



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:25 PM UTC

PDB ID : 4I5G / pdb_00004i5g
Title : Crystal structure of Ralstonia sp. alcohol dehydrogenase mutant N15G, G37D, R38V, R39S, A86N, S88A
Authors : Jarasch, A.; Lerchner, A.; Meining, W.; Schiefner, A.; Skerra, A.
Deposited on : 2012-11-28
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

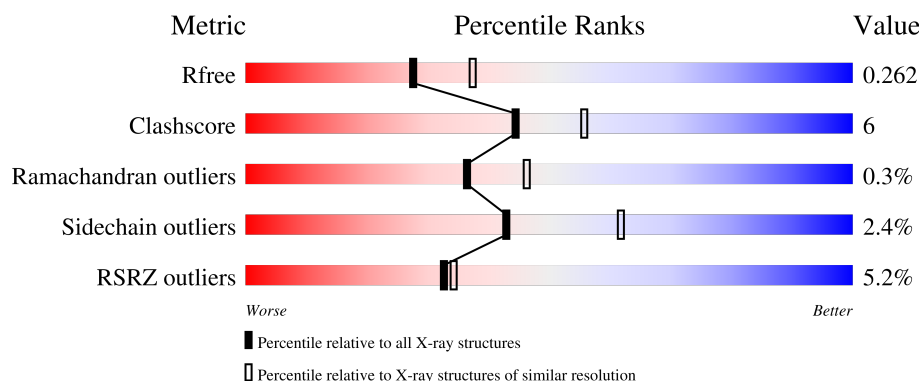
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	262	6% 76% 13% • 11%
1	B	262	4% 66% 19% • 11%
1	C	262	5% 76% 12% • 11%
1	D	262	5% 75% 12% • 11%
1	E	262	5% 74% 14% • 11%

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Mol	Chain	Length	Quality of chain
1	F	262	4%78%10% • 11%
1	G	262	3%71%16% • 11%
1	H	262	4%75%13% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14593 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 Alcohol dehydrogenase/short-chain dehydrogenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	0	0	0
			1745	1101	308	336			
1	B	233	Total	C	N	O	0	0	0
			1745	1101	308	336			
1	C	233	Total	C	N	O	0	0	0
			1745	1101	308	336			
1	D	233	Total	C	N	O	0	0	0
			1745	1101	308	336			
1	E	233	Total	C	N	O	0	0	0
			1745	1101	308	336			
1	F	233	Total	C	N	O	0	0	0
			1745	1101	308	336			
1	G	233	Total	C	N	O	0	0	0
			1745	1101	308	336			
1	H	233	Total	C	N	O	0	0	0
			1745	1101	308	336			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP C0IR58
A	-11	ALA	-	expression tag	UNP C0IR58
A	-10	SER	-	expression tag	UNP C0IR58
A	-9	ARG	-	expression tag	UNP C0IR58
A	-8	GLY	-	expression tag	UNP C0IR58
A	-7	SER	-	expression tag	UNP C0IR58
A	-6	HIS	-	expression tag	UNP C0IR58
A	-5	HIS	-	expression tag	UNP C0IR58
A	-4	HIS	-	expression tag	UNP C0IR58
A	-3	HIS	-	expression tag	UNP C0IR58
A	-2	HIS	-	expression tag	UNP C0IR58
A	-1	HIS	-	expression tag	UNP C0IR58
A	0	GLY	-	expression tag	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP C0IR58
A	15	GLY	ASN	engineered mutation	UNP C0IR58
A	37	ASP	GLY	engineered mutation	UNP C0IR58
A	38	VAL	ARG	engineered mutation	UNP C0IR58
A	39	SER	ARG	engineered mutation	UNP C0IR58
A	86	ASN	ALA	engineered mutation	UNP C0IR58
A	88	ALA	SER	engineered mutation	UNP C0IR58
B	-12	MET	-	expression tag	UNP C0IR58
B	-11	ALA	-	expression tag	UNP C0IR58
B	-10	SER	-	expression tag	UNP C0IR58
B	-9	ARG	-	expression tag	UNP C0IR58
B	-8	GLY	-	expression tag	UNP C0IR58
B	-7	SER	-	expression tag	UNP C0IR58
B	-6	HIS	-	expression tag	UNP C0IR58
B	-5	HIS	-	expression tag	UNP C0IR58
B	-4	HIS	-	expression tag	UNP C0IR58
B	-3	HIS	-	expression tag	UNP C0IR58
B	-2	HIS	-	expression tag	UNP C0IR58
B	-1	HIS	-	expression tag	UNP C0IR58
B	0	GLY	-	expression tag	UNP C0IR58
B	1	ALA	-	expression tag	UNP C0IR58
B	15	GLY	ASN	engineered mutation	UNP C0IR58
B	37	ASP	GLY	engineered mutation	UNP C0IR58
B	38	VAL	ARG	engineered mutation	UNP C0IR58
B	39	SER	ARG	engineered mutation	UNP C0IR58
B	86	ASN	ALA	engineered mutation	UNP C0IR58
B	88	ALA	SER	engineered mutation	UNP C0IR58
C	-12	MET	-	expression tag	UNP C0IR58
C	-11	ALA	-	expression tag	UNP C0IR58
C	-10	SER	-	expression tag	UNP C0IR58
C	-9	ARG	-	expression tag	UNP C0IR58
C	-8	GLY	-	expression tag	UNP C0IR58
C	-7	SER	-	expression tag	UNP C0IR58
C	-6	HIS	-	expression tag	UNP C0IR58
C	-5	HIS	-	expression tag	UNP C0IR58
C	-4	HIS	-	expression tag	UNP C0IR58
C	-3	HIS	-	expression tag	UNP C0IR58
C	-2	HIS	-	expression tag	UNP C0IR58
C	-1	HIS	-	expression tag	UNP C0IR58
C	0	GLY	-	expression tag	UNP C0IR58
C	1	ALA	-	expression tag	UNP C0IR58
C	15	GLY	ASN	engineered mutation	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
C	37	ASP	GLY	engineered mutation	UNP C0IR58
C	38	VAL	ARG	engineered mutation	UNP C0IR58
C	39	SER	ARG	engineered mutation	UNP C0IR58
C	86	ASN	ALA	engineered mutation	UNP C0IR58
C	88	ALA	SER	engineered mutation	UNP C0IR58
D	-12	MET	-	expression tag	UNP C0IR58
D	-11	ALA	-	expression tag	UNP C0IR58
D	-10	SER	-	expression tag	UNP C0IR58
D	-9	ARG	-	expression tag	UNP C0IR58
D	-8	GLY	-	expression tag	UNP C0IR58
D	-7	SER	-	expression tag	UNP C0IR58
D	-6	HIS	-	expression tag	UNP C0IR58
D	-5	HIS	-	expression tag	UNP C0IR58
D	-4	HIS	-	expression tag	UNP C0IR58
D	-3	HIS	-	expression tag	UNP C0IR58
D	-2	HIS	-	expression tag	UNP C0IR58
D	-1	HIS	-	expression tag	UNP C0IR58
D	0	GLY	-	expression tag	UNP C0IR58
D	1	ALA	-	expression tag	UNP C0IR58
D	15	GLY	ASN	engineered mutation	UNP C0IR58
D	37	ASP	GLY	engineered mutation	UNP C0IR58
D	38	VAL	ARG	engineered mutation	UNP C0IR58
D	39	SER	ARG	engineered mutation	UNP C0IR58
D	86	ASN	ALA	engineered mutation	UNP C0IR58
D	88	ALA	SER	engineered mutation	UNP C0IR58
E	-12	MET	-	expression tag	UNP C0IR58
E	-11	ALA	-	expression tag	UNP C0IR58
E	-10	SER	-	expression tag	UNP C0IR58
E	-9	ARG	-	expression tag	UNP C0IR58
E	-8	GLY	-	expression tag	UNP C0IR58
E	-7	SER	-	expression tag	UNP C0IR58
E	-6	HIS	-	expression tag	UNP C0IR58
E	-5	HIS	-	expression tag	UNP C0IR58
E	-4	HIS	-	expression tag	UNP C0IR58
E	-3	HIS	-	expression tag	UNP C0IR58
E	-2	HIS	-	expression tag	UNP C0IR58
E	-1	HIS	-	expression tag	UNP C0IR58
E	0	GLY	-	expression tag	UNP C0IR58
E	1	ALA	-	expression tag	UNP C0IR58
E	15	GLY	ASN	engineered mutation	UNP C0IR58
E	37	ASP	GLY	engineered mutation	UNP C0IR58
E	38	VAL	ARG	engineered mutation	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
E	39	SER	ARG	engineered mutation	UNP C0IR58
E	86	ASN	ALA	engineered mutation	UNP C0IR58
E	88	ALA	SER	engineered mutation	UNP C0IR58
F	-12	MET	-	expression tag	UNP C0IR58
F	-11	ALA	-	expression tag	UNP C0IR58
F	-10	SER	-	expression tag	UNP C0IR58
F	-9	ARG	-	expression tag	UNP C0IR58
F	-8	GLY	-	expression tag	UNP C0IR58
F	-7	SER	-	expression tag	UNP C0IR58
F	-6	HIS	-	expression tag	UNP C0IR58
F	-5	HIS	-	expression tag	UNP C0IR58
F	-4	HIS	-	expression tag	UNP C0IR58
F	-3	HIS	-	expression tag	UNP C0IR58
F	-2	HIS	-	expression tag	UNP C0IR58
F	-1	HIS	-	expression tag	UNP C0IR58
F	0	GLY	-	expression tag	UNP C0IR58
F	1	ALA	-	expression tag	UNP C0IR58
F	15	GLY	ASN	engineered mutation	UNP C0IR58
F	37	ASP	GLY	engineered mutation	UNP C0IR58
F	38	VAL	ARG	engineered mutation	UNP C0IR58
F	39	SER	ARG	engineered mutation	UNP C0IR58
F	86	ASN	ALA	engineered mutation	UNP C0IR58
F	88	ALA	SER	engineered mutation	UNP C0IR58
G	-12	MET	-	expression tag	UNP C0IR58
G	-11	ALA	-	expression tag	UNP C0IR58
G	-10	SER	-	expression tag	UNP C0IR58
G	-9	ARG	-	expression tag	UNP C0IR58
G	-8	GLY	-	expression tag	UNP C0IR58
G	-7	SER	-	expression tag	UNP C0IR58
G	-6	HIS	-	expression tag	UNP C0IR58
G	-5	HIS	-	expression tag	UNP C0IR58
G	-4	HIS	-	expression tag	UNP C0IR58
G	-3	HIS	-	expression tag	UNP C0IR58
G	-2	HIS	-	expression tag	UNP C0IR58
G	-1	HIS	-	expression tag	UNP C0IR58
G	0	GLY	-	expression tag	UNP C0IR58
G	1	ALA	-	expression tag	UNP C0IR58
G	15	GLY	ASN	engineered mutation	UNP C0IR58
G	37	ASP	GLY	engineered mutation	UNP C0IR58
G	38	VAL	ARG	engineered mutation	UNP C0IR58
G	39	SER	ARG	engineered mutation	UNP C0IR58
G	86	ASN	ALA	engineered mutation	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
G	88	ALA	SER	engineered mutation	UNP C0IR58
H	-12	MET	-	expression tag	UNP C0IR58
H	-11	ALA	-	expression tag	UNP C0IR58
H	-10	SER	-	expression tag	UNP C0IR58
H	-9	ARG	-	expression tag	UNP C0IR58
H	-8	GLY	-	expression tag	UNP C0IR58
H	-7	SER	-	expression tag	UNP C0IR58
H	-6	HIS	-	expression tag	UNP C0IR58
H	-5	HIS	-	expression tag	UNP C0IR58
H	-4	HIS	-	expression tag	UNP C0IR58
H	-3	HIS	-	expression tag	UNP C0IR58
H	-2	HIS	-	expression tag	UNP C0IR58
H	-1	HIS	-	expression tag	UNP C0IR58
H	0	GLY	-	expression tag	UNP C0IR58
H	1	ALA	-	expression tag	UNP C0IR58
H	15	GLY	ASN	engineered mutation	UNP C0IR58
H	37	ASP	GLY	engineered mutation	UNP C0IR58
H	38	VAL	ARG	engineered mutation	UNP C0IR58
H	39	SER	ARG	engineered mutation	UNP C0IR58
H	86	ASN	ALA	engineered mutation	UNP C0IR58
H	88	ALA	SER	engineered mutation	UNP C0IR58

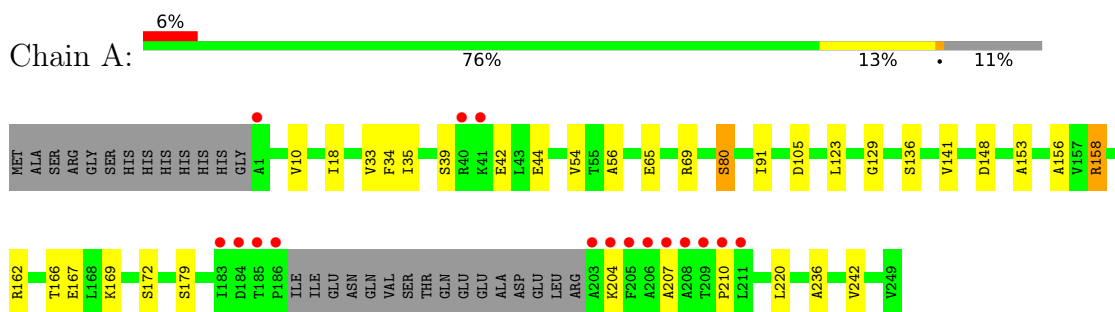
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	51	Total O 51 51	0	0
2	B	84	Total O 84 84	0	0
2	C	75	Total O 75 75	0	0
2	D	85	Total O 85 85	0	0
2	E	79	Total O 79 79	0	0
2	F	87	Total O 87 87	0	0
2	G	85	Total O 85 85	0	0
2	H	87	Total O 87 87	0	0

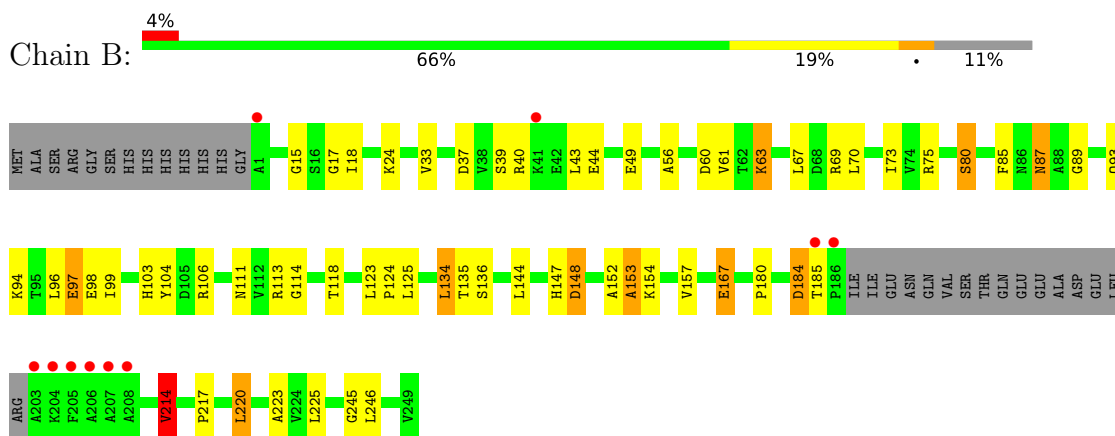
3 Residue-property plots [i](#)

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.

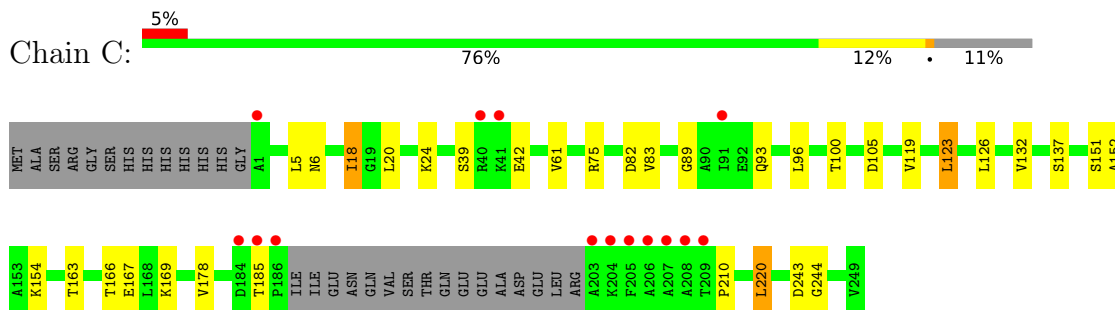
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



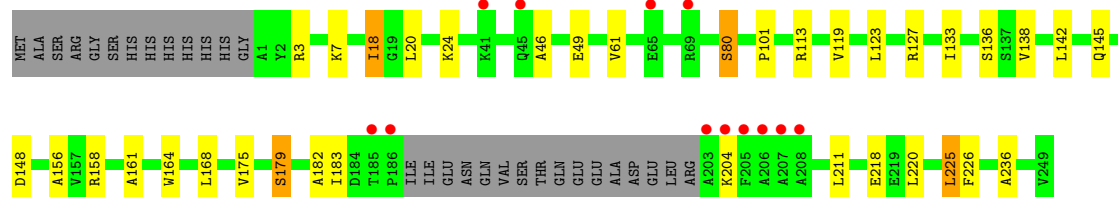
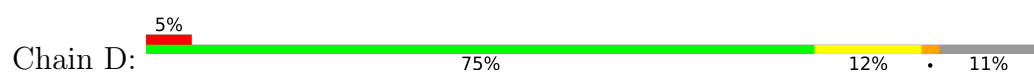
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



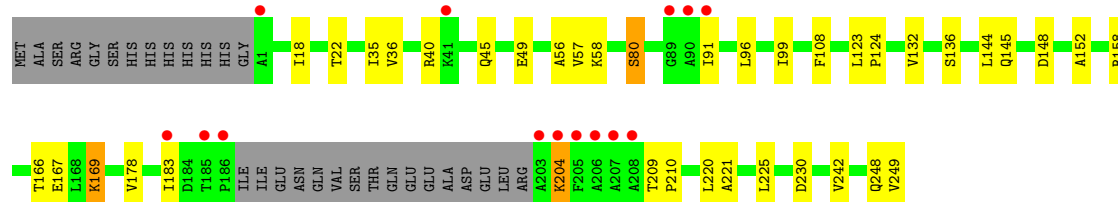
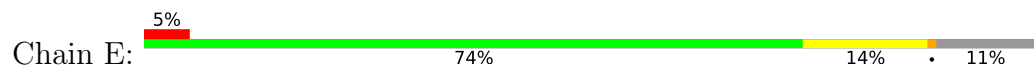
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



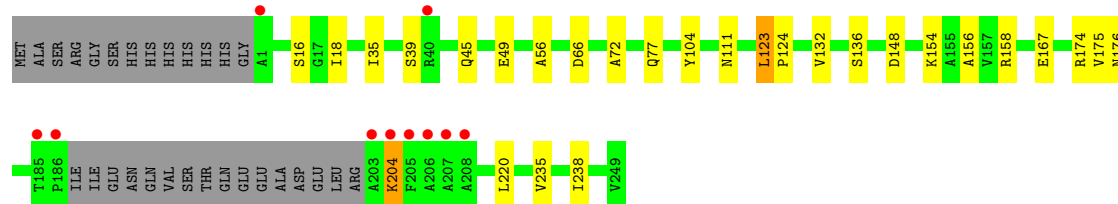
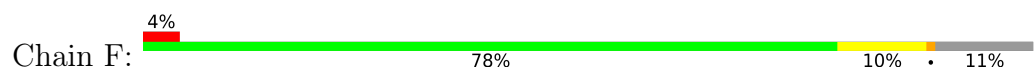
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



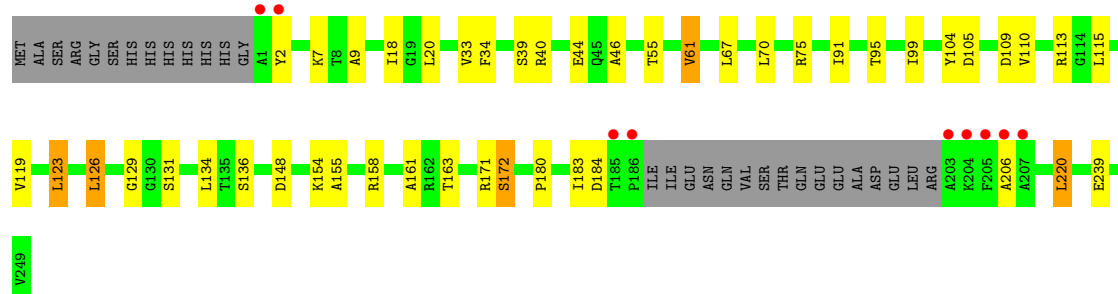
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

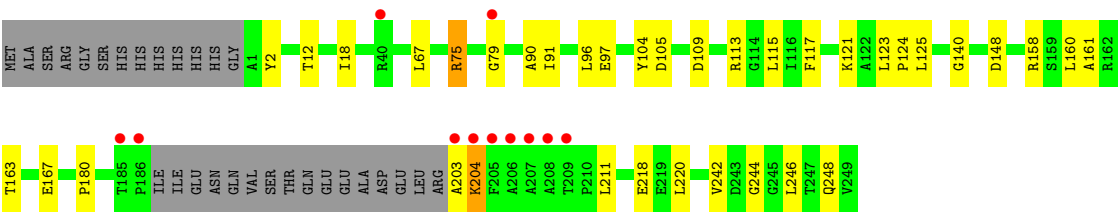


- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.47Å 122.14Å 133.54Å 90.00° 94.32° 90.00°	Depositor
Resolution (Å)	29.90 – 2.30 29.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-2.30) 98.1 (29.90-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.220 , 0.272 (Not available) , 0.262	Depositor DCC
R_{free} test set	5542 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14593	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 51.45 % 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 5.5968e-05. 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 ⓘ

5.1 Standard geometry ⓘ

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	1.23	4/1767 (0.2%)	1.25	4/2395 (0.2%)
1	B	1.42	9/1767 (0.5%)	1.37	8/2395 (0.3%)
1	C	1.42	9/1767 (0.5%)	1.30	9/2395 (0.4%)
1	D	1.38	3/1767 (0.2%)	1.34	7/2395 (0.3%)
1	E	1.29	4/1767 (0.2%)	1.32	10/2395 (0.4%)
1	F	1.33	2/1767 (0.1%)	1.28	5/2395 (0.2%)
1	G	1.41	9/1767 (0.5%)	1.29	7/2395 (0.3%)
1	H	1.34	6/1767 (0.3%)	1.25	4/2395 (0.2%)
All	All	1.35	46/14136 (0.3%)	1.30	54/19160 (0.3%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	VAL	CA-C	8.25	1.62	1.52
1	H	246	LEU	C-O	-7.75	1.15	1.24
1	A	141	VAL	C-O	-7.26	1.15	1.24
1	A	136	SER	CA-C	-7.18	1.49	1.53
1	E	136	SER	CA-C	-7.01	1.49	1.53
1	F	123	LEU	N-CA	6.42	1.52	1.46
1	E	242	VAL	C-O	6.33	1.31	1.24
1	H	140	GLY	C-O	6.31	1.30	1.24
1	D	133	ILE	C-O	6.25	1.30	1.24
1	C	83	VAL	C-O	-6.14	1.17	1.24
1	H	12	THR	C-O	5.99	1.30	1.23
1	G	119	VAL	N-CA	5.77	1.53	1.46
1	B	135	THR	N-CA	-5.75	1.38	1.46
1	G	155	ALA	N-CA	5.73	1.53	1.46
1	C	166	THR	N-CA	-5.67	1.39	1.46
1	B	134	LEU	C-O	5.64	1.30	1.23
1	D	225	LEU	C-O	-5.57	1.17	1.24
1	C	151	SER	N-CA	5.54	1.53	1.46
1	B	103	HIS	CG-CD2	5.45	1.41	1.35
1	B	111	ASN	N-CA	5.40	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	ASP	N-CA	-5.39	1.40	1.46
1	G	161	ALA	CA-C	-5.39	1.45	1.52
1	F	77	GLN	N-CA	5.38	1.53	1.46
1	B	103	HIS	ND1-CE1	5.38	1.38	1.32
1	H	161	ALA	N-CA	5.36	1.53	1.46
1	A	158	ARG	CA-CB	5.32	1.61	1.53
1	G	9	ALA	N-CA	5.26	1.52	1.46
1	B	152	ALA	CA-C	5.26	1.59	1.52
1	G	239	GLU	N-CA	5.22	1.53	1.46
1	H	160	LEU	N-CA	-5.21	1.40	1.46
1	B	220	LEU	CA-CB	5.21	1.61	1.53
1	E	248	GLN	CA-C	5.20	1.59	1.52
1	C	132	VAL	CA-CB	5.19	1.60	1.54
1	A	236	ALA	N-CA	5.17	1.52	1.46
1	E	136	SER	N-CA	5.16	1.49	1.46
1	C	154	LYS	C-O	-5.16	1.17	1.24
1	G	131	SER	C-O	5.15	1.29	1.23
1	G	126	LEU	CA-C	-5.14	1.46	1.52
1	C	137	SER	N-CA	5.13	1.52	1.46
1	G	158	ARG	C-O	5.12	1.30	1.24
1	B	225	LEU	C-O	5.10	1.30	1.24
1	G	119	VAL	C-O	-5.09	1.18	1.24
1	D	7	LYS	CA-C	-5.07	1.46	1.52
1	C	105	ASP	C-O	-5.03	1.18	1.24
1	B	153	ALA	C-O	5.01	1.29	1.24
1	H	90	ALA	N-CA	5.01	1.52	1.45

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	SER	N-CA-C	-10.32	100.32	108.78
1	A	162	ARG	N-CA-C	-9.87	100.08	111.03
1	B	97	GLU	N-CA-C	8.07	120.98	111.71
1	C	123	LEU	CA-C-N	-7.44	111.97	119.56
1	C	123	LEU	C-N-CA	-7.44	111.97	119.56
1	H	115	LEU	N-CA-C	-7.17	102.65	111.40
1	G	163	THR	N-CA-C	-7.12	103.60	111.36
1	B	33	VAL	N-CA-C	7.04	117.96	108.11
1	D	123	LEU	CA-C-N	-6.79	111.99	119.19
1	D	123	LEU	C-N-CA	-6.79	111.99	119.19
1	G	2	TYR	N-CA-C	6.20	119.91	111.17
1	B	214	VAL	CB-CA-C	6.02	118.19	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	ARG	CG-CD-NE	-5.86	99.10	112.00
1	B	114	GLY	N-CA-C	-5.84	105.72	112.73
1	B	167	GLU	N-CA-C	5.83	118.42	111.71
1	G	7	LYS	N-CA-C	-5.83	100.78	110.17
1	B	223	ALA	N-CA-C	-5.81	105.03	111.36
1	E	178	VAL	N-CA-C	-5.70	100.28	108.48
1	H	79	GLY	N-CA-C	5.66	122.28	114.92
1	E	152	ALA	N-CA-C	-5.62	105.24	111.36
1	E	136	SER	N-CA-C	-5.59	104.20	108.78
1	B	87	ASN	N-CA-C	5.56	120.37	111.81
1	C	89	GLY	CA-C-O	-5.56	118.31	122.37
1	B	89	GLY	CA-C-O	-5.44	116.88	122.26
1	D	113	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	G	172	SER	CB-CA-C	-5.41	103.89	111.80
1	C	100	THR	CA-C-N	5.41	124.87	119.24
1	C	100	THR	C-N-CA	5.41	124.87	119.24
1	A	179	SER	CA-C-N	5.38	125.29	119.85
1	A	179	SER	C-N-CA	5.38	125.29	119.85
1	E	132	VAL	CA-C-N	-5.36	116.54	123.19
1	E	132	VAL	C-N-CA	-5.36	116.54	123.19
1	E	230	ASP	N-CA-C	5.31	119.02	112.54
1	D	179	SER	CA-C-N	5.30	125.06	119.76
1	D	179	SER	C-N-CA	5.30	125.06	119.76
1	C	93	GLN	N-CA-C	5.28	118.22	109.46
1	F	72	ALA	N-CA-C	-5.24	105.65	111.36
1	E	108	PHE	N-CA-C	5.20	117.03	111.36
1	F	66	ASP	N-CA-C	-5.20	105.78	111.82
1	F	111	ASN	N-CA-C	5.20	118.79	112.23
1	F	16	SER	N-CA-C	5.20	115.21	107.88
1	E	209	THR	CA-C-N	-5.19	113.58	119.28
1	E	209	THR	C-N-CA	-5.19	113.58	119.28
1	H	67	LEU	N-CA-C	5.19	116.62	111.07
1	G	33	VAL	N-CA-C	5.16	115.39	108.17
1	F	156	ALA	N-CA-C	-5.12	105.88	111.82
1	C	119	VAL	N-CA-C	-5.12	105.42	111.00
1	H	2	TYR	N-CA-C	5.12	117.09	109.25
1	D	61	VAL	N-CA-C	5.10	119.24	112.76
1	C	82	ASP	N-CA-C	-5.06	107.24	113.41
1	C	18	ILE	N-CA-C	5.05	115.77	110.62
1	E	225	LEU	N-CA-C	-5.03	105.80	111.28
1	G	123	LEU	CA-C-N	-5.03	114.43	119.56
1	G	123	LEU	C-N-CA	-5.03	114.43	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1745	0	1786	26	0
1	B	1745	0	1786	33	0
1	C	1745	0	1786	15	0
1	D	1745	0	1786	23	0
1	E	1745	0	1786	25	0
1	F	1745	0	1786	14	0
1	G	1745	0	1786	26	0
1	H	1745	0	1786	26	0
2	A	51	0	0	2	0
2	B	84	0	0	1	0
2	C	75	0	0	1	0
2	D	85	0	0	3	0
2	E	79	0	0	3	0
2	F	87	0	0	0	0
2	G	85	0	0	2	0
2	H	87	0	0	0	0
All	All	14593	0	14288	168	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 (168) 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:ILE:HD13	1:A:220:LEU:CD2	1.87	1.03
1:A:18:ILE:HD13	1:A:220:LEU:HD22	1.49	0.94
1:F:18:ILE:HG12	1:F:220:LEU:HD23	1.56	0.88
1:E:18:ILE:HD13	1:E:220:LEU:CD2	2.08	0.84
1:G:18:ILE:HD13	1:G:220:LEU:CD2	2.08	0.83
1:B:60:ASP:HB3	1:B:63:LYS:HD2	1.61	0.82
1:A:18:ILE:CD1	1:A:220:LEU:HD22	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:ILE:HD13	1:H:220:LEU:HD23	1.64	0.78
1:H:123:LEU:HB2	1:H:124:PRO:HD3	1.67	0.75
1:C:18:ILE:HD13	1:C:220:LEU:HD22	1.69	0.74
1:B:18:ILE:HD13	1:B:220:LEU:HD23	1.70	0.72
1:C:61:VAL:HG23	2:C:318:HOH:O	1.88	0.72
1:B:93:GLN:O	1:B:94:LYS:HG2	1.89	0.72
1:G:180:PRO:HG3	1:G:220:LEU:HD21	1.74	0.69
1:E:18:ILE:HD13	1:E:220:LEU:HD23	1.74	0.68
1:G:18:ILE:HD13	1:G:220:LEU:HD22	1.75	0.68
1:B:80:SER:HB2	2:B:369:HOH:O	1.91	0.68
1:G:18:ILE:CD1	1:G:220:LEU:HD22	2.24	0.67
1:H:75:ARG:HB2	1:H:125:LEU:HD21	1.77	0.67
1:G:180:PRO:CG	1:G:220:LEU:HD21	2.27	0.65
1:E:18:ILE:CD1	1:E:220:LEU:HD23	2.27	0.65
1:G:105:ASP:OD1	1:H:113:ARG:NH2	2.30	0.64
1:F:204:LYS:HD2	1:F:204:LYS:H	1.63	0.64
1:B:15:GLY:HA3	1:B:37:ASP:OD2	1.99	0.62
1:E:18:ILE:CG1	1:E:220:LEU:HD23	2.29	0.62
1:B:18:ILE:HD13	1:B:220:LEU:CD2	2.28	0.62
1:E:166:THR:O	1:E:169:LYS:HG2	2.00	0.62
1:H:18:ILE:HD13	1:H:220:LEU:CD2	2.31	0.61
1:A:18:ILE:CD1	1:A:220:LEU:CD2	2.70	0.60
1:B:184:ASP:HB2	1:B:214:VAL:CG2	2.30	0.60
1:A:123:LEU:HD11	1:B:96:LEU:HD23	1.83	0.60
1:H:18:ILE:CD1	1:H:220:LEU:HD23	2.31	0.60
1:G:129:GLY:HA2	1:G:172:SER:O	2.02	0.60
1:E:18:ILE:CD1	1:E:220:LEU:CD2	2.77	0.59
1:A:39:SER:HB3	1:A:42:GLU:HB3	1.85	0.59
1:A:158:ARG:HD3	1:A:158:ARG:C	2.28	0.58
1:D:18:ILE:HG12	1:D:220:LEU:HD23	1.84	0.58
1:B:18:ILE:HG21	1:B:220:LEU:HD23	1.85	0.58
1:E:80:SER:HB2	2:E:363:HOH:O	2.02	0.58
1:G:123:LEU:HD11	1:H:96:LEU:HD23	1.86	0.58
1:G:18:ILE:HD13	1:G:220:LEU:HD23	1.85	0.57
1:A:18:ILE:CG2	1:A:220:LEU:HD23	2.34	0.57
1:H:180:PRO:HB3	1:H:220:LEU:HD21	1.86	0.57
1:D:18:ILE:HG12	1:D:220:LEU:CD2	2.35	0.57
1:H:203:ALA:HB3	1:H:204:LYS:HE2	1.86	0.57
1:D:136:SER:HB3	1:D:179:SER:OG	2.04	0.56
1:A:123:LEU:HD11	1:B:96:LEU:CD2	2.35	0.56
1:E:18:ILE:HG12	1:E:220:LEU:HD23	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:380:HOH:O	1:H:97:GLU:HG3	2.06	0.55
1:H:180:PRO:CG	1:H:220:LEU:HD21	2.36	0.55
1:A:167:GLU:OE2	1:B:148:ASP:OD1	2.25	0.54
1:D:18:ILE:CG2	1:D:220:LEU:HD23	2.38	0.54
1:H:180:PRO:HG3	1:H:220:LEU:HD21	1.89	0.54
1:G:18:ILE:HG21	1:G:220:LEU:HD23	1.90	0.54
1:G:148:ASP:OD1	1:H:167:GLU:OE2	2.25	0.53
1:F:158:ARG:NH2	1:H:248:GLN:OE1	2.41	0.53
1:B:123:LEU:HB2	1:B:124:PRO:HD3	1.91	0.53
1:B:136:SER:HA	1:B:154:LYS:HD2	1.91	0.53
1:G:115:LEU:HD11	1:G:134:LEU:HD22	1.92	0.52
1:H:218:GLU:H	1:H:218:GLU:CD	2.17	0.52
1:B:180:PRO:HG3	1:B:220:LEU:HD21	1.92	0.51
1:H:211:LEU:HD12	1:H:244:GLY:HA2	1.92	0.51
1:B:69:ARG:O	1:B:73:ILE:HD12	2.10	0.51
1:B:24:LYS:NZ	1:B:49:GLU:OE1	2.34	0.51
1:G:136:SER:HA	1:G:154:LYS:HD2	1.91	0.51
1:B:85:PHE:CZ	1:B:87:ASN:HB2	2.45	0.51
1:C:39:SER:HB3	1:C:42:GLU:CB	2.41	0.51
1:G:104:TYR:HD1	1:G:105:ASP:OD1	1.94	0.51
1:A:18:ILE:HG21	1:A:220:LEU:HD23	1.92	0.50
1:A:33:VAL:O	1:A:54:VAL:HA	2.10	0.50
1:H:123:LEU:HB2	1:H:124:PRO:CD	2.41	0.50
1:H:109:ASP:HA	1:H:113:ARG:HB3	1.94	0.50
1:A:153:ALA:O	1:A:156:ALA:HB3	2.12	0.49
1:D:138:VAL:O	1:D:142:LEU:HG	2.12	0.49
1:G:109:ASP:HA	1:G:113:ARG:HB3	1.95	0.49
1:H:18:ILE:CD1	1:H:220:LEU:CD2	2.90	0.49
1:D:225:LEU:O	1:D:226:PHE:C	2.54	0.49
1:E:148:ASP:OD1	1:F:167:GLU:OE2	2.29	0.49
1:D:3:ARG:HD3	2:D:355:HOH:O	2.12	0.49
1:H:104:TYR:CD1	1:H:104:TYR:C	2.91	0.49
1:E:167:GLU:OE2	1:F:148:ASP:OD1	2.30	0.49
1:G:148:ASP:HA	1:H:163:THR:HG21	1.95	0.49
1:D:24:LYS:NZ	1:D:49:GLU:HB3	2.27	0.49
1:D:236:ALA:HB1	2:D:342:HOH:O	2.13	0.49
1:B:184:ASP:HB2	1:B:214:VAL:HG23	1.94	0.48
1:C:5:LEU:O	1:C:6:ASN:HB2	2.12	0.48
1:B:40:ARG:NH1	1:B:44:GLU:OE2	2.46	0.48
1:E:58:LYS:NZ	2:E:355:HOH:O	2.46	0.48
1:G:113:ARG:NH2	1:H:105:ASP:OD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLU:O	1:B:99:ILE:C	2.57	0.47
1:B:67:LEU:O	1:B:70:LEU:HB3	2.14	0.47
1:C:210:PRO:HD2	1:C:244:GLY:O	2.15	0.47
1:A:129:GLY:HA2	1:A:172:SER:O	2.15	0.47
1:F:45:GLN:O	1:F:49:GLU:HG3	2.14	0.47
1:D:164:TRP:O	1:D:168:LEU:HB2	2.15	0.47
1:B:18:ILE:CG2	1:B:220:LEU:HD23	2.44	0.47
1:G:20:LEU:HD13	1:G:46:ALA:HB1	1.97	0.47
1:A:80:SER:HB2	2:A:351:HOH:O	2.14	0.46
1:A:18:ILE:HD13	1:A:220:LEU:HD23	1.87	0.46
1:A:210:PRO:O	1:C:169:LYS:HB2	2.16	0.46
1:B:153:ALA:O	1:B:157:VAL:HG23	2.16	0.46
1:E:210:PRO:HG3	1:E:249:VAL:HG21	1.96	0.46
1:H:180:PRO:CB	1:H:220:LEU:HD21	2.45	0.46
1:A:69:ARG:HD2	2:A:350:HOH:O	2.17	0.45
1:D:158:ARG:HD3	1:D:158:ARG:C	2.42	0.45
1:H:158:ARG:HD3	1:H:158:ARG:C	2.42	0.45
1:F:174:ARG:HD2	1:F:235:VAL:O	2.16	0.45
1:C:163:THR:HG21	1:D:148:ASP:HA	1.98	0.45
1:E:204:LYS:H	1:E:204:LYS:HG2	1.40	0.45
1:D:18:ILE:HG21	1:D:220:LEU:HD23	1.98	0.45
1:A:148:ASP:OD1	1:B:167:GLU:OE2	2.34	0.45
1:B:43:LEU:HB3	1:B:56:ALA:HB1	1.99	0.45
1:G:67:LEU:O	1:G:70:LEU:HB3	2.16	0.45
1:C:39:SER:HB3	1:C:42:GLU:HB3	1.98	0.44
1:D:20:LEU:HD13	1:D:46:ALA:HB1	1.98	0.44
1:B:134:LEU:HD23	1:B:134:LEU:N	2.32	0.44
1:F:35:ILE:HG13	1:F:56:ALA:HA	1.98	0.44
1:A:204:LYS:C	1:A:207:ALA:H	2.25	0.44
1:B:15:GLY:CA	1:B:37:ASP:OD2	2.66	0.44
1:A:166:THR:O	1:A:169:LYS:HG2	2.17	0.43
1:C:96:LEU:HD21	1:D:119:VAL:HG12	1.99	0.43
1:D:161:ALA:HA	1:D:175:VAL:HG12	2.00	0.43
1:E:22:THR:HA	1:E:221:ALA:HB1	2.00	0.43
1:E:144:LEU:O	1:E:145:GLN:C	2.62	0.43
1:G:61:VAL:HG23	2:G:336:HOH:O	2.18	0.43
1:C:39:SER:HB3	1:C:42:GLU:HB2	2.01	0.43
1:C:152:ALA:HB1	1:D:156:ALA:HB1	2.01	0.43
1:D:80:SER:HB2	2:D:321:HOH:O	2.18	0.43
1:G:184:ASP:OD1	1:G:184:ASP:C	2.61	0.43
1:H:220:LEU:HD12	1:H:242:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG13	1:A:56:ALA:HA	2.00	0.42
1:C:167:GLU:OE2	1:D:148:ASP:OD1	2.37	0.42
1:E:158:ARG:HD3	1:E:158:ARG:C	2.44	0.42
1:G:34:PHE:CD1	1:G:55:THR:HB	2.54	0.42
1:G:95:THR:O	1:G:99:ILE:HG13	2.20	0.42
1:D:101:PRO:HG2	1:E:40:ARG:CZ	2.49	0.42
1:G:183:ILE:HD11	1:G:220:LEU:HD13	2.01	0.42
1:A:10:VAL:HG22	1:A:34:PHE:HB2	2.01	0.42
1:B:104:TYR:CD1	1:B:104:TYR:C	2.96	0.42
1:E:45:GLN:O	1:E:49:GLU:HG3	2.19	0.42
1:F:136:SER:OG	1:F:154:LYS:O	2.36	0.42
1:A:220:LEU:HD12	1:A:242:VAL:HG11	2.01	0.42
1:D:218:GLU:H	1:D:218:GLU:CD	2.26	0.42
1:E:49:GLU:HA	2:E:374:HOH:O	2.19	0.42
1:C:123:LEU:HA	1:C:126:LEU:HD12	2.02	0.42
1:D:182:ALA:O	1:D:183:ILE:HD13	2.20	0.42
1:A:158:ARG:HD3	1:A:158:ARG:O	2.19	0.42
1:E:36:VAL:HA	1:E:57:VAL:O	2.18	0.42
1:A:105:ASP:OD1	1:B:113:ARG:NH2	2.52	0.42
1:E:18:ILE:HD11	1:E:183:ILE:HG13	2.02	0.42
1:C:167:GLU:HG2	1:D:145:GLN:OE1	2.20	0.42
1:E:35:ILE:HG13	1:E:56:ALA:HA	2.02	0.42
1:B:61:VAL:HB	1:B:118:THR:OG1	2.20	0.41
1:B:144:LEU:O	1:B:147:HIS:HB2	2.20	0.41
1:F:132:VAL:O	1:F:175:VAL:HA	2.20	0.41
1:G:126:LEU:O	1:G:171:ARG:NH2	2.54	0.41
1:F:123:LEU:HB2	1:F:124:PRO:HD3	2.02	0.41
1:H:117:PHE:O	1:H:121:LYS:HG3	2.20	0.41
1:B:245:GLY:O	1:B:246:LEU:C	2.64	0.41
1:C:20:LEU:HG	1:C:24:LYS:HE3	2.01	0.41
1:B:75:ARG:HB2	1:B:125:LEU:HD21	2.03	0.41
1:F:176:ASN:OD1	1:F:238:ILE:HG12	2.21	0.41
1:F:204:LYS:HD2	1:F:204:LYS:N	2.34	0.41
1:G:40:ARG:NH1	1:G:44:GLU:OE2	2.53	0.41
1:E:123:LEU:HB2	1:E:124:PRO:HD3	2.03	0.40
1:E:18:ILE:CG2	1:E:220:LEU:HD23	2.51	0.40
1:F:104:TYR:CD1	1:F:104:TYR:C	2.99	0.40
1:E:96:LEU:HA	1:E:99:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/262 (87%)	214 (93%)	15 (7%)	0	100	100
1	B	229/262 (87%)	214 (93%)	12 (5%)	3 (1%)	9	10
1	C	229/262 (87%)	218 (95%)	11 (5%)	0	100	100
1	D	229/262 (87%)	219 (96%)	10 (4%)	0	100	100
1	E	229/262 (87%)	210 (92%)	19 (8%)	0	100	100
1	F	229/262 (87%)	216 (94%)	13 (6%)	0	100	100
1	G	229/262 (87%)	213 (93%)	14 (6%)	2 (1%)	14	17
1	H	229/262 (87%)	215 (94%)	14 (6%)	0	100	100
All	All	1832/2096 (87%)	1719 (94%)	108 (6%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	ASP
1	G	206	ALA
1	B	17	GLY
1	G	61	VAL
1	B	148	ASP

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	179/204 (88%)	175 (98%)	4 (2%)	45	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	179/204 (88%)	171 (96%)	8 (4%)	24	37
1	C	179/204 (88%)	176 (98%)	3 (2%)	53	72
1	D	179/204 (88%)	175 (98%)	4 (2%)	45	65
1	E	179/204 (88%)	175 (98%)	4 (2%)	45	65
1	F	179/204 (88%)	177 (99%)	2 (1%)	65	81
1	G	179/204 (88%)	174 (97%)	5 (3%)	38	56
1	H	179/204 (88%)	175 (98%)	4 (2%)	45	65
All	All	1432/1632 (88%)	1398 (98%)	34 (2%)	43	62

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	65	GLU
1	A	80	SER
1	A	91	ILE
1	B	39	SER
1	B	63	LYS
1	B	80	SER
1	B	97	GLU
1	B	106	ARG
1	B	185	THR
1	B	214	VAL
1	B	217	PRO
1	C	75	ARG
1	C	185	THR
1	C	220	LEU
1	D	18	ILE
1	D	80	SER
1	D	204	LYS
1	D	211	LEU
1	E	80	SER
1	E	91	ILE
1	E	169	LYS
1	E	204	LYS
1	F	39	SER
1	F	204	LYS
1	G	39	SER
1	G	75	ARG
1	G	91	ILE

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Mol	Chain	Res	Type
1	G	110	VAL
1	G	220	LEU
1	H	75	ARG
1	H	91	ILE
1	H	148	ASP
1	H	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	B	93	GLN
1	C	77	GLN
1	C	93	GLN
1	E	6	ASN
1	E	87	ASN
1	E	120	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	233/262 (88%)	0.50	16 (6%)	23 25	1, 32, 62, 128	3 (1%)
1	B	233/262 (88%)	0.14	10 (4%)	40 41	14, 24, 46, 129	1 (0%)
1	C	233/262 (88%)	0.24	14 (6%)	27 29	15, 24, 51, 105	3 (1%)
1	D	233/262 (88%)	0.27	12 (5%)	33 34	1, 24, 47, 132	3 (1%)
1	E	233/262 (88%)	0.20	14 (6%)	27 29	15, 28, 51, 126	1 (0%)
1	F	233/262 (88%)	-0.10	10 (4%)	40 41	14, 24, 44, 120	1 (0%)
1	G	233/262 (88%)	0.13	9 (3%)	43 45	15, 25, 55, 85	0
1	H	233/262 (88%)	0.26	11 (4%)	36 38	14, 27, 57, 148	1 (0%)
All	All	1864/2096 (88%)	0.20	96 (5%)	33 34	1, 26, 55, 148	13 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	PHE	41.5
1	D	205	PHE	38.5
1	C	205	PHE	15.9
1	H	40	ARG	11.3
1	D	45	GLN	9.1
1	C	41	LYS	8.9
1	A	41	LYS	8.9
1	D	208	ALA	8.8
1	D	41	LYS	7.7
1	E	41	LYS	7.6
1	F	203	ALA	7.4
1	E	186	PRO	7.3
1	H	205	PHE	7.3
1	B	208	ALA	7.2
1	B	203	ALA	7.0
1	A	40	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
1	C	186	PRO	6.8
1	A	208	ALA	6.6
1	H	204	LYS	6.4
1	B	186	PRO	6.4
1	A	203	ALA	6.1
1	E	205	PHE	6.0
1	B	185	THR	6.0
1	B	41	LYS	5.9
1	H	209	THR	5.9
1	E	203	ALA	5.8
1	A	210	PRO	5.7
1	F	186	PRO	5.6
1	D	186	PRO	5.5
1	D	206	ALA	5.4
1	A	186	PRO	5.4
1	C	40	ARG	5.4
1	H	207	ALA	5.2
1	G	205	PHE	5.1
1	H	206	ALA	4.9
1	D	207	ALA	4.9
1	C	207	ALA	4.9
1	H	208	ALA	4.8
1	A	207	ALA	4.7
1	A	206	ALA	4.7
1	E	208	ALA	4.6
1	G	186	PRO	4.6
1	C	206	ALA	4.5
1	F	206	ALA	4.5
1	E	185	THR	4.5
1	E	90	ALA	4.4
1	G	185	THR	4.4
1	B	206	ALA	4.3
1	G	203	ALA	4.2
1	A	204	LYS	4.1
1	F	207	ALA	4.1
1	A	211	LEU	4.0
1	A	209	THR	4.0
1	B	207	ALA	3.9
1	C	203	ALA	3.9
1	E	1	ALA	3.8
1	G	1	ALA	3.8
1	H	186	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	183	ILE	3.8
1	F	40	ARG	3.8
1	B	205	PHE	3.7
1	D	185	THR	3.7
1	F	185	THR	3.7
1	E	207	ALA	3.7
1	E	91	ILE	3.6
1	C	185	THR	3.6
1	D	203	ALA	3.6
1	H	79	GLY	3.6
1	C	208	ALA	3.5
1	G	204	LYS	3.4
1	D	204	LYS	3.3
1	A	1	ALA	3.3
1	H	203	ALA	3.3
1	C	209	THR	3.3
1	F	205	PHE	3.2
1	F	204	LYS	3.2
1	H	185	THR	3.2
1	G	206	ALA	3.1
1	A	185	THR	3.1
1	B	204	LYS	3.0
1	F	208	ALA	2.9
1	B	1	ALA	2.7
1	E	204	LYS	2.6
1	A	184	ASP	2.6
1	G	2	TYR	2.6
1	C	204	LYS	2.5
1	E	89	GLY	2.5
1	D	65	GLU	2.4
1	E	183	ILE	2.4
1	D	69	ARG	2.3
1	C	184	ASP	2.3
1	C	1	ALA	2.3
1	C	91	ILE	2.3
1	G	207	ALA	2.2
1	E	206	ALA	2.1
1	F	1	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.