WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 01:15 AM EST

PDB ID	:	1QR7
Title	:	CRYSTAL STRUCTURE OF PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE FROM ESCHERICHIA COLI COMPLEXED WITH PB2+ AND PEP
Authors	:	Shumilin, I.A.; Kretsinger, R.H.; Bauerle, R.H.
Deposited on	:	1999-06-18
Resolution	:	2.60 Å(reported)

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

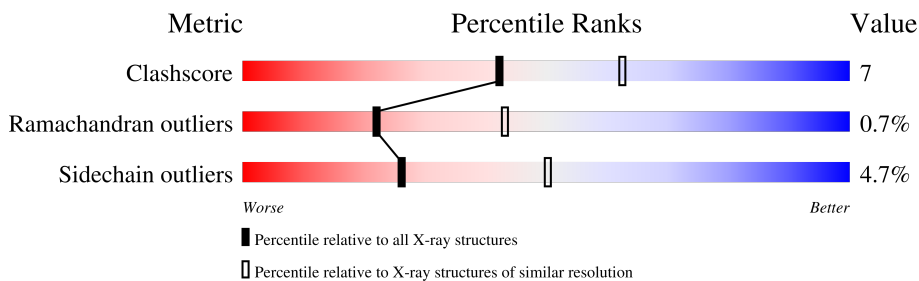|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et 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 2.60 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.7%
Sidechain outliers		4.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	350	75% 19% · ·
1	B	350	73% 20% · ·
1	C	350	75% 18% · ·
1	D	350	74% 19% · ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10359 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 PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO -HEPTULOSONATE-7-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2571	1617	459	481	14			
1	B	338	Total	C	N	O	S	0	0	0
			2571	1617	459	481	14			
1	C	338	Total	C	N	O	S	0	0	0
			2571	1617	459	481	14			
1	D	339	Total	C	N	O	S	0	0	0
			2578	1622	460	482	14			

- Molecule 2 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Pb	0	0
			1	1		
2	B	1	Total	Pb	0	0
			1	1		
2	C	1	Total	Pb	0	0
			1	1		
2	D	1	Total	Pb	0	0
			1	1		

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

SO4

O1

O3   O⁻ — S — O⁻ O4

S

O2

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

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).

PEP

O2'
HO

C1   O   O1

C3   C2

O3P

HO   P

P

OH
O2P

O

O1P
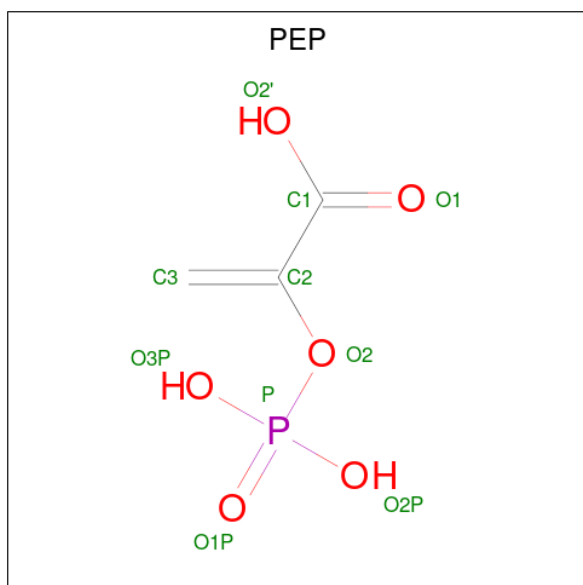
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 10	C 3	O 6	P 1	0	0
4	B	1	Total 10	C 3	O 6	P 1	0	0
4	C	1	Total 10	C 3	O 6	P 1	0	0
4	D	1	Total 10	C 3	O 6	P 1	0	0

• Molecule 5 is water.

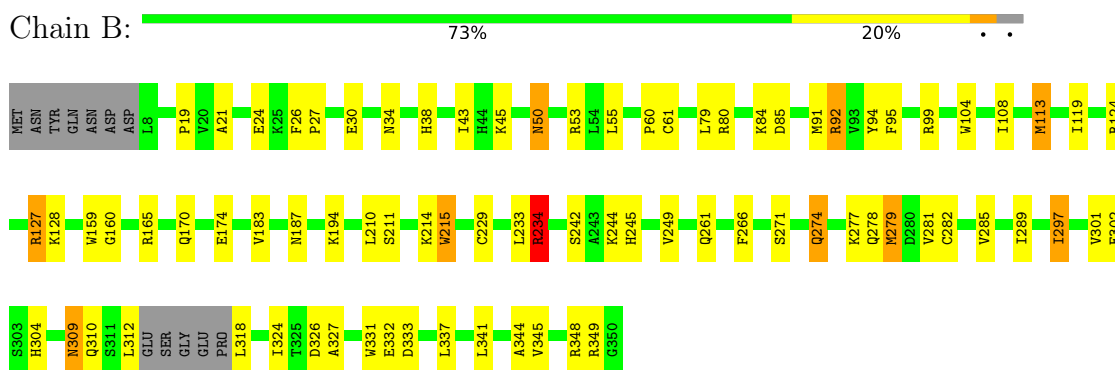| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	1	Total 1	O 1	0	0

3   Residue-property plots ⓘ

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

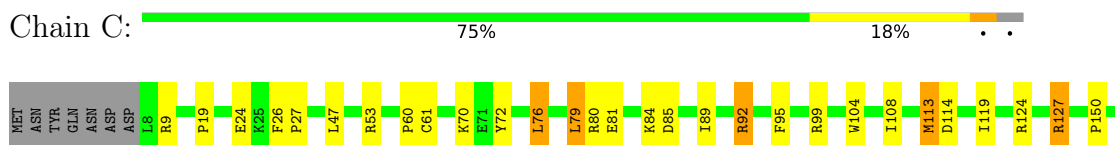Note EDS was not executed.

• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE
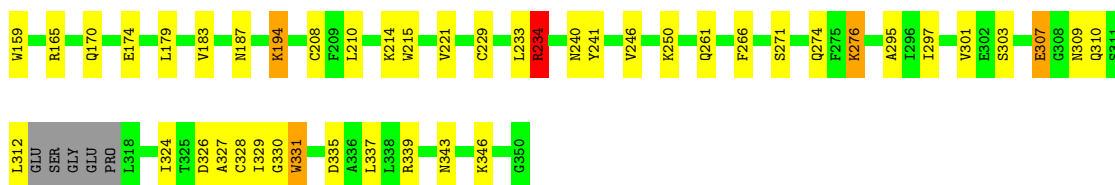
Chain A:

• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

Chain B:

• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

Chain C:

W159 R165 Q170 E174 L179 V183 N187 K194 C208 F209 L210 K214 W215 V221 C229 L233 R234 N240 Y241 V246 K250 Q261 F266 S271 Q274 F275 K276 A295 I296 I297 V301 E302 S303 E307 G308 N309 Q310 S311

L312 GLU SER GLY GLU PRO L318 I324 T325 D326 A327 C328 I329 G330 W331 D335 A336 L337 L338 R339 N343 K346 G350

• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE

Chain D:

74%   19%

MET ASN TYR GLN ASN ASP ASP L8 R9 E15 P19 V20 A21 F26 L47 R53 V57 P60 C61 R75 L76 R80 L83 K84 D85 I89 R92 V93 Y94 F95 W104 I108 H112 M113 D114 I119 R124 R127 P150 W159

G160 R165 Q170 V171 H172 R173 E174 V183 N187 K194 L210 K214 W215 C229 L233 R234 S242 A243 K244 H245 V246 K250 N254 Q261 F266 S271 Q274 F275 K276 D284 Q287 K294 I297 M300 V301 E302 S303 H304

E307 Q310 S311 L312 GLU SER GLY GLU P317 L318 A319 Y320 S323 I324 T325 D326 A327 C328 I329 G330 W331 E332 L337 N343 K346 R349 G350

4   Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.73Å 51.33Å 148.10Å 90.00° 116.43° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10359	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PEP, PB

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	0.80	0/2614	1.44	32/3532 (0.9%)
1	B	0.80	0/2614	1.45	26/3532 (0.7%)
1	C	0.82	0/2614	1.39	23/3532 (0.7%)
1	D	0.81	0/2622	1.40	32/3543 (0.9%)
All	All	0.81	0/10464	1.42	113/14139 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	92	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	B	127	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	B	92	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	C	92	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	C	127	ARG	NE-CZ-NH1	10.24	125.42	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	TYR	Sidechain

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	2571	0	2608	34	0
1	B	2571	0	2608	44	0
1	C	2571	0	2608	39	0
1	D	2578	0	2616	36	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
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	10	0	2	0	0
4	B	10	0	2	0	0
4	C	10	0	2	0	0
4	D	10	0	2	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	10359	0	10448	144	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 7.

The worst 5 of 144 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:276:LYS:HD3	1:C:276:LYS:H	1.56	0.71
1:B:278:GLN:HE22	1:B:302:GLU:H	1.40	0.68
1:A:194:LYS:HD2	1:A:194:LYS:H	1.60	0.67
1:A:276:LYS:HD3	1:A:276:LYS:H	1.60	0.67
1:B:312:LEU:HD11	1:B:324:ILE:HD12	1.76	0.66

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	334/350 (95%)	314 (94%)	17 (5%)	3 (1%)	17	35
1	B	334/350 (95%)	314 (94%)	17 (5%)	3 (1%)	17	35
1	C	334/350 (95%)	315 (94%)	17 (5%)	2 (1%)	25	47
1	D	335/350 (96%)	315 (94%)	18 (5%)	2 (1%)	25	47
All	All	1337/1400 (96%)	1258 (94%)	69 (5%)	10 (1%)	22	43

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	MET
1	A	320	TYR
1	B	50	ASN
1	B	113	MET
1	C	113	MET

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	272/283 (96%)	262 (96%)	10 (4%)	34	60
1	B	272/283 (96%)	259 (95%)	13 (5%)	25	49
1	C	272/283 (96%)	261 (96%)	11 (4%)	31	57
1	D	273/283 (96%)	256 (94%)	17 (6%)	18	37
All	All	1089/1132 (96%)	1038 (95%)	51 (5%)	26	50

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	150	PRO
1	D	75	ARG
1	D	332	GLU
1	C	234	ARG
1	C	297	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	278	GLN
1	C	170	GLN
1	D	187	ASN
1	D	38	HIS
1	D	170	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	PEP	B	2352	-	9,9,9	1.70	2 (22%)	11,13,13	3.20	5 (45%)
4	PEP	C	3352	-	9,9,9	1.82	3 (33%)	11,13,13	3.15	5 (45%)
3	SO4	A	1353	-	4,4,4	0.10	0	6,6,6	0.41	0
4	PEP	A	1352	-	9,9,9	2.03	3 (33%)	11,13,13	2.97	5 (45%)
4	PEP	D	4352	-	9,9,9	1.99	3 (33%)	11,13,13	3.08	5 (45%)
3	SO4	C	3353	-	4,4,4	0.07	0	6,6,6	0.87	0
3	SO4	B	2353	-	4,4,4	0.28	0	6,6,6	0.47	0
3	SO4	D	4353	-	4,4,4	0.25	0	6,6,6	0.61	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	PEP	A	1352	-	-	1/9/9/9	-
4	PEP	D	4352	-	-	0/9/9/9	-
4	PEP	C	3352	-	-	1/9/9/9	-
4	PEP	B	2352	-	-	0/9/9/9	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3352	PEP	O2'-C1	-3.36	1.20	1.30
4	D	4352	PEP	O2'-C1	-3.22	1.21	1.30
4	A	1352	PEP	C2-C1	3.10	1.52	1.49
4	D	4352	PEP	C2-C1	3.03	1.52	1.49
4	A	1352	PEP	O2'-C1	-3.02	1.21	1.30

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3352	PEP	O2'-C1-C2	5.96	124.07	113.91
4	B	2352	PEP	O2'-C1-C2	5.94	124.05	113.91
4	B	2352	PEP	O1-C1-C2	-5.93	112.85	121.79
4	D	4352	PEP	O2'-C1-C2	5.66	123.56	113.91
4	C	3352	PEP	O1-C1-C2	-5.54	113.44	121.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1352	PEP	C2-O2-P-O3P
4	C	3352	PEP	C2-O2-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.