W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 12:59 PM EDT

PDB ID	:	1F7T
Title	:	HOLO-(ACYL CARRIER PROTEIN) SYNTHASE AT 1.8A
Authors	:	Parris, K.D.; Lin, L.; Tam, A.; Mathew, R.; Hixon, J.; Stahl, M.; Fritz, C.C.; Seehra, J.; Somers, W.S.
Deposited on	:	2000-06-27
Resolution	:	1.80 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 (i) symbol.

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)	:	2.23.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.80 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.
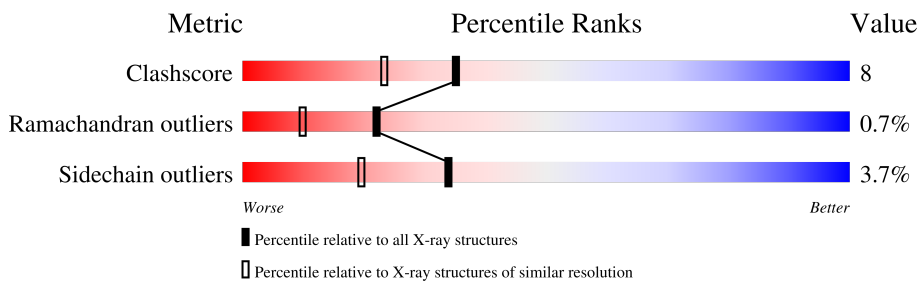
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 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	122	83% 13% • •
1	B	122	82% 12% • • •
1	C	122	85% 11% • •
1	D	122	81% 16% • •
1	E	122	80% 14% • •
1	F	122	80% 16% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTT	A	501	X	-	-	-
4	DTT	C	502	X	-	-	-
4	DTT	D	503	X	-	-	-
4	DTT	D	505	X	-	-	-
4	DTT	F	504	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6141 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 HOLO-(ACYL CARRIER PROTEIN) SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			928	588	165	173	2			
1	B	119	Total	C	N	O	S	0	0	0
			933	591	167	173	2			
1	C	119	Total	C	N	O	S	0	0	0
			929	590	166	171	2			
1	D	119	Total	C	N	O	S	0	0	0
			933	591	167	173	2			
1	E	118	Total	C	N	O	S	0	0	0
			933	592	167	172	2			
1	F	119	Total	C	N	O	S	0	0	0
			937	595	167	173	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P96618
B	0	GLY	-	expression tag	UNP P96618
C	0	GLY	-	expression tag	UNP P96618
D	0	GLY	-	expression tag	UNP P96618
E	0	GLY	-	expression tag	UNP P96618
F	0	GLY	-	expression tag	UNP P96618
A	1	GLY	-	expression tag	UNP P96618
B	1	GLY	-	expression tag	UNP P96618
C	1	GLY	-	expression tag	UNP P96618
D	1	GLY	-	expression tag	UNP P96618
E	1	GLY	-	expression tag	UNP P96618
F	1	GLY	-	expression tag	UNP P96618
A	96	PRO	GLN	engineered mutation	UNP P96618
B	96	PRO	GLN	engineered mutation	UNP P96618
C	96	PRO	GLN	engineered mutation	UNP P96618
D	96	PRO	GLN	engineered mutation	UNP P96618
E	96	PRO	GLN	engineered mutation	UNP P96618

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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
F	96	PRO	GLN	engineered mutation	UNP P96618

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	Cl 4	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	5	Total 5	Cl 5	0	0
3	D	4	Total 4	Cl 4	0	0
3	E	1	Total 1	Cl 1	0	0
3	F	3	Total 3	Cl 3	0	0

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).

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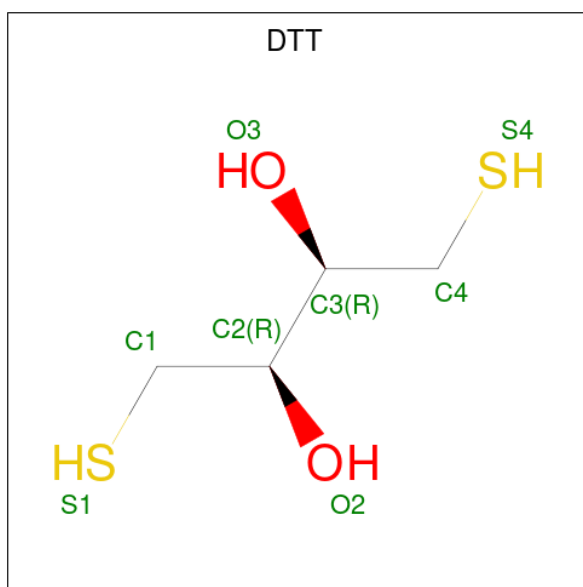
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 8	C 4	O 2	S 2	0	0
4	C	1	Total 8	C 4	O 2	S 2	0	0
4	D	1	Total 8	C 4	O 2	S 2	0	0
4	D	1	Total 8	C 4	O 2	S 2	0	0
4	F	1	Total 8	C 4	O 2	S 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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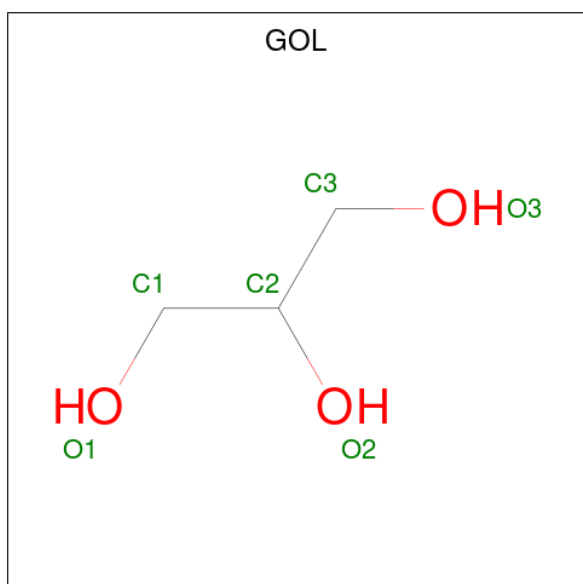
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total 76	O 76	0	0
6	B	78	Total 78	O 78	0	0
6	C	86	Total 86	O 86	0	0
6	D	67	Total 67	O 67	0	0
6	E	92	Total 92	O 92	0	0
6	F	70	Total 70	O 70	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: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain A:
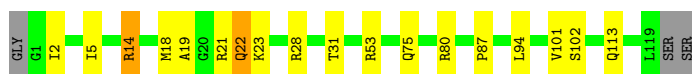
• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain B:

• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain C:

• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain D:

• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain E:

• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain F:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.26Å 76.16Å 85.69Å 90.00° 93.32° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	93.9 (50.00-1.80)	Depositor
R_{merge}	0.76	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.196 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6141	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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: GOL, CL, DTT, NA

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	0.39	0/942	0.65	0/1265
1	B	0.38	0/947	0.65	0/1269
1	C	0.38	0/943	0.68	0/1266
1	D	0.41	0/947	0.65	0/1269
1	E	0.39	0/947	0.63	0/1268
1	F	0.36	0/951	0.65	0/1275
All	All	0.39	0/5677	0.65	0/7612

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 ⓘ

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	928	0	930	12	0
1	B	933	0	945	18	0
1	C	929	0	938	16	0
1	D	933	0	945	17	0
1	E	933	0	953	20	0
1	F	937	0	953	23	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
3	F	3	0	0	0	0
4	A	8	0	8	0	0
4	C	8	0	8	0	0
4	D	16	0	16	0	0
4	F	8	0	8	0	0
5	B	6	0	8	0	0
5	D	6	0	8	1	0
6	A	76	0	0	0	0
6	B	78	0	0	0	0
6	C	86	0	0	0	0
6	D	67	0	0	1	0
6	E	92	0	0	2	0
6	F	70	0	0	1	0
All	All	6141	0	5720	93	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 8.

The worst 5 of 93 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:23:LYS:HD2	1:C:23:LYS:H	1.27	0.98
1:D:118:ARG:HB3	1:D:118:ARG:HH11	1.29	0.97
1:D:113:GLN:HE22	1:E:113:GLN:HE21	1.25	0.84
1:E:22:GLN:HE22	1:E:28:ARG:HH21	1.28	0.82
1:A:21:ARG:O	1:A:22:GLN:HG3	1.84	0.75

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	117/122 (96%)	111 (95%)	3 (3%)	3 (3%)	5	1
1	B	117/122 (96%)	113 (97%)	2 (2%)	2 (2%)	9	2
1	C	117/122 (96%)	117 (100%)	0	0	100	100
1	D	117/122 (96%)	117 (100%)	0	0	100	100
1	E	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
1	F	117/122 (96%)	117 (100%)	0	0	100	100
All	All	701/732 (96%)	688 (98%)	8 (1%)	5 (1%)	22	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	B	23	LYS
1	A	19	ALA
1	A	22	GLN
1	B	96	PRO

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	93/99 (94%)	90 (97%)	3 (3%)	39	25
1	B	94/99 (95%)	89 (95%)	5 (5%)	22	9
1	C	93/99 (94%)	90 (97%)	3 (3%)	39	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	94/99 (95%)	92 (98%)	2 (2%)	53	42
1	E	95/99 (96%)	91 (96%)	4 (4%)	30	15
1	F	95/99 (96%)	91 (96%)	4 (4%)	30	15
All	All	564/594 (95%)	543 (96%)	21 (4%)	34	19

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	45	ARG
1	F	72	LEU
1	F	94	LEU
1	F	80	ARG
1	E	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	83	GLN
1	F	47	ASN
1	E	47	ASN
1	F	37	GLN
1	E	22	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 34 ligands modelled in this entry, 27 are monoatomic - leaving 7 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	DTT	D	505	-	7,7,7	2.42	4 (57%)	4,8,8	1.76	1 (25%)
4	DTT	D	503	-	7,7,7	2.39	4 (57%)	4,8,8	1.81	1 (25%)
4	DTT	C	502	-	7,7,7	2.43	4 (57%)	4,8,8	1.82	1 (25%)
5	GOL	D	506	-	5,5,5	1.00	0	5,5,5	0.31	0
4	DTT	F	504	-	7,7,7	2.43	4 (57%)	4,8,8	1.76	1 (25%)
5	GOL	B	507	-	5,5,5	0.96	0	5,5,5	0.28	0
4	DTT	A	501	-	7,7,7	2.46	4 (57%)	4,8,8	1.76	1 (25%)

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	DTT	D	505	-	2/2/2/2	0/8/8/8	-
4	DTT	D	503	-	2/2/2/2	0/8/8/8	-
4	DTT	C	502	-	2/2/2/2	0/8/8/8	-
5	GOL	D	506	-	-	2/4/4/4	-
4	DTT	F	504	-	2/2/2/2	0/8/8/8	-
5	GOL	B	507	-	-	2/4/4/4	-
4	DTT	A	501	-	2/2/2/2	0/8/8/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	DTT	C3-C2	3.86	1.62	1.52
4	C	502	DTT	C3-C2	3.85	1.62	1.52
4	D	505	DTT	C3-C2	3.84	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	504	DTT	C3-C2	3.76	1.62	1.52
4	D	503	DTT	C3-C2	3.71	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	503	DTT	O2-C2-C3	-3.19	103.18	109.72
4	C	502	DTT	O2-C2-C3	-3.10	103.36	109.72
4	F	504	DTT	O2-C2-C3	-3.06	103.43	109.72
4	A	501	DTT	O2-C2-C3	-3.01	103.54	109.72
4	D	505	DTT	O2-C2-C3	-3.00	103.56	109.72

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	501	DTT	C3
4	A	501	DTT	C2
4	C	502	DTT	C3
4	C	502	DTT	C2
4	D	503	DTT	C3

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	507	GOL	O1-C1-C2-C3
5	D	506	GOL	O1-C1-C2-C3
5	B	507	GOL	O1-C1-C2-O2
5	D	506	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	506	GOL	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 ⓘ

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.