



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:11 PM GMT

PDB ID : 1NW4
Title : Crystal Structure of Plasmodium falciparum Purine Nucleoside Phosphorylase
in complex with ImmH and Sulfate
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 : 2003-02-05
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

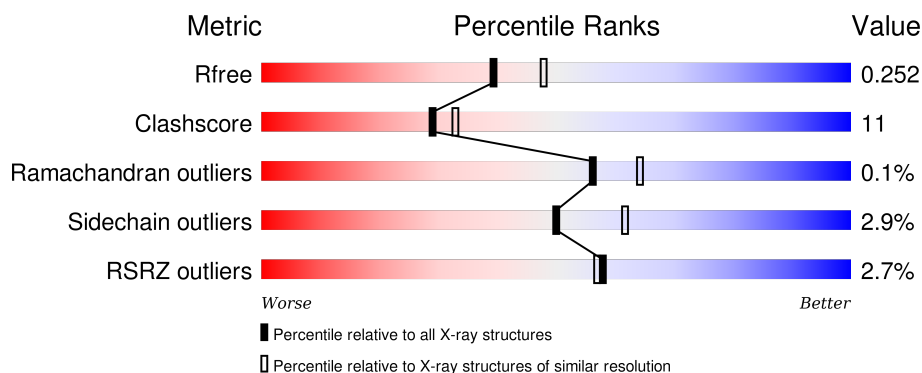
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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>3%</div> <div>63% 23% 12%</div> </div>
1	B	276	<div> <div>3%</div> <div>63% 23% 12%</div> </div>
1	C	276	<div> <div>3%</div> <div>67% 19% 12%</div> </div>
1	D	276	<div> <div>2%</div> <div>67% 20% 12%</div> </div>
1	E	276	<div> <div>2%</div> <div>66% 20% 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	276	 % 69% 18% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	F	415	-	-	-	X
4	IPA	A	510	-	-	-	X
4	IPA	B	501	-	-	-	X
4	IPA	B	508	-	-	-	X
4	IPA	C	504	-	-	-	X
4	IPA	D	514	-	-	-	X
4	IPA	E	506	-	-	-	X
4	IPA	E	513	-	-	-	X
4	IPA	F	505	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11683 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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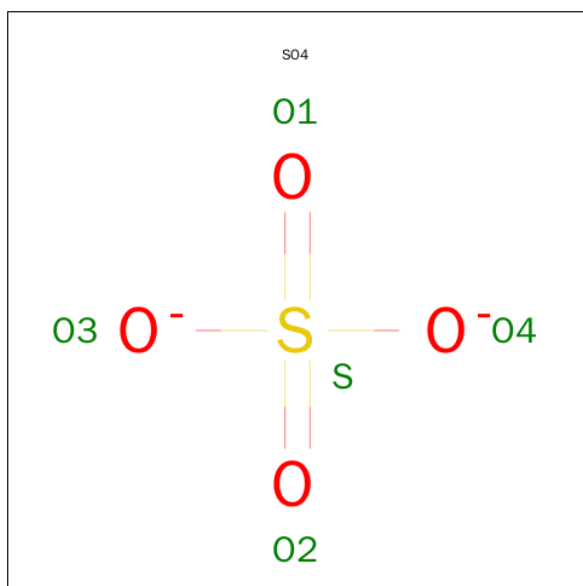
Chain	Residue	Modelled	Actual	Comment	Reference
E	263	LEU	-	CLONING ARTIFACT	UNP Q8I3X4
E	264	ASN	-	CLONING ARTIFACT	UNP Q8I3X4
E	265	SER	-	CLONING ARTIFACT	UNP Q8I3X4
E	266	ALA	-	CLONING ARTIFACT	UNP Q8I3X4
E	267	VAL	-	CLONING ARTIFACT	UNP Q8I3X4
E	268	ASP	-	CLONING ARTIFACT	UNP Q8I3X4
E	269	HIS	-	EXPRESSION 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).



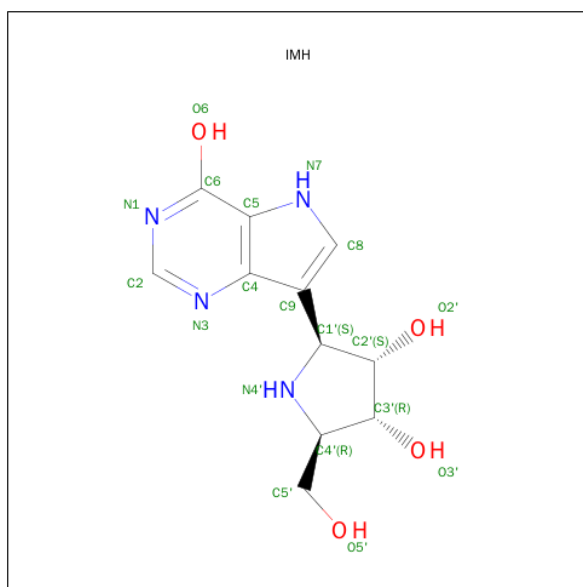
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total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

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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	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,4-DIDEOXY-4-AZA-1-(S)-(9-DEAZAHYPOXANTHIN-9-YL)-D-RIBITOL (three-letter code: IMH) (formula: C₁₁H₁₄N₄O₄).



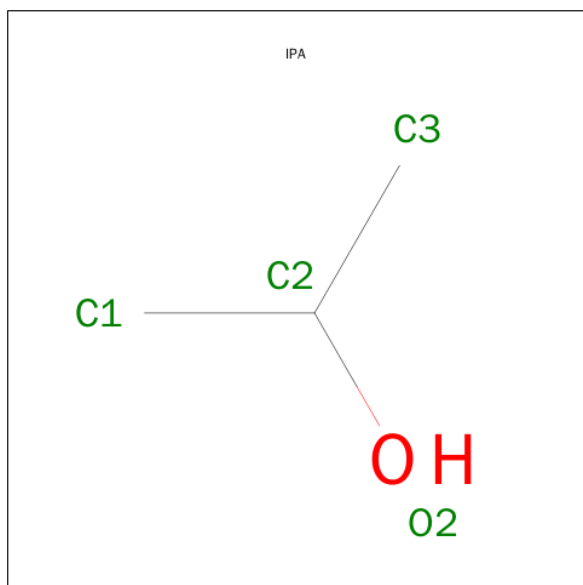
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	11	4	4		
3	B	1	Total	C	N	O	0	0
			19	11	4	4		
3	C	1	Total	C	N	O	0	0
			19	11	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			19	11	4	4		
3	E	1	Total	C	N	O	0	0
			19	11	4	4		
3	F	1	Total	C	N	O	0	0
			19	11	4	4		

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



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

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

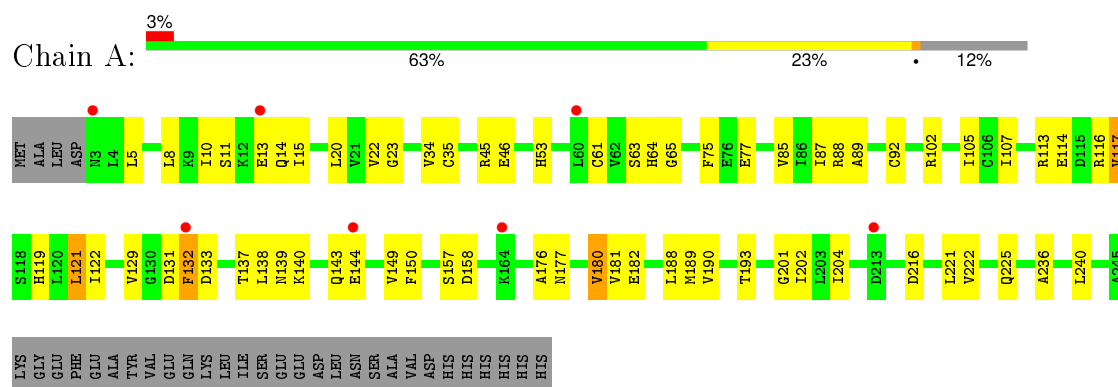
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	28	Total O 28 28	0	0
5	C	34	Total O 34 34	0	0
5	D	51	Total O 51 51	0	0
5	E	54	Total O 54 54	0	0
5	F	49	Total O 49 49	0	0

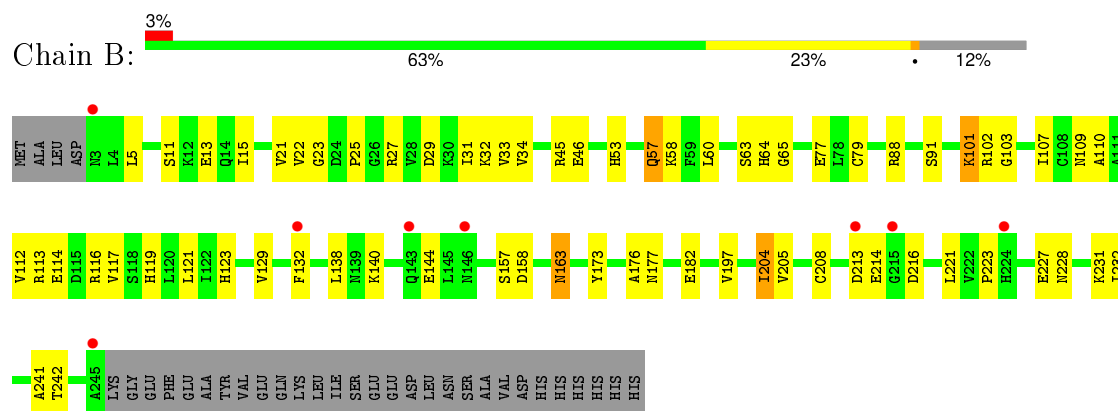
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

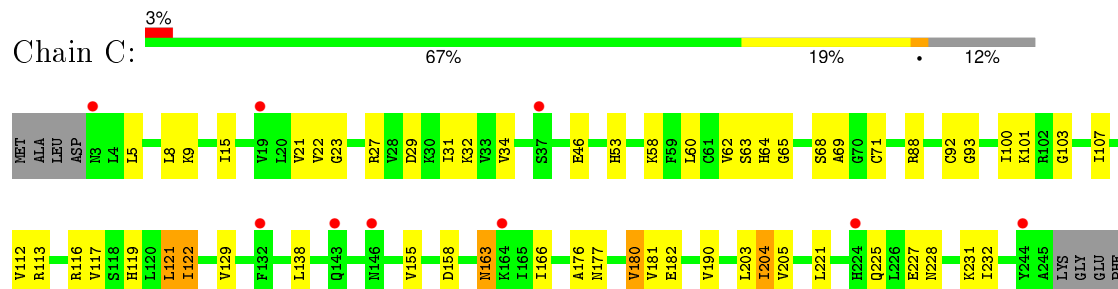
- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



GLU
ALA
TYR
VAL
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
SER
SER
ALA
VAL
ASP
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: uridine phosphorylase, putative

Chain D: 

MET ALA LEU ASP N3 L4 L5 E13 Q14 I15 T16 P17 V21 V22 R27 V28 D29 I31 K32 V33 V34 E46 E51 C52 H53 Q57 K58 F59 L60 G61 V62 S63 H64 G65 S68 C71 E77 S91 R102 V112 R113 E114 D115 R116 V117 S118 H119

L120 L121 D131 F132 D133 V134 T137 E138 K140 T16 E144 S157 D158 M163 K164 Y173 A176 N177 E182 G200 I204 I211 R212 D213 D216 L221 H224 Q225 L226 L230 K241 T242 K243 V244 A245 LYS GLY PHE GLU ALA TYR VAL GLN

LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
ALA
VAL
ASP
HIS
HIS
HIS
HIS

- Molecule 1: uridine phosphorylase, putative

Chain E: 

MET ALA LEU ASP N3 L4 L5 I10 E13 Q14 I15 L20 V21 V22 G23 D24 P25 G26 R27 V28 I31 V34 R45 E46 Y54 Q57 C61 V62 S63 H64 G65 S68 C71 F75 E77 V85 K101 R102 N109 V112 R113 E114

V117 S118 H119 L120 L121 I122 F132 D133 V134 Y135 D136 K140 V155 S156 S157 D158 M159 P162 R163 Y173 A176 N177 E182 L188 G200 D213 C214 E215 D216 L221 L226 L234 L240 A245 LYS GLY PHE GLU ALA TYR VAL GLN LYS

LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
SER
SER
ALA
VAL
ASP
HIS
HIS
HIS
HIS

- Molecule 1: uridine phosphorylase, putative

Chain F: 

MET ALA LEU ASP N3 L4 L5 I10 S11 K12 I15 L20 V21 V22 R27 K32 V33 V34 Y38 V39 D40 E46 V50 E51 K58 F59 L60 C61 V62 S63 H64 G65 E77 N81 R88 G93 I100 K101 R102 A110 A111 V112 R113 R116

V117 S118 H119 L120 L121 F132 K140 E144 L145 M146 D158 M163 K164 I165 Y173 A176 N177 V180 V181 E182 I202 V205 D216 V222 L60 P223 R224 Q225 M229 A245 LYS GLY PHE GLU ALA TYR VAL GLU GLN LYS ILE SER GLU ASP

LEU
ASN
SER
ALA
VAL
ASP
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.55Å 92.28Å 239.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.5 (20.00-2.20) 80.7 (19.97-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.248 0.212 , 0.252	Depositor DCC
R_{free} test set	3999 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 79211 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11683	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMH, 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	0.33	0/1893	0.61	0/2561
1	B	0.31	0/1893	0.58	0/2561
1	C	0.34	0/1893	0.61	0/2561
1	D	0.35	0/1893	0.60	0/2561
1	E	0.36	0/1893	0.62	0/2561
1	F	0.35	0/1893	0.61	0/2561
All	All	0.34	0/11358	0.61	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 [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	1861	0	1882	59	0
1	B	1861	0	1882	52	0
1	C	1861	0	1882	45	0
1	D	1861	0	1882	44	0
1	E	1861	0	1882	43	0
1	F	1861	0	1882	40	0
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	0	1	0
2	C	10	0	0	0	0
2	D	15	0	0	1	0
2	E	15	0	0	0	0
2	F	20	0	0	1	0
3	A	19	0	13	1	0
3	B	19	0	13	1	0
3	C	19	0	13	1	0
3	D	19	0	13	2	0
3	E	19	0	13	1	0
3	F	19	0	13	1	0
4	A	12	0	24	1	0
4	B	16	0	32	2	0
4	C	4	0	8	0	0
4	D	8	0	16	0	0
4	E	8	0	16	1	0
4	F	12	0	24	1	0
5	A	32	0	0	2	0
5	B	28	0	0	0	0
5	C	34	0	0	0	0
5	D	51	0	0	5	0
5	E	54	0	0	3	0
5	F	49	0	0	1	0
All	All	11683	0	11490	262	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 11.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD22	1:A:202:ILE:HD11	1.35	1.08
1:E:117:VAL:HG23	5:E:628:HOH:O	1.78	0.83
1:D:133:ASP:HB3	5:D:751:HOH:O	1.76	0.82
1:D:31:ILE:O	1:D:34:VAL:HG12	1.83	0.78
1:A:46:GLU:HB3	1:B:46:GLU:HB3	1.63	0.78
1:E:121:LEU:HD12	1:F:163:ASN:HB3	1.66	0.77
1:A:133:ASP:O	1:A:137:THR:HG23	1.85	0.76
1:E:46:GLU:HB3	1:F:46:GLU:HB3	1.68	0.75
1:C:117:VAL:HG22	1:D:158:ASP:HB3	1.69	0.73
1:D:15:ILE:HA	1:D:60:LEU:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:HD22	1:B:163:ASN:H	1.38	0.72
1:C:46:GLU:HB3	1:D:46:GLU:HB3	1.71	0.71
1:F:102:ARG:HD2	1:F:216:ASP:OD1	1.92	0.69
1:C:158:ASP:HB3	1:D:117:VAL:HG22	1.74	0.69
1:A:138:LEU:CD2	1:A:202:ILE:HD11	2.20	0.69
1:B:15:ILE:HA	1:B:60:LEU:HD11	1.75	0.69
1:A:138:LEU:HD22	1:A:202:ILE:CD1	2.19	0.68
1:E:163:ASN:HD22	1:E:163:ASN:C	1.96	0.68
5:E:612:HOH:O	1:F:117:VAL:HG23	1.93	0.68
1:F:5:LEU:HD13	1:F:77:GLU:HB3	1.76	0.66
1:B:31:ILE:O	1:B:34:VAL:HG22	1.96	0.65
1:A:140:LYS:O	1:A:144:GLU:HG3	1.96	0.65
1:B:102:ARG:HD2	1:B:216:ASP:OD1	1.98	0.64
1:C:204:ILE:HD12	1:C:221:LEU:HD22	1.80	0.64
1:A:102:ARG:HD2	1:A:216:ASP:OD1	1.97	0.64
1:A:64:HIS:HD2	1:A:65:GLY:O	1.81	0.64
1:A:117:VAL:HG22	5:A:793:HOH:O	1.97	0.64
1:E:158:ASP:HB3	1:F:117:VAL:HG22	1.81	0.63
1:D:64:HIS:HD2	1:D:65:GLY:O	1.82	0.63
1:D:102:ARG:HD2	1:D:216:ASP:OD1	1.97	0.63
1:B:5:LEU:HD13	1:B:77:GLU:HB3	1.81	0.62
1:F:51:GLU:OE2	1:F:58:LYS:HD3	1.98	0.62
1:E:5:LEU:HD11	1:E:15:ILE:HD11	1.80	0.62
1:A:132:PHE:CE1	1:F:132:PHE:HE1	2.18	0.61
1:D:117:VAL:HG23	5:D:644:HOH:O	2.00	0.61
1:B:228:ASN:O	1:B:232:ILE:HG13	2.01	0.61
1:D:140:LYS:O	1:D:144:GLU:HG3	1.99	0.61
1:C:180:VAL:HG13	1:C:181:VAL:N	2.16	0.60
1:E:25:PRO:O	1:E:28:VAL:HG13	2.01	0.60
1:E:31:ILE:O	1:E:34:VAL:HG22	2.01	0.60
1:D:13:GLU:H	1:D:13:GLU:CD	2.03	0.60
1:C:5:LEU:HD11	1:C:15:ILE:HD11	1.83	0.60
1:A:107:ILE:HD13	1:A:138:LEU:HB3	1.84	0.60
5:A:617:HOH:O	1:B:117:VAL:HG23	2.01	0.60
1:B:140:LYS:O	1:B:144:GLU:HG3	2.02	0.60
1:A:122:ILE:HD11	1:A:190:VAL:CG1	2.32	0.59
1:E:64:HIS:HD2	1:E:65:GLY:O	1.85	0.59
1:C:117:VAL:HG23	5:D:614:HOH:O	2.01	0.59
1:C:64:HIS:HD2	1:C:65:GLY:O	1.86	0.59
1:E:102:ARG:HD2	1:E:216:ASP:OD1	2.02	0.59
1:E:117:VAL:HG22	1:F:158:ASP:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ASP:HA	1:D:32:LYS:HE2	1.84	0.58
1:F:12:LYS:HG3	1:F:81:ASN:O	2.03	0.58
3:D:304:IMH:H2'	3:D:304:IMH:N3	2.18	0.58
1:A:122:ILE:HD11	1:A:190:VAL:HG11	1.86	0.58
3:E:305:IMH:H2'	3:E:305:IMH:N3	2.19	0.57
1:B:23:GLY:HA2	1:B:64:HIS:CD2	2.39	0.57
1:A:5:LEU:HD12	1:A:8:LEU:HD12	1.87	0.57
1:B:114:GLU:HB3	1:B:157:SER:HA	1.87	0.57
1:F:5:LEU:HD11	1:F:15:ILE:HD11	1.87	0.56
1:E:117:VAL:O	1:E:121:LEU:HD22	2.06	0.56
1:C:116:ARG:HB2	1:D:116:ARG:HB2	1.87	0.56
1:D:5:LEU:HD11	1:D:15:ILE:HD11	1.88	0.56
1:A:117:VAL:O	1:A:121:LEU:HD22	2.04	0.56
1:D:22:VAL:O	1:D:63:SER:HA	2.06	0.56
1:C:113:ARG:O	1:C:119:HIS:HE1	1.89	0.56
3:A:301:IMH:N3	3:A:301:IMH:H2'	2.21	0.56
1:A:117:VAL:HG13	1:B:158:ASP:O	2.06	0.55
3:C:303:IMH:H2'	3:C:303:IMH:N3	2.21	0.55
3:F:306:IMH:N3	3:F:306:IMH:H2'	2.20	0.55
1:D:132:PHE:HE1	1:E:132:PHE:HD1	1.54	0.55
1:F:64:HIS:HD2	1:F:65:GLY:O	1.89	0.55
1:A:22:VAL:O	1:A:63:SER:HA	2.07	0.55
1:B:53:HIS:ND1	1:B:58:LYS:HG2	2.22	0.55
1:F:93:GLY:O	1:F:180:VAL:HG22	2.06	0.55
1:E:163:ASN:C	1:E:163:ASN:ND2	2.60	0.55
1:C:180:VAL:CG1	1:C:181:VAL:N	2.70	0.55
1:C:228:ASN:O	1:C:232:ILE:HG13	2.07	0.55
1:D:5:LEU:HD13	1:D:77:GLU:HB3	1.89	0.54
1:D:27:ARG:NH1	1:D:226:LEU:HD21	2.23	0.54
1:E:221:LEU:HD13	1:E:226:LEU:HD13	1.89	0.53
1:A:132:PHE:CD1	1:F:132:PHE:HE1	2.25	0.53
3:B:302:IMH:N3	3:B:302:IMH:H2'	2.23	0.53
1:F:40:ASP:HA	1:F:50:VAL:HG22	1.90	0.53
1:F:140:LYS:O	1:F:144:GLU:HG3	2.08	0.53
1:A:189:MET:O	1:A:193:THR:HG23	2.09	0.53
1:F:27:ARG:NH2	2:F:415:SO4:O4	2.41	0.53
1:D:226:LEU:O	1:D:230:ILE:HG13	2.08	0.53
1:C:34:VAL:HG12	1:C:34:VAL:O	2.09	0.53
1:E:113:ARG:O	1:E:119:HIS:HE1	1.92	0.52
1:D:211:LYS:HE3	1:D:216:ASP:OD2	2.08	0.52
1:A:149:VAL:HG12	1:A:150:PHE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ASN:H	1:D:163:ASN:HD22	1.57	0.52
1:C:176:ALA:O	1:C:177:ASN:HB2	2.10	0.52
1:C:29:ASP:O	1:C:32:LYS:HG2	2.09	0.52
1:F:15:ILE:HA	1:F:60:LEU:HD11	1.92	0.52
1:C:93:GLY:O	1:C:180:VAL:HG22	2.10	0.51
1:A:5:LEU:HD13	1:A:77:GLU:HB3	1.92	0.51
1:C:227:GLU:HG2	1:C:231:LYS:HE3	1.91	0.51
1:D:51:GLU:OE2	1:D:58:LYS:HE2	2.10	0.51
1:A:92:CYS:HB2	1:A:180:VAL:HG13	1.93	0.51
1:A:107:ILE:HG12	1:A:202:ILE:HG23	1.92	0.51
1:E:119:HIS:HD2	5:E:806:HOH:O	1.93	0.51
1:B:163:ASN:ND2	1:B:163:ASN:H	2.06	0.51
1:D:53:HIS:HE1	1:D:58:LYS:HE3	1.75	0.51
1:B:27:ARG:O	1:B:31:ILE:HG13	2.11	0.51
1:D:29:ASP:O	1:D:32:LYS:HG2	2.12	0.50
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.77	0.50
1:F:180:VAL:HG13	1:F:181:VAL:N	2.26	0.50
1:E:20:LEU:O	1:E:61:CYS:HA	2.10	0.50
1:F:116:ARG:HE	4:F:511:IPA:H13	1.77	0.50
1:A:13:GLU:CD	1:A:13:GLU:H	2.14	0.50
1:D:133:ASP:O	1:D:137:THR:HG23	2.11	0.50
1:C:122:ILE:HD11	1:C:190:VAL:CG1	2.42	0.50
1:A:87:ILE:HD13	1:A:138:LEU:HD21	1.93	0.50
1:C:53:HIS:HE1	1:C:58:LYS:HE2	1.76	0.50
1:B:123:HIS:HA	4:B:508:IPA:H31	1.93	0.49
1:D:176:ALA:O	1:D:177:ASN:HB2	2.12	0.49
1:B:22:VAL:HG12	1:B:23:GLY:N	2.28	0.49
1:E:13:GLU:H	1:E:13:GLU:CD	2.15	0.49
1:C:112:VAL:HB	1:C:155:VAL:HA	1.93	0.49
1:C:103:GLY:HA2	1:C:204:ILE:HD11	1.95	0.49
1:A:222:VAL:HB	1:A:225:GLN:HB2	1.94	0.49
1:A:5:LEU:HD11	1:A:15:ILE:HD11	1.94	0.49
1:D:114:GLU:HB3	1:D:157:SER:HA	1.94	0.49
1:E:176:ALA:O	1:E:177:ASN:HB2	2.11	0.49
1:E:134:VAL:HG11	1:E:200:GLY:HA3	1.95	0.49
1:A:88:ARG:O	1:A:201:GLY:HA2	2.13	0.49
1:B:13:GLU:H	1:B:13:GLU:CD	2.17	0.49
1:C:100:ILE:HG22	1:C:205:VAL:HG21	1.94	0.49
1:B:57:GLN:NE2	1:B:242:THR:HA	2.28	0.49
1:E:5:LEU:HG	1:E:10:ILE:O	2.13	0.48
1:F:176:ALA:O	1:F:177:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:O	1:B:32:LYS:HG2	2.13	0.48
1:C:68:SER:HA	1:C:71:CYS:SG	2.54	0.48
1:A:23:GLY:HA2	1:A:64:HIS:CD2	2.49	0.48
1:B:227:GLU:HG2	1:B:231:LYS:HE3	1.94	0.48
1:A:149:VAL:HG12	1:A:150:PHE:N	2.28	0.48
1:C:69:ALA:HA	1:C:117:VAL:HG21	1.96	0.48
1:F:34:VAL:O	1:F:34:VAL:HG12	2.14	0.48
1:F:20:LEU:O	1:F:61:CYS:HA	2.14	0.48
1:A:113:ARG:O	1:A:119:HIS:HE1	1.96	0.48
1:C:27:ARG:O	1:C:31:ILE:HG13	2.13	0.48
1:A:114:GLU:HB3	1:A:157:SER:HA	1.95	0.48
1:D:131:ASP:OD1	1:D:133:ASP:HB2	2.13	0.48
1:C:22:VAL:O	1:C:63:SER:HA	2.13	0.48
1:A:107:ILE:HG13	1:A:149:VAL:HG11	1.96	0.47
1:E:46:GLU:CB	1:F:46:GLU:HB3	2.41	0.47
1:B:204:ILE:HD12	1:B:221:LEU:HD22	1.96	0.47
1:B:213:ASP:OD2	1:B:214:GLU:HG3	2.14	0.47
1:B:110:ALA:HB2	1:C:129:VAL:HG11	1.95	0.47
1:D:113:ARG:O	1:D:119:HIS:HE1	1.97	0.47
1:F:100:ILE:HG22	1:F:205:VAL:HG21	1.97	0.47
1:F:22:VAL:O	1:F:63:SER:HA	2.15	0.47
1:A:45:ARG:HB3	1:A:46:GLU:OE2	2.14	0.47
1:F:5:LEU:HG	1:F:10:ILE:O	2.15	0.47
1:B:208:CYS:HB3	1:B:216:ASP:OD2	2.15	0.47
1:B:113:ARG:O	1:B:119:HIS:HE1	1.98	0.47
1:E:159:MET:SD	1:F:121:LEU:HD13	2.55	0.47
1:E:159:MET:SD	1:E:162:PRO:HA	2.56	0.46
1:B:21:VAL:HG23	1:B:88:ARG:HA	1.97	0.46
1:A:11:SER:OG	1:A:14:GLN:HG3	2.16	0.46
1:B:64:HIS:HD2	1:B:65:GLY:O	1.99	0.46
1:C:21:VAL:HG23	1:C:88:ARG:HA	1.96	0.46
1:A:34:VAL:O	1:A:34:VAL:HG12	2.16	0.46
1:A:89:ALA:HA	1:A:202:ILE:O	2.15	0.46
1:C:163:ASN:C	1:C:163:ASN:ND2	2.69	0.46
1:F:163:ASN:HD21	1:F:165:ILE:HB	1.81	0.46
1:C:163:ASN:C	1:C:163:ASN:HD22	2.19	0.46
1:C:92:CYS:HB2	1:C:180:VAL:HG13	1.97	0.46
1:E:114:GLU:HB3	1:E:157:SER:HA	1.98	0.46
1:B:45:ARG:HE	4:B:501:IPA:H31	1.81	0.46
1:A:35:CYS:HB3	1:A:53:HIS:O	2.15	0.46
1:E:22:VAL:O	1:E:63:SER:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:CG1	1:A:181:VAL:N	2.80	0.45
1:B:204:ILE:HD13	1:B:205:VAL:N	2.31	0.45
1:F:113:ARG:O	1:F:119:HIS:HE1	2.00	0.45
1:C:46:GLU:CB	1:D:46:GLU:HB3	2.44	0.45
1:D:119:HIS:HD2	5:D:686:HOH:O	1.98	0.45
1:F:27:ARG:HG2	5:F:843:HOH:O	2.15	0.45
1:A:85:VAL:HG11	1:A:240:LEU:HD13	1.97	0.45
1:A:180:VAL:HG13	1:A:181:VAL:N	2.32	0.45
1:B:11:SER:HB2	1:B:13:GLU:OE2	2.17	0.45
1:A:139:ASN:O	1:A:143:GLN:HG3	2.17	0.45
1:D:91:SER:HA	1:D:204:ILE:O	2.16	0.45
1:C:204:ILE:HG23	1:C:221:LEU:HD22	1.98	0.45
1:B:112:VAL:HG11	1:B:173:TYR:CZ	2.52	0.45
1:A:64:HIS:HE1	1:A:88:ARG:HH11	1.64	0.45
1:C:225:GLN:OE1	1:C:225:GLN:HA	2.17	0.45
1:C:92:CYS:HB3	1:C:203:LEU:HD13	2.00	0.44
1:D:204:ILE:HG21	1:D:221:LEU:HD13	1.99	0.44
1:E:68:SER:HA	1:E:71:CYS:SG	2.58	0.44
1:D:132:PHE:HE1	1:E:132:PHE:CD1	2.35	0.44
1:E:109:ASN:HB3	1:E:135:TYR:CD1	2.52	0.44
1:D:68:SER:HA	1:D:71:CYS:SG	2.58	0.44
1:A:158:ASP:HB3	1:B:117:VAL:HG22	2.00	0.44
1:B:33:VAL:O	1:B:33:VAL:HG12	2.17	0.44
3:D:304:IMH:H2	5:D:835:HOH:O	2.18	0.44
1:F:112:VAL:HG11	1:F:173:TYR:CZ	2.52	0.44
1:E:5:LEU:HD13	1:E:77:GLU:HB3	1.99	0.44
1:A:5:LEU:HG	1:A:10:ILE:O	2.18	0.44
1:A:129:VAL:HG11	1:F:110:ALA:HB2	1.99	0.43
1:A:116:ARG:HE	4:A:509:IPA:H13	1.84	0.43
1:A:121:LEU:HD12	1:B:163:ASN:HB3	2.01	0.43
1:B:101:LYS:HB3	2:B:410:SO4:O4	2.17	0.43
1:A:20:LEU:O	1:A:61:CYS:HA	2.18	0.43
1:F:32:LYS:HD2	1:F:38:TYR:CE1	2.54	0.43
1:A:75:PHE:CE1	1:A:188:LEU:HB2	2.53	0.43
1:A:105:ILE:O	1:A:149:VAL:HG13	2.18	0.43
1:E:158:ASP:O	1:F:117:VAL:HG22	2.19	0.43
1:C:122:ILE:HD11	1:C:190:VAL:HG11	2.00	0.43
1:D:57:GLN:HG3	1:D:241:ALA:HB3	2.01	0.43
1:C:46:GLU:HB3	1:D:46:GLU:CB	2.45	0.43
1:B:5:LEU:HD11	1:B:15:ILE:HD11	2.00	0.43
1:B:57:GLN:CG	1:B:241:ALA:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:HG11	1:B:27:ARG:CG	2.49	0.43
1:D:112:VAL:HG11	1:D:173:TYR:CZ	2.54	0.43
1:A:204:ILE:HG21	1:A:221:LEU:HD13	2.00	0.42
1:D:21:VAL:HA	1:D:62:VAL:O	2.18	0.42
1:E:112:VAL:HG21	1:E:155:VAL:HG22	2.01	0.42
1:E:54:TYR:CE2	1:E:234:LEU:HB3	2.53	0.42
1:F:222:VAL:HB	1:F:225:GLN:HB2	2.01	0.42
1:E:24:ASP:O	1:E:27:ARG:HB3	2.18	0.42
1:E:75:PHE:CE1	1:E:188:LEU:HB2	2.54	0.42
1:A:116:ARG:HB2	1:B:116:ARG:HB2	2.01	0.42
1:A:176:ALA:O	1:A:177:ASN:HB2	2.19	0.42
1:A:131:ASP:OD1	1:A:133:ASP:HB2	2.19	0.42
1:E:46:GLU:HB3	1:F:46:GLU:CB	2.45	0.42
1:C:23:GLY:HA2	1:C:64:HIS:CD2	2.55	0.42
1:D:16:THR:HB	1:D:17:PRO:HD2	2.00	0.42
1:E:85:VAL:HG11	1:E:240:LEU:HD13	2.01	0.42
1:D:102:ARG:HD3	2:D:417:SO4:O3	2.19	0.42
1:B:57:GLN:HG2	1:B:241:ALA:HB3	2.02	0.42
1:D:57:GLN:CG	1:D:241:ALA:HB3	2.50	0.42
1:B:79:CYS:SG	1:B:197:VAL:HG21	2.60	0.42
1:A:46:GLU:HB3	1:B:46:GLU:CB	2.43	0.42
1:B:103:GLY:HA2	1:B:204:ILE:HD11	2.01	0.42
1:B:109:ASN:O	1:B:129:VAL:HG23	2.20	0.42
1:B:22:VAL:O	1:B:63:SER:HA	2.20	0.42
1:E:45:ARG:HE	4:E:506:IPA:H31	1.85	0.42
1:B:22:VAL:HG11	1:B:27:ARG:HB3	2.02	0.41
1:E:136:ASP:OD2	1:E:140:LYS:HE3	2.20	0.41
1:C:163:ASN:HD21	1:C:166:ILE:H	1.67	0.41
1:A:46:GLU:CB	1:B:46:GLU:HB3	2.43	0.41
1:D:134:VAL:HG11	1:D:200:GLY:HA3	2.03	0.41
1:A:138:LEU:HD23	1:A:236:ALA:CB	2.50	0.41
1:B:107:ILE:HD13	1:B:138:LEU:HB3	2.03	0.41
1:F:202:ILE:HG12	1:F:229:MET:HG3	2.03	0.41
1:C:117:VAL:O	1:C:121:LEU:HD22	2.21	0.41
1:B:25:PRO:HA	1:B:63:SER:HB3	2.02	0.41
1:C:15:ILE:HA	1:C:60:LEU:HD11	2.03	0.41
1:D:176:ALA:CB	1:E:122:ILE:HD12	2.51	0.41
1:F:225:GLN:HA	1:F:225:GLN:OE1	2.21	0.41
1:C:107:ILE:HD13	1:C:138:LEU:HB3	2.03	0.41
1:E:112:VAL:HG11	1:E:173:TYR:CZ	2.56	0.40
1:B:176:ALA:O	1:B:177:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ASP:OD2	1:E:214:GLU:HG3	2.22	0.40
1:B:91:SER:HA	1:B:204:ILE:O	2.22	0.40
1:C:181:VAL:HG13	1:C:181:VAL:O	2.21	0.40
1:C:21:VAL:HA	1:C:62:VAL:O	2.22	0.40
1:F:21:VAL:HG23	1:F:88:ARG:HA	2.03	0.40
1:C:8:LEU:O	1:C:9:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

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	241/276 (87%)	228 (95%)	13 (5%)	0	100	100
1	B	241/276 (87%)	229 (95%)	11 (5%)	1 (0%)	39	42
1	C	241/276 (87%)	233 (97%)	8 (3%)	0	100	100
1	D	241/276 (87%)	232 (96%)	9 (4%)	0	100	100
1	E	241/276 (87%)	233 (97%)	8 (3%)	0	100	100
1	F	241/276 (87%)	234 (97%)	7 (3%)	0	100	100
All	All	1446/1656 (87%)	1389 (96%)	56 (4%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	PRO

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	206/235 (88%)	201 (98%)	5 (2%)	57	69
1	B	206/235 (88%)	199 (97%)	7 (3%)	44	54
1	C	206/235 (88%)	199 (97%)	7 (3%)	44	54
1	D	206/235 (88%)	201 (98%)	5 (2%)	57	69
1	E	206/235 (88%)	198 (96%)	8 (4%)	39	48
1	F	206/235 (88%)	202 (98%)	4 (2%)	65	77
All	All	1236/1410 (88%)	1200 (97%)	36 (3%)	50	62

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	A	121	LEU
1	A	132	PHE
1	A	180	VAL
1	A	182	GLU
1	B	57	GLN
1	B	101	LYS
1	B	121	LEU
1	B	132	PHE
1	B	163	ASN
1	B	182	GLU
1	B	204	ILE
1	C	101	LYS
1	C	121	LEU
1	C	122	ILE
1	C	163	ASN
1	C	180	VAL
1	C	182	GLU
1	C	204	ILE
1	D	3	ASN
1	D	57	GLN
1	D	121	LEU
1	D	163	ASN
1	D	182	GLU
1	E	28	VAL
1	E	57	GLN

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Mol	Chain	Res	Type
1	E	101	LYS
1	E	121	LEU
1	E	132	PHE
1	E	133	ASP
1	E	163	ASN
1	E	182	GLU
1	F	101	LYS
1	F	121	LEU
1	F	180	VAL
1	F	182	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	57	GLN
1	A	64	HIS
1	A	119	HIS
1	A	139	ASN
1	B	57	GLN
1	B	64	HIS
1	B	119	HIS
1	C	44	ASN
1	C	53	HIS
1	C	64	HIS
1	C	119	HIS
1	C	163	ASN
1	C	224	HIS
1	C	228	ASN
1	D	44	ASN
1	D	53	HIS
1	D	57	GLN
1	D	64	HIS
1	D	119	HIS
1	D	163	ASN
1	D	219	ASN
1	E	44	ASN
1	E	57	GLN
1	E	64	HIS
1	E	119	HIS
1	E	151	ASN
1	E	163	ASN

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Mol	Chain	Res	Type
1	F	44	ASN
1	F	53	HIS
1	F	64	HIS
1	F	119	HIS
1	F	151	ASN
1	F	163	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

40 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	IMH	A	301	-	20,21,21	2.14	8 (40%)	12,31,31	3.24	4 (33%)
2	SO4	A	401	-	4,4,4	3.24	2 (50%)	6,6,6	0.97	0
2	SO4	A	411	-	4,4,4	3.25	2 (50%)	6,6,6	0.95	0
2	SO4	A	412	-	4,4,4	3.29	2 (50%)	6,6,6	0.96	0
2	SO4	A	413	-	4,4,4	3.22	2 (50%)	6,6,6	0.95	0
4	IPA	A	502	-	3,3,3	0.32	0	3,3,3	0.34	0
4	IPA	A	509	-	3,3,3	0.33	0	3,3,3	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IPA	A	510	-	3,3,3	0.33	0	3,3,3	0.35	0
3	IMH	B	302	-	20,21,21	2.06	7 (35%)	12,31,31	3.25	4 (33%)
2	SO4	B	402	-	4,4,4	3.25	2 (50%)	6,6,6	0.98	0
2	SO4	B	407	-	4,4,4	3.16	2 (50%)	6,6,6	0.96	0
2	SO4	B	410	-	4,4,4	3.27	2 (50%)	6,6,6	0.94	0
4	IPA	B	501	-	3,3,3	0.37	0	3,3,3	0.40	0
4	IPA	B	507	-	3,3,3	0.37	0	3,3,3	0.36	0
4	IPA	B	508	-	3,3,3	0.36	0	3,3,3	0.35	0
4	IPA	B	515	-	3,3,3	0.34	0	3,3,3	0.39	0
3	IMH	C	303	-	20,21,21	1.97	7 (35%)	12,31,31	3.22	4 (33%)
2	SO4	C	403	-	4,4,4	3.16	2 (50%)	6,6,6	0.91	0
2	SO4	C	418	-	4,4,4	3.24	2 (50%)	6,6,6	0.94	0
4	IPA	C	504	-	3,3,3	0.31	0	3,3,3	0.36	0
3	IMH	D	304	-	20,21,21	2.05	7 (35%)	12,31,31	3.40	4 (33%)
2	SO4	D	404	-	4,4,4	3.23	2 (50%)	6,6,6	0.97	0
2	SO4	D	408	-	4,4,4	3.20	2 (50%)	6,6,6	0.99	0
2	SO4	D	417	-	4,4,4	3.11	2 (50%)	6,6,6	0.95	0
4	IPA	D	503	-	3,3,3	0.30	0	3,3,3	0.32	0
4	IPA	D	514	-	3,3,3	0.23	0	3,3,3	0.29	0
3	IMH	E	305	-	20,21,21	2.08	7 (35%)	12,31,31	3.42	4 (33%)
2	SO4	E	405	-	4,4,4	3.30	2 (50%)	6,6,6	0.98	0
2	SO4	E	416	-	4,4,4	3.25	2 (50%)	6,6,6	0.88	0
2	SO4	E	419	-	4,4,4	3.28	2 (50%)	6,6,6	0.96	0
4	IPA	E	506	-	3,3,3	0.33	0	3,3,3	0.39	0
4	IPA	E	513	-	3,3,3	0.22	0	3,3,3	0.24	0
3	IMH	F	306	-	20,21,21	2.12	7 (35%)	12,31,31	3.31	4 (33%)
2	SO4	F	406	-	4,4,4	3.29	2 (50%)	6,6,6	0.92	0
2	SO4	F	409	-	4,4,4	3.16	2 (50%)	6,6,6	0.99	0
2	SO4	F	414	-	4,4,4	3.21	2 (50%)	6,6,6	0.96	0
2	SO4	F	415	-	4,4,4	3.24	2 (50%)	6,6,6	1.04	0
4	IPA	F	505	-	3,3,3	0.28	0	3,3,3	0.31	0
4	IPA	F	511	-	3,3,3	0.40	0	3,3,3	0.32	0
4	IPA	F	512	-	3,3,3	0.26	0	3,3,3	0.34	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	IMH	A	301	-	-	0/2/22/22	0/3/3/3
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	411	-	-	0/0/0/0	0/0/0/0
2	SO4	A	412	-	-	0/0/0/0	0/0/0/0
2	SO4	A	413	-	-	0/0/0/0	0/0/0/0
4	IPA	A	502	-	-	0/0/0/0	0/0/0/0
4	IPA	A	509	-	-	0/0/0/0	0/0/0/0
4	IPA	A	510	-	-	0/0/0/0	0/0/0/0
3	IMH	B	302	-	-	0/2/22/22	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
4	IPA	B	501	-	-	0/0/0/0	0/0/0/0
4	IPA	B	507	-	-	0/0/0/0	0/0/0/0
4	IPA	B	508	-	-	0/0/0/0	0/0/0/0
4	IPA	B	515	-	-	0/0/0/0	0/0/0/0
3	IMH	C	303	-	-	0/2/22/22	0/3/3/3
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	SO4	C	418	-	-	0/0/0/0	0/0/0/0
4	IPA	C	504	-	-	0/0/0/0	0/0/0/0
3	IMH	D	304	-	-	0/2/22/22	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	417	-	-	0/0/0/0	0/0/0/0
4	IPA	D	503	-	-	0/0/0/0	0/0/0/0
4	IPA	D	514	-	-	0/0/0/0	0/0/0/0
3	IMH	E	305	-	-	0/2/22/22	0/3/3/3
2	SO4	E	405	-	-	0/0/0/0	0/0/0/0
2	SO4	E	416	-	-	0/0/0/0	0/0/0/0
2	SO4	E	419	-	-	0/0/0/0	0/0/0/0
4	IPA	E	506	-	-	0/0/0/0	0/0/0/0
4	IPA	E	513	-	-	0/0/0/0	0/0/0/0
3	IMH	F	306	-	-	0/2/22/22	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	414	-	-	0/0/0/0	0/0/0/0
2	SO4	F	415	-	-	0/0/0/0	0/0/0/0
4	IPA	F	505	-	-	0/0/0/0	0/0/0/0
4	IPA	F	511	-	-	0/0/0/0	0/0/0/0
4	IPA	F	512	-	-	0/0/0/0	0/0/0/0

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	IMH	C3'-C4'	-4.73	1.49	1.53
2	E	405	SO4	O3-S	-4.71	1.30	1.47
2	A	401	SO4	O3-S	-4.68	1.30	1.47
2	F	406	SO4	O3-S	-4.66	1.30	1.47
2	D	404	SO4	O3-S	-4.64	1.30	1.47
2	B	402	SO4	O3-S	-4.62	1.30	1.47
2	F	415	SO4	O3-S	-4.56	1.31	1.47
2	A	412	SO4	O3-S	-4.52	1.31	1.47
2	B	410	SO4	O3-S	-4.51	1.31	1.47
2	E	419	SO4	O3-S	-4.51	1.31	1.47
2	C	403	SO4	O3-S	-4.49	1.31	1.47
2	A	413	SO4	O3-S	-4.48	1.31	1.47
2	A	411	SO4	O3-S	-4.47	1.31	1.47
2	E	416	SO4	O3-S	-4.45	1.31	1.47
2	F	409	SO4	O3-S	-4.43	1.31	1.47
2	F	414	SO4	O3-S	-4.39	1.31	1.47
2	C	418	SO4	O3-S	-4.37	1.31	1.47
2	D	417	SO4	O3-S	-4.34	1.31	1.47
2	B	407	SO4	O3-S	-4.28	1.32	1.47
2	D	408	SO4	O3-S	-4.22	1.32	1.47
3	F	306	IMH	C3'-C4'	-4.12	1.50	1.53
3	A	301	IMH	C1'-N4'	-4.10	1.42	1.47
3	E	305	IMH	C3'-C4'	-4.04	1.50	1.53
3	A	301	IMH	C3'-C4'	-3.89	1.50	1.53
3	F	306	IMH	C1'-N4'	-3.80	1.42	1.47
3	B	302	IMH	C3'-C4'	-3.47	1.50	1.53
3	B	302	IMH	C1'-N4'	-3.47	1.43	1.47
3	A	301	IMH	C4'-N4'	-3.44	1.42	1.48
3	F	306	IMH	C4'-N4'	-3.32	1.43	1.48
3	B	302	IMH	C4'-N4'	-3.19	1.43	1.48
3	C	303	IMH	C3'-C4'	-3.19	1.50	1.53
3	C	303	IMH	C4'-N4'	-3.18	1.43	1.48
3	E	305	IMH	C4'-N4'	-3.05	1.43	1.48
3	E	305	IMH	C1'-N4'	-2.98	1.43	1.47
3	D	304	IMH	C4'-N4'	-2.94	1.43	1.48
3	C	303	IMH	C1'-N4'	-2.87	1.43	1.47
3	D	304	IMH	C1'-N4'	-2.80	1.43	1.47
3	D	304	IMH	C8-N7	-2.80	1.30	1.36
3	B	302	IMH	C8-N7	-2.73	1.31	1.36
3	C	303	IMH	C8-N7	-2.72	1.31	1.36
3	F	306	IMH	C8-N7	-2.72	1.31	1.36
3	E	305	IMH	C8-N7	-2.45	1.31	1.36
3	A	301	IMH	C8-N7	-2.43	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	IMH	C9-C1'	2.22	1.54	1.52
3	A	301	IMH	C4-N3	2.35	1.40	1.37
3	B	302	IMH	C4-N3	2.40	1.40	1.37
3	D	304	IMH	C4-N3	2.61	1.40	1.37
3	E	305	IMH	C2-N3	2.72	1.37	1.32
3	F	306	IMH	C2-N3	2.80	1.37	1.32
3	D	304	IMH	C2-N3	2.84	1.37	1.32
3	C	303	IMH	C4-N3	2.85	1.40	1.37
3	F	306	IMH	C4-N3	2.87	1.40	1.37
3	E	305	IMH	C4-N3	2.93	1.41	1.37
3	C	303	IMH	C2-N3	3.04	1.37	1.32
3	A	301	IMH	C2-N3	3.07	1.37	1.32
3	B	302	IMH	C2-N3	3.40	1.38	1.32
3	D	304	IMH	C2-N1	3.44	1.40	1.33
3	C	303	IMH	C2-N1	3.52	1.40	1.33
3	A	301	IMH	C2-N1	3.54	1.40	1.33
3	B	302	IMH	C2-N1	3.64	1.40	1.33
3	F	306	IMH	C2-N1	3.89	1.41	1.33
3	E	305	IMH	C2-N1	4.07	1.41	1.33
2	A	401	SO4	O1-S	4.33	1.62	1.47
2	C	403	SO4	O1-S	4.34	1.62	1.47
2	D	417	SO4	O1-S	4.36	1.62	1.47
2	D	404	SO4	O1-S	4.37	1.62	1.47
2	F	409	SO4	O1-S	4.45	1.62	1.47
2	B	402	SO4	O1-S	4.47	1.62	1.47
2	E	405	SO4	O1-S	4.51	1.62	1.47
2	F	414	SO4	O1-S	4.54	1.62	1.47
2	F	415	SO4	O1-S	4.55	1.62	1.47
2	F	406	SO4	O1-S	4.55	1.62	1.47
2	B	407	SO4	O1-S	4.56	1.62	1.47
2	A	413	SO4	O1-S	4.59	1.62	1.47
2	C	418	SO4	O1-S	4.61	1.62	1.47
2	E	416	SO4	O1-S	4.62	1.63	1.47
2	B	410	SO4	O1-S	4.64	1.63	1.47
2	A	411	SO4	O1-S	4.65	1.63	1.47
2	E	419	SO4	O1-S	4.65	1.63	1.47
2	A	412	SO4	O1-S	4.65	1.63	1.47
2	D	408	SO4	O1-S	4.74	1.63	1.47

All (24) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	IMH	N3-C2-N1	-8.44	122.43	128.89
3	A	301	IMH	N3-C2-N1	-8.38	122.48	128.89
3	E	305	IMH	N3-C2-N1	-8.37	122.48	128.89
3	F	306	IMH	N3-C2-N1	-8.35	122.50	128.89
3	B	302	IMH	N3-C2-N1	-8.33	122.52	128.89
3	D	304	IMH	N3-C2-N1	-8.18	122.63	128.89
3	D	304	IMH	C9-C1'-N4'	-6.03	104.40	113.38
3	E	305	IMH	C9-C1'-N4'	-5.90	104.60	113.38
3	F	306	IMH	C9-C1'-N4'	-5.19	105.66	113.38
3	B	302	IMH	C9-C1'-N4'	-4.87	106.13	113.38
3	A	301	IMH	C9-C1'-N4'	-4.77	106.29	113.38
3	C	303	IMH	C9-C1'-N4'	-4.54	106.63	113.38
3	C	303	IMH	C9-C8-N7	3.26	115.01	108.79
3	B	302	IMH	C9-C8-N7	3.32	115.13	108.79
3	A	301	IMH	C9-C8-N7	3.34	115.16	108.79
3	E	305	IMH	C9-C8-N7	3.36	115.21	108.79
3	F	306	IMH	C9-C8-N7	3.37	115.23	108.79
3	D	304	IMH	C9-C8-N7	3.44	115.37	108.79
3	A	301	IMH	O6-C6-C5	3.90	127.00	119.85
3	C	303	IMH	O6-C6-C5	3.93	127.06	119.85
3	F	306	IMH	O6-C6-C5	3.97	127.14	119.85
3	E	305	IMH	O6-C6-C5	3.99	127.16	119.85
3	D	304	IMH	O6-C6-C5	3.99	127.16	119.85
3	B	302	IMH	O6-C6-C5	4.03	127.25	119.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	IMH	1	0
4	A	509	IPA	1	0
3	B	302	IMH	1	0
2	B	410	SO4	1	0
4	B	501	IPA	1	0
4	B	508	IPA	1	0
3	C	303	IMH	1	0
3	D	304	IMH	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	417	SO4	1	0
3	E	305	IMH	1	0
4	E	506	IPA	1	0
3	F	306	IMH	1	0
2	F	415	SO4	1	0
4	F	511	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

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	243/276 (88%)	-0.16	7 (2%) 55 54	15, 32, 47, 60	0
1	B	243/276 (88%)	-0.05	8 (3%) 50 49	19, 37, 54, 59	0
1	C	243/276 (88%)	-0.04	9 (3%) 45 44	17, 33, 50, 61	0
1	D	243/276 (88%)	-0.31	6 (2%) 61 60	16, 29, 43, 56	0
1	E	243/276 (88%)	-0.34	5 (2%) 67 65	12, 26, 42, 53	0
1	F	243/276 (88%)	-0.29	4 (1%) 74 73	16, 27, 43, 54	0
All	All	1458/1656 (88%)	-0.20	39 (2%) 58 57	12, 30, 49, 61	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	4.7
1	C	143	GLN	4.6
1	E	245	ALA	4.2
1	D	3	ASN	3.8
1	E	132	PHE	3.6
1	C	3	ASN	3.6
1	A	132	PHE	3.3
1	D	245	ALA	3.1
1	B	143	GLN	3.0
1	A	213	ASP	2.9
1	E	3	ASN	2.9
1	B	245	ALA	2.8
1	D	213	ASP	2.8
1	E	213	ASP	2.8
1	B	146	ASN	2.7
1	A	3	ASN	2.7
1	B	213	ASP	2.6
1	B	132	PHE	2.6
1	B	224	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	132	PHE	2.5
1	C	224	HIS	2.5
1	B	215	GLY	2.5
1	C	146	ASN	2.4
1	A	144	GLU	2.3
1	C	244	TYR	2.3
1	A	164	LYS	2.2
1	F	33	VAL	2.2
1	E	214	GLU	2.2
1	F	146	ASN	2.2
1	F	224	HIS	2.2
1	D	164	LYS	2.1
1	F	3	ASN	2.1
1	C	164	LYS	2.1
1	C	37	SER	2.1
1	D	243	LYS	2.1
1	C	19	VAL	2.1
1	A	13	GLU	2.0
1	A	60	LEU	2.0
1	D	224	HIS	2.0

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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	IPA	B	501	4/4	0.81	0.21	5.68	26,31,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	IPA	F	505	4/4	0.79	0.23	5.07	31,34,34,34	0
4	IPA	E	506	4/4	0.91	0.20	4.67	16,18,18,20	0
4	IPA	A	510	4/4	0.83	0.18	4.39	33,33,35,36	0
2	SO4	F	415	5/5	0.94	0.27	4.13	64,65,66,67	0
4	IPA	E	513	4/4	0.86	0.18	3.29	12,16,17,20	0
4	IPA	B	508	4/4	0.88	0.17	3.11	27,29,31,32	0
4	IPA	C	504	4/4	0.83	0.14	2.72	21,22,23,25	0
4	IPA	D	514	4/4	0.82	0.17	2.26	16,19,19,20	0
4	IPA	D	503	4/4	0.92	0.19	1.97	24,26,28,29	0
2	SO4	D	408	5/5	0.99	0.11	1.68	27,29,30,30	0
4	IPA	F	512	4/4	0.81	0.14	1.65	22,23,24,25	0
2	SO4	F	409	5/5	0.99	0.11	1.45	24,25,26,26	0
4	IPA	A	502	4/4	0.88	0.16	1.04	32,33,33,35	0
3	IMH	D	304	19/19	0.95	0.12	0.78	17,21,28,28	0
3	IMH	C	303	19/19	0.93	0.11	0.39	29,35,37,38	0
4	IPA	B	515	4/4	0.91	0.12	0.38	22,23,24,25	0
3	IMH	A	301	19/19	0.96	0.11	0.09	27,28,31,31	0
3	IMH	E	305	19/19	0.94	0.10	-0.08	25,27,29,31	0
2	SO4	B	407	5/5	0.99	0.08	-0.08	28,28,31,32	0
2	SO4	A	413	5/5	0.99	0.08	-0.23	24,25,27,28	0
3	IMH	F	306	19/19	0.97	0.09	-0.52	20,23,27,30	0
3	IMH	B	302	19/19	0.96	0.10	-0.60	31,35,38,39	0
2	SO4	D	404	5/5	0.98	0.09	-0.91	37,38,40,41	0
2	SO4	C	418	5/5	0.99	0.08	-1.15	30,30,32,33	0
2	SO4	A	401	5/5	0.99	0.08	-1.19	37,39,39,41	0
2	SO4	A	412	5/5	0.98	0.08	-1.47	49,50,51,51	0
2	SO4	D	417	5/5	0.99	0.06	-1.47	30,30,31,33	0
2	SO4	B	402	5/5	0.99	0.07	-1.69	42,42,43,44	0
2	SO4	C	403	5/5	0.99	0.07	-1.70	31,32,33,35	0
2	SO4	F	406	5/5	0.99	0.06	-1.83	28,29,30,31	0
2	SO4	E	405	5/5	0.99	0.05	-2.03	27,29,31,31	0
2	SO4	E	419	5/5	0.98	0.11	-	54,54,56,57	0
4	IPA	A	509	4/4	0.86	0.14	-	26,26,26,30	0
2	SO4	B	410	5/5	0.94	0.15	-	62,62,63,63	0
4	IPA	B	507	4/4	0.89	0.12	-	24,26,28,29	0
2	SO4	A	411	5/5	0.94	0.29	-	64,65,65,67	0
4	IPA	F	511	4/4	0.83	0.16	-	19,21,23,28	0
2	SO4	F	414	5/5	0.99	0.08	-	33,33,36,36	0
2	SO4	E	416	5/5	0.99	0.15	-	29,29,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.