



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:41 am BST

PDB ID : 5BUY  
Title : Crystal Structure of beta-hydroxyacyl-acyl carrier protein dehydratase (FabZ) from *Francisella tularensis*  
Authors : McGillick, B.; Kumaran, D.; Swaminathan, S.  
Deposited on : 2015-06-04  
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

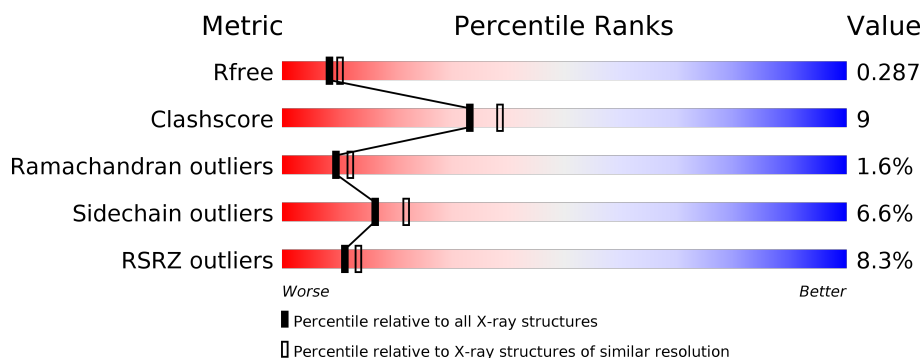
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	178	<div> <div>7%</div> <div>69%</div> <div>11%</div> <div>•</div> <div>18%</div> </div>
1	B	178	<div> <div>3%</div> <div>63%</div> <div>16%</div> <div>••</div> <div>20%</div> </div>
1	C	178	<div> <div>4%</div> <div>58%</div> <div>17%</div> <div>••</div> <div>22%</div> </div>
1	D	178	<div> <div>7%</div> <div>52%</div> <div>22%</div> <div>••</div> <div>23%</div> </div>
1	E	178	<div> <div>8%</div> <div>53%</div> <div>18%</div> <div>•</div> <div>27%</div> </div>
1	F	178	<div> <div>9%</div> <div>56%</div> <div>17%</div> <div>••</div> <div>24%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6560 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 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1139	734	193	203	9			
1	B	143	Total	C	N	O	S	0	0	0
			1114	718	186	201	9			
1	C	139	Total	C	N	O	S	0	0	0
			1079	694	183	193	9			
1	D	137	Total	C	N	O	S	0	0	0
			1066	687	179	191	9			
1	E	130	Total	C	N	O	S	0	0	0
			1003	647	167	180	9			
1	F	135	Total	C	N	O	S	0	0	0
			1049	677	176	187	9			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q5NEQ0
A	-13	HIS	-	expression tag	UNP Q5NEQ0
A	-12	HIS	-	expression tag	UNP Q5NEQ0
A	-11	HIS	-	expression tag	UNP Q5NEQ0
A	-10	HIS	-	expression tag	UNP Q5NEQ0
A	-9	HIS	-	expression tag	UNP Q5NEQ0
A	-8	SER	-	expression tag	UNP Q5NEQ0
A	-7	SER	-	expression tag	UNP Q5NEQ0
A	-6	GLY	-	expression tag	UNP Q5NEQ0
A	-5	LEU	-	expression tag	UNP Q5NEQ0
A	-4	VAL	-	expression tag	UNP Q5NEQ0
A	-3	PRO	-	expression tag	UNP Q5NEQ0
A	-2	ARG	-	expression tag	UNP Q5NEQ0
A	-1	GLY	-	expression tag	UNP Q5NEQ0
A	0	SER	-	expression tag	UNP Q5NEQ0
B	-14	HIS	-	expression tag	UNP Q5NEQ0
B	-13	HIS	-	expression tag	UNP Q5NEQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP Q5NEQ0
B	-11	HIS	-	expression tag	UNP Q5NEQ0
B	-10	HIS	-	expression tag	UNP Q5NEQ0
B	-9	HIS	-	expression tag	UNP Q5NEQ0
B	-8	SER	-	expression tag	UNP Q5NEQ0
B	-7	SER	-	expression tag	UNP Q5NEQ0
B	-6	GLY	-	expression tag	UNP Q5NEQ0
B	-5	LEU	-	expression tag	UNP Q5NEQ0
B	-4	VAL	-	expression tag	UNP Q5NEQ0
B	-3	PRO	-	expression tag	UNP Q5NEQ0
B	-2	ARG	-	expression tag	UNP Q5NEQ0
B	-1	GLY	-	expression tag	UNP Q5NEQ0
B	0	SER	-	expression tag	UNP Q5NEQ0
C	-14	HIS	-	expression tag	UNP Q5NEQ0
C	-13	HIS	-	expression tag	UNP Q5NEQ0
C	-12	HIS	-	expression tag	UNP Q5NEQ0
C	-11	HIS	-	expression tag	UNP Q5NEQ0
C	-10	HIS	-	expression tag	UNP Q5NEQ0
C	-9	HIS	-	expression tag	UNP Q5NEQ0
C	-8	SER	-	expression tag	UNP Q5NEQ0
C	-7	SER	-	expression tag	UNP Q5NEQ0
C	-6	GLY	-	expression tag	UNP Q5NEQ0
C	-5	LEU	-	expression tag	UNP Q5NEQ0
C	-4	VAL	-	expression tag	UNP Q5NEQ0
C	-3	PRO	-	expression tag	UNP Q5NEQ0
C	-2	ARG	-	expression tag	UNP Q5NEQ0
C	-1	GLY	-	expression tag	UNP Q5NEQ0
C	0	SER	-	expression tag	UNP Q5NEQ0
D	-14	HIS	-	expression tag	UNP Q5NEQ0
D	-13	HIS	-	expression tag	UNP Q5NEQ0
D	-12	HIS	-	expression tag	UNP Q5NEQ0
D	-11	HIS	-	expression tag	UNP Q5NEQ0
D	-10	HIS	-	expression tag	UNP Q5NEQ0
D	-9	HIS	-	expression tag	UNP Q5NEQ0
D	-8	SER	-	expression tag	UNP Q5NEQ0
D	-7	SER	-	expression tag	UNP Q5NEQ0
D	-6	GLY	-	expression tag	UNP Q5NEQ0
D	-5	LEU	-	expression tag	UNP Q5NEQ0
D	-4	VAL	-	expression tag	UNP Q5NEQ0
D	-3	PRO	-	expression tag	UNP Q5NEQ0
D	-2	ARG	-	expression tag	UNP Q5NEQ0
D	-1	GLY	-	expression tag	UNP Q5NEQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q5NEQ0
E	-14	HIS	-	expression tag	UNP Q5NEQ0
E	-13	HIS	-	expression tag	UNP Q5NEQ0
E	-12	HIS	-	expression tag	UNP Q5NEQ0
E	-11	HIS	-	expression tag	UNP Q5NEQ0
E	-10	HIS	-	expression tag	UNP Q5NEQ0
E	-9	HIS	-	expression tag	UNP Q5NEQ0
E	-8	SER	-	expression tag	UNP Q5NEQ0
E	-7	SER	-	expression tag	UNP Q5NEQ0
E	-6	GLY	-	expression tag	UNP Q5NEQ0
E	-5	LEU	-	expression tag	UNP Q5NEQ0
E	-4	VAL	-	expression tag	UNP Q5NEQ0
E	-3	PRO	-	expression tag	UNP Q5NEQ0
E	-2	ARG	-	expression tag	UNP Q5NEQ0
E	-1	GLY	-	expression tag	UNP Q5NEQ0
E	0	SER	-	expression tag	UNP Q5NEQ0
F	-14	HIS	-	expression tag	UNP Q5NEQ0
F	-13	HIS	-	expression tag	UNP Q5NEQ0
F	-12	HIS	-	expression tag	UNP Q5NEQ0
F	-11	HIS	-	expression tag	UNP Q5NEQ0
F	-10	HIS	-	expression tag	UNP Q5NEQ0
F	-9	HIS	-	expression tag	UNP Q5NEQ0
F	-8	SER	-	expression tag	UNP Q5NEQ0
F	-7	SER	-	expression tag	UNP Q5NEQ0
F	-6	GLY	-	expression tag	UNP Q5NEQ0
F	-5	LEU	-	expression tag	UNP Q5NEQ0
F	-4	VAL	-	expression tag	UNP Q5NEQ0
F	-3	PRO	-	expression tag	UNP Q5NEQ0
F	-2	ARG	-	expression tag	UNP Q5NEQ0
F	-1	GLY	-	expression tag	UNP Q5NEQ0
F	0	SER	-	expression tag	UNP Q5NEQ0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

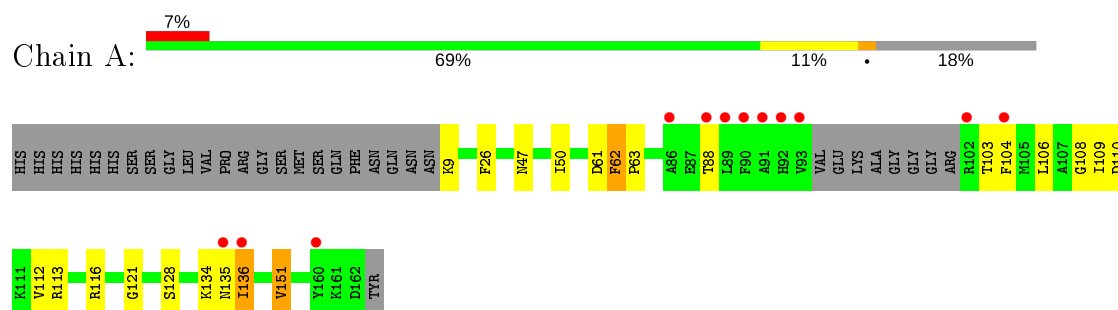
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	18	Total	O	0	0
			18	18		
3	C	23	Total	O	0	0
			23	23		
3	D	21	Total	O	0	0
			21	21		
3	E	9	Total	O	0	0
			9	9		
3	F	9	Total	O	0	0
			9	9		

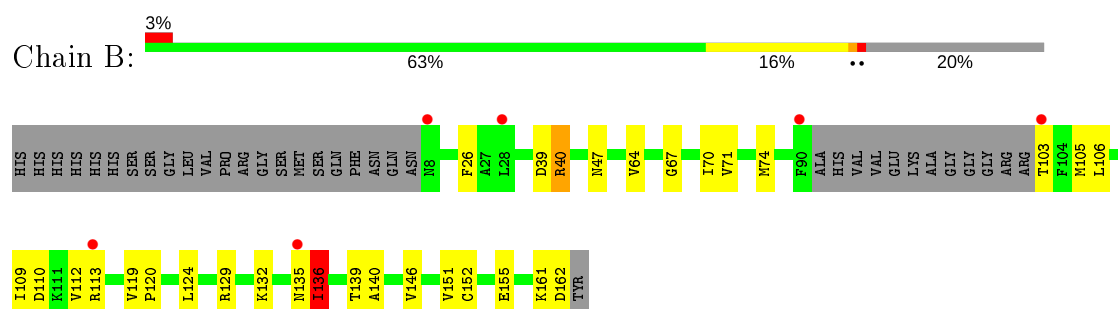
### 3 Residue-property plots [i](#)

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.

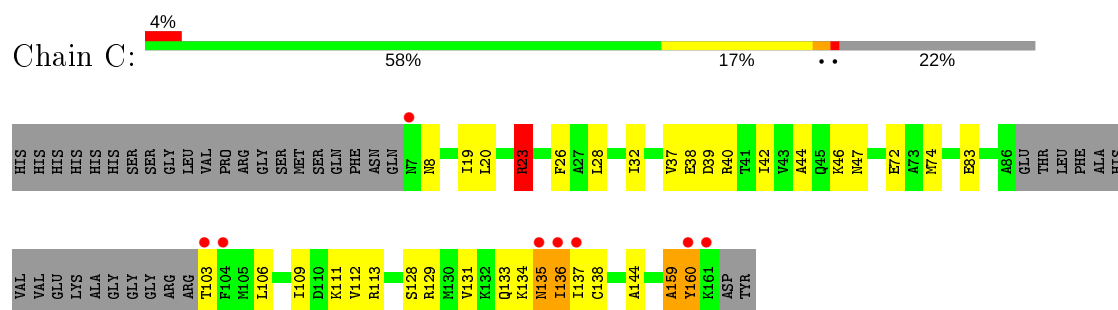
- Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ



- Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

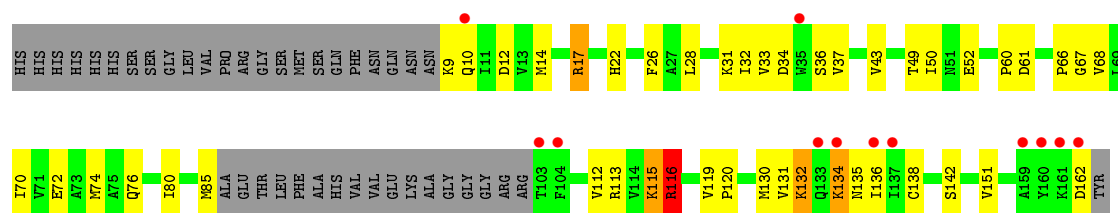


- Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

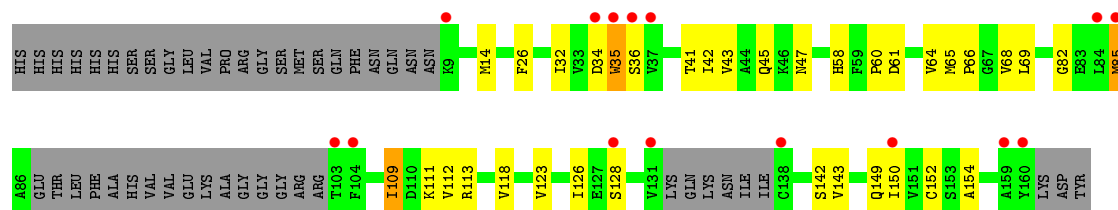


- Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

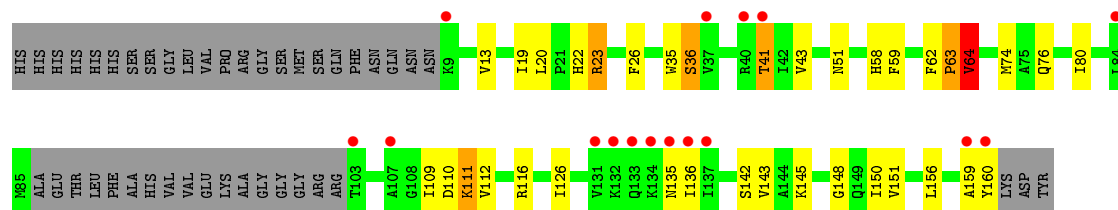




• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ



• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.71Å 56.03Å 140.09Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	45.22 – 2.55 45.18 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.22-2.55) 98.8 (45.18-2.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.209 , 0.281 0.217 , 0.287	Depositor DCC
$R_{free}$ test set	1614 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: SO4

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	0.65	0/1158	0.86	0/1566
1	B	0.70	0/1132	0.80	0/1531
1	C	0.70	0/1096	0.86	1/1482 (0.1%)
1	D	0.65	0/1083	0.86	3/1464 (0.2%)
1	E	0.59	0/1019	0.81	0/1379
1	F	0.57	0/1066	0.82	3/1442 (0.2%)
All	All	0.65	0/6554	0.84	7/8864 (0.1%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	64	VAL	CB-CA-C	-6.46	99.12	111.40
1	D	17	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	17	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	F	23	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	113	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	23	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	F	23	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	159	ALA	Peptide

## 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	1139	0	1182	16	0
1	B	1114	0	1154	16	2
1	C	1079	0	1123	25	2
1	D	1066	0	1110	23	0
1	E	1003	0	1035	26	0
1	F	1049	0	1093	20	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0
3	A	20	0	0	2	0
3	B	18	0	0	0	0
3	C	23	0	0	4	0
3	D	21	0	0	1	0
3	E	9	0	0	1	0
3	F	9	0	0	0	0
All	All	6560	0	6697	113	2

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 9.

All (113) 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:B:71:VAL:HA	1:B:74:MET:HE2	1.59	0.83
1:E:111:LYS:O	1:E:154:ALA:HA	1.94	0.68
1:F:62:PHE:CD2	1:F:64:VAL:HG22	2.31	0.65
1:D:17:ARG:O	3:D:301:HOH:O	2.14	0.65
1:C:74:MET:HE2	1:C:144:ALA:HB2	1.76	0.65
1:C:74:MET:CE	1:C:144:ALA:HB2	2.26	0.64
1:A:112:VAL:HB	1:B:109:ILE:HB	1.80	0.64
1:E:45:GLN:HE21	1:E:123:VAL:HG13	1.62	0.63
1:E:34:ASP:HB3	1:E:43:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:O	1:C:113:ARG:NH1	2.33	0.61
1:D:130:MET:SD	1:D:138:CYS:SG	2.99	0.61
1:F:20:LEU:O	1:F:23:ARG:NH2	2.34	0.61
1:D:14:MET:SD	1:F:63:PRO:HD2	2.41	0.61
1:F:22:HIS:O	1:F:23:ARG:NE	2.32	0.61
1:A:63:PRO:HD2	1:E:14:MET:SD	2.41	0.60
1:A:9:LYS:HB2	3:A:307:HOH:O	2.01	0.60
1:F:76:GLN:O	1:F:80:ILE:HG13	2.03	0.58
1:F:145:LYS:HD3	1:F:148:GLY:O	2.02	0.58
1:E:45:GLN:HE21	1:E:123:VAL:CG1	2.16	0.57
1:C:135:ASN:O	1:C:136:ILE:HG13	2.05	0.56
1:C:129:ARG:HG2	3:C:212:HOH:O	2.06	0.56
1:F:159:ALA:O	1:F:160:TYR:HB2	2.06	0.56
1:D:52:GLU:OE2	1:F:51:ASN:ND2	2.23	0.56
1:D:60:PRO:O	1:D:61:ASP:HB2	2.07	0.55
1:B:47:ASN:HB3	1:C:47:ASN:HB3	1.88	0.55
1:D:135:ASN:CG	1:D:136:ILE:H	2.10	0.55
1:E:34:ASP:HB2	1:E:43:VAL:CG2	2.37	0.55
1:E:82:GLY:O	1:E:85:MET:HB2	2.07	0.55
1:D:134:LYS:O	1:D:135:ASN:OD1	2.26	0.54
1:E:60:PRO:HA	3:E:207:HOH:O	2.06	0.54
1:D:115:LYS:O	1:D:116:ARG:HB2	2.06	0.54
1:D:37:VAL:HG23	1:D:85:MET:HG2	1.88	0.54
1:E:34:ASP:CB	1:E:43:VAL:HG22	2.38	0.54
1:E:109:ILE:HD11	1:E:112:VAL:CG2	2.37	0.53
1:E:109:ILE:HD11	1:E:112:VAL:HG22	1.91	0.53
1:E:32:ILE:HD12	1:E:42:ILE:HD11	1.90	0.53
1:D:115:LYS:O	1:D:151:VAL:O	2.27	0.52
1:B:70:ILE:HG23	1:B:124:LEU:HD21	1.90	0.52
1:B:132:LYS:HB2	1:B:139:THR:HB	1.91	0.52
1:C:106:LEU:HD21	1:C:109:ILE:HD11	1.91	0.52
1:C:46:LYS:NZ	3:C:201:HOH:O	2.42	0.51
1:C:37:VAL:HG12	3:C:221:HOH:O	2.11	0.51
1:C:131:VAL:HG23	3:C:212:HOH:O	2.10	0.51
1:D:22:HIS:CD2	1:D:76:GLN:NE2	2.79	0.51
1:E:58:HIS:ND1	1:E:64:VAL:O	2.40	0.51
1:D:70:ILE:HG22	1:D:74:MET:HE3	1.93	0.50
1:A:116:ARG:HB2	1:A:151:VAL:HG22	1.93	0.50
1:A:135:ASN:O	1:A:136:ILE:HB	2.11	0.50
1:B:135:ASN:O	1:B:136:ILE:HG22	2.11	0.50
1:A:61:ASP:O	1:A:62:PHE:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:VAL:HA	1:E:126:ILE:O	2.12	0.48
1:C:72:GLU:HB2	1:D:68:VAL:HG21	1.96	0.48
1:E:65:MET:HB3	1:E:118:VAL:HB	1.96	0.48
1:B:39:ASP:O	1:B:40:ARG:HG3	2.14	0.48
1:E:34:ASP:CB	1:E:43:VAL:CG2	2.91	0.48
1:C:106:LEU:HD11	1:C:109:ILE:CD1	2.44	0.48
1:B:106:LEU:HD21	1:B:109:ILE:HD11	1.96	0.47
1:C:135:ASN:O	1:C:137:ILE:N	2.46	0.47
1:F:19:ILE:HG21	1:F:80:ILE:HG23	1.95	0.47
1:F:36:SER:HB2	1:F:41:THR:HG22	1.95	0.47
1:C:20:LEU:O	1:C:23:ARG:NH2	2.47	0.47
1:E:143:VAL:HG11	1:E:150:ILE:HD12	1.97	0.47
1:A:135:ASN:O	1:A:135:ASN:ND2	2.48	0.46
1:B:113:ARG:O	1:B:152:CYS:HA	2.15	0.46
1:B:105:MET:HB3	1:B:161:LYS:HE2	1.97	0.46
1:E:42:ILE:HG22	1:E:128:SER:HB3	1.97	0.46
1:D:119:VAL:HB	1:D:120:PRO:HD2	1.97	0.46
1:C:32:ILE:HD13	1:C:44:ALA:HB2	1.97	0.46
1:C:19:ILE:HG23	1:C:83:GLU:HG2	1.98	0.46
1:C:28:LEU:HD12	1:C:72:GLU:HG3	1.98	0.46
1:F:143:VAL:HG11	1:F:150:ILE:HD12	1.97	0.46
1:D:66:PRO:O	1:D:67:GLY:C	2.54	0.46
1:F:62:PHE:HD2	1:F:64:VAL:HG22	1.79	0.46
1:E:35:TRP:HA	1:E:42:ILE:HA	1.97	0.45
1:A:110:ASP:O	1:B:110:ASP:OD1	2.35	0.45
1:C:159:ALA:O	1:C:160:TYR:CB	2.64	0.45
1:D:131:VAL:HG12	1:D:132:LYS:HG2	1.99	0.45
1:B:146:VAL:HG23	1:B:151:VAL:HG11	1.99	0.45
1:D:33:VAL:CG2	1:D:43:VAL:HG12	2.46	0.45
1:F:62:PHE:CE2	1:F:64:VAL:HG22	2.51	0.45
1:A:106:LEU:HD21	1:A:109:ILE:HD11	1.99	0.44
1:A:47:ASN:HB3	1:E:47:ASN:HB3	1.99	0.44
1:D:50:ILE:HD13	1:F:13:VAL:HG21	2.00	0.44
1:C:159:ALA:O	1:C:160:TYR:HB2	2.17	0.44
1:C:74:MET:HE3	1:C:144:ALA:HB2	1.99	0.44
1:A:116:ARG:HD2	3:A:312:HOH:O	2.18	0.44
1:A:50:ILE:HG13	1:A:50:ILE:O	2.17	0.44
1:E:109:ILE:HG23	1:F:112:VAL:CG1	2.47	0.44
1:C:106:LEU:HD11	1:C:109:ILE:HD11	1.99	0.43
1:E:60:PRO:O	1:E:61:ASP:HB2	2.17	0.43
1:E:66:PRO:HG2	1:E:69:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:VAL:HB	1:B:120:PRO:HD2	2.00	0.43
1:D:32:ILE:HD11	1:D:80:ILE:HD13	2.00	0.43
1:A:121:GLY:HA2	1:E:47:ASN:ND2	2.34	0.43
1:D:60:PRO:O	1:D:61:ASP:CB	2.67	0.43
1:F:109:ILE:HG22	1:F:156:LEU:HD22	2.00	0.43
1:E:113:ARG:O	1:E:152:CYS:HA	2.18	0.42
1:F:116:ARG:HB2	1:F:151:VAL:HG12	2.00	0.42
1:C:39:ASP:O	1:C:40:ARG:HB2	2.20	0.42
1:D:9:LYS:O	1:D:34:ASP:HA	2.20	0.42
1:A:135:ASN:O	1:A:136:ILE:CB	2.68	0.42
1:C:135:ASN:C	1:C:136:ILE:HG13	2.41	0.42
1:C:32:ILE:HD12	1:C:42:ILE:HD11	2.03	0.41
1:A:108:GLY:HA2	1:B:112:VAL:O	2.21	0.41
1:F:58:HIS:CE1	1:F:59:PHE:CZ	3.08	0.41
1:F:74:MET:HG2	1:F:142:SER:HB3	2.01	0.41
1:A:103:THR:O	1:A:104:PHE:HB2	2.21	0.41
1:B:140:ALA:O	1:B:155:GLU:HA	2.21	0.41
1:C:109:ILE:HB	1:D:112:VAL:HB	2.02	0.41
1:F:43:VAL:HA	1:F:126:ILE:O	2.21	0.41
1:D:28:LEU:HD12	1:D:72:GLU:CG	2.50	0.40
1:E:35:TRP:HA	1:E:41:THR:O	2.20	0.40
1:B:67:GLY:O	1:B:71:VAL:HG23	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ARG:NH2	1:C:38:GLU:OE2[2_555]	1.85	0.35
1:B:113:ARG:NH1	1:C:38:GLU:OE2[2_555]	2.13	0.07

## 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	142/178 (80%)	124 (87%)	15 (11%)	3 (2%)	7	7
1	B	139/178 (78%)	132 (95%)	6 (4%)	1 (1%)	22	30
1	C	135/178 (76%)	124 (92%)	8 (6%)	3 (2%)	6	7
1	D	133/178 (75%)	119 (90%)	13 (10%)	1 (1%)	19	27
1	E	124/178 (70%)	113 (91%)	9 (7%)	2 (2%)	9	12
1	F	131/178 (74%)	118 (90%)	10 (8%)	3 (2%)	6	6
All	All	804/1068 (75%)	730 (91%)	61 (8%)	13 (2%)	9	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ILE
1	B	136	ILE
1	C	135	ASN
1	E	36	SER
1	F	111	LYS
1	C	160	TYR
1	E	35	TRP
1	A	88	THR
1	F	136	ILE
1	C	136	ILE
1	D	116	ARG
1	A	62	PHE
1	F	63	PRO

### 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	125/151 (83%)	120 (96%)	5 (4%)	31	43
1	B	123/151 (82%)	116 (94%)	7 (6%)	20	27
1	C	119/151 (79%)	110 (92%)	9 (8%)	13	17
1	D	118/151 (78%)	106 (90%)	12 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	110/151 (73%)	104 (94%)	6 (6%)	21	29
1	F	116/151 (77%)	108 (93%)	8 (7%)	15	20
All	All	711/906 (78%)	664 (93%)	47 (7%)	16	22

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	113	ARG
1	A	128	SER
1	A	134	LYS
1	A	151	VAL
1	B	26	PHE
1	B	40	ARG
1	B	64	VAL
1	B	103	THR
1	B	129	ARG
1	B	136	ILE
1	B	162	ASP
1	C	8	ASN
1	C	23	ARG
1	C	26	PHE
1	C	103	THR
1	C	111	LYS
1	C	128	SER
1	C	133	GLN
1	C	134	LYS
1	C	138	CYS
1	D	10	GLN
1	D	12	ASP
1	D	26	PHE
1	D	31	LYS
1	D	36	SER
1	D	49	THR
1	D	115	LYS
1	D	116	ARG
1	D	132	LYS
1	D	134	LYS
1	D	142	SER
1	D	162	ASP
1	E	26	PHE

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Mol	Chain	Res	Type
1	E	68	VAL
1	E	85	MET
1	E	109	ILE
1	E	142	SER
1	E	149	GLN
1	F	26	PHE
1	F	35	TRP
1	F	36	SER
1	F	41	THR
1	F	64	VAL
1	F	110	ASP
1	F	111	LYS
1	F	135	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	C	135	ASN
1	D	22	HIS
1	D	56	ASN
1	F	22	HIS
1	F	135	ASN

### 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](#)

2 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	SO4	A	201	-	4,4,4	0.61	0	6,6,6	0.22	0
2	SO4	D	201	-	4,4,4	0.67	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	146/178 (82%)	0.28	12 (8%) 11 14	26, 43, 77, 89	0
1	B	143/178 (80%)	0.25	6 (4%) 36 42	20, 37, 76, 97	0
1	C	139/178 (78%)	0.11	8 (5%) 23 27	21, 35, 88, 106	0
1	D	137/178 (76%)	0.36	12 (8%) 10 11	26, 42, 87, 108	0
1	E	130/178 (73%)	0.50	15 (11%) 4 6	29, 56, 90, 99	0
1	F	135/178 (75%)	0.61	16 (11%) 4 5	29, 55, 97, 116	0
All	All	830/1068 (77%)	0.35	69 (8%) 11 13	20, 45, 89, 116	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	LEU	6.7
1	F	136	ILE	6.2
1	F	137	ILE	5.6
1	E	138	CYS	5.1
1	F	135	ASN	4.8
1	D	136	ILE	4.6
1	F	160	TYR	4.3
1	B	113	ARG	4.3
1	A	90	PHE	4.2
1	A	92	HIS	4.2
1	C	7	ASN	4.1
1	F	159	ALA	4.0
1	F	131	VAL	3.9
1	D	134	LYS	3.8
1	E	104	PHE	3.8
1	A	135	ASN	3.7
1	D	137	ILE	3.6
1	A	93	VAL	3.4
1	E	160	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	103	THR	3.3
1	F	107	ALA	3.3
1	E	34	ASP	3.3
1	D	160	TYR	3.3
1	A	91	ALA	3.2
1	D	104	PHE	3.1
1	B	8	ASN	3.1
1	F	103	THR	3.0
1	A	88	THR	3.0
1	B	90	PHE	3.0
1	C	136	ILE	3.0
1	E	35	TRP	3.0
1	E	103	THR	2.9
1	D	35	TRP	2.9
1	A	160	TYR	2.9
1	F	84	LEU	2.9
1	C	135	ASN	2.8
1	C	161	LYS	2.8
1	E	128	SER	2.8
1	E	37	VAL	2.7
1	F	41	THR	2.7
1	F	40	ARG	2.6
1	E	131	VAL	2.6
1	F	133	GLN	2.6
1	C	103	THR	2.5
1	F	9	LYS	2.5
1	E	150	ILE	2.5
1	C	160	TYR	2.5
1	E	84	LEU	2.5
1	F	134	LYS	2.5
1	E	85	MET	2.5
1	D	162	ASP	2.5
1	C	137	ILE	2.4
1	A	102	ARG	2.4
1	E	159	ALA	2.4
1	B	135	ASN	2.3
1	A	136	ILE	2.3
1	B	103	THR	2.3
1	F	132	LYS	2.3
1	A	86	ALA	2.2
1	B	28	LEU	2.2
1	E	9	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	37	VAL	2.2
1	A	104	PHE	2.2
1	C	104	PHE	2.1
1	E	36	SER	2.1
1	D	10	GLN	2.1
1	D	159	ALA	2.0
1	D	133	GLN	2.0
1	D	161	LYS	2.0

## 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. 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	201	5/5	0.89	0.31	66,70,78,92	0
2	SO4	D	201	5/5	0.89	0.29	60,64,71,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.