



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 08:43 pm BST

PDB ID : 1KFL
Title : Crystal structure of phenylalanine-regulated 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase (DAHP synthase) from E.coli complexed with Mn²⁺, PEP, and Phe
Authors : Shumilin, I.A.; Zhao, C.; Bauerle, R.; Kretsinger, R.H.
Deposited on : 2001-11-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

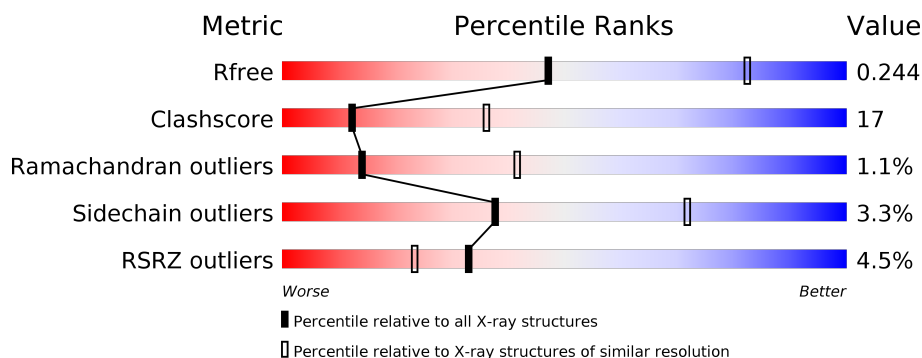
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	350	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>.</div> </div> </div>
1	B	350	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>31%</div> <div>.</div> </div> </div>
1	C	350	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div>.</div> </div> </div>
1	D	350	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>35%</div> <div>.</div> </div> </div>
1	E	350	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>33%</div> <div>..</div> </div> </div>
1	F	350	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	350	<div><div></div><div>4%</div><div>67%</div><div>32%</div><div></div></div>
1	H	350	<div><div></div><div>8%</div><div>67%</div><div>32%</div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21675 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 synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	Se	0	0	0
			2667	1672	474	506	7	8			
1	B	350	Total	C	N	O	S	Se	0	0	0
			2667	1672	474	506	7	8			
1	C	350	Total	C	N	O	S	Se	18	1	0
			2678	1678	478	507	7	8			
1	D	350	Total	C	N	O	S	Se	13	4	0
			2699	1691	481	512	7	8			
1	E	350	Total	C	N	O	S	Se	28	0	0
			2667	1672	474	506	7	8			
1	F	350	Total	C	N	O	S	Se	24	0	0
			2667	1672	474	506	7	8			
1	G	350	Total	C	N	O	S	Se	39	0	0
			2667	1672	474	506	7	8			
1	H	350	Total	C	N	O	S	Se	26	4	0
			2699	1691	481	512	7	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	CLONING ARTIFACT	UNP P00886
A	91	MSE	MET	CLONING ARTIFACT	UNP P00886
A	113	MSE	MET	CLONING ARTIFACT	UNP P00886
A	147	MSE	MET	CLONING ARTIFACT	UNP P00886
A	157	MSE	MET	CLONING ARTIFACT	UNP P00886
A	263	MSE	MET	CLONING ARTIFACT	UNP P00886
A	279	MSE	MET	CLONING ARTIFACT	UNP P00886
A	300	MSE	MET	CLONING ARTIFACT	UNP P00886
B	1	MSE	MET	CLONING ARTIFACT	UNP P00886
B	91	MSE	MET	CLONING ARTIFACT	UNP P00886
B	113	MSE	MET	CLONING ARTIFACT	UNP P00886
B	147	MSE	MET	CLONING ARTIFACT	UNP P00886
B	157	MSE	MET	CLONING ARTIFACT	UNP P00886

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	263	MSE	MET	CLONING ARTIFACT	UNP P00886
B	279	MSE	MET	CLONING ARTIFACT	UNP P00886
B	300	MSE	MET	CLONING ARTIFACT	UNP P00886
C	1	MSE	MET	CLONING ARTIFACT	UNP P00886
C	91	MSE	MET	CLONING ARTIFACT	UNP P00886
C	113	MSE	MET	CLONING ARTIFACT	UNP P00886
C	147	MSE	MET	CLONING ARTIFACT	UNP P00886
C	157	MSE	MET	CLONING ARTIFACT	UNP P00886
C	263	MSE	MET	CLONING ARTIFACT	UNP P00886
C	279	MSE	MET	CLONING ARTIFACT	UNP P00886
C	300	MSE	MET	CLONING ARTIFACT	UNP P00886
D	1	MSE	MET	CLONING ARTIFACT	UNP P00886
D	91	MSE	MET	CLONING ARTIFACT	UNP P00886
D	113	MSE	MET	CLONING ARTIFACT	UNP P00886
D	147	MSE	MET	CLONING ARTIFACT	UNP P00886
D	157	MSE	MET	CLONING ARTIFACT	UNP P00886
D	263	MSE	MET	CLONING ARTIFACT	UNP P00886
D	279	MSE	MET	CLONING ARTIFACT	UNP P00886
D	300	MSE	MET	CLONING ARTIFACT	UNP P00886
E	1	MSE	MET	CLONING ARTIFACT	UNP P00886
E	91	MSE	MET	CLONING ARTIFACT	UNP P00886
E	113	MSE	MET	CLONING ARTIFACT	UNP P00886
E	147	MSE	MET	CLONING ARTIFACT	UNP P00886
E	157	MSE	MET	CLONING ARTIFACT	UNP P00886
E	263	MSE	MET	CLONING ARTIFACT	UNP P00886
E	279	MSE	MET	CLONING ARTIFACT	UNP P00886
E	300	MSE	MET	CLONING ARTIFACT	UNP P00886
F	1	MSE	MET	CLONING ARTIFACT	UNP P00886
F	91	MSE	MET	CLONING ARTIFACT	UNP P00886
F	113	MSE	MET	CLONING ARTIFACT	UNP P00886
F	147	MSE	MET	CLONING ARTIFACT	UNP P00886
F	157	MSE	MET	CLONING ARTIFACT	UNP P00886
F	263	MSE	MET	CLONING ARTIFACT	UNP P00886
F	279	MSE	MET	CLONING ARTIFACT	UNP P00886
F	300	MSE	MET	CLONING ARTIFACT	UNP P00886
G	1	MSE	MET	CLONING ARTIFACT	UNP P00886
G	91	MSE	MET	CLONING ARTIFACT	UNP P00886
G	113	MSE	MET	CLONING ARTIFACT	UNP P00886
G	147	MSE	MET	CLONING ARTIFACT	UNP P00886
G	157	MSE	MET	CLONING ARTIFACT	UNP P00886
G	263	MSE	MET	CLONING ARTIFACT	UNP P00886
G	279	MSE	MET	CLONING ARTIFACT	UNP P00886

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	300	MSE	MET	CLONING ARTIFACT	UNP P00886
H	1	MSE	MET	CLONING ARTIFACT	UNP P00886
H	91	MSE	MET	CLONING ARTIFACT	UNP P00886
H	113	MSE	MET	CLONING ARTIFACT	UNP P00886
H	147	MSE	MET	CLONING ARTIFACT	UNP P00886
H	157	MSE	MET	CLONING ARTIFACT	UNP P00886
H	263	MSE	MET	CLONING ARTIFACT	UNP P00886
H	279	MSE	MET	CLONING ARTIFACT	UNP P00886
H	300	MSE	MET	CLONING ARTIFACT	UNP P00886

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



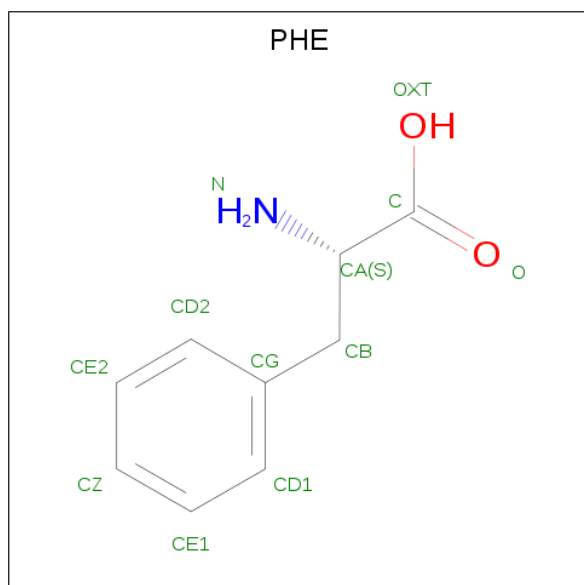
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total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

Continued on next page...

Continued from previous page...

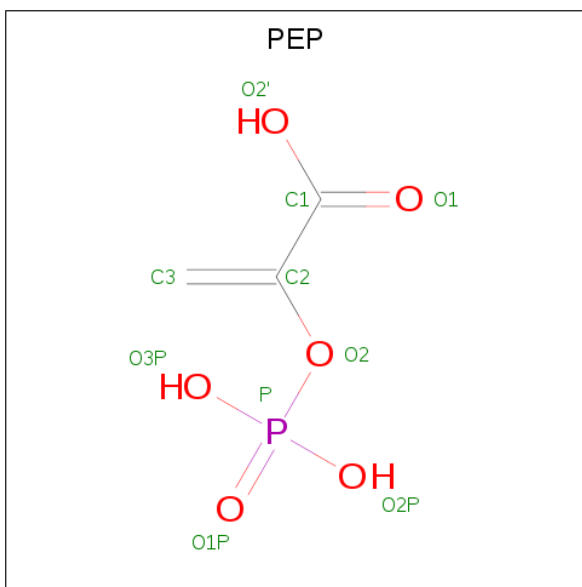
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		
4	B	1	Total	C	N	O	0	0
			12	9	1	2		
4	C	1	Total	C	N	O	0	0
			12	9	1	2		
4	D	1	Total	C	N	O	0	0
			12	9	1	2		
4	E	1	Total	C	N	O	0	0
			12	9	1	2		
4	F	1	Total	C	N	O	0	0
			12	9	1	2		
4	G	1	Total	C	N	O	0	0
			12	9	1	2		
4	H	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).

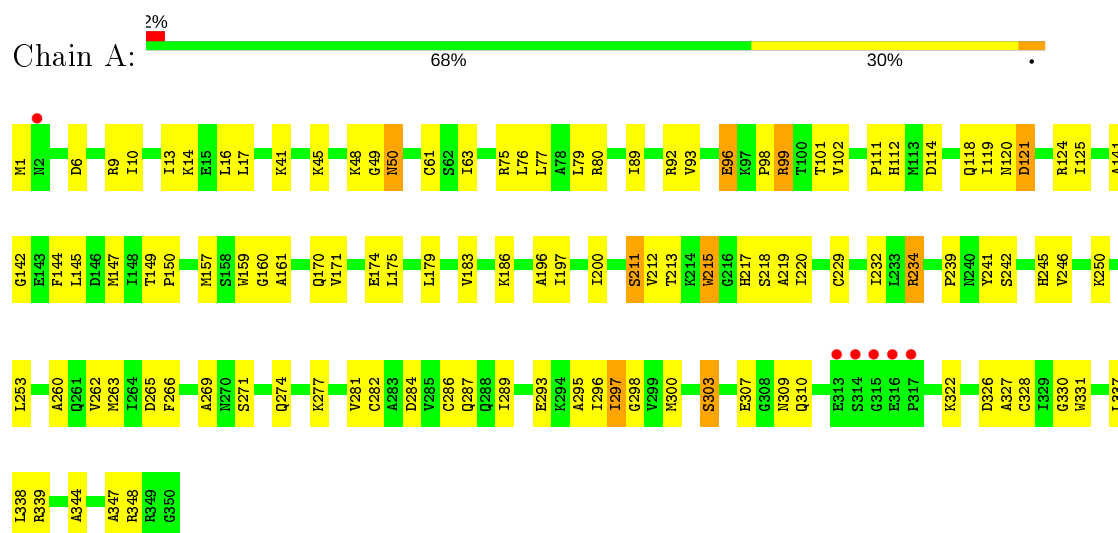


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			10	3	6	1		
5	B	1	Total	C	O	P	0	0
			10	3	6	1		
5	C	1	Total	C	O	P	0	0
			10	3	6	1		
5	D	1	Total	C	O	P	0	0
			10	3	6	1		
5	E	1	Total	C	O	P	0	0
			10	3	6	1		
5	F	1	Total	C	O	P	0	0
			10	3	6	1		
5	G	1	Total	C	O	P	0	0
			10	3	6	1		
5	H	1	Total	C	O	P	0	0
			10	3	6	1		

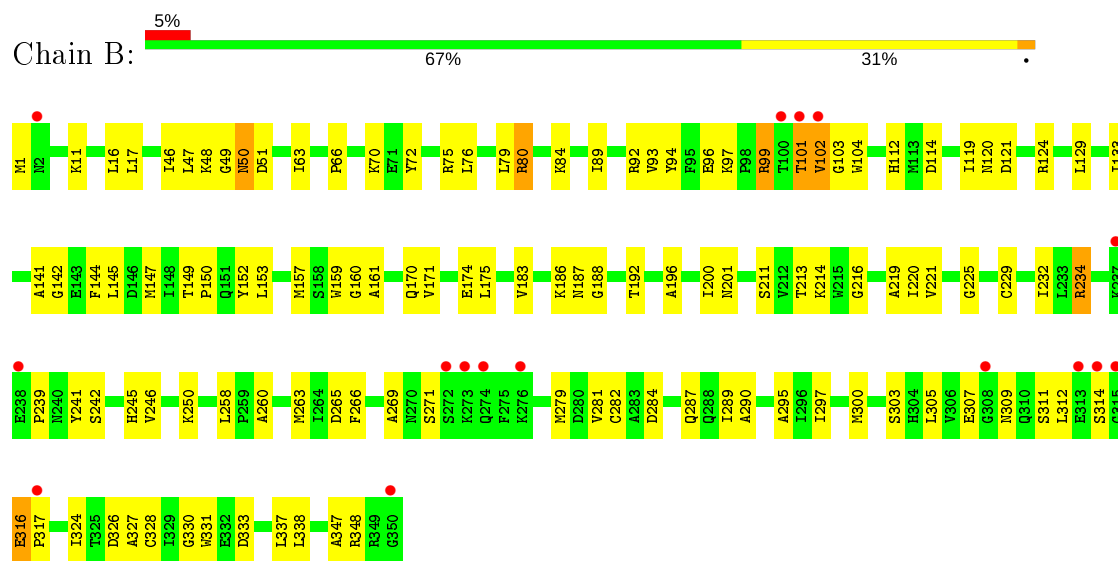
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 synthase

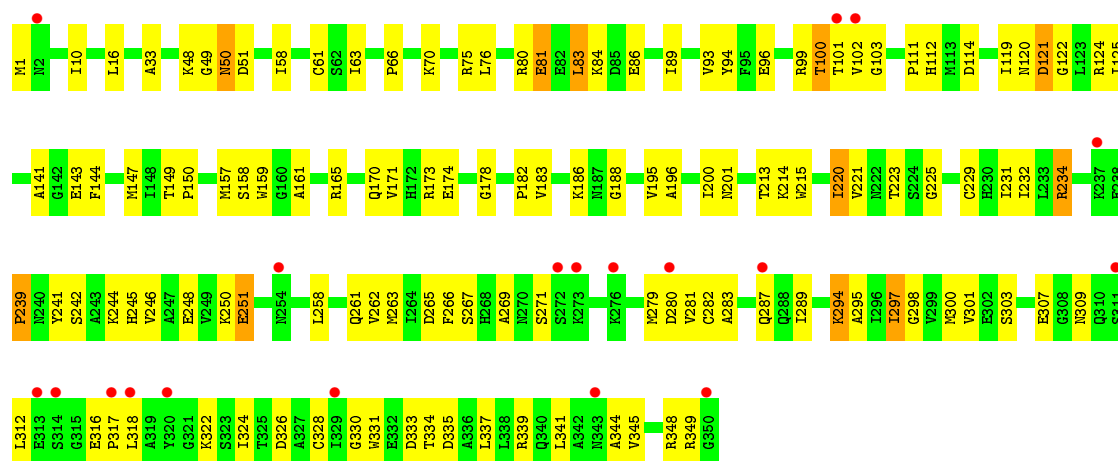


- Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

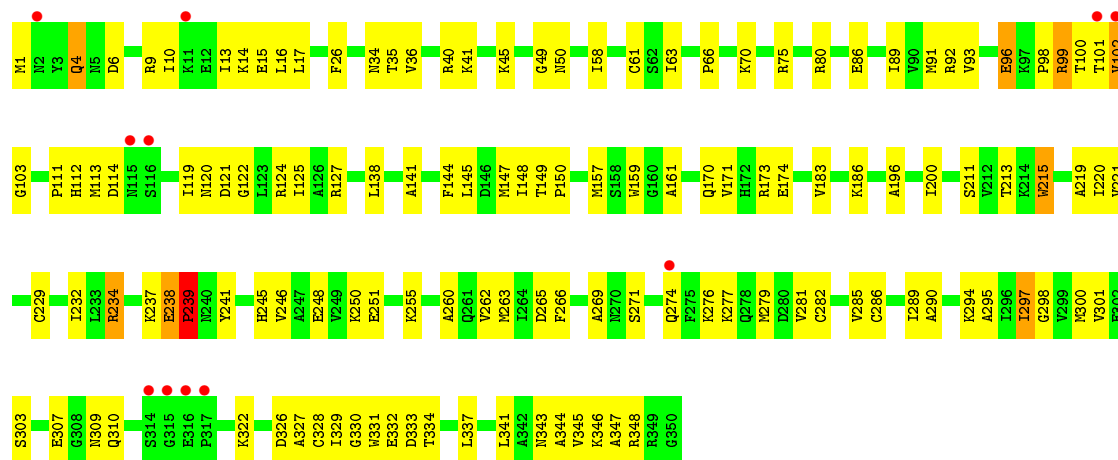


- Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

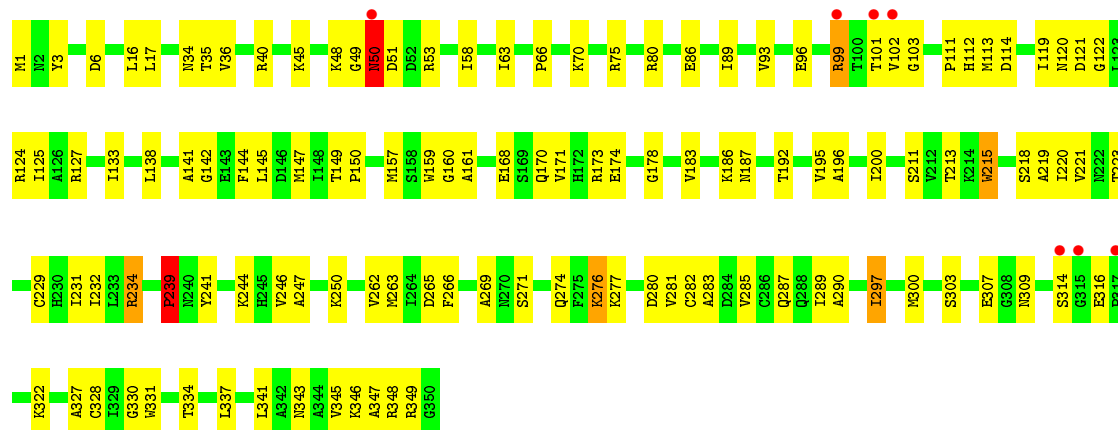




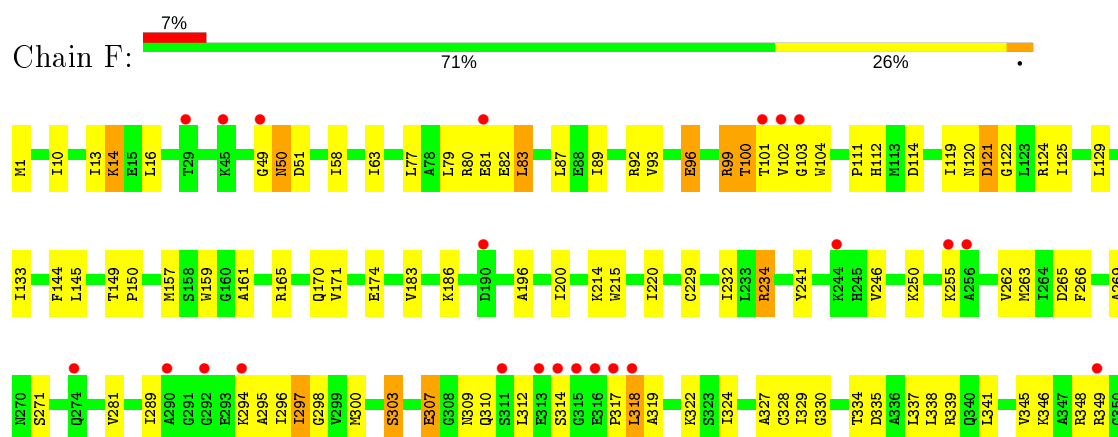
• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase



• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase



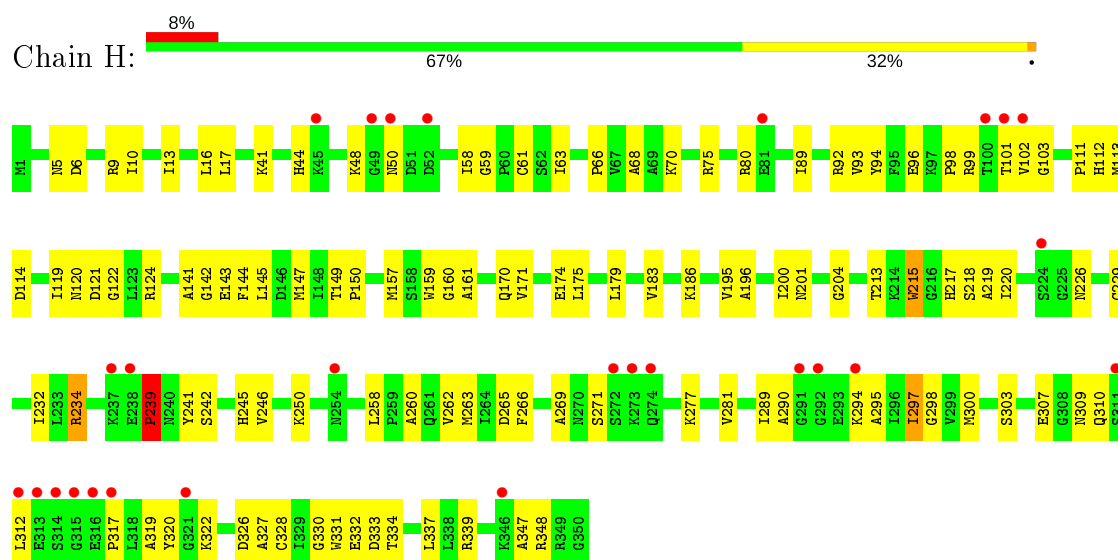
• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase



• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase



• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	290.10 Å 90.10 Å 155.80 Å 90.00° 120.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.80) 99.3 (20.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.79 Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.218 , 0.246 0.215 , 0.244	Depositor DCC
R_{free} test set	5052 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21675	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, PEP, 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	0.44	0/2706	0.67	0/3647
1	B	0.44	0/2706	0.66	0/3647
1	C	0.39	0/2717	0.63	0/3661
1	D	0.43	0/2738	0.64	0/3691
1	E	0.37	0/2706	0.62	0/3647
1	F	0.37	0/2706	0.62	0/3647
1	G	0.36	0/2706	0.60	0/3647
1	H	0.34	0/2738	0.58	0/3691
All	All	0.39	0/21723	0.63	0/29278

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2667	0	2684	107	0
1	B	2667	0	2684	104	0
1	C	2678	0	2696	121	0
1	D	2699	0	2718	128	0
1	E	2667	0	2684	94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2667	0	2684	84	0
1	G	2667	0	2685	83	0
1	H	2699	0	2718	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	5	0	0	0	0
3	H	15	0	0	0	0
4	A	12	0	8	0	0
4	B	12	0	8	0	0
4	C	12	0	8	0	0
4	D	12	0	8	0	0
4	E	12	0	8	0	0
4	F	12	0	8	0	0
4	G	12	0	8	0	0
4	H	12	0	8	0	0
5	A	10	0	2	0	0
5	B	10	0	2	1	0
5	C	10	0	2	1	0
5	D	10	0	2	1	0
5	E	10	0	2	1	0
5	F	10	0	2	1	0
5	G	10	0	2	0	0
5	H	10	0	2	0	0
All	All	21675	0	21633	727	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 17.

The worst 5 of 727 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:C:100:THR:HG23	1:C:165[A]:ARG:HH12	1.07	1.08
1:C:294:LYS:HD3	1:C:294:LYS:H	1.16	1.07
1:B:50:ASN:HD22	1:B:50:ASN:N	1.62	0.98
1:F:102:VAL:HG12	1:F:103:GLY:H	1.31	0.94
1:C:102:VAL:HG12	1:C:103:GLY:H	1.30	0.94

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	348/350 (99%)	322 (92%)	25 (7%)	1 (0%)	41	72
1	B	348/350 (99%)	326 (94%)	17 (5%)	5 (1%)	11	34
1	C	349/350 (100%)	323 (93%)	22 (6%)	4 (1%)	14	41
1	D	352/350 (101%)	323 (92%)	24 (7%)	5 (1%)	11	34
1	E	348/350 (99%)	323 (93%)	19 (6%)	6 (2%)	9	29
1	F	348/350 (99%)	318 (91%)	25 (7%)	5 (1%)	11	34
1	G	348/350 (99%)	327 (94%)	19 (6%)	2 (1%)	25	56
1	H	352/350 (101%)	319 (91%)	29 (8%)	4 (1%)	14	41
All	All	2793/2800 (100%)	2581 (92%)	180 (6%)	32 (1%)	14	41

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	50	ASN
1	F	318	LEU
1	H	101[A]	THR
1	H	101[B]	THR
1	C	50	ASN

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	283/275 (103%)	274 (97%)	9 (3%)	39	73
1	B	283/275 (103%)	276 (98%)	7 (2%)	47	80
1	C	284/275 (103%)	273 (96%)	11 (4%)	32	66
1	D	287/275 (104%)	277 (96%)	10 (4%)	36	70
1	E	283/275 (103%)	270 (95%)	13 (5%)	27	60
1	F	283/275 (103%)	273 (96%)	10 (4%)	36	70
1	G	283/275 (103%)	277 (98%)	6 (2%)	53	84
1	H	287/275 (104%)	279 (97%)	8 (3%)	43	77
All	All	2273/2200 (103%)	2199 (97%)	74 (3%)	38	72

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	234	ARG
1	E	121	ASP
1	H	121	ASP
1	D	238	GLU
1	E	45	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	254	ASN
1	E	254	ASN
1	H	240	ASN
1	D	261	GLN
1	E	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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
3	SO4	E	5355	-	4,4,4	0.28	0	6,6,6	0.10	0
5	PEP	A	1352	-	6,9,9	1.28	1 (16%)	8,13,13	2.24	3 (37%)
3	SO4	H	7355	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	A	1355	-	4,4,4	0.40	0	6,6,6	0.30	0
3	SO4	D	4355	-	4,4,4	0.30	0	6,6,6	0.20	0
3	SO4	F	6356	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	F	6355	-	4,4,4	0.30	0	6,6,6	0.15	0
5	PEP	H	8352	-	6,9,9	1.28	1 (16%)	8,13,13	2.27	3 (37%)
3	SO4	H	8356	-	4,4,4	0.26	0	6,6,6	0.15	0
5	PEP	F	6352	-	6,9,9	1.40	1 (16%)	8,13,13	2.38	3 (37%)
3	SO4	D	4356	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	C	3356	-	4,4,4	0.28	0	6,6,6	0.25	0
5	PEP	B	2352	-	6,9,9	1.32	0	8,13,13	2.22	3 (37%)
3	SO4	G	7356	-	4,4,4	0.27	0	6,6,6	0.14	0
3	SO4	E	5356	-	4,4,4	0.27	0	6,6,6	0.13	0
3	SO4	B	2355	-	4,4,4	0.26	0	6,6,6	0.22	0
5	PEP	G	7352	-	6,9,9	1.33	1 (16%)	8,13,13	2.33	3 (37%)
3	SO4	H	8355	-	4,4,4	0.36	0	6,6,6	0.14	0
3	SO4	C	3355	-	4,4,4	0.33	0	6,6,6	0.20	0
5	PEP	C	3352	-	6,9,9	1.23	1 (16%)	8,13,13	2.28	3 (37%)
5	PEP	D	4352	-	6,9,9	1.37	1 (16%)	8,13,13	2.31	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEP	E	5352	-	6,9,9	1.43	1 (16%)	8,13,13	2.34	3 (37%)
3	SO4	A	1356	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	B	2356	-	4,4,4	0.29	0	6,6,6	0.24	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	PEP	B	2352	-	-	2/5/9/9	-
5	PEP	C	3352	-	-	2/5/9/9	-
5	PEP	F	6352	-	-	2/5/9/9	-
5	PEP	A	1352	-	-	0/5/9/9	-
5	PEP	G	7352	-	-	2/5/9/9	-
5	PEP	D	4352	-	-	2/5/9/9	-
5	PEP	E	5352	-	-	2/5/9/9	-
5	PEP	H	8352	-	-	2/5/9/9	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	6352	PEP	C3-C2	2.25	1.37	1.33
5	G	7352	PEP	C3-C2	2.13	1.37	1.33
5	E	5352	PEP	C3-C2	2.13	1.37	1.33
5	D	4352	PEP	C3-C2	2.07	1.37	1.33
5	C	3352	PEP	C3-C2	2.03	1.36	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1352	PEP	C1-C2-C3	4.40	129.28	121.07
5	D	4352	PEP	C1-C2-C3	4.32	129.14	121.07
5	E	5352	PEP	C1-C2-C3	4.32	129.14	121.07
5	G	7352	PEP	C1-C2-C3	4.29	129.08	121.07
5	F	6352	PEP	C1-C2-C3	4.26	129.03	121.07

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	6352	PEP	C2-O2-P-O1P
5	D	4352	PEP	C2-O2-P-O1P
5	B	2352	PEP	C2-O2-P-O1P
5	G	7352	PEP	C2-O2-P-O1P
5	C	3352	PEP	C2-O2-P-O1P

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	6352	PEP	1	0
5	B	2352	PEP	1	0
5	C	3352	PEP	1	0
5	D	4352	PEP	1	0
5	E	5352	PEP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	342/350 (97%)	-0.55	6 (1%) 68 61	8, 29, 55, 111	0
1	B	342/350 (97%)	-0.28	16 (4%) 31 22	11, 37, 79, 104	0
1	C	342/350 (97%)	0.04	19 (5%) 24 16	14, 55, 92, 118	4 (1%)
1	D	342/350 (97%)	-0.34	11 (3%) 47 37	10, 40, 79, 118	3 (0%)
1	E	341/350 (97%)	-0.15	7 (2%) 63 54	27, 50, 78, 132	5 (1%)
1	F	341/350 (97%)	0.03	23 (6%) 17 10	20, 57, 90, 126	5 (1%)
1	G	341/350 (97%)	-0.04	13 (3%) 40 30	27, 57, 91, 127	6 (1%)
1	H	341/350 (97%)	0.13	27 (7%) 12 7	23, 65, 91, 125	5 (1%)
All	All	2732/2800 (97%)	-0.15	122 (4%) 33 23	8, 50, 88, 132	28 (1%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	350	GLY	12.0
1	G	314	SER	7.0
1	G	101	THR	7.0
1	B	350	GLY	7.0
1	C	350	GLY	6.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	H	8356	5/5	0.88	0.19	102,102,110,113	0
3	SO4	F	6356	5/5	0.90	0.21	82,93,94,107	0
3	SO4	C	3356	5/5	0.90	0.26	75,77,85,97	0
5	PEP	B	2352	10/10	0.90	0.21	55,71,80,81	0
5	PEP	C	3352	10/10	0.90	0.20	68,88,102,106	0
3	SO4	E	5356	5/5	0.91	0.17	68,74,78,88	0
3	SO4	E	5355	5/5	0.92	0.19	74,81,82,86	0
3	SO4	G	7356	5/5	0.93	0.26	87,88,90,103	0
4	PHE	H	8354	12/12	0.93	0.21	44,54,72,80	0
5	PEP	H	8352	10/10	0.93	0.21	84,94,97,99	0
5	PEP	G	7352	10/10	0.93	0.18	85,93,99,100	0
5	PEP	F	6352	10/10	0.93	0.20	54,76,91,103	0
4	PHE	F	6354	12/12	0.94	0.18	28,36,41,47	0
2	MN	G	7351	1/1	0.94	0.07	77,77,77,77	0
5	PEP	E	5352	10/10	0.94	0.18	71,76,77,85	0
3	SO4	B	2356	5/5	0.95	0.16	62,69,73,88	0
4	PHE	G	7354	12/12	0.95	0.15	19,25,48,49	0
3	SO4	D	4355	5/5	0.96	0.14	60,65,77,80	0
3	SO4	H	8355	5/5	0.96	0.17	49,62,73,74	0
3	SO4	A	1355	5/5	0.96	0.17	42,56,59,68	0
3	SO4	D	4356	5/5	0.96	0.16	60,65,75,90	0
4	PHE	E	5354	12/12	0.96	0.15	25,39,50,54	0
2	MN	H	8351	1/1	0.96	0.04	68,68,68,68	0
5	PEP	D	4352	10/10	0.96	0.14	56,69,77,78	0
5	PEP	A	1352	10/10	0.97	0.14	29,47,60,69	0
2	MN	E	5351	1/1	0.97	0.03	64,64,64,64	0
2	MN	C	3351	1/1	0.97	0.04	71,71,71,71	0
2	MN	F	6351	1/1	0.97	0.04	61,61,61,61	0
3	SO4	H	7355	5/5	0.97	0.19	85,95,98,99	0
3	SO4	A	1356	5/5	0.97	0.13	60,63,70,79	0
4	PHE	A	1354	12/12	0.97	0.13	1,15,32,33	0
4	PHE	B	2354	12/12	0.97	0.16	7,16,34,39	0
4	PHE	C	3354	12/12	0.98	0.12	15,26,37,51	0
2	MN	A	1351	1/1	0.98	0.06	33,33,33,33	0
2	MN	B	2351	1/1	0.98	0.07	57,57,57,57	0
4	PHE	D	4354	12/12	0.98	0.14	11,24,34,36	0
3	SO4	F	6355	5/5	0.98	0.11	63,66,71,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	D	4351	1/1	0.98	0.03	47,47,47,47	0
3	SO4	C	3355	5/5	0.99	0.09	26,33,44,46	0
3	SO4	B	2355	5/5	1.00	0.09	25,34,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.