



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 04:04 AM EST

PDB ID : 3GRK
Title : Crystal structure of short chain dehydrogenase reductase SDR glucose-ribitol dehydrogenase from *Brucella melitensis*
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2009-03-25
Resolution : 2.35 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

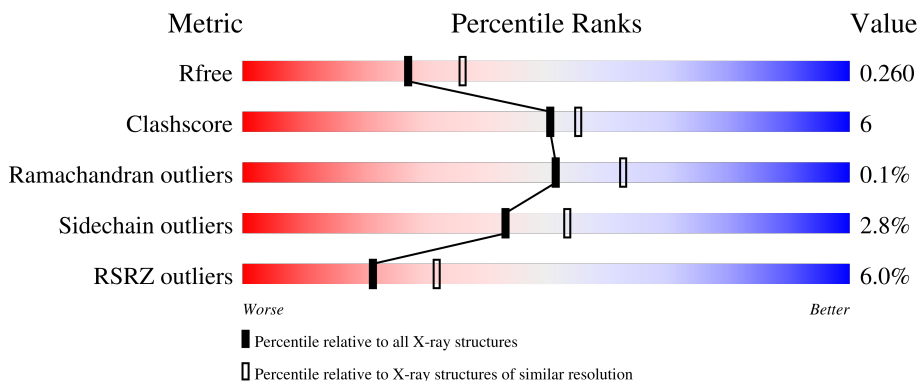
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



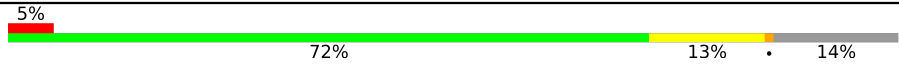

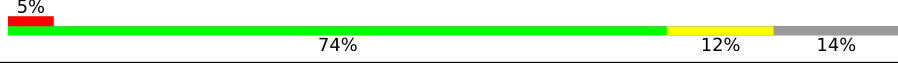
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 of 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 $\leq 5\%$. 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	293	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 73% 10% • 15%</p>
1	B	293	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 76% 9% • 14%</p>
1	C	293	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 69% 16% 15%</p>
1	D	293	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 73% 13% 14%</p>
1	E	293	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 76% 9% 15%</p>

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Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	
1	H	293	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15671 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 Enoyl-(acyl-carrier-protein) reductase (NADH).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	Total 1863	C 1184	N 314	O 359	S 6	0	0	0
1	B	252	Total 1904	C 1211	N 324	O 363	S 6	0	0	0
1	C	248	Total 1875	C 1191	N 320	O 358	S 6	0	0	0
1	D	251	Total 1909	C 1214	N 327	O 362	S 6	0	0	0
1	E	248	Total 1883	C 1196	N 322	O 359	S 6	0	0	0
1	F	252	Total 1907	C 1211	N 326	O 364	S 6	0	0	0
1	G	247	Total 1869	C 1189	N 320	O 354	S 6	0	0	0
1	H	252	Total 1898	C 1205	N 324	O 363	S 6	0	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q8YFK8
A	-19	ALA	-	expression tag	UNP Q8YFK8
A	-18	HIS	-	expression tag	UNP Q8YFK8
A	-17	HIS	-	expression tag	UNP Q8YFK8
A	-16	HIS	-	expression tag	UNP Q8YFK8
A	-15	HIS	-	expression tag	UNP Q8YFK8
A	-14	HIS	-	expression tag	UNP Q8YFK8
A	-13	HIS	-	expression tag	UNP Q8YFK8
A	-12	MET	-	expression tag	UNP Q8YFK8
A	-11	GLY	-	expression tag	UNP Q8YFK8
A	-10	THR	-	expression tag	UNP Q8YFK8
A	-9	LEU	-	expression tag	UNP Q8YFK8
A	-8	GLU	-	expression tag	UNP Q8YFK8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	expression tag	UNP Q8YFK8
A	-6	GLN	-	expression tag	UNP Q8YFK8
A	-5	THR	-	expression tag	UNP Q8YFK8
A	-4	GLN	-	expression tag	UNP Q8YFK8
A	-3	GLY	-	expression tag	UNP Q8YFK8
A	-2	PRO	-	expression tag	UNP Q8YFK8
A	-1	GLY	-	expression tag	UNP Q8YFK8
A	0	SER	-	expression tag	UNP Q8YFK8
B	-20	MET	-	expression tag	UNP Q8YFK8
B	-19	ALA	-	expression tag	UNP Q8YFK8
B	-18	HIS	-	expression tag	UNP Q8YFK8
B	-17	HIS	-	expression tag	UNP Q8YFK8
B	-16	HIS	-	expression tag	UNP Q8YFK8
B	-15	HIS	-	expression tag	UNP Q8YFK8
B	-14	HIS	-	expression tag	UNP Q8YFK8
B	-13	HIS	-	expression tag	UNP Q8YFK8
B	-12	MET	-	expression tag	UNP Q8YFK8
B	-11	GLY	-	expression tag	UNP Q8YFK8
B	-10	THR	-	expression tag	UNP Q8YFK8
B	-9	LEU	-	expression tag	UNP Q8YFK8
B	-8	GLU	-	expression tag	UNP Q8YFK8
B	-7	ALA	-	expression tag	UNP Q8YFK8
B	-6	GLN	-	expression tag	UNP Q8YFK8
B	-5	THR	-	expression tag	UNP Q8YFK8
B	-4	GLN	-	expression tag	UNP Q8YFK8
B	-3	GLY	-	expression tag	UNP Q8YFK8
B	-2	PRO	-	expression tag	UNP Q8YFK8
B	-1	GLY	-	expression tag	UNP Q8YFK8
B	0	SER	-	expression tag	UNP Q8YFK8
C	-20	MET	-	expression tag	UNP Q8YFK8
C	-19	ALA	-	expression tag	UNP Q8YFK8
C	-18	HIS	-	expression tag	UNP Q8YFK8
C	-17	HIS	-	expression tag	UNP Q8YFK8
C	-16	HIS	-	expression tag	UNP Q8YFK8
C	-15	HIS	-	expression tag	UNP Q8YFK8
C	-14	HIS	-	expression tag	UNP Q8YFK8
C	-13	HIS	-	expression tag	UNP Q8YFK8
C	-12	MET	-	expression tag	UNP Q8YFK8
C	-11	GLY	-	expression tag	UNP Q8YFK8
C	-10	THR	-	expression tag	UNP Q8YFK8
C	-9	LEU	-	expression tag	UNP Q8YFK8
C	-8	GLU	-	expression tag	UNP Q8YFK8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	expression tag	UNP Q8YFK8
C	-6	GLN	-	expression tag	UNP Q8YFK8
C	-5	THR	-	expression tag	UNP Q8YFK8
C	-4	GLN	-	expression tag	UNP Q8YFK8
C	-3	GLY	-	expression tag	UNP Q8YFK8
C	-2	PRO	-	expression tag	UNP Q8YFK8
C	-1	GLY	-	expression tag	UNP Q8YFK8
C	0	SER	-	expression tag	UNP Q8YFK8
D	-20	MET	-	expression tag	UNP Q8YFK8
D	-19	ALA	-	expression tag	UNP Q8YFK8
D	-18	HIS	-	expression tag	UNP Q8YFK8
D	-17	HIS	-	expression tag	UNP Q8YFK8
D	-16	HIS	-	expression tag	UNP Q8YFK8
D	-15	HIS	-	expression tag	UNP Q8YFK8
D	-14	HIS	-	expression tag	UNP Q8YFK8
D	-13	HIS	-	expression tag	UNP Q8YFK8
D	-12	MET	-	expression tag	UNP Q8YFK8
D	-11	GLY	-	expression tag	UNP Q8YFK8
D	-10	THR	-	expression tag	UNP Q8YFK8
D	-9	LEU	-	expression tag	UNP Q8YFK8
D	-8	GLU	-	expression tag	UNP Q8YFK8
D	-7	ALA	-	expression tag	UNP Q8YFK8
D	-6	GLN	-	expression tag	UNP Q8YFK8
D	-5	THR	-	expression tag	UNP Q8YFK8
D	-4	GLN	-	expression tag	UNP Q8YFK8
D	-3	GLY	-	expression tag	UNP Q8YFK8
D	-2	PRO	-	expression tag	UNP Q8YFK8
D	-1	GLY	-	expression tag	UNP Q8YFK8
D	0	SER	-	expression tag	UNP Q8YFK8
E	-20	MET	-	expression tag	UNP Q8YFK8
E	-19	ALA	-	expression tag	UNP Q8YFK8
E	-18	HIS	-	expression tag	UNP Q8YFK8
E	-17	HIS	-	expression tag	UNP Q8YFK8
E	-16	HIS	-	expression tag	UNP Q8YFK8
E	-15	HIS	-	expression tag	UNP Q8YFK8
E	-14	HIS	-	expression tag	UNP Q8YFK8
E	-13	HIS	-	expression tag	UNP Q8YFK8
E	-12	MET	-	expression tag	UNP Q8YFK8
E	-11	GLY	-	expression tag	UNP Q8YFK8
E	-10	THR	-	expression tag	UNP Q8YFK8
E	-9	LEU	-	expression tag	UNP Q8YFK8
E	-8	GLU	-	expression tag	UNP Q8YFK8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ALA	-	expression tag	UNP Q8YFK8
E	-6	GLN	-	expression tag	UNP Q8YFK8
E	-5	THR	-	expression tag	UNP Q8YFK8
E	-4	GLN	-	expression tag	UNP Q8YFK8
E	-3	GLY	-	expression tag	UNP Q8YFK8
E	-2	PRO	-	expression tag	UNP Q8YFK8
E	-1	GLY	-	expression tag	UNP Q8YFK8
E	0	SER	-	expression tag	UNP Q8YFK8
F	-20	MET	-	expression tag	UNP Q8YFK8
F	-19	ALA	-	expression tag	UNP Q8YFK8
F	-18	HIS	-	expression tag	UNP Q8YFK8
F	-17	HIS	-	expression tag	UNP Q8YFK8
F	-16	HIS	-	expression tag	UNP Q8YFK8
F	-15	HIS	-	expression tag	UNP Q8YFK8
F	-14	HIS	-	expression tag	UNP Q8YFK8
F	-13	HIS	-	expression tag	UNP Q8YFK8
F	-12	MET	-	expression tag	UNP Q8YFK8
F	-11	GLY	-	expression tag	UNP Q8YFK8
F	-10	THR	-	expression tag	UNP Q8YFK8
F	-9	LEU	-	expression tag	UNP Q8YFK8
F	-8	GLU	-	expression tag	UNP Q8YFK8
F	-7	ALA	-	expression tag	UNP Q8YFK8
F	-6	GLN	-	expression tag	UNP Q8YFK8
F	-5	THR	-	expression tag	UNP Q8YFK8
F	-4	GLN	-	expression tag	UNP Q8YFK8
F	-3	GLY	-	expression tag	UNP Q8YFK8
F	-2	PRO	-	expression tag	UNP Q8YFK8
F	-1	GLY	-	expression tag	UNP Q8YFK8
F	0	SER	-	expression tag	UNP Q8YFK8
G	-20	MET	-	expression tag	UNP Q8YFK8
G	-19	ALA	-	expression tag	UNP Q8YFK8
G	-18	HIS	-	expression tag	UNP Q8YFK8
G	-17	HIS	-	expression tag	UNP Q8YFK8
G	-16	HIS	-	expression tag	UNP Q8YFK8
G	-15	HIS	-	expression tag	UNP Q8YFK8
G	-14	HIS	-	expression tag	UNP Q8YFK8
G	-13	HIS	-	expression tag	UNP Q8YFK8
G	-12	MET	-	expression tag	UNP Q8YFK8
G	-11	GLY	-	expression tag	UNP Q8YFK8
G	-10	THR	-	expression tag	UNP Q8YFK8
G	-9	LEU	-	expression tag	UNP Q8YFK8
G	-8	GLU	-	expression tag	UNP Q8YFK8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	ALA	-	expression tag	UNP Q8YFK8
G	-6	GLN	-	expression tag	UNP Q8YFK8
G	-5	THR	-	expression tag	UNP Q8YFK8
G	-4	GLN	-	expression tag	UNP Q8YFK8
G	-3	GLY	-	expression tag	UNP Q8YFK8
G	-2	PRO	-	expression tag	UNP Q8YFK8
G	-1	GLY	-	expression tag	UNP Q8YFK8
G	0	SER	-	expression tag	UNP Q8YFK8
H	-20	MET	-	expression tag	UNP Q8YFK8
H	-19	ALA	-	expression tag	UNP Q8YFK8
H	-18	HIS	-	expression tag	UNP Q8YFK8
H	-17	HIS	-	expression tag	UNP Q8YFK8
H	-16	HIS	-	expression tag	UNP Q8YFK8
H	-15	HIS	-	expression tag	UNP Q8YFK8
H	-14	HIS	-	expression tag	UNP Q8YFK8
H	-13	HIS	-	expression tag	UNP Q8YFK8
H	-12	MET	-	expression tag	UNP Q8YFK8
H	-11	GLY	-	expression tag	UNP Q8YFK8
H	-10	THR	-	expression tag	UNP Q8YFK8
H	-9	LEU	-	expression tag	UNP Q8YFK8
H	-8	GLU	-	expression tag	UNP Q8YFK8
H	-7	ALA	-	expression tag	UNP Q8YFK8
H	-6	GLN	-	expression tag	UNP Q8YFK8
H	-5	THR	-	expression tag	UNP Q8YFK8
H	-4	GLN	-	expression tag	UNP Q8YFK8
H	-3	GLY	-	expression tag	UNP Q8YFK8
H	-2	PRO	-	expression tag	UNP Q8YFK8
H	-1	GLY	-	expression tag	UNP Q8YFK8
H	0	SER	-	expression tag	UNP Q8YFK8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	64	Total O 64 64	0	0
2	B	88	Total O 88 88	0	0
2	C	58	Total O 58 58	0	0
2	D	55	Total O 55 55	0	0
2	E	91	Total O 91 91	0	0

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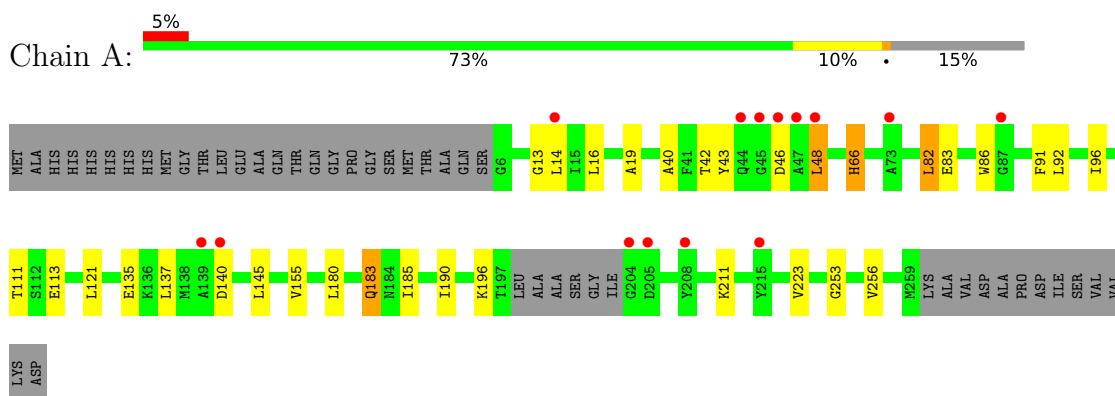
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	77	Total 77	O 77	0	0
2	G	56	Total 56	O 56	0	0
2	H	74	Total 74	O 74	0	0

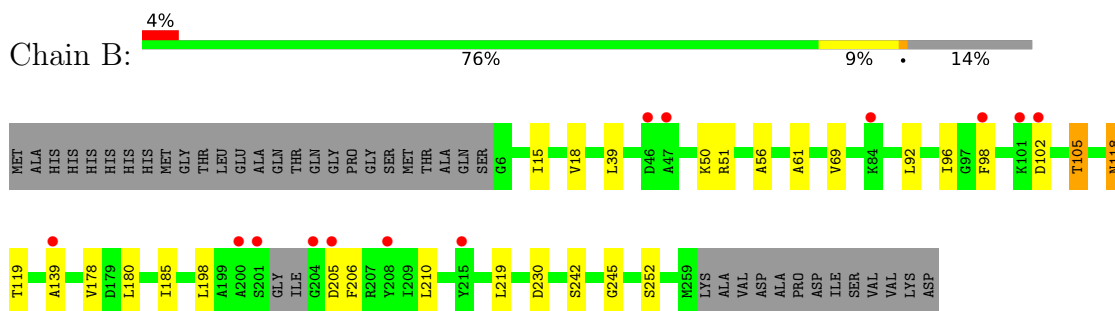
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

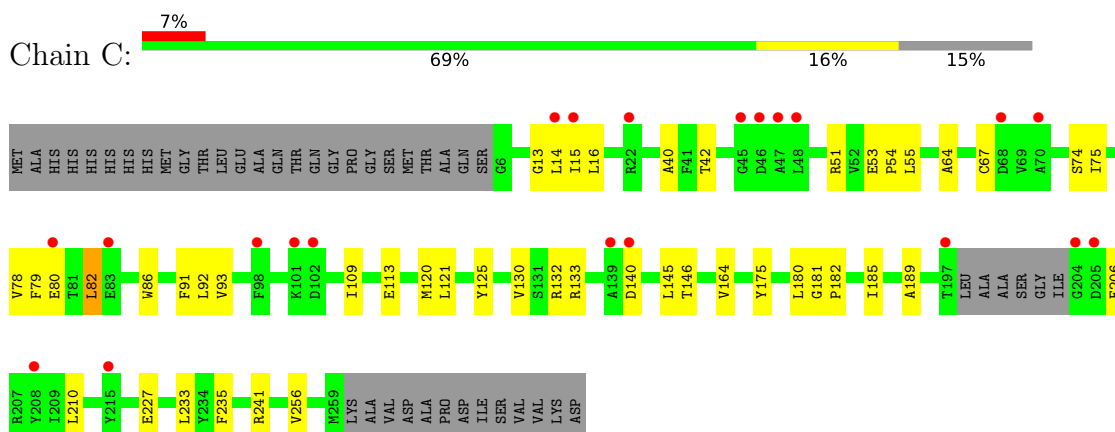
- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)



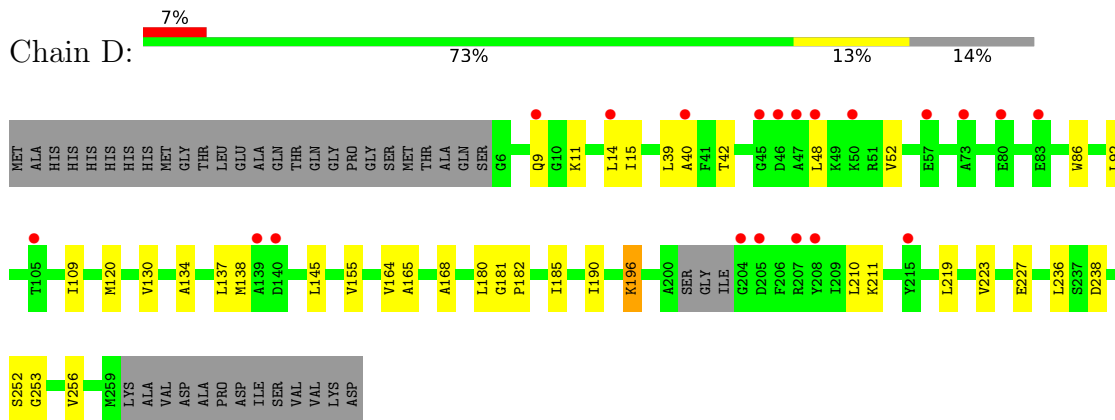
- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)



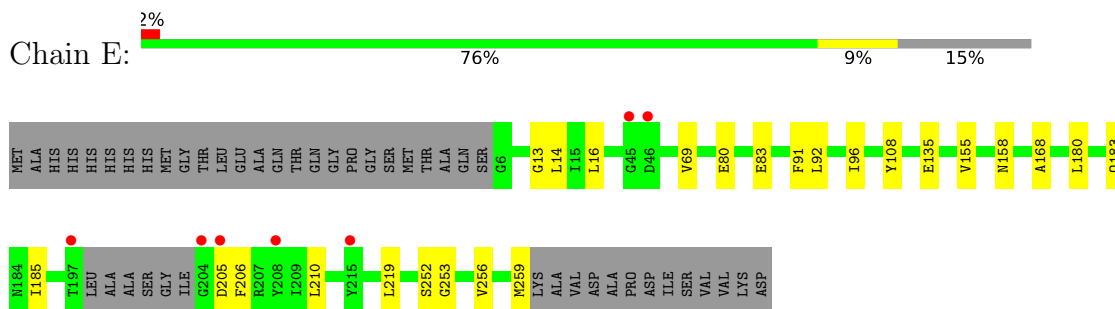
- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)



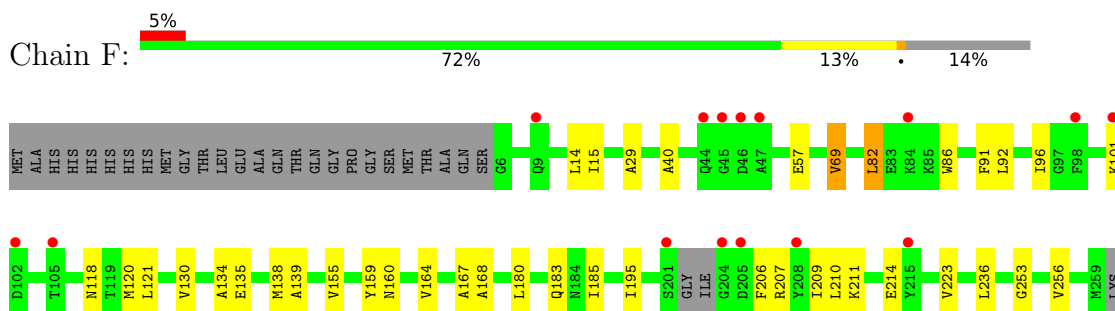
- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)



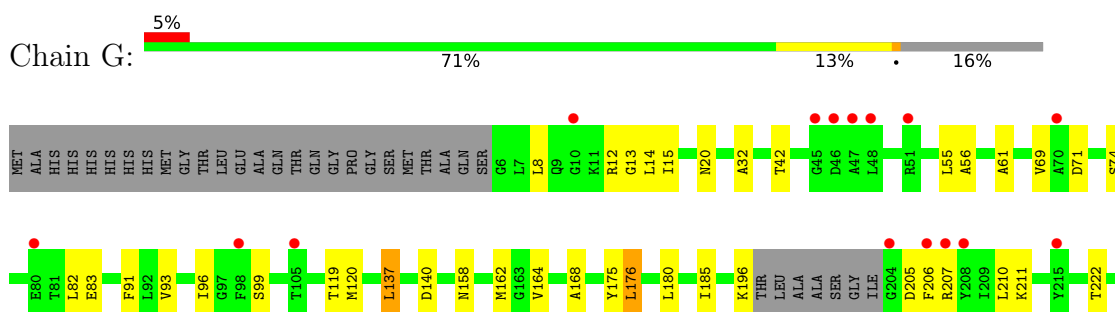
- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)

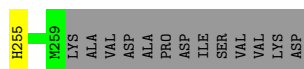


- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)

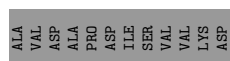
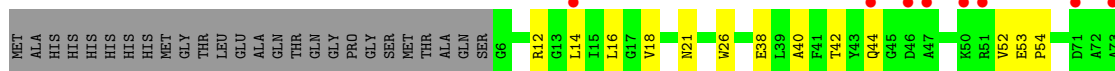
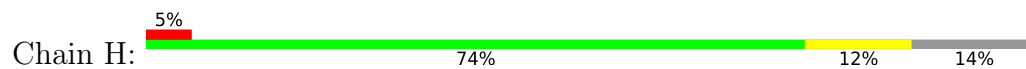


- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)





- Molecule 1: Enoyl-(acyl-carrier-protein) reductase (NADH)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.10Å 120.10Å 137.70Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	19.81 – 2.35 19.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.81-2.35) 95.3 (19.82-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.35Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.269 0.201 , 0.260	Depositor DCC
R_{free} test set	4211 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15671	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.22 % 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 3.8119e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/1896	0.58	0/2573
1	B	0.48	0/1937	0.59	0/2624
1	C	0.47	0/1908	0.60	0/2586
1	D	0.46	0/1942	0.59	0/2628
1	E	0.50	0/1916	0.60	0/2595
1	F	0.47	0/1940	0.59	0/2628
1	G	0.47	0/1902	0.59	0/2576
1	H	0.46	0/1931	0.59	0/2619
All	All	0.47	0/15372	0.59	0/20829

There are no bond length outliers.

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	1863	0	1822	20	0
1	B	1904	0	1889	20	0
1	C	1875	0	1849	37	0
1	D	1909	0	1909	24	0
1	E	1883	0	1866	16	0
1	F	1907	0	1892	28	0
1	G	1869	0	1851	26	0
1	H	1898	0	1867	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	64	0	0	1	0
2	B	88	0	0	2	0
2	C	58	0	0	0	0
2	D	55	0	0	1	0
2	E	91	0	0	0	0
2	F	77	0	0	1	0
2	G	56	0	0	2	0
2	H	74	0	0	0	0
All	All	15671	0	14945	171	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 6.

All (171) 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:F:92:LEU:HD11	1:F:130:VAL:CG1	2.10	0.81
1:D:11:LYS:NZ	1:D:238:ASP:OD1	2.15	0.79
1:F:134:ALA:HB1	1:F:138:MET:CE	2.13	0.77
1:F:92:LEU:HD11	1:F:130:VAL:HG12	1.65	0.76
1:C:92:LEU:HD11	1:C:130:VAL:CG1	2.16	0.74
1:D:14:LEU:HD11	1:D:42:THR:HG23	1.70	0.73
1:C:206:PHE:CE2	1:C:210:LEU:HD11	2.28	0.69
1:D:92:LEU:HD11	1:D:130:VAL:CG1	2.24	0.68
1:B:69:VAL:HG11	1:B:96:ILE:HD13	1.77	0.67
1:F:134:ALA:HB1	1:F:138:MET:HE2	1.76	0.66
1:G:120:MET:HE1	1:G:164:VAL:HG12	1.78	0.66
1:F:15:ILE:HD12	1:F:29:ALA:HB2	1.79	0.64
1:D:15:ILE:CD1	1:D:39:LEU:HD22	2.30	0.62
1:H:118:ASN:O	1:H:122:ILE:HD12	2.00	0.62
1:F:14:LEU:HD13	1:F:82:LEU:HD21	1.82	0.61
1:G:15:ILE:HD13	1:G:93:VAL:CG2	2.31	0.61
1:D:15:ILE:HD11	1:D:39:LEU:HD22	1.82	0.60
1:F:92:LEU:CD1	1:F:130:VAL:HG12	2.31	0.60
1:C:180:LEU:HB3	1:C:185:ILE:HB	1.84	0.59
1:G:83:GLU:HG3	1:G:137:LEU:HD11	1.83	0.59
1:A:113:GLU:HG3	1:C:121:LEU:HD11	1.84	0.59
1:A:16:LEU:HB3	1:A:96:ILE:HD11	1.82	0.59
1:G:180:LEU:HB3	1:G:185:ILE:HB	1.84	0.59
1:B:178:VAL:HG21	1:D:155:VAL:HG11	1.85	0.58
1:C:75:ILE:HG22	1:C:133:ARG:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:VAL:HG11	1:F:96:ILE:HD13	1.84	0.58
1:B:15:ILE:CD1	1:B:39:LEU:HD22	2.33	0.58
1:C:75:ILE:HG22	1:C:133:ARG:HD3	1.85	0.58
1:C:120:MET:HE1	1:C:164:VAL:HG12	1.86	0.58
1:D:145:LEU:HD11	1:D:190:ILE:HG13	1.86	0.57
1:H:120:MET:HE1	1:H:164:VAL:HG12	1.86	0.57
1:G:120:MET:CE	1:G:164:VAL:HG12	2.34	0.56
1:A:135:GLU:OE2	1:A:183:GLN:NE2	2.33	0.56
1:B:118:ASN:ND2	2:B:435:HOH:O	2.34	0.56
1:B:102:ASP:O	1:B:105:THR:CG2	2.54	0.56
1:D:180:LEU:HB3	1:D:185:ILE:HB	1.87	0.56
1:E:158:ASN:OD1	1:E:205:ASP:HB2	2.06	0.55
1:C:64:ALA:CB	1:C:82:LEU:HD11	2.36	0.55
1:H:120:MET:CE	1:H:164:VAL:HG12	2.37	0.55
1:D:134:ALA:HB1	1:D:138:MET:CE	2.37	0.55
1:D:219:LEU:HD12	1:D:252:SER:HA	1.89	0.55
1:B:15:ILE:HD11	1:B:39:LEU:HD22	1.89	0.54
1:C:40:ALA:HB2	1:C:86:TRP:CH2	2.42	0.54
1:B:180:LEU:HB3	1:B:185:ILE:HB	1.89	0.54
1:B:230:ASP:OD2	1:C:241:ARG:NH1	2.40	0.54
1:G:69:VAL:HG11	1:G:96:ILE:HD13	1.90	0.54
1:A:111:THR:O	1:C:132:ARG:NH2	2.39	0.54
1:A:14:LEU:HD11	1:A:42:THR:HG23	1.90	0.54
1:F:180:LEU:HB3	1:F:185:ILE:HB	1.89	0.54
1:D:92:LEU:C	1:D:92:LEU:HD23	2.29	0.53
1:E:253:GLY:O	1:E:256:VAL:HG22	2.07	0.53
1:G:119:THR:HG23	1:G:162:MET:HE1	1.90	0.53
1:C:64:ALA:HB1	1:C:82:LEU:HD11	1.90	0.53
1:A:180:LEU:HB3	1:A:185:ILE:HB	1.90	0.53
1:H:180:LEU:HB3	1:H:185:ILE:HB	1.90	0.53
1:D:134:ALA:HB1	1:D:138:MET:HE3	1.91	0.53
1:F:206:PHE:CE2	1:F:210:LEU:HD11	2.44	0.52
1:E:135:GLU:OE2	1:E:183:GLN:NE2	2.34	0.52
1:E:168:ALA:HB2	1:G:168:ALA:HB2	1.90	0.52
1:F:155:VAL:HG13	1:H:175:TYR:CE1	2.45	0.52
1:E:219:LEU:HD12	1:E:252:SER:HA	1.92	0.51
1:F:135:GLU:OE2	1:F:183:GLN:NE2	2.41	0.51
1:C:92:LEU:HD11	1:C:130:VAL:HG11	1.92	0.51
1:B:102:ASP:O	1:B:105:THR:HG23	2.11	0.51
1:G:14:LEU:HD11	1:G:42:THR:HG23	1.93	0.51
1:H:75:ILE:HG22	1:H:133:ARG:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:THR:OG1	2:G:280:HOH:O	2.16	0.50
1:G:206:PHE:CE2	1:G:210:LEU:HD11	2.47	0.50
1:H:12:ARG:HG2	1:H:38:GLU:HB2	1.93	0.49
1:E:206:PHE:CE2	1:E:210:LEU:HD11	2.47	0.49
1:D:48:LEU:O	1:D:52:VAL:HG23	2.12	0.49
1:F:253:GLY:O	1:F:256:VAL:HG22	2.13	0.49
1:E:108:TYR:CD2	1:G:176:LEU:HD13	2.47	0.49
1:A:180:LEU:HD21	1:C:109:ILE:CD1	2.43	0.48
1:H:92:LEU:HD11	1:H:130:VAL:CG1	2.43	0.48
1:D:92:LEU:HD11	1:D:130:VAL:HG11	1.95	0.48
1:D:165:ALA:O	1:D:168:ALA:HB3	2.14	0.48
1:E:259:MET:HE3	1:F:209:ILE:HG23	1.95	0.48
1:E:180:LEU:HB3	1:E:185:ILE:HB	1.96	0.47
1:B:139:ALA:N	2:B:309:HOH:O	2.47	0.47
1:E:108:TYR:CE2	1:G:176:LEU:HD13	2.49	0.47
1:E:259:MET:CE	1:F:209:ILE:HG23	2.44	0.47
1:B:92:LEU:C	1:B:92:LEU:HD23	2.35	0.47
1:E:92:LEU:C	1:E:92:LEU:HD23	2.35	0.47
1:D:253:GLY:O	1:D:256:VAL:HG22	2.15	0.47
1:H:135:GLU:OE2	1:H:183:GLN:NE2	2.35	0.47
1:D:120:MET:HE1	1:D:164:VAL:HG12	1.98	0.46
1:C:15:ILE:HD13	1:C:93:VAL:HB	1.97	0.46
1:G:8:LEU:HD12	1:G:32:ALA:HA	1.98	0.46
1:B:219:LEU:HD12	1:B:252:SER:HA	1.97	0.46
1:G:99:SER:HB2	1:G:162:MET:HE1	1.97	0.46
1:A:253:GLY:O	1:A:256:VAL:HG22	2.16	0.46
1:G:99:SER:HB2	1:G:162:MET:CE	2.46	0.46
1:H:16:LEU:HD23	1:H:42:THR:OG1	2.16	0.45
1:C:125:TYR:HH	1:C:132:ARG:HH22	1.60	0.45
1:H:91:PHE:CD1	1:H:236:LEU:HD22	2.51	0.45
1:C:13:GLY:HA3	1:C:91:PHE:CE1	2.51	0.45
1:C:78:VAL:O	1:C:82:LEU:HD13	2.17	0.44
1:C:120:MET:CE	1:C:164:VAL:HG12	2.46	0.44
1:C:79:PHE:HZ	1:C:130:VAL:HG13	1.82	0.44
1:B:102:ASP:O	1:B:105:THR:HG22	2.18	0.44
1:F:15:ILE:HD12	1:F:29:ALA:CB	2.46	0.44
1:A:155:VAL:HG13	1:C:175:TYR:CE1	2.53	0.44
1:A:19:ALA:HB1	1:A:48:LEU:HD11	1.99	0.43
1:C:16:LEU:HD11	1:C:130:VAL:HG11	2.00	0.43
1:F:195:ILE:HG12	1:F:223:VAL:HG23	2.00	0.43
1:E:14:LEU:HD21	1:E:16:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PHE:HE2	1:C:210:LEU:HD11	1.77	0.43
1:F:120:MET:CE	1:F:164:VAL:HG12	2.49	0.43
1:A:13:GLY:HA3	1:A:91:PHE:CZ	2.53	0.43
1:G:15:ILE:HD13	1:G:93:VAL:HG21	2.01	0.43
1:A:19:ALA:HB1	1:A:48:LEU:CD1	2.49	0.43
1:B:180:LEU:HD21	1:D:109:ILE:CD1	2.48	0.43
1:G:71:ASP:O	1:G:74:SER:HB3	2.19	0.43
1:G:14:LEU:HD13	1:G:82:LEU:HD11	2.00	0.43
1:C:14:LEU:HD11	1:C:42:THR:HG23	2.01	0.43
1:C:51:ARG:NH1	1:C:55:LEU:HD21	2.34	0.43
1:G:13:GLY:HA3	1:G:91:PHE:CZ	2.53	0.43
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.87	0.42
1:F:40:ALA:HB2	1:F:86:TRP:CH2	2.54	0.42
1:G:20:ASN:HA	1:G:55:LEU:HD11	2.02	0.42
1:H:21:ASN:HA	1:H:26:TRP:CG	2.54	0.42
1:A:113:GLU:CG	1:C:121:LEU:HD11	2.47	0.42
1:F:168:ALA:HB2	1:H:168:ALA:HB2	2.02	0.42
1:B:242:SER:HB3	1:C:227:GLU:HB3	2.01	0.42
1:G:158:ASN:ND2	1:G:205:ASP:HB3	2.34	0.42
1:E:155:VAL:HG13	1:G:175:TYR:CE1	2.55	0.42
1:F:91:PHE:HB2	1:F:236:LEU:HD22	2.02	0.42
1:C:145:LEU:HD13	1:C:235:PHE:HB3	2.02	0.42
1:D:181:GLY:N	1:D:182:PRO:CD	2.83	0.42
1:H:75:ILE:HG22	1:H:133:ARG:CD	2.50	0.42
1:E:69:VAL:HG11	1:E:96:ILE:HD13	2.02	0.42
1:B:206:PHE:CE2	1:B:210:LEU:HD11	2.55	0.42
1:C:64:ALA:HB2	1:C:82:LEU:HD11	2.02	0.42
1:D:223:VAL:HA	1:D:227:GLU:OE1	2.20	0.42
1:F:134:ALA:CB	1:F:138:MET:CE	2.94	0.42
1:A:40:ALA:HB2	1:A:86:TRP:CH2	2.55	0.41
1:A:223:VAL:HG22	2:A:287:HOH:O	2.19	0.41
1:C:53:GLU:N	1:C:54:PRO:HD2	2.35	0.41
1:F:167:ALA:CB	1:H:171:ALA:HB2	2.50	0.41
1:G:56:ALA:HA	1:G:61:ALA:HB3	2.02	0.41
1:B:245:GLY:HA3	1:C:256:VAL:HG11	2.01	0.41
1:C:146:THR:O	1:C:189:ALA:HA	2.20	0.41
1:C:181:GLY:N	1:C:182:PRO:CD	2.83	0.41
1:G:15:ILE:HD13	1:G:93:VAL:HB	2.02	0.41
1:E:13:GLY:HA3	1:E:91:PHE:CE1	2.55	0.41
1:G:255:HIS:HE1	2:G:276:HOH:O	2.03	0.41
1:A:43:TYR:CE1	1:A:66:HIS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PHE:CZ	1:C:130:VAL:HG13	2.55	0.41
1:D:40:ALA:HB2	1:D:86:TRP:CH2	2.56	0.41
1:A:145:LEU:HD11	1:A:190:ILE:HG13	2.02	0.41
1:F:121:LEU:HD11	1:H:113:GLU:HG3	2.02	0.41
1:F:139:ALA:N	2:F:287:HOH:O	2.53	0.41
1:F:155:VAL:HG13	1:H:175:TYR:CD1	2.55	0.41
1:H:18:VAL:O	1:H:52:VAL:HG22	2.21	0.41
1:A:121:LEU:HD11	1:C:113:GLU:HG3	2.02	0.41
1:B:56:ALA:HA	1:B:61:ALA:HB3	2.02	0.41
1:B:98:PHE:O	1:B:119:THR:HG23	2.21	0.41
1:H:219:LEU:HD12	1:H:252:SER:HA	2.03	0.41
1:D:223:VAL:HG22	2:D:284:HOH:O	2.21	0.41
1:F:211:LYS:HA	1:F:214:GLU:HG2	2.04	0.41
1:H:14:LEU:HD11	1:H:42:THR:HG23	2.02	0.41
1:H:40:ALA:HB2	1:H:86:TRP:CH2	2.56	0.41
1:H:53:GLU:N	1:H:54:PRO:HD2	2.35	0.41
1:D:120:MET:CE	1:D:164:VAL:HG12	2.51	0.40
1:C:67:CYS:HB2	1:C:78:VAL:HG21	2.04	0.40
1:C:233:LEU:O	1:C:233:LEU:HD12	2.22	0.40
1:A:92:LEU:HD23	1:A:92:LEU:C	2.41	0.40
1:F:159:TYR:O	1:F:160:ASN:C	2.60	0.40
1:B:15:ILE:HG22	1:B:18:VAL:HG23	2.03	0.40
1:D:196:LYS:HA	1:D:210:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	244/293 (83%)	237 (97%)	7 (3%)	0	100 100
1	B	248/293 (85%)	238 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	244/293 (83%)	235 (96%)	9 (4%)	0	100	100
1	D	247/293 (84%)	238 (96%)	9 (4%)	0	100	100
1	E	244/293 (83%)	236 (97%)	8 (3%)	0	100	100
1	F	248/293 (85%)	240 (97%)	7 (3%)	1 (0%)	34	38
1	G	243/293 (83%)	234 (96%)	9 (4%)	0	100	100
1	H	248/293 (85%)	240 (97%)	8 (3%)	0	100	100
All	All	1966/2344 (84%)	1898 (96%)	67 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	69	VAL

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	187/227 (82%)	177 (95%)	10 (5%)	22	26
1	B	192/227 (85%)	186 (97%)	6 (3%)	40	48
1	C	189/227 (83%)	185 (98%)	4 (2%)	53	65
1	D	194/227 (86%)	189 (97%)	5 (3%)	46	56
1	E	191/227 (84%)	189 (99%)	2 (1%)	76	85
1	F	193/227 (85%)	188 (97%)	5 (3%)	46	56
1	G	188/227 (83%)	181 (96%)	7 (4%)	34	42
1	H	190/227 (84%)	187 (98%)	3 (2%)	62	75
All	All	1524/1816 (84%)	1482 (97%)	42 (3%)	43	53

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP

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Mol	Chain	Res	Type
1	A	48	LEU
1	A	66	HIS
1	A	82	LEU
1	A	83	GLU
1	A	137	LEU
1	A	140	ASP
1	A	183	GLN
1	A	196	LYS
1	A	211	LYS
1	B	50	LYS
1	B	51	ARG
1	B	105	THR
1	B	118	ASN
1	B	198	LEU
1	B	205	ASP
1	C	74	SER
1	C	80	GLU
1	C	82	LEU
1	C	140	ASP
1	D	9	GLN
1	D	137	LEU
1	D	196	LYS
1	D	211	LYS
1	D	236	LEU
1	E	80	GLU
1	E	83	GLU
1	F	57	GLU
1	F	82	LEU
1	F	101	LYS
1	F	118	ASN
1	F	207	ARG
1	G	12	ARG
1	G	137	LEU
1	G	140	ASP
1	G	176	LEU
1	G	196	LYS
1	G	207	ARG
1	G	211	LYS
1	H	44	GLN
1	H	196	LYS
1	H	207	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	G	158	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/293 (84%)	0.40	14 (5%) 24 35	15, 29, 49, 59	0
1	B	252/293 (86%)	0.11	13 (5%) 27 39	10, 24, 40, 47	0
1	C	248/293 (84%)	0.34	21 (8%) 10 16	14, 27, 48, 57	0
1	D	251/293 (85%)	0.36	20 (7%) 12 18	13, 27, 51, 61	0
1	E	248/293 (84%)	-0.00	7 (2%) 53 64	11, 21, 34, 49	0
1	F	252/293 (86%)	0.27	15 (5%) 21 32	15, 27, 45, 53	0
1	G	247/293 (84%)	0.23	15 (6%) 21 31	12, 26, 48, 56	0
1	H	252/293 (86%)	0.27	14 (5%) 24 35	14, 26, 48, 58	0
All	All	1998/2344 (85%)	0.25	119 (5%) 21 32	10, 26, 47, 61	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	204	GLY	7.2
1	A	204	GLY	5.7
1	G	215	TYR	5.0
1	A	215	TYR	4.9
1	H	47	ALA	4.8
1	G	47	ALA	4.7
1	D	47	ALA	4.7
1	C	46	ASP	4.6
1	D	48	LEU	4.6
1	A	46	ASP	4.6
1	A	47	ALA	4.4
1	D	215	TYR	4.4
1	B	215	TYR	4.2
1	G	204	GLY	4.2
1	G	45	GLY	4.1
1	H	204	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	205	ASP	4.0
1	C	204	GLY	4.0
1	D	139	ALA	3.9
1	C	215	TYR	3.8
1	H	98	PHE	3.8
1	C	98	PHE	3.7
1	G	51	ARG	3.7
1	C	45	GLY	3.7
1	F	102	ASP	3.6
1	G	46	ASP	3.5
1	F	47	ALA	3.5
1	D	205	ASP	3.5
1	H	46	ASP	3.5
1	H	205	ASP	3.5
1	A	139	ALA	3.4
1	D	46	ASP	3.4
1	H	215	TYR	3.4
1	F	201	SER	3.4
1	H	73	ALA	3.3
1	E	208	TYR	3.2
1	B	201	SER	3.2
1	C	205	ASP	3.1
1	D	45	GLY	3.1
1	F	215	TYR	3.1
1	D	140	ASP	3.1
1	E	204	GLY	3.1
1	E	215	TYR	3.1
1	B	208	TYR	3.1
1	C	48	LEU	3.1
1	F	45	GLY	3.1
1	G	98	PHE	3.1
1	B	47	ALA	3.0
1	A	205	ASP	3.0
1	G	206	PHE	3.0
1	D	208	TYR	3.0
1	C	208	TYR	2.9
1	C	80	GLU	2.9
1	B	139	ALA	2.9
1	C	70	ALA	2.9
1	F	98	PHE	2.9
1	A	73	ALA	2.9
1	B	204	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	83	GLU	2.8
1	B	205	ASP	2.8
1	F	46	ASP	2.8
1	C	139	ALA	2.7
1	H	14	LEU	2.7
1	A	208	TYR	2.7
1	D	207	ARG	2.7
1	D	204	GLY	2.7
1	B	200	ALA	2.7
1	C	14	LEU	2.7
1	C	197	THR	2.7
1	C	68	ASP	2.6
1	F	9	GLN	2.6
1	G	208	TYR	2.6
1	C	140	ASP	2.6
1	D	50	LYS	2.6
1	D	80	GLU	2.6
1	F	84	LYS	2.5
1	C	47	ALA	2.5
1	E	197	THR	2.5
1	C	15	ILE	2.5
1	A	45	GLY	2.5
1	B	102	ASP	2.5
1	F	208	TYR	2.5
1	G	48	LEU	2.5
1	F	105	THR	2.4
1	D	9	GLN	2.4
1	A	140	ASP	2.4
1	E	46	ASP	2.4
1	A	48	LEU	2.4
1	D	73	ALA	2.4
1	A	44	GLN	2.4
1	C	102	ASP	2.4
1	G	105	THR	2.4
1	H	44	GLN	2.4
1	H	139	ALA	2.4
1	H	201	SER	2.4
1	B	101	LYS	2.3
1	F	101	LYS	2.3
1	G	70	ALA	2.3
1	C	101	LYS	2.3
1	F	44	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	45	GLY	2.2
1	B	84	LYS	2.2
1	D	83	GLU	2.2
1	E	205	ASP	2.2
1	C	22	ARG	2.2
1	D	14	LEU	2.2
1	B	46	ASP	2.2
1	H	50	LYS	2.2
1	B	98	PHE	2.1
1	D	40	ALA	2.1
1	G	10	GLY	2.1
1	D	57	GLU	2.1
1	G	80	GLU	2.1
1	A	14	LEU	2.1
1	G	207	ARG	2.1
1	H	71	ASP	2.1
1	D	105	THR	2.1
1	A	87	GLY	2.0
1	H	51	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.