wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 10:17 am GMT

PDB ID	:	5HUD
Title	:	Non-covalent complex of and DAHP synthase and chorismate mutase from Corynebacterium glutamicum with bound transition state analog
Authors	:	Burschowsky, D.; Heim, J.B.; Thorbjoernsrud, H.V.; Krengel, U.
Deposited on	:	2016-01-27
Resolution	:	2.15 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

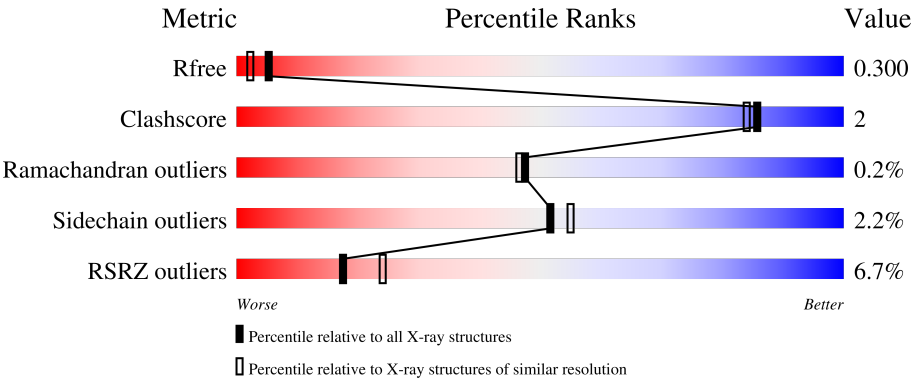
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	472	4% 89% 5% 6%
1	B	472	7% 88% 6% 6%
1	C	472	8% 88% 8%
1	D	472	6% 87% 10%
2	E	90	9% 88% 6% 7%

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Mol	Chain	Length	Quality of chain
2	F	90	9% 86% 7% 8%
2	G	90	7% 90% 8%
2	H	90	7% 89% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	509	-	-	-	X
3	GOL	C	510	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18279 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-Deoxy-D-arabino-heptulosonate 7-phosphate (DAHP) synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	1	0
			3445	2141	615	672	17			
1	B	444	Total	C	N	O	S	0	1	0
			3445	2141	615	672	17			
1	C	456	Total	C	N	O	S	0	1	0
			3537	2199	630	690	18			
1	D	457	Total	C	N	O	S	0	2	0
			3553	2209	634	692	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NNL5
A	2	HIS	-	expression tag	UNP Q8NNL5
A	3	HIS	-	expression tag	UNP Q8NNL5
A	4	HIS	-	expression tag	UNP Q8NNL5
A	5	HIS	-	expression tag	UNP Q8NNL5
A	6	HIS	-	expression tag	UNP Q8NNL5
A	7	HIS	-	expression tag	UNP Q8NNL5
A	8	SER	-	expression tag	UNP Q8NNL5
A	9	SER	-	expression tag	UNP Q8NNL5
A	10	GLY	-	expression tag	UNP Q8NNL5
B	1	MET	-	initiating methionine	UNP Q8NNL5
B	2	HIS	-	expression tag	UNP Q8NNL5
B	3	HIS	-	expression tag	UNP Q8NNL5
B	4	HIS	-	expression tag	UNP Q8NNL5
B	5	HIS	-	expression tag	UNP Q8NNL5
B	6	HIS	-	expression tag	UNP Q8NNL5
B	7	HIS	-	expression tag	UNP Q8NNL5
B	8	SER	-	expression tag	UNP Q8NNL5
B	9	SER	-	expression tag	UNP Q8NNL5
B	10	GLY	-	expression tag	UNP Q8NNL5

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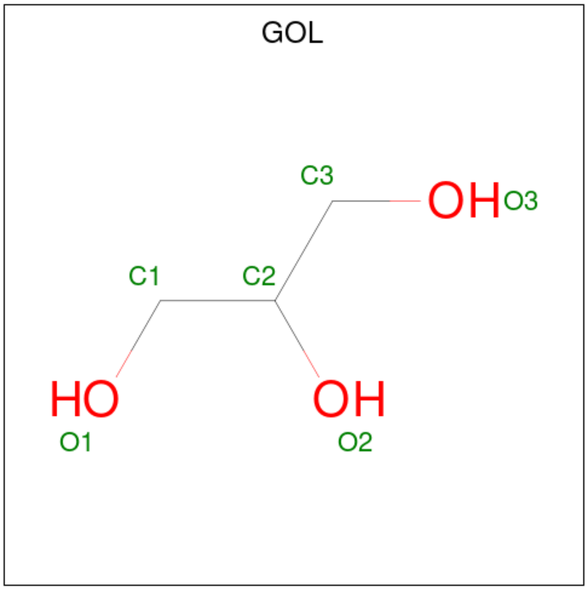
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP Q8NNL5
C	2	HIS	-	expression tag	UNP Q8NNL5
C	3	HIS	-	expression tag	UNP Q8NNL5
C	4	HIS	-	expression tag	UNP Q8NNL5
C	5	HIS	-	expression tag	UNP Q8NNL5
C	6	HIS	-	expression tag	UNP Q8NNL5
C	7	HIS	-	expression tag	UNP Q8NNL5
C	8	SER	-	expression tag	UNP Q8NNL5
C	9	SER	-	expression tag	UNP Q8NNL5
C	10	GLY	-	expression tag	UNP Q8NNL5
D	1	MET	-	initiating methionine	UNP Q8NNL5
D	2	HIS	-	expression tag	UNP Q8NNL5
D	3	HIS	-	expression tag	UNP Q8NNL5
D	4	HIS	-	expression tag	UNP Q8NNL5
D	5	HIS	-	expression tag	UNP Q8NNL5
D	6	HIS	-	expression tag	UNP Q8NNL5
D	7	HIS	-	expression tag	UNP Q8NNL5
D	8	SER	-	expression tag	UNP Q8NNL5
D	9	SER	-	expression tag	UNP Q8NNL5
D	10	GLY	-	expression tag	UNP Q8NNL5

- Molecule 2 is a protein called Chorismate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	84	Total	C	N	O	S	0	1	0
			672	411	130	129	2			
2	F	83	Total	C	N	O	S	0	1	0
			666	408	132	124	2			
2	G	83	Total	C	N	O	S	0	0	0
			655	402	128	123	2			
2	H	83	Total	C	N	O	S	0	0	0
			655	402	128	123	2			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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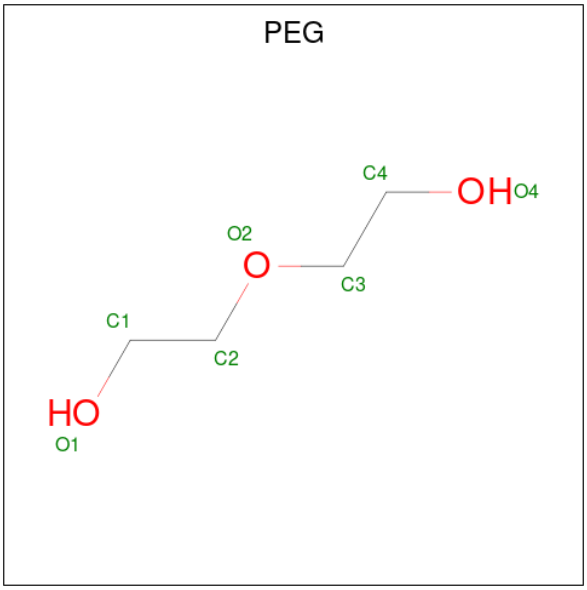
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0

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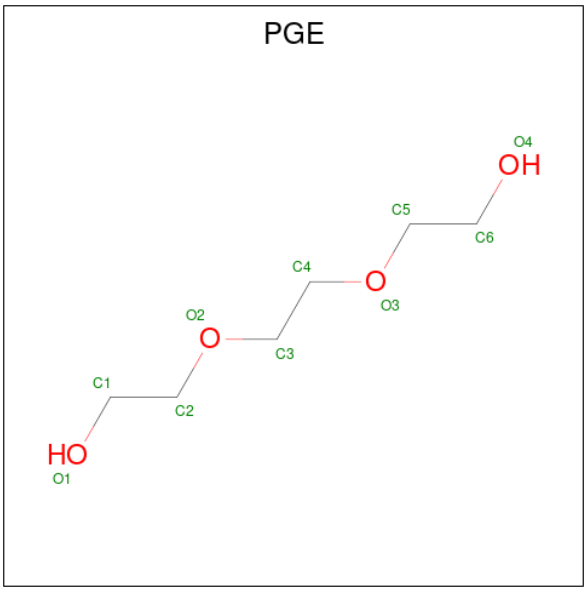
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

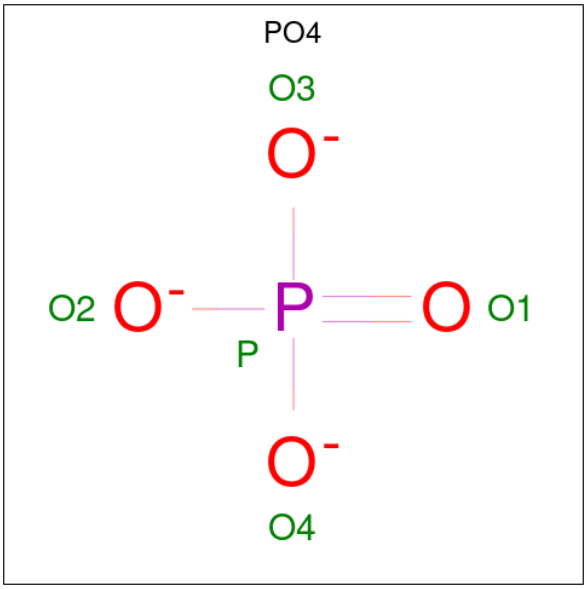


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	G	1	Total C O 10 6 4	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

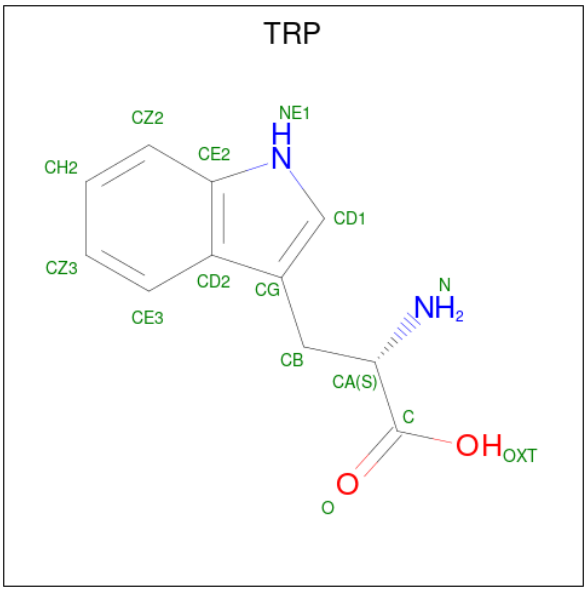
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mn 1 1	0	0
6	B	1	Total Mn 1 1	0	0
6	C	1	Total Mn 1 1	0	0
6	D	1	Total Mn 1 1	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



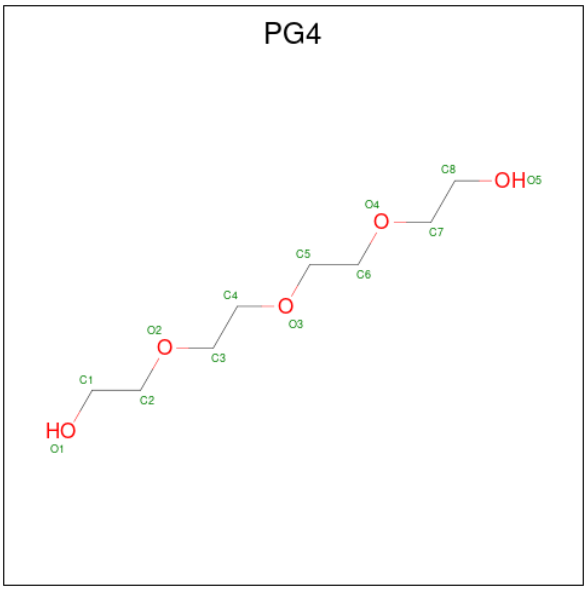
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0
7	C	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0

- Molecule 8 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



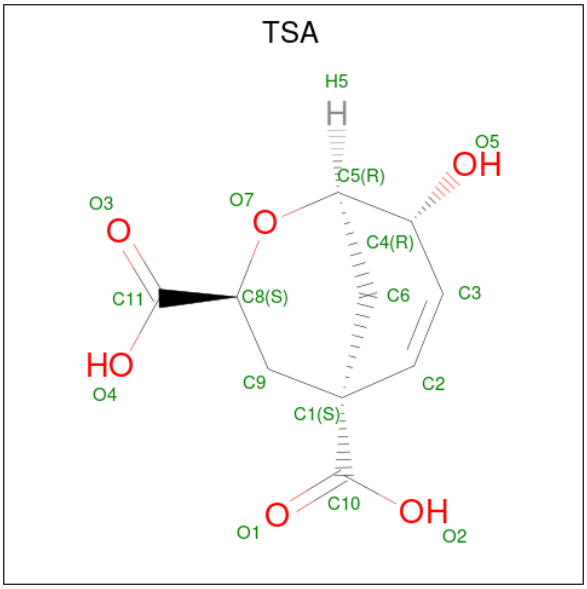
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 15 11 2 2	0	0
8	B	1	Total C N O 15 11 2 2	0	0
8	C	1	Total C N O 15 11 2 2	0	0
8	D	1	Total C N O 15 11 2 2	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 13 8 5	0	0
9	C	1	Total C O 13 8 5	0	0
9	D	1	Total C O 13 8 5	0	0
9	D	1	Total C O 13 8 5	0	0
9	D	1	Total C O 13 8 5	0	0

- Molecule 10 is 8-HYDROXY-2-OXA-BICYCLO[3.3.1]NON-6-ENE-3,5-DICARBOXYLIC ACID (three-letter code: TSA) (formula: $C_{10}H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total C O 16 10 6	0	0
10	F	1	Total C O 16 10 6	0	0
10	G	1	Total C O 16 10 6	0	0
10	H	1	Total C O 16 10 6	0	0

- Molecule 11 is water.

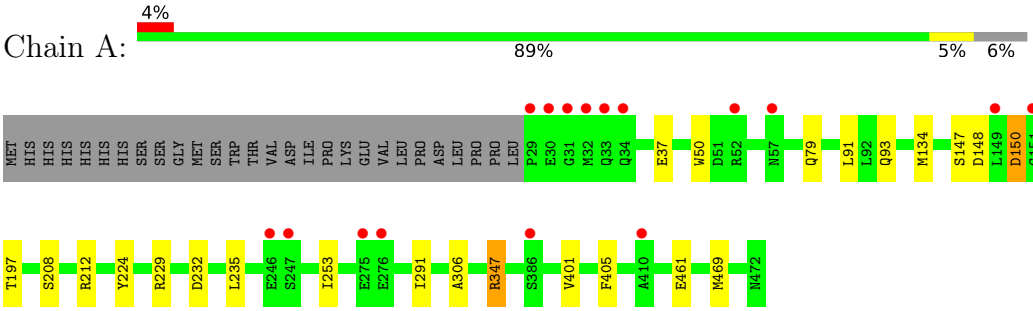
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	120	Total O 120 120	0	0
11	B	117	Total O 118 118	0	1
11	C	183	Total O 183 183	0	0
11	D	181	Total O 181 181	0	1
11	E	36	Total O 36 36	0	0
11	F	49	Total O 49 49	0	0
11	G	42	Total O 42 42	0	0
11	H	51	Total O 51 51	0	0

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.

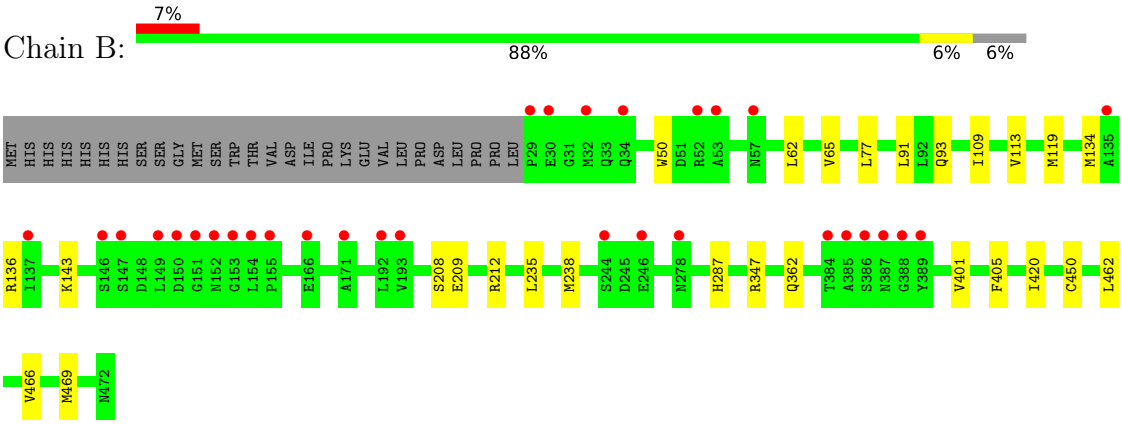
• Molecule 1: 3-Deoxy-D-arabino-heptulosonate 7-phosphate (DAHP) synthase

Chain A:



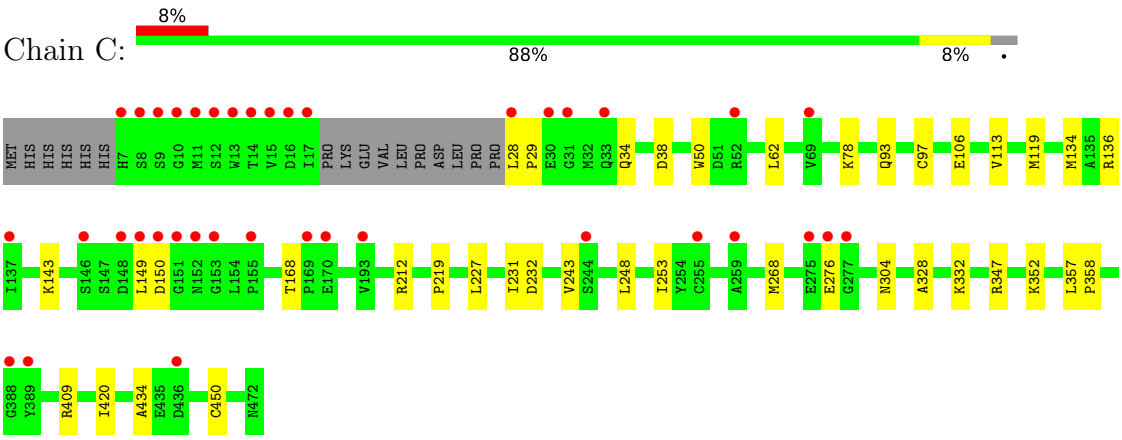
• Molecule 1: 3-Deoxy-D-arabino-heptulosonate 7-phosphate (DAHP) synthase

Chain B:



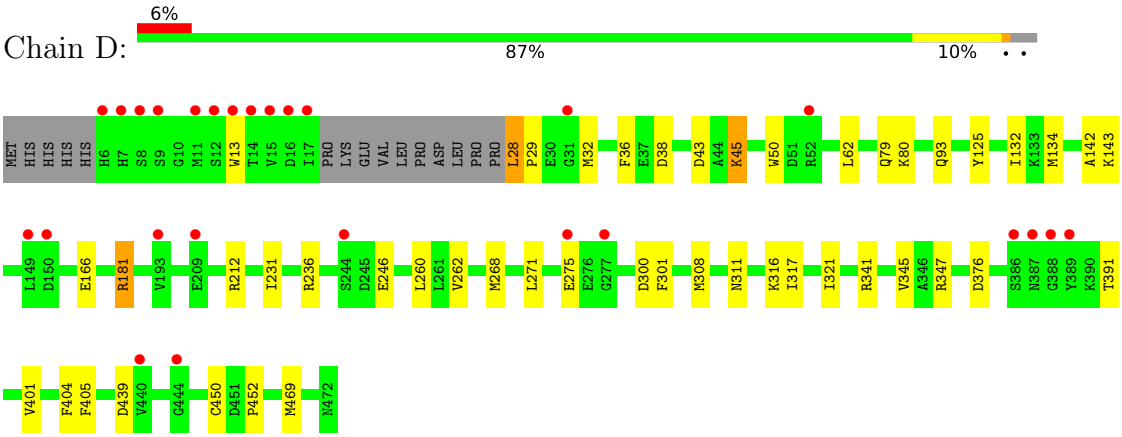
• Molecule 1: 3-Deoxy-D-arabino-heptulosonate 7-phosphate (DAHP) synthase

Chain C:



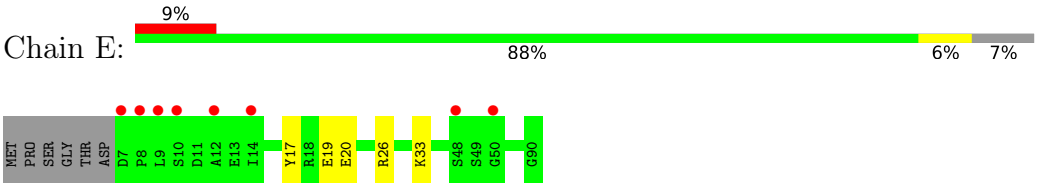
• Molecule 1: 3-Deoxy-D-arabino-heptulosonate 7-phosphate (DAHP) synthase

Chain D:



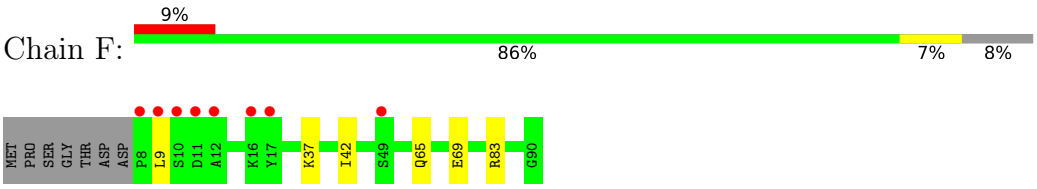
• Molecule 2: Chorismate mutase

Chain E:



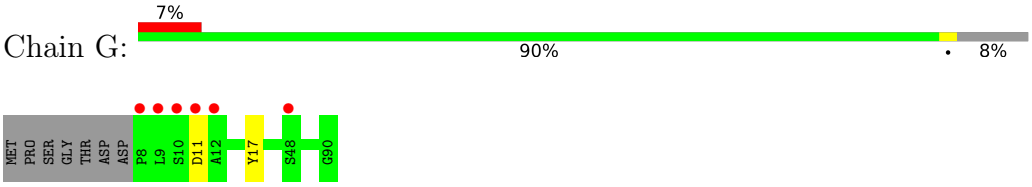
• Molecule 2: Chorismate mutase

Chain F:



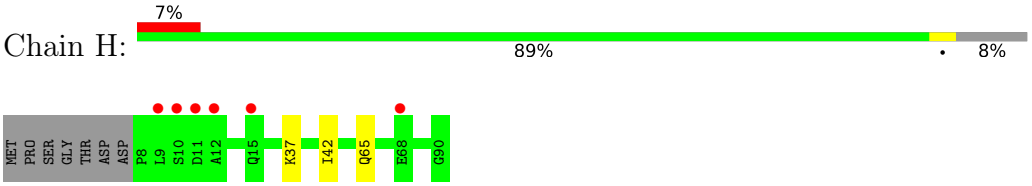
• Molecule 2: Chorismate mutase

Chain G:



• Molecule 2: Chorismate mutase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.62Å 110.48Å 134.65Å 90.00° 101.41° 90.00°	Depositor
Resolution (Å)	40.00 – 2.15 48.42 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.00-2.15) 98.0 (48.42-2.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.250 , 0.298 0.253 , 0.300	Depositor DCC
R_{free} test set	8847 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18279	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 22.63 % 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 5.4860e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: PG4, PGE, MN, TSA, GOL, PO4, PEG

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	0.50	0/3512	0.72	1/4759 (0.0%)
1	B	0.49	0/3512	0.71	1/4759 (0.0%)
1	C	0.62	0/3606	0.80	1/4887 (0.0%)
1	D	0.63	0/3626	0.79	4/4914 (0.1%)
2	E	0.57	0/676	0.74	0/900
2	F	0.64	0/670	0.82	1/890 (0.1%)
2	G	0.60	0/659	0.82	0/876
2	H	0.64	0/659	0.82	0/876
All	All	0.57	0/16920	0.76	8/22861 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	181	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	376	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	136	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	212	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	347	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	3445	0	3348	13	0
1	B	3445	0	3348	14	0
1	C	3537	0	3432	18	0
1	D	3553	0	3447	26	0
2	E	672	0	696	4	0
2	F	666	0	700	2	0
2	G	655	0	688	1	0
2	H	655	0	688	2	0
3	A	12	0	16	0	0
3	B	60	0	80	0	0
3	C	120	0	160	5	0
3	D	78	0	104	2	0
3	E	24	0	32	0	0
3	F	36	0	48	0	0
3	G	36	0	48	0	0
3	H	30	0	40	0	0
4	A	14	0	20	1	0
4	B	7	0	10	0	0
4	C	21	0	30	0	0
4	D	42	0	60	0	0
4	F	7	0	10	0	0
4	G	21	0	30	0	0
5	A	10	0	14	0	0
5	C	50	0	70	0	0
5	D	20	0	28	0	0
5	E	30	0	42	0	0
5	F	20	0	28	0	0
5	G	10	0	14	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	10	0	0	1	0
8	A	15	0	9	0	0
8	B	15	0	9	0	0
8	C	15	0	9	0	0
8	D	15	0	9	0	0
9	B	13	0	18	0	0
9	C	13	0	18	0	0
9	D	39	0	54	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	16	0	10	0	0
10	F	16	0	10	0	0
10	G	16	0	10	0	0
10	H	16	0	10	0	0
11	A	120	0	0	1	0
11	B	118	0	0	0	0
11	C	183	0	0	0	0
11	D	181	0	0	1	0
11	E	36	0	0	2	0
11	F	49	0	0	0	0
11	G	42	0	0	0	0
11	H	51	0	0	1	0
All	All	18279	0	17397	78	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 2.

The worst 5 of 78 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:E:20:GLU:CD	11:E:201:HOH:O	2.20	0.78
1:D:401:VAL:HG12	1:D:469:MET:HE1	1.67	0.77
1:A:401:VAL:HG12	1:A:469:MET:HE1	1.69	0.73
1:D:401:VAL:HG12	1:D:469:MET:CE	2.20	0.70
1:D:405:PHE:CD1	1:D:469:MET:HE2	2.29	0.67

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	443/472 (94%)	429 (97%)	12 (3%)	2 (0%)	29 22
1	B	443/472 (94%)	431 (97%)	12 (3%)	0	100 100
1	C	453/472 (96%)	435 (96%)	17 (4%)	1 (0%)	47 46
1	D	455/472 (96%)	439 (96%)	15 (3%)	1 (0%)	47 46
2	E	83/90 (92%)	81 (98%)	2 (2%)	0	100 100
2	F	82/90 (91%)	81 (99%)	1 (1%)	0	100 100
2	G	81/90 (90%)	80 (99%)	1 (1%)	0	100 100
2	H	81/90 (90%)	80 (99%)	1 (1%)	0	100 100
All	All	2121/2248 (94%)	2056 (97%)	61 (3%)	4 (0%)	47 46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
1	C	150	ASP
1	A	147	SER
1	D	246	GLU

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	363/389 (93%)	357 (98%)	6 (2%)	60 65
1	B	363/389 (93%)	360 (99%)	3 (1%)	81 86
1	C	374/389 (96%)	362 (97%)	12 (3%)	39 38
1	D	376/389 (97%)	365 (97%)	11 (3%)	42 42
2	E	71/75 (95%)	68 (96%)	3 (4%)	30 28
2	F	70/75 (93%)	67 (96%)	3 (4%)	29 27
2	G	69/75 (92%)	68 (99%)	1 (1%)	67 72
2	H	69/75 (92%)	68 (99%)	1 (1%)	67 72
All	All	1755/1856 (95%)	1715 (98%)	40 (2%)	52 53

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	166	GLU
2	F	9	LEU
1	D	275	GLU
2	E	19[A]	GLU
2	F	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	B	79	GLN
1	C	156	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)

Of 119 ligands modelled in this entry, 4 are monoatomic - leaving 115 for Mogul analysis.

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	$\#\|Z\|>2$
5	PGE	C	526	-	9,9,9	0.64	0	8,8,8	0.52	0
3	GOL	H	105	-	5,5,5	0.51	0	5,5,5	0.34	0
3	GOL	B	503	-	5,5,5	0.40	0	5,5,5	0.64	0
3	GOL	C	503	-	5,5,5	0.26	0	5,5,5	0.34	0
3	GOL	C	509	-	5,5,5	0.27	0	5,5,5	0.34	0
3	GOL	H	102	-	5,5,5	0.33	0	5,5,5	0.57	0
8	TRP	B	515	-	14,16,16	0.83	0	16,22,22	1.17	2 (12%)
3	GOL	F	106	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	H	101	-	5,5,5	0.46	0	5,5,5	0.47	0
5	PGE	C	525	-	9,9,9	0.52	0	8,8,8	0.52	0
3	GOL	C	505	-	5,5,5	0.56	0	5,5,5	0.47	0
5	PGE	F	109	-	9,9,9	0.62	0	8,8,8	0.39	0
10	TSA	E	108	-	16,17,17	1.21	1 (6%)	16,26,26	1.64	4 (25%)
9	PG4	D	522	-	12,12,12	0.68	0	11,11,11	1.02	1 (9%)
5	PGE	E	105	-	9,9,9	0.54	0	8,8,8	0.35	0
5	PGE	E	106	-	9,9,9	0.69	0	8,8,8	0.47	0
5	PGE	C	528	-	9,9,9	0.64	0	8,8,8	0.80	0
3	GOL	B	509	-	5,5,5	0.33	0	5,5,5	0.15	0
8	TRP	C	532	-	14,16,16	0.87	0	16,22,22	0.95	1 (6%)
3	GOL	D	502	-	5,5,5	0.54	0	5,5,5	0.79	0
3	GOL	C	518	-	5,5,5	0.55	0	5,5,5	0.62	0
3	GOL	D	509	-	5,5,5	0.34	0	5,5,5	0.36	0
3	GOL	H	104	-	5,5,5	0.67	0	5,5,5	0.60	0
3	GOL	B	510	-	5,5,5	0.25	0	5,5,5	0.32	0
3	GOL	C	512	-	5,5,5	0.23	0	5,5,5	0.33	0
3	GOL	G	104	-	5,5,5	0.41	0	5,5,5	0.55	0
9	PG4	D	524	-	12,12,12	0.61	0	11,11,11	0.92	0
9	PG4	C	529	-	12,12,12	0.65	0	11,11,11	0.54	0
5	PGE	C	527	-	9,9,9	0.63	0	8,8,8	0.69	0
3	GOL	D	501	-	5,5,5	0.49	0	5,5,5	0.23	0
4	PEG	D	515	-	6,6,6	0.59	0	5,5,5	0.50	0
3	GOL	G	102	-	5,5,5	0.70	0	5,5,5	0.61	0
3	GOL	D	504	-	5,5,5	0.48	0	5,5,5	0.52	0
3	GOL	B	507	-	5,5,5	0.28	0	5,5,5	0.46	0
4	PEG	A	503	-	6,6,6	0.42	0	5,5,5	0.30	0
3	GOL	D	512	-	5,5,5	0.39	0	5,5,5	0.39	0
8	TRP	A	509	-	14,16,16	0.85	1 (7%)	16,22,22	1.03	1 (6%)
3	GOL	C	506	-	5,5,5	0.30	0	5,5,5	0.28	0
4	PEG	D	514	-	6,6,6	0.59	0	5,5,5	1.11	0
3	GOL	C	520	-	5,5,5	0.41	0	5,5,5	0.39	0
7	PO4	B	514	-	4,4,4	0.91	0	6,6,6	0.51	0
3	GOL	H	103	-	5,5,5	0.37	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PEG	D	516	-	6,6,6	0.54	0	5,5,5	0.27	0
8	TRP	D	528	-	14,16,16	0.93	0	16,22,22	0.90	0
4	PEG	D	519	-	6,6,6	0.60	0	5,5,5	0.25	0
4	PEG	C	523	-	6,6,6	0.52	0	5,5,5	0.44	0
3	GOL	D	513	-	5,5,5	0.51	0	5,5,5	0.60	0
3	GOL	C	510	-	5,5,5	0.32	0	5,5,5	0.24	0
5	PGE	G	110	-	9,9,9	0.55	0	8,8,8	0.34	0
3	GOL	C	504	-	5,5,5	0.42	0	5,5,5	0.49	0
10	TSA	G	111	-	16,17,17	1.36	2 (12%)	16,26,26	1.57	6 (37%)
3	GOL	B	506	-	5,5,5	0.41	0	5,5,5	0.54	0
4	PEG	F	107	-	6,6,6	0.56	0	5,5,5	0.52	0
3	GOL	D	505	-	5,5,5	0.62	0	5,5,5	0.70	0
3	GOL	C	517	-	5,5,5	0.42	0	5,5,5	0.22	0
7	PO4	C	531	-	4,4,4	1.03	0	6,6,6	0.70	0
7	PO4	D	527	-	4,4,4	0.79	0	6,6,6	0.78	0
4	PEG	D	518	-	6,6,6	0.49	0	5,5,5	0.37	0
4	PEG	G	107	-	6,6,6	0.71	0	5,5,5	0.93	0
3	GOL	D	506	-	5,5,5	0.29	0	5,5,5	0.29	0
3	GOL	G	105	-	5,5,5	0.44	0	5,5,5	0.50	0
3	GOL	E	101	-	5,5,5	0.39	0	5,5,5	0.19	0
5	PGE	F	108	-	9,9,9	0.64	0	8,8,8	0.42	0
10	TSA	H	106	-	16,17,17	1.58	4 (25%)	16,26,26	1.74	4 (25%)
3	GOL	D	511	-	5,5,5	0.67	0	5,5,5	0.60	0
5	PGE	D	521	-	9,9,9	0.64	0	8,8,8	0.38	0
3	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	G	101	-	5,5,5	0.50	0	5,5,5	0.61	0
4	PEG	G	109	-	6,6,6	0.49	0	5,5,5	0.43	0
3	GOL	F	105	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	D	508	-	5,5,5	0.75	0	5,5,5	0.60	0
7	PO4	A	508	-	4,4,4	0.92	0	6,6,6	0.53	0
3	GOL	F	104	-	5,5,5	0.40	0	5,5,5	0.60	0
3	GOL	F	101	-	5,5,5	0.48	0	5,5,5	0.30	0
5	PGE	D	520	-	9,9,9	0.56	0	8,8,8	0.39	0
3	GOL	G	106	-	5,5,5	0.34	0	5,5,5	0.20	0
3	GOL	E	103	-	5,5,5	0.39	0	5,5,5	0.37	0
3	GOL	B	502	-	5,5,5	0.41	0	5,5,5	0.29	0
7	PO4	A	507	-	4,4,4	1.07	0	6,6,6	0.48	0
3	GOL	D	507	-	5,5,5	0.66	0	5,5,5	0.62	0
3	GOL	F	103	-	5,5,5	0.43	0	5,5,5	1.18	0
3	GOL	F	102	-	5,5,5	0.45	0	5,5,5	0.28	0
3	GOL	C	516	-	5,5,5	0.39	0	5,5,5	0.18	0
5	PGE	A	505	-	9,9,9	0.64	0	8,8,8	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	E	104	-	5,5,5	0.42	0	5,5,5	0.20	0
3	GOL	C	501	-	5,5,5	0.44	0	5,5,5	0.36	0
3	GOL	A	502	-	5,5,5	0.44	0	5,5,5	0.24	0
4	PEG	C	522	-	6,6,6	0.56	0	5,5,5	0.59	0
4	PEG	A	504	-	6,6,6	0.50	0	5,5,5	0.43	0
3	GOL	C	515	-	5,5,5	0.54	0	5,5,5	0.53	0
3	GOL	B	508	-	5,5,5	0.40	0	5,5,5	0.16	0
3	GOL	C	511	-	5,5,5	0.60	0	5,5,5	0.57	0
3	GOL	C	513	-	5,5,5	0.58	0	5,5,5	0.35	0
3	GOL	B	505	-	5,5,5	0.47	0	5,5,5	0.48	0
3	GOL	B	501	-	5,5,5	0.28	0	5,5,5	0.50	0
3	GOL	C	508	-	5,5,5	0.61	0	5,5,5	0.37	0
3	GOL	D	503	-	5,5,5	0.32	0	5,5,5	0.23	0
3	GOL	G	103	-	5,5,5	0.36	0	5,5,5	0.22	0
4	PEG	B	511	-	6,6,6	0.45	0	5,5,5	0.33	0
7	PO4	D	526	-	4,4,4	0.78	0	6,6,6	0.63	0
10	TSA	F	110	-	16,17,17	1.57	5 (31%)	16,26,26	1.47	2 (12%)
3	GOL	C	519	-	5,5,5	0.45	0	5,5,5	0.42	0
3	GOL	A	501	-	5,5,5	0.36	0	5,5,5	0.38	0
5	PGE	C	524	-	9,9,9	0.55	0	8,8,8	0.77	0
3	GOL	C	502	-	5,5,5	0.54	0	5,5,5	0.88	0
3	GOL	D	510	-	5,5,5	0.30	0	5,5,5	0.26	0
3	GOL	C	514	-	5,5,5	0.44	0	5,5,5	0.58	0
3	GOL	E	102	-	5,5,5	0.48	0	5,5,5	0.24	0
3	GOL	C	507	-	5,5,5	0.40	0	5,5,5	0.92	0
4	PEG	G	108	-	6,6,6	0.62	0	5,5,5	0.30	0
9	PG4	B	512	-	12,12,12	0.66	0	11,11,11	0.37	0
4	PEG	D	517	-	6,6,6	0.55	0	5,5,5	0.18	0
9	PG4	D	523	-	12,12,12	0.57	0	11,11,11	0.30	0
4	PEG	C	521	-	6,6,6	0.79	0	5,5,5	0.89	0
5	PGE	E	107	-	9,9,9	0.63	0	8,8,8	0.42	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
5	PGE	C	526	-	-	3/7/7/7	-
3	GOL	H	105	-	-	4/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	C	503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	509	-	-	0/4/4/4	-
3	GOL	H	102	-	-	1/4/4/4	-
8	TRP	B	515	-	-	0/7/8/8	0/2/2/2
3	GOL	F	106	-	-	2/4/4/4	-
3	GOL	H	101	-	-	2/4/4/4	-
5	PGE	C	525	-	-	4/7/7/7	-
3	GOL	C	505	-	-	2/4/4/4	-
5	PGE	F	109	-	-	2/7/7/7	-
10	TSA	E	108	-	-	1/10/34/34	1/3/2/2
9	PG4	D	522	-	-	6/10/10/10	-
5	PGE	E	105	-	-	2/7/7/7	-
5	PGE	E	106	-	-	3/7/7/7	-
5	PGE	C	528	-	-	5/7/7/7	-
3	GOL	B	509	-	-	2/4/4/4	-
8	TRP	C	532	-	-	0/7/8/8	0/2/2/2
3	GOL	D	502	-	-	1/4/4/4	-
3	GOL	C	518	-	-	2/4/4/4	-
3	GOL	D	509	-	-	2/4/4/4	-
3	GOL	H	104	-	-	2/4/4/4	-
3	GOL	B	510	-	-	3/4/4/4	-
3	GOL	C	512	-	-	2/4/4/4	-
3	GOL	G	104	-	-	2/4/4/4	-
9	PG4	D	524	-	-	4/10/10/10	-
9	PG4	C	529	-	-	7/10/10/10	-
5	PGE	C	527	-	-	3/7/7/7	-
3	GOL	D	501	-	-	4/4/4/4	-
4	PEG	D	515	-	-	1/4/4/4	-
3	GOL	G	102	-	-	2/4/4/4	-
3	GOL	D	504	-	-	4/4/4/4	-
3	GOL	B	507	-	-	2/4/4/4	-
4	PEG	A	503	-	-	2/4/4/4	-
3	GOL	D	512	-	-	2/4/4/4	-
8	TRP	A	509	-	-	1/7/8/8	0/2/2/2
3	GOL	C	506	-	-	2/4/4/4	-
4	PEG	D	514	-	-	3/4/4/4	-
3	GOL	C	520	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	H	103	-	-	1/4/4/4	-
4	PEG	D	516	-	-	3/4/4/4	-
8	TRP	D	528	-	-	0/7/8/8	0/2/2/2
4	PEG	D	519	-	-	1/4/4/4	-
4	PEG	C	523	-	-	1/4/4/4	-
3	GOL	D	513	-	-	2/4/4/4	-
3	GOL	C	510	-	-	0/4/4/4	-
5	PGE	G	110	-	-	3/7/7/7	-
3	GOL	C	504	-	-	2/4/4/4	-
10	TSA	G	111	-	-	0/10/34/34	1/3/2/2
3	GOL	B	506	-	-	0/4/4/4	-
4	PEG	F	107	-	-	3/4/4/4	-
3	GOL	D	505	-	-	4/4/4/4	-
3	GOL	C	517	-	-	2/4/4/4	-
4	PEG	D	518	-	-	2/4/4/4	-
4	PEG	G	107	-	-	2/4/4/4	-
3	GOL	D	506	-	-	0/4/4/4	-
3	GOL	G	105	-	-	0/4/4/4	-
3	GOL	E	101	-	-	0/4/4/4	-
5	PGE	F	108	-	-	4/7/7/7	-
10	TSA	H	106	-	-	0/10/34/34	1/3/2/2
3	GOL	D	511	-	-	4/4/4/4	-
5	PGE	D	521	-	-	3/7/7/7	-
3	GOL	B	504	-	-	4/4/4/4	-
3	GOL	G	101	-	-	0/4/4/4	-
4	PEG	G	109	-	-	3/4/4/4	-
3	GOL	F	105	-	-	2/4/4/4	-
3	GOL	D	508	-	-	4/4/4/4	-
3	GOL	F	104	-	-	4/4/4/4	-
3	GOL	F	101	-	-	4/4/4/4	-
5	PGE	D	520	-	-	5/7/7/7	-
3	GOL	G	106	-	-	3/4/4/4	-
3	GOL	E	103	-	-	1/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	D	507	-	-	2/4/4/4	-
3	GOL	F	103	-	-	2/4/4/4	-
3	GOL	F	102	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	516	-	-	2/4/4/4	-
5	PGE	A	505	-	-	5/7/7/7	-
3	GOL	E	104	-	-	4/4/4/4	-
3	GOL	C	501	-	-	2/4/4/4	-
3	GOL	A	502	-	-	3/4/4/4	-
4	PEG	C	522	-	-	1/4/4/4	-
4	PEG	A	504	-	-	3/4/4/4	-
3	GOL	C	515	-	-	2/4/4/4	-
3	GOL	B	508	-	-	2/4/4/4	-
3	GOL	C	511	-	-	2/4/4/4	-
3	GOL	C	513	-	-	3/4/4/4	-
3	GOL	B	505	-	-	0/4/4/4	-
3	GOL	B	501	-	-	4/4/4/4	-
3	GOL	C	508	-	-	4/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	G	103	-	-	2/4/4/4	-
4	PEG	B	511	-	-	0/4/4/4	-
10	TSA	F	110	-	-	0/10/34/34	1/3/2/2
3	GOL	C	519	-	-	4/4/4/4	-
3	GOL	A	501	-	-	2/4/4/4	-
5	PGE	C	524	-	-	5/7/7/7	-
3	GOL	C	502	-	-	4/4/4/4	-
3	GOL	D	510	-	-	0/4/4/4	-
3	GOL	C	514	-	-	2/4/4/4	-
3	GOL	E	102	-	-	0/4/4/4	-
3	GOL	C	507	-	-	2/4/4/4	-
4	PEG	G	108	-	-	2/4/4/4	-
9	PG4	B	512	-	-	1/10/10/10	-
4	PEG	D	517	-	-	2/4/4/4	-
9	PG4	D	523	-	-	5/10/10/10	-
4	PEG	C	521	-	-	2/4/4/4	-
5	PGE	E	107	-	-	2/7/7/7	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	106	TSA	C8-C11	-3.13	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	110	TSA	C9-C1	-2.63	1.51	1.55
10	H	106	TSA	C3-C2	2.60	1.36	1.32
10	G	111	TSA	C6-C1	-2.55	1.51	1.55
10	F	110	TSA	C3-C2	2.53	1.36	1.32

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	106	TSA	O7-C8-C9	3.81	115.54	109.92
10	F	110	TSA	O7-C8-C9	3.38	114.92	109.92
10	E	108	TSA	O7-C8-C9	3.38	114.91	109.92
10	E	108	TSA	O4-C11-C8	2.97	121.52	113.03
10	H	106	TSA	O4-C11-C8	2.72	120.78	113.03

There are no chirality outliers.

5 of 243 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GOL	O1-C1-C2-O2
3	A	501	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-C3

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	110	TSA	C1-C2-C3-C4-C5-C8-C9-O7
10	H	106	TSA	C1-C2-C3-C4-C5-C8-C9-O7
10	E	108	TSA	C1-C2-C3-C4-C5-C8-C9-O7
10	G	111	TSA	C1-C2-C3-C4-C5-C8-C9-O7

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	512	GOL	1	0
4	A	503	PEG	1	0
3	D	513	GOL	1	0
7	D	527	PO4	1	0
3	D	511	GOL	1	0
3	C	508	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	444/472 (94%)	0.19	19 (4%)	35	45	19, 30, 63, 99	0
1	B	444/472 (94%)	0.42	31 (6%)	16	22	20, 34, 68, 93	0
1	C	456/472 (96%)	0.56	38 (8%)	11	15	13, 25, 71, 111	0
1	D	457/472 (96%)	0.35	26 (5%)	23	32	13, 24, 63, 100	0
2	E	84/90 (93%)	0.23	8 (9%)	8	12	22, 33, 57, 81	0
2	F	83/90 (92%)	0.36	8 (9%)	8	11	20, 28, 76, 102	0
2	G	83/90 (92%)	0.16	6 (7%)	15	21	19, 28, 54, 71	0
2	H	83/90 (92%)	0.35	6 (7%)	15	21	18, 25, 63, 98	0
All	All	2134/2248 (94%)	0.36	142 (6%)	17	24	13, 29, 67, 111	0

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	ILE	12.4
1	C	13	TRP	11.9
1	C	17	ILE	11.8
1	A	152	ASN	8.5
1	D	13	TRP	8.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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
3	GOL	D	507	6/6	0.38	0.28	57,61,63,64	0
3	GOL	E	103	6/6	0.62	0.23	56,58,60,60	0
5	PGE	A	505	10/10	0.64	0.19	53,65,67,68	0
5	PGE	C	527	10/10	0.64	0.23	44,51,58,58	0
3	GOL	C	511	6/6	0.67	0.17	60,62,63,64	0
5	PGE	C	524	10/10	0.68	0.21	53,66,70,71	0
5	PGE	E	106	10/10	0.68	0.18	63,66,68,69	0
5	PGE	E	107	10/10	0.68	0.20	56,63,65,66	0
3	GOL	C	520	6/6	0.69	0.33	46,49,51,52	0
3	GOL	D	504	6/6	0.69	0.23	55,60,61,62	0
3	GOL	C	517	6/6	0.69	0.25	58,65,68,69	0
3	GOL	C	519	6/6	0.69	0.32	54,56,58,58	0
3	GOL	G	104	6/6	0.69	0.16	49,54,56,57	0
8	TRP	D	528	15/15	0.69	0.25	55,57,61,63	0
3	GOL	C	518	6/6	0.71	0.21	53,53,55,55	0
3	GOL	D	508	6/6	0.71	0.24	49,56,57,61	0
3	GOL	G	105	6/6	0.71	0.20	53,58,59,59	0
3	GOL	F	101	6/6	0.72	0.20	48,51,52,52	0
9	PG4	B	512	13/13	0.72	0.15	50,57,60,61	0
3	GOL	F	106	6/6	0.73	0.21	45,47,48,49	0
3	GOL	C	505	6/6	0.73	0.27	43,49,50,52	0
3	GOL	C	508	6/6	0.75	0.17	46,51,53,54	0
4	PEG	D	516	7/7	0.75	0.17	46,52,58,59	0
3	GOL	D	511	6/6	0.75	0.31	50,51,55,55	0
9	PG4	C	529	13/13	0.75	0.21	48,53,61,62	0
3	GOL	B	506	6/6	0.76	0.30	60,65,66,66	0
5	PGE	D	520	10/10	0.76	0.24	43,51,53,54	0
3	GOL	H	101	6/6	0.76	0.23	50,54,56,57	0
4	PEG	D	515	7/7	0.76	0.17	41,42,45,45	0
3	GOL	C	510	6/6	0.76	0.43	58,60,65,66	0
3	GOL	G	103	6/6	0.76	0.22	57,61,62,65	0
3	GOL	C	507	6/6	0.76	0.21	39,45,49,50	0
3	GOL	H	105	6/6	0.77	0.24	54,56,58,59	0
5	PGE	G	110	10/10	0.77	0.20	45,65,69,70	0
3	GOL	F	105	6/6	0.77	0.24	50,53,53,54	0
3	GOL	B	509	6/6	0.77	0.41	59,64,66,67	0
3	GOL	B	502	6/6	0.77	0.20	51,56,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	G	106	6/6	0.78	0.33	67,68,68,68	0
5	PGE	F	109	10/10	0.78	0.17	56,61,64,65	0
3	GOL	D	512	6/6	0.78	0.37	51,56,59,59	0
8	TRP	A	509	15/15	0.78	0.26	58,61,64,67	0
4	PEG	D	517	7/7	0.78	0.18	52,56,58,59	0
5	PGE	D	521	10/10	0.78	0.16	51,54,57,58	0
3	GOL	C	513	6/6	0.78	0.17	54,58,58,59	0
3	GOL	E	102	6/6	0.79	0.26	48,54,57,58	0
3	GOL	B	507	6/6	0.79	0.25	50,51,52,55	0
3	GOL	E	104	6/6	0.79	0.19	50,52,53,53	0
5	PGE	E	105	10/10	0.79	0.27	58,64,65,66	0
3	GOL	H	103	6/6	0.79	0.18	46,53,54,55	0
3	GOL	D	510	6/6	0.79	0.30	47,49,55,58	0
3	GOL	B	505	6/6	0.80	0.30	54,54,56,58	0
4	PEG	C	523	7/7	0.80	0.23	46,49,50,51	0
4	PEG	D	514	7/7	0.80	0.16	47,49,50,51	0
3	GOL	G	101	6/6	0.80	0.27	40,45,45,47	0
4	PEG	G	109	7/7	0.81	0.21	49,53,57,57	0
3	GOL	C	515	6/6	0.81	0.17	57,62,63,63	0
3	GOL	B	503	6/6	0.81	0.17	44,50,55,59	0
3	GOL	C	504	6/6	0.81	0.14	56,57,58,60	0
4	PEG	F	107	7/7	0.81	0.21	42,48,50,51	0
9	PG4	D	524	13/13	0.81	0.18	51,52,60,63	0
4	PEG	C	521	7/7	0.82	0.28	34,41,46,47	0
4	PEG	G	107	7/7	0.82	0.14	41,45,49,51	0
5	PGE	C	526	10/10	0.82	0.21	39,47,50,51	0
3	GOL	D	505	6/6	0.82	0.18	38,41,43,43	0
3	GOL	C	503	6/6	0.83	0.18	55,56,57,59	0
5	PGE	C	525	10/10	0.83	0.16	42,49,55,56	0
3	GOL	B	504	6/6	0.84	0.22	57,62,64,65	0
3	GOL	B	510	6/6	0.84	0.15	55,60,63,65	0
4	PEG	G	108	7/7	0.84	0.14	49,51,53,54	0
8	TRP	B	515	15/15	0.84	0.18	62,64,65,65	0
8	TRP	C	532	15/15	0.84	0.20	47,51,54,55	0
3	GOL	C	502	6/6	0.84	0.20	36,39,40,42	0
3	GOL	B	501	6/6	0.84	0.21	45,49,50,50	0
3	GOL	H	104	6/6	0.84	0.20	31,37,37,39	0
9	PG4	D	522	13/13	0.84	0.20	28,35,56,56	0
9	PG4	D	523	13/13	0.84	0.17	57,62,67,67	0
3	GOL	C	516	6/6	0.84	0.23	50,55,56,57	0
3	GOL	A	501	6/6	0.85	0.21	48,49,56,59	0
4	PEG	A	504	7/7	0.85	0.30	52,53,59,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	501	6/6	0.85	0.15	35,37,39,41	0
3	GOL	D	513	6/6	0.86	0.14	36,41,42,44	0
5	PGE	C	528	10/10	0.86	0.21	43,47,48,48	0
3	GOL	H	102	6/6	0.86	0.13	38,42,43,47	0
3	GOL	A	502	6/6	0.86	0.21	44,48,48,49	0
3	GOL	C	514	6/6	0.86	0.23	41,43,43,46	0
3	GOL	C	512	6/6	0.86	0.27	57,61,63,65	0
3	GOL	D	506	6/6	0.87	0.22	41,45,47,48	0
4	PEG	D	518	7/7	0.87	0.17	47,51,53,53	0
5	PGE	F	108	10/10	0.88	0.17	43,50,56,58	0
3	GOL	F	103	6/6	0.88	0.16	47,48,51,53	0
3	GOL	F	104	6/6	0.89	0.16	32,37,39,45	0
4	PEG	B	511	7/7	0.89	0.20	40,40,44,44	0
3	GOL	D	503	6/6	0.89	0.15	42,45,46,47	0
3	GOL	G	102	6/6	0.89	0.19	31,34,35,36	0
7	PO4	D	527	5/5	0.90	0.12	52,56,59,61	0
4	PEG	C	522	7/7	0.90	0.18	39,43,46,49	0
4	PEG	D	519	7/7	0.90	0.14	44,47,47,48	0
3	GOL	C	509	6/6	0.90	0.26	54,56,57,58	0
3	GOL	D	502	6/6	0.90	0.17	38,42,44,46	0
3	GOL	B	508	6/6	0.91	0.33	47,51,51,52	0
3	GOL	E	101	6/6	0.91	0.29	53,55,56,57	0
3	GOL	F	102	6/6	0.92	0.15	35,36,38,38	0
10	TSA	G	111	16/16	0.92	0.14	27,28,29,29	0
3	GOL	C	506	6/6	0.93	0.11	57,59,64,71	0
3	GOL	D	509	6/6	0.93	0.23	43,47,49,50	0
3	GOL	D	501	6/6	0.93	0.10	34,37,39,41	0
10	TSA	E	108	16/16	0.93	0.10	31,33,34,35	0
4	PEG	A	503	7/7	0.93	0.17	33,36,42,42	0
10	TSA	F	110	16/16	0.96	0.10	16,18,23,24	0
7	PO4	A	508	5/5	0.96	0.13	68,68,70,72	0
10	TSA	H	106	16/16	0.96	0.10	15,17,22,23	0
6	MN	A	506	1/1	0.98	0.05	40,40,40,40	0
7	PO4	B	514	5/5	0.98	0.08	33,34,35,35	0
6	MN	B	513	1/1	0.99	0.06	40,40,40,40	0
6	MN	C	530	1/1	0.99	0.09	29,29,29,29	0
7	PO4	C	531	5/5	0.99	0.10	28,29,30,30	0
7	PO4	D	526	5/5	0.99	0.09	26,27,28,28	0
6	MN	D	525	1/1	0.99	0.09	27,27,27,27	0
7	PO4	A	507	5/5	0.99	0.08	31,32,33,34	0

6.5 Other polymers (i)

There are no such residues in this entry.