



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID : 3AZ8  
Title : Beta-Hydroxyacyl-Acyl Carrier Protein Dehydratase (FabZ) from Plasmodium falciparum in complex with NAS21  
Authors : Maity, K.; Venkata, B.S.; Kapoor, N.; Surolia, N.; Surolia, A.; Suguna, K.  
Deposited on : 2011-05-20  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

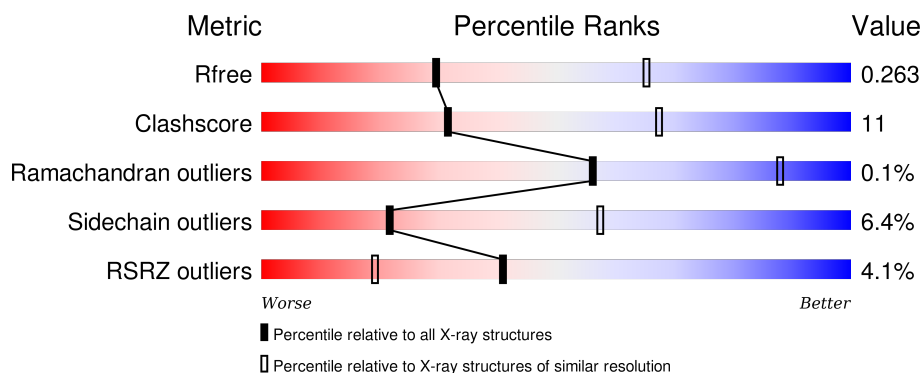
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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>4%</div> <div>73% 21% • 6%</div> </div>
1	B	154	<div> <div>%</div> <div>75% 16% 8%</div> </div>
1	C	154	<div> <div>%</div> <div>75% 18% • 6%</div> </div>
1	D	154	<div> <div>3%</div> <div>77% 14% 9%</div> </div>
1	E	154	<div> <div>%</div> <div>74% 18% • 7%</div> </div>

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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
3	PEG	I	20	-	-	-	X
3	PEG	S	19	-	-	-	X
5	S21	D	231	-	-	X	-
5	S21	F	231	-	-	X	X
5	S21	P	4	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	S21	R	1	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27454 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	145	Total	C	N	O	S	0	0	0
			1121	731	184	201	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	143	Total	C	N	O	S	0	0	0
			1109	722	182	200	5			
1	F	146	Total	C	N	O	S	0	1	0
			1136	736	188	207	5			
1	G	145	Total	C	N	O	S	0	0	0
			1111	722	183	201	5			
1	H	141	Total	C	N	O	S	0	0	0
			1090	710	179	196	5			
1	I	143	Total	C	N	O	S	0	1	0
			1118	732	183	198	5			
1	J	144	Total	C	N	O	S	0	0	0
			1098	714	180	199	5			
1	K	145	Total	C	N	O	S	0	0	0
			1123	731	184	203	5			
1	L	146	Total	C	N	O	S	0	0	0
			1124	728	186	205	5			
1	M	145	Total	C	N	O	S	0	0	0
			1123	731	184	203	5			
1	N	145	Total	C	N	O	S	0	0	0
			1114	724	184	201	5			
1	O	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	P	145	Total	C	N	O	S	0	0	0
			1099	714	181	199	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	1	0
			1133	740	184	204	5			
1	T	142	Total	C	N	O	S	0	0	0
			1098	715	181	197	5			
1	U	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	V	144	Total	C	N	O	S	0	0	0
			1098	713	180	200	5			
1	W	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	X	145	Total	C	N	O	S	0	0	0
			1119	727	185	202	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

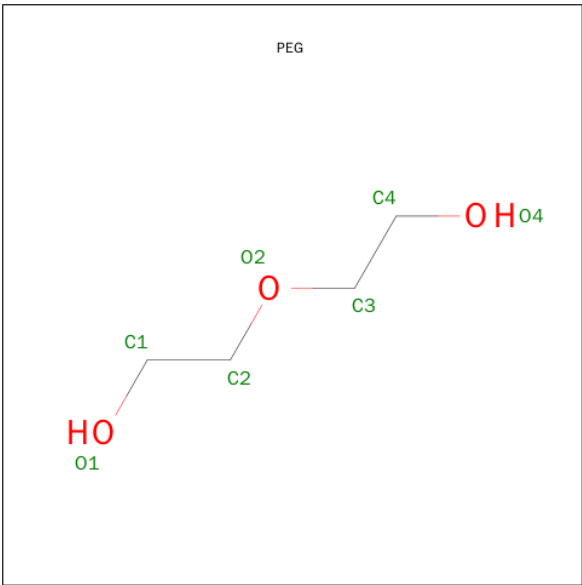
- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





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	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	L	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	P	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	W	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		
3	H	1	Total	C	O	0	0
			7	4	3		
3	I	1	Total	C	O	0	0
			7	4	3		
3	I	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	Q	1	Total C O 7 4 3	0	0
3	Q	1	Total C O 7 4 3	0	0
3	Q	1	Total C O 7 4 3	0	0
3	R	1	Total C O 7 4 3	0	0
3	R	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	U	1	Total C O 7 4 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

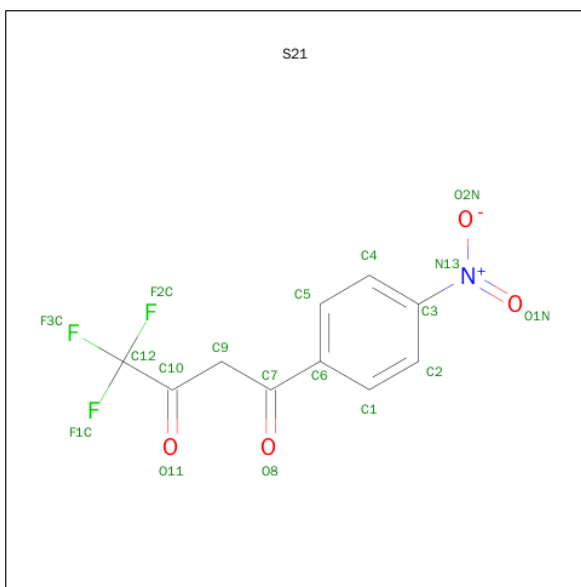
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

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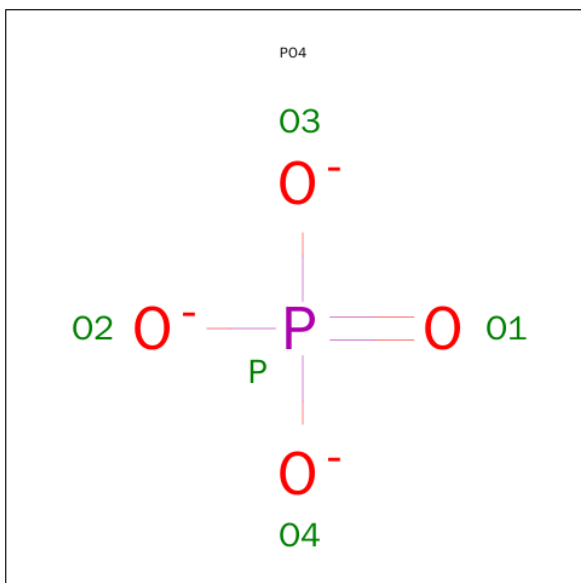
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	I	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	V	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	T	1	Total Cl 1 1	0	0
4	N	1	Total Cl 1 1	0	0
4	U	1	Total Cl 1 1	0	0
4	O	1	Total Cl 1 1	0	0
4	R	1	Total Cl 1 1	0	0
4	L	1	Total Cl 1 1	0	0
4	S	1	Total Cl 1 1	0	0
4	M	1	Total Cl 1 1	0	0

- Molecule 5 is 4,4,4-TRIFLUORO-1-(4-NITROPHENYL)BUTANE-1,3-DIONE (three-letter code: S21) (formula: C<sub>10</sub>H<sub>6</sub>F<sub>3</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	F	N	O	0	0
			18	10	3	1	4		
5	F	1	Total	C	F	N	O	0	0
			18	10	3	1	4		
5	P	1	Total	C	F	N	O	0	0
			18	10	3	1	4		
5	R	1	Total	C	F	N	O	0	0
			18	10	3	1	4		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	10	Total	O		0	0
			10	10			
7	B	21	Total	O		0	0
			21	21			
7	C	27	Total	O		0	0
			27	27			
7	D	19	Total	O		0	0
			19	19			
7	E	21	Total	O		0	0
			21	21			
7	F	25	Total	O		0	0
			25	25			
7	G	18	Total	O		0	0
			18	18			
7	H	16	Total	O		0	0
			16	16			
7	I	10	Total	O		0	0
			10	10			
7	J	23	Total	O		0	0
			23	23			
7	K	12	Total	O		0	0
			12	12			
7	L	15	Total	O		0	0
			15	15			
7	M	9	Total	O		0	0
			9	9			
7	N	18	Total	O		0	0
			18	18			
7	O	19	Total	O		0	0
			19	19			
7	P	22	Total	O		0	0
			22	22			
7	Q	16	Total	O		0	0
			16	16			
7	R	26	Total	O		0	0
			26	26			
7	S	9	Total	O		0	0
			9	9			

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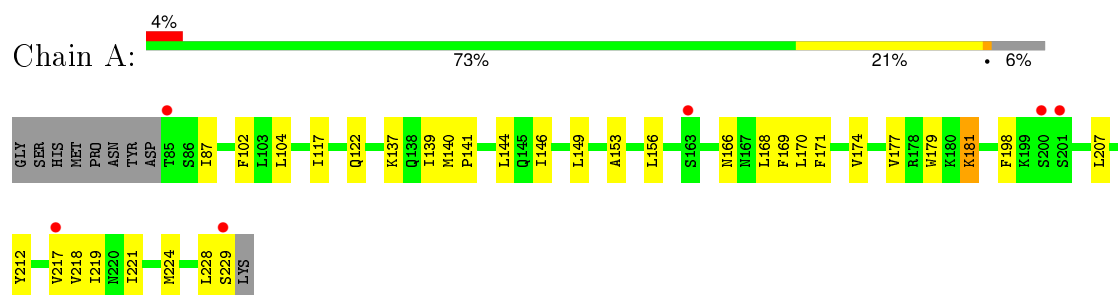
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	19	Total 19	O 19	0	0
7	U	18	Total 18	O 18	0	0
7	V	13	Total 13	O 13	0	0
7	W	12	Total 12	O 12	0	0
7	X	17	Total 17	O 17	0	0

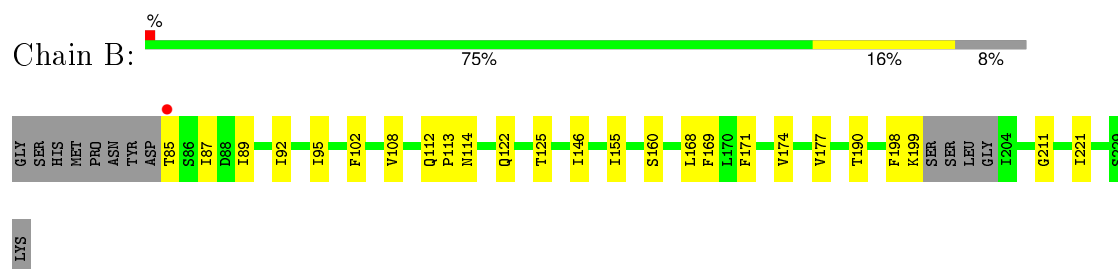
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

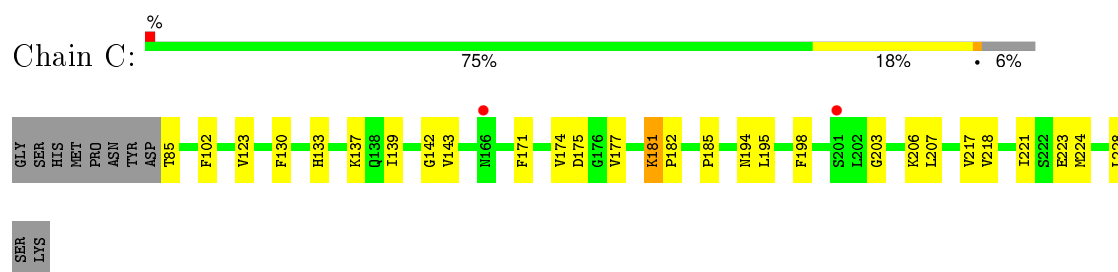
#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase



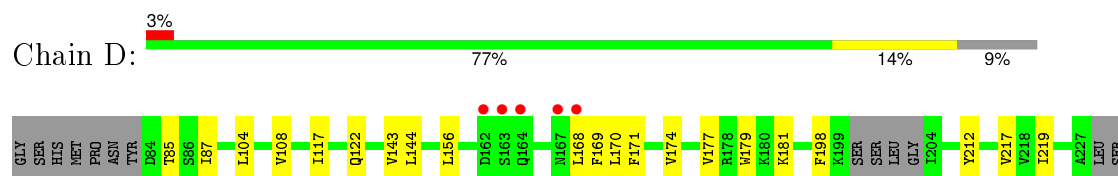
#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase



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




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






LYS

- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain E: 

A227  
L228  
SER  
LYS

- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain F: 

L207  
V210  
V218  
V219  
N220  
A227  
L228  
S229  
LYS

- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain G: 

N166  
F171  
V177  
V178  
M179  
K180  
K181  
V183  
V184  
L185  
G186  
D187  
T188  
L189  
M191  
T196  
S197  
F198  
S201  
L202  
G203  
L204  
S208  
Y212  
V213  
N214  
G215  
K216  
V217  
V218  
I219  
I221  
L228  
S229  
LYS

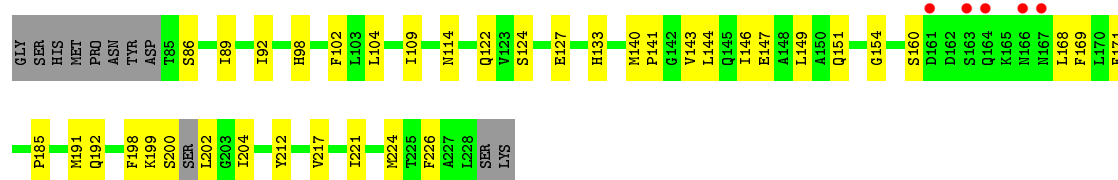
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain H: 

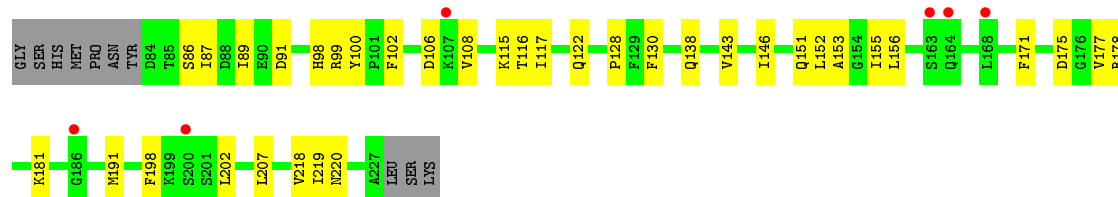
G142  
V143  
L144  
Q145  
I146  
E147  
A148  
L149  
A150  
Q151  
L152  
A153  
S160  
S163  
Q164  
K165  
N166  
M167  
L168  
F169  
L170  
F171  
V174  
V177  
G186  
L195  
F198  
K199  
SER  
SER  
LEU  
GLY  
I204  
A205  
K206  
L207  
Y212  
V213  
N214  
G215  
K216  
V217  
V218  
I219  
N220  
I221  
S222  
E223  
S229  
LYS

- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

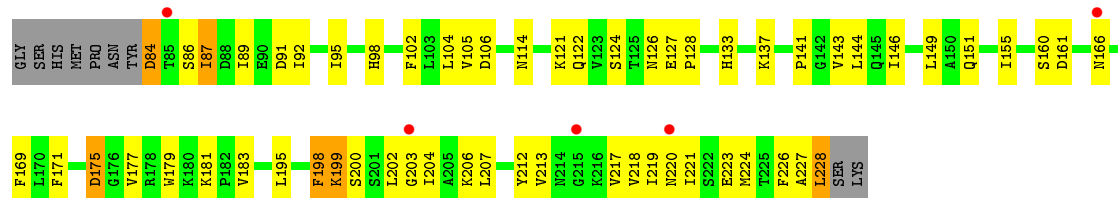
Chain I: 



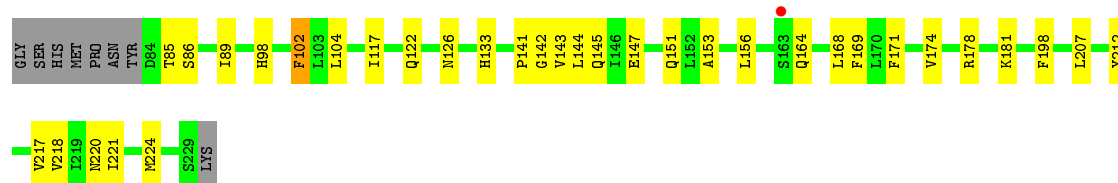
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



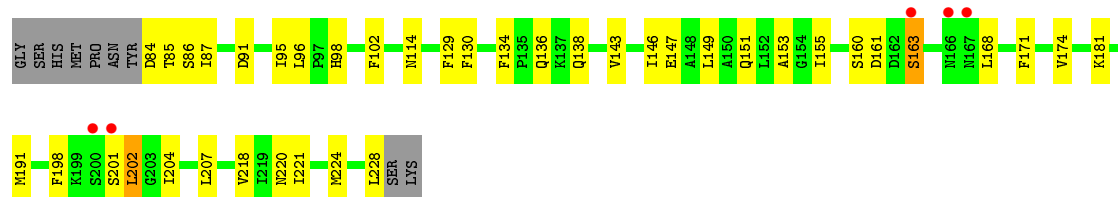
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



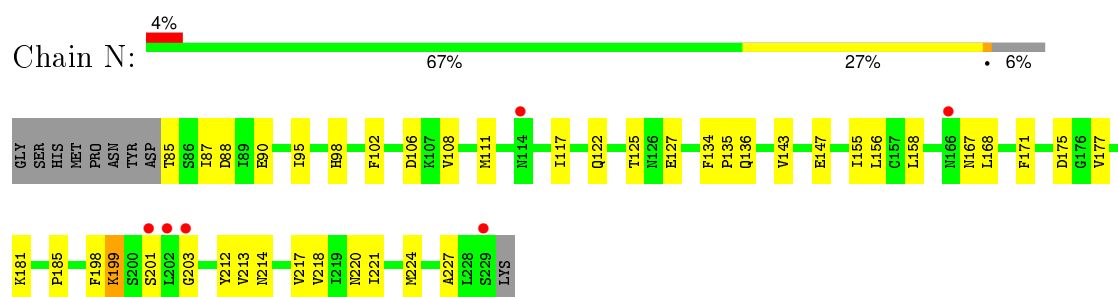
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



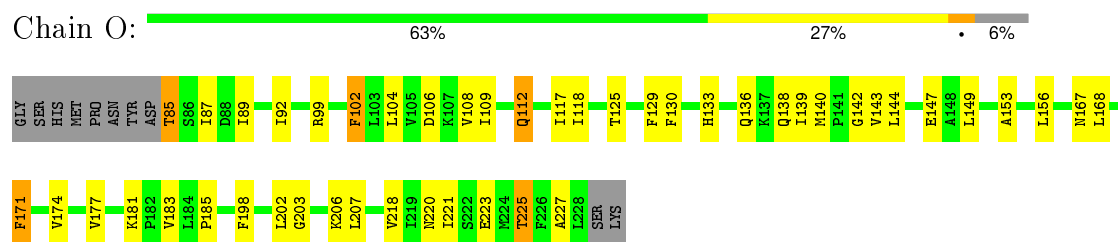
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



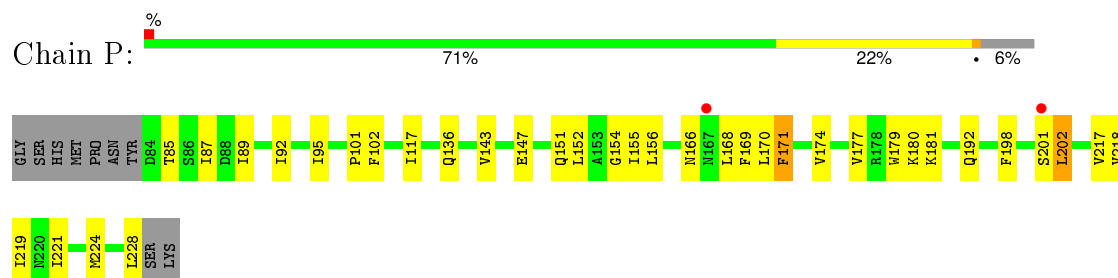
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



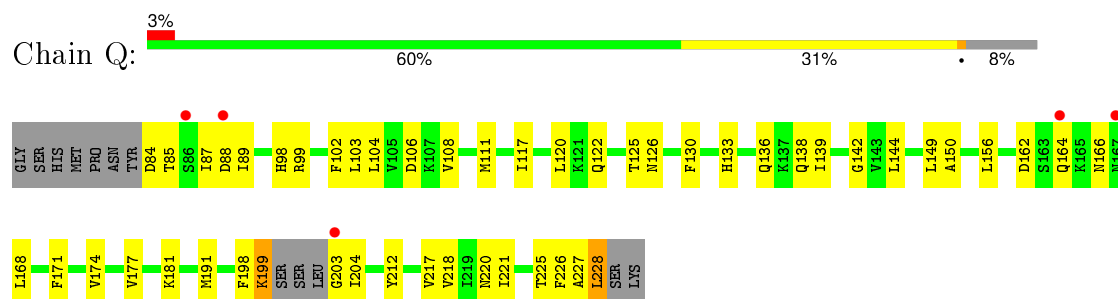
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



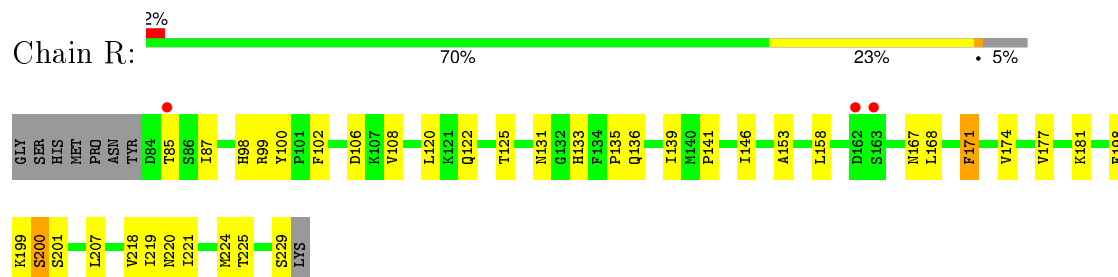
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



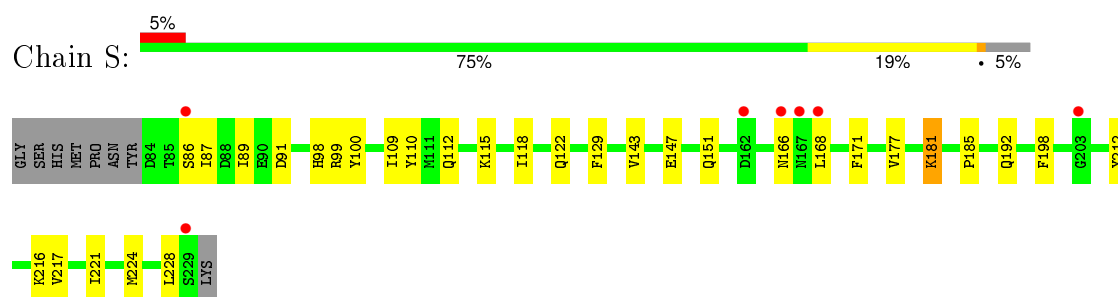
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



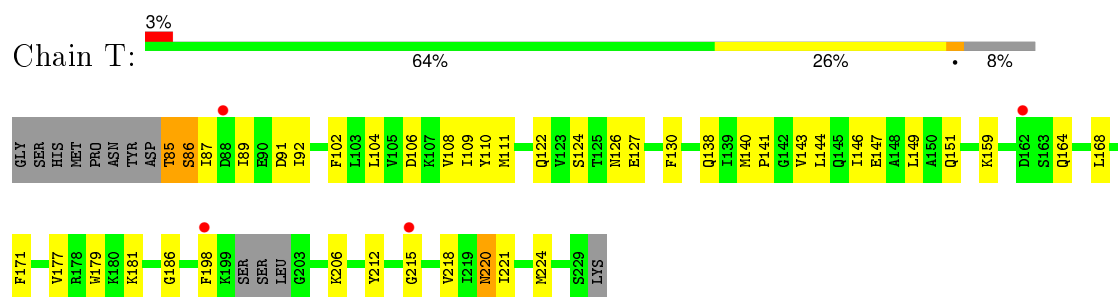
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



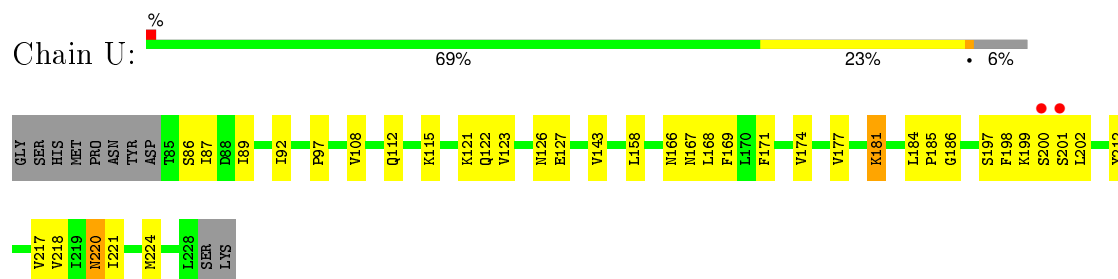
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



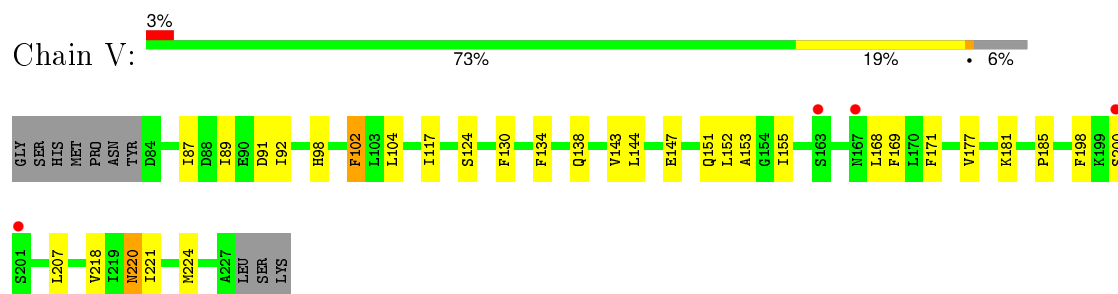
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



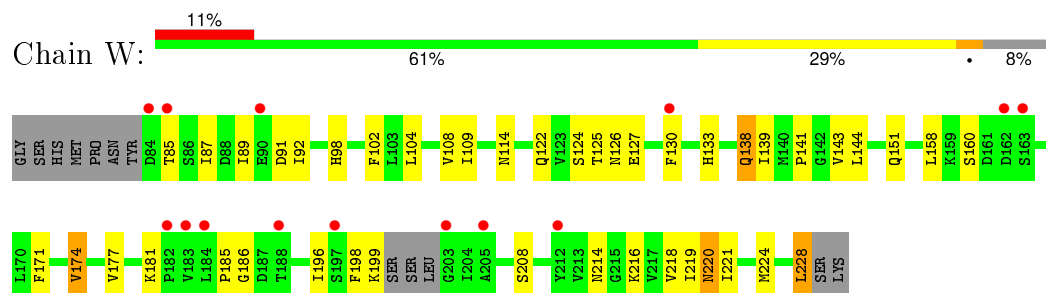
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



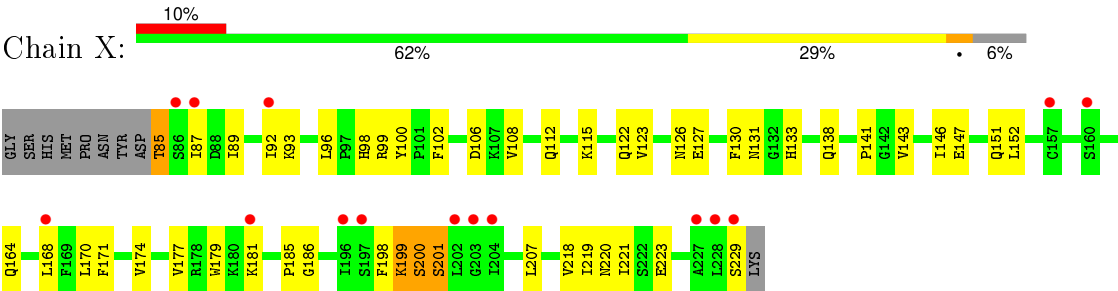
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- 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, $\alpha$ , $\beta$ , $\gamma$	218.99Å 218.99Å 157.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.62 – 3.10 51.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (51.62-3.10) 99.6 (51.62-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.206 , 0.266 0.203 , 0.263	Depositor DCC
$R_{free}$ test set	3394 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 13.2	EDS
Estimated twinning fraction	0.558 for H, K, L 0.442 for -H, K, -L 0.419 for -k,-h,-l	Xtriage
Reported twinning fraction	0.558 for H, K, L 0.442 for -H, K, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 66984 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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 40.61 % 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 2.6688e-04.*

<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, 0.375 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: PEG, GOL, PO4, S21, CL

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	0.55	0/1143	0.57	0/1546
1	B	0.61	0/1115	0.58	0/1508
1	C	0.53	0/1138	0.60	0/1539
1	D	0.59	0/1096	0.60	0/1485
1	E	0.54	0/1130	0.61	0/1528
1	F	0.58	0/1158	0.60	0/1566
1	G	0.72	1/1132 (0.1%)	0.63	0/1533
1	H	0.65	0/1111	0.61	0/1504
1	I	0.57	0/1143	0.59	0/1544
1	J	0.67	0/1120	0.62	0/1520
1	K	0.63	0/1145	0.59	0/1550
1	L	0.57	0/1146	0.59	0/1550
1	M	0.62	0/1145	0.62	0/1550
1	N	0.57	0/1136	0.57	0/1538
1	O	0.54	0/1138	0.61	0/1539
1	P	0.60	0/1121	0.62	0/1520
1	Q	0.57	0/1124	0.62	0/1520
1	R	0.57	0/1149	0.63	0/1554
1	S	0.60	0/1159	0.61	0/1569
1	T	0.65	0/1119	0.60	0/1513
1	U	0.64	1/1138 (0.1%)	0.61	0/1539
1	V	0.61	0/1120	0.63	0/1519
1	W	0.73	0/1124	0.63	0/1520
1	X	0.67	1/1141 (0.1%)	0.59	0/1543
All	All	0.61	3/27191 (0.0%)	0.61	0/36797

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	166	ASN	CG-ND2	5.61	1.46	1.32
1	X	85	THR	N-CA	5.10	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	181	LYS	CE-NZ	5.08	1.61	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1121	0	1172	18	0
1	B	1094	0	1133	13	0
1	C	1116	0	1164	22	0
1	D	1075	0	1092	14	0
1	E	1109	0	1149	23	0
1	F	1136	0	1171	24	0
1	G	1111	0	1154	33	0
1	H	1090	0	1122	59	0
1	I	1118	0	1167	26	0
1	J	1098	0	1112	20	0
1	K	1123	0	1166	45	0
1	L	1124	0	1155	19	0
1	M	1123	0	1166	26	0
1	N	1114	0	1146	24	0
1	O	1116	0	1164	37	0
1	P	1099	0	1113	33	0
1	Q	1103	0	1144	30	0
1	R	1127	0	1164	29	0
1	S	1133	0	1174	25	0
1	T	1098	0	1136	40	0
1	U	1116	0	1164	24	0
1	V	1098	0	1114	18	0
1	W	1103	0	1144	42	0
1	X	1119	0	1160	37	0
2	A	6	0	8	0	0
2	D	6	0	8	0	0
2	F	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	6	0	8	2	0
2	I	6	0	8	0	0
2	L	6	0	8	1	0
2	M	6	0	8	1	0
2	O	6	0	8	1	0
2	P	6	0	8	1	0
2	R	6	0	8	0	0
2	S	6	0	8	2	0
2	U	6	0	8	0	0
2	W	6	0	8	0	0
3	A	28	0	40	0	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	E	7	0	10	0	0
3	F	21	0	30	3	0
3	G	7	0	10	0	0
3	H	7	0	10	0	0
3	I	14	0	20	1	0
3	N	7	0	10	0	0
3	O	28	0	40	6	0
3	Q	21	0	30	1	0
3	R	14	0	20	0	0
3	S	28	0	40	8	0
3	U	7	0	10	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	G	1	0	0	1	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	1	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
5	D	18	0	6	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	18	0	6	10	0
5	P	18	0	6	11	0
5	R	18	0	6	12	0
6	E	5	0	0	1	0
7	A	10	0	0	0	0
7	B	21	0	0	2	0
7	C	27	0	0	2	0
7	D	19	0	0	0	0
7	E	21	0	0	1	0
7	F	25	0	0	0	0
7	G	18	0	0	0	0
7	H	16	0	0	1	0
7	I	10	0	0	0	0
7	J	23	0	0	0	0
7	K	12	0	0	1	0
7	L	15	0	0	0	0
7	M	9	0	0	0	0
7	N	18	0	0	0	0
7	O	19	0	0	1	0
7	P	22	0	0	1	0
7	Q	16	0	0	0	0
7	R	26	0	0	0	0
7	S	9	0	0	0	0
7	T	19	0	0	0	0
7	U	18	0	0	2	0
7	V	13	0	0	0	0
7	W	12	0	0	0	0
7	X	17	0	0	1	0
All	All	27454	0	27964	590	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 590 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:R:171:PHE:CB	5:R:1:S21:H5	1.61	1.31
1:R:171:PHE:HB2	5:R:1:S21:C5	1.69	1.21
1:F:171:PHE:HB2	5:F:231:S21:H5	1.13	1.08
1:J:87:ILE:HG23	1:J:91:ASP:HB2	1.42	1.02
1:M:84:ASP:O	1:M:85:THR:HG22	1.62	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
1	B	137/154 (89%)	127 (93%)	10 (7%)	0	100	100
1	C	142/154 (92%)	132 (93%)	10 (7%)	0	100	100
1	D	136/154 (88%)	127 (93%)	9 (7%)	0	100	100
1	E	139/154 (90%)	130 (94%)	9 (6%)	0	100	100
1	F	145/154 (94%)	133 (92%)	11 (8%)	1 (1%)	26	65
1	G	143/154 (93%)	133 (93%)	10 (7%)	0	100	100
1	H	137/154 (89%)	122 (89%)	15 (11%)	0	100	100
1	I	140/154 (91%)	131 (94%)	9 (6%)	0	100	100
1	J	142/154 (92%)	130 (92%)	12 (8%)	0	100	100
1	K	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
1	L	144/154 (94%)	134 (93%)	10 (7%)	0	100	100
1	M	143/154 (93%)	127 (89%)	15 (10%)	1 (1%)	26	65
1	N	143/154 (93%)	131 (92%)	12 (8%)	0	100	100
1	O	142/154 (92%)	128 (90%)	14 (10%)	0	100	100
1	P	143/154 (93%)	132 (92%)	11 (8%)	0	100	100
1	Q	138/154 (90%)	128 (93%)	10 (7%)	0	100	100
1	R	144/154 (94%)	134 (93%)	9 (6%)	1 (1%)	26	65
1	S	145/154 (94%)	132 (91%)	13 (9%)	0	100	100
1	T	138/154 (90%)	127 (92%)	11 (8%)	0	100	100
1	U	142/154 (92%)	125 (88%)	17 (12%)	0	100	100
1	V	142/154 (92%)	130 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	138/154 (90%)	128 (93%)	10 (7%)	0	100	100
1	X	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
All	All	3392/3696 (92%)	3123 (92%)	266 (8%)	3 (0%)	56	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	201	SER
1	R	200	SER
1	F	168	LEU

### 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%)	26	62
1	B	122/135 (90%)	116 (95%)	6 (5%)	31	68
1	C	125/135 (93%)	119 (95%)	6 (5%)	31	69
1	D	118/135 (87%)	113 (96%)	5 (4%)	36	73
1	E	124/135 (92%)	116 (94%)	8 (6%)	21	57
1	F	127/135 (94%)	123 (97%)	4 (3%)	47	80
1	G	124/135 (92%)	119 (96%)	5 (4%)	38	75
1	H	121/135 (90%)	113 (93%)	8 (7%)	21	56
1	I	125/135 (93%)	117 (94%)	8 (6%)	22	57
1	J	119/135 (88%)	112 (94%)	7 (6%)	24	60
1	K	126/135 (93%)	115 (91%)	11 (9%)	13	44
1	L	125/135 (93%)	116 (93%)	9 (7%)	18	53
1	M	126/135 (93%)	118 (94%)	8 (6%)	22	58
1	N	123/135 (91%)	114 (93%)	9 (7%)	17	52
1	O	125/135 (93%)	115 (92%)	10 (8%)	15	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	119/135 (88%)	112 (94%)	7 (6%)	24	60
1	Q	123/135 (91%)	108 (88%)	15 (12%)	6	24
1	R	126/135 (93%)	116 (92%)	10 (8%)	15	49
1	S	127/135 (94%)	123 (97%)	4 (3%)	47	80
1	T	122/135 (90%)	114 (93%)	8 (7%)	21	56
1	U	125/135 (93%)	118 (94%)	7 (6%)	26	62
1	V	120/135 (89%)	113 (94%)	7 (6%)	25	61
1	W	123/135 (91%)	111 (90%)	12 (10%)	10	36
1	X	125/135 (93%)	115 (92%)	10 (8%)	15	48
All	All	2966/3240 (92%)	2775 (94%)	191 (6%)	22	57

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	163	SER
1	O	171	PHE
1	W	174	VAL
1	M	171	PHE
1	N	175	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	192	GLN
1	K	114	ASN
1	U	214	ASN
1	J	98	HIS
1	J	214	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 17 are monoatomic - leaving 47 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	$\# Z  > 2$
2	GOL	A	1	-	5,5,5	0.29	0	5,5,5	0.40	0
3	PEG	A	18	-	6,6,6	0.57	0	5,5,5	0.33	0
3	PEG	A	26	-	6,6,6	0.63	0	5,5,5	0.31	0
3	PEG	A	27	-	6,6,6	0.64	0	5,5,5	0.35	0
3	PEG	A	5	-	6,6,6	0.59	0	5,5,5	0.27	0
3	PEG	B	3	-	6,6,6	0.56	0	5,5,5	0.28	0
3	PEG	C	1	-	6,6,6	0.69	0	5,5,5	0.21	0
2	GOL	D	2	-	5,5,5	0.23	0	5,5,5	0.51	0
5	S21	D	231	-	15,18,18	0.67	0	22,26,26	1.07	2 (9%)
6	PO4	E	1	-	4,4,4	0.15	0	6,6,6	0.28	0
3	PEG	E	17	-	6,6,6	0.66	0	5,5,5	0.24	0
3	PEG	F	2	-	6,6,6	0.63	0	5,5,5	0.24	0
5	S21	F	231	-	15,18,18	0.71	0	22,26,26	1.19	2 (9%)
3	PEG	F	24	-	6,6,6	0.59	0	5,5,5	0.28	0
3	PEG	F	25	-	6,6,6	0.59	0	5,5,5	0.29	0
2	GOL	F	3	-	5,5,5	0.25	0	5,5,5	0.46	0
3	PEG	G	6	-	6,6,6	0.58	0	5,5,5	0.43	0
3	PEG	H	231	-	6,6,6	0.51	0	5,5,5	0.42	0
2	GOL	H	4	-	5,5,5	0.39	0	5,5,5	0.37	0
3	PEG	I	11	-	6,6,6	0.52	0	5,5,5	0.30	0
3	PEG	I	20	-	6,6,6	0.38	0	5,5,5	0.32	0
2	GOL	I	5	-	5,5,5	0.32	0	5,5,5	0.35	0
2	GOL	L	6	-	5,5,5	0.34	0	5,5,5	0.23	0
2	GOL	M	7	-	5,5,5	0.33	0	5,5,5	0.35	0
3	PEG	N	14	-	6,6,6	0.72	0	5,5,5	0.37	0
3	PEG	O	10	-	6,6,6	0.56	0	5,5,5	0.38	0
3	PEG	O	22	-	6,6,6	0.61	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	O	23	-	6,6,6	0.59	0	5,5,5	0.72	0
3	PEG	O	28	-	6,6,6	0.43	0	5,5,5	0.33	0
2	GOL	O	8	-	5,5,5	0.34	0	5,5,5	0.33	0
2	GOL	P	13	-	5,5,5	0.36	0	5,5,5	0.58	0
5	S21	P	4	-	15,18,18	0.59	0	22,26,26	0.92	0
3	PEG	Q	16	-	6,6,6	0.76	0	5,5,5	0.43	0
3	PEG	Q	7	-	6,6,6	0.68	0	5,5,5	0.32	0
3	PEG	Q	9	-	6,6,6	0.58	0	5,5,5	0.22	0
5	S21	R	1	-	15,18,18	0.57	0	22,26,26	1.11	1 (4%)
3	PEG	R	15	-	6,6,6	0.53	0	5,5,5	0.47	0
3	PEG	R	29	-	6,6,6	0.72	0	5,5,5	0.21	0
2	GOL	R	9	-	5,5,5	0.32	0	5,5,5	0.39	0
2	GOL	S	10	-	5,5,5	0.45	0	5,5,5	1.00	0
3	PEG	S	12	-	6,6,6	0.55	0	5,5,5	0.48	0
3	PEG	S	13	-	6,6,6	0.49	0	5,5,5	0.38	0
3	PEG	S	19	-	6,6,6	0.68	0	5,5,5	0.21	0
3	PEG	S	8	-	6,6,6	0.69	0	5,5,5	0.42	0
2	GOL	U	11	-	5,5,5	0.31	0	5,5,5	0.32	0
3	PEG	U	21	-	6,6,6	0.79	0	5,5,5	0.48	0
2	GOL	W	12	-	5,5,5	0.25	0	5,5,5	0.37	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	-	-	0/4/4/4	0/0/0/0
3	PEG	A	18	-	-	0/4/4/4	0/0/0/0
3	PEG	A	26	-	-	0/4/4/4	0/0/0/0
3	PEG	A	27	-	-	0/4/4/4	0/0/0/0
3	PEG	A	5	-	-	0/4/4/4	0/0/0/0
3	PEG	B	3	-	-	0/4/4/4	0/0/0/0
3	PEG	C	1	-	-	0/4/4/4	0/0/0/0
2	GOL	D	2	-	-	0/4/4/4	0/0/0/0
5	S21	D	231	-	-	0/18/18/18	0/1/1/1
6	PO4	E	1	-	-	0/0/0/0	0/0/0/0
3	PEG	E	17	-	-	0/4/4/4	0/0/0/0
3	PEG	F	2	-	-	0/4/4/4	0/0/0/0
5	S21	F	231	-	-	0/18/18/18	0/1/1/1
3	PEG	F	24	-	-	0/4/4/4	0/0/0/0
3	PEG	F	25	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	F	3	-	-	0/4/4/4	0/0/0/0
3	PEG	G	6	-	-	0/4/4/4	0/0/0/0
3	PEG	H	231	-	-	0/4/4/4	0/0/0/0
2	GOL	H	4	-	-	0/4/4/4	0/0/0/0
3	PEG	I	11	-	-	0/4/4/4	0/0/0/0
3	PEG	I	20	-	-	0/4/4/4	0/0/0/0
2	GOL	I	5	-	-	0/4/4/4	0/0/0/0
2	GOL	L	6	-	-	0/4/4/4	0/0/0/0
2	GOL	M	7	-	-	0/4/4/4	0/0/0/0
3	PEG	N	14	-	-	0/4/4/4	0/0/0/0
3	PEG	O	10	-	-	0/4/4/4	0/0/0/0
3	PEG	O	22	-	-	0/4/4/4	0/0/0/0
3	PEG	O	23	-	-	0/4/4/4	0/0/0/0
3	PEG	O	28	-	-	0/4/4/4	0/0/0/0
2	GOL	O	8	-	-	0/4/4/4	0/0/0/0
2	GOL	P	13	-	-	0/4/4/4	0/0/0/0
5	S21	P	4	-	-	0/18/18/18	0/1/1/1
3	PEG	Q	16	-	-	0/4/4/4	0/0/0/0
3	PEG	Q	7	-	-	0/4/4/4	0/0/0/0
3	PEG	Q	9	-	-	0/4/4/4	0/0/0/0
5	S21	R	1	-	-	0/18/18/18	0/1/1/1
3	PEG	R	15	-	-	0/4/4/4	0/0/0/0
3	PEG	R	29	-	-	0/4/4/4	0/0/0/0
2	GOL	R	9	-	-	0/4/4/4	0/0/0/0
2	GOL	S	10	-	-	0/4/4/4	0/0/0/0
3	PEG	S	12	-	-	0/4/4/4	0/0/0/0
3	PEG	S	13	-	-	0/4/4/4	0/0/0/0
3	PEG	S	19	-	-	0/4/4/4	0/0/0/0
3	PEG	S	8	-	-	0/4/4/4	0/0/0/0
2	GOL	U	11	-	-	0/4/4/4	0/0/0/0
3	PEG	U	21	-	-	0/4/4/4	0/0/0/0
2	GOL	W	12	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	231	S21	F1C-C12-C10	-2.24	106.54	112.67
5	F	231	S21	C2-C3-N13	2.05	121.14	119.48
5	F	231	S21	C4-C3-N13	2.29	121.33	119.48
5	R	1	S21	C2-C3-N13	2.40	121.42	119.48
5	D	231	S21	C2-C3-N13	2.62	121.60	119.48



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	231	S21	9	0
6	E	1	PO4	1	0
5	F	231	S21	10	0
3	F	24	PEG	1	0
3	F	25	PEG	3	0
2	F	3	GOL	2	0
2	H	4	GOL	2	0
3	I	11	PEG	1	0
2	L	6	GOL	1	0
2	M	7	GOL	1	0
3	O	10	PEG	1	0
3	O	23	PEG	3	0
3	O	28	PEG	2	0
2	O	8	GOL	1	0
2	P	13	GOL	1	0
5	P	4	S21	11	0
3	Q	9	PEG	1	0
5	R	1	S21	12	0
2	S	10	GOL	2	0
3	S	12	PEG	1	0
3	S	13	PEG	3	0
3	S	19	PEG	1	0
3	S	8	PEG	3	0
3	U	21	PEG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	145/154 (94%)	0.10	6 (4%) 41 19	32, 56, 71, 72	0
1	B	141/154 (91%)	-0.03	1 (0%) 89 78	33, 56, 72, 77	0
1	C	144/154 (93%)	-0.13	2 (1%) 78 60	28, 41, 65, 70	0
1	D	140/154 (90%)	-0.11	5 (3%) 46 23	32, 46, 67, 71	1 (0%)
1	E	143/154 (92%)	-0.14	1 (0%) 89 78	28, 42, 65, 71	0
1	F	146/154 (94%)	-0.07	3 (2%) 67 44	29, 44, 64, 73	0
1	G	145/154 (94%)	0.82	27 (18%) 2 1	49, 61, 73, 79	0
1	H	141/154 (91%)	0.34	10 (7%) 19 7	48, 61, 74, 77	0
1	I	143/154 (92%)	-0.06	5 (3%) 48 23	41, 53, 71, 77	0
1	J	144/154 (93%)	0.32	6 (4%) 40 19	45, 59, 73, 78	1 (0%)
1	K	145/154 (94%)	0.22	5 (3%) 49 24	46, 58, 73, 78	0
1	L	146/154 (94%)	0.17	1 (0%) 89 78	42, 61, 76, 80	0
1	M	145/154 (94%)	0.01	5 (3%) 49 24	35, 55, 70, 73	0
1	N	145/154 (94%)	0.06	6 (4%) 41 19	31, 52, 71, 74	0
1	O	144/154 (93%)	-0.15	0 100 100	29, 44, 62, 68	0
1	P	145/154 (94%)	-0.09	2 (1%) 78 60	33, 50, 66, 73	1 (0%)
1	Q	142/154 (92%)	-0.04	5 (3%) 48 23	26, 44, 67, 73	0
1	R	146/154 (94%)	-0.07	3 (2%) 67 44	30, 47, 69, 76	0
1	S	146/154 (94%)	0.11	7 (4%) 34 15	39, 51, 73, 79	0
1	T	142/154 (92%)	0.11	4 (2%) 56 32	41, 59, 73, 79	0
1	U	144/154 (93%)	0.10	2 (1%) 78 60	41, 57, 72, 76	0
1	V	144/154 (93%)	0.05	4 (2%) 56 32	40, 55, 74, 79	1 (0%)
1	W	142/154 (92%)	0.72	17 (11%) 6 2	48, 63, 78, 85	0
1	X	145/154 (94%)	0.46	15 (10%) 9 3	46, 62, 77, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3453/3696 (93%)	0.11	142 (4%)	41	19	26, 54, 72, 85	4 (0%)

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	167	ASN	6.7
1	S	168	LEU	6.0
1	G	163	SER	5.6
1	A	201	SER	5.6
1	W	167	ASN	5.2

## 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	I	20	7/7	0.73	0.37	5.23	74,74,74,75	0
5	S21	F	231	18/18	0.74	0.30	2.56	66,70,73,73	6
3	PEG	S	19	7/7	0.78	0.31	2.18	34,37,39,39	0
2	GOL	U	11	6/6	0.91	0.25	1.40	40,41,42,43	0
5	S21	P	4	18/18	0.88	0.26	1.27	63,65,66,67	0
3	PEG	O	28	7/7	0.90	0.23	1.21	29,30,32,33	0
5	S21	D	231	18/18	0.89	0.25	1.18	50,55,57,57	0
3	PEG	O	23	7/7	0.93	0.25	0.95	27,32,37,38	0
2	GOL	A	1	6/6	0.90	0.24	0.90	45,46,46,46	0
2	GOL	W	12	6/6	0.89	0.28	0.89	54,55,55,56	0
3	PEG	S	13	7/7	0.92	0.25	0.58	46,47,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	F	3	6/6	0.94	0.23	0.57	27,29,29,29	0
2	GOL	R	9	6/6	0.97	0.22	0.56	28,29,31,33	0
3	PEG	A	26	7/7	0.81	0.26	0.50	51,52,53,53	0
4	CL	C	5	1/1	0.96	0.24	0.47	51,51,51,51	0
5	S21	R	1	18/18	0.91	0.25	0.46	44,46,52,53	0
2	GOL	H	4	6/6	0.95	0.27	0.45	25,28,29,29	0
3	PEG	S	8	7/7	0.85	0.23	0.40	55,56,56,56	0
3	PEG	O	22	7/7	0.90	0.21	0.39	52,53,54,55	0
3	PEG	O	10	7/7	0.91	0.22	0.12	46,47,48,48	0
2	GOL	S	10	6/6	0.95	0.20	0.07	36,37,38,39	0
2	GOL	D	2	6/6	0.95	0.19	-0.05	29,30,30,30	0
4	CL	U	2	1/1	0.96	0.20	-0.12	52,52,52,52	0
3	PEG	I	11	7/7	0.91	0.22	-0.14	51,51,53,53	0
4	CL	A	3	1/1	0.95	0.19	-0.35	55,55,55,55	0
4	CL	V	17	1/1	0.95	0.19	-0.40	39,39,39,39	0
4	CL	K	10	1/1	0.90	0.17	-0.43	53,53,53,53	0
4	CL	O	1	1/1	0.95	0.19	-0.51	45,45,45,45	0
2	GOL	O	8	6/6	0.95	0.18	-0.58	23,24,25,26	0
4	CL	J	9	1/1	0.91	0.17	-0.60	49,49,49,49	0
3	PEG	A	27	7/7	0.89	0.19	-0.61	52,54,55,55	0
4	CL	L	11	1/1	0.91	0.21	-0.62	50,50,50,50	0
3	PEG	U	21	7/7	0.88	0.18	-0.62	37,40,41,42	0
3	PEG	R	15	7/7	0.91	0.18	-0.77	36,40,43,44	0
4	CL	B	4	1/1	0.76	0.14	-0.89	49,49,49,49	0
6	PO4	E	1	5/5	0.95	0.18	-1.00	42,43,44,44	0
3	PEG	E	17	7/7	0.89	0.19	-1.05	59,60,60,60	0
2	GOL	I	5	6/6	0.95	0.16	-1.06	58,59,60,60	0
4	CL	H	6	1/1	0.98	0.15	-1.09	44,44,44,44	0
3	PEG	S	12	7/7	0.93	0.15	-1.10	28,28,30,31	0
4	CL	S	15	1/1	0.93	0.15	-1.24	43,43,43,43	0
2	GOL	P	13	6/6	0.94	0.15	-1.31	27,30,30,31	0
4	CL	N	13	1/1	0.97	0.15	-1.35	66,66,66,66	0
4	CL	M	12	1/1	0.97	0.16	-1.38	39,39,39,39	0
3	PEG	Q	7	7/7	0.90	0.16	-1.41	56,58,59,59	0
2	GOL	L	6	6/6	0.95	0.17	-1.46	35,38,38,39	0
4	CL	T	16	1/1	0.93	0.17	-1.49	50,50,50,50	0
4	CL	I	8	1/1	0.96	0.15	-1.54	46,46,46,46	0
3	PEG	C	1	7/7	0.91	0.18	-1.55	36,37,39,39	0
3	PEG	G	6	7/7	0.94	0.13	-1.56	29,29,30,30	0
2	GOL	M	7	6/6	0.96	0.15	-1.92	29,30,30,31	0
4	CL	G	7	1/1	0.82	0.12	-2.30	57,57,57,57	0
4	CL	R	14	1/1	0.98	0.11	-2.43	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	H	231	7/7	0.91	0.14	-2.47	52,52,55,55	0
3	PEG	B	3	7/7	0.86	0.17	-	40,41,41,41	0
3	PEG	Q	16	7/7	0.88	0.20	-	48,49,50,50	0
3	PEG	A	18	7/7	0.85	0.20	-	53,56,58,58	0
3	PEG	N	14	7/7	0.96	0.10	-	29,34,35,36	0
3	PEG	F	24	7/7	0.90	0.20	-	38,41,42,42	0
3	PEG	R	29	7/7	0.86	0.23	-	40,43,43,43	0
3	PEG	F	25	7/7	0.72	0.24	-	63,63,64,64	0
3	PEG	A	5	7/7	0.76	0.24	-	57,58,58,59	0
3	PEG	F	2	7/7	0.89	0.18	-	42,42,43,43	0
3	PEG	Q	9	7/7	0.86	0.21	-	40,41,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.