



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:36 AM UTC

PDB ID : 4I5F / pdb_00004i5f
Title : Crystal structure of Ralstonia sp. alcohol dehydrogenase mutant N15G, G37D, R38V, R39S
Authors : Jarasch, A.; Lerchner, A.; Meining, W.; Schiefner, A.; Skerra, A.
Deposited on : 2012-11-28
Resolution : 2.10 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:

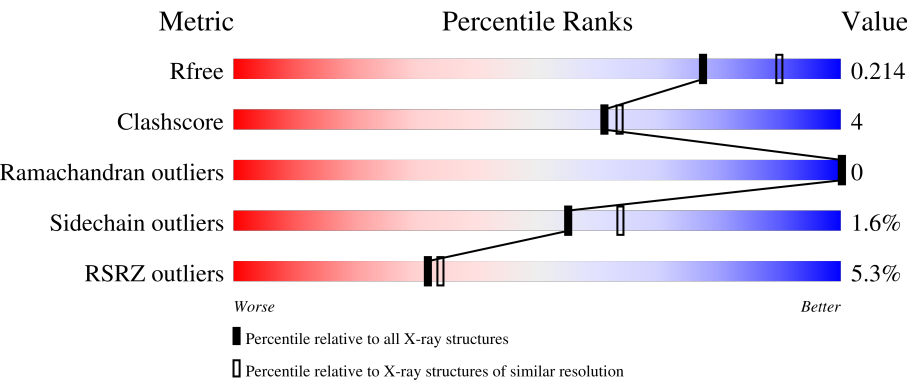
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 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	4% 77% 10% • 11%
1	B	262	4% 78% 10% 11%
1	C	262	5% 79% 10% 11%
1	D	262	4% 80% 9% 11%
1	E	262	3% 74% 13% • 11%

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Mol	Chain	Length	Quality of chain
1	F	262	5% 74%13%11%
1	G	262	8% 79%10%11%
1	H	262	4% 79%9%11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14580 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
			1743	1100	307	336			
1	B	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	C	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	D	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	E	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	F	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	G	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	H	233	Total	C	N	O	0	0	0
			1743	1100	307	336			

There are 144 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
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
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
C	37	ASP	GLY	engineered mutation	UNP C0IR58
C	38	VAL	ARG	engineered mutation	UNP C0IR58
C	39	SER	ARG	engineered mutation	UNP C0IR58
D	-12	MET	-	expression tag	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
E	39	SER	ARG	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

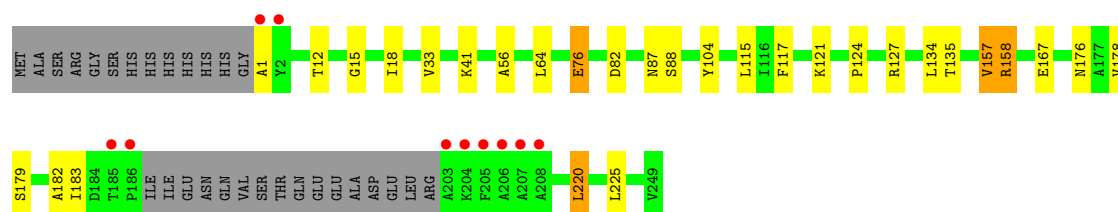
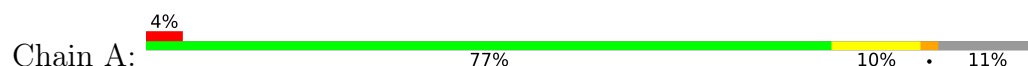
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	89	Total O 89 89	0	0
2	B	84	Total O 84 84	0	0
2	C	80	Total O 80 80	0	0
2	D	85	Total O 85 85	0	0
2	E	87	Total O 87 87	0	0
2	F	74	Total O 74 74	0	0
2	G	65	Total O 65 65	0	0
2	H	72	Total O 72 72	0	0

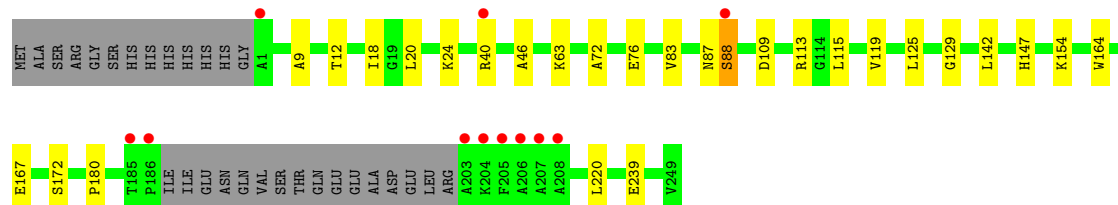
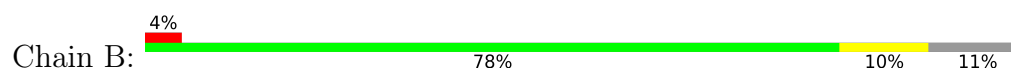
3 Residue-property plots [i](#)

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.

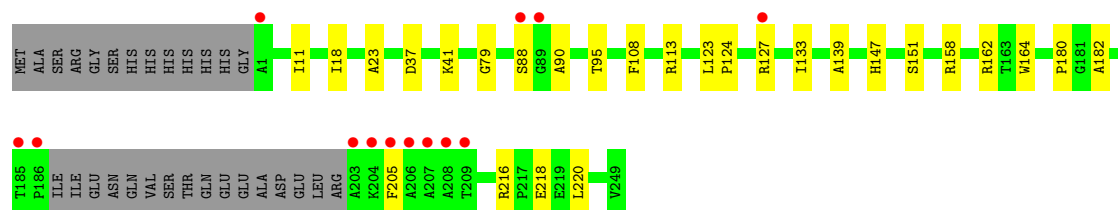
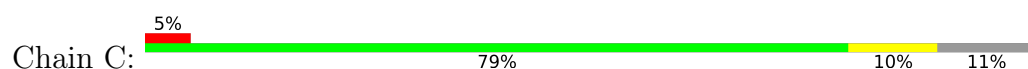
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



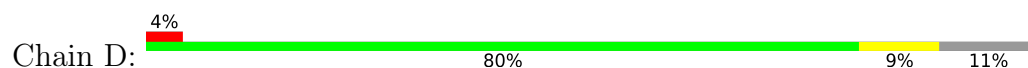
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

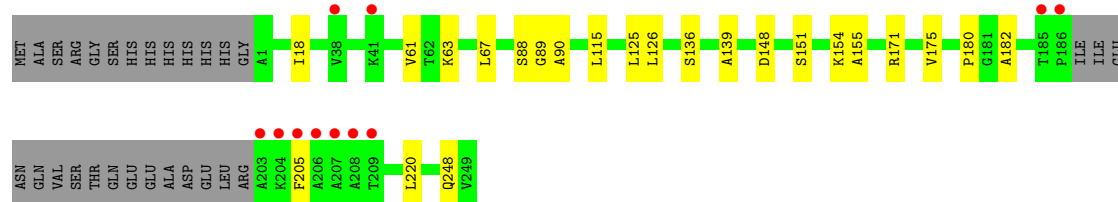


- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

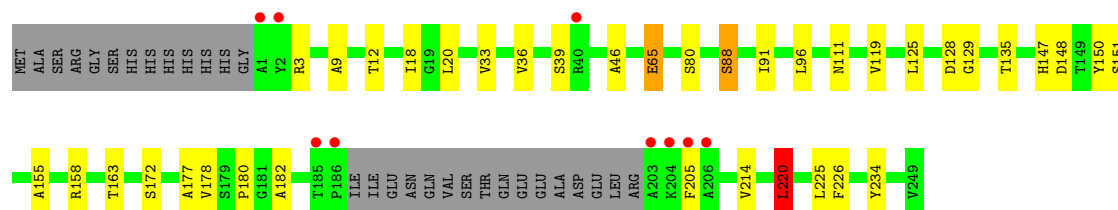
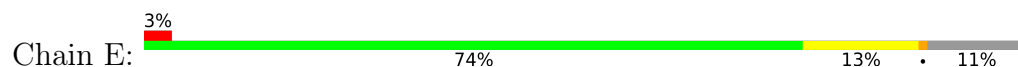


- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

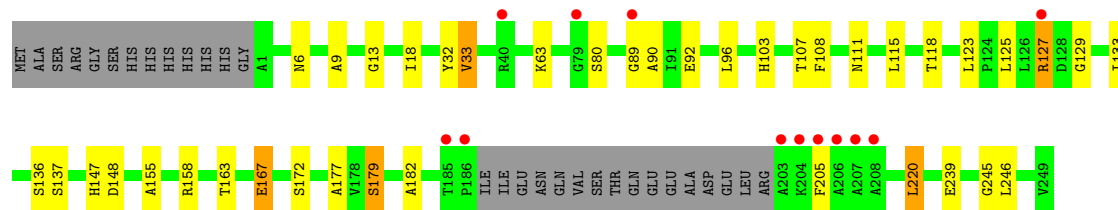
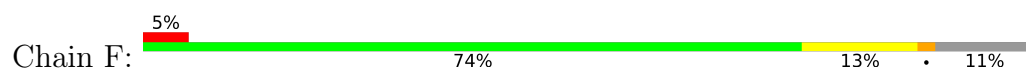




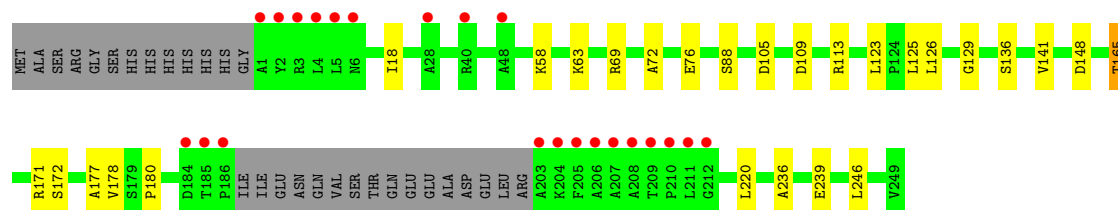
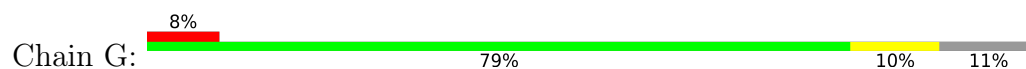
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



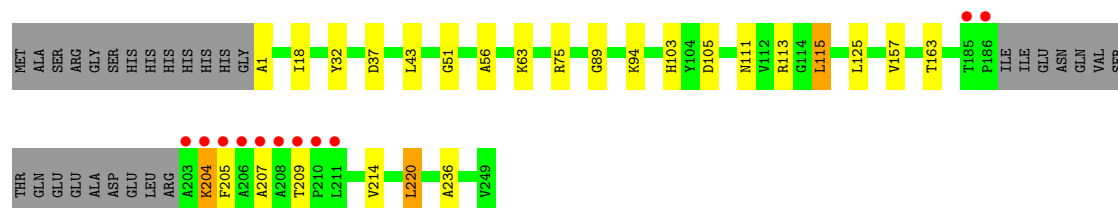
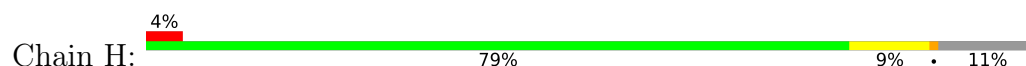
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



- 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	Depositor
Cell constants a, b, c, α , β , γ	72.80Å 72.97Å 132.89Å 80.74° 86.53° 64.18°	Depositor
Resolution (Å)	29.58 – 2.10 29.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.58-2.10) 96.5 (29.58-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.244 (Not available) , 0.214	Depositor DCC
R_{free} test set	6862 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14580	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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	1.38	11/1765 (0.6%)	1.32	8/2392 (0.3%)
1	B	1.24	2/1765 (0.1%)	1.22	3/2392 (0.1%)
1	C	1.32	3/1765 (0.2%)	1.28	4/2392 (0.2%)
1	D	1.29	1/1765 (0.1%)	1.21	3/2392 (0.1%)
1	E	1.38	8/1765 (0.5%)	1.33	8/2392 (0.3%)
1	F	1.28	11/1765 (0.6%)	1.24	10/2392 (0.4%)
1	G	1.25	5/1765 (0.3%)	1.24	7/2392 (0.3%)
1	H	1.22	3/1765 (0.2%)	1.16	2/2392 (0.1%)
All	All	1.30	44/14120 (0.3%)	1.25	45/19136 (0.2%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	136	SER	CA-C	-7.47	1.49	1.53
1	F	239	GLU	C-O	6.87	1.31	1.24
1	E	234	TYR	CA-CB	6.76	1.62	1.53
1	F	246	LEU	C-O	-6.59	1.15	1.24
1	A	158	ARG	N-CA	6.56	1.54	1.46
1	A	178	VAL	C-O	6.12	1.31	1.24
1	E	111	ASN	N-CA	6.09	1.54	1.46
1	A	135	THR	C-O	6.06	1.31	1.24
1	E	225	LEU	C-O	6.02	1.31	1.24
1	F	179	SER	CA-C	5.96	1.58	1.52
1	G	177	ALA	C-O	-5.80	1.17	1.23
1	D	175	VAL	C-O	5.80	1.30	1.24
1	E	178	VAL	C-O	5.67	1.30	1.24
1	F	92	GLU	CA-C	5.59	1.59	1.52
1	C	147	HIS	CG-CD2	5.55	1.42	1.35
1	A	225	LEU	C-O	5.55	1.30	1.24
1	G	141	VAL	C-O	-5.53	1.17	1.24
1	F	155	ALA	N-CA	5.52	1.53	1.46
1	F	177	ALA	C-O	5.50	1.30	1.24
1	B	142	LEU	N-CA	5.48	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	56	ALA	C-O	-5.47	1.17	1.24
1	F	137	SER	CA-C	-5.40	1.45	1.52
1	E	135	THR	C-O	5.39	1.30	1.24
1	A	56	ALA	C-O	-5.39	1.17	1.24
1	A	157	VAL	CA-CB	5.36	1.61	1.54
1	F	90	ALA	CA-C	-5.33	1.46	1.52
1	G	178	VAL	C-O	5.30	1.30	1.24
1	G	177	ALA	N-CA	5.29	1.52	1.46
1	F	147	HIS	CG-CD2	5.28	1.41	1.35
1	H	75	ARG	CA-C	5.22	1.59	1.52
1	E	147	HIS	CG-CD2	5.18	1.41	1.35
1	A	124	PRO	C-O	-5.18	1.17	1.24
1	A	176	ASN	CA-C	-5.16	1.46	1.52
1	E	177	ALA	CA-C	5.16	1.59	1.52
1	C	164	TRP	CD2-CE2	5.15	1.50	1.41
1	C	133	ILE	C-O	5.15	1.29	1.24
1	A	88	SER	C-O	5.14	1.30	1.23
1	F	127	ARG	C-O	5.14	1.30	1.23
1	B	147	HIS	CG-CD2	5.10	1.41	1.35
1	A	33	VAL	CA-C	5.09	1.58	1.52
1	F	103	HIS	CG-CD2	5.09	1.41	1.35
1	E	12	THR	C-O	5.07	1.30	1.23
1	A	135	THR	CA-CB	-5.07	1.46	1.53
1	H	103	HIS	CG-CD2	5.01	1.41	1.35

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	123	LEU	CA-C-N	-9.68	109.58	120.04
1	G	123	LEU	C-N-CA	-9.68	109.58	120.04
1	A	88	SER	N-CA-C	-8.80	95.88	109.52
1	B	88	SER	N-CA-C	-7.66	96.97	108.99
1	G	88	SER	N-CA-C	-6.46	99.50	109.52
1	D	88	SER	N-CA-C	-6.42	99.39	108.96
1	F	167	GLU	N-CA-C	6.33	119.16	111.82
1	B	154	LYS	N-CA-C	6.30	118.15	111.28
1	F	179	SER	CA-C-N	6.26	126.02	119.76
1	F	179	SER	C-N-CA	6.26	126.02	119.76
1	E	220	LEU	CA-CB-CG	-6.17	94.69	116.30
1	C	108	PHE	N-CA-C	6.09	118.89	111.82
1	H	51	GLY	N-CA-C	6.08	123.15	115.42
1	E	155	ALA	N-CA-C	-6.03	104.79	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ALA	N-CA-C	-6.01	98.05	108.69
1	E	88	SER	N-CA-C	-5.97	100.17	109.72
1	H	32	TYR	N-CA-C	-5.76	100.32	109.76
1	A	76	GLU	CB-CA-C	-5.76	101.06	110.85
1	G	165	THR	N-CA-C	-5.70	104.97	111.07
1	F	155	ALA	N-CA-C	-5.64	105.21	111.36
1	F	107	THR	N-CA-C	5.63	117.09	111.07
1	D	90	ALA	N-CA-C	-5.60	98.40	108.48
1	E	226	PHE	N-CA-C	-5.60	105.26	111.36
1	F	118	THR	N-CA-C	-5.58	105.19	111.28
1	E	180	PRO	CB-CA-C	-5.54	104.14	111.23
1	A	167	GLU	N-CA-C	5.54	117.39	111.36
1	E	128	ASP	N-CA-C	-5.45	102.33	110.23
1	F	33	VAL	N-CA-C	5.44	115.95	108.12
1	G	246	LEU	N-CA-C	5.41	116.86	111.07
1	G	239	GLU	CA-C-N	-5.39	115.84	122.84
1	G	239	GLU	C-N-CA	-5.39	115.84	122.84
1	F	133	ILE	N-CA-C	-5.38	100.58	108.11
1	C	216	ARG	N-CA-C	-5.35	102.90	110.29
1	E	214	VAL	N-CA-C	-5.30	104.27	110.05
1	C	95	THR	N-CA-C	-5.29	103.70	110.53
1	F	32	TYR	N-CA-C	-5.26	101.14	109.76
1	A	15	GLY	N-CA-C	5.25	122.20	115.32
1	A	33	VAL	N-CA-C	5.20	116.07	108.53
1	A	179	SER	CA-C-N	5.20	125.13	119.78
1	A	179	SER	C-N-CA	5.20	125.13	119.78
1	D	155	ALA	N-CA-C	-5.20	105.70	111.36
1	E	151	SER	N-CA-C	5.19	117.34	111.11
1	B	239	GLU	N-CA-C	-5.12	100.06	108.41
1	A	1	ALA	N-CA-C	-5.04	96.89	111.00
1	F	108	PHE	N-CA-C	5.03	116.85	111.36

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	1743	0	1785	14	0
1	B	1743	0	1785	21	0
1	C	1743	0	1785	19	0
1	D	1743	0	1785	14	0
1	E	1743	0	1785	16	0
1	F	1743	0	1785	23	0
1	G	1743	0	1785	12	0
1	H	1743	0	1785	15	0
2	A	89	0	0	1	0
2	B	84	0	0	1	0
2	C	80	0	0	0	0
2	D	85	0	0	1	0
2	E	87	0	0	2	0
2	F	74	0	0	4	0
2	G	65	0	0	2	0
2	H	72	0	0	3	0
All	All	14580	0	14280	119	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 4.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HG2	1:B:40:ARG:HH11	1.46	0.80
1:B:18:ILE:HG21	1:B:220:LEU:HD23	1.63	0.80
1:D:18:ILE:HD12	1:D:220:LEU:HD22	1.64	0.80
1:D:18:ILE:HD12	1:D:220:LEU:CD2	2.14	0.78
1:B:72:ALA:O	1:B:76:GLU:HG3	1.86	0.75
1:H:214:VAL:HG22	2:H:345:HOH:O	1.88	0.72
1:A:18:ILE:HD12	1:A:220:LEU:CD2	2.20	0.71
1:C:18:ILE:HB	1:C:220:LEU:HD23	1.74	0.70
1:C:18:ILE:HD12	1:C:220:LEU:CD2	2.23	0.68
1:C:18:ILE:HG21	1:C:220:LEU:HD22	1.74	0.68
1:C:18:ILE:CD1	1:C:220:LEU:CD2	2.74	0.66
1:B:180:PRO:HG3	1:B:220:LEU:HD21	1.78	0.64
1:G:236:ALA:HB1	2:G:321:HOH:O	1.99	0.62
1:F:18:ILE:HD12	1:F:220:LEU:CD2	2.31	0.61
1:F:18:ILE:HD12	1:F:220:LEU:HD22	1.82	0.61
1:H:18:ILE:HD12	1:H:220:LEU:HD22	1.81	0.60
1:A:64:LEU:HD22	1:A:121:LYS:HE3	1.82	0.60
1:H:1:ALA:N	2:H:372:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:LEU:N	1:H:125:LEU:HD12	2.18	0.58
1:B:40:ARG:HG2	1:B:40:ARG:NH1	2.17	0.58
1:H:115:LEU:HD22	1:H:157:VAL:HG22	1.85	0.58
1:E:91:ILE:HB	1:E:150:TYR:CD1	2.38	0.58
1:E:129:GLY:HA2	1:E:172:SER:O	2.05	0.57
1:E:18:ILE:HD12	1:E:220:LEU:HD22	1.86	0.57
1:D:61:VAL:HG12	1:D:67:LEU:HD21	1.87	0.57
1:B:119:VAL:HG21	1:B:164:TRP:CZ3	2.40	0.56
1:H:18:ILE:HD12	1:H:220:LEU:CD2	2.36	0.56
1:F:89:GLY:HA2	1:F:111:ASN:OD1	2.06	0.56
1:G:72:ALA:O	1:G:76:GLU:HG3	2.06	0.55
1:B:18:ILE:HG21	1:B:220:LEU:CD2	2.35	0.55
1:D:18:ILE:CD1	1:D:220:LEU:HD22	2.34	0.55
1:E:20:LEU:HD13	1:E:46:ALA:HB1	1.86	0.55
1:D:182:ALA:HB2	1:D:205:PHE:HD2	1.72	0.55
1:E:148:ASP:OD1	1:F:167:GLU:OE2	2.25	0.55
1:B:180:PRO:CG	1:B:220:LEU:HD21	2.37	0.54
1:A:76:GLU:HG3	2:A:313:HOH:O	2.06	0.54
1:A:115:LEU:HD22	1:A:157:VAL:HG22	1.90	0.54
1:G:125:LEU:HD12	1:G:125:LEU:N	2.23	0.54
1:F:80:SER:HB2	1:F:125:LEU:O	2.08	0.53
1:G:58:LYS:O	1:G:69:ARG:NH2	2.40	0.53
1:D:126:LEU:O	1:D:171:ARG:NH2	2.42	0.52
1:A:104:TYR:CE2	1:C:113:ARG:HB2	2.44	0.52
1:H:205:PHE:O	1:H:209:THR:OG1	2.25	0.52
1:G:109:ASP:HA	1:G:113:ARG:HB3	1.91	0.51
1:G:105:ASP:OD1	1:H:113:ARG:NH2	2.44	0.51
1:F:18:ILE:CD1	1:F:220:LEU:HD22	2.39	0.51
1:F:63:LYS:HA	2:F:358:HOH:O	2.11	0.50
1:B:88:SER:HA	2:B:352:HOH:O	2.11	0.49
1:F:13:GLY:N	2:F:347:HOH:O	2.44	0.49
1:B:167:GLU:OE2	1:D:148:ASP:OD1	2.30	0.49
1:F:136:SER:HB3	1:F:179:SER:OG	2.12	0.49
1:C:79:GLY:O	1:F:6:ASN:HB3	2.12	0.49
1:B:129:GLY:HA2	1:B:172:SER:O	2.13	0.49
1:F:158:ARG:C	1:F:158:ARG:HD3	2.38	0.49
1:E:163:THR:HG21	1:F:148:ASP:HA	1.95	0.48
1:D:125:LEU:HD12	1:D:125:LEU:N	2.29	0.48
1:A:82:ASP:OD1	1:A:127:ARG:NE	2.22	0.48
1:F:13:GLY:HA2	2:F:347:HOH:O	2.13	0.48
1:B:40:ARG:HH11	1:B:40:ARG:CG	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:CD1	1:A:220:LEU:HD22	2.44	0.47
1:C:18:ILE:HD12	1:C:220:LEU:HD23	1.96	0.47
1:A:158:ARG:HD3	1:A:158:ARG:C	2.39	0.47
1:E:148:ASP:HA	1:F:163:THR:HG21	1.96	0.47
1:G:126:LEU:O	1:G:171:ARG:NH2	2.48	0.47
1:G:180:PRO:HG3	1:G:220:LEU:HD21	1.96	0.47
1:B:18:ILE:CG2	1:B:220:LEU:HD23	2.39	0.47
1:D:182:ALA:HB2	1:D:205:PHE:CD2	2.50	0.47
1:G:148:ASP:HA	1:H:163:THR:HG21	1.96	0.47
1:A:18:ILE:HD12	1:A:220:LEU:HD22	1.96	0.46
1:H:204:LYS:O	1:H:207:ALA:HB3	2.15	0.46
1:D:89:GLY:HA3	2:D:373:HOH:O	2.15	0.46
1:E:3:ARG:HD3	2:E:326:HOH:O	2.16	0.46
1:E:119:VAL:HG12	1:F:96:LEU:HD21	1.96	0.46
1:C:139:ALA:HB1	1:C:151:SER:OG	2.16	0.45
1:C:182:ALA:HB2	1:C:205:PHE:HD2	1.81	0.45
1:F:129:GLY:HA2	1:F:172:SER:O	2.16	0.45
1:B:18:ILE:CD1	1:B:220:LEU:HD23	2.46	0.45
1:E:9:ALA:HB3	1:E:33:VAL:HG22	1.99	0.45
1:C:18:ILE:HD12	1:C:220:LEU:HD21	1.97	0.45
1:G:113:ARG:NH2	1:H:105:ASP:OD1	2.50	0.45
1:E:182:ALA:HB2	1:E:205:PHE:HD2	1.81	0.45
1:A:115:LEU:HD11	1:A:134:LEU:HD22	2.00	0.44
1:C:127:ARG:CZ	1:F:127:ARG:NH1	2.80	0.44
1:A:182:ALA:O	1:A:183:ILE:HD13	2.17	0.44
1:B:12:THR:O	1:B:87:ASN:HB3	2.17	0.44
1:E:96:LEU:HD23	1:F:123:LEU:HD11	2.00	0.44
1:E:158:ARG:HD3	1:E:158:ARG:C	2.43	0.44
1:C:218:GLU:H	1:C:218:GLU:CD	2.26	0.44
1:F:182:ALA:HB2	1:F:205:PHE:HB3	1.99	0.44
1:C:180:PRO:HB3	1:C:220:LEU:HD13	1.99	0.44
1:D:139:ALA:O	1:D:151:SER:HB3	2.17	0.44
1:F:9:ALA:HB3	1:F:33:VAL:HG22	2.00	0.44
1:B:125:LEU:HD12	1:B:125:LEU:N	2.33	0.43
1:E:80:SER:HB2	1:E:125:LEU:O	2.17	0.43
1:B:20:LEU:HD13	1:B:46:ALA:HB1	2.00	0.43
1:G:129:GLY:HA2	1:G:172:SER:O	2.18	0.43
1:A:64:LEU:HD21	1:A:117:PHE:CG	2.54	0.43
1:C:11:ILE:HD12	1:C:23:ALA:HB2	2.01	0.43
1:B:109:ASP:HA	1:B:113:ARG:HB3	1.99	0.43
1:C:162:ARG:HD3	1:D:248:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:ASP:O	1:H:43:LEU:HD11	2.18	0.43
1:A:18:ILE:CD1	1:A:220:LEU:CD2	2.96	0.43
1:A:12:THR:O	1:A:87:ASN:HB3	2.19	0.42
1:B:9:ALA:HA	1:B:83:VAL:O	2.19	0.42
1:D:180:PRO:HB3	1:D:220:LEU:HD13	2.01	0.42
1:C:158:ARG:HD3	1:C:158:ARG:C	2.45	0.42
1:F:245:GLY:HA2	1:H:236:ALA:O	2.20	0.42
1:E:65:GLU:CD	1:E:65:GLU:H	2.28	0.42
1:C:18:ILE:HD13	1:C:220:LEU:CD2	2.47	0.41
1:C:123:LEU:HB2	1:C:124:PRO:HD3	2.01	0.41
1:H:89:GLY:HA2	1:H:111:ASN:OD1	2.20	0.41
1:D:136:SER:OG	1:D:154:LYS:O	2.36	0.41
1:G:165:THR:HG23	2:G:321:HOH:O	2.19	0.41
1:C:127:ARG:NH2	1:F:127:ARG:NH1	2.69	0.40
1:E:88:SER:HA	2:E:379:HOH:O	2.21	0.40
1:F:13:GLY:CA	2:F:347:HOH:O	2.67	0.40
1:B:40:ARG:NH1	1:B:40:ARG:CG	2.77	0.40
1:B:20:LEU:HG	1:B:24:LYS:HE3	2.03	0.40
1:H:94:LYS:NZ	2:H:354:HOH:O	2.51	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%)	218 (95%)	11 (5%)	0	100	100
1	B	229/262 (87%)	219 (96%)	10 (4%)	0	100	100
1	C	229/262 (87%)	217 (95%)	12 (5%)	0	100	100
1	D	229/262 (87%)	222 (97%)	7 (3%)	0	100	100
1	E	229/262 (87%)	217 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	229/262 (87%)	219 (96%)	10 (4%)	0	100	100
1	G	229/262 (87%)	218 (95%)	11 (5%)	0	100	100
1	H	229/262 (87%)	221 (96%)	8 (4%)	0	100	100
All	All	1832/2096 (87%)	1751 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	173/204 (85%)	171 (99%)	2 (1%)	63	72
1	B	179/204 (88%)	177 (99%)	2 (1%)	65	74
1	C	179/204 (88%)	176 (98%)	3 (2%)	53	62
1	D	179/204 (88%)	177 (99%)	2 (1%)	65	74
1	E	179/204 (88%)	175 (98%)	4 (2%)	45	53
1	F	144/204 (71%)	142 (99%)	2 (1%)	59	67
1	G	157/204 (77%)	155 (99%)	2 (1%)	61	69
1	H	145/204 (71%)	141 (97%)	4 (3%)	38	43
All	All	1335/1632 (82%)	1314 (98%)	21 (2%)	55	64

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	220	LEU
1	B	63	LYS
1	B	115	LEU
1	C	37	ASP
1	C	41	LYS
1	C	88	SER
1	D	63	LYS

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Mol	Chain	Res	Type
1	D	115	LEU
1	E	36	VAL
1	E	39	SER
1	E	65	GLU
1	E	220	LEU
1	F	115	LEU
1	F	220	LEU
1	G	18	ILE
1	G	63	LYS
1	H	63	LYS
1	H	115	LEU
1	H	204	LYS
1	H	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	87	ASN
1	F	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%)	0.10	10 (4%) 40 41	16, 26, 52, 175	0
1	B	233/262 (88%)	0.25	11 (4%) 36 38	18, 34, 57, 126	0
1	C	233/262 (88%)	0.13	13 (5%) 30 32	17, 29, 50, 129	0
1	D	233/262 (88%)	0.08	11 (4%) 36 38	17, 30, 50, 117	0
1	E	233/262 (88%)	0.02	9 (3%) 43 45	18, 27, 51, 109	0
1	F	233/262 (88%)	0.23	12 (5%) 33 35	19, 32, 58, 126	0
1	G	233/262 (88%)	0.45	22 (9%) 14 14	18, 36, 95, 119	0
1	H	233/262 (88%)	0.28	11 (4%) 36 38	20, 33, 60, 159	0
All	All	1864/2096 (88%)	0.19	99 (5%) 32 34	16, 31, 60, 175	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	210	PRO	7.8
1	B	207	ALA	7.5
1	A	208	ALA	7.3
1	A	205	PHE	7.2
1	B	208	ALA	6.9
1	C	208	ALA	6.8
1	F	205	PHE	6.6
1	B	205	PHE	6.5
1	G	1	ALA	6.5
1	G	207	ALA	6.5
1	H	186	PRO	6.5
1	B	206	ALA	6.5
1	C	186	PRO	6.5
1	H	185	THR	6.4
1	G	205	PHE	6.4
1	A	185	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	209	THR	5.9
1	H	211	LEU	5.8
1	F	186	PRO	5.7
1	B	186	PRO	5.7
1	F	208	ALA	5.6
1	C	209	THR	5.6
1	G	209	THR	5.5
1	A	186	PRO	5.5
1	G	210	PRO	5.5
1	A	207	ALA	5.5
1	C	207	ALA	5.5
1	H	205	PHE	5.5
1	G	3	ARG	5.4
1	G	186	PRO	5.3
1	A	203	ALA	5.3
1	G	208	ALA	5.3
1	E	186	PRO	5.2
1	H	208	ALA	5.2
1	D	186	PRO	5.1
1	G	5	LEU	5.1
1	H	207	ALA	5.1
1	G	211	LEU	5.0
1	C	205	PHE	4.9
1	C	206	ALA	4.8
1	E	205	PHE	4.8
1	G	2	TYR	4.8
1	D	208	ALA	4.6
1	F	207	ALA	4.6
1	G	203	ALA	4.6
1	H	209	THR	4.5
1	D	207	ALA	4.5
1	E	203	ALA	4.5
1	D	185	THR	4.5
1	F	185	THR	4.5
1	D	203	ALA	4.4
1	G	206	ALA	4.2
1	G	4	LEU	4.2
1	D	206	ALA	4.2
1	F	203	ALA	4.2
1	B	203	ALA	4.1
1	E	206	ALA	4.1
1	H	203	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	204	LYS	3.9
1	A	1	ALA	3.9
1	C	203	ALA	3.9
1	C	185	THR	3.8
1	E	1	ALA	3.7
1	A	206	ALA	3.6
1	A	204	LYS	3.6
1	D	205	PHE	3.5
1	G	212	GLY	3.4
1	H	206	ALA	3.3
1	C	89	GLY	3.3
1	A	2	TYR	3.3
1	H	204	LYS	3.3
1	E	2	TYR	3.2
1	E	185	THR	3.2
1	C	88	SER	3.2
1	B	204	LYS	3.2
1	D	204	LYS	3.2
1	E	204	LYS	3.0
1	F	204	LYS	2.9
1	B	88	SER	2.9
1	B	185	THR	2.8
1	G	6	ASN	2.8
1	G	184	ASP	2.7
1	G	48	ALA	2.7
1	D	41	LYS	2.6
1	F	40	ARG	2.5
1	G	40	ARG	2.5
1	B	1	ALA	2.4
1	F	127	ARG	2.3
1	G	185	THR	2.3
1	C	127	ARG	2.2
1	E	40	ARG	2.2
1	F	89	GLY	2.2
1	F	79	GLY	2.1
1	C	1	ALA	2.1
1	F	206	ALA	2.1
1	C	204	LYS	2.1
1	D	38	VAL	2.1
1	G	28	ALA	2.1
1	B	40	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 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.