



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID : 3AZA
Title : Beta-Hydroxyacyl-Acyl Carrier Protein Dehydratase (FabZ) from Plasmodium falciparum in complex with NAS91-10
Authors : Maity, K.; Venkata, B.S.; Kapoor, N.; Surolia, N.; Surolia, A.; Suguna, K.
Deposited on : 2011-05-21
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

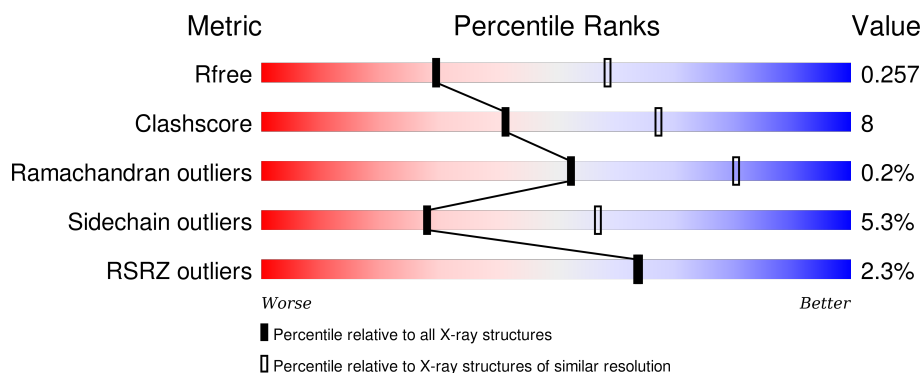
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	154	 2% 81% 14% • 5%
1	B	154	 1% 81% 10% • 9%
1	C	154	 1% 79% 14% • 6%
1	D	154	 1% 81% 12% • 6%
1	E	154	 79% 12% • 8%

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Mol	Chain	Length	Quality of chain
1	F	154	
1	G	154	
1	H	154	
1	I	154	
1	J	154	
1	K	154	
1	L	154	
1	M	154	
1	N	154	
1	O	154	
1	P	154	
1	Q	154	
1	R	154	
1	S	154	
1	T	154	
1	U	154	
1	V	154	
1	W	154	
1	X	154	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	1	-	-	-	X
2	GOL	W	11	-	-	-	X
3	KM0	B	2	-	-	X	-
3	KM0	C	3	-	-	X	X
3	KM0	D	1	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	KM0	M	4	-	-	X	-
3	KM0	O	5	-	-	X	-
3	KM0	P	6	-	-	X	-
3	KM0	Q	7	-	-	X	-
3	KM0	U	8	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27042 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 Beta-hydroxyacyl-ACP dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1125	732	184	204	5			
1	B	140	Total	C	N	O	S	0	0	0
			1082	704	179	194	5			
1	C	144	Total	C	N	O	S	0	1	0
			1127	733	188	201	5			
1	D	144	Total	C	N	O	S	0	0	0
			1093	709	179	200	5			
1	E	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	F	146	Total	C	N	O	S	0	0	0
			1127	731	186	205	5			
1	G	146	Total	C	N	O	S	0	0	0
			1125	732	184	204	5			
1	H	141	Total	C	N	O	S	0	0	0
			1094	713	180	196	5			
1	I	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	J	144	Total	C	N	O	S	0	0	0
			1096	710	180	201	5			
1	K	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	L	146	Total	C	N	O	S	0	0	0
			1127	731	186	205	5			
1	M	146	Total	C	N	O	S	0	0	0
			1125	732	184	204	5			
1	N	141	Total	C	N	O	S	0	0	0
			1094	713	180	196	5			
1	O	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	P	144	Total	C	N	O	S	0	0	0
			1096	710	180	201	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	R	146	Total	C	N	O	S	0	0	0
			1127	731	186	205	5			
1	S	146	Total	C	N	O	S	0	0	0
			1125	732	184	204	5			
1	T	141	Total	C	N	O	S	0	0	0
			1094	713	180	196	5			
1	U	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	V	140	Total	C	N	O	S	0	0	0
			1075	699	176	195	5			
1	W	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	X	146	Total	C	N	O	S	0	1	0
			1131	732	186	208	5			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	EXPRESSION TAG	UNP Q965D7
A	78	SER	-	EXPRESSION TAG	UNP Q965D7
A	79	HIS	-	EXPRESSION TAG	UNP Q965D7
A	80	MET	-	EXPRESSION TAG	UNP Q965D7
B	77	GLY	-	EXPRESSION TAG	UNP Q965D7
B	78	SER	-	EXPRESSION TAG	UNP Q965D7
B	79	HIS	-	EXPRESSION TAG	UNP Q965D7
B	80	MET	-	EXPRESSION TAG	UNP Q965D7
C	77	GLY	-	EXPRESSION TAG	UNP Q965D7
C	78	SER	-	EXPRESSION TAG	UNP Q965D7
C	79	HIS	-	EXPRESSION TAG	UNP Q965D7
C	80	MET	-	EXPRESSION TAG	UNP Q965D7
D	77	GLY	-	EXPRESSION TAG	UNP Q965D7
D	78	SER	-	EXPRESSION TAG	UNP Q965D7
D	79	HIS	-	EXPRESSION TAG	UNP Q965D7
D	80	MET	-	EXPRESSION TAG	UNP Q965D7
E	77	GLY	-	EXPRESSION TAG	UNP Q965D7
E	78	SER	-	EXPRESSION TAG	UNP Q965D7
E	79	HIS	-	EXPRESSION TAG	UNP Q965D7
E	80	MET	-	EXPRESSION TAG	UNP Q965D7
F	77	GLY	-	EXPRESSION TAG	UNP Q965D7
F	78	SER	-	EXPRESSION TAG	UNP Q965D7
F	79	HIS	-	EXPRESSION TAG	UNP Q965D7

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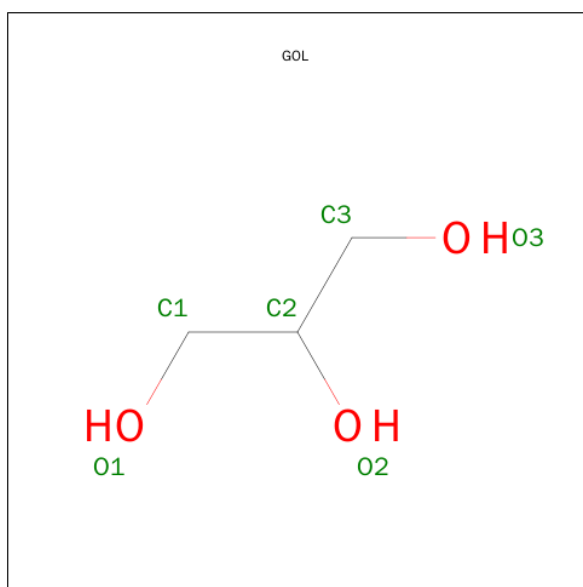
Chain	Residue	Modelled	Actual	Comment	Reference
F	80	MET	-	EXPRESSION TAG	UNP Q965D7
G	77	GLY	-	EXPRESSION TAG	UNP Q965D7
G	78	SER	-	EXPRESSION TAG	UNP Q965D7
G	79	HIS	-	EXPRESSION TAG	UNP Q965D7
G	80	MET	-	EXPRESSION TAG	UNP Q965D7
H	77	GLY	-	EXPRESSION TAG	UNP Q965D7
H	78	SER	-	EXPRESSION TAG	UNP Q965D7
H	79	HIS	-	EXPRESSION TAG	UNP Q965D7
H	80	MET	-	EXPRESSION TAG	UNP Q965D7
I	77	GLY	-	EXPRESSION TAG	UNP Q965D7
I	78	SER	-	EXPRESSION TAG	UNP Q965D7
I	79	HIS	-	EXPRESSION TAG	UNP Q965D7
I	80	MET	-	EXPRESSION TAG	UNP Q965D7
J	77	GLY	-	EXPRESSION TAG	UNP Q965D7
J	78	SER	-	EXPRESSION TAG	UNP Q965D7
J	79	HIS	-	EXPRESSION TAG	UNP Q965D7
J	80	MET	-	EXPRESSION TAG	UNP Q965D7
K	77	GLY	-	EXPRESSION TAG	UNP Q965D7
K	78	SER	-	EXPRESSION TAG	UNP Q965D7
K	79	HIS	-	EXPRESSION TAG	UNP Q965D7
K	80	MET	-	EXPRESSION TAG	UNP Q965D7
L	77	GLY	-	EXPRESSION TAG	UNP Q965D7
L	78	SER	-	EXPRESSION TAG	UNP Q965D7
L	79	HIS	-	EXPRESSION TAG	UNP Q965D7
L	80	MET	-	EXPRESSION TAG	UNP Q965D7
M	77	GLY	-	EXPRESSION TAG	UNP Q965D7
M	78	SER	-	EXPRESSION TAG	UNP Q965D7
M	79	HIS	-	EXPRESSION TAG	UNP Q965D7
M	80	MET	-	EXPRESSION TAG	UNP Q965D7
N	77	GLY	-	EXPRESSION TAG	UNP Q965D7
N	78	SER	-	EXPRESSION TAG	UNP Q965D7
N	79	HIS	-	EXPRESSION TAG	UNP Q965D7
N	80	MET	-	EXPRESSION TAG	UNP Q965D7
O	77	GLY	-	EXPRESSION TAG	UNP Q965D7
O	78	SER	-	EXPRESSION TAG	UNP Q965D7
O	79	HIS	-	EXPRESSION TAG	UNP Q965D7
O	80	MET	-	EXPRESSION TAG	UNP Q965D7
P	77	GLY	-	EXPRESSION TAG	UNP Q965D7
P	78	SER	-	EXPRESSION TAG	UNP Q965D7
P	79	HIS	-	EXPRESSION TAG	UNP Q965D7
P	80	MET	-	EXPRESSION TAG	UNP Q965D7
Q	77	GLY	-	EXPRESSION TAG	UNP Q965D7

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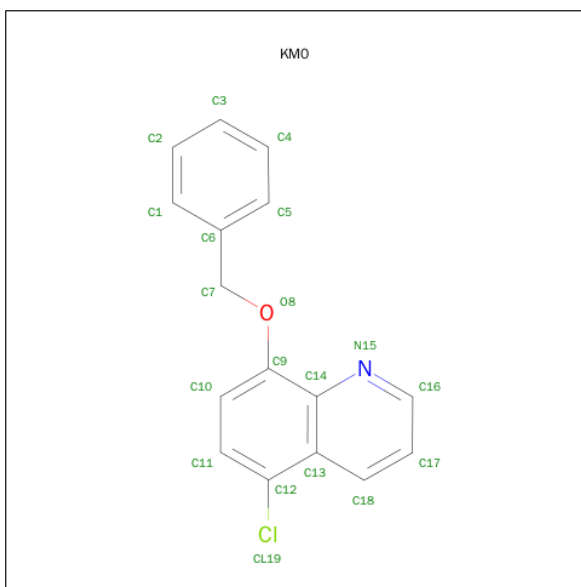
Chain	Residue	Modelled	Actual	Comment	Reference
Q	78	SER	-	EXPRESSION TAG	UNP Q965D7
Q	79	HIS	-	EXPRESSION TAG	UNP Q965D7
Q	80	MET	-	EXPRESSION TAG	UNP Q965D7
R	77	GLY	-	EXPRESSION TAG	UNP Q965D7
R	78	SER	-	EXPRESSION TAG	UNP Q965D7
R	79	HIS	-	EXPRESSION TAG	UNP Q965D7
R	80	MET	-	EXPRESSION TAG	UNP Q965D7
S	77	GLY	-	EXPRESSION TAG	UNP Q965D7
S	78	SER	-	EXPRESSION TAG	UNP Q965D7
S	79	HIS	-	EXPRESSION TAG	UNP Q965D7
S	80	MET	-	EXPRESSION TAG	UNP Q965D7
T	77	GLY	-	EXPRESSION TAG	UNP Q965D7
T	78	SER	-	EXPRESSION TAG	UNP Q965D7
T	79	HIS	-	EXPRESSION TAG	UNP Q965D7
T	80	MET	-	EXPRESSION TAG	UNP Q965D7
U	77	GLY	-	EXPRESSION TAG	UNP Q965D7
U	78	SER	-	EXPRESSION TAG	UNP Q965D7
U	79	HIS	-	EXPRESSION TAG	UNP Q965D7
U	80	MET	-	EXPRESSION TAG	UNP Q965D7
V	77	GLY	-	EXPRESSION TAG	UNP Q965D7
V	78	SER	-	EXPRESSION TAG	UNP Q965D7
V	79	HIS	-	EXPRESSION TAG	UNP Q965D7
V	80	MET	-	EXPRESSION TAG	UNP Q965D7
W	77	GLY	-	EXPRESSION TAG	UNP Q965D7
W	78	SER	-	EXPRESSION TAG	UNP Q965D7
W	79	HIS	-	EXPRESSION TAG	UNP Q965D7
W	80	MET	-	EXPRESSION TAG	UNP Q965D7
X	77	GLY	-	EXPRESSION TAG	UNP Q965D7
X	78	SER	-	EXPRESSION TAG	UNP Q965D7
X	79	HIS	-	EXPRESSION TAG	UNP Q965D7
X	80	MET	-	EXPRESSION TAG	UNP Q965D7

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		
2	W	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 8-(BENZYLOXY)-5-CHLOROQUINOLINE (three-letter code: KM0) (formula: C₁₆H₁₂ClNO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	
			19	16	1	1	1	
3	C	1	Total	C	Cl	N	O	
			19	16	1	1	1	
3	D	1	Total	C	Cl	N	O	
			19	16	1	1	1	
3	M	1	Total	C	Cl	N	O	
			19	16	1	1	1	
3	O	1	Total	C	Cl	N	O	
			19	16	1	1	1	
3	P	1	Total	C	Cl	N	O	
			19	16	1	1	1	
3	Q	1	Total	C	Cl	N	O	
			19	16	1	1	1	
3	U	1	Total	C	Cl	N	O	
			19	16	1	1	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O		
			5	5	0	0
4	B	11	Total	O		
			11	11	0	0
4	C	13	Total	O		
			13	13	0	0
4	D	8	Total	O		
			8	8	0	0

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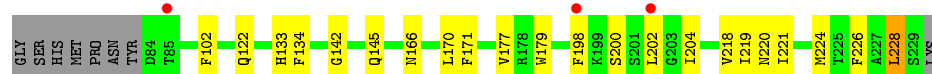
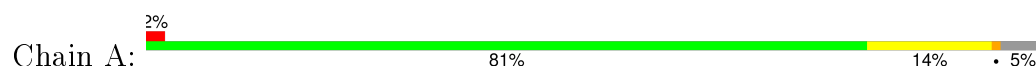
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	12	Total 12	O 12	0	0
4	F	13	Total 13	O 13	0	0
4	G	4	Total 4	O 4	0	0
4	H	11	Total 11	O 11	0	0
4	I	5	Total 5	O 5	0	0
4	J	9	Total 9	O 9	0	0
4	K	11	Total 11	O 11	0	0
4	L	8	Total 8	O 8	0	0
4	M	12	Total 12	O 12	0	0
4	N	8	Total 8	O 8	0	0
4	O	12	Total 12	O 12	0	0
4	P	4	Total 4	O 4	0	0
4	Q	3	Total 3	O 3	0	0
4	R	8	Total 8	O 8	0	0
4	S	6	Total 6	O 6	0	0
4	T	10	Total 10	O 10	0	0
4	U	11	Total 11	O 11	0	0
4	V	2	Total 2	O 2	0	0
4	W	7	Total 7	O 7	0	0
4	X	8	Total 8	O 8	0	0

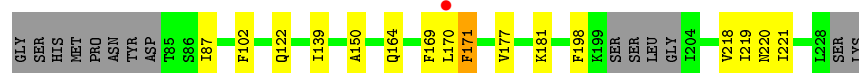
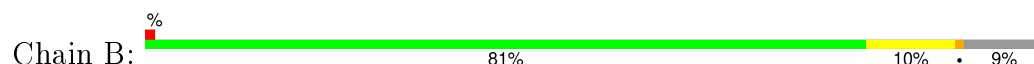
3 Residue-property plots [i](#)

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

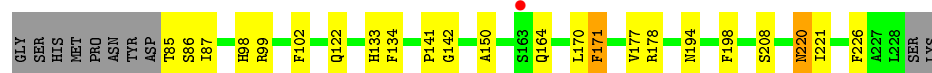
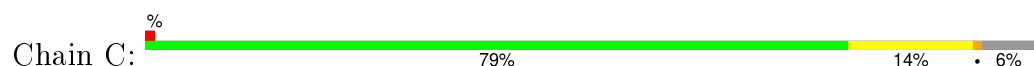
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



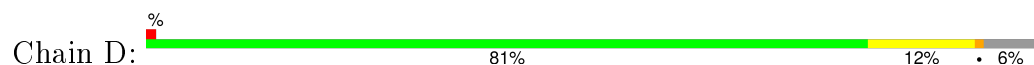
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



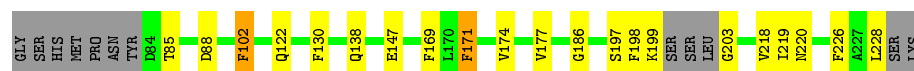
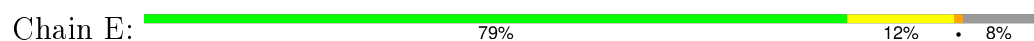
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

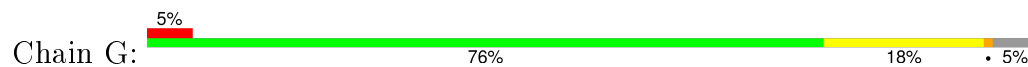


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

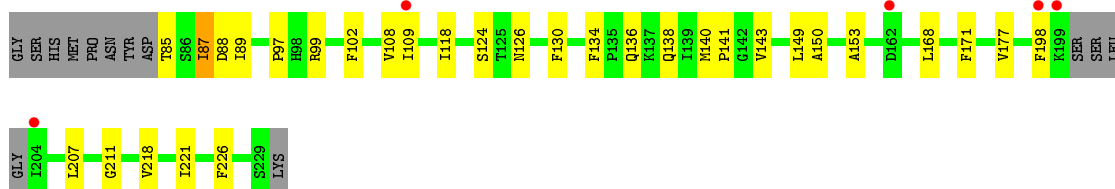




• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



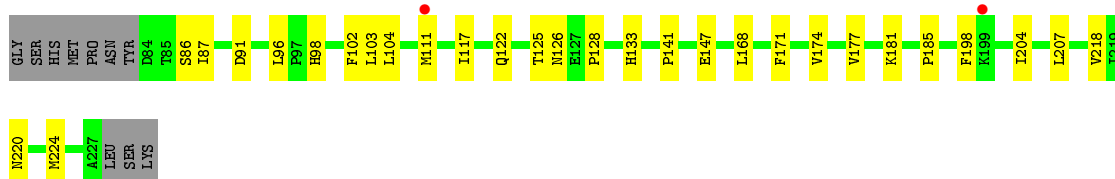
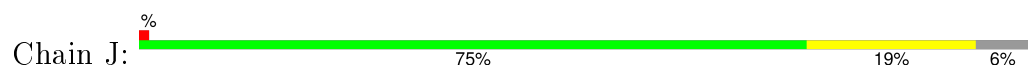
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



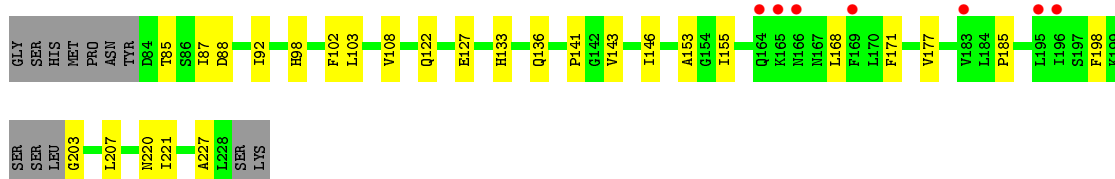
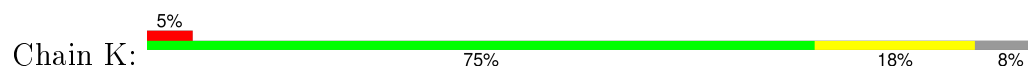
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



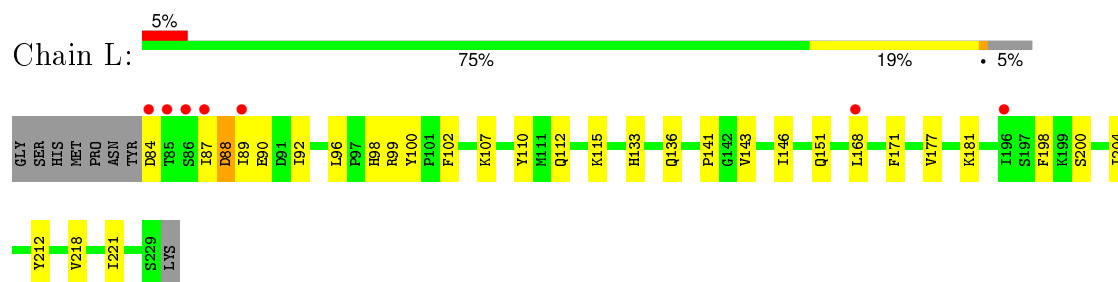
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



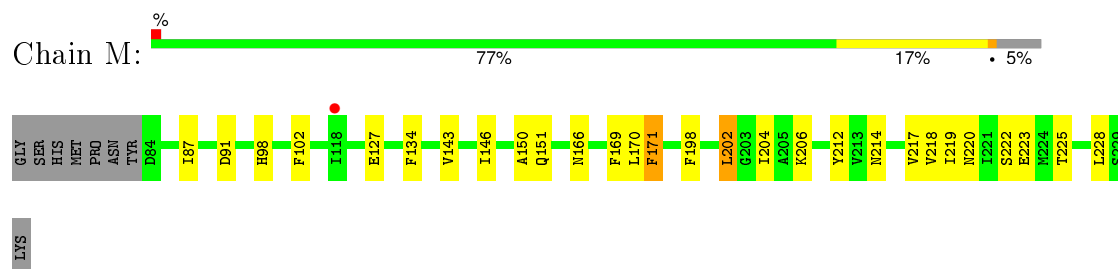
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



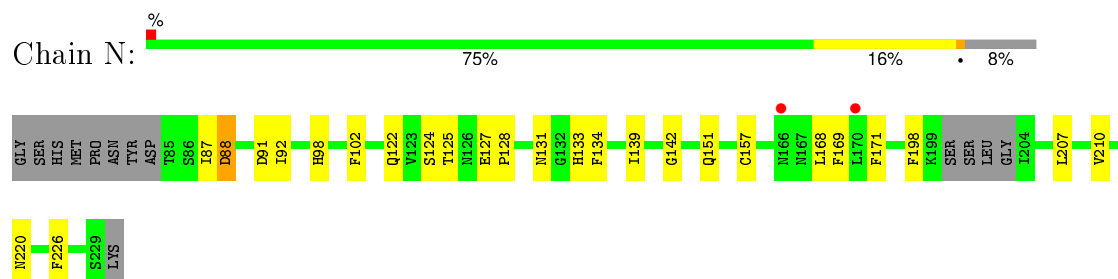
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



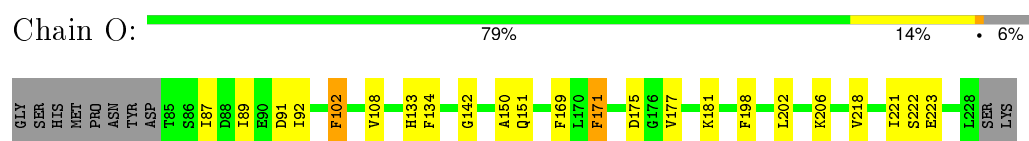
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



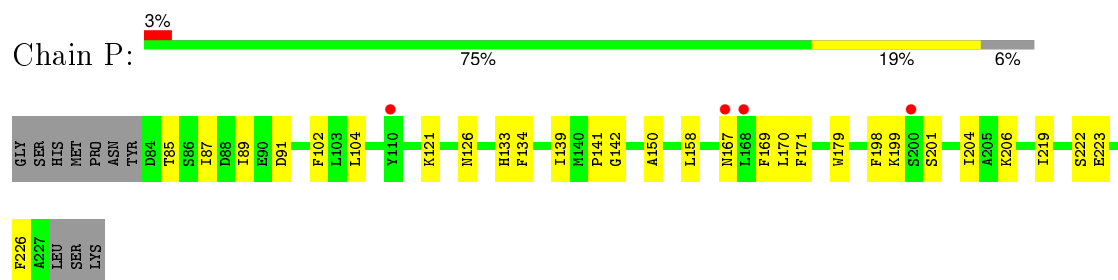
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



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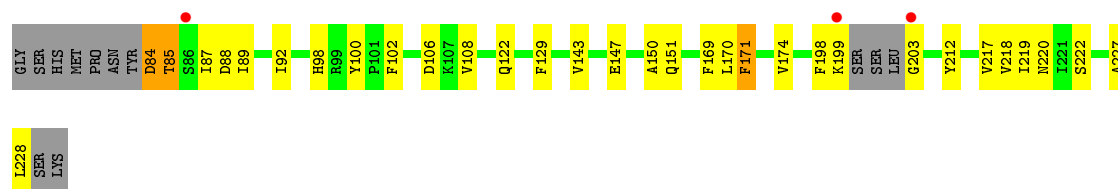


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

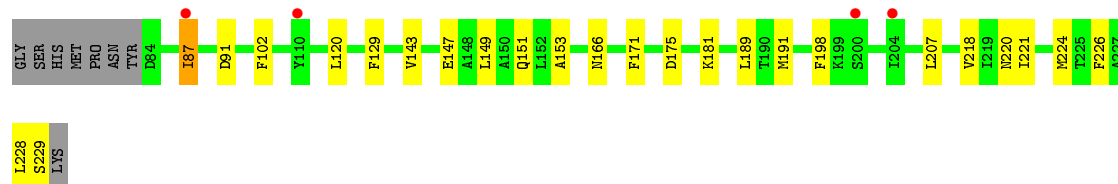




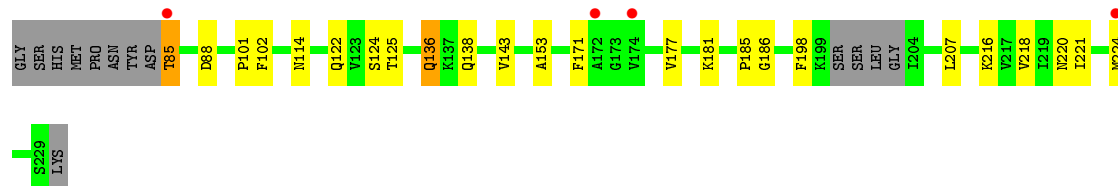
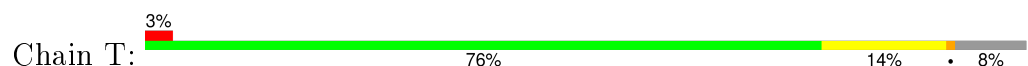
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



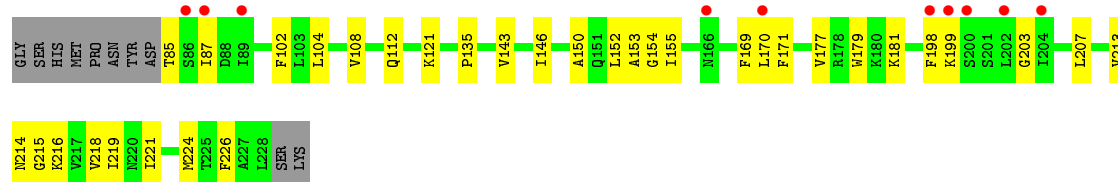
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



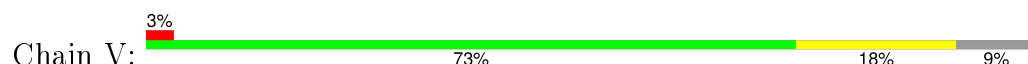
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

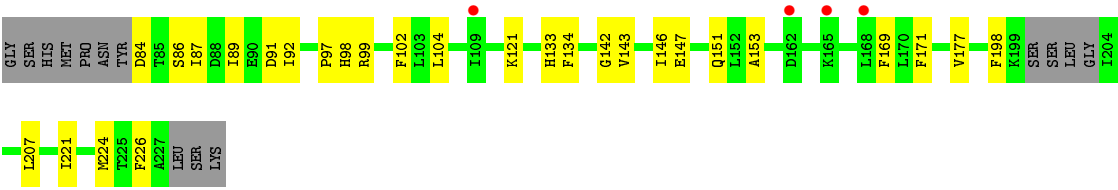


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

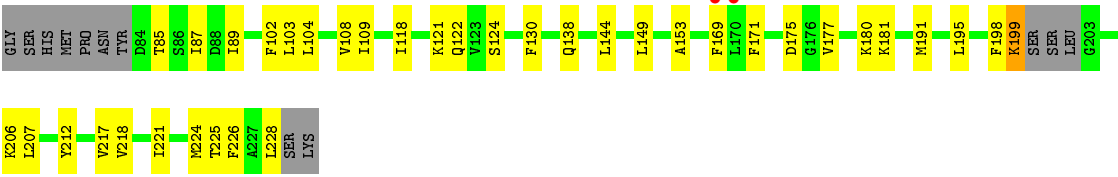


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

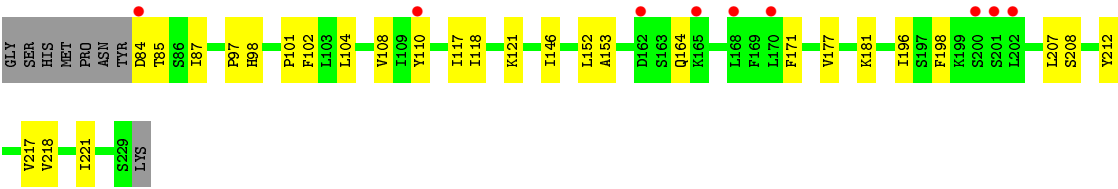
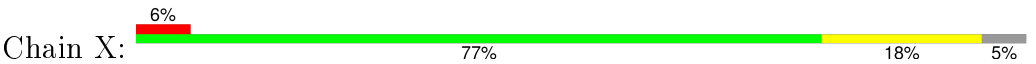




• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	219.21Å 219.21Å 156.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.91 – 2.70 51.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (51.91-2.70) 99.9 (51.91-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.222 , 0.273 0.220 , 0.257	Depositor DCC
R_{free} test set	5062 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 15.8	EDS
Estimated twinning fraction	0.504 for H, K, L 0.496 for -H, K, -L 0.457 for -k,-h,-l	Xtriage
Reported twinning fraction	0.504 for H, K, L 0.496 for -H, K, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 101381 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27042	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 30.41 % 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 1.3151e-03.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, KM0

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	0/1147	0.56	0/1553
1	B	0.51	0/1102	0.55	0/1491
1	C	0.46	0/1149	0.57	0/1553
1	D	0.50	0/1115	0.57	0/1512
1	E	0.45	0/1124	0.53	0/1520
1	F	0.46	1/1149 (0.1%)	0.54	0/1554
1	G	0.44	0/1147	0.52	0/1553
1	H	0.50	0/1115	0.55	0/1508
1	I	0.46	0/1138	0.54	0/1539
1	J	0.48	0/1118	0.54	0/1516
1	K	0.47	0/1124	0.53	0/1520
1	L	0.51	0/1149	0.54	0/1554
1	M	0.46	0/1147	0.58	0/1553
1	N	0.50	0/1115	0.54	0/1508
1	O	0.43	0/1138	0.56	0/1539
1	P	0.46	0/1118	0.56	0/1516
1	Q	0.42	0/1124	0.57	1/1520 (0.1%)
1	R	0.48	0/1149	0.56	0/1554
1	S	0.50	1/1147 (0.1%)	0.55	0/1553
1	T	0.50	1/1115 (0.1%)	0.52	0/1508
1	U	0.52	0/1138	0.54	0/1539
1	V	0.46	0/1096	0.54	0/1485
1	W	0.51	0/1124	0.55	0/1520
1	X	0.53	0/1153	0.55	0/1561
All	All	0.48	3/27141 (0.0%)	0.55	1/36729 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	229	SER	CB-OG	5.92	1.50	1.42
1	F	181	LYS	CD-CE	5.52	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	136	GLN	CG-CD	5.11	1.62	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	85	THR	N-CA-C	-5.59	95.92	111.00

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	1125	0	1165	15	0
1	B	1082	0	1121	22	0
1	C	1127	0	1176	24	0
1	D	1093	0	1104	22	0
1	E	1103	0	1144	13	0
1	F	1127	0	1164	14	0
1	G	1125	0	1165	26	0
1	H	1094	0	1133	17	0
1	I	1116	0	1164	15	0
1	J	1096	0	1108	17	0
1	K	1103	0	1144	13	0
1	L	1127	0	1164	17	0
1	M	1125	0	1165	26	0
1	N	1094	0	1133	17	0
1	O	1116	0	1164	25	0
1	P	1096	0	1108	32	0
1	Q	1103	0	1144	28	0
1	R	1127	0	1164	16	0
1	S	1125	0	1165	14	0
1	T	1094	0	1133	17	0
1	U	1116	0	1164	32	0
1	V	1075	0	1092	29	0
1	W	1103	0	1144	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1131	0	1156	14	0
2	A	6	0	8	0	0
2	C	6	0	8	1	0
2	E	6	0	8	0	0
2	G	6	0	8	1	0
2	J	6	0	8	0	0
2	N	6	0	8	1	0
2	P	6	0	8	0	0
2	Q	6	0	8	3	0
2	T	6	0	8	3	0
2	V	6	0	8	0	0
2	W	6	0	8	1	0
3	B	19	0	12	22	0
3	C	19	0	12	17	0
3	D	19	0	12	18	0
3	M	19	0	12	15	0
3	O	19	0	12	24	0
3	P	19	0	12	23	0
3	Q	19	0	12	16	0
3	U	19	0	12	25	0
4	A	5	0	0	0	0
4	B	11	0	0	0	0
4	C	13	0	0	0	0
4	D	8	0	0	0	0
4	E	12	0	0	1	0
4	F	13	0	0	1	0
4	G	4	0	0	1	0
4	H	11	0	0	0	0
4	I	5	0	0	0	0
4	J	9	0	0	0	0
4	K	11	0	0	0	0
4	L	8	0	0	1	0
4	M	12	0	0	1	0
4	N	8	0	0	0	0
4	O	12	0	0	0	0
4	P	4	0	0	0	0
4	Q	3	0	0	0	0
4	R	8	0	0	0	0
4	S	6	0	0	0	0
4	T	10	0	0	1	0
4	U	11	0	0	0	0
4	V	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	W	7	0	0	1	0
4	X	8	0	0	0	0
All	All	27042	0	27668	462	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 462 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:150:ALA:CB	3:C:3:KM0:H17	1.62	1.27
1:O:150:ALA:HB1	3:O:5:KM0:C17	1.77	1.14
1:P:150:ALA:CB	3:P:6:KM0:H17	1.76	1.14
1:D:150:ALA:HB1	3:D:1:KM0:H17	1.21	1.13
1:U:150:ALA:HB1	3:U:8:KM0:H17	1.23	1.12

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	144/154 (94%)	132 (92%)	11 (8%)	1 (1%)	26	55
1	B	136/154 (88%)	125 (92%)	11 (8%)	0	100	100
1	C	143/154 (93%)	132 (92%)	11 (8%)	0	100	100
1	D	142/154 (92%)	129 (91%)	12 (8%)	1 (1%)	26	55
1	E	138/154 (90%)	130 (94%)	8 (6%)	0	100	100
1	F	144/154 (94%)	132 (92%)	11 (8%)	1 (1%)	26	55
1	G	144/154 (94%)	135 (94%)	9 (6%)	0	100	100
1	H	137/154 (89%)	128 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	142/154 (92%)	132 (93%)	10 (7%)	0	100	100
1	J	142/154 (92%)	129 (91%)	12 (8%)	1 (1%)	26	55
1	K	138/154 (90%)	132 (96%)	6 (4%)	0	100	100
1	L	144/154 (94%)	130 (90%)	13 (9%)	1 (1%)	26	55
1	M	144/154 (94%)	133 (92%)	11 (8%)	0	100	100
1	N	137/154 (89%)	131 (96%)	6 (4%)	0	100	100
1	O	142/154 (92%)	132 (93%)	10 (7%)	0	100	100
1	P	142/154 (92%)	129 (91%)	12 (8%)	1 (1%)	26	55
1	Q	138/154 (90%)	129 (94%)	9 (6%)	0	100	100
1	R	144/154 (94%)	137 (95%)	7 (5%)	0	100	100
1	S	144/154 (94%)	134 (93%)	10 (7%)	0	100	100
1	T	137/154 (89%)	127 (93%)	10 (7%)	0	100	100
1	U	142/154 (92%)	131 (92%)	11 (8%)	0	100	100
1	V	136/154 (88%)	124 (91%)	12 (9%)	0	100	100
1	W	138/154 (90%)	127 (92%)	11 (8%)	0	100	100
1	X	145/154 (94%)	137 (94%)	8 (6%)	0	100	100
All	All	3383/3696 (92%)	3137 (93%)	240 (7%)	6 (0%)	52	80

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	204	ILE
1	J	204	ILE
1	P	204	ILE
1	A	200	SER
1	F	200	SER

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	126/135 (93%)	121 (96%)	5 (4%)	38	69
1	B	120/135 (89%)	114 (95%)	6 (5%)	30	60
1	C	126/135 (93%)	120 (95%)	6 (5%)	31	62
1	D	119/135 (88%)	114 (96%)	5 (4%)	36	68
1	E	123/135 (91%)	115 (94%)	8 (6%)	21	46
1	F	126/135 (93%)	117 (93%)	9 (7%)	18	41
1	G	126/135 (93%)	117 (93%)	9 (7%)	18	41
1	H	122/135 (90%)	114 (93%)	8 (7%)	21	45
1	I	125/135 (93%)	120 (96%)	5 (4%)	38	69
1	J	120/135 (89%)	116 (97%)	4 (3%)	45	76
1	K	123/135 (91%)	116 (94%)	7 (6%)	25	53
1	L	126/135 (93%)	119 (94%)	7 (6%)	26	54
1	M	126/135 (93%)	120 (95%)	6 (5%)	31	62
1	N	122/135 (90%)	117 (96%)	5 (4%)	37	69
1	O	125/135 (93%)	119 (95%)	6 (5%)	31	62
1	P	120/135 (89%)	114 (95%)	6 (5%)	30	60
1	Q	123/135 (91%)	113 (92%)	10 (8%)	15	33
1	R	126/135 (93%)	113 (90%)	13 (10%)	9	20
1	S	126/135 (93%)	120 (95%)	6 (5%)	31	62
1	T	122/135 (90%)	116 (95%)	6 (5%)	31	61
1	U	125/135 (93%)	120 (96%)	5 (4%)	38	69
1	V	118/135 (87%)	115 (98%)	3 (2%)	55	84
1	W	123/135 (91%)	116 (94%)	7 (6%)	25	53
1	X	126/135 (93%)	121 (96%)	5 (4%)	38	69
All	All	2964/3240 (92%)	2807 (95%)	157 (5%)	28	57

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	198	PHE
1	N	168	LEU
1	W	85	THR
1	L	102	PHE
1	M	102	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	164	GLN
1	K	214	ASN
1	P	145	GLN
1	J	138	GLN
1	K	98	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	2	-	5,5,5	0.31	0	5,5,5	0.26	0
3	KM0	B	2	-	21,21,21	1.16	1 (4%)	28,28,28	1.61	7 (25%)
2	GOL	C	1	-	5,5,5	0.30	0	5,5,5	0.42	0
3	KM0	C	3	-	21,21,21	1.27	1 (4%)	28,28,28	1.58	5 (17%)
3	KM0	D	1	-	21,21,21	1.13	1 (4%)	28,28,28	1.62	6 (21%)
2	GOL	E	3	-	5,5,5	0.35	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	G	4	-	5,5,5	0.38	0	5,5,5	0.39	0
2	GOL	J	5	-	5,5,5	0.41	0	5,5,5	0.88	0
3	KM0	M	4	-	21,21,21	1.17	1 (4%)	28,28,28	1.71	8 (28%)
2	GOL	N	6	-	5,5,5	0.32	0	5,5,5	0.23	0
3	KM0	O	5	-	21,21,21	1.25	2 (9%)	28,28,28	1.46	5 (17%)
3	KM0	P	6	-	21,21,21	1.11	1 (4%)	28,28,28	1.67	6 (21%)
2	GOL	P	7	-	5,5,5	0.32	0	5,5,5	0.25	0
3	KM0	Q	7	-	21,21,21	0.98	1 (4%)	28,28,28	1.43	5 (17%)
2	GOL	Q	8	-	5,5,5	0.28	0	5,5,5	0.30	0
2	GOL	T	9	-	5,5,5	0.27	0	5,5,5	0.41	0
3	KM0	U	8	-	21,21,21	1.14	1 (4%)	28,28,28	1.77	8 (28%)
2	GOL	V	10	-	5,5,5	0.36	0	5,5,5	0.25	0
2	GOL	W	11	-	5,5,5	0.35	0	5,5,5	0.32	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
2	GOL	A	2	-	-	0/4/4/4	0/0/0/0
3	KM0	B	2	-	-	0/5/5/5	0/3/3/3
2	GOL	C	1	-	-	0/4/4/4	0/0/0/0
3	KM0	C	3	-	-	0/5/5/5	0/3/3/3
3	KM0	D	1	-	-	0/5/5/5	0/3/3/3
2	GOL	E	3	-	-	0/4/4/4	0/0/0/0
2	GOL	G	4	-	-	0/4/4/4	0/0/0/0
2	GOL	J	5	-	-	0/4/4/4	0/0/0/0
3	KM0	M	4	-	-	0/5/5/5	0/3/3/3
2	GOL	N	6	-	-	0/4/4/4	0/0/0/0
3	KM0	O	5	-	-	0/5/5/5	0/3/3/3
3	KM0	P	6	-	-	0/5/5/5	0/3/3/3
2	GOL	P	7	-	-	0/4/4/4	0/0/0/0
3	KM0	Q	7	-	-	0/5/5/5	0/3/3/3
2	GOL	Q	8	-	-	0/4/4/4	0/0/0/0
2	GOL	T	9	-	-	0/4/4/4	0/0/0/0
3	KM0	U	8	-	-	0/5/5/5	0/3/3/3
2	GOL	V	10	-	-	0/4/4/4	0/0/0/0
2	GOL	W	11	-	-	0/4/4/4	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	KM0	C9-C14	-3.76	1.37	1.42
3	O	5	KM0	C9-C14	-3.75	1.37	1.42
3	M	4	KM0	C9-C14	-3.21	1.38	1.42
3	B	2	KM0	C9-C14	-3.19	1.38	1.42
3	D	1	KM0	C9-C14	-3.17	1.38	1.42

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	KM0	C17-C16-N15	-3.40	118.62	123.94
3	U	8	KM0	C17-C16-N15	-3.35	118.69	123.94
3	B	2	KM0	C17-C16-N15	-3.05	119.15	123.94
3	D	1	KM0	C17-C16-N15	-3.00	119.24	123.94
3	M	4	KM0	C17-C16-N15	-2.97	119.28	123.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 170 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	KM0	22	0
2	C	1	GOL	1	0
3	C	3	KM0	17	0
3	D	1	KM0	18	0
2	G	4	GOL	1	0
3	M	4	KM0	15	0
2	N	6	GOL	1	0
3	O	5	KM0	24	0
3	P	6	KM0	23	0
3	Q	7	KM0	16	0
2	Q	8	GOL	3	0
2	T	9	GOL	3	0
3	U	8	KM0	25	0
2	W	11	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	146/154 (94%)	0.20	3 (2%) 67 68	31, 46, 64, 70	0
1	B	140/154 (90%)	0.07	1 (0%) 89 90	31, 45, 62, 65	0
1	C	144/154 (93%)	0.27	1 (0%) 89 90	31, 45, 64, 65	0
1	D	144/154 (93%)	0.08	2 (1%) 78 77	31, 45, 64, 65	1 (0%)
1	E	142/154 (92%)	0.07	0 100 100	31, 45, 62, 65	0
1	F	146/154 (94%)	0.21	0 100 100	31, 45, 63, 65	0
1	G	146/154 (94%)	0.22	7 (4%) 34 33	34, 47, 62, 66	0
1	H	141/154 (91%)	0.28	5 (3%) 48 48	35, 46, 62, 66	0
1	I	144/154 (93%)	0.10	0 100 100	34, 47, 62, 66	0
1	J	144/154 (93%)	0.23	2 (1%) 78 77	35, 47, 64, 69	1 (0%)
1	K	142/154 (92%)	0.37	7 (4%) 33 32	34, 46, 62, 66	0
1	L	146/154 (94%)	0.40	7 (4%) 34 33	35, 47, 65, 75	0
1	M	146/154 (94%)	0.09	1 (0%) 89 90	32, 46, 63, 66	0
1	N	141/154 (91%)	0.13	2 (1%) 78 77	32, 46, 62, 65	0
1	O	144/154 (93%)	0.16	0 100 100	32, 45, 62, 65	0
1	P	144/154 (93%)	0.15	4 (2%) 56 57	32, 46, 64, 66	1 (0%)
1	Q	142/154 (92%)	0.16	3 (2%) 67 68	32, 46, 62, 68	0
1	R	146/154 (94%)	0.16	1 (0%) 89 90	31, 45, 62, 66	0
1	S	146/154 (94%)	0.16	4 (2%) 58 58	35, 47, 63, 66	0
1	T	141/154 (91%)	0.12	4 (2%) 56 57	35, 47, 63, 65	0
1	U	144/154 (93%)	0.41	10 (6%) 20 18	35, 47, 64, 71	0
1	V	140/154 (90%)	0.11	4 (2%) 55 55	34, 47, 64, 66	1 (0%)
1	W	142/154 (92%)	0.31	2 (1%) 78 77	35, 47, 64, 68	0
1	X	146/154 (94%)	0.48	9 (6%) 24 23	34, 47, 63, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3447/3696 (93%)	0.21	79 (2%) 64 64	31, 46, 64, 75	4 (0%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	168	LEU	5.5
1	V	162	ASP	4.4
1	P	110	TYR	4.1
1	U	170	LEU	3.8
1	U	166	ASN	3.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	C	1	6/6	0.90	0.24	3.72	41,42,45,46	0
2	GOL	W	11	6/6	0.94	0.31	3.69	27,31,37,41	0
3	KM0	C	3	19/19	0.89	0.27	2.76	52,56,60,60	0
3	KM0	B	2	19/19	0.92	0.27	1.52	37,46,53,54	4
3	KM0	Q	7	19/19	0.91	0.26	1.47	46,51,55,55	0
3	KM0	U	8	19/19	0.89	0.29	1.17	44,54,58,59	0
2	GOL	E	3	6/6	0.97	0.20	0.86	18,27,30,38	0
3	KM0	M	4	19/19	0.94	0.22	0.76	48,51,54,54	0
2	GOL	A	2	6/6	0.92	0.18	0.48	36,41,43,44	0
3	KM0	O	5	19/19	0.91	0.20	0.42	35,45,50,50	0
2	GOL	N	6	6/6	0.91	0.17	0.23	38,40,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	P	7	6/6	0.93	0.17	0.17	39,43,46,49	0
3	KM0	P	6	19/19	0.89	0.21	0.13	43,53,57,58	0
3	KM0	D	1	19/19	0.92	0.20	0.10	45,52,59,59	0
2	GOL	G	4	6/6	0.97	0.16	-0.06	37,38,38,39	0
2	GOL	T	9	6/6	0.92	0.14	-0.53	42,47,50,52	0
2	GOL	V	10	6/6	0.98	0.16	-0.59	23,28,30,33	0
2	GOL	Q	8	6/6	0.97	0.16	-0.69	17,23,25,27	0
2	GOL	J	5	6/6	0.94	0.14	-1.15	33,34,36,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.