Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 PM GMT

PDB ID	:	4FYM
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

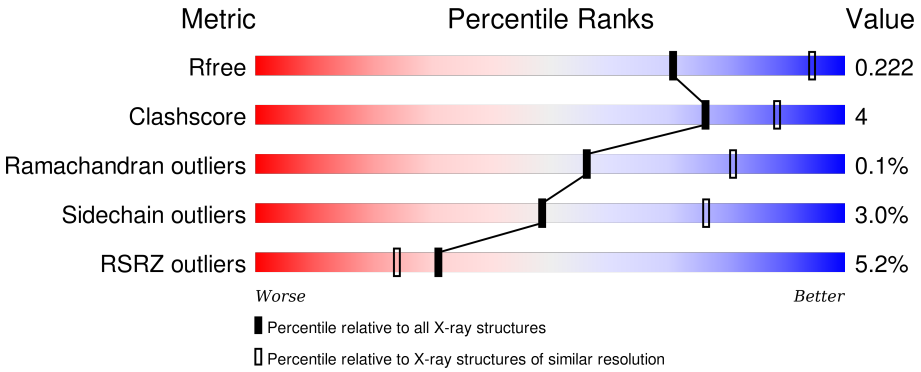
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 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 <=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	4% 76% 7% • 16%
1	B	266	2% 73% 8% • 18%
1	C	266	4% 75% 7% • 17%
1	D	266	3% 76% 9% • 15%
1	E	266	5% 71% 12% • 17%

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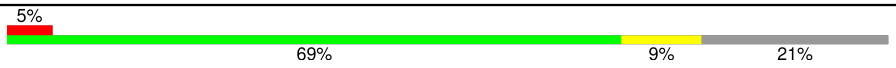
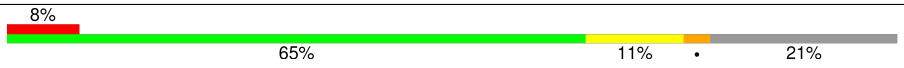
Mol	Chain	Length	Quality of chain
1	F	266	
1	G	266	
1	H	266	

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	SO4	E	304	-	-	-	X

2 Entry composition (i)

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

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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

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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	?	-	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

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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

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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

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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	?	-	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

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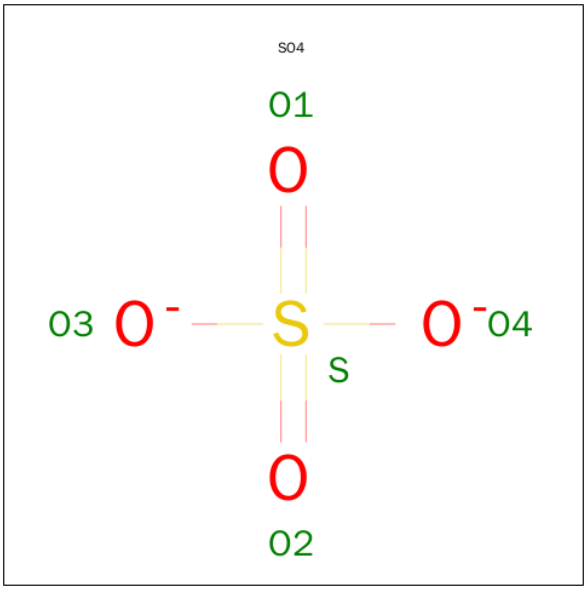
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ASP	DELETION	UNP Q8N0R1
H	?	-	ASP	DELETION	UNP Q8N0R1
H	?	-	ASP	DELETION	UNP Q8N0R1
H	?	-	ASN	DELETION	UNP Q8N0R1
H	?	-	ASN	DELETION	UNP Q8N0R1
H	?	-	TYR	DELETION	UNP Q8N0R1
H	?	-	ASP	DELETION	UNP Q8N0R1
H	?	-	ASP	DELETION	UNP Q8N0R1
H	?	-	ASP	DELETION	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 (three-letter code: SO4) (formula: O_4S).



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

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

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

- Molecule 3 is water.

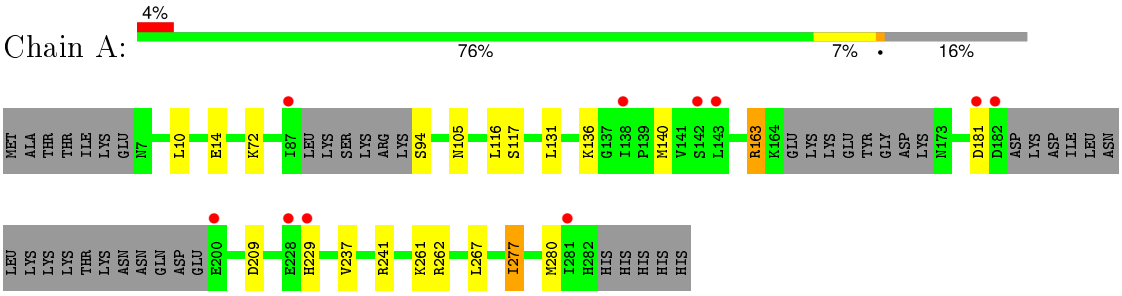
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	56	Total O 56 56	0	0
3	B	68	Total O 68 68	0	0
3	C	39	Total O 39 39	0	0
3	D	53	Total O 53 53	0	0
3	E	13	Total O 13 13	0	0
3	F	15	Total O 15 15	0	0
3	G	19	Total O 19 19	0	0
3	H	1	Total O 1 1	0	0

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.

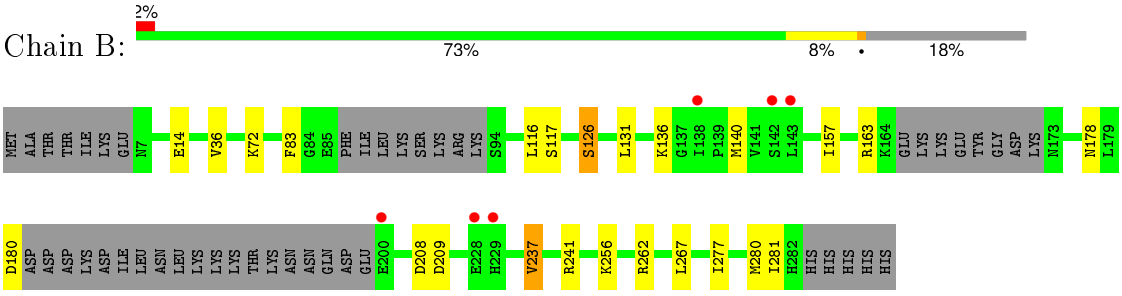
- Molecule 1: Orotate phosphoribosyltransferase

Chain A:



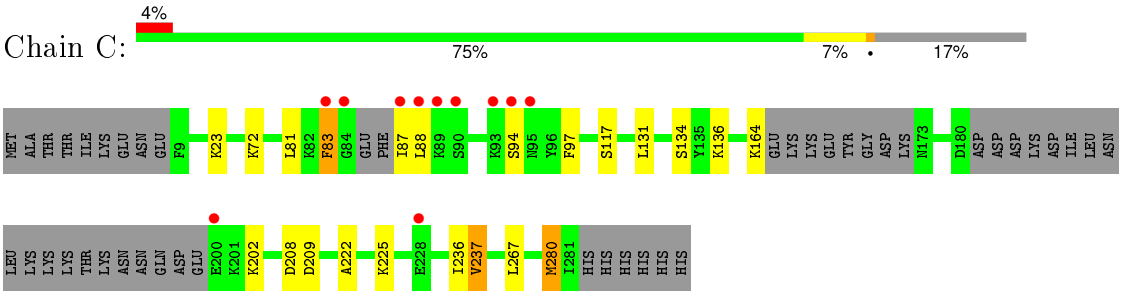
- Molecule 1: Orotate phosphoribosyltransferase

Chain B:



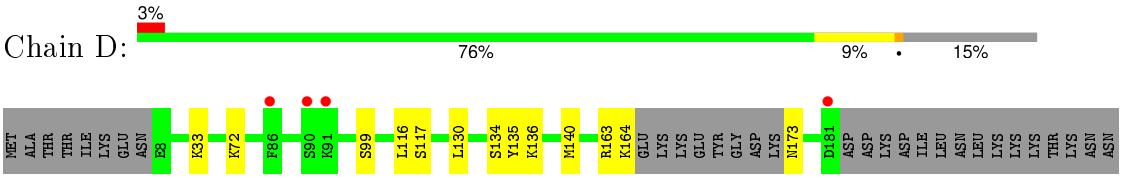
- Molecule 1: Orotate phosphoribosyltransferase

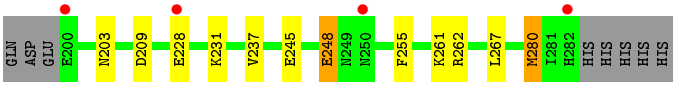
Chain C:



- Molecule 1: Orotate phosphoribosyltransferase

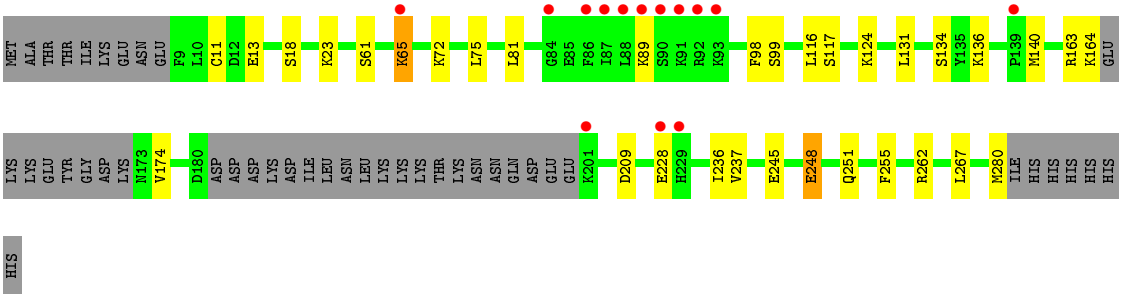
Chain D:





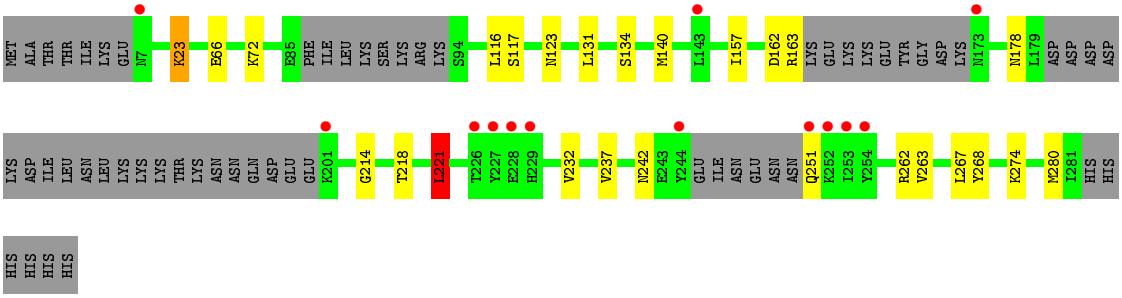
• Molecule 1: Orotate phosphoribosyltransferase

Chain E:



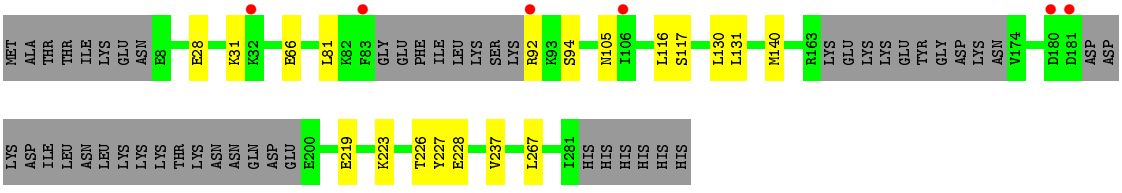
• Molecule 1: Orotate phosphoribosyltransferase

Chain F:



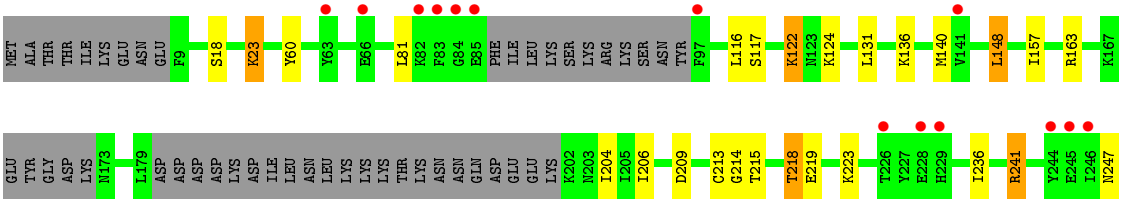
• Molecule 1: Orotate phosphoribosyltransferase

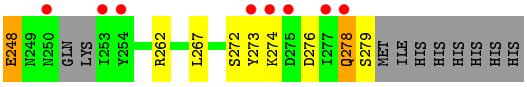
Chain G:



• Molecule 1: Orotate phosphoribosyltransferase

Chain H:




E248
N249
N250
GLN
LYS
T253
Y254
R262
L267
S272
Y273
K274
D275
D276
I277
Q278
S279
MET
ILE
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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 40.44 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.47-2.60) 98.6 (40.44-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.197 , 0.218 0.199 , 0.222	Depositor DCC
R_{free} test set	4570 reflections (5.34%)	DCC
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 , 36.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 90553 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.91	0/1878	0.87	4/2517 (0.2%)
1	B	0.99	4/1842 (0.2%)	0.92	4/2468 (0.2%)
1	C	0.82	0/1865	0.85	3/2495 (0.1%)
1	D	0.85	0/1915	0.90	2/2564 (0.1%)
1	E	0.76	0/1870	0.88	3/2503 (0.1%)
1	F	0.80	0/1754	0.87	4/2348 (0.2%)
1	G	0.82	2/1821 (0.1%)	0.89	3/2439 (0.1%)
1	H	0.71	0/1753	0.93	8/2346 (0.3%)
All	All	0.84	6/14698 (0.0%)	0.89	31/19680 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	SER	CB-OG	-6.12	1.34	1.42
1	B	180	ASP	CB-CG	5.75	1.63	1.51
1	B	14	GLU	CD-OE2	5.67	1.31	1.25
1	G	66	GLU	CD-OE2	-5.58	1.19	1.25
1	B	14	GLU	CG-CD	5.48	1.60	1.51
1	G	219	GLU	CG-CD	5.11	1.59	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	262	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	C	280	MET	CG-SD-CE	9.34	115.14	100.20
1	F	221	LEU	CA-CB-CG	7.39	132.29	115.30
1	H	276	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	277	ILE	CG1-CB-CG2	-7.09	95.81	111.40
1	B	262	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	F	23	LYS	CD-CE-NZ	6.60	126.88	111.70
1	E	163	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	163	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	H	148	LEU	CA-CB-CG	6.08	129.27	115.30
1	C	83	PHE	CB-CA-C	6.06	122.52	110.40
1	C	202	LYS	CD-CE-NZ	6.04	125.59	111.70
1	A	14	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	H	262	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	H	23	LYS	CD-CE-NZ	5.89	125.25	111.70
1	H	241	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	280	MET	CG-SD-CE	5.77	109.43	100.20
1	B	163	ARG	CB-CG-CD	5.74	126.53	111.60
1	E	262	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	H	218	THR	N-CA-CB	5.66	121.05	110.30
1	B	163	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	G	228	GLU	N-CA-C	-5.46	96.25	111.00
1	G	66	GLU	CG-CD-OE1	5.43	129.16	118.30
1	F	262	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	262	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	H	122	LYS	CA-CB-CG	-5.30	101.75	113.40
1	G	28	GLU	CG-CD-OE1	5.20	128.70	118.30
1	H	213	CYS	CA-CB-SG	5.16	123.28	114.00
1	F	163	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	D	228	GLU	N-CA-C	-5.08	97.29	111.00
1	E	251	GLN	N-CA-CB	-5.01	101.58	110.60

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 (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	1846	0	1901	12	0
1	B	1811	0	1873	16	0
1	C	1835	0	1927	13	0
1	D	1882	0	1960	15	0
1	E	1838	0	1926	17	0
1	F	1725	0	1801	19	0
1	G	1791	0	1862	9	0
1	H	1725	0	1801	17	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	113	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 (113) 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:72:LYS:HD2	1:A:280:MET:HE2	1.56	0.88
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:251:GLN:HG3	1:F:251:GLN:O	1.97	0.64
1:B:116:LEU:HD11	1:B:140:MET:CE	2.27	0.64
1:F:72:LYS:HE3	1:F:280:MET:HE2	1.80	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: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:H:23:LYS:NZ	2:H:302:SO4:O4	2.32	0.62
1:C:136:LYS:HD2	1:C:209:ASP:OD2	2.00	0.62
1:F:72:LYS:HE3	1:F:280:MET:CE	2.29	0.62
1:B:256:LYS:HE3	3:B:417:HOH:O	2.00	0.62
1:C:72:LYS:HD3	1:C:280:MET:HE2	1.81	0.61
1:B:241:ARG:NH1	3:B:448:HOH:O	2.24	0.60
1:F:263:VAL:O	1:F:263:VAL:HG22	2.02	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: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:72:LYS:HD2	1:D:280:MET:HE2	1.86	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:E:11:CYS:SG	1:E:13:GLU:OE1	2.62	0.56
1:A:131:LEU:HD23	1:A:131:LEU:C	2.26	0.56
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:116:LEU:HD11	1:G:140:MET:HE3	1.88	0.55
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
1:H:116:LEU:HD11	1:H:140:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:SO4:O3	1:H:163:ARG:NH1	2.38	0.53
1:B:36:VAL:HG11	1:F:66:GLU:HG3	1.91	0.52
1:B:131:LEU:C	1:B:131:LEU:HD23	2.29	0.52
1:F:116:LEU:HD11	1:F:140:MET:HE3	1.90	0.52
1:E:116:LEU:HD11	1:E:140:MET:HE3	1.90	0.52
1:H:278:GLN:O	1:H:279:SER:CB	2.57	0.51
1:F:23:LYS:NZ	2:F:304:SO4:O2	2.38	0.51
1:D:72:LYS:HD2	1:D:280:MET:CE	2.41	0.51
1:F:123:ASN:OD1	1:F:123:ASN:N	2.43	0.50
1:C:72:LYS:HD3	1:C:280:MET:CE	2.40	0.50
1:A:116:LEU:HD11	1:A:140:MET:HE3	1.93	0.50
1:G:131:LEU:HD23	1:G:131:LEU:C	2.33	0.49
1:E:136:LYS:HD2	1:E:209:ASP:OD2	2.13	0.49
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:D:116:LEU:HD11	1:D:140:MET:HE3	1.97	0.47
1:F:221:LEU:HD12	1:F:232:VAL:HG11	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: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:C:134:SER:OG	1:C:164:LYS:HE2	2.16	0.45
1:B:72:LYS:HB3	1:B:280:MET:CE	2.46	0.45
1:F:242:ASN:ND2	1:F:274:LYS:H	2.14	0.45
1:B:72:LYS:HD2	1:B:280:MET:CE	2.47	0.45
1:D:245:GLU:HG2	1:D:255:PHE:CZ	2.51	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:C:131:LEU:HD23	1:C:131:LEU:C	2.37	0.45
1:E:72:LYS:HB3	1:E:280:MET:CE	2.47	0.44
1:B:72:LYS:HD2	1:B:280:MET:HE3	1.98	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
1:F:131:LEU:C	1:F:131:LEU:HD23	2.38	0.44
1:H:204:ILE:HG22	1:H:206:ILE:HD13	2.00	0.44
1:B:116:LEU:HD11	1:B:140:MET:HE3	1.98	0.43
1:D:72:LYS:HB3	1:D:280:MET:CE	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:HD22	1:B:178:ASN:HD21	1.66	0.43
1:F:123:ASN:ND2	1:F:268:TYR:CE2	2.86	0.43
1:G:81:LEU:HA	1:G:81:LEU:HD12	1.88	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:B:136:LYS:HD3	1:B:209:ASP:OD2	2.20	0.42
1:E:136:LYS:HE2	2:E:301:SO4:O1	2.21	0.41
1:C:208:ASP:O	1:C:237:VAL:HA	2.20	0.41
1:H:148:LEU:HD23	1:H:157:ILE:HD13	2.02	0.41
1:G:31:LYS:HA	1:G:31:LYS:HD2	1.88	0.41
1:D:262:ARG:NE	3:D:451:HOH:O	2.37	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:C:81:LEU:HA	1:C:81:LEU:HD12	1.90	0.41
1:E:131:LEU:HD23	1:E:131:LEU:C	2.41	0.41
1:B:136:LYS:CE	2:B:305:SO4:O4	2.65	0.41
1:B:208:ASP:O	1:B:237:VAL:HA	2.21	0.41
1:A:277:ILE:HD12	1:A:277:ILE:N	2.36	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
1:F:72:LYS:HE3	1:F:280:MET:HE3	2.02	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	215/266 (81%)	210 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	34	60
All	All	1683/2128 (79%)	1653 (98%)	29 (2%)	1 (0%)	56	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	278	GLN

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	211/252 (84%)	206 (98%)	5 (2%)	57	82
1	B	207/252 (82%)	201 (97%)	6 (3%)	50	77
1	C	210/252 (83%)	206 (98%)	4 (2%)	65	86
1	D	215/252 (85%)	208 (97%)	7 (3%)	45	73
1	E	210/252 (83%)	200 (95%)	10 (5%)	31	58
1	F	197/252 (78%)	192 (98%)	5 (2%)	55	81
1	G	205/252 (81%)	201 (98%)	4 (2%)	63	85
1	H	197/252 (78%)	188 (95%)	9 (5%)	33	61
All	All	1652/2016 (82%)	1602 (97%)	50 (3%)	48	76

All (50) 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	237	VAL
1	A	267	LEU
1	B	117	SER
1	B	126	SER
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	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	267	LEU
1	F	117	SER
1	F	157	ILE
1	F	221	LEU
1	F	237	VAL
1	F	267	LEU
1	G	117	SER
1	G	130	LEU
1	G	237	VAL
1	G	267	LEU
1	H	18	SER
1	H	117	SER

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Mol	Chain	Res	Type
1	H	124	LYS
1	H	215	THR
1	H	236	ILE
1	H	241	ARG
1	H	248	GLU
1	H	267	LEU
1	H	272	SER

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

Mol	Chain	Res	Type
1	B	178	ASN
1	F	178	ASN
1	F	242	ASN
1	H	173	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

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	A	301	-	4,4,4	0.69	0	6,6,6	1.31	1 (16%)
2	SO4	A	302	-	4,4,4	0.55	0	6,6,6	0.16	0
2	SO4	A	303	-	4,4,4	1.46	1 (25%)	6,6,6	1.24	1 (16%)
2	SO4	A	304	-	4,4,4	1.26	1 (25%)	6,6,6	0.81	0
2	SO4	B	301	-	4,4,4	0.78	0	6,6,6	0.59	0
2	SO4	B	302	-	4,4,4	0.65	0	6,6,6	0.56	0
2	SO4	B	303	-	4,4,4	0.74	0	6,6,6	0.99	1 (16%)
2	SO4	B	304	-	4,4,4	1.17	0	6,6,6	1.17	1 (16%)
2	SO4	B	305	-	4,4,4	0.95	0	6,6,6	1.35	1 (16%)
2	SO4	C	301	-	4,4,4	0.78	0	6,6,6	0.46	0
2	SO4	C	302	-	4,4,4	0.73	0	6,6,6	0.51	0
2	SO4	C	303	-	4,4,4	0.45	0	6,6,6	0.28	0
2	SO4	C	304	-	4,4,4	0.75	0	6,6,6	0.49	0
2	SO4	C	305	-	4,4,4	0.44	0	6,6,6	0.46	0
2	SO4	D	301	-	4,4,4	0.71	0	6,6,6	0.61	0
2	SO4	D	302	-	4,4,4	0.42	0	6,6,6	0.80	0
2	SO4	D	303	-	4,4,4	0.22	0	6,6,6	0.66	0
2	SO4	D	304	-	4,4,4	0.09	0	6,6,6	0.86	0
2	SO4	D	305	-	4,4,4	1.27	0	6,6,6	2.04	2 (33%)
2	SO4	E	301	-	4,4,4	0.75	0	6,6,6	1.04	1 (16%)
2	SO4	E	302	-	4,4,4	0.59	0	6,6,6	0.56	0
2	SO4	E	303	-	4,4,4	0.86	0	6,6,6	0.32	0
2	SO4	E	304	-	4,4,4	0.74	0	6,6,6	0.40	0
2	SO4	F	301	-	4,4,4	0.31	0	6,6,6	0.94	0
2	SO4	F	302	-	4,4,4	0.81	0	6,6,6	0.76	0
2	SO4	F	303	-	4,4,4	0.64	0	6,6,6	0.57	0
2	SO4	F	304	-	4,4,4	0.62	0	6,6,6	0.35	0
2	SO4	G	301	-	4,4,4	0.79	0	6,6,6	0.44	0
2	SO4	G	302	-	4,4,4	0.53	0	6,6,6	0.20	0
2	SO4	G	303	-	4,4,4	0.44	0	6,6,6	0.35	0
2	SO4	H	301	-	4,4,4	0.84	0	6,6,6	0.38	0
2	SO4	H	302	-	4,4,4	0.76	0	6,6,6	0.53	0
2	SO4	H	303	-	4,4,4	0.85	0	6,6,6	0.43	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
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	303	-	-	0/0/0/0	0/0/0/0
2	SO4	A	304	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	303	-	-	0/0/0/0	0/0/0/0
2	SO4	B	304	-	-	0/0/0/0	0/0/0/0
2	SO4	B	305	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	SO4	C	303	-	-	0/0/0/0	0/0/0/0
2	SO4	C	304	-	-	0/0/0/0	0/0/0/0
2	SO4	C	305	-	-	0/0/0/0	0/0/0/0
2	SO4	D	301	-	-	0/0/0/0	0/0/0/0
2	SO4	D	302	-	-	0/0/0/0	0/0/0/0
2	SO4	D	303	-	-	0/0/0/0	0/0/0/0
2	SO4	D	304	-	-	0/0/0/0	0/0/0/0
2	SO4	D	305	-	-	0/0/0/0	0/0/0/0
2	SO4	E	301	-	-	0/0/0/0	0/0/0/0
2	SO4	E	302	-	-	0/0/0/0	0/0/0/0
2	SO4	E	303	-	-	0/0/0/0	0/0/0/0
2	SO4	E	304	-	-	0/0/0/0	0/0/0/0
2	SO4	F	301	-	-	0/0/0/0	0/0/0/0
2	SO4	F	302	-	-	0/0/0/0	0/0/0/0
2	SO4	F	303	-	-	0/0/0/0	0/0/0/0
2	SO4	F	304	-	-	0/0/0/0	0/0/0/0
2	SO4	G	301	-	-	0/0/0/0	0/0/0/0
2	SO4	G	302	-	-	0/0/0/0	0/0/0/0
2	SO4	G	303	-	-	0/0/0/0	0/0/0/0
2	SO4	H	301	-	-	0/0/0/0	0/0/0/0
2	SO4	H	302	-	-	0/0/0/0	0/0/0/0
2	SO4	H	303	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	303	SO4	O1-S	2.02	1.54	1.47
2	A	304	SO4	O1-S	2.44	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	305	SO4	O2-S-O1	-3.72	97.72	109.50
2	D	305	SO4	O4-S-O3	-2.91	97.16	108.98
2	A	301	SO4	O2-S-O1	-2.53	101.47	109.50
2	B	304	SO4	O4-S-O3	-2.37	99.35	108.98
2	B	303	SO4	O2-S-O1	-2.21	102.49	109.50
2	A	303	SO4	O4-S-O3	-2.09	100.49	108.98
2	E	301	SO4	O4-S-O3	2.34	118.49	108.98
2	B	305	SO4	O2-S-O1	2.96	118.86	109.50

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	B	305	SO4	2	0
2	C	305	SO4	1	0
2	E	301	SO4	3	0
2	E	304	SO4	1	0
2	F	304	SO4	1	0
2	H	302	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	223/266 (83%)	-0.15	10 (4%) 37 29	27, 44, 87, 130	0
1	B	219/266 (82%)	-0.23	6 (2%) 58 51	29, 43, 79, 108	0
1	C	222/266 (83%)	-0.13	11 (4%) 32 26	35, 52, 98, 144	0
1	D	227/266 (85%)	-0.11	8 (3%) 48 40	32, 47, 84, 120	0
1	E	222/266 (83%)	0.08	14 (6%) 23 17	45, 65, 105, 131	0
1	F	209/266 (78%)	-0.02	13 (6%) 24 18	39, 62, 105, 131	0
1	G	216/266 (81%)	-0.16	6 (2%) 56 49	41, 58, 100, 124	0
1	H	209/266 (78%)	0.52	22 (10%) 8 5	48, 82, 133, 169	0
All	All	1747/2128 (82%)	-0.03	90 (5%) 31 24	27, 57, 109, 169	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	244	TYR	5.9
1	E	86	PHE	5.8
1	E	87	ILE	5.6
1	H	250	ASN	5.6
1	H	246	ILE	5.5
1	H	253	ILE	4.8
1	F	252	LYS	4.8
1	H	83	PHE	4.6
1	A	182	ASP	4.4
1	E	88	LEU	4.3
1	F	244	TYR	4.3
1	F	173	ASN	4.3
1	E	90	SER	4.2
1	F	253	ILE	4.2
1	E	91	LYS	4.2
1	H	278	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	228	GLU	3.8
1	E	92	ARG	3.8
1	H	229	HIS	3.7
1	D	181	ASP	3.7
1	H	84	GLY	3.6
1	C	83	PHE	3.6
1	C	89	LYS	3.6
1	H	82	LYS	3.5
1	H	274	LYS	3.5
1	F	228	GLU	3.5
1	E	229	HIS	3.5
1	E	89	LYS	3.4
1	D	282	HIS	3.4
1	C	88	LEU	3.4
1	H	97	PHE	3.3
1	F	229	HIS	3.3
1	C	90	SER	3.3
1	C	84	GLY	3.2
1	F	254	TYR	3.2
1	D	200	GLU	3.2
1	G	181	ASP	3.1
1	C	200	GLU	3.1
1	H	63	TYR	3.1
1	A	229	HIS	3.0
1	A	181	ASP	3.0
1	D	86	PHE	2.9
1	F	201	LYS	2.9
1	E	93	LYS	2.9
1	B	228	GLU	2.8
1	F	226	THR	2.8
1	H	228	GLU	2.7
1	B	200	GLU	2.7
1	H	66	GLU	2.7
1	A	228	GLU	2.7
1	B	229	HIS	2.7
1	C	95	ASN	2.7
1	E	201	LYS	2.7
1	F	227	TYR	2.6
1	F	7	ASN	2.6
1	G	92	ARG	2.6
1	F	251	GLN	2.6
1	D	91	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	85	GLU	2.5
1	C	87	ILE	2.5
1	H	277	ILE	2.5
1	B	143	LEU	2.5
1	G	32	LYS	2.4
1	A	281	ILE	2.4
1	A	200	GLU	2.4
1	E	84	GLY	2.4
1	C	228	GLU	2.4
1	D	228	GLU	2.4
1	D	250	ASN	2.4
1	C	94	SER	2.3
1	A	143	LEU	2.3
1	E	65	LYS	2.3
1	H	245	GLU	2.3
1	B	142	SER	2.3
1	H	275	ASP	2.2
1	E	139	PRO	2.2
1	H	226	THR	2.2
1	A	87	ILE	2.1
1	G	83	PHE	2.1
1	G	180	ASP	2.1
1	B	138	ILE	2.1
1	A	142	SER	2.1
1	F	143	LEU	2.1
1	G	106	ILE	2.1
1	H	273	TYR	2.1
1	D	90	SER	2.1
1	H	141	VAL	2.1
1	C	93	LYS	2.1
1	A	138	ILE	2.0
1	H	254	TYR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	E	304	5/5	0.70	0.27	5.72	103,103,132,141	0
2	SO4	D	301	5/5	0.99	0.17	1.89	53,55,58,61	0
2	SO4	D	305	5/5	0.86	0.24	1.81	74,79,102,106	0
2	SO4	F	302	5/5	0.97	0.18	1.09	78,79,89,97	0
2	SO4	D	303	5/5	0.99	0.14	0.10	44,45,48,48	0
2	SO4	A	303	5/5	0.94	0.16	-0.31	53,57,66,70	0
2	SO4	A	301	5/5	0.98	0.12	-0.36	54,54,58,59	0
2	SO4	F	301	5/5	0.98	0.12	-0.36	65,68,74,75	0
2	SO4	F	304	5/5	0.97	0.14	-0.44	67,67,73,87	0
2	SO4	A	304	5/5	0.98	0.10	-0.45	53,54,60,60	0
2	SO4	C	302	5/5	0.99	0.08	-0.71	46,47,48,48	0
2	SO4	H	302	5/5	0.94	0.14	-0.71	86,88,89,91	0
2	SO4	F	303	5/5	0.96	0.08	-0.80	76,79,81,81	0
2	SO4	G	303	5/5	0.95	0.10	-0.93	83,83,86,94	0
2	SO4	G	302	5/5	0.99	0.08	-0.94	48,48,51,52	0
2	SO4	B	302	5/5	0.98	0.11	-0.95	55,59,62,64	0
2	SO4	B	303	5/5	0.98	0.09	-1.05	47,54,57,60	0
2	SO4	G	301	5/5	0.95	0.11	-1.11	72,86,89,89	0
2	SO4	D	302	5/5	0.98	0.10	-1.17	66,71,79,79	0
2	SO4	E	303	5/5	0.99	0.09	-1.22	48,51,52,54	0
2	SO4	B	304	5/5	0.96	0.12	-1.28	54,62,62,65	0
2	SO4	E	301	5/5	0.96	0.11	-1.28	69,69,73,82	0
2	SO4	C	305	5/5	0.95	0.11	-1.39	72,75,87,87	0
2	SO4	C	301	5/5	0.96	0.11	-1.40	69,70,76,82	0
2	SO4	D	304	5/5	0.98	0.12	-1.53	64,72,77,77	0
2	SO4	H	303	5/5	0.91	0.12	-1.80	84,93,100,104	0
2	SO4	B	301	5/5	0.99	0.09	-2.18	42,43,48,50	0
2	SO4	A	302	5/5	0.99	0.07	-2.43	46,46,48,52	0
2	SO4	H	301	5/5	0.97	0.07	-3.27	84,87,89,98	0
2	SO4	B	305	5/5	0.94	0.11	-3.45	77,82,86,94	0
2	SO4	C	303	5/5	0.99	0.08	-	63,66,69,70	0
2	SO4	E	302	5/5	0.85	0.20	-	112,116,123,124	0
2	SO4	C	304	5/5	0.80	0.34	-	121,122,126,127	0

6.5 Other polymers (i)

There are no such residues in this entry.