



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2022 – 08:48 am GMT

PDB ID : 7PKC
Title : Streptococcus pyogenes Apo-GapN C284S variant
Authors : Schindelin, H.; Albert, L.
Deposited on : 2021-08-25
Resolution : 1.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

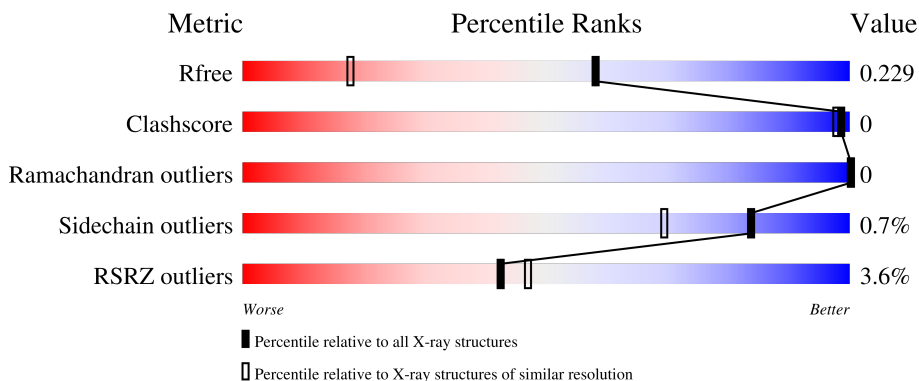
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	496	 2% 94%
1	B	496	 3% 94%
1	C	496	 % 94%
1	D	496	 % 95%
1	E	496	 5% 94%

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Mol	Chain	Length	Quality of chain
1	F	496	 2% 93% . .
1	G	496	 % 94% . .
1	H	496	 2% 94% . .
1	I	496	 12% 94% . .
1	J	496	 4% 93% . .
1	K	496	 % 94% . .
1	L	496	 % 94% . .
1	M	496	 10% 93% . .
1	N	496	 7% 95% . .
1	O	496	 % 94% . .
1	P	496	 % 95% . .

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
3	GOL	J	504	-	-	-	X
3	GOL	P	504	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 123923 atoms, of which 59318 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 Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	474	7306	2307	3697	596	697	9	3697	11	0
1	B	474	7377	2328	3743	596	702	8	3743	17	0
1	C	475	7307	2303	3699	593	703	9	3702	12	0
1	D	476	7347	2314	3723	600	700	10	3723	13	0
1	E	474	7355	2319	3720	598	708	10	3720	20	0
1	F	474	7310	2310	3695	593	704	8	3695	14	0
1	G	474	7308	2299	3700	596	703	10	3700	15	0
1	H	476	7357	2318	3722	597	711	9	3722	18	0
1	I	476	7289	2298	3684	598	700	9	3689	9	0
1	J	474	7397	2333	3757	596	703	8	3757	19	0
1	K	476	7372	2321	3736	600	705	10	3736	15	0
1	L	476	7289	2299	3686	594	701	9	3686	10	0
1	M	476	7243	2287	3658	593	696	9	3658	5	0
1	N	474	7230	2286	3648	591	697	8	3648	7	0
1	O	476	7355	2317	3727	598	703	10	3727	14	0
1	P	476	7349	2318	3723	596	702	10	3723	14	0

There are 400 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
A	-19	SER	-	expression tag	UNP A0A7G1J7Q1
A	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
A	-17	SER	-	expression tag	UNP A0A7G1J7Q1
A	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
A	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
A	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
A	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
A	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
A	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
A	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
A	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
A	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
A	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
A	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
A	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
A	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
A	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
A	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
A	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
A	0	PHE	-	expression tag	UNP A0A7G1J7Q1
A	58	THR	ALA	conflict	UNP A0A7G1J7Q1
A	170	ALA	SER	conflict	UNP A0A7G1J7Q1
A	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
A	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
B	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
B	-19	SER	-	expression tag	UNP A0A7G1J7Q1
B	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
B	-17	SER	-	expression tag	UNP A0A7G1J7Q1
B	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
B	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
B	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
B	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
B	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
B	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
B	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
B	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
B	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
B	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
B	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
B	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
B	-4	ARG	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
B	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
B	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
B	0	PHE	-	expression tag	UNP A0A7G1J7Q1
B	58	THR	ALA	conflict	UNP A0A7G1J7Q1
B	170	ALA	SER	conflict	UNP A0A7G1J7Q1
B	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
B	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
C	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
C	-19	SER	-	expression tag	UNP A0A7G1J7Q1
C	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
C	-17	SER	-	expression tag	UNP A0A7G1J7Q1
C	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
C	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
C	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
C	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
C	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
C	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
C	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
C	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
C	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
C	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
C	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
C	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
C	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
C	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
C	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
C	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
C	0	PHE	-	expression tag	UNP A0A7G1J7Q1
C	58	THR	ALA	conflict	UNP A0A7G1J7Q1
C	170	ALA	SER	conflict	UNP A0A7G1J7Q1
C	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
C	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
D	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
D	-19	SER	-	expression tag	UNP A0A7G1J7Q1
D	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
D	-17	SER	-	expression tag	UNP A0A7G1J7Q1
D	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
D	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
D	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
D	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
D	-12	GLU	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
D	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
D	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
D	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
D	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
D	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
D	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
D	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
D	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
D	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
D	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
D	0	PHE	-	expression tag	UNP A0A7G1J7Q1
D	58	THR	ALA	conflict	UNP A0A7G1J7Q1
D	170	ALA	SER	conflict	UNP A0A7G1J7Q1
D	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
D	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
E	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
E	-19	SER	-	expression tag	UNP A0A7G1J7Q1
E	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
E	-17	SER	-	expression tag	UNP A0A7G1J7Q1
E	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
E	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
E	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
E	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
E	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
E	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
E	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
E	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
E	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
E	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
E	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
E	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
E	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
E	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
E	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
E	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
E	0	PHE	-	expression tag	UNP A0A7G1J7Q1
E	58	THR	ALA	conflict	UNP A0A7G1J7Q1
E	170	ALA	SER	conflict	UNP A0A7G1J7Q1
E	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
E	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
F	-20	ALA	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	SER	-	expression tag	UNP A0A7G1J7Q1
F	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
F	-17	SER	-	expression tag	UNP A0A7G1J7Q1
F	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
F	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
F	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
F	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
F	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
F	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
F	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
F	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
F	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
F	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
F	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
F	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
F	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
F	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
F	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
F	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
F	0	PHE	-	expression tag	UNP A0A7G1J7Q1
F	58	THR	ALA	conflict	UNP A0A7G1J7Q1
F	170	ALA	SER	conflict	UNP A0A7G1J7Q1
F	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
F	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
G	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
G	-19	SER	-	expression tag	UNP A0A7G1J7Q1
G	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
G	-17	SER	-	expression tag	UNP A0A7G1J7Q1
G	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
G	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
G	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
G	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
G	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
G	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
G	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
G	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
G	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
G	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
G	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
G	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
G	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
G	-3	GLY	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
G	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
G	0	PHE	-	expression tag	UNP A0A7G1J7Q1
G	58	THR	ALA	conflict	UNP A0A7G1J7Q1
G	170	ALA	SER	conflict	UNP A0A7G1J7Q1
G	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
G	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
H	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
H	-19	SER	-	expression tag	UNP A0A7G1J7Q1
H	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
H	-17	SER	-	expression tag	UNP A0A7G1J7Q1
H	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
H	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
H	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
H	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
H	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
H	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
H	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
H	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
H	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
H	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
H	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
H	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
H	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
H	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
H	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
H	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
H	0	PHE	-	expression tag	UNP A0A7G1J7Q1
H	58	THR	ALA	conflict	UNP A0A7G1J7Q1
H	170	ALA	SER	conflict	UNP A0A7G1J7Q1
H	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
H	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
I	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
I	-19	SER	-	expression tag	UNP A0A7G1J7Q1
I	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
I	-17	SER	-	expression tag	UNP A0A7G1J7Q1
I	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
I	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
I	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
I	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
I	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
I	-11	LYS	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
I	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
I	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
I	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
I	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
I	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
I	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
I	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
I	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
I	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
I	0	PHE	-	expression tag	UNP A0A7G1J7Q1
I	58	THR	ALA	conflict	UNP A0A7G1J7Q1
I	170	ALA	SER	conflict	UNP A0A7G1J7Q1
I	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
I	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
J	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
J	-19	SER	-	expression tag	UNP A0A7G1J7Q1
J	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
J	-17	SER	-	expression tag	UNP A0A7G1J7Q1
J	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
J	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
J	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
J	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
J	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
J	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
J	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
J	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
J	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
J	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
J	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
J	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
J	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
J	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
J	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
J	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
J	0	PHE	-	expression tag	UNP A0A7G1J7Q1
J	58	THR	ALA	conflict	UNP A0A7G1J7Q1
J	170	ALA	SER	conflict	UNP A0A7G1J7Q1
J	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
J	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
K	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
K	-19	SER	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
K	-17	SER	-	expression tag	UNP A0A7G1J7Q1
K	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
K	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
K	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
K	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
K	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
K	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
K	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
K	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
K	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
K	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
K	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
K	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
K	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
K	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
K	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
K	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
K	0	PHE	-	expression tag	UNP A0A7G1J7Q1
K	58	THR	ALA	conflict	UNP A0A7G1J7Q1
K	170	ALA	SER	conflict	UNP A0A7G1J7Q1
K	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
K	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
L	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
L	-19	SER	-	expression tag	UNP A0A7G1J7Q1
L	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
L	-17	SER	-	expression tag	UNP A0A7G1J7Q1
L	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
L	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
L	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
L	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
L	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
L	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
L	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
L	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
L	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
L	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
L	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
L	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
L	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
L	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
L	-2	PRO	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
L	0	PHE	-	expression tag	UNP A0A7G1J7Q1
L	58	THR	ALA	conflict	UNP A0A7G1J7Q1
L	170	ALA	SER	conflict	UNP A0A7G1J7Q1
L	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
L	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
M	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
M	-19	SER	-	expression tag	UNP A0A7G1J7Q1
M	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
M	-17	SER	-	expression tag	UNP A0A7G1J7Q1
M	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
M	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
M	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
M	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
M	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
M	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
M	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
M	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
M	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
M	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
M	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
M	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
M	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
M	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
M	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
M	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
M	0	PHE	-	expression tag	UNP A0A7G1J7Q1
M	58	THR	ALA	conflict	UNP A0A7G1J7Q1
M	170	ALA	SER	conflict	UNP A0A7G1J7Q1
M	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
M	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
N	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
N	-19	SER	-	expression tag	UNP A0A7G1J7Q1
N	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
N	-17	SER	-	expression tag	UNP A0A7G1J7Q1
N	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
N	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
N	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
N	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
N	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
N	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
N	-10	ILE	-	expression tag	UNP A0A7G1J7Q1

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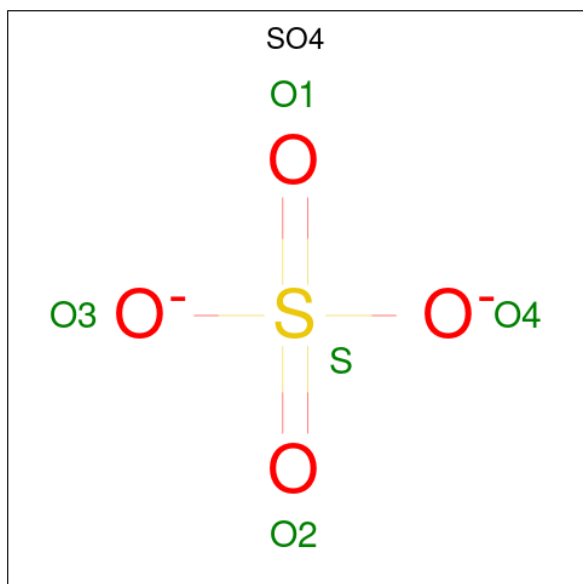
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N	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
N	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
N	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
N	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
N	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
N	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
N	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
N	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
N	0	PHE	-	expression tag	UNP A0A7G1J7Q1
N	58	THR	ALA	conflict	UNP A0A7G1J7Q1
N	170	ALA	SER	conflict	UNP A0A7G1J7Q1
N	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
N	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
O	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
O	-19	SER	-	expression tag	UNP A0A7G1J7Q1
O	-18	TRP	-	expression tag	UNP A0A7G1J7Q1
O	-17	SER	-	expression tag	UNP A0A7G1J7Q1
O	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
O	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
O	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
O	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
O	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
O	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
O	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
O	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
O	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
O	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
O	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
O	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
O	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
O	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
O	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
O	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
O	0	PHE	-	expression tag	UNP A0A7G1J7Q1
O	58	THR	ALA	conflict	UNP A0A7G1J7Q1
O	170	ALA	SER	conflict	UNP A0A7G1J7Q1
O	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
O	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1
P	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
P	-19	SER	-	expression tag	UNP A0A7G1J7Q1
P	-18	TRP	-	expression tag	UNP A0A7G1J7Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-17	SER	-	expression tag	UNP A0A7G1J7Q1
P	-16	HIS	-	expression tag	UNP A0A7G1J7Q1
P	-15	PRO	-	expression tag	UNP A0A7G1J7Q1
P	-14	GLN	-	expression tag	UNP A0A7G1J7Q1
P	-13	PHE	-	expression tag	UNP A0A7G1J7Q1
P	-12	GLU	-	expression tag	UNP A0A7G1J7Q1
P	-11	LYS	-	expression tag	UNP A0A7G1J7Q1
P	-10	ILE	-	expression tag	UNP A0A7G1J7Q1
P	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
P	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
P	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
P	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
P	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
P	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
P	-3	GLY	-	expression tag	UNP A0A7G1J7Q1
P	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
P	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
P	0	PHE	-	expression tag	UNP A0A7G1J7Q1
P	58	THR	ALA	conflict	UNP A0A7G1J7Q1
P	170	ALA	SER	conflict	UNP A0A7G1J7Q1
P	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
P	284	SER	CYS	engineered mutation	UNP A0A7G1J7Q1

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



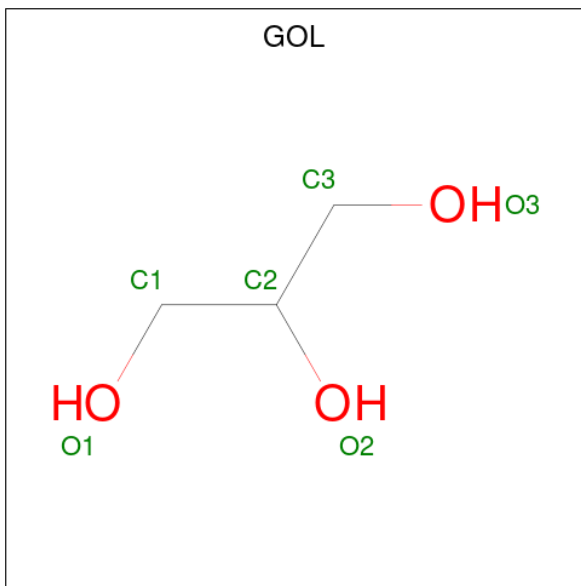
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	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	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	I	1	Total 6	C 3	O 3	0	0
3	J	1	Total 6	C 3	O 3	0	0
3	J	1	Total 6	C 3	O 3	0	0
3	J	1	Total 6	C 3	O 3	0	0
3	K	1	Total 6	C 3	O 3	0	0
3	L	1	Total 6	C 3	O 3	0	0
3	L	1	Total 6	C 3	O 3	0	0
3	M	1	Total 6	C 3	O 3	0	0
3	N	1	Total 6	C 3	O 3	0	0
3	O	1	Total 6	C 3	O 3	0	0
3	P	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	P	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		

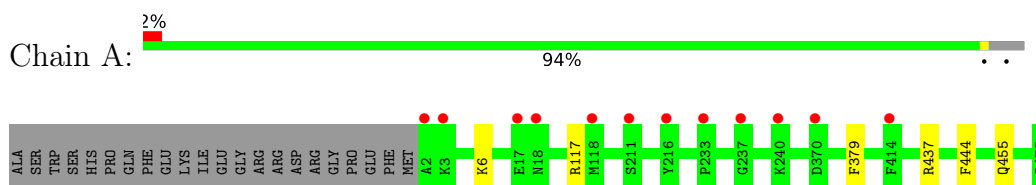
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	364	Total	O	0	5
			369	369		
4	B	426	Total	O	0	7
			433	433		
4	C	469	Total	O	0	6
			475	475		
4	D	456	Total	O	0	4
			460	460		
4	E	327	Total	O	0	4
			331	331		
4	F	444	Total	O	0	6
			450	450		
4	G	450	Total	O	0	3
			453	453		
4	H	417	Total	O	0	4
			421	421		
4	I	281	Total	O	0	6
			287	287		
4	J	392	Total	O	0	6
			398	398		
4	K	459	Total	O	0	2
			461	461		
4	L	440	Total	O	0	2
			442	442		
4	M	289	Total	O	0	1
			290	290		
4	N	295	Total	O	0	3
			298	298		
4	O	402	Total	O	0	7
			409	409		
4	P	450	Total	O	0	0
			450	450		

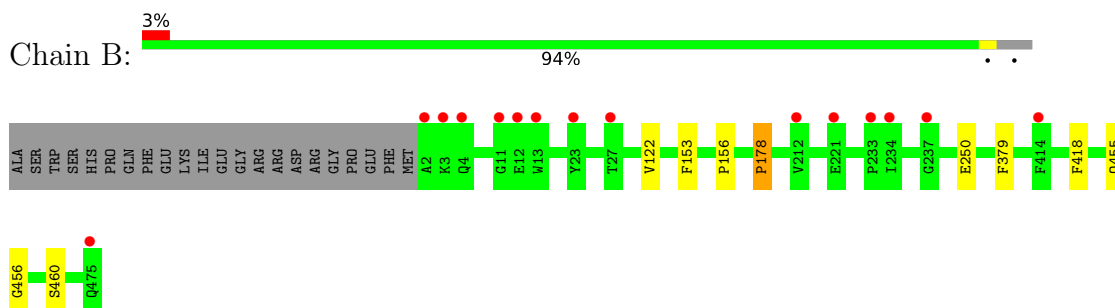
3 Residue-property plots [i](#)

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.

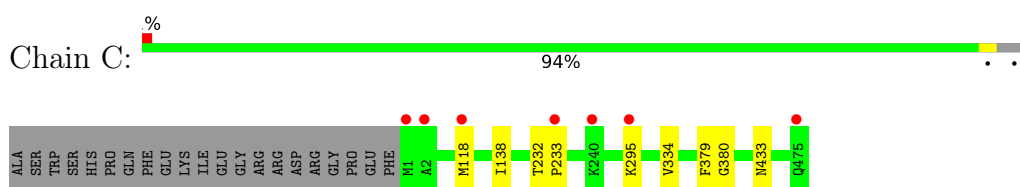
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



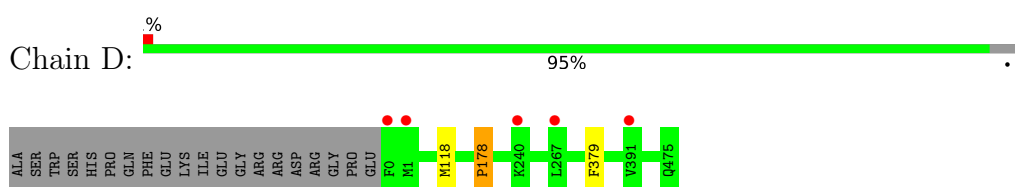
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

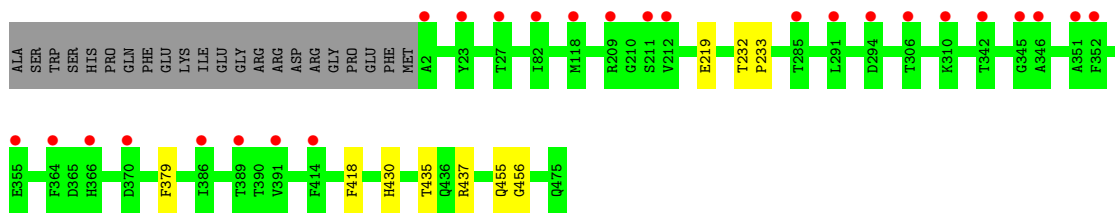


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

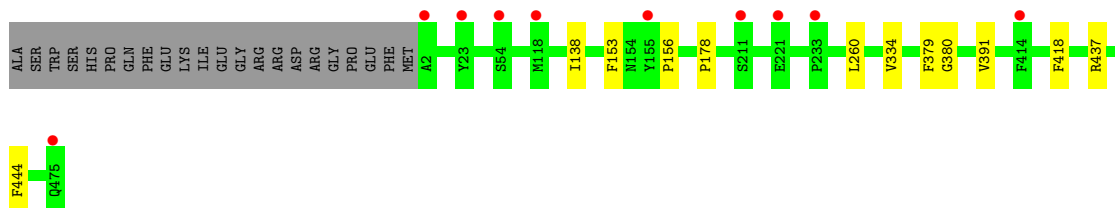


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

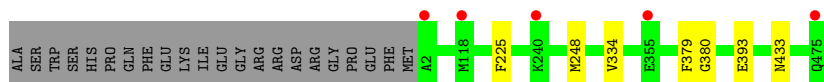




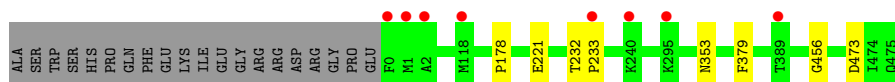
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



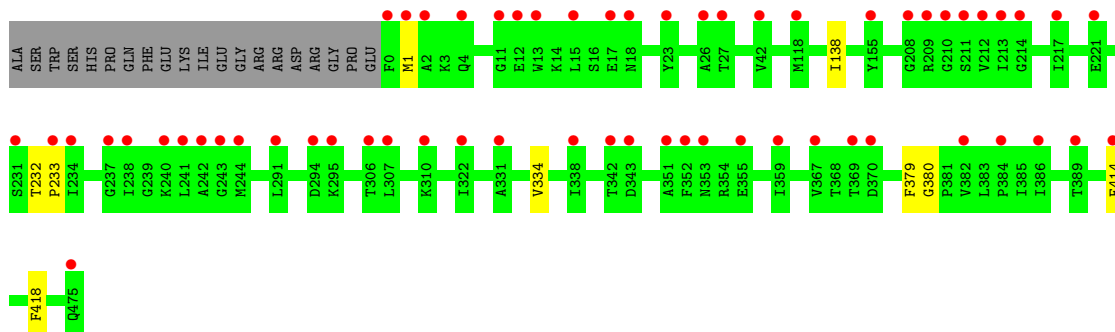
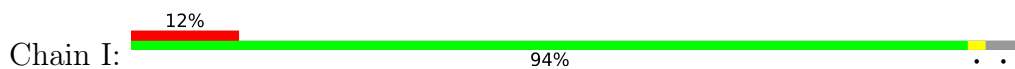
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



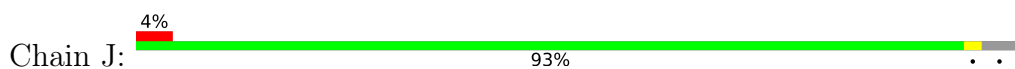
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

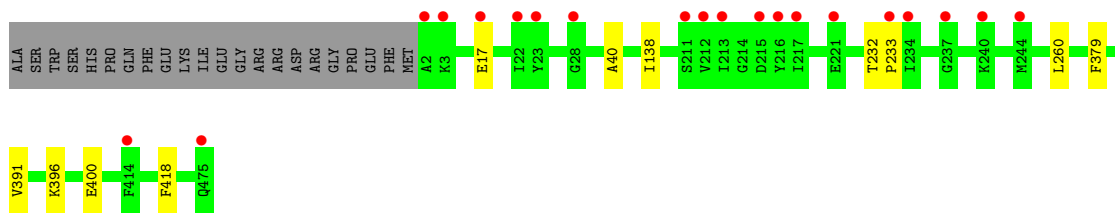


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

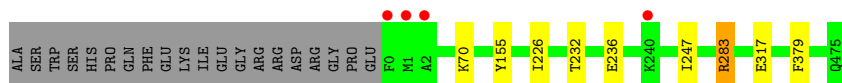
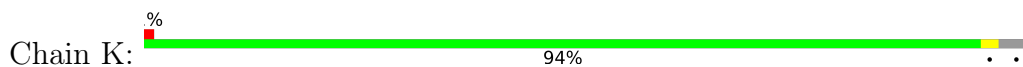


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

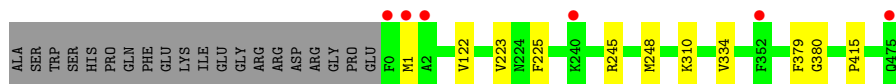
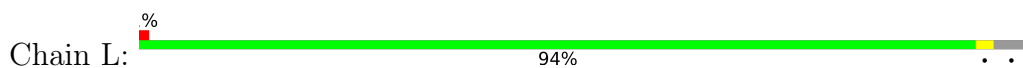




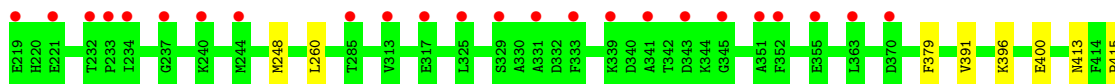
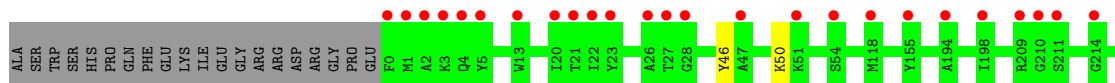
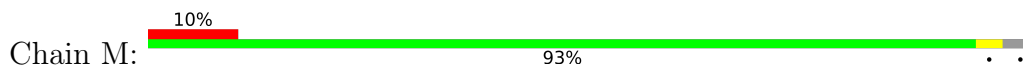
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



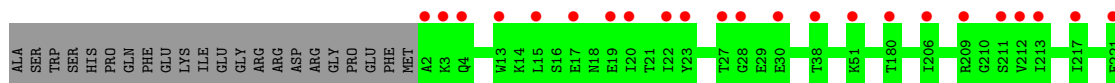
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

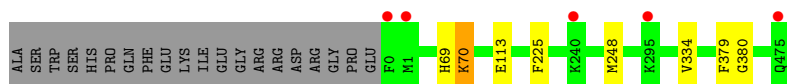


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

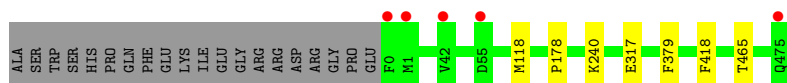


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase





- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.67Å 126.04Å 148.39Å 96.36° 104.81° 84.23°	Depositor
Resolution (Å)	19.97 – 1.50 19.97 – 1.50	Depositor EDS
% Data completeness (in resolution range)	68.6 (19.97-1.50) 68.6 (19.97-1.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.50Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.200 , 0.232 0.196 , 0.229	Depositor DCC
R_{free} test set	18412 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	123923	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.34 % 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 2.4010e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.41	0/3701	0.59	0/5016
1	B	0.43	0/3744	0.60	1/5074 (0.0%)
1	C	0.43	0/3701	0.59	0/5017
1	D	0.44	0/3721	0.59	0/5042
1	E	0.42	0/3750	0.60	2/5082 (0.0%)
1	F	0.43	0/3716	0.58	0/5039
1	G	0.43	0/3708	0.59	0/5023
1	H	0.43	0/3746	0.59	1/5078 (0.0%)
1	I	0.39	0/3690	0.56	0/5001
1	J	0.41	0/3756	0.57	0/5091
1	K	0.43	0/3739	0.59	0/5064
1	L	0.43	0/3691	0.59	0/5004
1	M	0.40	0/3658	0.57	0/4959
1	N	0.40	0/3662	0.56	0/4965
1	O	0.43	0/3728	0.58	0/5051
1	P	0.42	0/3727	0.59	0/5051
All	All	0.42	0/59438	0.58	4/80557 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	456[A]	GLY	N-CA-C	-6.26	97.46	113.10
1	E	456[B]	GLY	N-CA-C	-6.26	97.46	113.10
1	H	456	GLY	N-CA-C	-5.69	98.88	113.10
1	B	456	GLY	N-CA-C	-5.69	98.88	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3609	3697	3697	2	0
1	B	3634	3743	3743	5	0
1	C	3608	3699	3701	3	0
1	D	3624	3723	3725	1	0
1	E	3635	3720	3688	4	0
1	F	3615	3695	3695	6	0
1	G	3608	3700	3696	4	0
1	H	3635	3722	3718	3	0
1	I	3605	3684	3686	4	0
1	J	3640	3757	3757	5	0
1	K	3636	3736	3738	4	0
1	L	3603	3686	3688	5	0
1	M	3585	3658	3660	6	0
1	N	3582	3648	3648	1	0
1	O	3628	3727	3729	4	0
1	P	3626	3723	3725	2	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	5	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	0	0
2	L	15	0	0	0	0
2	M	10	0	0	0	0
2	N	5	0	0	0	0
2	O	10	0	0	0	0
2	P	10	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	12	0	16	1	0
3	G	6	0	8	0	0
3	H	24	0	32	0	0
3	I	6	0	8	0	0
3	J	18	0	24	1	0
3	K	6	0	8	0	0
3	L	12	0	16	0	0
3	M	6	0	8	0	0
3	N	6	0	8	0	0
3	O	6	0	8	0	0
3	P	18	0	24	0	0
4	A	369	0	0	1	0
4	B	433	0	0	1	0
4	C	475	0	0	0	0
4	D	460	0	0	1	0
4	E	331	0	0	1	0
4	F	450	0	0	2	0
4	G	453	0	0	0	0
4	H	421	0	0	1	0
4	I	287	0	0	0	0
4	J	398	0	0	0	0
4	K	461	0	0	1	0
4	L	442	0	0	0	0
4	M	290	0	0	0	0
4	N	298	0	0	0	0
4	O	409	0	0	0	0
4	P	450	0	0	1	0
All	All	64605	59318	59494	55	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 0.

The worst 5 of 55 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:D:178:PRO:HB3	4:D:611:HOH:O	1.94	0.67
1:K:317[A]:GLU:HG3	4:K:965:HOH:O	2.04	0.58
1:B:178:PRO:HB3	4:B:606:HOH:O	2.05	0.57
1:I:138:ILE:HG23	1:L:122:VAL:HG21	1.88	0.56
1:F:178:PRO:HB3	4:F:605:HOH:O	2.06	0.55

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	483/496 (97%)	473 (98%)	10 (2%)	0	100	100
1	B	489/496 (99%)	479 (98%)	10 (2%)	0	100	100
1	C	485/496 (98%)	476 (98%)	9 (2%)	0	100	100
1	D	487/496 (98%)	476 (98%)	11 (2%)	0	100	100
1	E	492/496 (99%)	479 (97%)	13 (3%)	0	100	100
1	F	486/496 (98%)	477 (98%)	9 (2%)	0	100	100
1	G	487/496 (98%)	474 (97%)	13 (3%)	0	100	100
1	H	492/496 (99%)	482 (98%)	10 (2%)	0	100	100
1	I	483/496 (97%)	472 (98%)	11 (2%)	0	100	100
1	J	491/496 (99%)	480 (98%)	11 (2%)	0	100	100
1	K	489/496 (99%)	475 (97%)	14 (3%)	0	100	100
1	L	484/496 (98%)	473 (98%)	11 (2%)	0	100	100
1	M	479/496 (97%)	468 (98%)	11 (2%)	0	100	100
1	N	479/496 (97%)	466 (97%)	13 (3%)	0	100	100
1	O	488/496 (98%)	477 (98%)	11 (2%)	0	100	100
1	P	488/496 (98%)	478 (98%)	10 (2%)	0	100	100
All	All	7782/7936 (98%)	7605 (98%)	177 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	380/388 (98%)	377 (99%)	3 (1%)	81	66
1	B	386/388 (100%)	383 (99%)	3 (1%)	81	66
1	C	382/388 (98%)	378 (99%)	4 (1%)	76	57
1	D	383/388 (99%)	379 (99%)	4 (1%)	76	57
1	E	385/388 (99%)	383 (100%)	2 (0%)	88	78
1	F	383/388 (99%)	381 (100%)	2 (0%)	88	78
1	G	383/388 (99%)	382 (100%)	1 (0%)	92	85
1	H	387/388 (100%)	382 (99%)	5 (1%)	69	44
1	I	380/388 (98%)	377 (99%)	3 (1%)	81	66
1	J	388/388 (100%)	385 (99%)	3 (1%)	81	66
1	K	386/388 (100%)	382 (99%)	4 (1%)	76	57
1	L	381/388 (98%)	378 (99%)	3 (1%)	81	66
1	M	376/388 (97%)	374 (100%)	2 (0%)	88	78
1	N	376/388 (97%)	373 (99%)	3 (1%)	81	66
1	O	385/388 (99%)	383 (100%)	2 (0%)	88	78
1	P	385/388 (99%)	381 (99%)	4 (1%)	76	57
All	All	6126/6208 (99%)	6078 (99%)	48 (1%)	84	66

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	379	PHE
1	L	310	LYS
1	J	418	PHE
1	K	283[B]	ARG
1	M	379	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

56 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	E	502	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	F	502	-	4,4,4	0.17	0	6,6,6	0.12	0
3	GOL	H	504	-	5,5,5	0.04	0	5,5,5	0.15	0
3	GOL	K	503	-	5,5,5	0.06	0	5,5,5	0.49	0
2	SO4	I	501	-	4,4,4	0.19	0	6,6,6	0.22	0
2	SO4	K	502	-	4,4,4	0.24	0	6,6,6	0.45	0
3	GOL	H	506	-	5,5,5	0.05	0	5,5,5	0.26	0
2	SO4	K	501	-	4,4,4	0.21	0	6,6,6	0.11	0
3	GOL	M	503	-	5,5,5	0.04	0	5,5,5	0.18	0
3	GOL	H	503	-	5,5,5	0.03	0	5,5,5	0.14	0
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	H	502	-	4,4,4	0.16	0	6,6,6	0.16	0
3	GOL	I	502	-	5,5,5	0.04	0	5,5,5	0.14	0
2	SO4	F	501	-	4,4,4	0.20	0	6,6,6	0.25	0
2	SO4	P	502	-	4,4,4	0.27	0	6,6,6	0.26	0
2	SO4	G	502	-	4,4,4	0.26	0	6,6,6	0.46	0
2	SO4	B	501	-	4,4,4	0.20	0	6,6,6	0.29	0
2	SO4	L	502	-	4,4,4	0.25	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	P	501	-	4,4,4	0.19	0	6,6,6	0.22	0
2	SO4	C	502	-	4,4,4	0.29	0	6,6,6	0.60	0
3	GOL	F	503	-	5,5,5	0.06	0	5,5,5	0.22	0
3	GOL	J	504	-	5,5,5	0.06	0	5,5,5	0.20	0
2	SO4	C	501	-	4,4,4	0.21	0	6,6,6	0.26	0
3	GOL	D	503	-	5,5,5	0.03	0	5,5,5	0.18	0
2	SO4	M	501	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	J	501	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	G	501	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	D	502	-	4,4,4	0.25	0	6,6,6	0.16	0
3	GOL	P	505	-	5,5,5	0.08	0	5,5,5	0.23	0
2	SO4	M	502	-	4,4,4	0.17	0	6,6,6	0.14	0
3	GOL	J	503	-	5,5,5	0.05	0	5,5,5	0.18	0
2	SO4	J	502	-	4,4,4	0.26	0	6,6,6	0.26	0
3	GOL	L	504	-	5,5,5	0.05	0	5,5,5	0.15	0
2	SO4	N	501	-	4,4,4	0.22	0	6,6,6	0.27	0
3	GOL	C	503	-	5,5,5	0.05	0	5,5,5	0.18	0
3	GOL	F	504	-	5,5,5	0.10	0	5,5,5	0.43	0
3	GOL	L	505	-	5,5,5	0.06	0	5,5,5	0.17	0
3	GOL	O	503	-	5,5,5	0.05	0	5,5,5	0.16	0
2	SO4	H	501	-	4,4,4	0.24	0	6,6,6	0.40	0
2	SO4	O	502	-	4,4,4	0.31	0	6,6,6	0.51	0
3	GOL	N	502	-	5,5,5	0.05	0	5,5,5	0.24	0
2	SO4	B	502	-	4,4,4	0.17	0	6,6,6	0.05	0
3	GOL	J	505	-	5,5,5	0.08	0	5,5,5	0.38	0
3	GOL	A	503	-	5,5,5	0.05	0	5,5,5	0.24	0
2	SO4	A	502	-	4,4,4	0.13	0	6,6,6	0.09	0
3	GOL	B	503	-	5,5,5	0.04	0	5,5,5	0.11	0
2	SO4	L	501	-	4,4,4	0.20	0	6,6,6	0.17	0
3	GOL	H	505	-	5,5,5	0.06	0	5,5,5	0.19	0
3	GOL	P	503	-	5,5,5	0.05	0	5,5,5	0.21	0
3	GOL	G	503	-	5,5,5	0.05	0	5,5,5	0.12	0
2	SO4	L	503	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	O	501	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	E	501	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.35	0
3	GOL	P	504	-	5,5,5	0.04	0	5,5,5	0.19	0
3	GOL	E	503	-	5,5,5	0.06	0	5,5,5	0.17	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	GOL	H	504	-	-	0/4/4/4	-
3	GOL	K	503	-	-	0/4/4/4	-
3	GOL	H	506	-	-	0/4/4/4	-
3	GOL	M	503	-	-	0/4/4/4	-
3	GOL	H	503	-	-	0/4/4/4	-
3	GOL	I	502	-	-	0/4/4/4	-
3	GOL	J	504	-	-	0/4/4/4	-
3	GOL	D	503	-	-	3/4/4/4	-
3	GOL	P	505	-	-	3/4/4/4	-
3	GOL	E	503	-	-	0/4/4/4	-
3	GOL	J	503	-	-	0/4/4/4	-
3	GOL	L	504	-	-	0/4/4/4	-
3	GOL	F	504	-	-	3/4/4/4	-
3	GOL	L	505	-	-	0/4/4/4	-
3	GOL	O	503	-	-	0/4/4/4	-
3	GOL	N	502	-	-	0/4/4/4	-
3	GOL	J	505	-	-	0/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	B	503	-	-	0/4/4/4	-
3	GOL	H	505	-	-	3/4/4/4	-
3	GOL	P	503	-	-	1/4/4/4	-
3	GOL	G	503	-	-	0/4/4/4	-
3	GOL	C	503	-	-	0/4/4/4	-
3	GOL	P	504	-	-	0/4/4/4	-
3	GOL	F	503	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	503	GOL	O1-C1-C2-O2
3	H	505	GOL	C1-C2-C3-O3
3	P	505	GOL	O1-C1-C2-C3
3	D	503	GOL	O1-C1-C2-C3
3	F	504	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	504	GOL	1	0
3	J	505	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/496 (95%)	0.30	12 (2%) 57 62	8, 16, 25, 36	0
1	B	474/496 (95%)	0.27	15 (3%) 47 52	8, 13, 22, 32	0
1	C	475/496 (95%)	0.09	7 (1%) 73 78	8, 11, 21, 45	1 (0%)
1	D	476/496 (95%)	0.13	5 (1%) 80 84	8, 12, 22, 35	0
1	E	474/496 (95%)	0.45	26 (5%) 25 27	8, 17, 29, 35	0
1	F	474/496 (95%)	0.17	10 (2%) 63 68	8, 13, 21, 28	0
1	G	474/496 (95%)	0.07	5 (1%) 80 84	8, 12, 21, 33	0
1	H	476/496 (95%)	0.18	8 (1%) 70 75	8, 13, 23, 36	0
1	I	476/496 (95%)	0.87	60 (12%) 3 3	8, 20, 35, 52	0
1	J	474/496 (95%)	0.32	20 (4%) 36 40	8, 14, 30, 42	0
1	K	476/496 (95%)	0.10	4 (0%) 86 89	8, 11, 21, 42	0
1	L	476/496 (95%)	0.11	6 (1%) 77 81	8, 12, 21, 37	0
1	M	476/496 (95%)	0.90	49 (10%) 6 6	11, 19, 31, 49	0
1	N	474/496 (95%)	0.64	35 (7%) 14 15	11, 18, 36, 46	0
1	O	476/496 (95%)	0.12	5 (1%) 80 84	8, 13, 22, 37	0
1	P	476/496 (95%)	0.13	5 (1%) 80 84	8, 14, 22, 41	0
All	All	7601/7936 (95%)	0.30	272 (3%) 42 47	8, 14, 27, 52	1 (0%)

The worst 5 of 272 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	10.3
1	I	0	PHE	10.1
1	N	2	ALA	9.7
1	C	1	MET	9.3
1	J	2	ALA	9.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	GOL	P	504	6/6	0.37	0.48	88,88,89,89	0
2	SO4	M	501	5/5	0.38	0.33	113,114,114,114	0
3	GOL	C	503	6/6	0.39	0.27	59,60,60,60	0
3	GOL	E	503	6/6	0.40	0.19	67,67,67,67	0
3	GOL	J	505	6/6	0.45	0.37	42,42,43,43	0
3	GOL	J	504	6/6	0.46	0.41	49,49,50,50	0
3	GOL	G	503	6/6	0.48	0.25	57,57,57,57	0
3	GOL	O	503	6/6	0.50	0.32	74,74,74,74	0
3	GOL	H	504	6/6	0.52	0.30	56,56,56,56	0
3	GOL	F	503	6/6	0.53	0.21	54,55,55,55	0
3	GOL	P	505	6/6	0.59	0.20	35,36,36,37	0
3	GOL	D	503	6/6	0.60	0.18	45,46,46,46	0
3	GOL	J	503	6/6	0.62	0.15	53,53,54,54	0
3	GOL	P	503	6/6	0.63	0.16	44,44,44,44	0
3	GOL	H	505	6/6	0.65	0.18	40,41,41,41	0
3	GOL	F	504	6/6	0.65	0.16	38,38,38,38	0
3	GOL	K	503	6/6	0.66	0.23	47,47,47,47	0
3	GOL	I	502	6/6	0.67	0.18	63,63,63,63	0
3	GOL	M	503	6/6	0.68	0.27	54,54,54,55	0
3	GOL	N	502	6/6	0.68	0.25	57,57,57,57	0
3	GOL	B	503	6/6	0.69	0.21	58,58,58,58	0
3	GOL	H	506	6/6	0.70	0.35	59,59,59,59	0
3	GOL	L	504	6/6	0.71	0.12	56,56,56,56	0
2	SO4	D	502	5/5	0.76	0.30	45,45,45,45	0
3	GOL	A	503	6/6	0.76	0.20	48,48,48,48	0
2	SO4	E	502	5/5	0.79	0.28	83,84,84,84	0
2	SO4	A	502	5/5	0.80	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	E	501	5/5	0.81	0.20	53,53,53,53	0
2	SO4	F	502	5/5	0.82	0.29	56,56,56,56	0
2	SO4	J	501	5/5	0.82	0.24	59,59,59,59	0
2	SO4	L	503	5/5	0.83	0.24	64,64,64,64	0
2	SO4	L	502	5/5	0.83	0.17	33,34,34,34	0
3	GOL	H	503	6/6	0.83	0.15	44,44,44,44	0
2	SO4	L	501	5/5	0.84	0.19	51,51,51,51	0
3	GOL	L	505	6/6	0.85	0.18	47,47,47,47	0
2	SO4	P	502	5/5	0.86	0.17	31,32,32,32	0
2	SO4	P	501	5/5	0.87	0.22	34,34,35,35	0
2	SO4	H	502	5/5	0.87	0.19	53,54,54,54	0
2	SO4	C	501	5/5	0.87	0.21	31,32,33,33	0
2	SO4	B	502	5/5	0.88	0.31	57,57,57,57	0
2	SO4	F	501	5/5	0.88	0.13	44,44,44,44	0
2	SO4	O	501	5/5	0.89	0.21	34,34,34,35	0
2	SO4	J	502	5/5	0.89	0.17	35,35,35,36	0
2	SO4	K	501	5/5	0.89	0.24	39,39,40,40	0
2	SO4	N	501	5/5	0.89	0.18	36,37,37,37	0
2	SO4	H	501	5/5	0.90	0.16	22,23,24,25	0
2	SO4	I	501	5/5	0.90	0.18	32,33,33,34	0
2	SO4	M	502	5/5	0.91	0.14	43,43,43,43	0
2	SO4	A	501	5/5	0.92	0.14	48,48,48,48	0
2	SO4	O	502	5/5	0.93	0.12	25,25,26,26	0
2	SO4	D	501	5/5	0.93	0.13	24,24,25,25	0
2	SO4	G	502	5/5	0.94	0.11	25,25,25,26	0
2	SO4	B	501	5/5	0.94	0.12	43,43,43,44	0
2	SO4	G	501	5/5	0.95	0.18	39,39,40,40	0
2	SO4	K	502	5/5	0.96	0.11	22,22,23,23	0
2	SO4	C	502	5/5	0.96	0.12	22,22,22,22	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.