



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 12:40 pm GMT

PDB ID : 1Q1G
Title : Crystal structure of Plasmodium falciparum PNP with 5'-methylthio-immucillin-H
Authors : Shi, W.; Ting, L.M.; Kicska, G.A.; Lewandowicz, A.; Tyler, P.C.; Evans, G.B.; Furneaux, R.H.; Kim, K.; Almo, S.C.; Schramm, V.L.
Deposited on : 2003-07-19
Resolution : 2.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

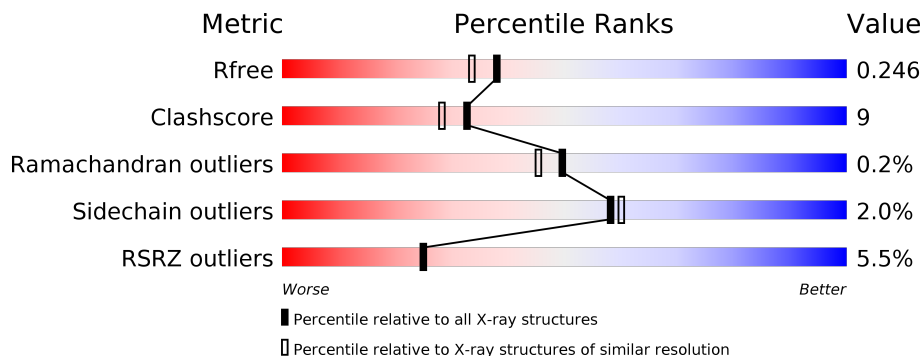
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	111664	9172 (2.04-2.00)
Clashscore	122126	10355 (2.04-2.00)
Ramachandran outliers	120053	10237 (2.04-2.00)
Sidechain outliers	120020	10236 (2.04-2.00)
RSRZ outliers	108989	8961 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	276	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>12%</div> </div> </div>
1	B	276	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>• 12%</div> </div> </div>
1	C	276	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>• 12%</div> </div> </div>
1	D	276	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>12%</div> </div> </div>
1	E	276	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>• 12%</div> </div> </div>
1	F	276	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>• 12%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11789 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 Uridine phosphorylase putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1861	1179	319	347	16			
1	B	243	Total	C	N	O	S	0	0	0
			1861	1179	319	347	16			
1	C	243	Total	C	N	O	S	0	0	0
			1861	1179	319	347	16			
1	D	243	Total	C	N	O	S	0	0	0
			1861	1179	319	347	16			
1	E	243	Total	C	N	O	S	0	0	0
			1861	1179	319	347	16			
1	F	243	Total	C	N	O	S	0	0	0
			1861	1179	319	347	16			

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
A	1	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
A	246	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
A	247	GLY	-	CLONING ARTIFACT	UNP Q8I3X4
A	248	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
A	249	PHE	-	CLONING ARTIFACT	UNP Q8I3X4
A	250	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
A	251	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
A	252	TYR	-	CLONING ARTIFACT	UNP Q8I3X4
A	253	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
A	254	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
A	255	GLN	-	CLONING ARTIFACT	UNP Q8I3X4
A	256	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
A	257	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
A	258	ILE	-	CLONING ARTIFACT	UNP Q8I3X4
A	259	SER	-	CLONING ARTIFACT	UNP Q8I3X4
A	260	GLU	-	CLONING ARTIFACT	UNP Q8I3X4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
A	262	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
A	263	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
A	264	ASN	-	CLONING ARTIFACT	UNP Q8I3X4
A	265	SER	-	CLONING ARTIFACT	UNP Q8I3X4
A	266	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
A	267	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
A	268	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
A	269	HIS	-	EXPRESSION TAG	UNP Q8I3X4
A	270	HIS	-	EXPRESSION TAG	UNP Q8I3X4
A	271	HIS	-	EXPRESSION TAG	UNP Q8I3X4
A	272	HIS	-	EXPRESSION TAG	UNP Q8I3X4
A	273	HIS	-	EXPRESSION TAG	UNP Q8I3X4
A	274	HIS	-	EXPRESSION TAG	UNP Q8I3X4
B	0	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
B	1	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
B	246	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
B	247	GLY	-	CLONING ARTIFACT	UNP Q8I3X4
B	248	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
B	249	PHE	-	CLONING ARTIFACT	UNP Q8I3X4
B	250	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
B	251	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
B	252	TYR	-	CLONING ARTIFACT	UNP Q8I3X4
B	253	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
B	254	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
B	255	GLN	-	CLONING ARTIFACT	UNP Q8I3X4
B	256	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
B	257	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
B	258	ILE	-	CLONING ARTIFACT	UNP Q8I3X4
B	259	SER	-	CLONING ARTIFACT	UNP Q8I3X4
B	260	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
B	261	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
B	262	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
B	263	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
B	264	ASN	-	CLONING ARTIFACT	UNP Q8I3X4
B	265	SER	-	CLONING ARTIFACT	UNP Q8I3X4
B	266	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
B	267	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
B	268	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
B	269	HIS	-	EXPRESSION TAG	UNP Q8I3X4
B	270	HIS	-	EXPRESSION TAG	UNP Q8I3X4
B	271	HIS	-	EXPRESSION TAG	UNP Q8I3X4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	272	HIS	-	EXPRESSION TAG	UNP Q8I3X4
B	273	HIS	-	EXPRESSION TAG	UNP Q8I3X4
B	274	HIS	-	EXPRESSION TAG	UNP Q8I3X4
C	0	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
C	1	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
C	246	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
C	247	GLY	-	CLONING ARTIFACT	UNP Q8I3X4
C	248	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
C	249	PHE	-	CLONING ARTIFACT	UNP Q8I3X4
C	250	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
C	251	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
C	252	TYR	-	CLONING ARTIFACT	UNP Q8I3X4
C	253	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
C	254	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
C	255	GLN	-	CLONING ARTIFACT	UNP Q8I3X4
C	256	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
C	257	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
C	258	ILE	-	CLONING ARTIFACT	UNP Q8I3X4
C	259	SER	-	CLONING ARTIFACT	UNP Q8I3X4
C	260	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
C	261	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
C	262	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
C	263	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
C	264	ASN	-	CLONING ARTIFACT	UNP Q8I3X4
C	265	SER	-	CLONING ARTIFACT	UNP Q8I3X4
C	266	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
C	267	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
C	268	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
C	269	HIS	-	EXPRESSION TAG	UNP Q8I3X4
C	270	HIS	-	EXPRESSION TAG	UNP Q8I3X4
C	271	HIS	-	EXPRESSION TAG	UNP Q8I3X4
C	272	HIS	-	EXPRESSION TAG	UNP Q8I3X4
C	273	HIS	-	EXPRESSION TAG	UNP Q8I3X4
C	274	HIS	-	EXPRESSION TAG	UNP Q8I3X4
D	0	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
D	1	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
D	246	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
D	247	GLY	-	CLONING ARTIFACT	UNP Q8I3X4
D	248	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
D	249	PHE	-	CLONING ARTIFACT	UNP Q8I3X4
D	250	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
D	251	ALA	-	CLONING ARTIFACT	UNP Q8I3X4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	252	TYR	-	CLONING ARTIFACT	UNP Q8I3X4
D	253	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
D	254	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
D	255	GLN	-	CLONING ARTIFACT	UNP Q8I3X4
D	256	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
D	257	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
D	258	ILE	-	CLONING ARTIFACT	UNP Q8I3X4
D	259	SER	-	CLONING ARTIFACT	UNP Q8I3X4
D	260	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
D	261	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
D	262	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
D	263	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
D	264	ASN	-	CLONING ARTIFACT	UNP Q8I3X4
D	265	SER	-	CLONING ARTIFACT	UNP Q8I3X4
D	266	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
D	267	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
D	268	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
D	269	HIS	-	EXPRESSION TAG	UNP Q8I3X4
D	270	HIS	-	EXPRESSION TAG	UNP Q8I3X4
D	271	HIS	-	EXPRESSION TAG	UNP Q8I3X4
D	272	HIS	-	EXPRESSION TAG	UNP Q8I3X4
D	273	HIS	-	EXPRESSION TAG	UNP Q8I3X4
D	274	HIS	-	EXPRESSION TAG	UNP Q8I3X4
E	0	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
E	1	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
E	246	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
E	247	GLY	-	CLONING ARTIFACT	UNP Q8I3X4
E	248	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
E	249	PHE	-	CLONING ARTIFACT	UNP Q8I3X4
E	250	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
E	251	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
E	252	TYR	-	CLONING ARTIFACT	UNP Q8I3X4
E	253	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
E	254	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
E	255	GLN	-	CLONING ARTIFACT	UNP Q8I3X4
E	256	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
E	257	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
E	258	ILE	-	CLONING ARTIFACT	UNP Q8I3X4
E	259	SER	-	CLONING ARTIFACT	UNP Q8I3X4
E	260	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
E	261	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
E	262	ASP	-	CLONING ARTIFACT	UNP Q8I3X4

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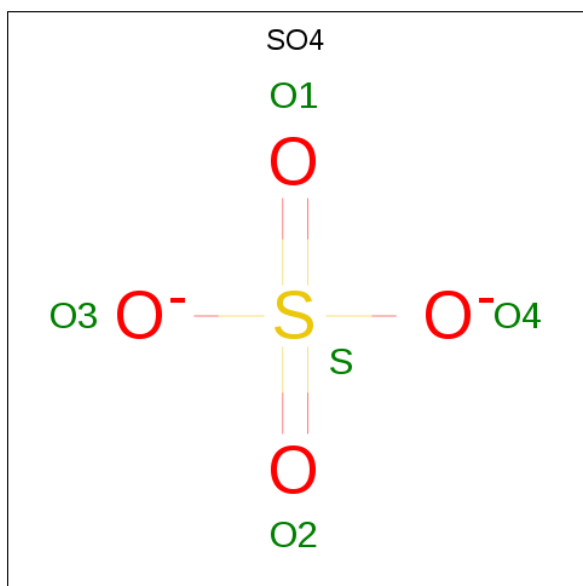
Chain	Residue	Modelled	Actual	Comment	Reference
E	263	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
E	264	ASN	-	CLONING ARTIFACT	UNP Q8I3X4
E	265	SER	-	CLONING ARTIFACT	UNP Q8I3X4
E	266	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
E	267	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
E	268	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
E	269	HIS	-	EXPRESSION TAG	UNP Q8I3X4
E	270	HIS	-	EXPRESSION TAG	UNP Q8I3X4
E	271	HIS	-	EXPRESSION TAG	UNP Q8I3X4
E	272	HIS	-	EXPRESSION TAG	UNP Q8I3X4
E	273	HIS	-	EXPRESSION TAG	UNP Q8I3X4
E	274	HIS	-	EXPRESSION TAG	UNP Q8I3X4
F	0	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
F	1	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
F	246	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
F	247	GLY	-	CLONING ARTIFACT	UNP Q8I3X4
F	248	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
F	249	PHE	-	CLONING ARTIFACT	UNP Q8I3X4
F	250	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
F	251	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
F	252	TYR	-	CLONING ARTIFACT	UNP Q8I3X4
F	253	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
F	254	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
F	255	GLN	-	CLONING ARTIFACT	UNP Q8I3X4
F	256	LYS	-	CLONING ARTIFACT	UNP Q8I3X4
F	257	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
F	258	ILE	-	CLONING ARTIFACT	UNP Q8I3X4
F	259	SER	-	CLONING ARTIFACT	UNP Q8I3X4
F	260	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
F	261	GLU	-	CLONING ARTIFACT	UNP Q8I3X4
F	262	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
F	263	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
F	264	ASN	-	CLONING ARTIFACT	UNP Q8I3X4
F	265	SER	-	CLONING ARTIFACT	UNP Q8I3X4
F	266	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
F	267	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
F	268	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
F	269	HIS	-	EXPRESSION TAG	UNP Q8I3X4
F	270	HIS	-	EXPRESSION TAG	UNP Q8I3X4
F	271	HIS	-	EXPRESSION TAG	UNP Q8I3X4
F	272	HIS	-	EXPRESSION TAG	UNP Q8I3X4
F	273	HIS	-	EXPRESSION TAG	UNP Q8I3X4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	274	HIS	-	EXPRESSION TAG	UNP Q8I3X4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



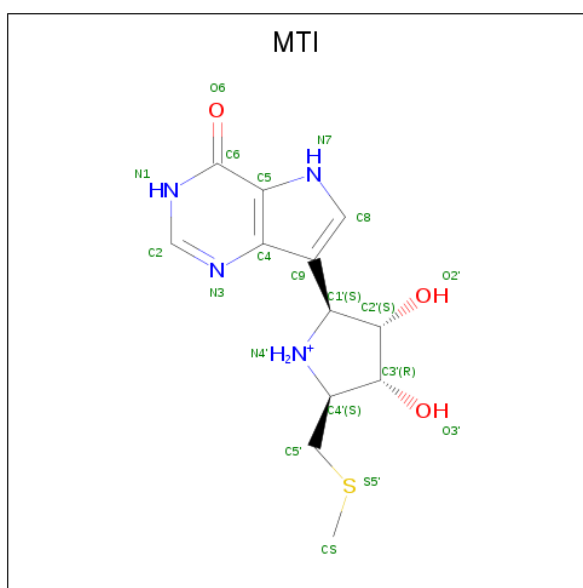
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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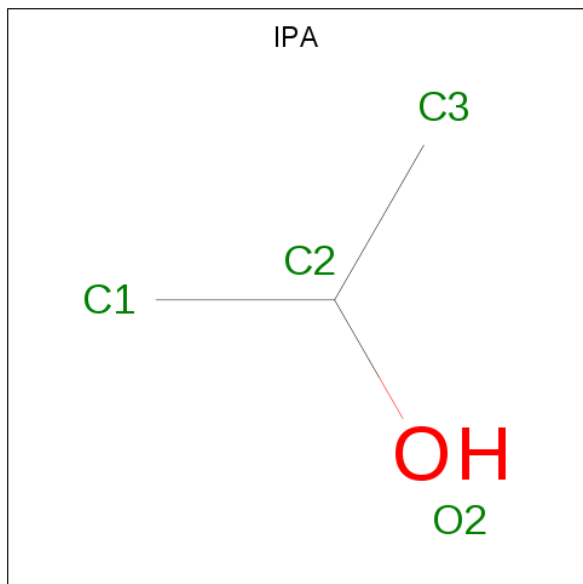
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3,4-DIHYDROXY-2-[(METHYLSULFANYL)METHYL]-5-(4-OXO-4,5-DIHYDRO-3H-PYRROLO[3,2-D]PYRIMIDIN-7-YL)PYRROLIDINIUM (three-letter code: MTI) (formula: $C_{12}H_{17}N_4O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	12	4	3	1		
3	B	1	Total	C	N	O	S	0	0
			20	12	4	3	1		
3	C	1	Total	C	N	O	S	0	0
			20	12	4	3	1		
3	D	1	Total	C	N	O	S	0	0
			20	12	4	3	1		
3	E	1	Total	C	N	O	S	0	0
			20	12	4	3	1		
3	F	1	Total	C	N	O	S	0	0
			20	12	4	3	1		

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	D	1	Total	C	O	0	0
			4	3	1		
4	D	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	3	1		
4	F	1	Total	C	O	0	0
			4	3	1		
4	F	1	Total	C	O	0	0
			4	3	1		

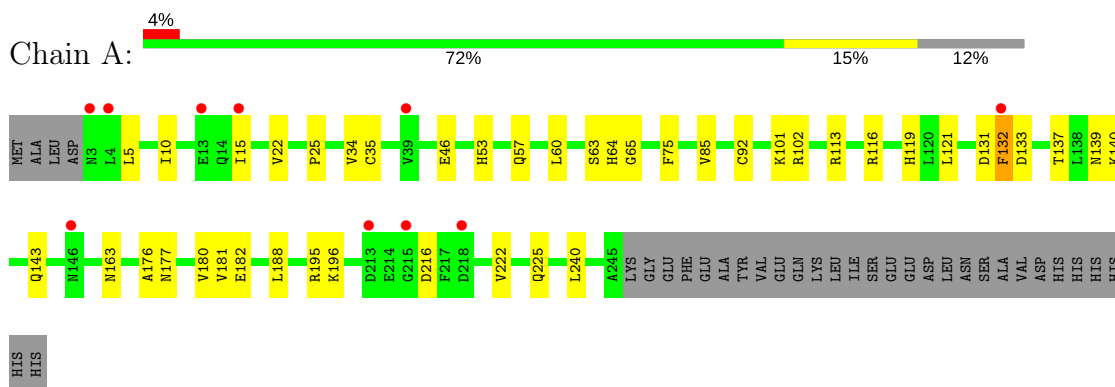
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	45	Total	O	0	0
			45	45		
5	C	51	Total	O	0	0
			51	51		
5	D	61	Total	O	0	0
			61	61		
5	E	65	Total	O	0	0
			65	65		
5	F	79	Total	O	0	0
			79	79		

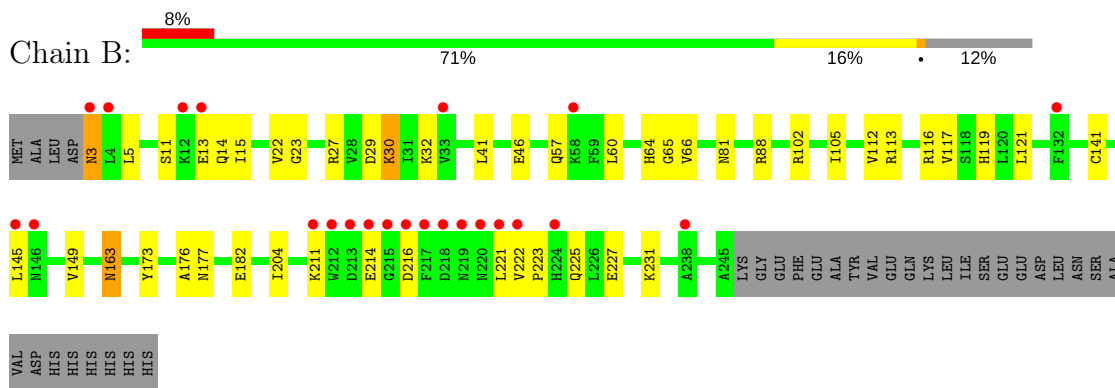
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

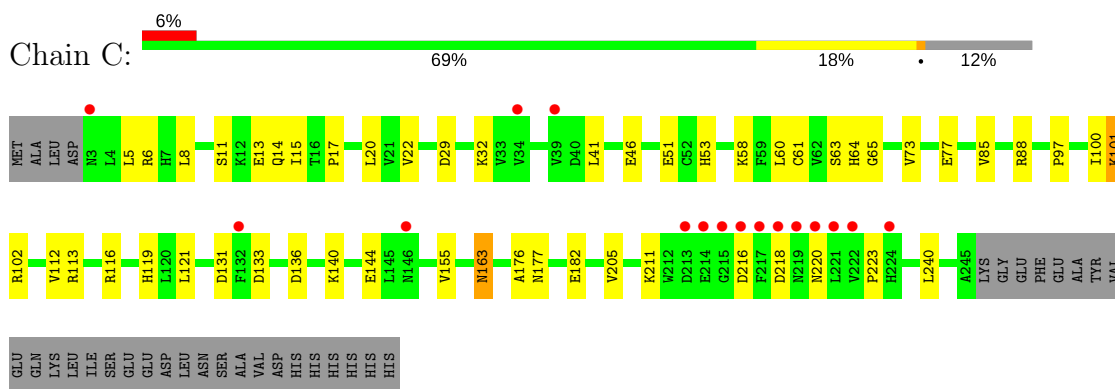
- Molecule 1: Uridine phosphorylase putative



- Molecule 1: Uridine phosphorylase putative



- Molecule 1: Uridine phosphorylase putative



Chain D:

[illegible]

Figure 1: Chain F: A horizontal bar chart showing the percentage of amino acids in Chain F. The bar is color-coded: green for 70%, yellow for 17%, and grey for 12%. The amino acids are listed on the left, and their corresponding percentages are shown on the right.

Amino Acid	Percentage
MET	12%
HIS	12%
HIS	12%
HIS	12%
HIS	12%
LEU	17%
ASP	17%
R3	70%
L4	70%
L5	70%
E13	70%
E14	70%
I15	70%
V22	70%
G23	70%
D24	70%
P25	70%
V34	70%
V39	70%
D40	70%
L41	70%
E46	70%
E51	70%
Q57	70%
L60	70%
S63	70%
H64	70%
G65	70%
V73	70%
E77	70%
N81	70%
C92	70%
G93	70%
I100	70%
K101	70%
R102	70%
R113	70%
R116	70%
V117	70%
S118	70%
H119	70%
L120	70%
L121	70%
Y135	70%
V140	70%
E144	70%
L145	70%
N146	70%
Y160	70%
A176	70%
N177	70%
V180	70%
V181	70%
E192	70%
V205	70%
D216	70%
F217	70%
D218	70%
N219	70%
N220	70%
L221	70%
V222	70%
P223	70%
H224	70%
Q225	70%
L226	70%
E227	70%
I230	70%
K231	70%
A241	70%
A245	70%
LYS	17%
GLY	17%
GLU	17%
PHE	17%
GLU	17%
ALA	17%
TYR	17%
VAL	17%
GLU	17%
GLN	17%
LYS	17%
LEU	17%
ILE	17%
SER	17%
GLU	17%
ASP	17%
LEU	17%
ASN	17%
SER	17%
ALA	17%
VAL	17%
ASP	17%
HIS	17%

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.44Å 91.73Å 238.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.02 45.87 – 2.02	Depositor EDS
% Data completeness (in resolution range)	88.8 (30.00-2.02) 91.5 (45.87-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.03Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.242 0.215 , 0.246	Depositor DCC
R_{free} test set	11403 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11789	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: MTI, IPA, SO4

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	0.32	0/1893	0.58	0/2561
1	B	0.30	0/1893	0.56	0/2561
1	C	0.31	0/1893	0.57	0/2561
1	D	0.31	0/1893	0.59	0/2561
1	E	0.33	0/1893	0.59	0/2561
1	F	0.33	0/1893	0.59	0/2561
All	All	0.32	0/11358	0.58	0/15366

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1861	0	1882	35	0
1	B	1861	0	1882	38	0
1	C	1861	0	1882	35	0
1	D	1861	0	1882	41	0
1	E	1861	0	1882	38	0
1	F	1861	0	1882	40	0
2	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	0	0	0
2	C	15	0	0	0	0
2	D	20	0	0	1	0
2	E	15	0	0	0	0
2	F	20	0	0	0	0
3	A	20	0	17	0	0
3	B	20	0	17	2	0
3	C	20	0	17	1	0
3	D	20	0	17	0	0
3	E	20	0	17	2	0
3	F	20	0	17	1	0
4	A	4	0	8	0	0
4	B	12	0	24	1	0
4	D	8	0	16	1	0
4	E	4	0	8	0	0
4	F	8	0	16	1	0
5	A	56	0	0	2	0
5	B	45	0	0	1	0
5	C	51	0	0	1	0
5	D	61	0	0	3	0
5	E	65	0	0	3	0
5	F	79	0	0	2	0
All	All	11789	0	11466	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 215 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:C:5:LEU:HD11	1:C:15:ILE:HD11	1.49	0.94
1:D:163:ASN:HD22	1:D:164:LYS:H	1.20	0.89
1:E:102:ARG:HH11	1:E:102:ARG:HB2	1.37	0.86
1:A:133:ASP:O	1:A:137:THR:HG23	1.76	0.84
1:B:5:LEU:HD11	1:B:15:ILE:HD11	1.61	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/276 (87%)	231 (96%)	10 (4%)	0	100	100
1	B	241/276 (87%)	234 (97%)	6 (2%)	1 (0%)	36	30
1	C	241/276 (87%)	228 (95%)	12 (5%)	1 (0%)	36	30
1	D	241/276 (87%)	230 (95%)	11 (5%)	0	100	100
1	E	241/276 (87%)	234 (97%)	6 (2%)	1 (0%)	36	30
1	F	241/276 (87%)	233 (97%)	8 (3%)	0	100	100
All	All	1446/1656 (87%)	1390 (96%)	53 (4%)	3 (0%)	49	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	PRO
1	E	223	PRO
1	C	223	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/235 (88%)	203 (98%)	3 (2%)	67	71
1	B	206/235 (88%)	201 (98%)	5 (2%)	52	52
1	C	206/235 (88%)	202 (98%)	4 (2%)	60	62
1	D	206/235 (88%)	203 (98%)	3 (2%)	67	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	206/235 (88%)	201 (98%)	5 (2%)	52	52
1	F	206/235 (88%)	201 (98%)	5 (2%)	52	52
All	All	1236/1410 (88%)	1211 (98%)	25 (2%)	58	60

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	182	GLU
1	D	163	ASN
1	F	180	VAL
1	D	121	LEU
1	D	182	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	228	ASN
1	D	64	HIS
1	F	64	HIS
1	D	57	GLN
1	D	119	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

37 ligands 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$
3	MTI	A	301	-	18,22,22	2.82	9 (50%)	15,32,32	2.86	5 (33%)
2	SO4	A	401	-	4,4,4	1.87	1 (25%)	6,6,6	0.86	0
2	SO4	A	413	-	4,4,4	1.91	1 (25%)	6,6,6	0.89	0
2	SO4	A	414	-	4,4,4	1.91	1 (25%)	6,6,6	0.82	0
2	SO4	A	418	-	4,4,4	1.93	1 (25%)	6,6,6	0.90	0
4	IPA	A	503	-	3,3,3	0.32	0	3,3,3	0.38	0
3	MTI	B	302	-	18,22,22	2.80	9 (50%)	15,32,32	2.94	5 (33%)
2	SO4	B	402	-	4,4,4	1.85	1 (25%)	6,6,6	0.89	0
2	SO4	B	407	-	4,4,4	1.88	1 (25%)	6,6,6	0.93	0
2	SO4	B	410	-	4,4,4	1.91	1 (25%)	6,6,6	0.90	0
2	SO4	B	417	-	4,4,4	1.89	1 (25%)	6,6,6	0.90	0
4	IPA	B	501	-	3,3,3	0.30	0	3,3,3	0.35	0
4	IPA	B	502	-	3,3,3	0.33	0	3,3,3	0.36	0
4	IPA	B	508	-	3,3,3	0.36	0	3,3,3	0.37	0
3	MTI	C	303	-	18,22,22	2.73	9 (50%)	15,32,32	3.00	5 (33%)
2	SO4	C	403	-	4,4,4	1.87	1 (25%)	6,6,6	0.83	0
2	SO4	C	416	-	4,4,4	1.91	1 (25%)	6,6,6	0.86	0
2	SO4	C	422	-	4,4,4	1.91	1 (25%)	6,6,6	0.89	0
3	MTI	D	304	-	18,22,22	2.71	9 (50%)	15,32,32	2.97	5 (33%)
2	SO4	D	404	-	4,4,4	1.90	1 (25%)	6,6,6	0.87	0
2	SO4	D	408	-	4,4,4	1.83	1 (25%)	6,6,6	0.85	0
2	SO4	D	412	-	4,4,4	1.89	1 (25%)	6,6,6	0.91	0
2	SO4	D	421	-	4,4,4	1.94	1 (25%)	6,6,6	0.91	0
4	IPA	D	507	-	3,3,3	0.29	0	3,3,3	0.34	0
4	IPA	D	509	-	3,3,3	0.32	0	3,3,3	0.34	0
3	MTI	E	305	-	18,22,22	2.76	9 (50%)	15,32,32	2.89	5 (33%)
2	SO4	E	405	-	4,4,4	1.89	1 (25%)	6,6,6	0.87	0
2	SO4	E	415	-	4,4,4	1.85	1 (25%)	6,6,6	0.90	0
2	SO4	E	420	-	4,4,4	1.92	1 (25%)	6,6,6	0.91	0
4	IPA	E	506	-	3,3,3	0.24	0	3,3,3	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MTI	F	306	-	18,22,22	2.71	9 (50%)	15,32,32	2.94	5 (33%)
2	SO4	F	406	-	4,4,4	1.85	1 (25%)	6,6,6	0.82	0
2	SO4	F	409	-	4,4,4	1.88	1 (25%)	6,6,6	0.89	0
2	SO4	F	411	-	4,4,4	1.83	1 (25%)	6,6,6	0.90	0
2	SO4	F	419	-	4,4,4	1.93	1 (25%)	6,6,6	0.91	0
4	IPA	F	504	-	3,3,3	0.30	0	3,3,3	0.33	0
4	IPA	F	505	-	3,3,3	0.32	0	3,3,3	0.36	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	MTI	A	301	-	-	0/3/23/23	0/3/3/3
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	413	-	-	0/0/0/0	0/0/0/0
2	SO4	A	414	-	-	0/0/0/0	0/0/0/0
2	SO4	A	418	-	-	0/0/0/0	0/0/0/0
4	IPA	A	503	-	-	0/0/0/0	0/0/0/0
3	MTI	B	302	-	-	0/3/23/23	0/3/3/3
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	407	-	-	0/0/0/0	0/0/0/0
2	SO4	B	410	-	-	0/0/0/0	0/0/0/0
2	SO4	B	417	-	-	0/0/0/0	0/0/0/0
4	IPA	B	501	-	-	0/0/0/0	0/0/0/0
4	IPA	B	502	-	-	0/0/0/0	0/0/0/0
4	IPA	B	508	-	-	0/0/0/0	0/0/0/0
3	MTI	C	303	-	-	0/3/23/23	0/3/3/3
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	SO4	C	416	-	-	0/0/0/0	0/0/0/0
2	SO4	C	422	-	-	0/0/0/0	0/0/0/0
3	MTI	D	304	-	-	0/3/23/23	0/3/3/3
2	SO4	D	404	-	-	0/0/0/0	0/0/0/0
2	SO4	D	408	-	-	0/0/0/0	0/0/0/0
2	SO4	D	412	-	-	0/0/0/0	0/0/0/0
2	SO4	D	421	-	-	0/0/0/0	0/0/0/0
4	IPA	D	507	-	-	0/0/0/0	0/0/0/0
4	IPA	D	509	-	-	0/0/0/0	0/0/0/0
3	MTI	E	305	-	-	0/3/23/23	0/3/3/3
2	SO4	E	405	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	415	-	-	0/0/0/0	0/0/0/0
2	SO4	E	420	-	-	0/0/0/0	0/0/0/0
4	IPA	E	506	-	-	0/0/0/0	0/0/0/0
3	MTI	F	306	-	-	0/3/23/23	0/3/3/3
2	SO4	F	406	-	-	0/0/0/0	0/0/0/0
2	SO4	F	409	-	-	0/0/0/0	0/0/0/0
2	SO4	F	411	-	-	0/0/0/0	0/0/0/0
2	SO4	F	419	-	-	0/0/0/0	0/0/0/0
4	IPA	F	504	-	-	0/0/0/0	0/0/0/0
4	IPA	F	505	-	-	0/0/0/0	0/0/0/0

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	MTI	C8-N7	-2.63	1.31	1.36
3	C	303	MTI	C8-N7	-2.48	1.31	1.36
3	D	304	MTI	C8-N7	-2.45	1.31	1.36
3	B	302	MTI	C8-N7	-2.31	1.31	1.36
3	E	305	MTI	C8-N7	-2.30	1.31	1.36

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	MTI	N3-C2-N1	-8.72	121.40	128.86
3	D	304	MTI	N3-C2-N1	-8.63	121.47	128.86
3	F	306	MTI	N3-C2-N1	-8.57	121.53	128.86
3	B	302	MTI	N3-C2-N1	-8.53	121.56	128.86
3	A	301	MTI	N3-C2-N1	-8.38	121.69	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	413	SO4	1	0
3	B	302	MTI	2	0
4	B	501	IPA	1	0
3	C	303	MTI	1	0
2	D	412	SO4	1	0
4	D	509	IPA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	305	MTI	2	0
3	F	306	MTI	1	0
4	F	504	IPA	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	243/276 (88%)	0.21	10 (4%) 37 37	14, 29, 47, 57	0
1	B	243/276 (88%)	0.56	23 (9%) 8 8	14, 33, 51, 62	0
1	C	243/276 (88%)	0.46	16 (6%) 18 18	12, 29, 48, 62	0
1	D	243/276 (88%)	0.36	12 (4%) 29 29	11, 28, 47, 58	0
1	E	243/276 (88%)	0.20	15 (6%) 20 20	10, 24, 45, 63	0
1	F	243/276 (88%)	0.19	4 (1%) 72 71	11, 24, 41, 51	0
All	All	1458/1656 (88%)	0.33	80 (5%) 25 25	10, 27, 48, 63	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	5.3
1	C	3	ASN	5.3
1	A	132	PHE	5.1
1	E	213	ASP	5.0
1	C	219	ASN	4.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IPA	B	501	4/4	0.49	0.30	29,30,30,31	0
4	IPA	D	509	4/4	0.62	0.27	24,24,24,27	0
4	IPA	F	505	4/4	0.66	0.28	24,26,27,28	0
4	IPA	B	508	4/4	0.73	0.23	24,24,25,26	0
4	IPA	F	504	4/4	0.79	0.25	15,18,21,23	0
4	IPA	B	502	4/4	0.82	0.20	21,21,22,24	0
4	IPA	E	506	4/4	0.83	0.20	23,24,26,26	0
4	IPA	A	503	4/4	0.85	0.15	23,24,25,26	0
4	IPA	D	507	4/4	0.88	0.16	19,21,22,22	0
2	SO4	B	410	5/5	0.90	0.25	69,70,70,70	0
2	SO4	A	413	5/5	0.91	0.33	65,65,66,66	0
2	SO4	F	419	5/5	0.92	0.18	48,51,52,52	0
3	MTI	C	303	20/20	0.92	0.15	25,30,41,44	0
3	MTI	B	302	20/20	0.92	0.13	27,34,46,48	0
2	SO4	B	417	5/5	0.93	0.16	69,70,70,71	0
3	MTI	E	305	20/20	0.93	0.14	26,28,37,42	0
3	MTI	A	301	20/20	0.94	0.12	19,22,34,36	0
2	SO4	E	420	5/5	0.94	0.14	44,46,47,48	0
2	SO4	A	418	5/5	0.94	0.16	59,59,59,62	0
3	MTI	F	306	20/20	0.95	0.14	18,20,32,34	0
2	SO4	C	422	5/5	0.95	0.10	44,45,48,48	0
3	MTI	D	304	20/20	0.95	0.15	19,20,33,36	0
2	SO4	D	421	5/5	0.95	0.19	56,57,58,58	0
2	SO4	D	412	5/5	0.95	0.16	52,52,54,54	0
2	SO4	F	411	5/5	0.96	0.13	40,41,44,44	0
2	SO4	F	406	5/5	0.96	0.10	23,24,26,27	0
2	SO4	B	402	5/5	0.96	0.11	40,40,42,42	0
2	SO4	A	401	5/5	0.97	0.12	32,32,35,35	0
2	SO4	D	408	5/5	0.97	0.09	18,25,25,27	0
2	SO4	C	403	5/5	0.97	0.13	30,31,34,35	0
2	SO4	D	404	5/5	0.97	0.12	29,29,30,30	0
2	SO4	B	407	5/5	0.98	0.10	25,27,29,31	0
2	SO4	F	409	5/5	0.98	0.06	20,23,29,30	0
2	SO4	C	416	5/5	0.98	0.07	25,26,27,29	0
2	SO4	E	415	5/5	0.98	0.09	20,22,26,27	0
2	SO4	E	405	5/5	0.98	0.11	26,27,27,28	0
2	SO4	A	414	5/5	0.98	0.08	22,26,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.