Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:08 am BST

PDB ID	:	6HRD
Title	:	Crystal structure of M. tuberculosis FadB2 (Rv0468)
Authors	:	Cox, J.A.G.; Besra, G.S.; Futterer, K.
Deposited on	:	2018-09-26
Resolution	:	2.11 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

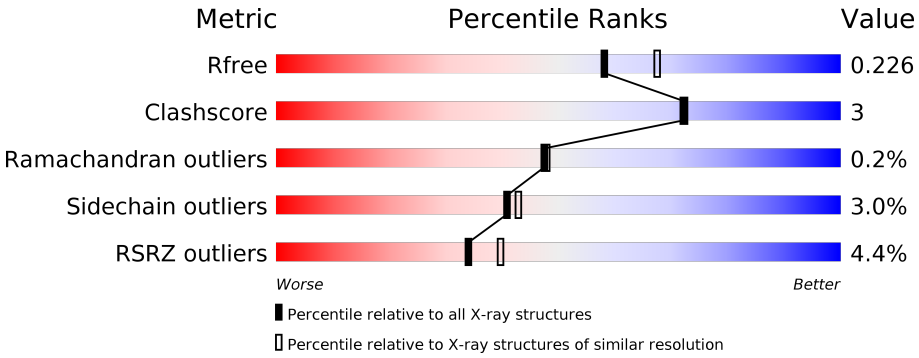
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	317	82% 7% • 10%
1	B	317	% 81% 7% • 10%
1	C	317	80% 8% • 10%
1	D	317	% 80% 9% • 10%
1	E	317	83% 5% • 10%
1	F	317	21% 76% 13% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13117 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-hydroxybutyryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2117	1345	368	397	7			
1	B	285	Total	C	N	O	S	0	0	0
			2112	1342	369	394	7			
1	C	285	Total	C	N	O	S	0	0	0
			2108	1340	366	395	7			
1	D	285	Total	C	N	O	S	0	0	0
			2118	1344	369	398	7			
1	E	285	Total	C	N	O	S	0	0	0
			2112	1341	369	395	7			
1	F	285	Total	C	N	O	S	0	0	0
			2108	1340	368	393	7			

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WNP7
A	-18	GLY	-	expression tag	UNP P9WNP7
A	-17	SER	-	expression tag	UNP P9WNP7
A	-16	SER	-	expression tag	UNP P9WNP7
A	-15	HIS	-	expression tag	UNP P9WNP7
A	-14	HIS	-	expression tag	UNP P9WNP7
A	-13	HIS	-	expression tag	UNP P9WNP7
A	-12	HIS	-	expression tag	UNP P9WNP7
A	-11	HIS	-	expression tag	UNP P9WNP7
A	-10	HIS	-	expression tag	UNP P9WNP7
A	-9	SER	-	expression tag	UNP P9WNP7
A	-8	SER	-	expression tag	UNP P9WNP7
A	-7	GLY	-	expression tag	UNP P9WNP7
A	-6	LEU	-	expression tag	UNP P9WNP7
A	-5	VAL	-	expression tag	UNP P9WNP7
A	-4	PRO	-	expression tag	UNP P9WNP7
A	-3	ARG	-	expression tag	UNP P9WNP7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P9WNP7
A	-1	SER	-	expression tag	UNP P9WNP7
A	0	HIS	-	expression tag	UNP P9WNP7
A	287	ALA	-	expression tag	UNP P9WNP7
A	288	ALA	-	expression tag	UNP P9WNP7
A	289	ALA	-	expression tag	UNP P9WNP7
A	290	LEU	-	expression tag	UNP P9WNP7
A	291	GLU	-	expression tag	UNP P9WNP7
A	292	HIS	-	expression tag	UNP P9WNP7
A	293	HIS	-	expression tag	UNP P9WNP7
A	294	HIS	-	expression tag	UNP P9WNP7
A	295	HIS	-	expression tag	UNP P9WNP7
A	296	HIS	-	expression tag	UNP P9WNP7
A	297	HIS	-	expression tag	UNP P9WNP7
B	-19	MET	-	initiating methionine	UNP P9WNP7
B	-18	GLY	-	expression tag	UNP P9WNP7
B	-17	SER	-	expression tag	UNP P9WNP7
B	-16	SER	-	expression tag	UNP P9WNP7
B	-15	HIS	-	expression tag	UNP P9WNP7
B	-14	HIS	-	expression tag	UNP P9WNP7
B	-13	HIS	-	expression tag	UNP P9WNP7
B	-12	HIS	-	expression tag	UNP P9WNP7
B	-11	HIS	-	expression tag	UNP P9WNP7
B	-10	HIS	-	expression tag	UNP P9WNP7
B	-9	SER	-	expression tag	UNP P9WNP7
B	-8	SER	-	expression tag	UNP P9WNP7
B	-7	GLY	-	expression tag	UNP P9WNP7
B	-6	LEU	-	expression tag	UNP P9WNP7
B	-5	VAL	-	expression tag	UNP P9WNP7
B	-4	PRO	-	expression tag	UNP P9WNP7
B	-3	ARG	-	expression tag	UNP P9WNP7
B	-2	GLY	-	expression tag	UNP P9WNP7
B	-1	SER	-	expression tag	UNP P9WNP7
B	0	HIS	-	expression tag	UNP P9WNP7
B	287	ALA	-	expression tag	UNP P9WNP7
B	288	ALA	-	expression tag	UNP P9WNP7
B	289	ALA	-	expression tag	UNP P9WNP7
B	290	LEU	-	expression tag	UNP P9WNP7
B	291	GLU	-	expression tag	UNP P9WNP7
B	292	HIS	-	expression tag	UNP P9WNP7
B	293	HIS	-	expression tag	UNP P9WNP7
B	294	HIS	-	expression tag	UNP P9WNP7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	295	HIS	-	expression tag	UNP P9WNP7
B	296	HIS	-	expression tag	UNP P9WNP7
B	297	HIS	-	expression tag	UNP P9WNP7
C	-19	MET	-	initiating methionine	UNP P9WNP7
C	-18	GLY	-	expression tag	UNP P9WNP7
C	-17	SER	-	expression tag	UNP P9WNP7
C	-16	SER	-	expression tag	UNP P9WNP7
C	-15	HIS	-	expression tag	UNP P9WNP7
C	-14	HIS	-	expression tag	UNP P9WNP7
C	-13	HIS	-	expression tag	UNP P9WNP7
C	-12	HIS	-	expression tag	UNP P9WNP7
C	-11	HIS	-	expression tag	UNP P9WNP7
C	-10	HIS	-	expression tag	UNP P9WNP7
C	-9	SER	-	expression tag	UNP P9WNP7
C	-8	SER	-	expression tag	UNP P9WNP7
C	-7	GLY	-	expression tag	UNP P9WNP7
C	-6	LEU	-	expression tag	UNP P9WNP7
C	-5	VAL	-	expression tag	UNP P9WNP7
C	-4	PRO	-	expression tag	UNP P9WNP7
C	-3	ARG	-	expression tag	UNP P9WNP7
C	-2	GLY	-	expression tag	UNP P9WNP7
C	-1	SER	-	expression tag	UNP P9WNP7
C	0	HIS	-	expression tag	UNP P9WNP7
C	287	ALA	-	expression tag	UNP P9WNP7
C	288	ALA	-	expression tag	UNP P9WNP7
C	289	ALA	-	expression tag	UNP P9WNP7
C	290	LEU	-	expression tag	UNP P9WNP7
C	291	GLU	-	expression tag	UNP P9WNP7
C	292	HIS	-	expression tag	UNP P9WNP7
C	293	HIS	-	expression tag	UNP P9WNP7
C	294	HIS	-	expression tag	UNP P9WNP7
C	295	HIS	-	expression tag	UNP P9WNP7
C	296	HIS	-	expression tag	UNP P9WNP7
C	297	HIS	-	expression tag	UNP P9WNP7
D	-19	MET	-	initiating methionine	UNP P9WNP7
D	-18	GLY	-	expression tag	UNP P9WNP7
D	-17	SER	-	expression tag	UNP P9WNP7
D	-16	SER	-	expression tag	UNP P9WNP7
D	-15	HIS	-	expression tag	UNP P9WNP7
D	-14	HIS	-	expression tag	UNP P9WNP7
D	-13	HIS	-	expression tag	UNP P9WNP7
D	-12	HIS	-	expression tag	UNP P9WNP7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	expression tag	UNP P9WNP7
D	-10	HIS	-	expression tag	UNP P9WNP7
D	-9	SER	-	expression tag	UNP P9WNP7
D	-8	SER	-	expression tag	UNP P9WNP7
D	-7	GLY	-	expression tag	UNP P9WNP7
D	-6	LEU	-	expression tag	UNP P9WNP7
D	-5	VAL	-	expression tag	UNP P9WNP7
D	-4	PRO	-	expression tag	UNP P9WNP7
D	-3	ARG	-	expression tag	UNP P9WNP7
D	-2	GLY	-	expression tag	UNP P9WNP7
D	-1	SER	-	expression tag	UNP P9WNP7
D	0	HIS	-	expression tag	UNP P9WNP7
D	287	ALA	-	expression tag	UNP P9WNP7
D	288	ALA	-	expression tag	UNP P9WNP7
D	289	ALA	-	expression tag	UNP P9WNP7
D	290	LEU	-	expression tag	UNP P9WNP7
D	291	GLU	-	expression tag	UNP P9WNP7
D	292	HIS	-	expression tag	UNP P9WNP7
D	293	HIS	-	expression tag	UNP P9WNP7
D	294	HIS	-	expression tag	UNP P9WNP7
D	295	HIS	-	expression tag	UNP P9WNP7
D	296	HIS	-	expression tag	UNP P9WNP7
D	297	HIS	-	expression tag	UNP P9WNP7
E	-19	MET	-	initiating methionine	UNP P9WNP7
E	-18	GLY	-	expression tag	UNP P9WNP7
E	-17	SER	-	expression tag	UNP P9WNP7
E	-16	SER	-	expression tag	UNP P9WNP7
E	-15	HIS	-	expression tag	UNP P9WNP7
E	-14	HIS	-	expression tag	UNP P9WNP7
E	-13	HIS	-	expression tag	UNP P9WNP7
E	-12	HIS	-	expression tag	UNP P9WNP7
E	-11	HIS	-	expression tag	UNP P9WNP7
E	-10	HIS	-	expression tag	UNP P9WNP7
E	-9	SER	-	expression tag	UNP P9WNP7
E	-8	SER	-	expression tag	UNP P9WNP7
E	-7	GLY	-	expression tag	UNP P9WNP7
E	-6	LEU	-	expression tag	UNP P9WNP7
E	-5	VAL	-	expression tag	UNP P9WNP7
E	-4	PRO	-	expression tag	UNP P9WNP7
E	-3	ARG	-	expression tag	UNP P9WNP7
E	-2	GLY	-	expression tag	UNP P9WNP7
E	-1	SER	-	expression tag	UNP P9WNP7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P9WNP7
E	287	ALA	-	expression tag	UNP P9WNP7
E	288	ALA	-	expression tag	UNP P9WNP7
E	289	ALA	-	expression tag	UNP P9WNP7
E	290	LEU	-	expression tag	UNP P9WNP7
E	291	GLU	-	expression tag	UNP P9WNP7
E	292	HIS	-	expression tag	UNP P9WNP7
E	293	HIS	-	expression tag	UNP P9WNP7
E	294	HIS	-	expression tag	UNP P9WNP7
E	295	HIS	-	expression tag	UNP P9WNP7
E	296	HIS	-	expression tag	UNP P9WNP7
E	297	HIS	-	expression tag	UNP P9WNP7
F	-19	MET	-	initiating methionine	UNP P9WNP7
F	-18	GLY	-	expression tag	UNP P9WNP7
F	-17	SER	-	expression tag	UNP P9WNP7
F	-16	SER	-	expression tag	UNP P9WNP7
F	-15	HIS	-	expression tag	UNP P9WNP7
F	-14	HIS	-	expression tag	UNP P9WNP7
F	-13	HIS	-	expression tag	UNP P9WNP7
F	-12	HIS	-	expression tag	UNP P9WNP7
F	-11	HIS	-	expression tag	UNP P9WNP7
F	-10	HIS	-	expression tag	UNP P9WNP7
F	-9	SER	-	expression tag	UNP P9WNP7
F	-8	SER	-	expression tag	UNP P9WNP7
F	-7	GLY	-	expression tag	UNP P9WNP7
F	-6	LEU	-	expression tag	UNP P9WNP7
F	-5	VAL	-	expression tag	UNP P9WNP7
F	-4	PRO	-	expression tag	UNP P9WNP7
F	-3	ARG	-	expression tag	UNP P9WNP7
F	-2	GLY	-	expression tag	UNP P9WNP7
F	-1	SER	-	expression tag	UNP P9WNP7
F	0	HIS	-	expression tag	UNP P9WNP7
F	287	ALA	-	expression tag	UNP P9WNP7
F	288	ALA	-	expression tag	UNP P9WNP7
F	289	ALA	-	expression tag	UNP P9WNP7
F	290	LEU	-	expression tag	UNP P9WNP7
F	291	GLU	-	expression tag	UNP P9WNP7
F	292	HIS	-	expression tag	UNP P9WNP7
F	293	HIS	-	expression tag	UNP P9WNP7
F	294	HIS	-	expression tag	UNP P9WNP7
F	295	HIS	-	expression tag	UNP P9WNP7
F	296	HIS	-	expression tag	UNP P9WNP7

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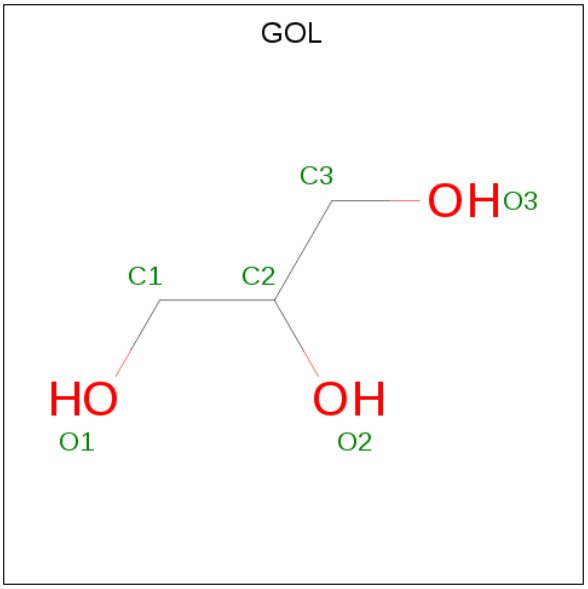
Chain	Residue	Modelled	Actual	Comment	Reference
F	297	HIS	-	expression tag	UNP P9WNP7

- 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 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

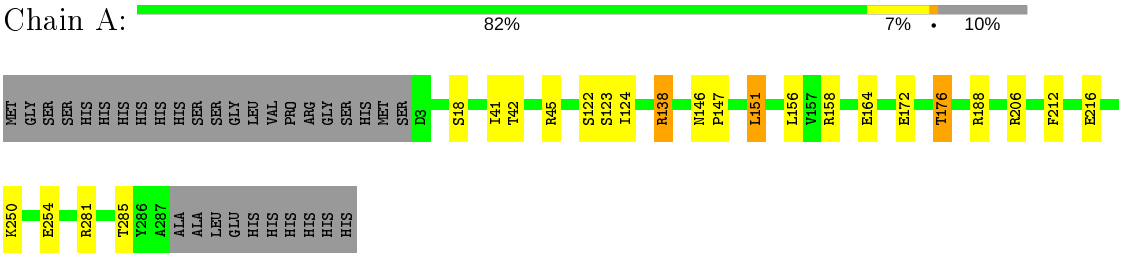
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	B	87	Total O 87 87	0	0
3	C	69	Total O 69 69	0	0
3	D	50	Total O 50 50	0	0
3	E	66	Total O 66 66	0	0
3	F	43	Total O 43 43	0	0

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.

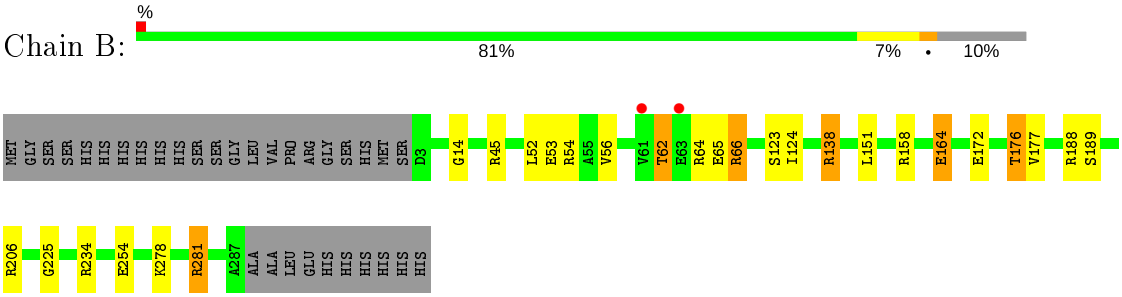
- Molecule 1: 3-hydroxybutyryl-CoA dehydrogenase

Chain A:



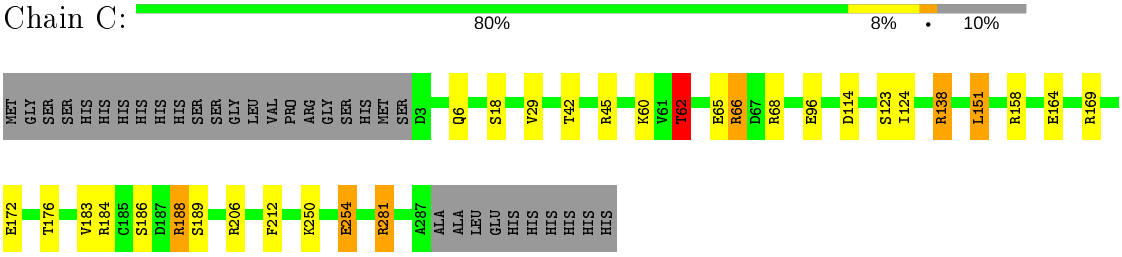
- Molecule 1: 3-hydroxybutyryl-CoA dehydrogenase

Chain B:



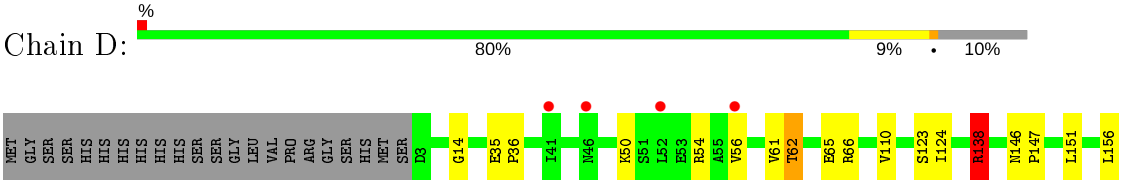
- Molecule 1: 3-hydroxybutyryl-CoA dehydrogenase

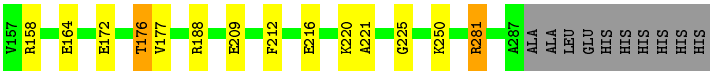
Chain C:



- Molecule 1: 3-hydroxybutyryl-CoA dehydrogenase

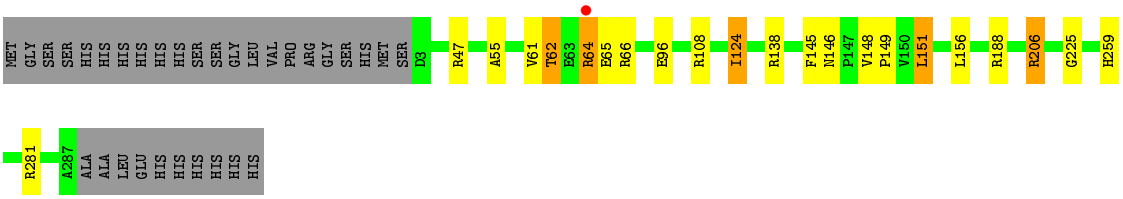
Chain D:





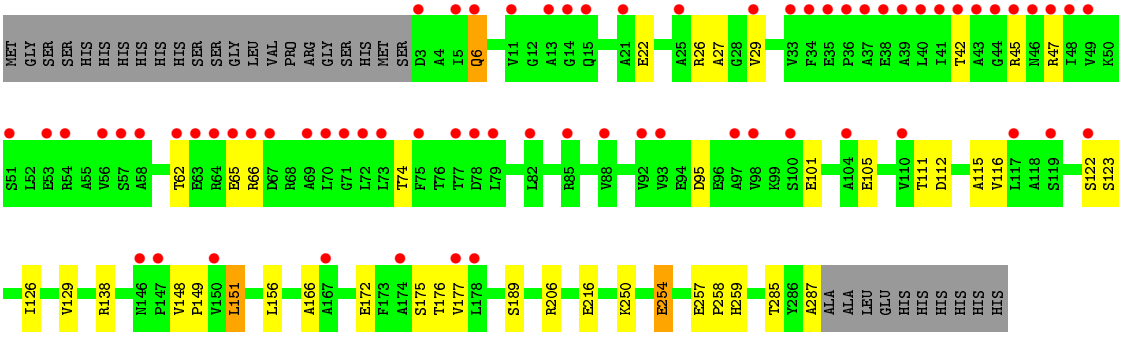
• Molecule 1: 3-hydroxybutyryl-CoA dehydrogenase

Chain E:



• Molecule 1: 3-hydroxybutyryl-CoA dehydrogenase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	90.22Å 90.22Å 284.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.20 – 2.11 90.22 – 2.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.20-2.11) 100.0 (90.22-2.11)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.190 , 0.221 0.199 , 0.226	Depositor DCC
R_{free} test set	6484 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13117	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.75	1/2148 (0.0%)	0.87	3/2920 (0.1%)
1	B	0.74	0/2143	0.80	1/2913 (0.0%)
1	C	0.72	1/2139 (0.0%)	0.83	3/2909 (0.1%)
1	D	0.71	1/2149 (0.0%)	0.80	2/2920 (0.1%)
1	E	0.68	0/2143	0.81	1/2911 (0.0%)
1	F	0.64	2/2139 (0.1%)	0.72	1/2907 (0.0%)
All	All	0.71	5/12861 (0.0%)	0.81	11/17480 (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	A	0	4
1	B	0	6
1	C	0	4
1	D	0	3
1	E	0	5
1	F	0	4
All	All	0	26

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	GLU	CD-OE2	-6.55	1.18	1.25
1	F	216	GLU	CD-OE1	6.38	1.32	1.25
1	D	216	GLU	CD-OE1	5.88	1.32	1.25
1	F	254	GLU	CD-OE2	-5.45	1.19	1.25
1	A	216	GLU	CD-OE1	5.20	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	E	206	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	138	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	138	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	138	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	285	THR	CA-CB-OG1	-5.53	97.39	109.00
1	A	138	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	F	285	THR	CA-CB-OG1	-5.42	97.62	109.00
1	C	188	ARG	CB-CA-C	-5.12	100.16	110.40
1	C	254	GLU	CB-CA-C	-5.10	100.20	110.40
1	C	62	THR	N-CA-CB	-5.02	100.75	110.30

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	206	ARG	Sidechain
1	A	281	ARG	Sidechain
1	A	45	ARG	Sidechain
1	B	138	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	234	ARG	Sidechain
1	B	281	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	54	ARG	Sidechain
1	C	138	ARG	Sidechain
1	C	206	ARG	Sidechain
1	C	281	ARG	Sidechain
1	C	66	ARG	Sidechain
1	D	138	ARG	Sidechain
1	D	281	ARG	Sidechain
1	D	66	ARG	Sidechain
1	E	108	ARG	Sidechain
1	E	138	ARG	Sidechain
1	E	206	ARG	Sidechain
1	E	64	ARG	Sidechain
1	E	66	ARG	Sidechain
1	F	122	SER	Peptide
1	F	138	ARG	Sidechain
1	F	206	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	47	ARG	Sidechain

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	2117	0	2150	14	1
1	B	2112	0	2144	14	0
1	C	2108	0	2140	22	0
1	D	2118	0	2146	16	1
1	E	2112	0	2149	11	0
1	F	2108	0	2136	19	0
2	A	6	0	8	0	0
2	C	6	0	8	0	0
2	E	6	0	8	3	0
3	A	109	0	0	4	0
3	B	87	0	0	1	0
3	C	69	0	0	9	0
3	D	50	0	0	0	0
3	E	66	0	0	1	0
3	F	43	0	0	1	0
All	All	13117	0	12889	87	1

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 3.

All (87) 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:A:18:SER:CB	3:A:446:HOH:O	1.72	1.29
1:F:287:ALA:O	3:F:301:HOH:O	1.66	1.12
1:A:158:ARG:NH1	1:A:164:GLU:OE1	1.82	1.12
1:C:18:SER:CB	3:C:401:HOH:O	2.01	1.07
1:B:158:ARG:NH1	1:B:164:GLU:OE2	2.00	0.94
1:E:62:THR:HG22	1:E:65:GLU:H	1.40	0.86
1:C:60:LYS:CB	3:C:462:HOH:O	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:THR:HG22	1:C:65:GLU:H	1.44	0.82
1:C:189:SER:HB2	1:C:254:GLU:HG3	1.65	0.79
2:E:301:GOL:H11	1:F:259:HIS:ND1	1.97	0.79
1:A:122:SER:HB2	3:A:502:HOH:O	1.85	0.76
1:C:184:ARG:HD2	3:C:429:HOH:O	1.90	0.70
1:D:158:ARG:NH1	1:D:164:GLU:OE1	2.20	0.70
1:B:189:SER:HB2	1:B:254:GLU:HG3	1.76	0.68
1:C:212:PHE:CE1	1:D:188:ARG:HD3	2.27	0.68
1:A:212:PHE:CE1	1:B:188:ARG:HD3	2.30	0.66
1:F:123:SER:HB2	1:F:250:LYS:HG3	1.77	0.65
1:D:50:LYS:CB	1:D:54:ARG:HH12	2.09	0.65
1:C:158:ARG:HD2	1:C:184:ARG:HH12	1.64	0.61
1:C:68:ARG:HG3	3:C:464:HOH:O	2.00	0.61
1:C:96:GLU:CG	3:C:455:HOH:O	2.47	0.61
1:A:146:ASN:ND2	1:A:147:PRO:HA	2.16	0.61
1:D:146:ASN:ND2	1:D:147:PRO:HA	2.17	0.60
1:E:146:ASN:ND2	3:E:402:HOH:O	2.34	0.60
1:B:52:LEU:O	1:B:56:VAL:HG23	2.03	0.59
1:D:176:THR:HG22	1:D:177:VAL:HG23	1.84	0.59
1:C:164:GLU:CB	3:C:410:HOH:O	2.51	0.58
1:A:42:THR:HG21	3:C:461:HOH:O	2.04	0.56
1:F:6:GLN:HE22	1:F:29:VAL:HA	1.71	0.55
1:D:172:GLU:O	1:D:176:THR:HB	2.08	0.55
3:A:411:HOH:O	1:E:188:ARG:HD2	2.08	0.53
1:C:138:ARG:HD3	3:C:415:HOH:O	2.09	0.53
1:C:158:ARG:HD2	1:C:184:ARG:NH1	2.24	0.53
1:D:110:VAL:O	1:D:138:ARG:NH2	2.35	0.53
2:E:301:GOL:C1	1:F:259:HIS:ND1	2.72	0.52
1:C:212:PHE:CD1	1:D:188:ARG:HD3	2.43	0.52
1:E:62:THR:HG22	1:E:65:GLU:N	2.18	0.52
1:F:42:THR:HG22	1:F:45:ARG:HH21	1.75	0.52
1:A:123:SER:HB3	3:A:502:HOH:O	2.09	0.51
1:A:151:LEU:HD21	1:B:225:GLY:HA2	1.93	0.51
1:A:172:GLU:O	1:A:176:THR:HB	2.10	0.51
1:A:123:SER:HB2	1:A:250:LYS:HG3	1.93	0.50
1:D:123:SER:HB2	1:D:250:LYS:HG3	1.91	0.50
1:B:172:GLU:O	1:B:176:THR:HB	2.12	0.50
1:F:22:GLU:OE2	1:F:26:ARG:NH1	2.44	0.49
1:D:56:VAL:HG22	1:D:61:VAL:HG23	1.95	0.48
1:E:145:PHE:HB2	1:E:151:LEU:HD22	1.96	0.48
1:B:176:THR:HG22	1:B:177:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:THR:HG22	1:D:65:GLU:H	1.79	0.47
1:E:124:ILE:N	1:E:124:ILE:HD13	2.30	0.47
1:C:42:THR:HG22	1:C:45:ARG:HH21	1.80	0.47
1:B:254:GLU:HG2	3:B:339:HOH:O	2.13	0.47
1:B:53:GLU:CG	1:B:66:ARG:HH21	2.28	0.47
1:C:123:SER:HB2	1:C:250:LYS:HG3	1.97	0.46
1:B:62:THR:HG22	1:B:65:GLU:H	1.81	0.46
1:C:6:GLN:O	1:C:29:VAL:HG13	2.15	0.46
1:A:42:THR:CG2	3:C:461:HOH:O	2.61	0.46
1:A:212:PHE:CD1	1:B:188:ARG:HD3	2.51	0.45
1:F:189:SER:HB2	1:F:254:GLU:HG3	1.98	0.45
1:A:156:LEU:C	1:A:156:LEU:HD23	2.38	0.45
1:C:172:GLU:O	1:C:176:THR:HB	2.17	0.45
1:F:62:THR:HG22	1:F:65:GLU:CD	2.36	0.44
1:E:55:ALA:HB1	1:E:61:VAL:HG13	1.98	0.44
1:A:41:ILE:HA	1:A:41:ILE:HD13	1.80	0.44
1:F:27:ALA:HB1	1:F:177:VAL:O	2.17	0.44
1:E:156:LEU:HD23	1:E:156:LEU:C	2.38	0.44
1:C:114:ASP:O	1:C:169:ARG:NH2	2.51	0.43
1:D:156:LEU:HD23	1:D:156:LEU:C	2.38	0.43
1:F:148:VAL:N	1:F:149:PRO:CD	2.81	0.43
1:F:116:VAL:HG22	1:F:166:ALA:HB1	2.01	0.43
1:B:189:SER:CB	1:B:254:GLU:HG3	2.48	0.43
1:E:259:HIS:N	2:E:301:GOL:O3	2.51	0.43
1:C:189:SER:CB	1:C:254:GLU:HG3	2.43	0.42
1:C:188:ARG:HD3	1:D:212:PHE:CE1	2.54	0.42
1:C:151:LEU:HD21	1:D:225:GLY:HA2	2.02	0.42
1:B:124:ILE:N	1:B:124:ILE:HD12	2.35	0.42
1:F:257:GLU:HA	1:F:258:PRO:HD3	1.95	0.42
1:D:35:GLU:OE1	1:D:36:PRO:HD2	2.20	0.41
1:C:183:VAL:HG21	1:D:221:ALA:HB2	2.03	0.41
1:F:6:GLN:NE2	1:F:29:VAL:HA	2.34	0.41
1:F:62:THR:HG22	1:F:65:GLU:CG	2.51	0.41
1:F:101:GLU:O	1:F:105:GLU:HG3	2.21	0.41
1:E:148:VAL:N	1:E:149:PRO:CD	2.84	0.41
1:F:126:ILE:O	1:F:129:VAL:HG22	2.21	0.41
1:F:112:ASP:HB3	1:F:115:ALA:HB2	2.03	0.41
1:E:225:GLY:HA2	1:F:151:LEU:HD21	2.03	0.40
1:B:123:SER:OG	1:B:124:ILE:HD12	2.21	0.40

All (1) 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:A:188:ARG:NH1	1:D:209:GLU:OE2[1_455]	2.18	0.02

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	283/317 (89%)	275 (97%)	8 (3%)	0	100	100
1	B	283/317 (89%)	274 (97%)	8 (3%)	1 (0%)	34	32
1	C	283/317 (89%)	278 (98%)	5 (2%)	0	100	100
1	D	283/317 (89%)	271 (96%)	11 (4%)	1 (0%)	34	32
1	E	283/317 (89%)	277 (98%)	6 (2%)	0	100	100
1	F	283/317 (89%)	267 (94%)	15 (5%)	1 (0%)	34	32
All	All	1698/1902 (89%)	1642 (97%)	53 (3%)	3 (0%)	47	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14	GLY
1	F	176	THR
1	B	14	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/258 (85%)	216 (98%)	4 (2%)	59	63
1	B	219/258 (85%)	211 (96%)	8 (4%)	34	34
1	C	219/258 (85%)	213 (97%)	6 (3%)	44	47
1	D	221/258 (86%)	215 (97%)	6 (3%)	44	47
1	E	221/258 (86%)	214 (97%)	7 (3%)	39	40
1	F	218/258 (84%)	209 (96%)	9 (4%)	30	30
All	All	1318/1548 (85%)	1278 (97%)	40 (3%)	41	43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ILE
1	A	151	LEU
1	A	176	THR
1	A	254	GLU
1	B	62	THR
1	B	64	ARG
1	B	66	ARG
1	B	151	LEU
1	B	164	GLU
1	B	176	THR
1	B	278	LYS
1	B	281	ARG
1	C	62	THR
1	C	66	ARG
1	C	124	ILE
1	C	151	LEU
1	C	186	SER
1	C	281	ARG
1	D	62	THR
1	D	124	ILE
1	D	151	LEU
1	D	176	THR
1	D	220	LYS
1	D	281	ARG
1	E	47	ARG
1	E	62	THR
1	E	64	ARG
1	E	96	GLU
1	E	124	ILE
1	E	151	LEU

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Mol	Chain	Res	Type
1	E	281	ARG
1	F	6	GLN
1	F	66	ARG
1	F	74	THR
1	F	95	ASP
1	F	111	THR
1	F	151	LEU
1	F	156	LEU
1	F	172	GLU
1	F	175	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	181	GLN
1	B	80	ASN
1	B	146	ASN
1	C	6	GLN
1	C	146	ASN
1	C	181	GLN
1	D	80	ASN
1	D	146	ASN
1	D	181	GLN
1	E	181	GLN
1	E	259	HIS
1	F	6	GLN
1	F	146	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 (i)

3 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	301	-	5,5,5	0.20	0	5,5,5	0.71	0
2	GOL	C	301	-	5,5,5	0.26	0	5,5,5	1.20	1 (20%)
2	GOL	E	301	-	5,5,5	0.16	0	5,5,5	0.63	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	301	-	-	3/4/4/4	-
2	GOL	C	301	-	-	4/4/4/4	-
2	GOL	E	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	GOL	C3-C2-C1	-2.35	102.58	111.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	C1-C2-C3-O3
2	C	301	GOL	C1-C2-C3-O3
2	E	301	GOL	C1-C2-C3-O3
2	C	301	GOL	O1-C1-C2-C3
2	A	301	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	301	GOL	O1-C1-C2-O2
2	C	301	GOL	O2-C2-C3-O3
2	E	301	GOL	O2-C2-C3-O3
2	A	301	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	GOL	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	285/317 (89%)	-0.11	0 100 100	20, 28, 42, 75	0
1	B	285/317 (89%)	-0.03	2 (0%) 87 89	22, 34, 75, 98	0
1	C	285/317 (89%)	-0.09	0 100 100	23, 34, 50, 78	0
1	D	285/317 (89%)	0.04	4 (1%) 75 78	23, 37, 86, 97	0
1	E	285/317 (89%)	-0.11	1 (0%) 92 93	25, 36, 57, 83	0
1	F	285/317 (89%)	1.16	68 (23%) 0 0	24, 69, 118, 138	0
All	All	1710/1902 (89%)	0.14	75 (4%) 34 40	20, 35, 92, 138	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	40	LEU	8.7
1	F	36	PRO	7.3
1	F	46	ASN	7.2
1	F	57	SER	7.0
1	F	37	ALA	7.0
1	F	42	THR	6.7
1	F	43	ALA	5.9
1	F	62	THR	5.8
1	F	82	LEU	5.8
1	F	13	ALA	5.2
1	F	93	VAL	5.0
1	F	11	VAL	5.0
1	F	79	LEU	4.9
1	F	69	ALA	4.8
1	F	5	ILE	4.8
1	F	70	LEU	4.7
1	F	178	LEU	4.7
1	F	66	ARG	4.1
1	F	49	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	117	LEU	4.1
1	F	177	VAL	4.0
1	F	47	ARG	3.9
1	F	64	ARG	3.8
1	F	174	ALA	3.8
1	F	29	VAL	3.6
1	B	63	GLU	3.6
1	F	54	ARG	3.6
1	F	58	ALA	3.4
1	F	150	VAL	3.4
1	F	104	ALA	3.3
1	F	41	ILE	3.1
1	F	45	ARG	3.1
1	F	33	VAL	3.1
1	F	56	VAL	3.1
1	F	67	ASP	3.0
1	F	14	GLY	2.9
1	F	146	ASN	2.9
1	F	48	ILE	2.9
1	F	75	PHE	2.9
1	F	25	ALA	2.9
1	F	88	VAL	2.8
1	F	35	GLU	2.8
1	F	100	SER	2.8
1	F	51	SER	2.8
1	F	122	SER	2.8
1	F	167	ALA	2.8
1	F	39	ALA	2.7
1	F	92	VAL	2.7
1	F	44	GLY	2.7
1	F	38	GLU	2.6
1	D	56	VAL	2.6
1	F	3	ASP	2.6
1	F	119	SER	2.5
1	B	61	VAL	2.5
1	D	46	ASN	2.5
1	F	97	ALA	2.4
1	F	34	PHE	2.4
1	F	73	LEU	2.4
1	F	15	GLN	2.4
1	F	53	GLU	2.3
1	F	21	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	71	GLY	2.3
1	D	41	ILE	2.3
1	F	85	ARG	2.2
1	D	52	LEU	2.2
1	F	6	GLN	2.2
1	F	110	VAL	2.2
1	F	78	ASP	2.2
1	F	63	GLU	2.1
1	F	147	PRO	2.1
1	F	65	GLU	2.1
1	F	77	THR	2.1
1	E	64	ARG	2.1
1	F	98	VAL	2.1
1	F	72	LEU	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^{th} 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^2)	Q<0.9
2	GOL	A	301	6/6	0.82	0.21	52,53,61,61	0
2	GOL	C	301	6/6	0.83	0.26	55,56,57,63	0
2	GOL	E	301	6/6	0.85	0.22	52,54,60,61	0

6.5 Other polymers (i)

There are no such residues in this entry.