Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2022 – 09:36 pm GMT

PDB ID	:	7PKJ
Title	:	Streptococcus pyogenes apo GapN
Authors	:	Schindelin, H.; Albert, L.
Deposited on	:	2021-08-25
Resolution	:	1.99 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 (i) symbol.

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

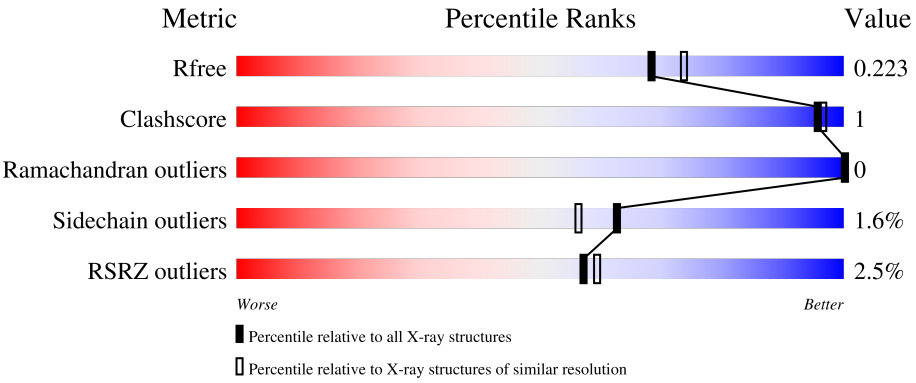
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.99 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	4% 92%
1	B	496	% 93%
1	C	496	% 93%
1	D	496	2% 92%
1	E	496	4% 93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	496	5% 92%
1	G	496	% 92%
1	H	496	% 92%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BME	D	601[A]	-	-	-	X
2	BME	D	601[B]	-	-	-	X
4	GOL	B	606	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 60189 atoms, of which 29098 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	3628	4	0
			7192	2270	3628	591	694	9			
1	B	474	Total	C	H	N	O	S	3648	6	0
			7229	2287	3648	591	694	9			
1	C	475	Total	C	H	N	O	S	3632	3	0
			7189	2266	3629	592	692	10			
1	D	475	Total	C	H	N	O	S	3653	7	0
			7236	2282	3653	593	697	11			
1	E	475	Total	C	H	N	O	S	3630	1	0
			7180	2264	3624	593	689	10			
1	F	474	Total	C	H	N	O	S	3627	4	0
			7190	2271	3627	591	691	10			
1	G	475	Total	C	H	N	O	S	3647	4	0
			7220	2276	3644	596	694	10			
1	H	475	Total	C	H	N	O	S	3645	5	0
			7221	2277	3645	593	696	10			

There are 192 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
F	-20	ALA	-	expression tag	UNP A0A7G1J7Q1
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

Continued on next page...

Continued from previous page...

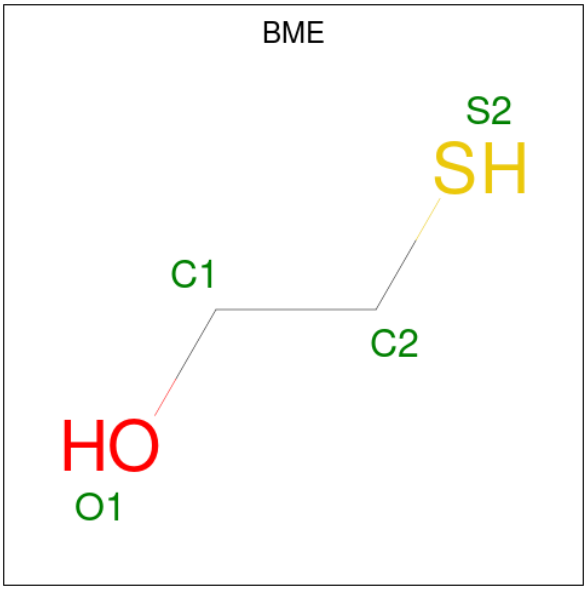
Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	PRO	-	expression tag	UNP A0A7G1J7Q1
F	-1	GLU	-	expression tag	UNP A0A7G1J7Q1
F	0	PHE	-	expression tag	UNP A0A7G1J7Q1
F	58	THR	ALA	conflict	UNP A0A7G1J7Q1
F	170	ALA	SER	conflict	UNP A0A7G1J7Q1
F	266	ALA	VAL	conflict	UNP A0A7G1J7Q1
G	-20	ALA	-	expression 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
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



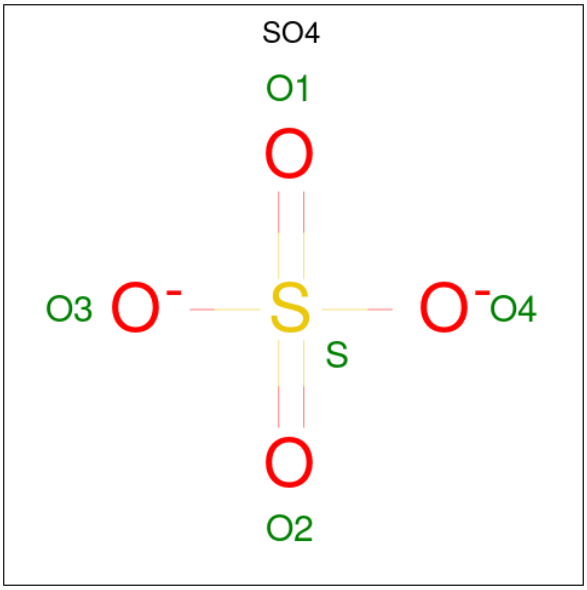
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	1
			8	4	2	2		
2	E	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O S 8 4 2 2	0	1
2	G	1	Total C O S 4 2 1 1	0	0
2	H	1	Total C O S 4 2 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



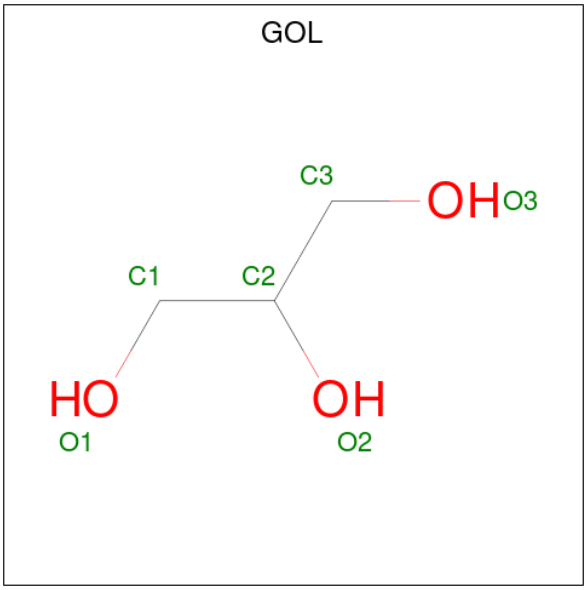
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

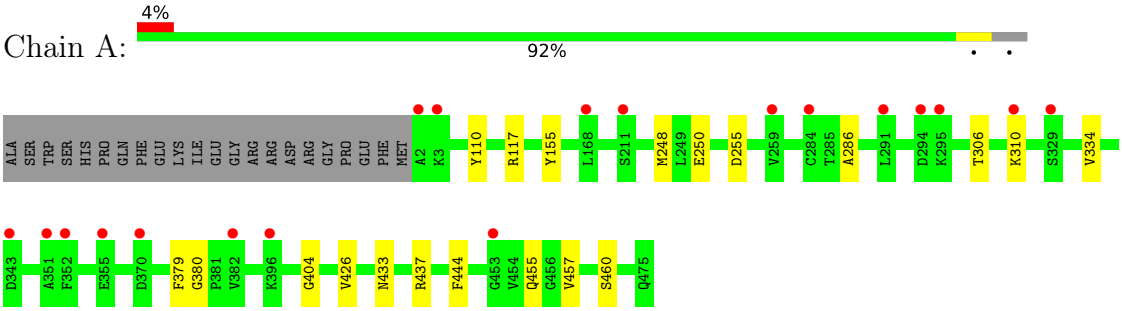
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	272	Total O 272 272	0	0
5	B	311	Total O 315 315	0	4
5	C	295	Total O 296 296	0	1
5	D	289	Total O 289 289	0	0
5	E	234	Total O 234 234	0	0
5	F	210	Total O 211 211	0	1
5	G	314	Total O 316 316	0	2
5	H	318	Total O 319 319	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

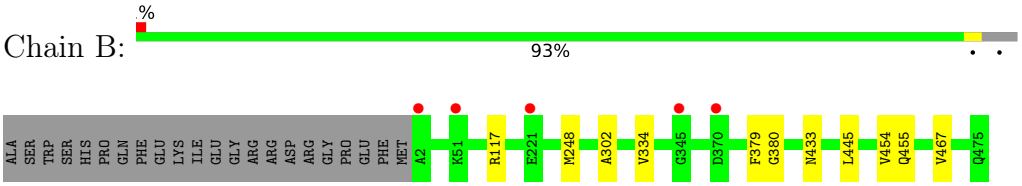
• Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain A:



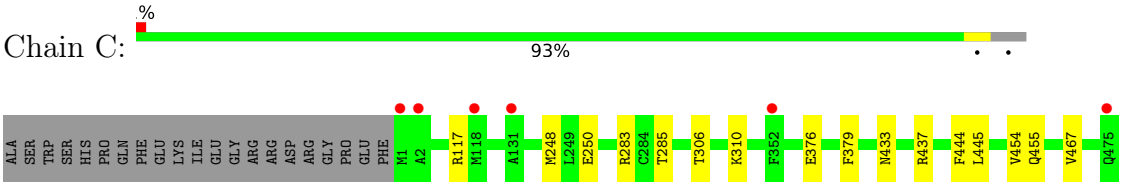
• Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain B:



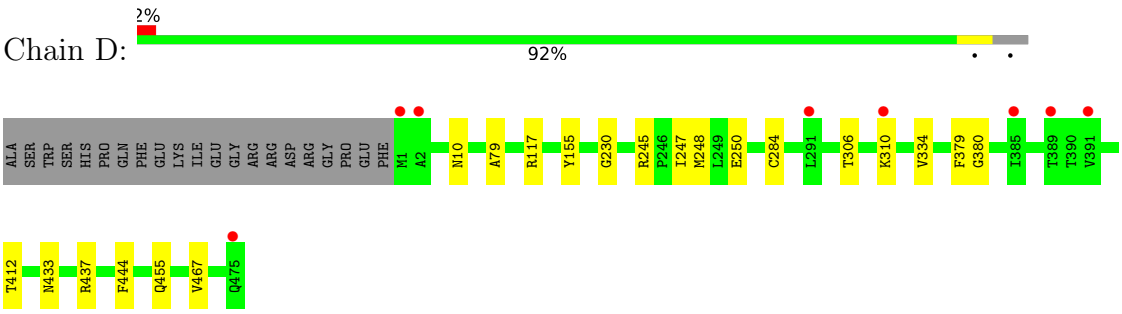
• Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain C:



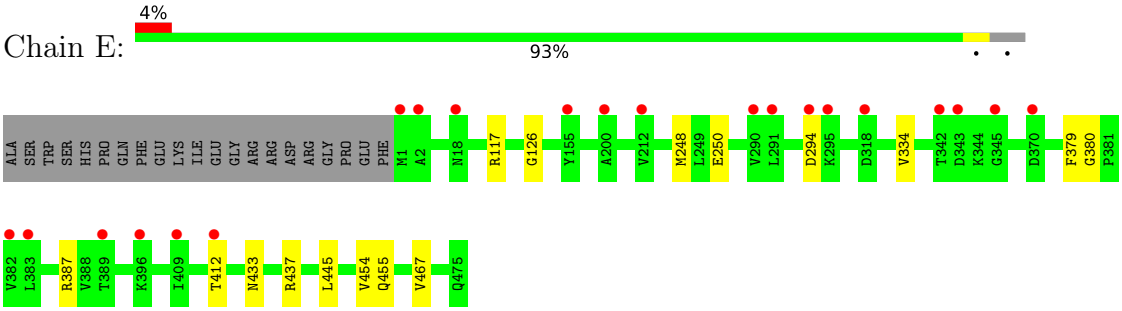
• Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain D:



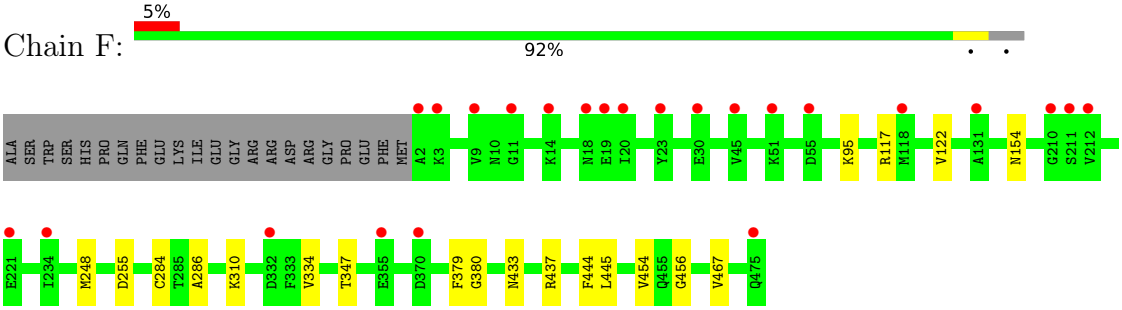
• Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain E:



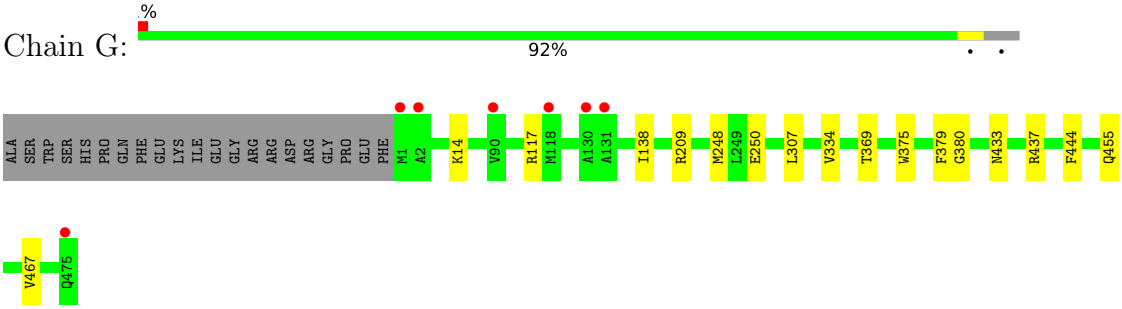
• Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain F:



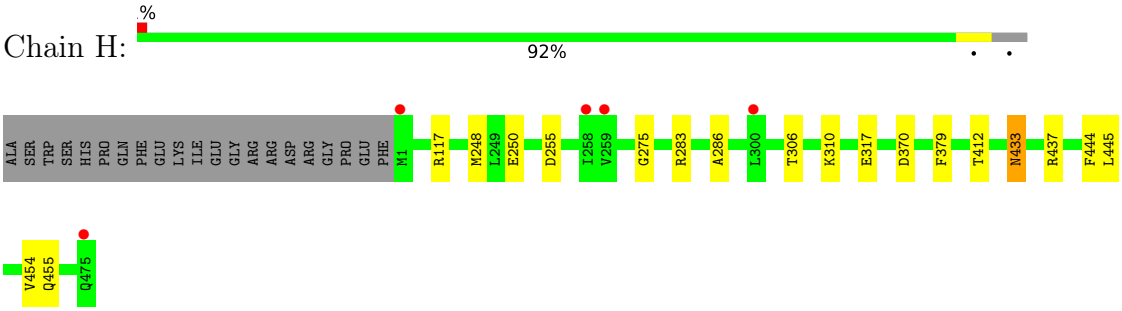
• Molecule 1: Putative NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	97.75Å 99.89Å 106.18Å 77.67° 75.19° 67.12°	Depositor
Resolution (Å)	20.03 – 1.99 20.03 – 1.99	Depositor EDS
% Data completeness (in resolution range)	62.9 (20.03-1.99) 62.9 (20.03-1.99)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 1.99Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.192 , 0.232 0.185 , 0.223	Depositor DCC
R_{free} test set	7387 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	60189	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BME, 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	0/3633	0.58	0/4926
1	B	0.41	0/3658	0.58	0/4960
1	C	0.42	0/3626	0.58	0/4916
1	D	0.42	0/3661	0.58	0/4963
1	E	0.40	0/3616	0.58	0/4901
1	F	0.41	0/3633	0.59	1/4927 (0.0%)
1	G	0.44	0/3645	0.60	0/4940
1	H	0.43	0/3648	0.59	0/4945
All	All	0.42	0/29120	0.59	1/39478 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	456	GLY	N-CA-C	-5.07	100.43	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	3564	3628	3628	10	0
1	B	3581	3648	3648	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3560	3629	3631	8	0
1	D	3583	3653	3655	13	0
1	E	3556	3624	3626	7	0
1	F	3563	3627	3627	11	0
1	G	3576	3644	3646	10	0
1	H	3576	3645	3647	8	0
2	A	4	0	5	1	0
2	B	4	0	5	0	0
2	C	4	0	6	0	0
2	D	8	0	10	2	0
2	E	4	0	5	0	0
2	F	8	0	9	2	0
2	G	4	0	5	0	0
2	H	4	0	5	0	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
3	G	10	0	0	1	0
3	H	10	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	2	0
4	D	36	0	48	3	0
4	E	12	0	16	0	0
4	F	12	0	16	1	0
4	G	42	0	56	1	0
4	H	12	0	16	0	0
5	A	272	0	0	0	0
5	B	315	0	0	0	0
5	C	296	0	0	0	0
5	D	289	0	0	0	0
5	E	234	0	0	1	0
5	F	211	0	0	0	0
5	G	316	0	0	1	0
5	H	319	0	0	2	0
All	All	31091	29098	29358	66	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 1.

All (66) 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)
2:F:601[B]:BME:H12	4:F:603:GOL:H2	1.61	0.82
1:D:230:GLY:HA2	2:D:601[B]:BME:H11	1.69	0.75
1:A:250:GLU:OE2	1:A:455:GLN:HG3	1.87	0.73
1:E:250:GLU:OE2	1:E:437:ARG:NH1	2.23	0.71
1:D:10:ASN:ND2	1:F:95:LYS:HZ2	1.89	0.71
1:D:10:ASN:ND2	1:F:95:LYS:NZ	2.42	0.68
1:E:294:ASP:OD1	1:E:387:ARG:HB3	1.95	0.65
1:D:79:ALA:HB3	4:D:608:GOL:H2	1.82	0.62
1:C:285:THR:O	1:C:285:THR:HG23	2.00	0.61
1:D:247:ILE:HG12	4:D:609:GOL:H11	1.82	0.61
1:E:250:GLU:OE2	1:E:455:GLN:HG3	2.02	0.60
1:C:376:GLU:HA	4:C:606:GOL:H31	1.83	0.59
1:G:307:LEU:HD22	4:G:605:GOL:H31	1.83	0.59
1:C:250:GLU:OE2	1:C:455:GLN:HG3	2.03	0.58
1:H:250:GLU:OE2	1:H:455:GLN:HG3	2.05	0.57
1:H:275:GLY:O	1:H:283:ARG:NH1	2.39	0.55
1:G:369:THR:HG23	1:G:375:TRP:HZ2	1.73	0.54
1:A:437:ARG:NH2	1:A:444:PHE:CE2	2.77	0.52
1:G:250:GLU:OE2	1:G:455:GLN:HG3	2.09	0.52
1:F:445:LEU:HD13	1:F:454:VAL:HG22	1.92	0.51
1:H:255:ASP:HB2	1:H:286:ALA:O	2.11	0.51
1:D:245:ARG:O	4:D:609:GOL:H12	2.11	0.50
1:F:437:ARG:NH2	1:F:444:PHE:CE2	2.81	0.49
1:D:155:TYR:CD2	2:D:601[A]:BME:H22	2.48	0.49
1:A:455:GLN:OE1	1:A:460:SER:OG	2.26	0.49
1:D:250[A]:GLU:OE2	1:D:455:GLN:HG3	2.14	0.48
1:G:437:ARG:NH2	1:G:444:PHE:CE2	2.82	0.48
1:A:437:ARG:NH2	1:A:444:PHE:CD2	2.82	0.47
1:A:255:ASP:HB2	1:A:286:ALA:O	2.14	0.47
1:E:437:ARG:NH2	5:E:713:HOH:O	2.48	0.47
1:H:433:ASN:ND2	5:H:710:HOH:O	2.48	0.47
1:C:437:ARG:NH2	1:C:444:PHE:CE2	2.83	0.46
1:F:255:ASP:HB2	1:F:286:ALA:O	2.15	0.46
1:D:437:ARG:NH2	1:D:444:PHE:CE2	2.84	0.46
1:G:209[A]:ARG:NH2	3:G:603:SO4:O2	2.41	0.46
1:G:14:LYS:NZ	5:G:708:HOH:O	2.43	0.45
1:C:376:GLU:HG2	4:C:606:GOL:H31	1.98	0.45
1:D:10:ASN:HD22	1:F:95:LYS:NZ	2.11	0.45
1:A:306:THR:O	1:A:310:LYS:HG2	2.17	0.45
1:H:437:ARG:NH2	1:H:444:PHE:CE2	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:THR:O	1:C:285:THR:CG2	2.64	0.45
1:D:306:THR:O	1:D:310:LYS:HG2	2.17	0.44
1:H:306:THR:O	1:H:310:LYS:HG2	2.17	0.44
1:A:404:GLY:O	1:A:426:VAL:HA	2.17	0.44
1:E:126:GLY:HA3	5:H:955:HOH:O	2.16	0.44
1:B:302:ALA:HB1	1:G:369:THR:HG22	2.00	0.43
1:G:334:VAL:HG21	1:G:380:GLY:HA3	2.00	0.43
1:A:110:TYR:HD1	1:A:457:VAL:HG11	1.84	0.43
1:F:437:ARG:NH2	1:F:444:PHE:CD2	2.87	0.43
1:E:334:VAL:HG21	1:E:380:GLY:HA3	2.01	0.42
1:C:306:THR:O	1:C:310:LYS:HG2	2.19	0.42
1:A:155:TYR:CE2	2:A:601:BME:H12	2.54	0.41
1:B:445:LEU:HD13	1:B:454:VAL:HG22	2.02	0.41
1:B:334:VAL:HG21	1:B:380:GLY:HA3	2.01	0.41
1:F:334:VAL:HG21	1:F:380:GLY:HA3	2.02	0.41
1:A:334:VAL:HG21	1:A:380:GLY:HA3	2.02	0.41
1:F:154:ASN:ND2	2:F:601[A]:BME:S2	2.94	0.41
1:D:334:VAL:HG21	1:D:380:GLY:HA3	2.01	0.41
1:F:122:VAL:HG21	1:G:138:ILE:HG23	2.03	0.41
1:E:445:LEU:HD13	1:E:454:VAL:HG22	2.04	0.40
1:D:437:ARG:NH2	1:D:444:PHE:CD2	2.89	0.40
1:H:445:LEU:HD13	1:H:454:VAL:HG22	2.04	0.40
1:C:445:LEU:HD13	1:C:454:VAL:HG22	2.04	0.40
1:H:437:ARG:NH2	1:H:444:PHE:CD2	2.89	0.40
1:G:437:ARG:NH2	1:G:444:PHE:CD2	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/496 (96%)	465 (98%)	11 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	478/496 (96%)	467 (98%)	11 (2%)	0	100	100
1	C	476/496 (96%)	465 (98%)	11 (2%)	0	100	100
1	D	480/496 (97%)	467 (97%)	13 (3%)	0	100	100
1	E	474/496 (96%)	462 (98%)	12 (2%)	0	100	100
1	F	476/496 (96%)	463 (97%)	13 (3%)	0	100	100
1	G	477/496 (96%)	464 (97%)	13 (3%)	0	100	100
1	H	478/496 (96%)	467 (98%)	11 (2%)	0	100	100
All	All	3815/3968 (96%)	3720 (98%)	95 (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	373/388 (96%)	369 (99%)	4 (1%)	73	70
1	B	375/388 (97%)	369 (98%)	6 (2%)	62	56
1	C	373/388 (96%)	367 (98%)	6 (2%)	62	56
1	D	377/388 (97%)	368 (98%)	9 (2%)	49	41
1	E	371/388 (96%)	365 (98%)	6 (2%)	62	56
1	F	373/388 (96%)	365 (98%)	8 (2%)	53	47
1	G	374/388 (96%)	369 (99%)	5 (1%)	69	64
1	H	375/388 (97%)	366 (98%)	9 (2%)	49	41
All	All	2991/3104 (96%)	2938 (98%)	53 (2%)	62	51

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

Mol	Chain	Res	Type
1	A	117	ARG
1	A	248	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	379	PHE
1	A	433	ASN
1	B	117	ARG
1	B	248	MET
1	B	379	PHE
1	B	433	ASN
1	B	455	GLN
1	B	467	VAL
1	C	117	ARG
1	C	248	MET
1	C	283	ARG
1	C	379	PHE
1	C	433	ASN
1	C	467	VAL
1	D	117	ARG
1	D	248	MET
1	D	284[A]	CYS
1	D	284[B]	CYS
1	D	379	PHE
1	D	412	THR
1	D	433[A]	ASN
1	D	433[B]	ASN
1	D	467	VAL
1	E	117	ARG
1	E	248	MET
1	E	379	PHE
1	E	412	THR
1	E	433	ASN
1	E	467	VAL
1	F	117	ARG
1	F	248	MET
1	F	284[A]	CYS
1	F	284[B]	CYS
1	F	347	THR
1	F	379	PHE
1	F	433	ASN
1	F	467	VAL
1	G	117	ARG
1	G	248	MET
1	G	379	PHE
1	G	433	ASN
1	G	467	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	117	ARG
1	H	248	MET
1	H	317[A]	GLU
1	H	317[B]	GLU
1	H	370[A]	ASP
1	H	370[B]	ASP
1	H	379	PHE
1	H	412	THR
1	H	433	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	B	433	ASN
1	D	10	ASN
1	E	94	HIS
1	F	455	GLN
1	G	433	ASN
1	H	433	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

53 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	H	603	-	4,4,4	0.26	0	6,6,6	0.34	0
4	GOL	F	604	-	5,5,5	0.04	0	5,5,5	0.27	0
4	GOL	G	605	-	5,5,5	0.14	0	5,5,5	0.45	0
2	BME	F	601[A]	1	3,3,3	0.21	0	1,2,2	0.26	0
4	GOL	G	607	-	5,5,5	0.14	0	5,5,5	0.41	0
4	GOL	D	609	-	5,5,5	0.13	0	5,5,5	0.26	0
3	SO4	B	602	-	4,4,4	0.17	0	6,6,6	0.16	0
4	GOL	G	608	-	5,5,5	0.08	0	5,5,5	0.22	0
2	BME	C	601	-	3,3,3	0.16	0	1,2,2	0.02	0
4	GOL	A	605	-	5,5,5	0.04	0	5,5,5	0.12	0
3	SO4	C	602	-	4,4,4	0.24	0	6,6,6	0.18	0
4	GOL	D	605	-	5,5,5	0.14	0	5,5,5	0.30	0
2	BME	G	601	-	3,3,3	0.19	0	1,2,2	0.16	0
3	SO4	G	603	-	4,4,4	0.11	0	6,6,6	0.15	0
2	BME	D	601[A]	1	3,3,3	0.15	0	1,2,2	0.04	0
4	GOL	D	608	-	5,5,5	0.14	0	5,5,5	0.22	0
3	SO4	A	603	-	4,4,4	0.19	0	6,6,6	0.17	0
3	SO4	B	603	-	4,4,4	0.21	0	6,6,6	0.31	0
4	GOL	B	606	-	5,5,5	0.10	0	5,5,5	0.20	0
4	GOL	C	605	-	5,5,5	0.07	0	5,5,5	0.14	0
2	BME	A	601	-	3,3,3	0.19	0	1,2,2	0.36	0
3	SO4	C	604	-	4,4,4	0.17	0	6,6,6	0.19	0
4	GOL	G	610	-	5,5,5	0.11	0	5,5,5	0.28	0
4	GOL	E	605	-	5,5,5	0.11	0	5,5,5	0.22	0
4	GOL	H	605	-	5,5,5	0.09	0	5,5,5	0.14	0
4	GOL	F	603	-	5,5,5	0.03	0	5,5,5	0.16	0
2	BME	H	601	-	3,3,3	0.19	0	1,2,2	0.05	0
3	SO4	F	602	-	4,4,4	0.11	0	6,6,6	0.17	0
2	BME	F	601[B]	1	3,3,3	0.20	0	1,2,2	0.41	0
2	BME	B	601	-	3,3,3	0.25	0	1,2,2	0.32	0
3	SO4	C	603	-	4,4,4	0.27	0	6,6,6	0.32	0
3	SO4	E	603	-	4,4,4	0.21	0	6,6,6	0.22	0
4	GOL	B	605	-	5,5,5	0.05	0	5,5,5	0.43	0
3	SO4	G	602	-	4,4,4	0.23	0	6,6,6	0.32	0
4	GOL	A	604	-	5,5,5	0.05	0	5,5,5	0.27	0
2	BME	E	601	-	3,3,3	0.22	0	1,2,2	0.43	0
4	GOL	G	609	-	5,5,5	0.10	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	H	602	-	4,4,4	0.29	0	6,6,6	0.30	0
3	SO4	D	604	-	4,4,4	0.13	0	6,6,6	0.10	0
4	GOL	H	604	-	5,5,5	0.05	0	5,5,5	0.22	0
2	BME	D	601[B]	1	3,3,3	0.18	0	1,2,2	0.49	0
3	SO4	D	602	-	4,4,4	0.14	0	6,6,6	0.25	0
4	GOL	C	606	-	5,5,5	0.18	0	5,5,5	0.75	0
4	GOL	G	604	-	5,5,5	0.06	0	5,5,5	0.32	0
3	SO4	B	604	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	E	602	-	4,4,4	0.15	0	6,6,6	0.20	0
4	GOL	D	610	-	5,5,5	0.09	0	5,5,5	0.19	0
4	GOL	E	604	-	5,5,5	0.05	0	5,5,5	0.15	0
4	GOL	D	607	-	5,5,5	0.08	0	5,5,5	0.21	0
3	SO4	A	602	-	4,4,4	0.23	0	6,6,6	0.23	0
3	SO4	D	603	-	4,4,4	0.15	0	6,6,6	0.30	0
4	GOL	G	606	-	5,5,5	0.08	0	5,5,5	0.16	0
4	GOL	D	606	-	5,5,5	0.11	0	5,5,5	0.21	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
4	GOL	F	604	-	-	0/4/4/4	-
4	GOL	G	605	-	-	3/4/4/4	-
2	BME	F	601[A]	1	-	0/1/1/1	-
4	GOL	G	607	-	-	0/4/4/4	-
4	GOL	D	609	-	-	2/4/4/4	-
4	GOL	G	608	-	-	0/4/4/4	-
2	BME	C	601	-	-	0/1/1/1	-
4	GOL	A	605	-	-	0/4/4/4	-
4	GOL	D	605	-	-	0/4/4/4	-
2	BME	G	601	-	-	1/1/1/1	-
2	BME	D	601[A]	1	-	0/1/1/1	-
4	GOL	D	608	-	-	4/4/4/4	-
4	GOL	B	606	-	-	2/4/4/4	-
4	GOL	G	610	-	-	0/4/4/4	-
4	GOL	C	605	-	-	0/4/4/4	-
2	BME	A	601	-	-	0/1/1/1	-
4	GOL	E	605	-	-	0/4/4/4	-
4	GOL	H	605	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	603	-	-	2/4/4/4	-
2	BME	H	601	-	-	1/1/1/1	-
2	BME	F	601[B]	1	-	0/1/1/1	-
2	BME	B	601	-	-	1/1/1/1	-
4	GOL	B	605	-	-	0/4/4/4	-
4	GOL	A	604	-	-	0/4/4/4	-
2	BME	E	601	-	-	1/1/1/1	-
4	GOL	G	609	-	-	2/4/4/4	-
4	GOL	H	604	-	-	1/4/4/4	-
2	BME	D	601[B]	1	-	0/1/1/1	-
4	GOL	G	604	-	-	0/4/4/4	-
4	GOL	C	606	-	-	2/4/4/4	-
4	GOL	D	610	-	-	0/4/4/4	-
4	GOL	E	604	-	-	0/4/4/4	-
4	GOL	D	607	-	-	2/4/4/4	-
4	GOL	G	606	-	-	0/4/4/4	-
4	GOL	D	606	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	BME	O1-C1-C2-S2
2	H	601	BME	O1-C1-C2-S2
4	D	608	GOL	O1-C1-C2-O2
4	D	608	GOL	O1-C1-C2-C3
4	D	608	GOL	C1-C2-C3-O3
4	D	609	GOL	O1-C1-C2-C3
4	G	605	GOL	C1-C2-C3-O3
4	G	609	GOL	O1-C1-C2-C3
4	C	606	GOL	C1-C2-C3-O3
4	D	607	GOL	O1-C1-C2-C3
4	G	605	GOL	O1-C1-C2-C3
4	H	605	GOL	O1-C1-C2-C3
4	C	606	GOL	O2-C2-C3-O3
4	H	605	GOL	O1-C1-C2-O2
4	G	609	GOL	O1-C1-C2-O2
4	D	609	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	601	BME	O1-C1-C2-S2
4	D	608	GOL	O2-C2-C3-O3
2	G	601	BME	O1-C1-C2-S2
4	D	607	GOL	O1-C1-C2-O2
4	G	605	GOL	O2-C2-C3-O3
4	B	606	GOL	O1-C1-C2-C3
4	B	606	GOL	C1-C2-C3-O3
4	F	603	GOL	C1-C2-C3-O3
4	F	603	GOL	O1-C1-C2-C3
4	H	604	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	605	GOL	1	0
2	F	601[A]	BME	1	0
4	D	609	GOL	2	0
3	G	603	SO4	1	0
2	D	601[A]	BME	1	0
4	D	608	GOL	1	0
2	A	601	BME	1	0
4	F	603	GOL	1	0
2	F	601[B]	BME	1	0
2	D	601[B]	BME	1	0
4	C	606	GOL	2	0

5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	474/496 (95%)	0.25	19 (4%)	38	40	11, 24, 39, 49	0
1	B	474/496 (95%)	0.15	5 (1%)	80	82	13, 22, 31, 49	0
1	C	475/496 (95%)	0.11	6 (1%)	77	78	14, 21, 31, 52	1 (0%)
1	D	475/496 (95%)	0.12	8 (1%)	70	71	14, 21, 32, 56	0
1	E	475/496 (95%)	0.37	21 (4%)	34	36	12, 27, 41, 57	2 (0%)
1	F	474/496 (95%)	0.42	24 (5%)	28	30	16, 30, 48, 61	0
1	G	475/496 (95%)	0.04	7 (1%)	73	75	12, 19, 29, 55	1 (0%)
1	H	475/496 (95%)	0.10	5 (1%)	80	82	13, 20, 32, 47	0
All	All	3797/3968 (95%)	0.20	95 (2%)	57	59	11, 22, 38, 61	4 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	12.8
1	C	1	MET	8.5
1	G	1	MET	8.3
1	F	2	ALA	8.3
1	E	1	MET	7.0
1	H	1	MET	6.4
1	D	1	MET	5.6
1	E	2	ALA	5.4
1	A	2	ALA	5.3
1	D	2	ALA	5.3
1	G	2	ALA	4.9
1	F	211	SER	4.4
1	G	475	GLN	3.8
1	C	475	GLN	3.7
1	B	370	ASP	3.4
1	E	294	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	131	ALA	3.4
1	F	355[A]	GLU	3.3
1	F	212	VAL	3.3
1	A	294[A]	ASP	3.3
1	G	118	MET	3.3
1	G	131	ALA	3.3
1	F	475	GLN	3.3
1	E	342	THR	3.2
1	H	475	GLN	3.2
1	E	396	LYS	3.2
1	F	23	TYR	3.1
1	F	51	LYS	3.1
1	F	18	ASN	3.0
1	D	389	THR	2.9
1	A	343	ASP	2.9
1	A	295	LYS	2.9
1	A	355	GLU	2.9
1	E	295	LYS	2.9
1	E	291	LEU	2.8
1	D	391	VAL	2.8
1	F	19	GLU	2.7
1	E	389	THR	2.7
1	C	2	ALA	2.7
1	E	212	VAL	2.7
1	A	329	SER	2.7
1	F	11	GLY	2.6
1	F	221	GLU	2.6
1	F	332	ASP	2.6
1	F	3	LYS	2.6
1	A	370	ASP	2.6
1	F	14	LYS	2.5
1	E	318	ASP	2.5
1	A	3	LYS	2.5
1	H	258	ILE	2.5
1	F	20	ILE	2.4
1	E	412	THR	2.4
1	E	370	ASP	2.4
1	A	396	LYS	2.4
1	F	45	VAL	2.4
1	F	234	ILE	2.4
1	A	291	LEU	2.4
1	A	259	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	343	ASP	2.3
1	C	118	MET	2.3
1	E	345	GLY	2.3
1	B	51	LYS	2.3
1	F	131	ALA	2.3
1	E	409	ILE	2.3
1	G	130	ALA	2.3
1	H	259	VAL	2.2
1	F	370	ASP	2.2
1	D	310	LYS	2.2
1	E	290	VAL	2.2
1	E	155	TYR	2.2
1	A	352	PHE	2.2
1	F	9	VAL	2.2
1	A	168	LEU	2.2
1	E	383	LEU	2.2
1	H	300	LEU	2.2
1	F	30	GLU	2.2
1	A	284	CYS	2.2
1	D	291	LEU	2.1
1	A	211	SER	2.1
1	B	221	GLU	2.1
1	A	453	GLY	2.1
1	F	55	ASP	2.1
1	F	210	GLY	2.1
1	A	310	LYS	2.1
1	C	352	PHE	2.1
1	G	90	VAL	2.1
1	B	345	GLY	2.1
1	F	118	MET	2.1
1	E	200	ALA	2.1
1	E	382	VAL	2.0
1	D	385	ILE	2.0
1	D	475	GLN	2.0
1	A	382	VAL	2.0
1	A	351	ALA	2.0
1	E	18	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	606	6/6	0.38	0.43	67,67,67,67	0
4	GOL	A	605	6/6	0.40	0.27	58,58,59,59	0
4	GOL	E	605	6/6	0.53	0.25	52,53,53,53	0
4	GOL	A	604	6/6	0.66	0.37	61,61,61,62	0
3	SO4	B	602	5/5	0.68	0.34	108,108,108,108	0
2	BME	H	601	4/4	0.70	0.22	44,44,44,44	0
4	GOL	D	605	6/6	0.71	0.23	42,42,43,43	0
4	GOL	D	610	6/6	0.72	0.22	55,55,56,56	0
4	GOL	C	606	6/6	0.72	0.33	52,53,53,53	0
4	GOL	F	603	6/6	0.73	0.26	55,55,55,55	0
4	GOL	G	608	6/6	0.73	0.16	40,41,41,41	0
4	GOL	E	604	6/6	0.74	0.30	62,62,62,62	0
3	SO4	D	602	5/5	0.75	0.20	86,86,86,86	0
2	BME	D	601[A]	4/4	0.75	0.42	39,40,40,40	4
2	BME	D	601[B]	4/4	0.75	0.42	38,38,38,38	4
4	GOL	G	605	6/6	0.75	0.26	49,49,50,50	0
4	GOL	B	605	6/6	0.75	0.17	52,52,52,52	0
2	BME	G	601	4/4	0.76	0.20	46,46,47,47	0
2	BME	A	601	4/4	0.80	0.14	53,53,54,54	0
2	BME	E	601	4/4	0.81	0.17	51,51,51,51	0
4	GOL	F	604	6/6	0.81	0.18	52,52,52,53	0
2	BME	C	601	4/4	0.82	0.25	71,72,72,72	0
3	SO4	C	602	5/5	0.83	0.21	83,83,83,83	0
4	GOL	C	605	6/6	0.84	0.13	52,52,53,53	0
3	SO4	C	603	5/5	0.84	0.20	60,61,61,61	0
4	GOL	G	610	6/6	0.84	0.19	46,46,47,47	0
3	SO4	F	602	5/5	0.85	0.15	78,78,78,78	0
3	SO4	D	604	5/5	0.86	0.31	93,93,93,93	0
4	GOL	G	609	6/6	0.86	0.25	49,50,50,51	0
4	GOL	G	607	6/6	0.86	0.17	38,38,39,39	0
2	BME	F	601[B]	4/4	0.87	0.35	38,38,38,38	4
2	BME	F	601[A]	4/4	0.87	0.35	36,36,36,37	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	G	604	6/6	0.87	0.18	49,50,50,50	0
4	GOL	D	607	6/6	0.87	0.15	36,37,37,37	0
4	GOL	G	606	6/6	0.88	0.21	45,46,46,46	0
2	BME	B	601	4/4	0.89	0.16	47,48,48,48	0
4	GOL	D	608	6/6	0.89	0.22	41,42,42,42	0
3	SO4	E	602	5/5	0.90	0.16	76,76,76,76	0
3	SO4	A	603	5/5	0.90	0.14	73,73,73,73	0
3	SO4	G	602	5/5	0.90	0.23	53,54,54,54	0
3	SO4	H	603	5/5	0.90	0.24	56,56,56,56	0
3	SO4	B	604	5/5	0.90	0.17	83,83,83,83	0
4	GOL	D	606	6/6	0.91	0.11	40,40,40,40	0
3	SO4	B	603	5/5	0.91	0.14	71,71,71,71	0
3	SO4	D	603	5/5	0.91	0.22	56,57,57,57	0
3	SO4	A	602	5/5	0.91	0.18	74,74,74,74	0
3	SO4	H	602	5/5	0.91	0.14	57,57,57,57	0
4	GOL	D	609	6/6	0.92	0.14	39,39,39,40	0
4	GOL	H	604	6/6	0.92	0.22	39,39,40,40	0
4	GOL	H	605	6/6	0.92	0.11	43,43,43,43	0
3	SO4	E	603	5/5	0.93	0.18	64,64,64,65	0
3	SO4	C	604	5/5	0.93	0.20	69,69,69,69	0
3	SO4	G	603	5/5	0.97	0.21	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.