	PHE	2.6
1	C	228	SER	2.5
1	F	389	ASN	2.5
1	K	272	TYR	2.5
1	E	389	ASN	2.5
1	C	644	LYS	2.5
1	K	428	ASP	2.4
1	A	390	TYR	2.4
1	K	380	TYR	2.4
1	J	639	LYS	2.4
1	I	596	THR	2.4
1	F	644	LYS	2.4
1	I	388	SER	2.4
1	J	377	ALA	2.3
1	A	429	GLU	2.3
1	C	390	TYR	2.3
1	K	430	LYS	2.3
1	K	454	LEU	2.3
1	J	403	GLU	2.3
1	E	290	GLN	2.3
1	K	444	VAL	2.3
1	H	228	SER	2.3
1	J	389	ASN	2.2
1	K	460	SER	2.2
1	K	279	VAL	2.2
1	K	442	SER	2.2
1	H	644	LYS	2.2
1	K	626	PHE	2.2
1	K	463	ASP	2.2
1	H	643	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	227	SER	2.2
1	K	377	ALA	2.2
1	K	487	ASP	2.2
1	J	331	GLY	2.1
1	C	389	ASN	2.1
1	D	641	ASN	2.1
1	K	425	TYR	2.1
1	J	384	GLU	2.1
1	K	245	ASN	2.1
1	K	429	GLU	2.1
1	K	461	PHE	2.1
1	K	458	VAL	2.0
1	J	381	ASP	2.0
1	K	522	GLN	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, 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
1	TPO	K	307	11/12	0.94	0.10	47,60,71,72	0
1	TPO	H	307	11/12	0.97	0.09	22,26,31,32	0
1	TPO	C	307	11/12	0.98	0.09	19,21,25,28	0
1	TPO	D	307	11/12	0.98	0.11	20,22,26,26	0
1	TPO	E	307	11/12	0.98	0.10	22,24,28,29	0
1	TPO	F	307	11/12	0.98	0.08	18,23,31,31	0
1	TPO	G	307	11/12	0.98	0.13	22,24,32,40	0
1	TPO	A	307	11/12	0.98	0.12	20,23,27,32	0
1	TPO	I	307	11/12	0.98	0.09	26,30,32,35	0
1	TPO	J	307	11/12	0.98	0.11	26,32,39,40	0
1	TPO	B	307	11/12	0.98	0.12	20,24,28,32	0

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
2	MG	K	699	1/1	0.58	0.10	69,69,69,69	0
2	MG	J	699	1/1	0.84	0.42	54,54,54,54	0
3	GP9	K	700	10/10	0.89	0.27	72,79,88,89	0
2	MG	E	699	1/1	0.91	0.40	41,41,41,41	0
2	MG	C	699	1/1	0.91	0.20	40,40,40,40	0
2	MG	B	699	1/1	0.92	0.17	46,46,46,46	0
2	MG	G	699	1/1	0.93	0.11	40,40,40,40	0
2	MG	I	699	1/1	0.94	0.15	47,47,47,47	0
2	MG	H	699	1/1	0.94	0.15	40,40,40,40	0
3	GP9	B	700	10/10	0.95	0.17	24,35,39,44	0
2	MG	F	699	1/1	0.95	0.21	43,43,43,43	0
2	MG	A	699	1/1	0.96	0.11	40,40,40,40	0
3	GP9	D	700	10/10	0.97	0.13	20,24,33,44	0
3	GP9	J	700	10/10	0.97	0.15	28,32,40,46	0
3	GP9	C	700	10/10	0.97	0.11	26,29,41,44	0
3	GP9	F	700	10/10	0.98	0.10	22,29,38,42	0
3	GP9	G	700	10/10	0.98	0.11	27,33,47,55	0
3	GP9	H	700	10/10	0.98	0.13	29,33,43,47	0
3	GP9	I	700	10/10	0.98	0.14	29,34,47,48	0
2	MG	D	699	1/1	0.98	0.10	36,36,36,36	0
3	GP9	E	700	10/10	0.98	0.10	23,29,39,45	0
3	GP9	A	700	10/10	0.99	0.11	19,25,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.