



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:41 PM UTC

PDB ID : 7PKC / pdb_00007pkc
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

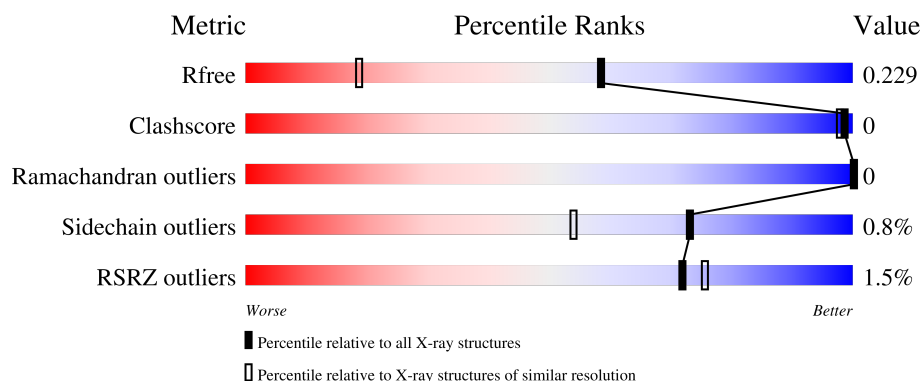
1 Overall quality at a glance

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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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	
1	B	496	
1	C	496	
1	D	496	
1	E	496	

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Mol	Chain	Length	Quality of chain
1	F	496	 93% . .
1	G	496	%  93% . .
1	H	496	%  94% . .
1	I	496	4%  93% . .
1	J	496	2%  92% . .
1	K	496	%  93% . .
1	L	496	 93% . .
1	M	496	3%  92% . .
1	N	496	5%  94% . .
1	O	496	%  94% . .
1	P	496	%  94% . .

2 Entry composition

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

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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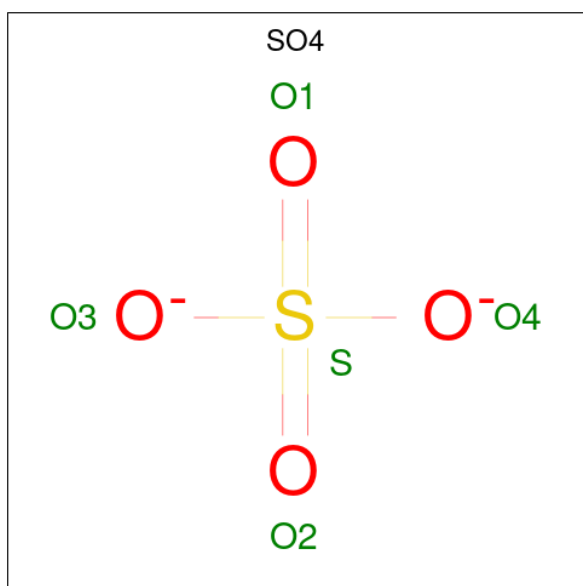
Chain	Residue	Modelled	Actual	Comment	Reference
N	-9	GLU	-	expression tag	UNP A0A7G1J7Q1
N	-8	GLY	-	expression tag	UNP A0A7G1J7Q1
N	-7	ARG	-	expression tag	UNP A0A7G1J7Q1
N	-6	ARG	-	expression tag	UNP A0A7G1J7Q1
N	-5	ASP	-	expression tag	UNP A0A7G1J7Q1
N	-4	ARG	-	expression tag	UNP A0A7G1J7Q1
N	-3	GLY	-	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 (CCD ID: SO4) (formula: O₄S).



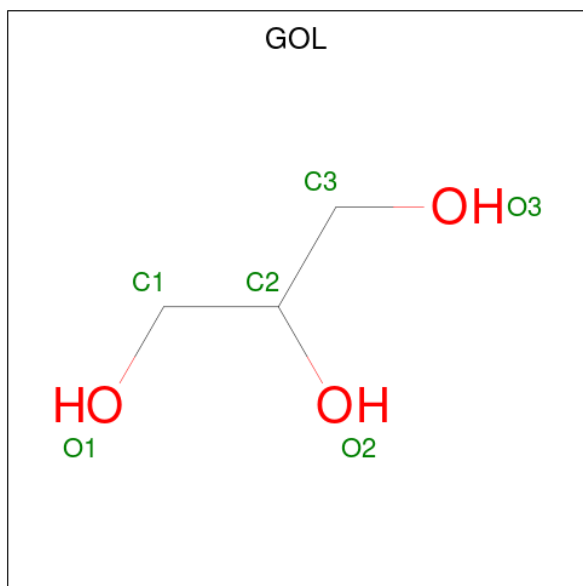
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0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

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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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

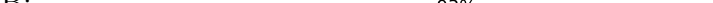
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

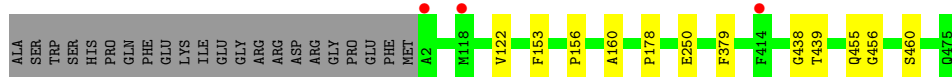
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain A: 93% ...

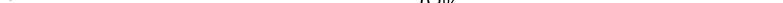


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain B:  93%



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

Chain C:  93%

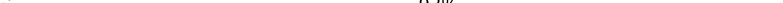


- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain D: 94%



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

Chain E:  93%





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

Chain F: 93%



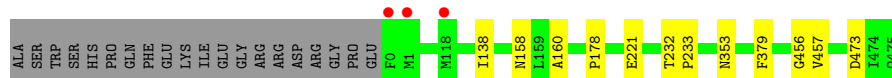
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain G: 93%



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

Chain H: 94%



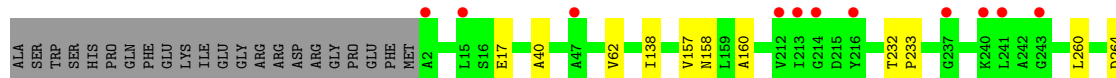
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain I: 93%



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

Chain J: 92%



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

Chain K: 93%



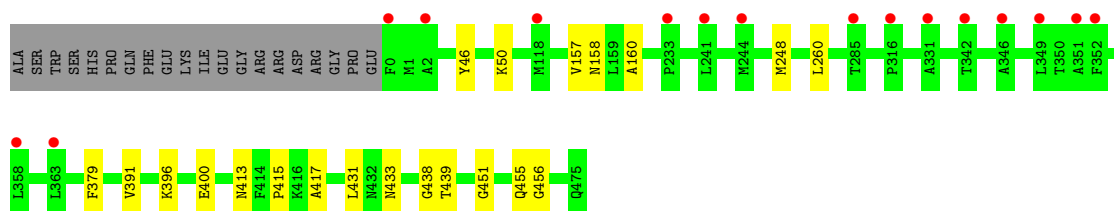
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain L: 93%



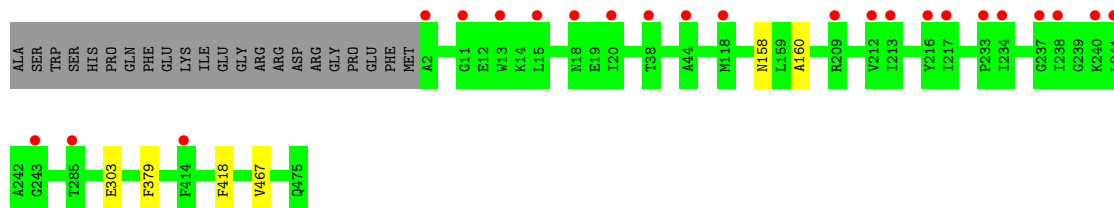
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain M: 92%



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

Chain N: 94%



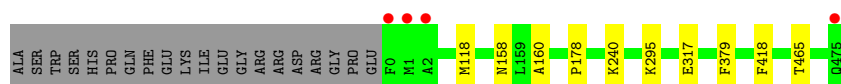
- Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain O: 94%



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

Chain P: 94%



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)	Xtriage
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	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: SO4, GOL

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	0.72	0/3701	0.94	6/5016 (0.1%)
1	B	0.73	0/3744	0.92	2/5074 (0.0%)
1	C	0.72	0/3701	0.90	3/5017 (0.1%)
1	D	0.74	0/3721	0.91	4/5042 (0.1%)
1	E	0.72	0/3750	0.93	4/5082 (0.1%)
1	F	0.72	0/3716	0.91	2/5039 (0.0%)
1	G	0.73	1/3708 (0.0%)	0.91	5/5023 (0.1%)
1	H	0.74	1/3746 (0.0%)	0.91	4/5078 (0.1%)
1	I	0.70	0/3690	0.93	2/5001 (0.0%)
1	J	0.72	0/3756	0.92	4/5091 (0.1%)
1	K	0.74	0/3739	0.90	4/5064 (0.1%)
1	L	0.73	0/3691	0.91	3/5004 (0.1%)
1	M	0.71	0/3658	0.95	5/4959 (0.1%)
1	N	0.71	0/3662	0.92	2/4965 (0.0%)
1	O	0.73	0/3728	0.90	3/5051 (0.1%)
1	P	0.72	0/3727	0.91	2/5051 (0.0%)
All	All	0.72	2/59438 (0.0%)	0.91	55/80557 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	138	ILE	CG1-CD1	-5.67	1.29	1.51
1	G	160	ALA	CA-C	5.21	1.57	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	456	GLY	N-CA-C	-9.29	101.24	112.48
1	F	456	GLY	N-CA-C	-8.57	100.70	112.18
1	C	456	GLY	N-CA-C	-8.50	102.19	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	456	GLY	N-CA-C	-8.29	101.07	112.18
1	J	158	ASN	CA-CB-CG	8.24	120.84	112.60
1	M	160	ALA	N-CA-C	-7.91	102.16	112.68
1	A	456	GLY	N-CA-C	-7.84	101.67	112.18
1	D	160	ALA	N-CA-C	-7.80	102.30	112.68
1	H	158	ASN	CA-CB-CG	7.71	120.31	112.60
1	M	456	GLY	N-CA-C	-7.67	101.91	112.18
1	L	160	ALA	N-CA-C	-7.63	102.78	112.93
1	I	160	ALA	N-CA-C	-7.56	102.62	112.68
1	N	160	ALA	N-CA-C	-7.51	102.69	112.68
1	P	160	ALA	N-CA-C	-7.50	102.70	112.68
1	E	160	ALA	N-CA-C	-7.50	102.71	112.68
1	C	160	ALA	N-CA-C	-7.44	102.78	112.68
1	B	160	ALA	N-CA-C	-7.38	102.87	112.68
1	L	158	ASN	CA-CB-CG	7.32	119.92	112.60
1	J	160	ALA	N-CA-C	-7.26	101.72	111.96
1	G	160	ALA	N-CA-C	-7.19	103.37	112.93
1	G	158	ASN	CA-CB-CG	7.09	119.69	112.60
1	O	160	ALA	N-CA-C	-6.88	103.53	112.68
1	H	160	ALA	N-CA-C	-6.79	103.65	112.68
1	A	160	ALA	N-CA-C	-6.78	103.67	112.68
1	E	456[A]	GLY	N-CA-C	-6.63	97.46	113.18
1	E	456[B]	GLY	N-CA-C	-6.63	97.46	113.18
1	K	158	ASN	CA-CB-CG	6.59	119.19	112.60
1	K	160	ALA	N-CA-C	-6.54	104.23	112.93
1	F	160	ALA	N-CA-C	-6.51	104.02	112.68
1	C	158	ASN	CA-CB-CG	6.40	119.00	112.60
1	D	158	ASN	CA-CB-CG	6.37	118.97	112.60
1	P	158	ASN	CA-CB-CG	6.10	118.70	112.60
1	M	451	GLY	N-CA-C	6.05	118.97	110.38
1	H	456	GLY	N-CA-C	-6.04	98.88	113.18
1	B	456	GLY	N-CA-C	-6.03	98.88	113.18
1	O	158	ASN	CA-CB-CG	5.85	118.45	112.60
1	E	451	GLY	N-CA-C	5.76	117.75	110.38
1	M	158	ASN	CA-CB-CG	5.66	118.26	112.60
1	D	457	VAL	N-CA-C	5.57	116.02	110.23
1	H	457	VAL	N-CA-C	5.44	115.89	110.23
1	A	327	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	451	GLY	N-CA-C	5.32	117.61	110.43
1	A	438	GLY	N-CA-C	5.32	118.18	112.33
1	G	451	GLY	N-CA-C	5.32	118.24	110.63
1	K	456	GLY	N-CA-C	-5.27	100.70	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	154	ASN	CA-CB-CG	5.24	117.84	112.60
1	J	157	VAL	N-CA-C	-5.21	107.08	111.56
1	O	456	GLY	N-CA-C	-5.16	100.95	113.18
1	G	457	VAL	N-CA-C	5.16	115.59	110.23
1	J	264	ASP	CA-CB-CG	5.09	117.69	112.60
1	L	456	GLY	N-CA-C	-5.08	101.14	113.18
1	M	157	VAL	N-CA-C	-5.07	106.85	111.67
1	A	457	VAL	N-CA-C	5.06	115.50	110.23
1	N	158	ASN	CA-CB-CG	5.05	117.65	112.60
1	G	456	GLY	N-CA-C	-5.01	101.31	113.18

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	6	0
1	C	3608	3699	3701	3	0
1	D	3624	3723	3725	2	0
1	E	3635	3720	3688	4	0
1	F	3615	3695	3695	6	0
1	G	3608	3700	3696	5	0
1	H	3635	3722	3718	3	0
1	I	3605	3684	3686	5	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	7	0
1	N	3582	3648	3648	1	0
1	O	3628	3727	3729	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	59	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.

All (59) 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
1:F:138:ILE:HD12	1:F:138:ILE:N	2.22	0.54
1:B:250[B]:GLU:OE2	1:B:455[B]:GLN:HG3	2.07	0.54
1:J:396:LYS:O	1:J:400:GLU:HG3	2.09	0.52
1:B:455[B]:GLN:OE1	1:B:460:SER:OG	2.24	0.51
1:P:178:PRO:HB3	4:P:611:HOH:O	2.11	0.50
1:D:118[B]:MET:HE2	4:D:666[B]:HOH:O	2.13	0.49
1:M:260:LEU:HD22	1:M:391:VAL:HG12	1.95	0.48
1:J:138:ILE:N	1:J:138:ILE:HD12	2.29	0.48
1:K:155:TYR:OH	1:K:283[A]:ARG:HD3	2.14	0.48
1:H:178:PRO:HB3	4:H:605:HOH:O	2.13	0.47
1:P:118[A]:MET:HE1	1:P:465:THR:HG21	1.97	0.47
1:A:455:GLN:NE2	4:A:603:HOH:O	2.46	0.47
1:J:40:ALA:HB3	3:J:505:GOL:H31	1.98	0.46
1:J:260:LEU:HD22	1:J:391[A]:VAL:HG12	1.97	0.46
1:O:70:LYS:O	1:O:70:LYS:HD3	2.16	0.46
1:G:225:PHE:CZ	1:G:248:MET:HG3	2.52	0.45
1:M:396:LYS:O	1:M:400:GLU:HG3	2.17	0.44
1:B:153:PHE:O	1:B:156:PRO:HD3	2.17	0.44
1:F:153:PHE:O	1:F:156:PRO:HD3	2.18	0.44
1:F:260:LEU:HD22	1:F:391[A]:VAL:HG12	1.99	0.44
1:M:248:MET:HG2	1:M:455:GLN:NE2	2.33	0.44
1:A:437[B]:ARG:NH2	1:A:444:PHE:CE2	2.85	0.44
1:I:232:THR:N	1:I:233:PRO:HD2	2.33	0.43
1:K:226:ILE:HB	1:K:247:ILE:HG22	2.00	0.43
1:G:334:VAL:HG21	1:G:380:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:438:GLY:HA2	1:I:439:THR:C	2.44	0.43
1:O:225:PHE:CZ	1:O:248:MET:HG3	2.54	0.43
1:O:334:VAL:HG21	1:O:380:GLY:HA3	2.00	0.43
1:I:334:VAL:HG21	1:I:380:GLY:HA3	2.01	0.42
1:M:46:TYR:O	1:M:50:LYS:HG2	2.19	0.42
1:E:430:HIS:CD2	1:E:435:THR:HA	2.55	0.42
1:L:334:VAL:HG21	1:L:380:GLY:HA3	2.01	0.42
1:B:438:GLY:HA2	1:B:439:THR:C	2.45	0.42
1:J:232:THR:N	1:J:233:PRO:HD2	2.35	0.42
1:L:225:PHE:CZ	1:L:248:MET:HG3	2.55	0.42
1:M:438:GLY:HA2	1:M:439:THR:C	2.45	0.42
1:K:232:THR:O	1:K:236:GLU:HG3	2.20	0.41
1:F:334:VAL:HG21	1:F:380:GLY:HA3	2.01	0.41
1:G:393:GLU:OE2	1:N:303:GLU:OE1	2.38	0.41
1:C:232:THR:N	1:C:233:PRO:HD2	2.35	0.41
1:E:232:THR:N	1:E:233:PRO:HD2	2.35	0.41
1:F:437:ARG:NH2	1:F:444:PHE:CE2	2.89	0.41
3:F:504:GOL:H31	4:F:622:HOH:O	2.20	0.41
1:H:232:THR:N	1:H:233:PRO:HD2	2.35	0.41
1:B:122:VAL:HG21	1:C:138:ILE:HG23	2.03	0.41
1:C:334:VAL:HG21	1:C:380:GLY:HA3	2.03	0.41
1:E:219[A]:GLU:HG3	4:E:782:HOH:O	2.21	0.41
1:M:413:ASN:OD1	1:M:415:PRO:HD2	2.21	0.41
1:G:433:ASN:ND2	1:H:473:ASP:OD2	2.46	0.40
1:I:414:PHE:CZ	1:L:415:PRO:HG3	2.56	0.40
1:E:437:ARG:HH12	1:E:455[B]:GLN:NE2	2.18	0.40
1:G:438:GLY:HA2	1:G:439:THR:C	2.47	0.40
1:L:223:VAL:O	1:L:245:ARG:HD2	2.21	0.40
1:M:417:ALA:HB1	1:M:431:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	73	54
1	B	386/388 (100%)	385 (100%)	1 (0%)	86	75
1	C	382/388 (98%)	376 (98%)	6 (2%)	55	28
1	D	383/388 (99%)	379 (99%)	4 (1%)	68	45
1	E	385/388 (99%)	381 (99%)	4 (1%)	68	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	383/388 (99%)	381 (100%)	2 (0%)	81	66
1	G	383/388 (99%)	382 (100%)	1 (0%)	86	75
1	H	387/388 (100%)	382 (99%)	5 (1%)	61	35
1	I	380/388 (98%)	377 (99%)	3 (1%)	73	54
1	J	388/388 (100%)	384 (99%)	4 (1%)	68	45
1	K	386/388 (100%)	382 (99%)	4 (1%)	68	45
1	L	381/388 (98%)	378 (99%)	3 (1%)	73	54
1	M	376/388 (97%)	374 (100%)	2 (0%)	81	66
1	N	376/388 (97%)	373 (99%)	3 (1%)	73	54
1	O	385/388 (99%)	382 (99%)	3 (1%)	73	54
1	P	385/388 (99%)	380 (99%)	5 (1%)	61	35
All	All	6126/6208 (99%)	6073 (99%)	53 (1%)	73	49

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	379	PHE
1	A	416	LYS
1	B	379	PHE
1	C	70[A]	LYS
1	C	70[B]	LYS
1	C	118	MET
1	C	295	LYS
1	C	379	PHE
1	C	433	ASN
1	D	118[A]	MET
1	D	118[B]	MET
1	D	267	LEU
1	D	379	PHE
1	E	118[A]	MET
1	E	118[B]	MET
1	E	379	PHE
1	E	418	PHE
1	F	379	PHE
1	F	418	PHE
1	G	379	PHE
1	H	221[A]	GLU

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Mol	Chain	Res	Type
1	H	221[B]	GLU
1	H	353[A]	ASN
1	H	353[B]	ASN
1	H	379	PHE
1	I	1	MET
1	I	379	PHE
1	I	418	PHE
1	J	17	GLU
1	J	62	VAL
1	J	379	PHE
1	J	418	PHE
1	K	70	LYS
1	K	283[A]	ARG
1	K	283[B]	ARG
1	K	379	PHE
1	L	1	MET
1	L	310	LYS
1	L	379	PHE
1	M	379	PHE
1	M	433	ASN
1	N	379	PHE
1	N	418	PHE
1	N	467	VAL
1	O	70	LYS
1	O	306	THR
1	O	379	PHE
1	P	240	LYS
1	P	295	LYS
1	P	317	GLU
1	P	379	PHE
1	P	418	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	ASN
1	C	39	GLN
1	D	18	ASN
1	D	271	ASN
1	F	94	HIS
1	G	18	ASN
1	G	475	GLN

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Mol	Chain	Res	Type
1	H	18	ASN
1	H	423	GLN
1	I	39	GLN
1	J	433	ASN
1	L	10	ASN
1	L	39	GLN
1	L	436	GLN
1	M	39	GLN
1	N	18	ASN
1	N	94	HIS
1	N	433	ASN
1	O	18	ASN
1	O	39	GLN
1	O	353	ASN
1	O	366	HIS
1	O	475	GLN
1	P	18	ASN
1	P	423	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 oligosaccharides 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	A	502	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	L	503	-	4,4,4	0.31	0	6,6,6	0.12	0
3	GOL	G	503	-	5,5,5	0.06	0	5,5,5	0.12	0
3	GOL	K	503	-	5,5,5	0.07	0	5,5,5	0.52	0
2	SO4	N	501	-	4,4,4	0.33	0	6,6,6	0.28	0
3	GOL	J	503	-	5,5,5	0.06	0	5,5,5	0.19	0
2	SO4	G	502	-	4,4,4	0.37	0	6,6,6	0.47	0
3	GOL	O	503	-	5,5,5	0.07	0	5,5,5	0.17	0
2	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.29	0
2	SO4	O	501	-	4,4,4	0.32	0	6,6,6	0.33	0
3	GOL	H	503	-	5,5,5	0.04	0	5,5,5	0.14	0
2	SO4	E	502	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	D	502	-	4,4,4	0.36	0	6,6,6	0.17	0
2	SO4	H	501	-	4,4,4	0.32	0	6,6,6	0.39	0
2	SO4	M	501	-	4,4,4	0.26	0	6,6,6	0.08	0
3	GOL	J	505	-	5,5,5	0.08	0	5,5,5	0.40	0
2	SO4	I	501	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	E	501	-	4,4,4	0.19	0	6,6,6	0.20	0
3	GOL	L	505	-	5,5,5	0.07	0	5,5,5	0.17	0
2	SO4	K	502	-	4,4,4	0.35	0	6,6,6	0.48	0
2	SO4	P	502	-	4,4,4	0.36	0	6,6,6	0.28	0
2	SO4	M	502	-	4,4,4	0.28	0	6,6,6	0.15	0
3	GOL	B	503	-	5,5,5	0.05	0	5,5,5	0.10	0
2	SO4	H	502	-	4,4,4	0.27	0	6,6,6	0.19	0
3	GOL	F	503	-	5,5,5	0.07	0	5,5,5	0.23	0
2	SO4	F	502	-	4,4,4	0.28	0	6,6,6	0.13	0
3	GOL	J	504	-	5,5,5	0.07	0	5,5,5	0.20	0
3	GOL	M	503	-	5,5,5	0.05	0	5,5,5	0.19	0
2	SO4	K	501	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	P	501	-	4,4,4	0.30	0	6,6,6	0.21	0
3	GOL	F	504	-	5,5,5	0.10	0	5,5,5	0.43	0
2	SO4	O	502	-	4,4,4	0.41	0	6,6,6	0.53	0
3	GOL	H	504	-	5,5,5	0.05	0	5,5,5	0.15	0
3	GOL	P	505	-	5,5,5	0.09	0	5,5,5	0.22	0
2	SO4	L	502	-	4,4,4	0.36	0	6,6,6	0.37	0
2	SO4	B	502	-	4,4,4	0.29	0	6,6,6	0.09	0
3	GOL	C	503	-	5,5,5	0.06	0	5,5,5	0.19	0
2	SO4	F	501	-	4,4,4	0.31	0	6,6,6	0.23	0
3	GOL	N	502	-	5,5,5	0.06	0	5,5,5	0.25	0
3	GOL	A	503	-	5,5,5	0.06	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	501	-	4,4,4	0.29	0	6,6,6	0.28	0
2	SO4	C	501	-	4,4,4	0.32	0	6,6,6	0.30	0
3	GOL	D	503	-	5,5,5	0.03	0	5,5,5	0.18	0
3	GOL	H	505	-	5,5,5	0.07	0	5,5,5	0.19	0
3	GOL	E	503	-	5,5,5	0.07	0	5,5,5	0.17	0
2	SO4	J	501	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	L	501	-	4,4,4	0.31	0	6,6,6	0.19	0
3	GOL	I	502	-	5,5,5	0.05	0	5,5,5	0.14	0
3	GOL	P	504	-	5,5,5	0.05	0	5,5,5	0.19	0
2	SO4	D	501	-	4,4,4	0.34	0	6,6,6	0.36	0
2	SO4	G	501	-	4,4,4	0.29	0	6,6,6	0.22	0
2	SO4	J	502	-	4,4,4	0.36	0	6,6,6	0.28	0
3	GOL	H	506	-	5,5,5	0.06	0	5,5,5	0.28	0
3	GOL	L	504	-	5,5,5	0.06	0	5,5,5	0.16	0
3	GOL	P	503	-	5,5,5	0.05	0	5,5,5	0.22	0
2	SO4	C	502	-	4,4,4	0.40	0	6,6,6	0.60	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	G	503	-	-	0/4/4/4	-
3	GOL	K	503	-	-	0/4/4/4	-
3	GOL	O	503	-	-	0/4/4/4	-
3	GOL	J	503	-	-	0/4/4/4	-
3	GOL	H	503	-	-	0/4/4/4	-
3	GOL	J	505	-	-	0/4/4/4	-
3	GOL	L	505	-	-	0/4/4/4	-
3	GOL	B	503	-	-	0/4/4/4	-
3	GOL	F	503	-	-	0/4/4/4	-
3	GOL	J	504	-	-	0/4/4/4	-
3	GOL	F	504	-	-	3/4/4/4	-
3	GOL	H	504	-	-	0/4/4/4	-
3	GOL	P	505	-	-	2/4/4/4	-
3	GOL	C	503	-	-	0/4/4/4	-
3	GOL	N	502	-	-	0/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	D	503	-	-	3/4/4/4	-
3	GOL	H	505	-	-	3/4/4/4	-
3	GOL	E	503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	I	502	-	-	0/4/4/4	-
3	GOL	P	504	-	-	0/4/4/4	-
3	GOL	H	506	-	-	0/4/4/4	-
3	GOL	L	504	-	-	0/4/4/4	-
3	GOL	P	503	-	-	2/4/4/4	-
3	GOL	M	503	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/496 (95%)	-0.00	2 (0%) 88 90	2, 8, 14, 18	11 (2%)
1	B	474/496 (95%)	-0.16	3 (0%) 85 88	2, 6, 12, 17	17 (3%)
1	C	475/496 (95%)	-0.33	4 (0%) 82 86	2, 6, 11, 21	13 (2%)
1	D	476/496 (95%)	-0.23	4 (0%) 82 86	2, 6, 12, 18	13 (2%)
1	E	474/496 (95%)	0.21	10 (2%) 63 67	2, 8, 16, 21	16 (3%)
1	F	474/496 (95%)	-0.19	2 (0%) 88 90	2, 6, 11, 17	14 (2%)
1	G	474/496 (95%)	-0.30	3 (0%) 85 88	3, 6, 12, 18	14 (2%)
1	H	476/496 (95%)	-0.14	3 (0%) 85 88	2, 6, 13, 19	17 (3%)
1	I	476/496 (95%)	0.46	22 (4%) 37 41	4, 10, 19, 28	9 (1%)
1	J	474/496 (95%)	-0.02	11 (2%) 61 65	3, 7, 16, 22	19 (4%)
1	K	476/496 (95%)	-0.30	3 (0%) 85 88	2, 6, 11, 22	15 (3%)
1	L	476/496 (95%)	-0.25	2 (0%) 88 90	2, 6, 12, 19	10 (2%)
1	M	476/496 (95%)	0.51	16 (3%) 48 52	3, 10, 17, 26	5 (1%)
1	N	474/496 (95%)	0.47	23 (4%) 35 38	4, 9, 19, 26	7 (1%)
1	O	476/496 (95%)	-0.16	3 (0%) 85 88	2, 6, 12, 18	14 (2%)
1	P	476/496 (95%)	-0.16	4 (0%) 82 86	3, 7, 13, 21	14 (2%)
All	All	7601/7936 (95%)	-0.04	115 (1%) 72 75	2, 7, 14, 28	208 (2%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	5.4
1	B	2	ALA	5.1
1	I	0	PHE	5.1
1	M	0	PHE	4.8
1	F	2	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	O	240[A]	LYS	4.3
1	C	1	MET	4.3
1	K	0	PHE	4.3
1	J	2	ALA	4.3
1	K	2	ALA	3.9
1	M	2	ALA	3.7
1	J	212	VAL	3.6
1	P	0	PHE	3.6
1	K	1	MET	3.4
1	I	352	PHE	3.4
1	I	2	ALA	3.2
1	P	1	MET	3.2
1	I	351	ALA	3.2
1	H	118	MET	3.1
1	N	209	ARG	3.1
1	N	241	LEU	3.0
1	G	2	ALA	2.9
1	H	0	PHE	2.9
1	P	2	ALA	2.9
1	A	2	ALA	2.8
1	N	2	ALA	2.8
1	D	1	MET	2.8
1	N	285	THR	2.8
1	I	118	MET	2.7
1	M	118	MET	2.7
1	J	47	ALA	2.7
1	F	118	MET	2.7
1	I	1	MET	2.7
1	I	212	VAL	2.7
1	J	237	GLY	2.6
1	J	240	LYS	2.6
1	I	238	ILE	2.6
1	N	11	GLY	2.6
1	N	243	GLY	2.6
1	E	351	ALA	2.6
1	N	44	ALA	2.6
1	E	306	THR	2.6
1	N	237	GLY	2.6
1	N	20	ILE	2.6
1	M	363	LEU	2.6
1	I	313	VAL	2.6
1	J	213	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	414[A]	PHE	2.5
1	I	349	LEU	2.5
1	N	234	ILE	2.5
1	I	119	GLU	2.5
1	M	244	MET	2.5
1	A	237	GLY	2.5
1	J	214	GLY	2.5
1	N	233	PRO	2.5
1	E	285[A]	THR	2.5
1	N	15	LEU	2.4
1	D	0	PHE	2.4
1	M	352	PHE	2.4
1	N	38	THR	2.4
1	N	212	VAL	2.4
1	M	346	ALA	2.4
1	C	475	GLN	2.4
1	N	213	ILE	2.4
1	J	216	TYR	2.4
1	I	211	SER	2.4
1	C	118	MET	2.4
1	P	475	GLN	2.4
1	G	240	LYS	2.4
1	O	0	PHE	2.4
1	M	351	ALA	2.3
1	N	217	ILE	2.3
1	M	241	LEU	2.3
1	N	216	TYR	2.3
1	M	342	THR	2.3
1	E	267	LEU	2.3
1	I	234	ILE	2.3
1	N	414[A]	PHE	2.3
1	I	367	VAL	2.3
1	I	343	ASP	2.3
1	M	358	LEU	2.3
1	M	331	ALA	2.2
1	N	18	ASN	2.2
1	E	352	PHE	2.2
1	J	243	GLY	2.2
1	J	15	LEU	2.2
1	J	241	LEU	2.2
1	G	475	GLN	2.2
1	E	307	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	241	LEU	2.2
1	N	238	ILE	2.2
1	M	233	PRO	2.2
1	I	306	THR	2.2
1	O	475	GLN	2.2
1	E	348	ALA	2.1
1	I	359	ILE	2.1
1	D	285	THR	2.1
1	L	1	MET	2.1
1	N	118	MET	2.1
1	B	414[A]	PHE	2.1
1	L	0	PHE	2.1
1	E	370	ASP	2.1
1	I	285	THR	2.1
1	M	285	THR	2.1
1	N	240	LYS	2.1
1	I	23	TYR	2.1
1	N	13	TRP	2.1
1	E	346	ALA	2.0
1	M	349	LEU	2.0
1	I	345	GLY	2.0
1	D	240	LYS	2.0
1	M	316	PRO	2.0
1	I	346	ALA	2.0
1	B	118	MET	2.0
1	H	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	P	504	6/6	0.59	0.30	88,88,89,89	0
2	SO4	M	501	5/5	0.62	0.23	113,114,114,114	0
3	GOL	N	502	6/6	0.63	0.19	57,57,57,57	0
3	GOL	I	502	6/6	0.63	0.19	63,63,63,63	0
3	GOL	O	503	6/6	0.64	0.30	74,74,74,74	0
3	GOL	B	503	6/6	0.64	0.24	58,58,58,58	0
2	SO4	E	502	5/5	0.65	0.20	83,84,84,84	0
3	GOL	J	504	6/6	0.66	0.21	49,49,50,50	0
3	GOL	E	503	6/6	0.66	0.19	67,67,67,67	0
3	GOL	L	504	6/6	0.67	0.19	56,56,56,56	0
3	GOL	G	503	6/6	0.69	0.21	57,57,57,57	0
3	GOL	F	503	6/6	0.70	0.23	54,55,55,55	0
2	SO4	L	503	5/5	0.70	0.18	64,64,64,64	0
3	GOL	F	504	6/6	0.72	0.19	38,38,38,38	0
2	SO4	F	502	5/5	0.72	0.14	56,56,56,56	0
3	GOL	H	504	6/6	0.72	0.17	56,56,56,56	0
3	GOL	C	503	6/6	0.73	0.22	59,60,60,60	0
3	GOL	L	505	6/6	0.74	0.16	47,47,47,47	0
3	GOL	J	505	6/6	0.74	0.17	42,42,43,43	0
3	GOL	K	503	6/6	0.75	0.16	47,47,47,47	0
3	GOL	A	503	6/6	0.75	0.16	48,48,48,48	0
3	GOL	H	503	6/6	0.75	0.18	44,44,44,44	0
2	SO4	J	501	5/5	0.76	0.15	59,59,59,59	0
3	GOL	D	503	6/6	0.76	0.17	45,46,46,46	0
3	GOL	H	506	6/6	0.76	0.18	59,59,59,59	0
3	GOL	P	503	6/6	0.77	0.17	44,44,44,44	0
2	SO4	D	502	5/5	0.77	0.14	45,45,45,45	0
3	GOL	P	505	6/6	0.77	0.16	35,36,36,37	0
3	GOL	M	503	6/6	0.78	0.16	54,54,54,55	0
2	SO4	A	502	5/5	0.79	0.16	75,75,75,75	0
3	GOL	J	503	6/6	0.80	0.16	53,53,54,54	0
3	GOL	H	505	6/6	0.83	0.14	40,41,41,41	0
2	SO4	B	501	5/5	0.83	0.17	43,43,43,44	0
2	SO4	L	501	5/5	0.83	0.13	51,51,51,51	0
2	SO4	A	501	5/5	0.84	0.15	48,48,48,48	0
2	SO4	J	502	5/5	0.84	0.12	35,35,35,36	0
2	SO4	H	502	5/5	0.84	0.12	53,54,54,54	0
2	SO4	F	501	5/5	0.85	0.14	44,44,44,44	0
2	SO4	E	501	5/5	0.85	0.14	53,53,53,53	0
2	SO4	B	502	5/5	0.85	0.12	57,57,57,57	0
2	SO4	P	501	5/5	0.86	0.11	34,34,35,35	0
2	SO4	L	502	5/5	0.86	0.11	33,34,34,34	0
2	SO4	P	502	5/5	0.87	0.11	31,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	O	501	5/5	0.87	0.12	34,34,34,35	0
2	SO4	M	502	5/5	0.88	0.11	43,43,43,43	0
2	SO4	N	501	5/5	0.88	0.11	36,37,37,37	0
2	SO4	C	501	5/5	0.89	0.10	31,32,33,33	0
2	SO4	I	501	5/5	0.90	0.10	32,33,33,34	0
2	SO4	H	501	5/5	0.91	0.12	22,23,24,25	0
2	SO4	K	501	5/5	0.91	0.09	39,39,40,40	0
2	SO4	G	501	5/5	0.92	0.10	39,39,40,40	0
2	SO4	O	502	5/5	0.94	0.09	25,25,26,26	0
2	SO4	D	501	5/5	0.94	0.10	24,24,25,25	0
2	SO4	G	502	5/5	0.95	0.08	25,25,25,26	0
2	SO4	C	502	5/5	0.95	0.08	22,22,22,22	0
2	SO4	K	502	5/5	0.96	0.10	22,22,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.