



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:56 PM UTC

PDB ID : 4FYM / pdb_00004fym
Title : Crystal structure of Plasmodium falciparum orotate phosphoribosyltransferase
Authors : Rathod, P.K.; Kumar, S.
Deposited on : 2012-07-05
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

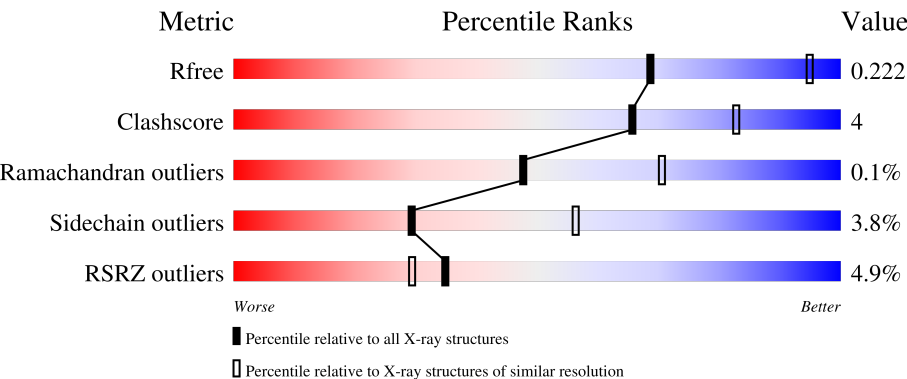
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	2% 75% 8% • 16%
1	B	266	2% 73% 8% 18%
1	C	266	5% 75% 7% • 17%
1	D	266	2% 73% 12% 15%
1	E	266	4% 70% 13% • 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	266	
1	G	266	
1	H	266	

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	B	305	-	-	X	-
2	SO4	E	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14882 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 Orotate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1846	1214	288	337	7			
1	B	219	Total	C	N	O	S	0	0	0
			1811	1191	284	329	7			
1	C	222	Total	C	N	O	S	0	0	0
			1835	1210	290	328	7			
1	D	227	Total	C	N	O	S	0	0	0
			1882	1239	297	339	7			
1	E	222	Total	C	N	O	S	0	0	0
			1838	1213	290	328	7			
1	F	209	Total	C	N	O	S	0	0	0
			1725	1142	268	308	7			
1	G	216	Total	C	N	O	S	0	0	0
			1791	1180	280	324	7			
1	H	209	Total	C	N	O	S	0	0	0
			1725	1140	269	310	6			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q8N0R1
A	1	ALA	-	expression tag	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	ILE	deletion	UNP Q8N0R1
A	?	-	ASP	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	VAL	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	PHE	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	ASP	deletion	UNP Q8N0R1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q8N0R1
A	?	-	ASP	deletion	UNP Q8N0R1
A	?	-	ASP	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	?	-	TYR	deletion	UNP Q8N0R1
A	?	-	ASP	deletion	UNP Q8N0R1
A	?	-	ASP	deletion	UNP Q8N0R1
A	?	-	ASP	deletion	UNP Q8N0R1
A	?	-	GLY	deletion	UNP Q8N0R1
A	?	-	ASN	deletion	UNP Q8N0R1
A	282	HIS	-	expression tag	UNP Q8N0R1
A	283	HIS	-	expression tag	UNP Q8N0R1
A	284	HIS	-	expression tag	UNP Q8N0R1
A	285	HIS	-	expression tag	UNP Q8N0R1
A	286	HIS	-	expression tag	UNP Q8N0R1
A	287	HIS	-	expression tag	UNP Q8N0R1
B	0	MET	-	expression tag	UNP Q8N0R1
B	1	ALA	-	expression tag	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	ILE	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	VAL	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	PHE	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	?	-	TYR	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	ASP	deletion	UNP Q8N0R1
B	?	-	GLY	deletion	UNP Q8N0R1
B	?	-	ASN	deletion	UNP Q8N0R1
B	282	HIS	-	expression tag	UNP Q8N0R1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	283	HIS	-	expression tag	UNP Q8N0R1
B	284	HIS	-	expression tag	UNP Q8N0R1
B	285	HIS	-	expression tag	UNP Q8N0R1
B	286	HIS	-	expression tag	UNP Q8N0R1
B	287	HIS	-	expression tag	UNP Q8N0R1
C	0	MET	-	expression tag	UNP Q8N0R1
C	1	ALA	-	expression tag	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	ILE	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	VAL	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	PHE	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	?	-	TYR	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	ASP	deletion	UNP Q8N0R1
C	?	-	GLY	deletion	UNP Q8N0R1
C	?	-	ASN	deletion	UNP Q8N0R1
C	282	HIS	-	expression tag	UNP Q8N0R1
C	283	HIS	-	expression tag	UNP Q8N0R1
C	284	HIS	-	expression tag	UNP Q8N0R1
C	285	HIS	-	expression tag	UNP Q8N0R1
C	286	HIS	-	expression tag	UNP Q8N0R1
C	287	HIS	-	expression tag	UNP Q8N0R1
D	0	MET	-	expression tag	UNP Q8N0R1
D	1	ALA	-	expression tag	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	ILE	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	VAL	deletion	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	PHE	deletion	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	?	-	TYR	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1
D	?	-	ASP	deletion	UNP Q8N0R1
D	?	-	GLY	deletion	UNP Q8N0R1
D	?	-	ASN	deletion	UNP Q8N0R1
D	282	HIS	-	expression tag	UNP Q8N0R1
D	283	HIS	-	expression tag	UNP Q8N0R1
D	284	HIS	-	expression tag	UNP Q8N0R1
D	285	HIS	-	expression tag	UNP Q8N0R1
D	286	HIS	-	expression tag	UNP Q8N0R1
D	287	HIS	-	expression tag	UNP Q8N0R1
E	0	MET	-	expression tag	UNP Q8N0R1
E	1	ALA	-	expression tag	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	ILE	deletion	UNP Q8N0R1
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	VAL	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	PHE	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	?	-	TYR	deletion	UNP Q8N0R1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	ASP	deletion	UNP Q8N0R1
E	?	-	GLY	deletion	UNP Q8N0R1
E	?	-	ASN	deletion	UNP Q8N0R1
E	282	HIS	-	expression tag	UNP Q8N0R1
E	283	HIS	-	expression tag	UNP Q8N0R1
E	284	HIS	-	expression tag	UNP Q8N0R1
E	285	HIS	-	expression tag	UNP Q8N0R1
E	286	HIS	-	expression tag	UNP Q8N0R1
E	287	HIS	-	expression tag	UNP Q8N0R1
F	0	MET	-	expression tag	UNP Q8N0R1
F	1	ALA	-	expression tag	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	ILE	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	VAL	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	PHE	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	?	-	TYR	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	ASP	deletion	UNP Q8N0R1
F	?	-	GLY	deletion	UNP Q8N0R1
F	?	-	ASN	deletion	UNP Q8N0R1
F	282	HIS	-	expression tag	UNP Q8N0R1
F	283	HIS	-	expression tag	UNP Q8N0R1
F	284	HIS	-	expression tag	UNP Q8N0R1
F	285	HIS	-	expression tag	UNP Q8N0R1
F	286	HIS	-	expression tag	UNP Q8N0R1
F	287	HIS	-	expression tag	UNP Q8N0R1
G	0	MET	-	expression tag	UNP Q8N0R1

Continued on next page...

Continued from previous page...

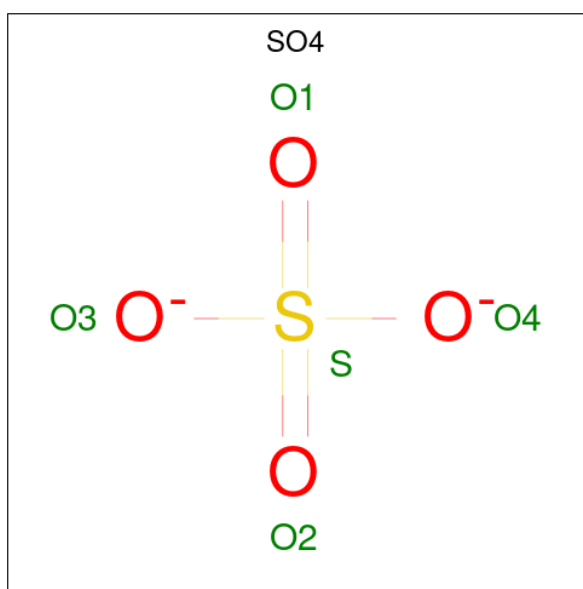
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	expression tag	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	ILE	deletion	UNP Q8N0R1
G	?	-	ASP	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	VAL	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	PHE	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	ASP	deletion	UNP Q8N0R1
G	?	-	ASP	deletion	UNP Q8N0R1
G	?	-	ASP	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	?	-	TYR	deletion	UNP Q8N0R1
G	?	-	ASP	deletion	UNP Q8N0R1
G	?	-	ASP	deletion	UNP Q8N0R1
G	?	-	ASP	deletion	UNP Q8N0R1
G	?	-	GLY	deletion	UNP Q8N0R1
G	?	-	ASN	deletion	UNP Q8N0R1
G	282	HIS	-	expression tag	UNP Q8N0R1
G	283	HIS	-	expression tag	UNP Q8N0R1
G	284	HIS	-	expression tag	UNP Q8N0R1
G	285	HIS	-	expression tag	UNP Q8N0R1
G	286	HIS	-	expression tag	UNP Q8N0R1
G	287	HIS	-	expression tag	UNP Q8N0R1
H	0	MET	-	expression tag	UNP Q8N0R1
H	1	ALA	-	expression tag	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	ILE	deletion	UNP Q8N0R1
H	?	-	ASP	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	VAL	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	PHE	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	ASP	deletion	UNP Q8N0R1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ASP	deletion	UNP Q8N0R1
H	?	-	ASP	deletion	UNP Q8N0R1
H	?	-	ASP	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	?	-	TYR	deletion	UNP Q8N0R1
H	?	-	ASP	deletion	UNP Q8N0R1
H	?	-	ASP	deletion	UNP Q8N0R1
H	?	-	ASP	deletion	UNP Q8N0R1
H	?	-	GLY	deletion	UNP Q8N0R1
H	?	-	ASN	deletion	UNP Q8N0R1
H	282	HIS	-	expression tag	UNP Q8N0R1
H	283	HIS	-	expression tag	UNP Q8N0R1
H	284	HIS	-	expression tag	UNP Q8N0R1
H	285	HIS	-	expression tag	UNP Q8N0R1
H	286	HIS	-	expression tag	UNP Q8N0R1
H	287	HIS	-	expression tag	UNP Q8N0R1

- Molecule 2 is SULFATE ION (CCD ID: 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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

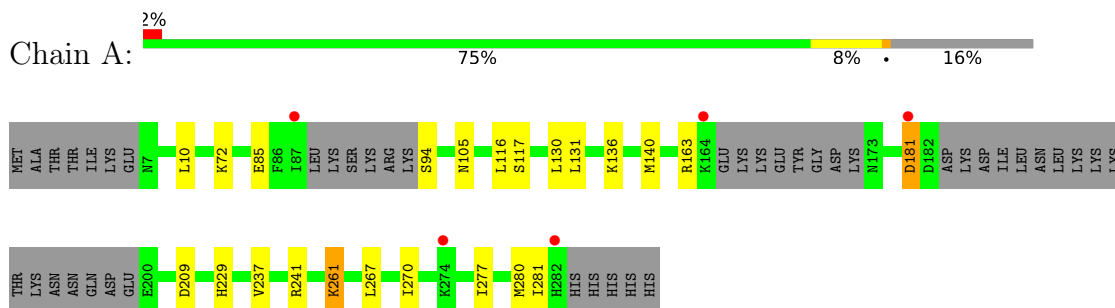
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	68	Total	O	0	0
			68	68		
3	C	39	Total	O	0	0
			39	39		
3	D	53	Total	O	0	0
			53	53		
3	E	13	Total	O	0	0
			13	13		
3	F	15	Total	O	0	0
			15	15		
3	G	19	Total	O	0	0
			19	19		
3	H	1	Total	O	0	0
			1	1		

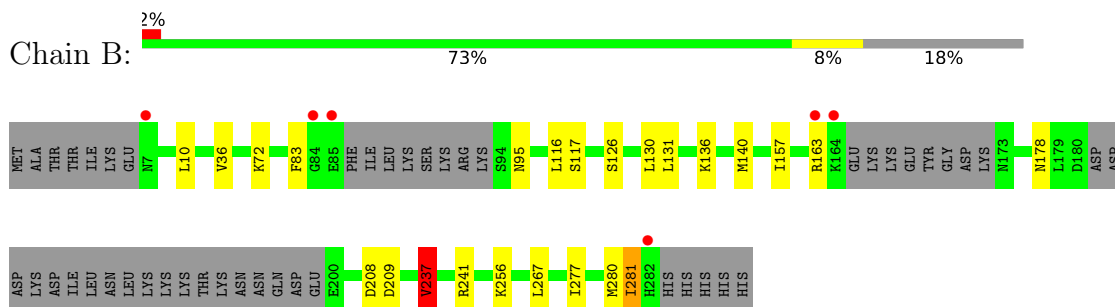
3 Residue-property plots [i](#)

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.

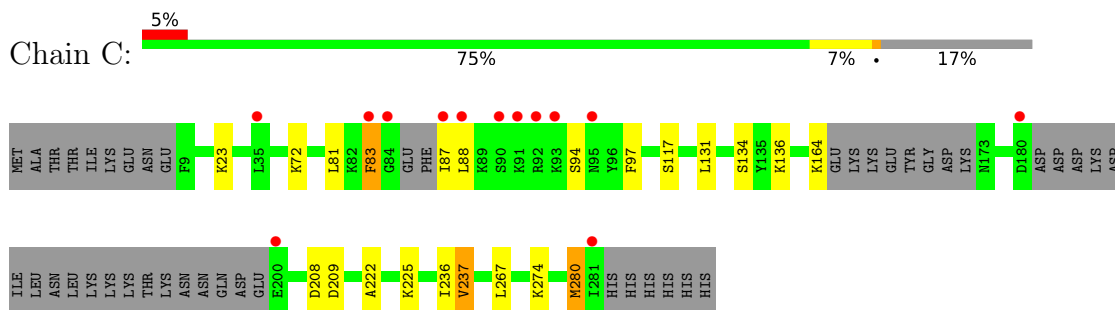
- Molecule 1: Orotate phosphoribosyltransferase



- Molecule 1: Orotate phosphoribosyltransferase

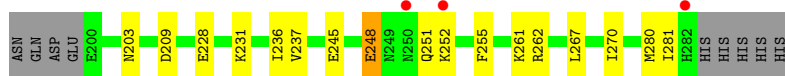
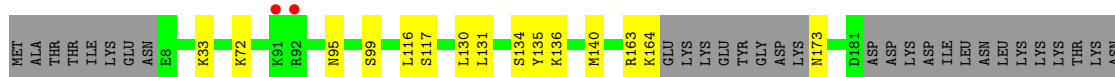


- Molecule 1: Orotate phosphoribosyltransferase

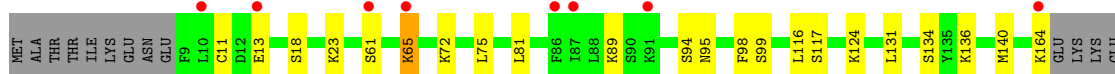


- Molecule 1: Orotate phosphoribosyltransferase



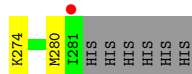
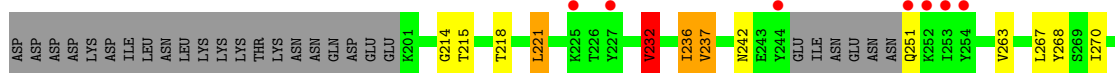


● Molecule 1: Orotate phosphoribosyltransferase

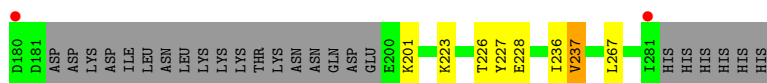
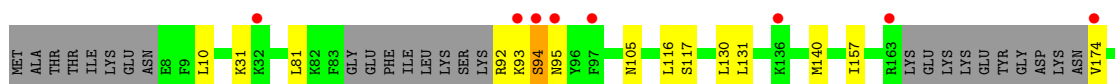


HIS

● Molecule 1: Orotate phosphoribosyltransferase

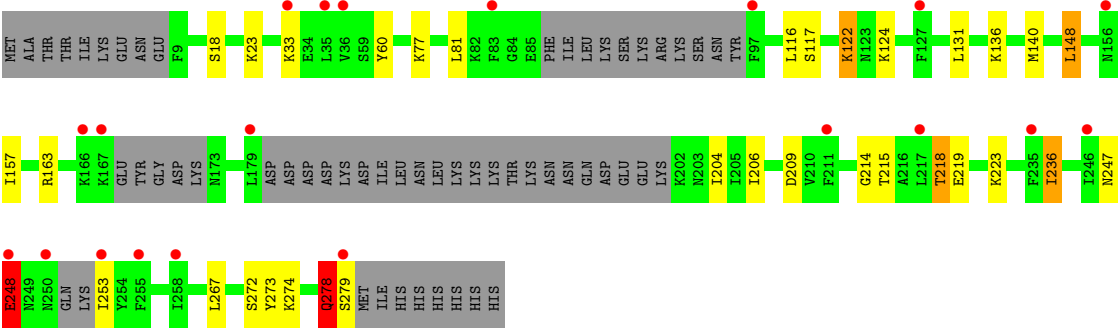


● Molecule 1: Orotate phosphoribosyltransferase



● Molecule 1: Orotate phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.77Å 152.49Å 167.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.47 – 2.60 40.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.47-2.60) 98.9 (40.47-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.218 0.199 , 0.222	Depositor DCC
R_{free} test set	4589 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14882	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2757e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.15	1/1878 (0.1%)	1.02	3/2517 (0.1%)
1	B	1.21	1/1842 (0.1%)	1.05	3/2468 (0.1%)
1	C	1.05	0/1865	1.00	3/2495 (0.1%)
1	D	1.09	1/1915 (0.1%)	1.07	6/2564 (0.2%)
1	E	0.96	0/1870	1.03	4/2503 (0.2%)
1	F	1.03	3/1754 (0.2%)	0.99	3/2348 (0.1%)
1	G	1.02	3/1821 (0.2%)	1.00	3/2439 (0.1%)
1	H	0.93	1/1753 (0.1%)	1.07	8/2346 (0.3%)
All	All	1.06	10/14698 (0.1%)	1.03	33/19680 (0.2%)

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	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	94	SER	CA-C	7.67	1.63	1.53
1	G	93	LYS	CA-C	6.71	1.62	1.52
1	F	215	THR	CA-CB	6.49	1.63	1.53
1	H	278	GLN	CA-C	5.99	1.60	1.52
1	G	95	ASN	N-CA	5.89	1.54	1.46
1	F	270	ILE	C-O	-5.71	1.17	1.24
1	A	85	GLU	CA-C	5.29	1.58	1.52
1	B	95	ASN	CA-C	5.19	1.60	1.52
1	F	237	VAL	N-CA	-5.12	1.40	1.46
1	D	270	ILE	C-O	-5.07	1.18	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	228	GLU	N-CA-C	-8.83	96.25	110.20
1	D	228	GLU	N-CA-C	-8.17	97.29	110.20
1	D	281	ILE	N-CA-C	8.09	118.10	110.74
1	H	218	THR	N-CA-CB	7.43	121.05	110.12
1	F	232	VAL	CB-CA-C	7.03	119.47	110.96
1	C	83	PHE	CB-CA-C	6.67	122.52	111.31
1	B	281	ILE	N-CA-C	6.63	116.77	110.74
1	B	163	ARG	CB-CG-CD	6.62	126.53	111.30
1	A	281	ILE	N-CA-C	6.59	116.74	110.74
1	H	77	LYS	CG-CD-CE	6.58	126.42	111.30
1	C	280	MET	CG-SD-CE	6.47	115.14	100.90
1	E	179	LEU	CA-C-N	6.24	132.93	121.70
1	E	179	LEU	C-N-CA	6.24	132.93	121.70
1	H	122	LYS	CA-CB-CG	-6.17	101.75	114.10
1	D	95	ASN	N-CA-C	-6.05	103.85	111.11
1	E	252	LYS	CG-CD-CE	5.72	124.45	111.30
1	F	215	THR	CB-CA-C	5.70	119.83	110.88
1	A	181	ASP	N-CA-C	5.68	117.47	108.67
1	E	251	GLN	N-CA-CB	-5.66	101.58	110.69
1	H	236	ILE	CB-CG1-CD1	5.65	125.67	113.80
1	F	236	ILE	CB-CG1-CD1	5.61	125.59	113.80
1	D	95	ASN	CB-CA-C	5.57	119.72	110.81
1	H	248	GLU	N-CA-C	-5.55	104.25	111.02
1	H	122	LYS	CB-CG-CD	5.30	123.49	111.30
1	D	251	GLN	N-CA-CB	-5.24	102.26	110.69
1	G	201	LYS	N-CA-C	5.19	117.42	109.07
1	C	274	LYS	CB-CG-CD	5.17	123.19	111.30
1	G	237	VAL	N-CA-CB	-5.09	102.39	111.92
1	H	33	LYS	N-CA-CB	-5.09	104.56	112.30
1	B	237	VAL	N-CA-CB	-5.07	102.45	111.92
1	H	124	LYS	CA-CB-CG	5.07	124.23	114.10
1	A	270	ILE	N-CA-C	-5.06	105.77	110.53
1	D	252	LYS	CG-CD-CE	5.00	122.81	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	83	PHE	Peptide

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	1846	0	1901	13	0
1	B	1811	0	1873	15	0
1	C	1835	0	1927	12	0
1	D	1882	0	1960	15	0
1	E	1838	0	1926	19	0
1	F	1725	0	1801	18	0
1	G	1791	0	1862	9	0
1	H	1725	0	1801	18	0
2	A	20	0	0	0	0
2	B	25	0	0	2	0
2	C	25	0	0	1	0
2	D	25	0	0	0	0
2	E	20	0	0	4	0
2	F	20	0	0	1	0
2	G	15	0	0	0	0
2	H	15	0	0	1	0
3	A	56	0	0	2	0
3	B	68	0	0	4	0
3	C	39	0	0	2	0
3	D	53	0	0	1	0
3	E	13	0	0	0	0
3	F	15	0	0	0	0
3	G	19	0	0	0	0
3	H	1	0	0	0	0
All	All	14882	0	15051	114	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 4.

All (114) 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:72:LYS:HD3	1:C:280:MET:HE2	1.46	0.97
1:D:72:LYS:HD2	1:D:280:MET:HE3	1.50	0.93
1:B:72:LYS:HD2	1:B:280:MET:HE3	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LEU:HD22	1:C:97:PHE:HB2	1.58	0.84
1:F:134:SER:OG	1:F:162:ASP:O	1.96	0.82
1:A:72:LYS:HD2	1:A:280:MET:CE	2.14	0.77
1:F:72:LYS:HE3	1:F:280:MET:HE2	1.68	0.76
1:C:88:LEU:CD2	1:C:97:PHE:HB2	2.16	0.74
1:C:87:ILE:HA	1:C:94:SER:O	1.88	0.72
1:A:261:LYS:HE2	3:A:450:HOH:O	1.89	0.72
1:A:72:LYS:HD2	1:A:280:MET:HE2	1.72	0.70
1:A:163:ARG:HD3	3:B:462:HOH:O	1.93	0.69
1:B:136:LYS:HE3	2:B:305:SO4:O4	1.94	0.68
1:H:60:TYR:CE2	1:H:122:LYS:HD2	2.27	0.68
1:C:23:LYS:HE2	2:C:305:SO4:O2	1.94	0.67
1:H:278:GLN:O	1:H:279:SER:HB2	1.95	0.67
1:E:116:LEU:HD11	1:E:140:MET:CE	2.26	0.66
1:H:116:LEU:HD11	1:H:140:MET:CE	2.25	0.65
1:E:23:LYS:NZ	2:E:304:SO4:O2	2.30	0.65
1:B:116:LEU:HD11	1:B:140:MET:CE	2.27	0.64
1:A:116:LEU:HD11	1:A:140:MET:CE	2.27	0.64
1:G:116:LEU:HD11	1:G:140:MET:CE	2.27	0.64
1:F:251:GLN:HG3	1:F:251:GLN:O	1.97	0.64
1:D:116:LEU:HD11	1:D:140:MET:CE	2.28	0.63
1:A:136:LYS:HD2	1:A:209:ASP:OD2	1.99	0.63
1:F:116:LEU:HD11	1:F:140:MET:CE	2.28	0.63
1:H:136:LYS:HD2	1:H:209:ASP:OD2	2.00	0.62
1:C:136:LYS:HD2	1:C:209:ASP:OD2	2.00	0.62
1:H:23:LYS:NZ	2:H:302:SO4:O4	2.32	0.62
1:B:256:LYS:HE3	3:B:417:HOH:O	2.00	0.62
1:F:72:LYS:HE3	1:F:280:MET:CE	2.29	0.62
1:A:131:LEU:C	1:A:131:LEU:HD23	2.26	0.60
1:B:241:ARG:NH1	3:B:448:HOH:O	2.24	0.60
1:F:214:GLY:O	1:F:218:THR:HG23	2.02	0.59
1:C:222:ALA:O	1:C:225:LYS:HG2	2.02	0.59
1:F:263:VAL:O	1:F:263:VAL:HG22	2.02	0.59
1:H:247:ASN:OD1	1:H:248:GLU:N	2.35	0.58
1:F:221:LEU:HD21	1:F:263:VAL:HG21	1.85	0.58
1:B:241:ARG:HD2	3:B:448:HOH:O	2.02	0.58
1:D:99:SER:HA	1:E:248:GLU:HG3	1.84	0.58
1:G:223:LYS:O	1:G:226:THR:HG22	2.04	0.58
1:B:131:LEU:HD23	1:B:131:LEU:C	2.29	0.57
1:E:11:CYS:SG	1:E:13:GLU:OE1	2.62	0.56
1:F:23:LYS:NZ	2:F:304:SO4:O2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:SER:OG	1:D:164:LYS:HE2	2.06	0.56
1:A:241:ARG:NH1	3:A:438:HOH:O	2.29	0.55
1:G:131:LEU:C	1:G:131:LEU:HD23	2.33	0.54
1:E:81:LEU:HD12	1:E:98:PHE:HD1	1.73	0.53
1:H:273:TYR:HD2	1:H:274:LYS:HD2	1.73	0.53
1:A:181:ASP:HB3	1:A:229:HIS:HB2	1.89	0.53
2:E:301:SO4:O3	1:H:163:ARG:NH1	2.38	0.53
1:E:72:LYS:HB3	1:E:280:MET:HE1	1.91	0.53
1:B:36:VAL:HG11	1:F:66:GLU:HG3	1.91	0.52
1:G:116:LEU:HD11	1:G:140:MET:HE3	1.91	0.52
1:H:278:GLN:O	1:H:279:SER:CB	2.57	0.51
1:F:123:ASN:N	1:F:123:ASN:OD1	2.43	0.50
1:A:72:LYS:HD2	1:A:280:MET:HE3	1.94	0.50
1:C:131:LEU:C	1:C:131:LEU:HD23	2.37	0.49
1:H:116:LEU:HD11	1:H:140:MET:HE3	1.94	0.49
1:E:136:LYS:HD2	1:E:209:ASP:OD2	2.13	0.49
1:F:131:LEU:C	1:F:131:LEU:HD23	2.38	0.48
1:E:116:LEU:HD11	1:E:140:MET:HE3	1.96	0.48
1:D:248:GLU:HG3	1:E:99:SER:HA	1.95	0.47
1:F:242:ASN:HD22	1:F:274:LYS:H	1.61	0.47
1:E:61:SER:O	1:E:65:LYS:HG2	2.14	0.47
1:E:134:SER:OG	1:E:164:LYS:HE2	2.14	0.47
1:F:221:LEU:HD12	1:F:232:VAL:HG11	1.96	0.47
1:F:116:LEU:HD11	1:F:140:MET:HE3	1.96	0.47
1:G:92:ARG:HB2	1:G:94:SER:O	2.15	0.47
1:E:75:LEU:HB3	1:E:81:LEU:HD13	1.97	0.46
1:H:219:GLU:OE1	1:H:223:LYS:HE3	2.15	0.46
1:E:131:LEU:C	1:E:131:LEU:HD23	2.41	0.46
1:G:226:THR:HG23	1:G:227:TYR:CD2	2.51	0.45
1:H:214:GLY:O	1:H:218:THR:HG23	2.17	0.45
1:B:72:LYS:HB3	1:B:280:MET:CE	2.46	0.45
1:C:134:SER:OG	1:C:164:LYS:HE2	2.16	0.45
1:D:245:GLU:HG2	1:D:255:PHE:CZ	2.51	0.45
1:F:242:ASN:ND2	1:F:274:LYS:H	2.14	0.45
1:E:65:LYS:HA	1:E:65:LYS:HD3	1.83	0.45
3:C:434:HOH:O	1:D:163:ARG:HD3	2.15	0.45
1:F:178:ASN:HD21	1:G:105:ASN:HD22	1.64	0.45
1:E:94:SER:O	1:E:95:ASN:C	2.59	0.45
1:E:72:LYS:HB3	1:E:280:MET:CE	2.47	0.44
1:C:136:LYS:HE2	3:C:408:HOH:O	2.18	0.44
1:E:245:GLU:HG2	1:E:255:PHE:CZ	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:ILE:HG22	1:H:206:ILE:HD13	2.00	0.44
1:A:105:ASN:HD22	1:B:178:ASN:HD21	1.66	0.43
1:D:72:LYS:HB3	1:D:280:MET:CE	2.47	0.43
1:F:123:ASN:ND2	1:F:268:TYR:CE2	2.86	0.43
1:G:81:LEU:HD12	1:G:81:LEU:HA	1.88	0.43
1:B:116:LEU:HD11	1:B:140:MET:HE3	1.98	0.43
1:D:163:ARG:NH1	1:D:173:ASN:O	2.50	0.43
1:H:131:LEU:HB3	1:H:206:ILE:CD1	2.49	0.43
1:A:116:LEU:HD11	1:A:140:MET:HE3	1.98	0.43
1:D:116:LEU:HD11	1:D:140:MET:HE3	2.00	0.42
1:H:131:LEU:C	1:H:131:LEU:HD23	2.44	0.42
1:D:131:LEU:C	1:D:131:LEU:HD23	2.45	0.42
1:B:136:LYS:HD3	1:B:209:ASP:OD2	2.20	0.42
1:C:208:ASP:O	1:C:237:VAL:HA	2.20	0.41
1:E:136:LYS:HE2	2:E:301:SO4:O1	2.21	0.41
1:H:148:LEU:HD23	1:H:157:ILE:HD13	2.02	0.41
1:G:31:LYS:HD2	1:G:31:LYS:HA	1.88	0.41
1:D:262:ARG:NE	3:D:451:HOH:O	2.37	0.41
1:C:81:LEU:HD12	1:C:81:LEU:HA	1.90	0.41
2:E:301:SO4:S	1:H:163:ARG:NH1	2.93	0.41
1:H:81:LEU:HD12	1:H:81:LEU:HA	1.90	0.41
1:B:136:LYS:CE	2:B:305:SO4:O4	2.65	0.41
1:A:277:ILE:HD12	1:A:277:ILE:N	2.36	0.41
1:B:208:ASP:O	1:B:237:VAL:HA	2.21	0.41
1:E:174:VAL:O	1:E:174:VAL:HG12	2.21	0.40
1:B:83:PHE:CD1	1:B:281:ILE:HD13	2.56	0.40
1:D:136:LYS:HD3	1:D:209:ASP:OD2	2.21	0.40
1:D:134:SER:HA	1:D:135:TYR:HA	1.85	0.40
1:D:203:ASN:OD1	1:D:231:LYS:HE3	2.21	0.40

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	215/266 (81%)	210 (98%)	5 (2%)	0	100	100
1	B	211/266 (79%)	209 (99%)	2 (1%)	0	100	100
1	C	214/266 (80%)	211 (99%)	3 (1%)	0	100	100
1	D	221/266 (83%)	215 (97%)	6 (3%)	0	100	100
1	E	216/266 (81%)	212 (98%)	4 (2%)	0	100	100
1	F	199/266 (75%)	197 (99%)	2 (1%)	0	100	100
1	G	208/266 (78%)	205 (99%)	3 (1%)	0	100	100
1	H	199/266 (75%)	194 (98%)	4 (2%)	1 (0%)	24	46
All	All	1683/2128 (79%)	1653 (98%)	29 (2%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	278	GLN

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	211/252 (84%)	204 (97%)	7 (3%)	33	61
1	B	207/252 (82%)	199 (96%)	8 (4%)	28	55
1	C	210/252 (83%)	206 (98%)	4 (2%)	50	75
1	D	215/252 (85%)	207 (96%)	8 (4%)	30	57
1	E	210/252 (83%)	199 (95%)	11 (5%)	21	44
1	F	197/252 (78%)	189 (96%)	8 (4%)	27	54
1	G	205/252 (81%)	197 (96%)	8 (4%)	28	55
1	H	197/252 (78%)	188 (95%)	9 (5%)	24	49
All	All	1652/2016 (82%)	1589 (96%)	63 (4%)	29	56

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	94	SER
1	A	117	SER
1	A	130	LEU
1	A	237	VAL
1	A	261	LYS
1	A	267	LEU
1	B	10	LEU
1	B	117	SER
1	B	126	SER
1	B	130	LEU
1	B	157	ILE
1	B	237	VAL
1	B	267	LEU
1	B	277	ILE
1	C	117	SER
1	C	236	ILE
1	C	237	VAL
1	C	267	LEU
1	D	33	LYS
1	D	117	SER
1	D	130	LEU
1	D	236	ILE
1	D	237	VAL
1	D	248	GLU
1	D	261	LYS
1	D	267	LEU
1	E	18	SER
1	E	65	LYS
1	E	89	LYS
1	E	117	SER
1	E	124	LYS
1	E	228	GLU
1	E	236	ILE
1	E	237	VAL
1	E	248	GLU
1	E	261	LYS
1	E	267	LEU
1	F	35	LEU
1	F	117	SER
1	F	157	ILE
1	F	221	LEU
1	F	232	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	236	ILE
1	F	237	VAL
1	F	267	LEU
1	G	10	LEU
1	G	117	SER
1	G	130	LEU
1	G	157	ILE
1	G	174	VAL
1	G	236	ILE
1	G	237	VAL
1	G	267	LEU
1	H	18	SER
1	H	117	SER
1	H	148	LEU
1	H	215	THR
1	H	236	ILE
1	H	248	GLU
1	H	253	ILE
1	H	267	LEU
1	H	272	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	178	ASN
1	B	203	ASN
1	D	282	HIS
1	F	178	ASN
1	F	242	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

33 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	$\# Z > 2$
2	SO4	C	304	-	4,4,4	0.63	0	6,6,6	0.49	0
2	SO4	E	301	-	4,4,4	0.46	0	6,6,6	1.00	0
2	SO4	B	303	-	4,4,4	0.47	0	6,6,6	0.78	0
2	SO4	C	302	-	4,4,4	0.70	0	6,6,6	0.62	0
2	SO4	D	302	-	4,4,4	0.37	0	6,6,6	0.62	0
2	SO4	F	304	-	4,4,4	0.48	0	6,6,6	0.59	0
2	SO4	H	302	-	4,4,4	0.62	0	6,6,6	0.66	0
2	SO4	E	302	-	4,4,4	0.46	0	6,6,6	0.48	0
2	SO4	G	301	-	4,4,4	0.64	0	6,6,6	0.71	0
2	SO4	H	301	-	4,4,4	0.64	0	6,6,6	0.44	0
2	SO4	C	305	-	4,4,4	0.48	0	6,6,6	0.75	0
2	SO4	D	303	-	4,4,4	0.37	0	6,6,6	0.59	0
2	SO4	E	304	-	4,4,4	0.60	0	6,6,6	0.66	0
2	SO4	B	305	-	4,4,4	0.81	0	6,6,6	0.99	0
2	SO4	C	301	-	4,4,4	0.69	0	6,6,6	0.68	0
2	SO4	F	303	-	4,4,4	0.60	0	6,6,6	0.81	0
2	SO4	B	301	-	4,4,4	0.64	0	6,6,6	0.81	0
2	SO4	H	303	-	4,4,4	0.63	0	6,6,6	0.61	0
2	SO4	G	302	-	4,4,4	0.43	0	6,6,6	0.20	0
2	SO4	E	303	-	4,4,4	0.70	0	6,6,6	0.41	0
2	SO4	D	304	-	4,4,4	0.26	0	6,6,6	0.57	0
2	SO4	A	301	-	4,4,4	0.59	0	6,6,6	1.02	0
2	SO4	B	304	-	4,4,4	0.84	0	6,6,6	1.26	1 (16%)
2	SO4	B	302	-	4,4,4	0.35	0	6,6,6	0.38	0
2	SO4	D	301	-	4,4,4	0.68	0	6,6,6	0.43	0
2	SO4	F	301	-	4,4,4	0.42	0	6,6,6	1.00	0
2	SO4	A	302	-	4,4,4	0.43	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	304	-	4,4,4	0.90	0	6,6,6	1.04	1 (16%)
2	SO4	D	305	-	4,4,4	0.84	0	6,6,6	1.67	2 (33%)
2	SO4	A	303	-	4,4,4	0.96	0	6,6,6	1.36	1 (16%)
2	SO4	G	303	-	4,4,4	0.40	0	6,6,6	0.48	0
2	SO4	C	303	-	4,4,4	0.51	0	6,6,6	0.29	0
2	SO4	F	302	-	4,4,4	0.56	0	6,6,6	0.76	0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	305	SO4	O4-S-O2	2.70	123.66	109.56
2	B	304	SO4	O4-S-O2	2.36	121.92	109.56
2	A	304	SO4	O4-S-O2	-2.25	97.80	109.56
2	A	303	SO4	O3-S-O2	2.24	121.29	109.56
2	D	305	SO4	O4-S-O3	-2.06	97.16	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	SO4	3	0
2	F	304	SO4	1	0
2	H	302	SO4	1	0
2	C	305	SO4	1	0
2	E	304	SO4	1	0
2	B	305	SO4	2	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	223/266 (83%)	-0.23	5 (2%) 62 57	27, 44, 87, 130	0
1	B	219/266 (82%)	-0.27	6 (2%) 56 50	29, 43, 79, 108	0
1	C	222/266 (83%)	-0.04	13 (5%) 28 23	35, 52, 98, 144	0
1	D	227/266 (85%)	-0.24	5 (2%) 62 57	32, 47, 84, 120	0
1	E	222/266 (83%)	0.31	10 (4%) 38 32	45, 65, 105, 131	0
1	F	209/266 (78%)	0.19	16 (7%) 19 15	39, 62, 105, 131	0
1	G	216/266 (81%)	0.06	10 (4%) 37 32	41, 58, 100, 124	0
1	H	209/266 (78%)	0.76	20 (9%) 13 10	48, 82, 133, 169	0
All	All	1747/2128 (82%)	0.06	85 (4%) 35 29	27, 56, 109, 169	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	246	ILE	4.9
1	H	253	ILE	4.9
1	A	87	ILE	4.7
1	H	97	PHE	4.1
1	F	244	TYR	4.1
1	F	134	SER	4.0
1	C	87	ILE	3.8
1	C	92	ARG	3.7
1	G	163	ARG	3.7
1	F	253	ILE	3.6
1	C	91	LYS	3.5
1	E	65	LYS	3.5
1	F	135	TYR	3.5
1	H	167	LYS	3.5
1	E	86	PHE	3.4
1	H	250	ASN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	282	HIS	3.3
1	C	93	LYS	3.2
1	G	94	SER	3.2
1	G	32	LYS	3.2
1	B	84	GLY	3.1
1	B	163	ARG	3.0
1	C	88	LEU	3.0
1	F	133	ALA	3.0
1	A	282	HIS	3.0
1	D	91	LYS	3.0
1	G	93	LYS	2.9
1	D	282	HIS	2.9
1	H	36	VAL	2.9
1	D	92	ARG	2.9
1	E	10	LEU	2.9
1	G	97	PHE	2.9
1	H	166	LYS	2.9
1	G	95	ASN	2.8
1	G	281	ILE	2.7
1	H	33	LYS	2.7
1	E	164	LYS	2.7
1	E	87	ILE	2.7
1	D	250	ASN	2.7
1	E	13	GLU	2.7
1	F	251	GLN	2.6
1	H	235	PHE	2.6
1	C	84	GLY	2.6
1	F	173	ASN	2.6
1	H	279	SER	2.6
1	H	35	LEU	2.6
1	A	274	LYS	2.5
1	H	83	PHE	2.5
1	F	252	LYS	2.5
1	F	281	ILE	2.5
1	C	83	PHE	2.5
1	D	252	LYS	2.4
1	H	255	PHE	2.4
1	E	274	LYS	2.4
1	F	225	LYS	2.4
1	C	95	ASN	2.3
1	G	180	ASP	2.3
1	F	137	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	180	ASP	2.3
1	F	132	GLY	2.3
1	B	7	ASN	2.3
1	A	181	ASP	2.3
1	C	180	ASP	2.3
1	C	35	LEU	2.3
1	E	61	SER	2.2
1	A	164	LYS	2.2
1	E	91	LYS	2.2
1	B	85	GLU	2.2
1	F	85	GLU	2.2
1	F	7	ASN	2.2
1	G	174	VAL	2.2
1	H	211	PHE	2.2
1	F	227	TYR	2.1
1	F	254	TYR	2.1
1	H	217	LEU	2.1
1	G	136	LYS	2.1
1	H	179	LEU	2.1
1	H	258	ILE	2.1
1	H	248	GLU	2.0
1	B	164	LYS	2.0
1	C	200	GLU	2.0
1	H	127	PHE	2.0
1	C	90	SER	2.0
1	C	281	ILE	2.0
1	H	156	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	304	5/5	0.53	0.14	121,122,126,127	0
2	SO4	E	302	5/5	0.71	0.10	112,116,123,124	0
2	SO4	E	304	5/5	0.77	0.16	103,103,132,141	0
2	SO4	D	305	5/5	0.81	0.17	74,79,102,106	0
2	SO4	H	303	5/5	0.83	0.12	84,93,100,104	0
2	SO4	F	303	5/5	0.91	0.09	76,79,81,81	0
2	SO4	H	301	5/5	0.91	0.13	84,87,89,98	0
2	SO4	H	302	5/5	0.91	0.10	86,88,89,91	0
2	SO4	B	305	5/5	0.91	0.14	77,82,86,94	0
2	SO4	A	303	5/5	0.92	0.11	53,57,66,70	0
2	SO4	G	301	5/5	0.93	0.11	72,86,89,89	0
2	SO4	C	301	5/5	0.94	0.12	69,70,76,82	0
2	SO4	F	302	5/5	0.95	0.11	78,79,89,97	0
2	SO4	B	304	5/5	0.95	0.10	54,62,62,65	0
2	SO4	E	301	5/5	0.95	0.09	69,69,73,82	0
2	SO4	G	303	5/5	0.95	0.07	83,83,86,94	0
2	SO4	C	305	5/5	0.95	0.13	72,75,87,87	0
2	SO4	D	304	5/5	0.95	0.16	64,72,77,77	0
2	SO4	F	301	5/5	0.95	0.10	65,68,74,75	0
2	SO4	F	304	5/5	0.96	0.09	67,67,73,87	0
2	SO4	G	302	5/5	0.97	0.06	48,48,51,52	0
2	SO4	D	301	5/5	0.97	0.11	53,55,58,61	0
2	SO4	D	302	5/5	0.97	0.09	66,71,79,79	0
2	SO4	B	302	5/5	0.97	0.06	55,59,62,64	0
2	SO4	A	304	5/5	0.97	0.08	53,54,60,60	0
2	SO4	B	303	5/5	0.98	0.05	47,54,57,60	0
2	SO4	A	301	5/5	0.98	0.06	54,54,58,59	0
2	SO4	C	303	5/5	0.98	0.07	63,66,69,70	0
2	SO4	E	303	5/5	0.98	0.06	48,51,52,54	0
2	SO4	B	301	5/5	0.98	0.06	42,43,48,50	0
2	SO4	A	302	5/5	0.99	0.05	46,46,48,52	0
2	SO4	D	303	5/5	0.99	0.04	44,45,48,48	0
2	SO4	C	302	5/5	0.99	0.05	46,47,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.