WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 03:07 PM EDT

PDB ID	:	4I5G
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)

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	:	2.35.1
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)	:	2.35.1

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 2.30 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		3.1%
RSRZ outliers		4.6%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
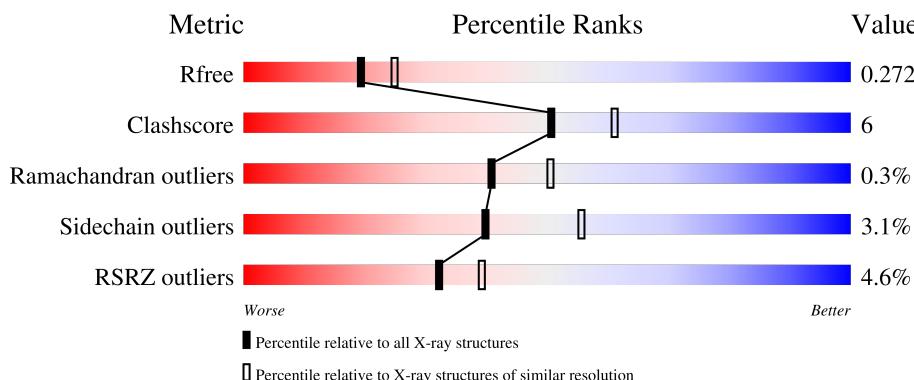
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	8% / 76% 11% · 11%
1	B	262	4% / 69% 18% · 11%
1	C	262	2% / 80% 9% 11%
1	D	262	3% / 75% 12% · 11%
1	E	262	5% / 77% 11% · 11%

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Mol	Chain	Length	Quality of chain
1	F	262	2% 81% 8% 11%
1	G	262	4% 74% 14% 11%
1	H	262	5% 77% 10% 11%
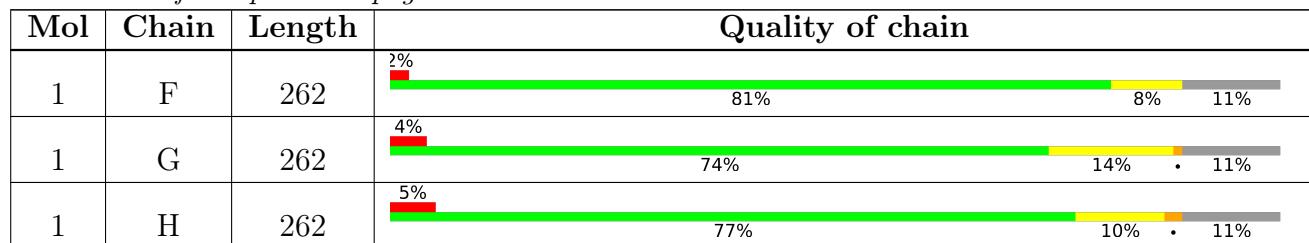
2 Entry composition ⓘ

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 Alclohol 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 51	O 51	0	0
2	B	84	Total 84	O 84	0	0
2	C	75	Total 75	O 75	0	0
2	D	85	Total 85	O 85	0	0
2	E	79	Total 79	O 79	0	0
2	F	87	Total 87	O 87	0	0
2	G	85	Total 85	O 85	0	0
2	H	87	Total 87	O 87	0	0

3 Residue-property plots ⓘ

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: Alclohol dehydrogenase/short-chain dehydrogenase
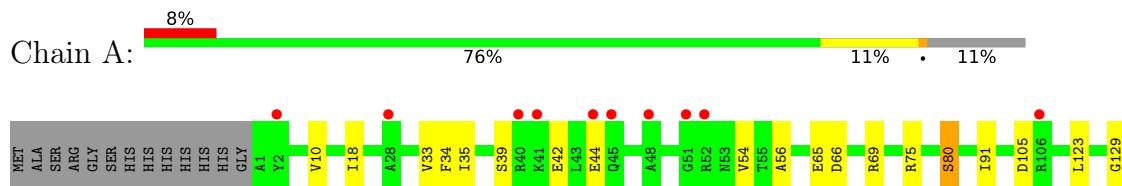
Chain A:

- Molecule 1: Alclohol dehydrogenase/short-chain dehydrogenase

Chain B:

- Molecule 1: Alclohol dehydrogenase/short-chain dehydrogenase

Chain C:

- Molecule 1: Alclohol dehydrogenase/short-chain dehydrogenase

Chain D:

Chain D residue plot (3%, 75%, 12%, 11%)

- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

Chain E:

Chain E residue plot (5%, 77%, 11%, 11%)

- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

Chain F:

Chain F residue plot (2%, 81%, 8%, 11%)

- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

Chain G:

Chain G residue plot (4%, 74%, 14%, 11%)

- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

Chain H:

Chain H residue plot (5%, 77%, 10%, 11%)
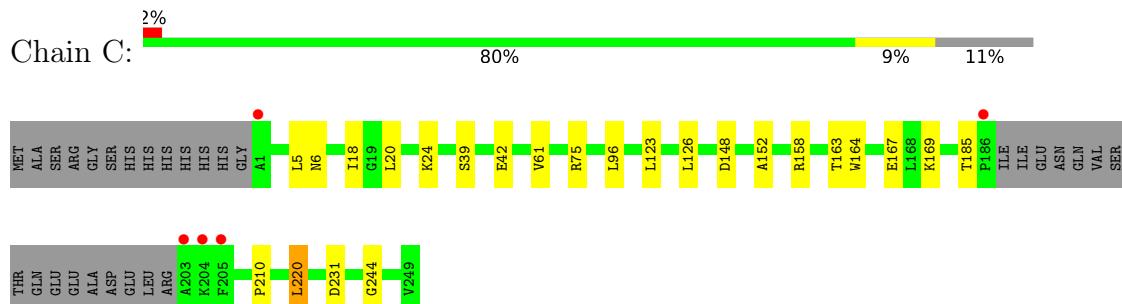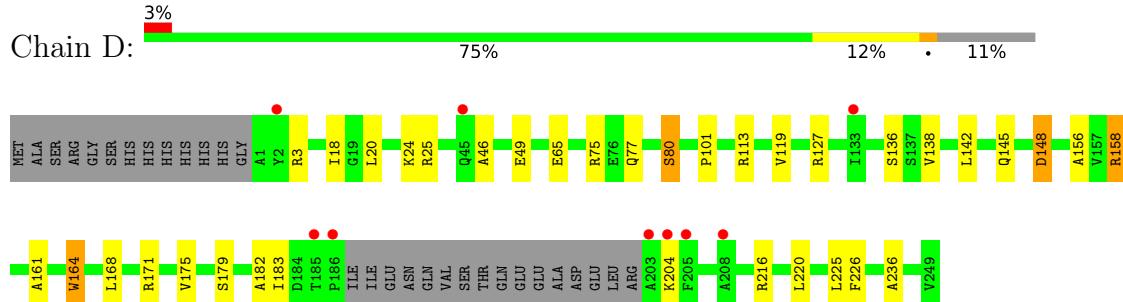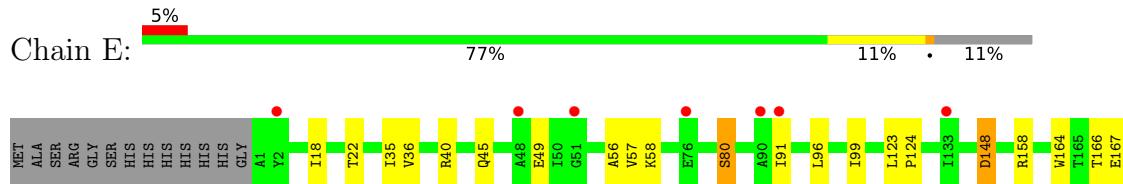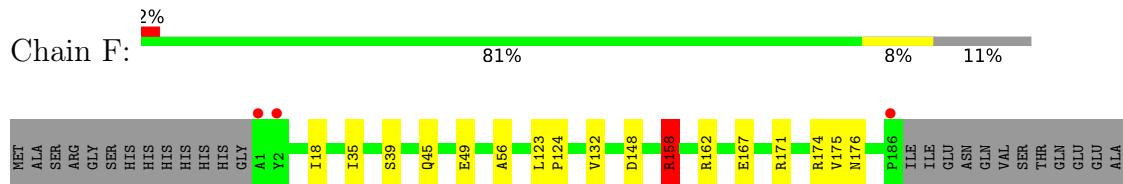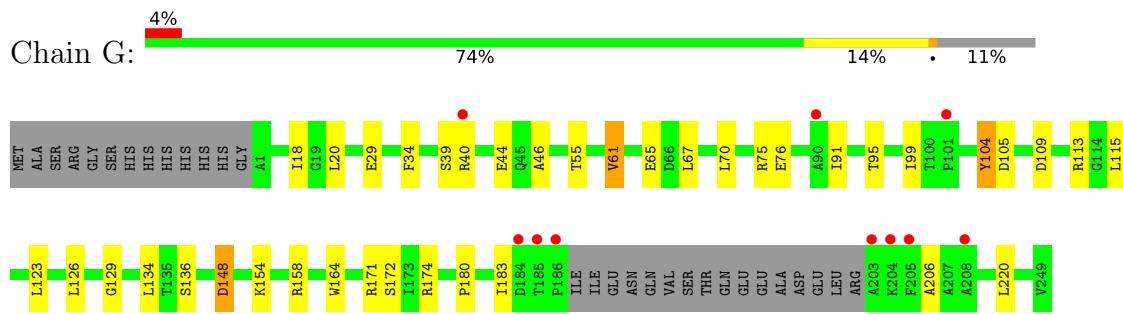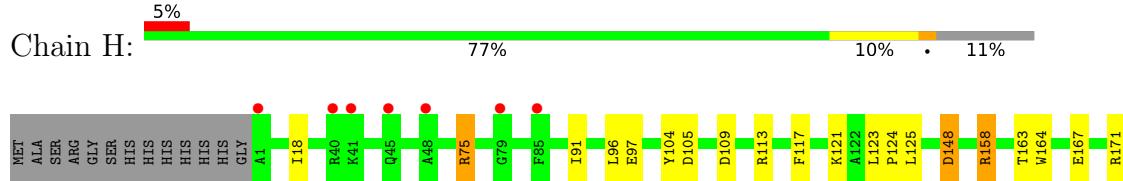
4   Data and refinement statistics   ⓘ

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 29.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-2.30) 98.1 (29.80-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.220 , 0.272 0.221 , 0.272	Depositor DCC
R_{free} test set	5542 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.5	EDS
L-test for twinning[2]	$< |L| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.89	1/1767 (0.1%)	0.92	2/2395 (0.1%)
1	B	1.09	1/1767 (0.1%)	1.08	4/2395 (0.2%)
1	C	1.07	1/1767 (0.1%)	1.00	1/2395 (0.0%)
1	D	1.04	1/1767 (0.1%)	1.07	7/2395 (0.3%)
1	E	0.96	1/1767 (0.1%)	1.02	4/2395 (0.2%)
1	F	0.98	0/1767	1.02	5/2395 (0.2%)
1	G	1.05	5/1767 (0.3%)	1.03	1/2395 (0.0%)
1	H	1.01	2/1767 (0.1%)	1.02	2/2395 (0.1%)
All	All	1.01	12/14136 (0.1%)	1.02	26/19160 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	239	GLU	CD-OE2	7.90	1.34	1.25
1	C	164	TRP	CD2-CE2	6.49	1.49	1.41
1	B	164	TRP	CD2-CE2	5.95	1.48	1.41
1	G	76	GLU	CD-OE1	5.64	1.31	1.25
1	A	164	TRP	CD2-CE2	5.54	1.48	1.41
1	G	164	TRP	CD2-CE2	5.45	1.47	1.41
1	E	164	TRP	CD2-CE2	5.44	1.47	1.41
1	D	164	TRP	CD2-CE2	5.42	1.47	1.41
1	G	104	TYR	CG-CD1	5.40	1.46	1.39
1	G	29	GLU	CG-CD	5.25	1.59	1.51
1	H	164	TRP	CD2-CE2	5.19	1.47	1.41
1	G	65	GLU	CG-CD	5.02	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	171	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	D	113	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	D	171	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	F	158	ARG	NE-CZ-NH1	-7.40	116.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	25	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	E	171	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	171	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	B	216	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	230	ASP	CB-CG-OD2	6.36	124.02	118.30
1	C	231	ASP	CB-CG-OD1	6.30	123.97	118.30
1	D	75	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	F	231	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	127	ARG	CG-CD-NE	-6.05	99.10	111.80
1	H	148	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	171	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	F	231	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	216	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	25	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	H	171	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	E	174	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	E	171	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	G	174	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	213	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	F	162	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	B	113	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	66	ASP	CB-CG-OD1	5.02	122.82	118.30

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	1745	0	1786	25	0
1	B	1745	0	1786	31	0
1	C	1745	0	1786	15	0
1	D	1745	0	1786	22	0
1	E	1745	0	1786	23	0
1	F	1745	0	1786	12	0
1	G	1745	0	1786	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	159	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 (159) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:158:ARG:HD3	1:A:158:ARG:C	2.28	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:H:218:GLU:H	1:H:218:GLU:CD	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:LEU:O	1:G:70:LEU:HB3	2.16	0.45
1:B:24:LYS:NZ	1:B:49:GLU:OE1	2.34	0.44
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:D:225:LEU:O	1:D:226:PHE:C	2.54	0.44
1:H:104:TYR:CD1	1:H:104:TYR:C	2.91	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: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: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:H:220:LEU:HD12	1:H:242:VAL:HG11	1.99	0.43
1:A:35:ILE:HG13	1:A:56:ALA:HA	2.00	0.42
1:B:98:GLU:O	1:B:99:ILE:C	2.57	0.42
1:C:167:GLU:OE2	1:D:148:ASP:OD1	2.37	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:E:45:GLN:O	1:E:49:GLU:HG3	2.19	0.42
1:A:220:LEU:HD12	1:A:242:VAL:HG11	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:158:ARG:C	1:D:158:ARG:HD3	2.42	0.40
1:E:18:ILE:CG2	1:E:220:LEU:HD23	2.51	0.40
1:H:158:ARG:C	1:H:158:ARG:HD3	2.42	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%)	12	12
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%)	17	20
1	H	229/262 (87%)	215 (94%)	14 (6%)	0	100	100
All	All	1832/2096 (87%)	1719 (94%)	108 (6%)	5 (0%)	41	50

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%)	171 (96%)	8 (4%)	27	39
1	B	179/204 (88%)	172 (96%)	7 (4%)	32	46
1	C	179/204 (88%)	174 (97%)	5 (3%)	43	60
1	D	179/204 (88%)	173 (97%)	6 (3%)	37	51
1	E	179/204 (88%)	174 (97%)	5 (3%)	43	60
1	F	179/204 (88%)	176 (98%)	3 (2%)	60	76
1	G	179/204 (88%)	174 (97%)	5 (3%)	43	60
1	H	179/204 (88%)	174 (97%)	5 (3%)	43	60
All	All	1432/1632 (88%)	1388 (97%)	44 (3%)	40	55

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	65	GLU
1	A	75	ARG
1	A	80	SER
1	A	91	ILE
1	A	148	ASP
1	A	158	ARG
1	A	205	PHE
1	B	39	SER
1	B	63	LYS
1	B	80	SER

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Mol	Chain	Res	Type
1	B	97	GLU
1	B	106	ARG
1	B	158	ARG
1	B	185	THR
1	C	75	ARG
1	C	148	ASP
1	C	158	ARG
1	C	185	THR
1	C	220	LEU
1	D	65	GLU
1	D	77	GLN
1	D	80	SER
1	D	148	ASP
1	D	158	ARG
1	D	204	LYS
1	E	80	SER
1	E	91	ILE
1	E	148	ASP
1	E	158	ARG
1	E	204	LYS
1	F	39	SER
1	F	158	ARG
1	F	204	LYS
1	G	39	SER
1	G	75	ARG
1	G	91	ILE
1	G	148	ASP
1	G	158	ARG
1	H	75	ARG
1	H	91	ILE
1	H	148	ASP
1	H	158	ARG
1	H	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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(Å²)	Q<0.9
1	A	233/262 (88%)	0.32	20 (8%)	10	14	17, 32, 83, 128	3 (1%)
1	B	233/262 (88%)	0.10	10 (4%)	35	42	14, 24, 46, 129	1 (0%)
1	C	233/262 (88%)	-0.02	5 (2%)	63	70	15, 24, 55, 105	3 (1%)
1	D	233/262 (88%)	0.06	9 (3%)	39	46	13, 24, 48, 132	3 (1%)
1	E	233/262 (88%)	0.09	14 (6%)	21	28	15, 28, 51, 126	1 (0%)
1	F	233/262 (88%)	-0.15	6 (2%)	56	63	14, 24, 44, 120	1 (0%)
1	G	233/262 (88%)	0.07	10 (4%)	35	42	15, 25, 55, 85	0
1	H	233/262 (88%)	0.17	12 (5%)	27	34	14, 27, 57, 148	1 (0%)
All	All	1864/2096 (88%)	0.08	86 (4%)	32	39	13, 26, 55, 148	13 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	205	PHE	24.1
1	A	205	PHE	19.0
1	H	205	PHE	7.2
1	G	186	PRO	6.4
1	G	185	THR	6.3
1	E	186	PRO	6.3
1	C	205	PHE	6.3
1	G	205	PHE	6.2
1	H	203	ALA	5.9
1	H	186	PRO	5.9
1	F	186	PRO	5.8
1	A	203	ALA	5.7
1	G	204	LYS	5.6
1	B	186	PRO	5.6
1	F	203	ALA	5.3
1	D	186	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	185	THR	5.0
1	D	208	ALA	4.8
1	H	185	THR	4.8
1	A	186	PRO	4.7
1	E	205	PHE	4.7
1	B	203	ALA	4.4
1	E	203	ALA	4.2
1	H	204	LYS	4.2
1	B	204	LYS	4.1
1	C	186	PRO	4.0
1	H	40	ARG	4.0
1	G	203	ALA	4.0
1	E	2	TYR	3.7
1	A	2	TYR	3.7
1	C	203	ALA	3.4
1	A	204	LYS	3.4
1	B	185	THR	3.4
1	D	203	ALA	3.3
1	G	40	ARG	3.3
1	H	1	ALA	3.3
1	A	51	GLY	3.1
1	A	48	ALA	3.0
1	C	204	LYS	3.0
1	D	204	LYS	3.0
1	E	90	ALA	2.9
1	A	208	ALA	2.9
1	H	79	GLY	2.9
1	E	48	ALA	2.8
1	F	2	TYR	2.8
1	F	205	PHE	2.8
1	G	208	ALA	2.7
1	A	185	THR	2.7
1	A	41	LYS	2.7
1	G	184	ASP	2.7
1	H	45	GLN	2.7
1	A	40	ARG	2.7
1	C	1	ALA	2.7
1	A	44	GLU	2.7
1	F	1	ALA	2.6
1	H	41	LYS	2.6
1	A	212	GLY	2.6
1	E	51	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	132	VAL	2.5
1	E	91	ILE	2.5
1	A	45	GLN	2.5
1	D	45	GLN	2.5
1	F	204	LYS	2.5
1	E	133	ILE	2.5
1	B	1	ALA	2.4
1	B	100	THR	2.4
1	B	212	GLY	2.4
1	A	28	ALA	2.4
1	B	134	LEU	2.4
1	E	185	THR	2.4
1	B	133	ILE	2.4
1	A	132	VAL	2.4
1	D	133	ILE	2.4
1	G	101	PRO	2.3
1	A	106	ARG	2.3
1	G	90	ALA	2.3
1	A	52	ARG	2.2
1	E	224	VAL	2.1
1	H	48	ALA	2.1
1	D	2	TYR	2.1
1	E	183	ILE	2.1
1	E	207	ALA	2.0
1	H	85	PHE	2.0
1	A	133	ILE	2.0
1	E	76	GLU	2.0
1	A	210	PRO	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.