



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 09:43 pm BST

PDB ID : 3AZB  
Title : Beta-Hydroxyacyl-Acyl Carrier Protein Dehydratase (FabZ) from Plasmodium falciparum in complex with NAS91-11  
Authors : Maity, K.; Venkata, B.S.; Kapoor, N.; Surolia, N.; Surolia, A.; Suguna, K.  
Deposited on : 2011-05-21  
Resolution : 2.60 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](mailto: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.

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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  
buster-report : 1.1.7 (2018)  
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

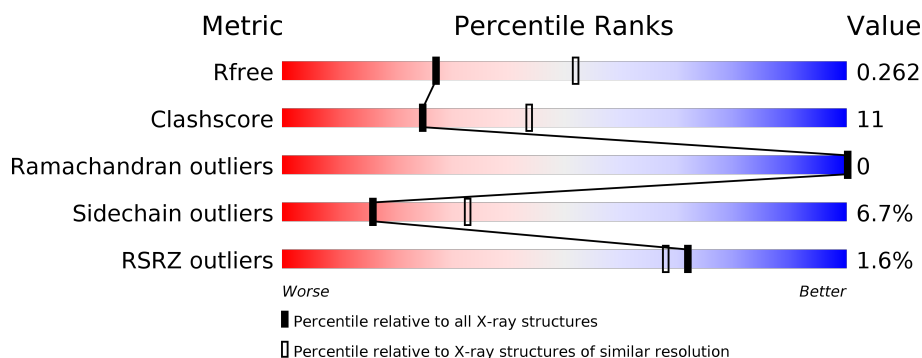
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	154	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	B	154	<div> <div>70%</div> <div>21%</div> <div>• 8%</div> </div>
1	C	154	<div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	D	154	<div> <div>%</div> <div>68%</div> <div>21%</div> <div>• 9%</div> </div>
1	E	154	<div> <div>%</div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div>
1	F	154	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
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	Q	9	-	-	X	-
3	KM1	D	1	-	-	X	-
3	KM1	G	2	-	-	X	-
3	KM1	H	3	-	-	X	-
3	KM1	J	4	-	-	X	-
3	KM1	P	5	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27276 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	141	Total	C	N	O	S	0	0	0
			1094	713	180	196	5			
1	C	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	D	140	Total	C	N	O	S	0	0	0
			1075	699	176	195	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
			1091	710	180	196	5			
1	I	143	Total	C	N	O	S	0	0	0
			1109	723	183	198	5			
1	J	140	Total	C	N	O	S	0	0	0
			1079	702	177	195	5			
1	K	142	Total	C	N	O	S	0	0	0
			1099	716	180	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
			1087	708	179	195	5			
1	O	144	Total	C	N	O	S	0	0	0
			1110	723	183	199	5			
1	P	140	Total	C	N	O	S	0	0	0
			1070	697	176	192	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	S	0	0	0
			1097	713	181	198	5			
1	R	146	Total	C	N	O	S	0	0	0
			1130	734	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
			1090	710	179	196	5			
1	U	143	Total	C	N	O	S	0	0	0
			1106	722	183	196	5			
1	V	140	Total	C	N	O	S	0	0	0
			1079	702	177	195	5			
1	W	142	Total	C	N	O	S	0	0	0
			1100	716	181	198	5			
1	X	146	Total	C	N	O	S	0	0	0
			1130	734	186	205	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

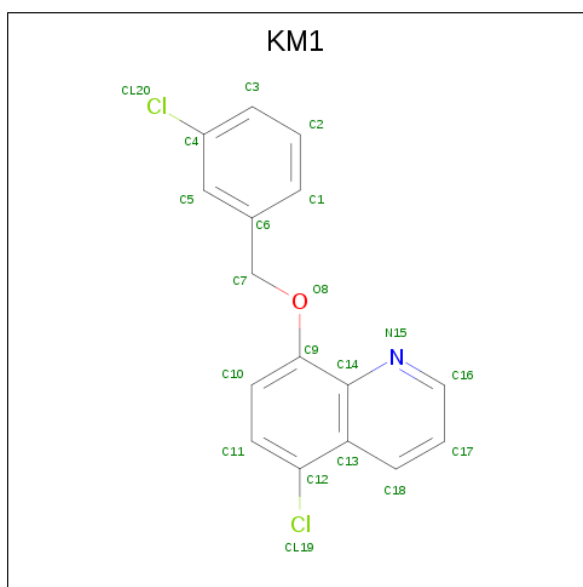
- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	D	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	I	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		
2	X	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 5-chloro-8-[(3-chlorobenzyl)oxy]quinoline (three-letter code: KM1) (formula: C<sub>16</sub>H<sub>11</sub>Cl<sub>2</sub>NO).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	Cl	N	O	
			20	16	2	1	1	
3	G	1	Total	C	Cl	N	O	
			20	16	2	1	1	
3	H	1	Total	C	Cl	N	O	
			20	16	2	1	1	
3	J	1	Total	C	Cl	N	O	
			20	16	2	1	1	
3	P	1	Total	C	Cl	N	O	
			20	16	2	1	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O		
			28	28	0	0
4	B	25	Total	O		
			25	25	0	0
4	C	30	Total	O		
			30	30	0	0
4	D	21	Total	O		
			21	21	0	0
4	E	27	Total	O		
			27	27	0	0
4	F	27	Total	O		
			27	27	0	0
4	G	22	Total	O		
			22	22	0	0

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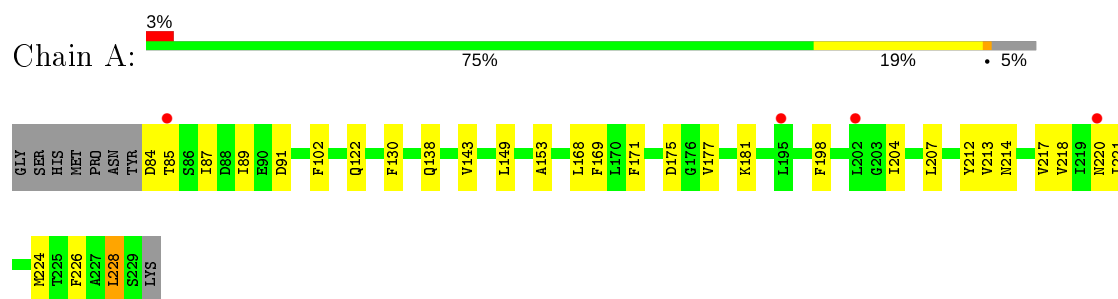
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	18	Total 18	O 18	0	0
4	I	30	Total 30	O 30	0	0
4	J	23	Total 23	O 23	0	0
4	K	28	Total 28	O 28	0	0
4	L	22	Total 22	O 22	0	0
4	M	21	Total 21	O 21	0	0
4	N	29	Total 29	O 29	0	0
4	O	16	Total 16	O 16	0	0
4	P	24	Total 24	O 24	0	0
4	Q	17	Total 17	O 17	0	0
4	R	27	Total 27	O 27	0	0
4	S	21	Total 21	O 21	0	0
4	T	31	Total 31	O 31	0	0
4	U	23	Total 23	O 23	0	0
4	V	23	Total 23	O 23	0	0
4	W	27	Total 27	O 27	0	0
4	X	25	Total 25	O 25	0	0

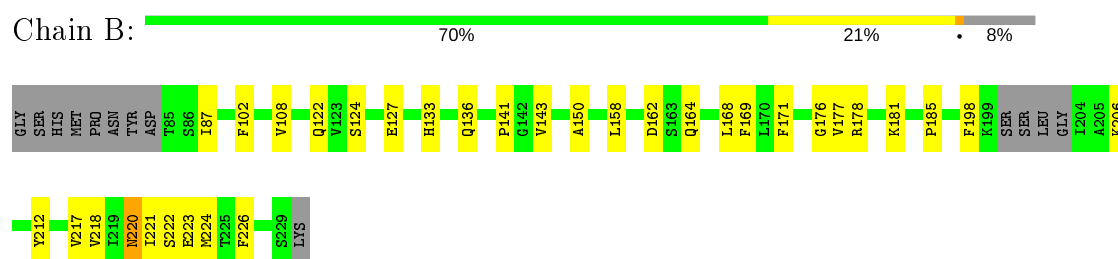
### 3 Residue-property plots [i](#)

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

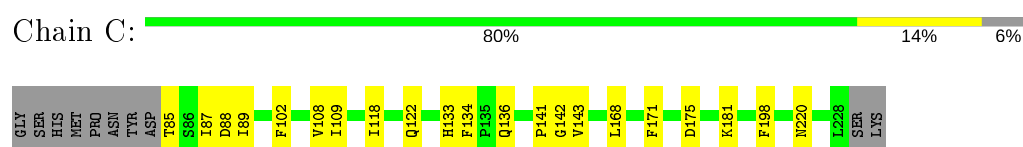
#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase



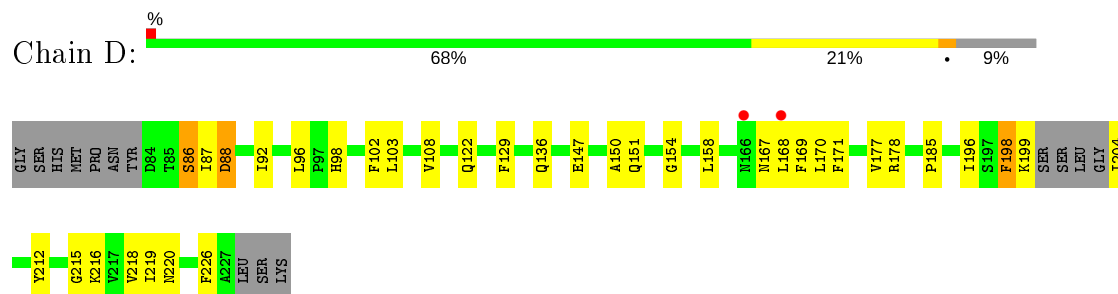
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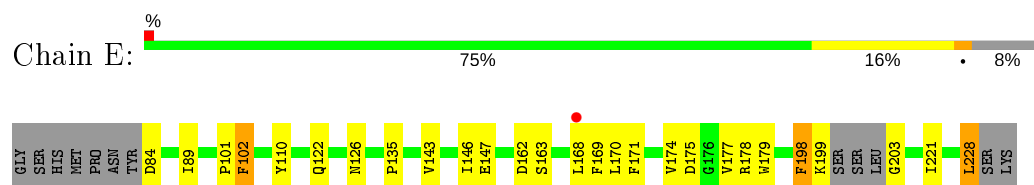
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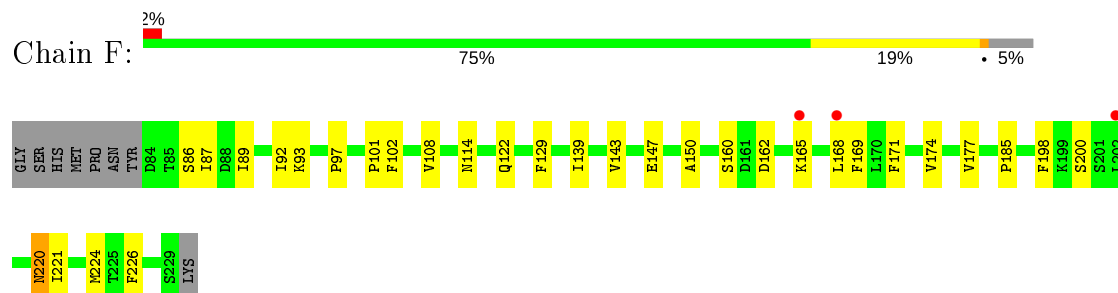
#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase



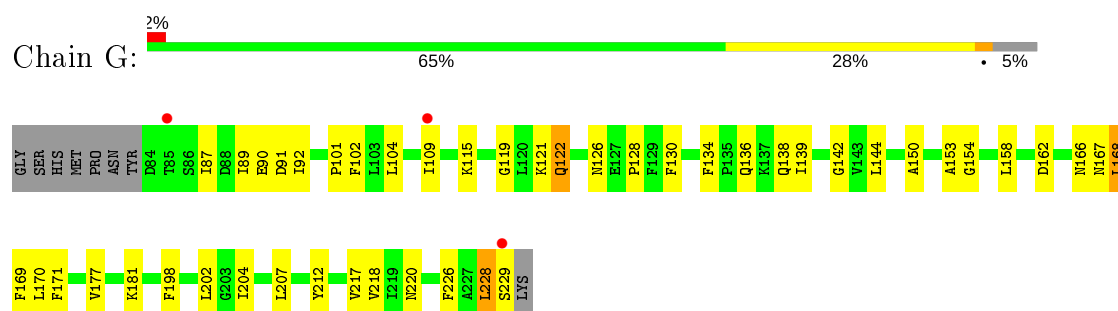
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



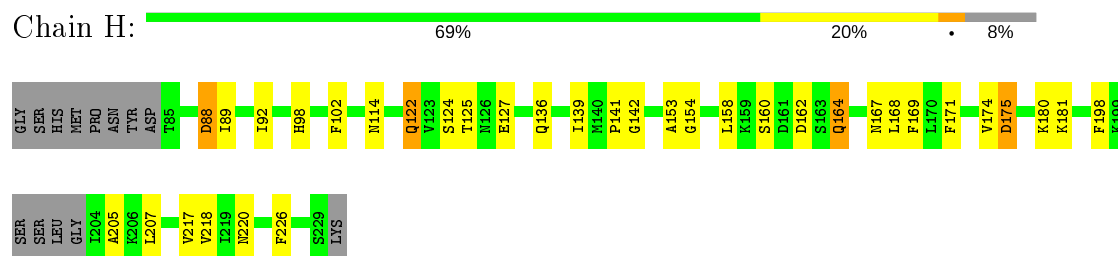
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



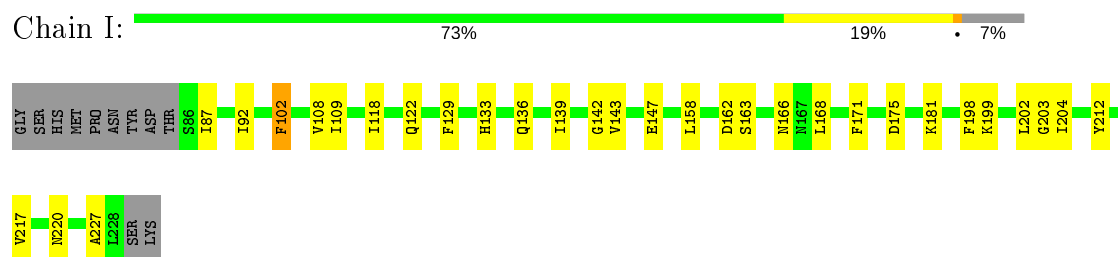
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



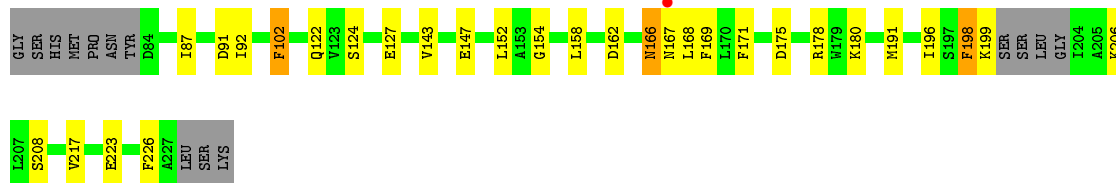
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



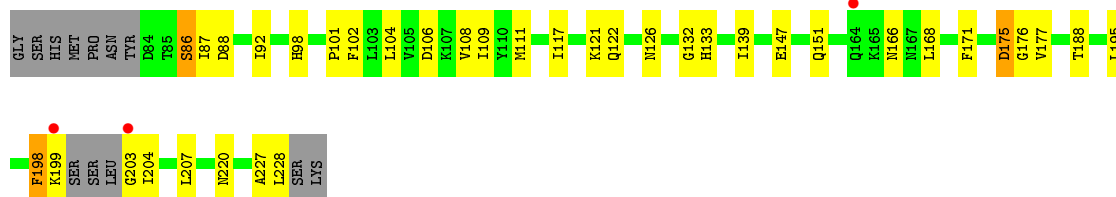
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



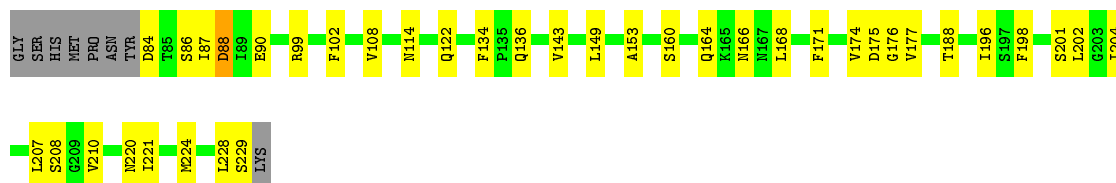
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



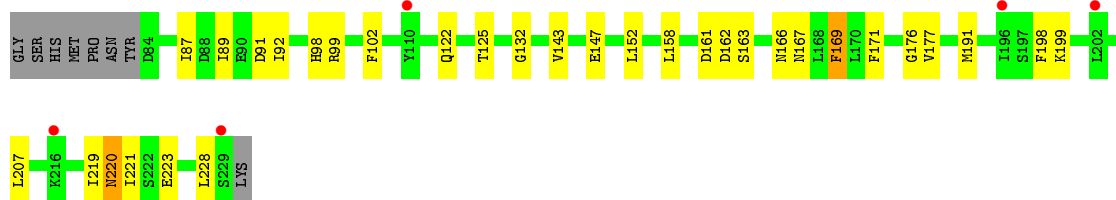
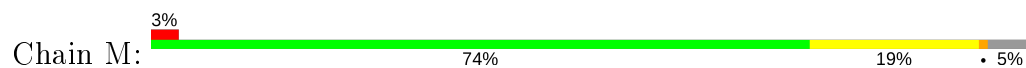
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



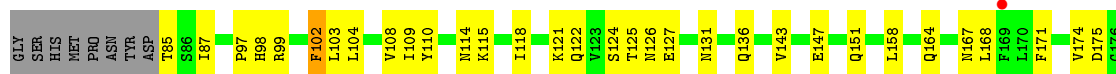
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

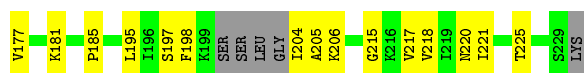


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

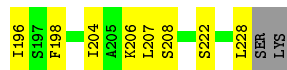


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase





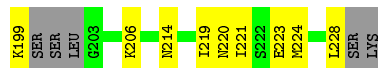
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

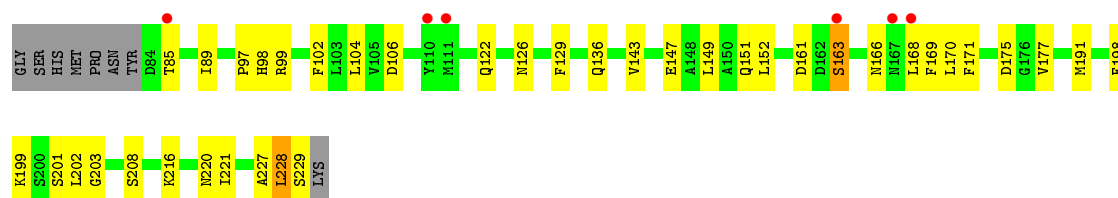


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

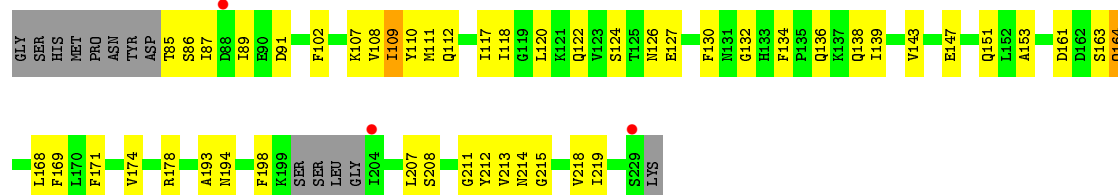


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

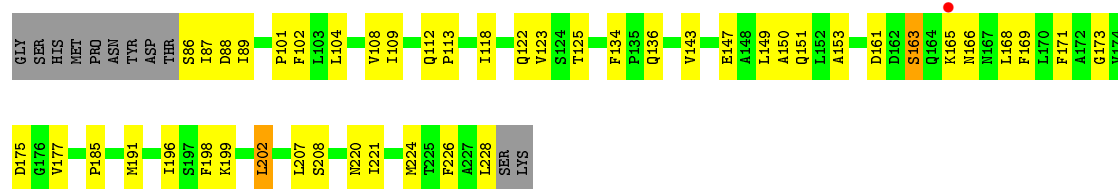




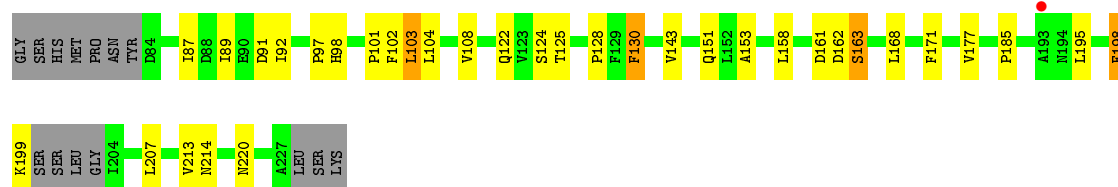
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



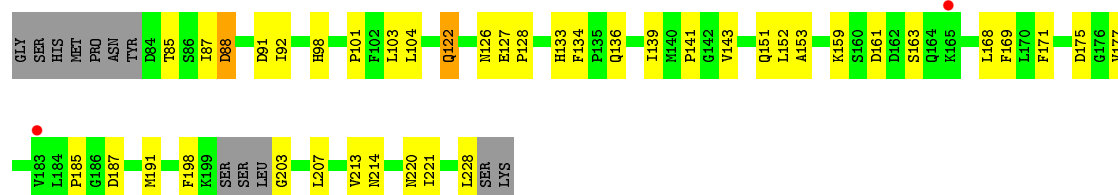
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



● Molecule 1: Beta-hydroxyacyl-ACP dehydratase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.05Å 217.05Å 157.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.85 – 2.60 41.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.85-2.60) 96.2 (41.85-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.226 , 0.264 0.225 , 0.262	Depositor DCC
$R_{free}$ test set	5371 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 18.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.368 for -k,-h,-l	Xtriage
Reported twinning fraction	0.525 for H, K, L 0.475 for -H, K, -L	Depositor
Outliers	0 of 107501 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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 30.39 % 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 1.3187e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, KM1

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	0.62	1/1553 (0.1%)
1	B	0.51	0/1115	0.59	0/1508
1	C	0.49	0/1138	0.63	0/1539
1	D	0.49	0/1096	0.63	0/1485
1	E	0.45	0/1124	0.61	0/1520
1	F	0.47	0/1149	0.57	0/1554
1	G	0.51	0/1147	0.65	1/1553 (0.1%)
1	H	0.50	0/1112	0.62	0/1504
1	I	0.44	0/1131	0.59	0/1529
1	J	0.46	0/1100	0.62	0/1489
1	K	0.51	0/1120	0.60	0/1516
1	L	0.43	0/1148	0.63	0/1553
1	M	0.51	0/1147	0.61	0/1553
1	N	0.51	0/1108	0.66	0/1499
1	O	0.49	0/1132	0.65	0/1532
1	P	0.52	0/1091	0.64	0/1477
1	Q	0.48	0/1117	0.61	0/1511
1	R	0.49	0/1152	0.62	0/1558
1	S	0.49	0/1147	0.63	0/1553
1	T	0.51	0/1111	0.62	0/1504
1	U	0.51	0/1128	0.59	0/1525
1	V	0.50	0/1100	0.62	0/1489
1	W	0.50	0/1121	0.61	0/1516
1	X	0.52	0/1152	0.62	0/1558
All	All	0.49	0/27033	0.62	2/36578 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	LEU	CA-CB-CG	5.79	128.61	115.30
1	G	228	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1125	0	1165	20	0
1	B	1094	0	1133	19	0
1	C	1116	0	1164	20	0
1	D	1075	0	1092	42	0
1	E	1103	0	1144	22	0
1	F	1127	0	1164	22	0
1	G	1125	0	1165	42	0
1	H	1091	0	1124	33	0
1	I	1109	0	1157	24	0
1	J	1079	0	1103	25	0
1	K	1099	0	1133	24	0
1	L	1127	0	1175	21	0
1	M	1125	0	1165	24	0
1	N	1087	0	1118	49	0
1	O	1110	0	1148	29	0
1	P	1070	0	1088	29	0
1	Q	1097	0	1137	27	0
1	R	1130	0	1173	23	0
1	S	1125	0	1165	33	0
1	T	1090	0	1122	50	0
1	U	1106	0	1155	28	0
1	V	1079	0	1103	23	0
1	W	1100	0	1135	35	0
1	X	1130	0	1173	22	0
2	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	0	8	1	0
2	E	6	0	8	3	0
2	G	6	0	8	2	0
2	I	6	0	8	1	0
2	K	6	0	8	2	0
2	M	6	0	8	0	0
2	O	6	0	8	1	0
2	Q	6	0	8	4	0
2	S	6	0	8	1	0
2	V	6	0	8	2	0
2	X	6	0	8	1	0
3	D	20	0	11	31	0
3	G	20	0	11	20	0
3	H	20	0	11	19	0
3	J	20	0	11	14	0
3	P	20	0	11	25	0
4	A	28	0	0	0	0
4	B	25	0	0	0	0
4	C	30	0	0	1	0
4	D	21	0	0	2	0
4	E	27	0	0	1	0
4	F	27	0	0	1	0
4	G	22	0	0	1	0
4	H	18	0	0	2	0
4	I	30	0	0	1	0
4	J	23	0	0	4	0
4	K	28	0	0	1	0
4	L	22	0	0	1	0
4	M	21	0	0	1	0
4	N	29	0	0	1	0
4	O	16	0	0	0	0
4	P	24	0	0	0	0
4	Q	17	0	0	1	0
4	R	27	0	0	2	0
4	S	21	0	0	1	0
4	T	31	0	0	2	0
4	U	23	0	0	2	0
4	V	23	0	0	0	0
4	W	27	0	0	1	0
4	X	25	0	0	1	0
All	All	27276	0	27552	584	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 11.

The worst 5 of 584 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:G:154:GLY:HA3	3:G:2:KM1:CL19	1.30	1.59
1:J:154:GLY:HA3	3:J:4:KM1:CL19	1.47	1.51
1:H:154:GLY:HA3	3:H:3:KM1:CL19	1.68	1.31
1:I:139:ILE:HG21	3:J:4:KM1:CL20	1.69	1.29
1:P:154:GLY:CA	3:P:5:KM1:CL19	2.21	1.24

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%)	137 (95%)	7 (5%)	0	100	100
1	B	137/154 (89%)	131 (96%)	6 (4%)	0	100	100
1	C	142/154 (92%)	137 (96%)	5 (4%)	0	100	100
1	D	136/154 (88%)	129 (95%)	7 (5%)	0	100	100
1	E	138/154 (90%)	131 (95%)	7 (5%)	0	100	100
1	F	144/154 (94%)	132 (92%)	12 (8%)	0	100	100
1	G	144/154 (94%)	135 (94%)	9 (6%)	0	100	100
1	H	137/154 (89%)	128 (93%)	9 (7%)	0	100	100
1	I	141/154 (92%)	134 (95%)	7 (5%)	0	100	100
1	J	136/154 (88%)	129 (95%)	7 (5%)	0	100	100
1	K	138/154 (90%)	132 (96%)	6 (4%)	0	100	100
1	L	144/154 (94%)	135 (94%)	9 (6%)	0	100	100
1	M	144/154 (94%)	137 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	137/154 (89%)	128 (93%)	9 (7%)	0	100	100
1	O	142/154 (92%)	134 (94%)	8 (6%)	0	100	100
1	P	136/154 (88%)	127 (93%)	9 (7%)	0	100	100
1	Q	138/154 (90%)	132 (96%)	6 (4%)	0	100	100
1	R	144/154 (94%)	135 (94%)	9 (6%)	0	100	100
1	S	144/154 (94%)	134 (93%)	10 (7%)	0	100	100
1	T	137/154 (89%)	129 (94%)	8 (6%)	0	100	100
1	U	141/154 (92%)	134 (95%)	7 (5%)	0	100	100
1	V	136/154 (88%)	129 (95%)	7 (5%)	0	100	100
1	W	138/154 (90%)	131 (95%)	7 (5%)	0	100	100
1	X	144/154 (94%)	135 (94%)	9 (6%)	0	100	100
All	All	3362/3696 (91%)	3175 (94%)	187 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	119 (94%)	7 (6%)	21	42
1	B	122/135 (90%)	115 (94%)	7 (6%)	20	41
1	C	125/135 (93%)	117 (94%)	8 (6%)	17	35
1	D	118/135 (87%)	111 (94%)	7 (6%)	19	39
1	E	123/135 (91%)	117 (95%)	6 (5%)	25	48
1	F	126/135 (93%)	119 (94%)	7 (6%)	21	42
1	G	126/135 (93%)	118 (94%)	8 (6%)	18	36
1	H	121/135 (90%)	111 (92%)	10 (8%)	11	22
1	I	124/135 (92%)	116 (94%)	8 (6%)	17	34
1	J	119/135 (88%)	113 (95%)	6 (5%)	24	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	122/135 (90%)	113 (93%)	9 (7%)	13	28
1	L	127/135 (94%)	116 (91%)	11 (9%)	10	20
1	M	126/135 (93%)	120 (95%)	6 (5%)	25	49
1	N	120/135 (89%)	113 (94%)	7 (6%)	20	40
1	O	123/135 (91%)	114 (93%)	9 (7%)	14	28
1	P	116/135 (86%)	108 (93%)	8 (7%)	15	31
1	Q	122/135 (90%)	114 (93%)	8 (7%)	16	33
1	R	127/135 (94%)	117 (92%)	10 (8%)	12	24
1	S	126/135 (93%)	116 (92%)	10 (8%)	12	24
1	T	121/135 (90%)	112 (93%)	9 (7%)	13	28
1	U	123/135 (91%)	112 (91%)	11 (9%)	9	19
1	V	119/135 (88%)	111 (93%)	8 (7%)	16	33
1	W	122/135 (90%)	113 (93%)	9 (7%)	13	28
1	X	127/135 (94%)	117 (92%)	10 (8%)	12	24
All	All	2951/3240 (91%)	2752 (93%)	199 (7%)	16	33

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	171	PHE
1	O	171	PHE
1	W	136	GLN
1	L	204	ILE
1	N	136	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	220	ASN
1	Q	114	ASN
1	X	122	GLN
1	N	151	GLN
1	N	220	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 ⓘ

17 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	1	-	5,5,5	0.37	0	5,5,5	0.66	0
2	GOL	K	6	-	5,5,5	0.35	0	5,5,5	0.54	0
3	KM1	P	5	-	22,22,22	1.17	2 (9%)	30,30,30	1.95	8 (26%)
2	GOL	V	11	-	5,5,5	0.35	0	5,5,5	0.33	0
2	GOL	X	12	-	5,5,5	0.51	0	5,5,5	0.43	0
2	GOL	Q	9	-	5,5,5	0.37	0	5,5,5	0.61	0
2	GOL	M	7	-	5,5,5	0.36	0	5,5,5	0.33	0
3	KM1	G	2	-	22,22,22	1.20	3 (13%)	30,30,30	1.83	9 (30%)
2	GOL	S	10	-	5,5,5	0.47	0	5,5,5	0.32	0
3	KM1	H	3	-	22,22,22	1.30	2 (9%)	30,30,30	2.18	12 (40%)
3	KM1	D	1	-	22,22,22	1.40	3 (13%)	30,30,30	1.82	8 (26%)
2	GOL	E	3	-	5,5,5	0.41	0	5,5,5	0.80	0
2	GOL	G	4	-	5,5,5	0.38	0	5,5,5	0.52	0
3	KM1	J	4	-	22,22,22	1.02	1 (4%)	30,30,30	2.15	7 (23%)
2	GOL	O	8	-	5,5,5	0.37	0	5,5,5	0.25	0
2	GOL	I	5	-	5,5,5	0.27	0	5,5,5	0.29	0
2	GOL	D	2	-	5,5,5	0.41	0	5,5,5	0.48	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	1	-	-	4/4/4/4	-
2	GOL	K	6	-	-	4/4/4/4	-
3	KM1	P	5	-	-	3/5/5/5	0/3/3/3
2	GOL	V	11	-	-	2/4/4/4	-
2	GOL	X	12	-	-	2/4/4/4	-
2	GOL	Q	9	-	-	4/4/4/4	-
2	GOL	M	7	-	-	1/4/4/4	-
3	KM1	G	2	-	-	2/5/5/5	0/3/3/3
2	GOL	S	10	-	-	4/4/4/4	-
3	KM1	H	3	-	-	3/5/5/5	0/3/3/3
3	KM1	D	1	-	-	2/5/5/5	0/3/3/3
2	GOL	E	3	-	-	2/4/4/4	-
2	GOL	G	4	-	-	3/4/4/4	-
3	KM1	J	4	-	-	3/5/5/5	0/3/3/3
2	GOL	O	8	-	-	2/4/4/4	-
2	GOL	I	5	-	-	2/4/4/4	-
2	GOL	D	2	-	-	2/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	KM1	C9-C14	-3.36	1.38	1.42
3	D	1	KM1	C4-CL20	3.12	1.81	1.74
3	P	5	KM1	C4-CL20	2.80	1.80	1.74
3	H	3	KM1	C4-CL20	2.78	1.80	1.74
3	H	3	KM1	C12-C13	-2.63	1.37	1.42

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	4	KM1	O8-C9-C14	6.66	123.35	115.16
3	P	5	KM1	O8-C9-C14	5.76	122.24	115.16
3	H	3	KM1	O8-C7-C6	5.33	125.14	109.16
3	G	2	KM1	O8-C9-C14	4.32	120.47	115.16
3	H	3	KM1	C18-C13-C12	-3.86	118.19	125.06

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	GOL	C1-C2-C3-O3
2	K	6	GOL	O1-C1-C2-C3
2	K	6	GOL	C1-C2-C3-O3
2	K	6	GOL	O2-C2-C3-O3
2	V	11	GOL	C1-C2-C3-O3

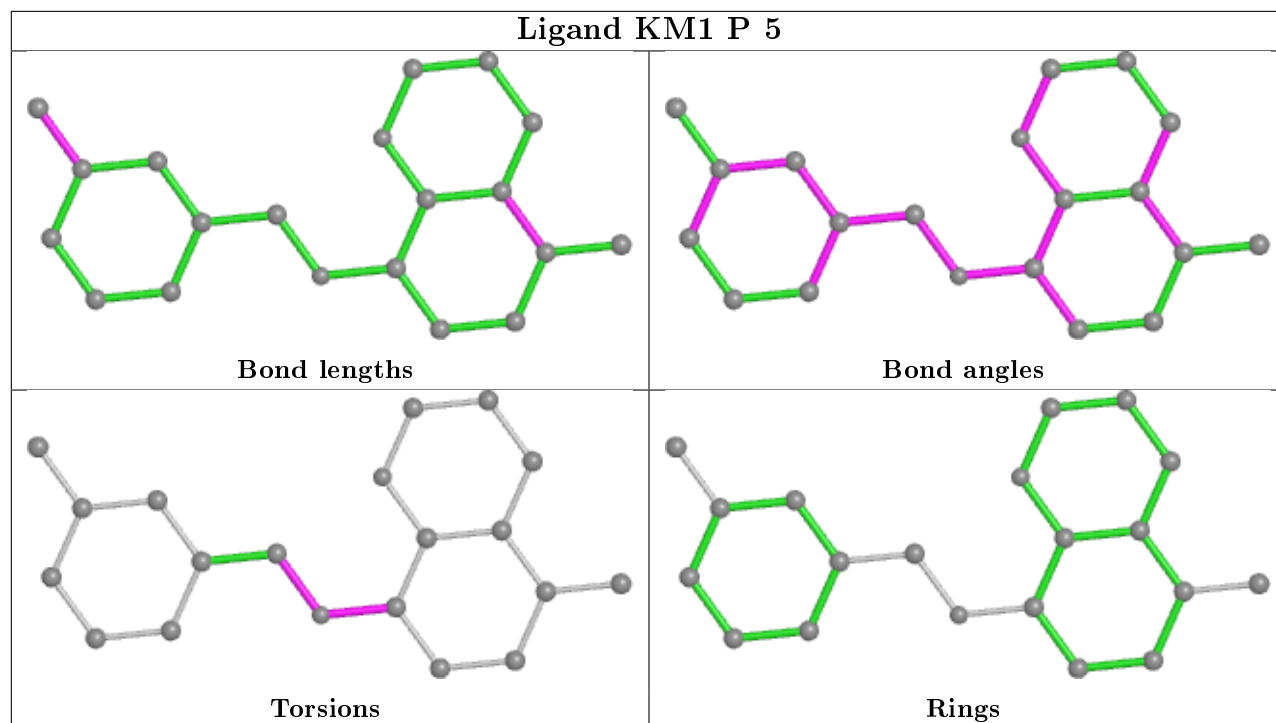
There are no ring outliers.

15 monomers are involved in 127 short contacts:

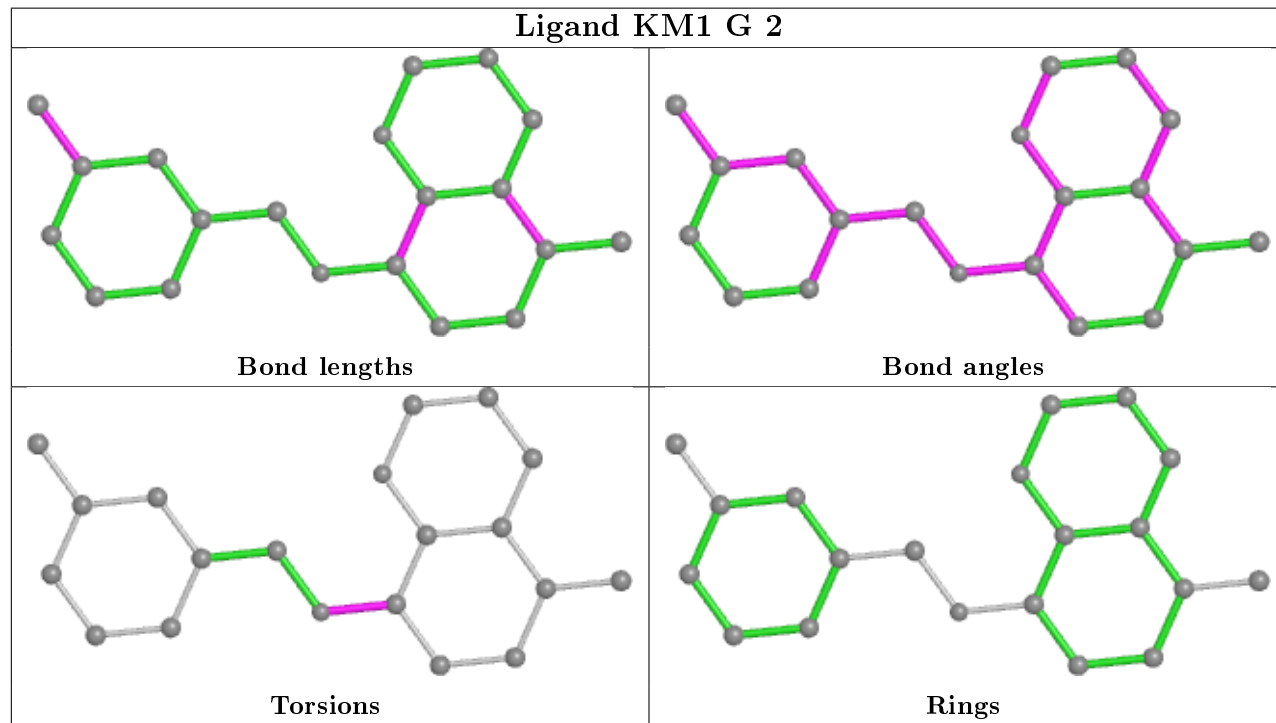
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	6	GOL	2	0
3	P	5	KM1	25	0
2	V	11	GOL	2	0
2	X	12	GOL	1	0
2	Q	9	GOL	4	0
3	G	2	KM1	20	0
2	S	10	GOL	1	0
3	H	3	KM1	19	0
3	D	1	KM1	31	0
2	E	3	GOL	3	0
2	G	4	GOL	2	0
3	J	4	KM1	14	0
2	O	8	GOL	1	0
2	I	5	GOL	1	0
2	D	2	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

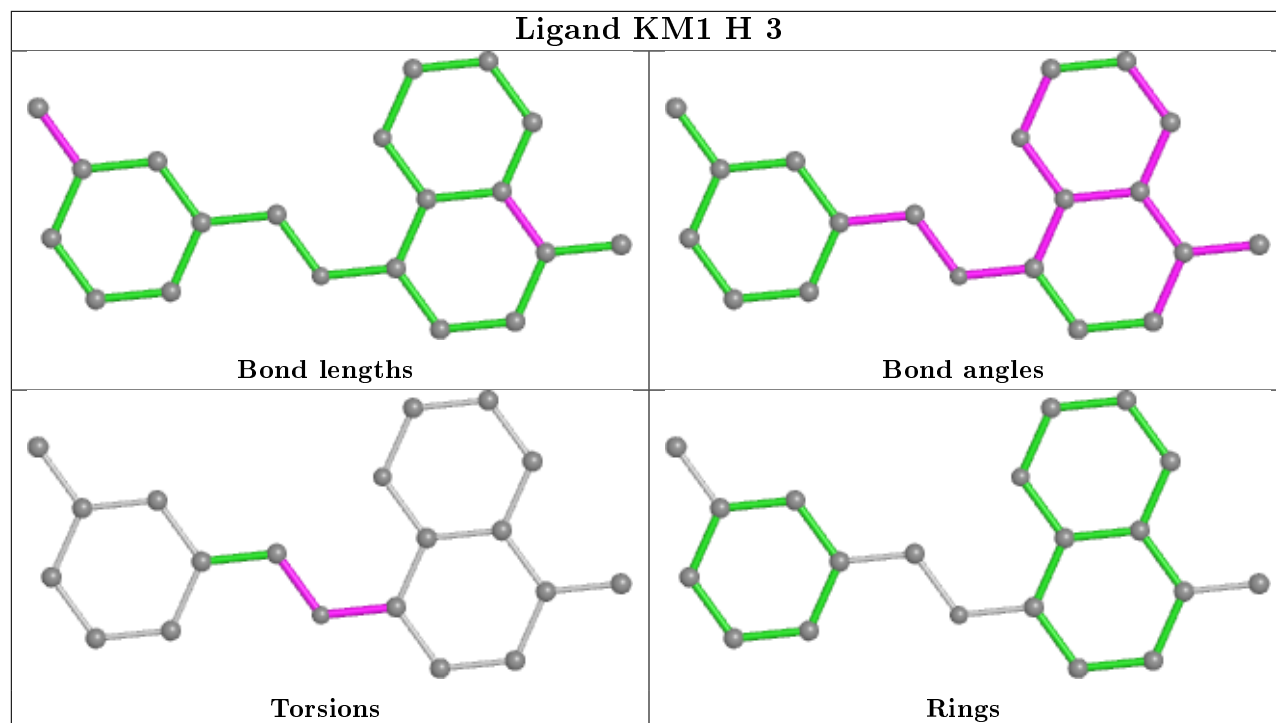
## Ligand KM1 P 5



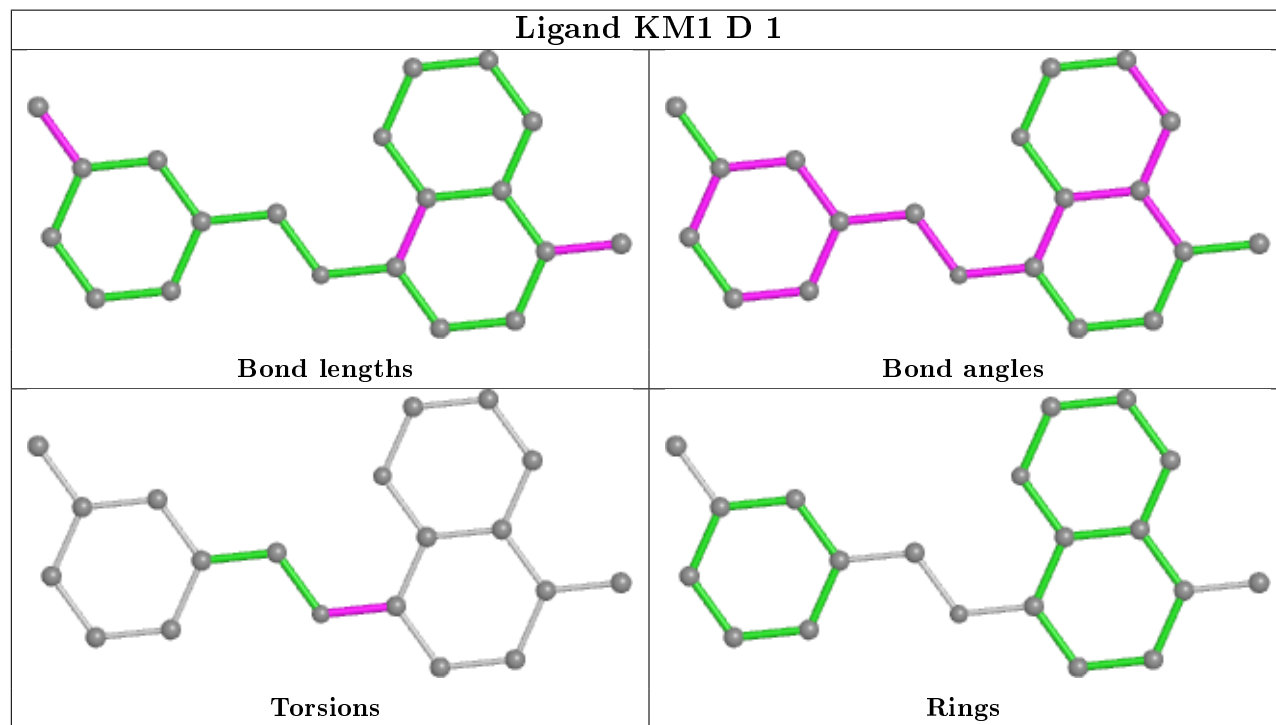
## Ligand KM1 G 2

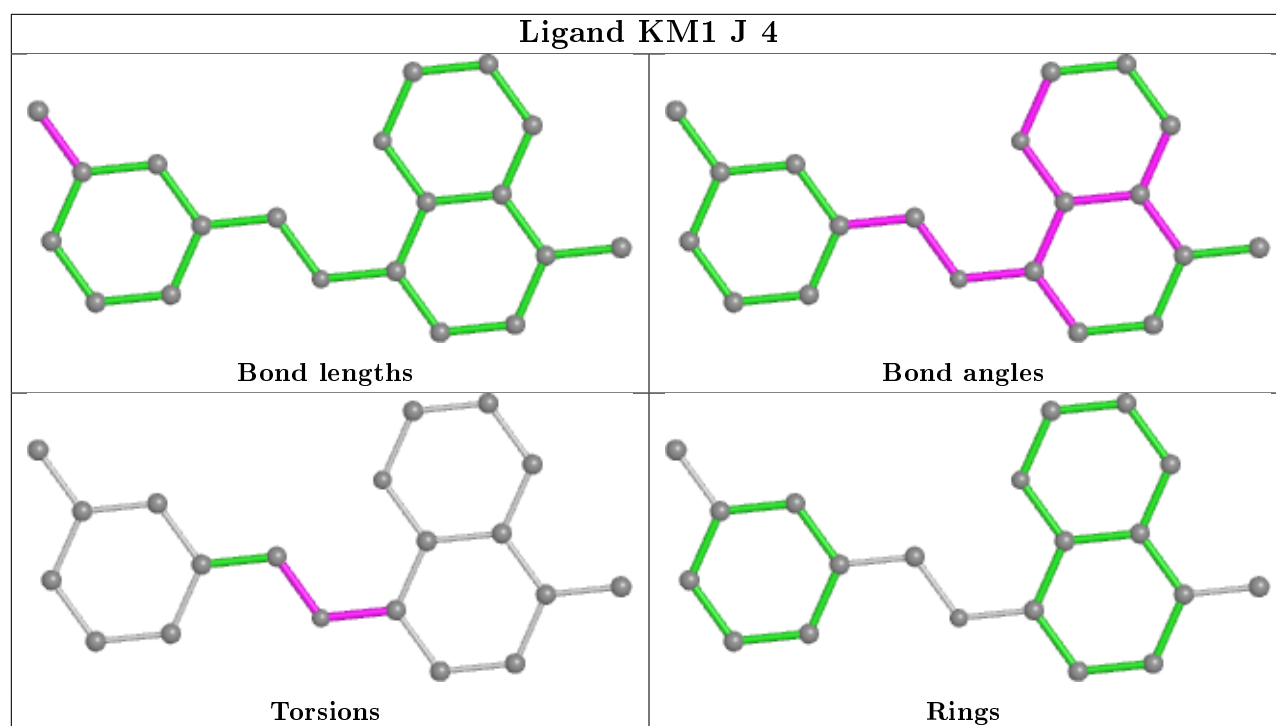


## Ligand KM1 H 3



## Ligand KM1 D 1





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	146/154 (94%)	-0.01	4 (2%) 54 48	30, 44, 60, 65	0
1	B	141/154 (91%)	-0.16	0 100 100	31, 43, 58, 62	0
1	C	144/154 (93%)	-0.16	0 100 100	30, 42, 59, 63	0
1	D	140/154 (90%)	-0.12	2 (1%) 75 71	31, 43, 60, 62	1 (0%)
1	E	142/154 (92%)	-0.22	1 (0%) 87 86	30, 43, 58, 61	0
1	F	146/154 (94%)	-0.08	3 (2%) 63 58	30, 43, 61, 62	0
1	G	146/154 (94%)	-0.10	3 (2%) 63 58	30, 44, 60, 62	1 (0%)
1	H	141/154 (91%)	-0.24	0 100 100	30, 43, 58, 63	0
1	I	143/154 (92%)	-0.16	0 100 100	30, 43, 59, 62	0
1	J	140/154 (90%)	-0.13	1 (0%) 87 86	30, 43, 59, 62	1 (0%)
1	K	142/154 (92%)	-0.05	3 (2%) 63 58	30, 43, 59, 64	2 (1%)
1	L	146/154 (94%)	-0.14	0 100 100	30, 43, 59, 63	0
1	M	146/154 (94%)	0.21	5 (3%) 45 38	33, 44, 61, 63	0
1	N	141/154 (91%)	-0.12	1 (0%) 87 86	32, 44, 60, 62	1 (0%)
1	O	144/154 (93%)	-0.13	4 (2%) 53 46	32, 44, 60, 63	0
1	P	140/154 (90%)	0.05	6 (4%) 35 28	33, 45, 60, 64	1 (0%)
1	Q	142/154 (92%)	-0.16	1 (0%) 87 86	32, 44, 58, 62	0
1	R	146/154 (94%)	0.01	3 (2%) 63 58	32, 45, 60, 61	0
1	S	146/154 (94%)	0.00	6 (4%) 37 30	33, 44, 60, 63	0
1	T	141/154 (91%)	-0.01	3 (2%) 63 58	34, 44, 58, 61	0
1	U	143/154 (92%)	-0.14	1 (0%) 87 86	33, 44, 60, 63	1 (0%)
1	V	140/154 (90%)	-0.08	1 (0%) 87 86	33, 44, 61, 63	0
1	W	142/154 (92%)	0.05	2 (1%) 75 71	34, 45, 58, 62	0
1	X	146/154 (94%)	0.14	6 (4%) 37 30	33, 44, 61, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3434/3696 (92%)	-0.07	56 (1%) 72 68	30, 44, 60, 65	8 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	85	THR	5.3
1	P	164	GLN	5.0
1	P	166	ASN	4.7
1	P	227	ALA	4.6
1	O	163	SER	4.3

## 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, 95<sup>th</sup> 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.

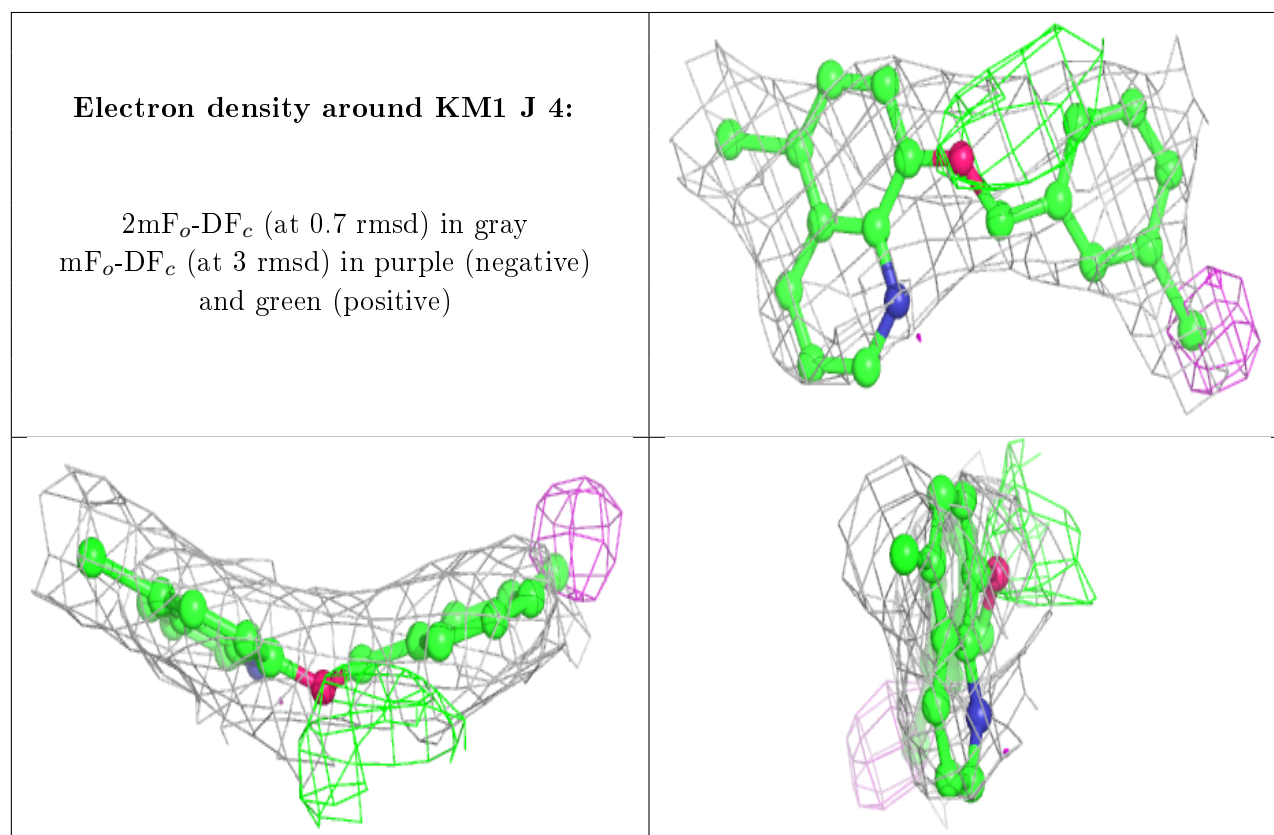
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	KM1	J	4	20/20	0.85	0.25	48,51,53,54	2
3	KM1	P	5	20/20	0.86	0.16	46,48,51,53	0
3	KM1	G	2	20/20	0.87	0.24	40,45,47,49	4
3	KM1	H	3	20/20	0.89	0.23	38,41,41,44	16
3	KM1	D	1	20/20	0.90	0.15	51,52,54,56	0
2	GOL	Q	9	6/6	0.91	0.15	37,39,40,43	0
2	GOL	E	3	6/6	0.92	0.24	35,36,37,39	0
2	GOL	X	12	6/6	0.92	0.16	49,50,51,52	0
2	GOL	G	4	6/6	0.95	0.17	25,27,28,30	0
2	GOL	K	6	6/6	0.95	0.14	41,43,43,44	0
2	GOL	I	5	6/6	0.95	0.17	42,42,43,46	0
2	GOL	O	8	6/6	0.96	0.13	29,31,32,36	0
2	GOL	M	7	6/6	0.96	0.24	51,51,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	S	10	6/6	0.97	0.14	41,42,43,44	0
2	GOL	V	11	6/6	0.97	0.16	34,35,36,36	0
2	GOL	D	2	6/6	0.97	0.15	31,32,33,33	0
2	GOL	A	1	6/6	0.98	0.16	39,40,41,42	0

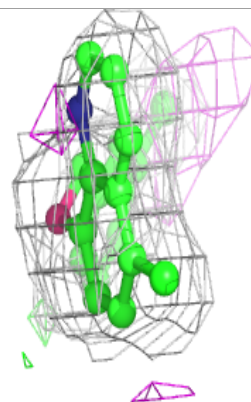
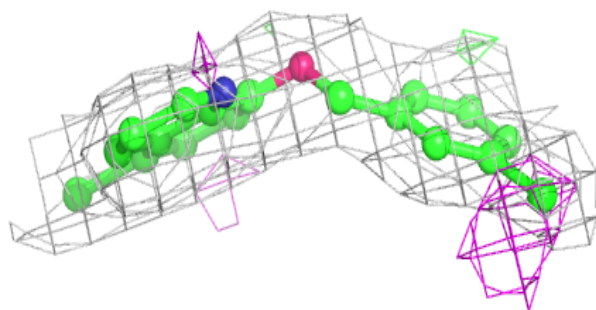
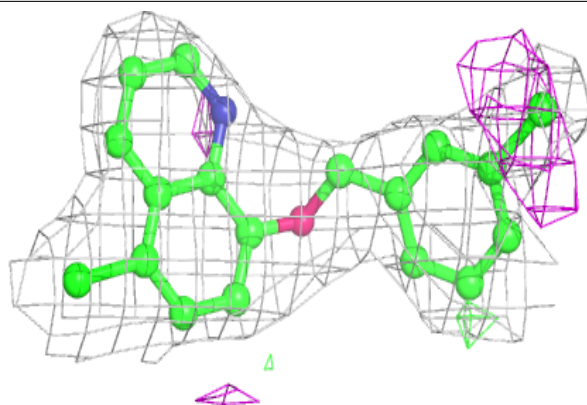
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



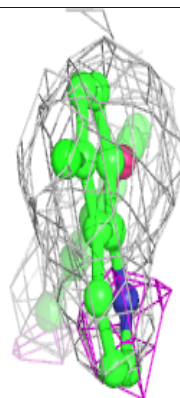
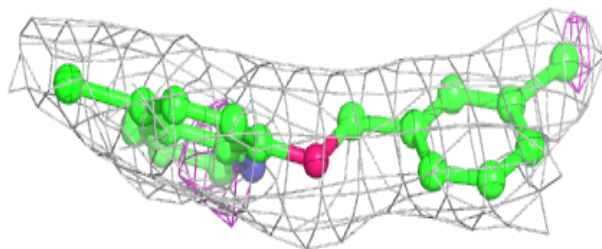
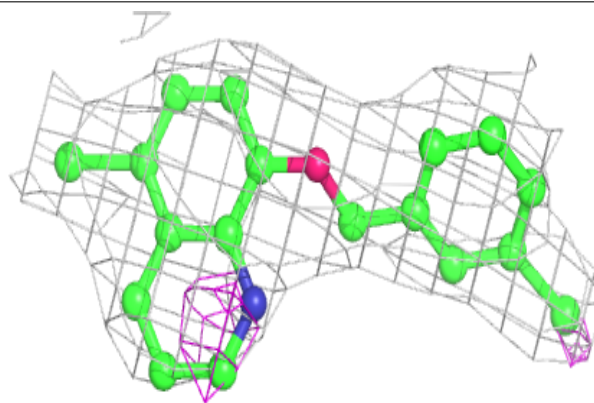


**Electron density around KM1 P 5:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

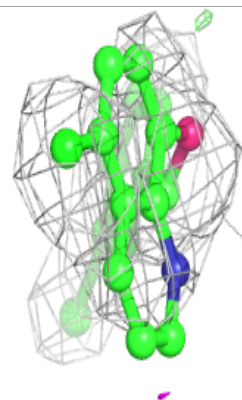
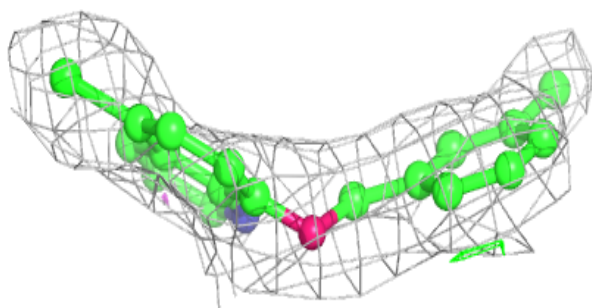
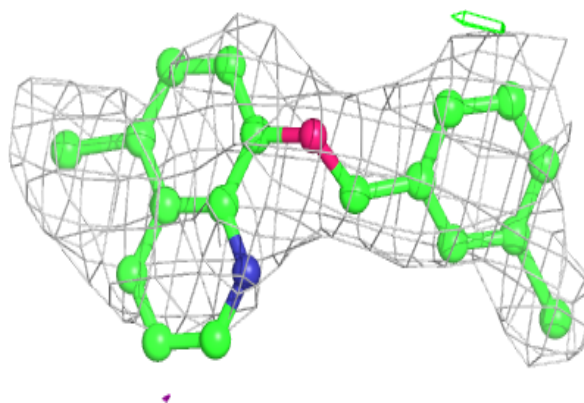
**Electron density around KM1 G 2:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

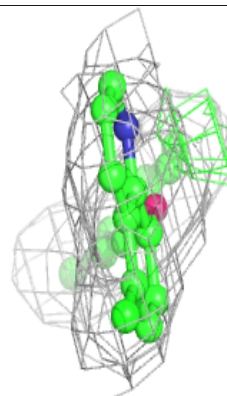
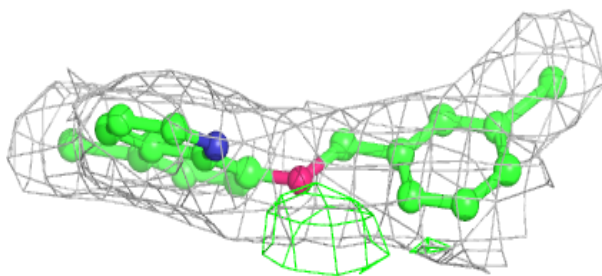
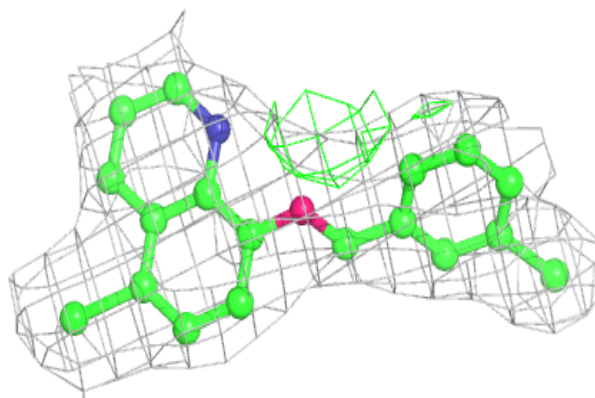


**Electron density around KM1 H 3:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around KM1 D 1:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.