



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:27 AM UTC

PDB ID : 6QAK / pdb_00006qak
Title : Structure of human ALDH9 in P21212 space group
Authors : Morera, S.; Vigouroux, A.; Kopečný, D.
Deposited on : 2018-12-19
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

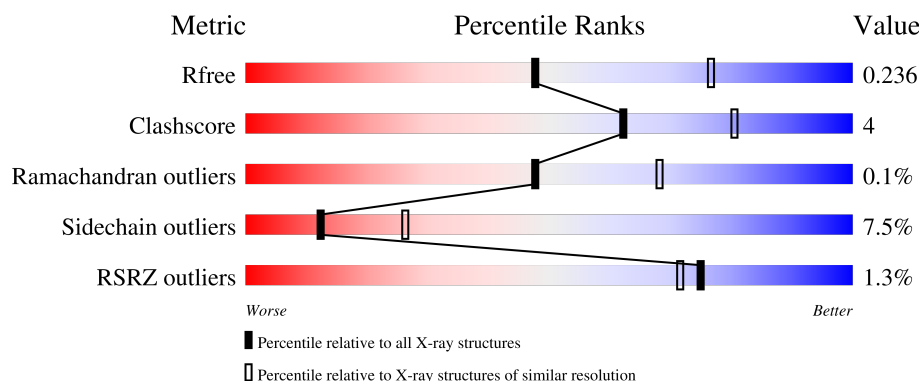
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	508	% 77% 14% • 7%
1	B	508	% 76% 16% • 7%
1	C	508	 77% 14% • 7%
1	D	508	% 77% 15% • 7%
1	E	508	3% 73% 18% • 7%

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Mol	Chain	Length	Quality of chain
1	F	508	2% 74% 17% 7%
1	G	508	1% 76% 16% 7%
1	H	508	1% 75% 15% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28938 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 4-trimethylaminobutyraldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	B	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	C	471	Total	C	N	O	S	0	2	0
			3614	2288	618	679	29			
1	D	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	E	471	Total	C	N	O	S	0	1	0
			3611	2286	618	679	28			
1	F	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	G	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	H	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P49189
A	-12	GLY	-	expression tag	UNP P49189
A	-11	SER	-	expression tag	UNP P49189
A	-10	SER	-	expression tag	UNP P49189
A	-9	HIS	-	expression tag	UNP P49189
A	-8	HIS	-	expression tag	UNP P49189
A	-7	HIS	-	expression tag	UNP P49189
A	-6	HIS	-	expression tag	UNP P49189
A	-5	HIS	-	expression tag	UNP P49189
A	-4	HIS	-	expression tag	UNP P49189
A	-3	SER	-	expression tag	UNP P49189
A	-2	GLN	-	expression tag	UNP P49189
A	-1	ASP	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP P49189
B	-13	MET	-	initiating methionine	UNP P49189
B	-12	GLY	-	expression tag	UNP P49189
B	-11	SER	-	expression tag	UNP P49189
B	-10	SER	-	expression tag	UNP P49189
B	-9	HIS	-	expression tag	UNP P49189
B	-8	HIS	-	expression tag	UNP P49189
B	-7	HIS	-	expression tag	UNP P49189
B	-6	HIS	-	expression tag	UNP P49189
B	-5	HIS	-	expression tag	UNP P49189
B	-4	HIS	-	expression tag	UNP P49189
B	-3	SER	-	expression tag	UNP P49189
B	-2	GLN	-	expression tag	UNP P49189
B	-1	ASP	-	expression tag	UNP P49189
B	0	PRO	-	expression tag	UNP P49189
C	-13	MET	-	initiating methionine	UNP P49189
C	-12	GLY	-	expression tag	UNP P49189
C	-11	SER	-	expression tag	UNP P49189
C	-10	SER	-	expression tag	UNP P49189
C	-9	HIS	-	expression tag	UNP P49189
C	-8	HIS	-	expression tag	UNP P49189
C	-7	HIS	-	expression tag	UNP P49189
C	-6	HIS	-	expression tag	UNP P49189
C	-5	HIS	-	expression tag	UNP P49189
C	-4	HIS	-	expression tag	UNP P49189
C	-3	SER	-	expression tag	UNP P49189
C	-2	GLN	-	expression tag	UNP P49189
C	-1	ASP	-	expression tag	UNP P49189
C	0	PRO	-	expression tag	UNP P49189
D	-13	MET	-	initiating methionine	UNP P49189
D	-12	GLY	-	expression tag	UNP P49189
D	-11	SER	-	expression tag	UNP P49189
D	-10	SER	-	expression tag	UNP P49189
D	-9	HIS	-	expression tag	UNP P49189
D	-8	HIS	-	expression tag	UNP P49189
D	-7	HIS	-	expression tag	UNP P49189
D	-6	HIS	-	expression tag	UNP P49189
D	-5	HIS	-	expression tag	UNP P49189
D	-4	HIS	-	expression tag	UNP P49189
D	-3	SER	-	expression tag	UNP P49189
D	-2	GLN	-	expression tag	UNP P49189
D	-1	ASP	-	expression tag	UNP P49189

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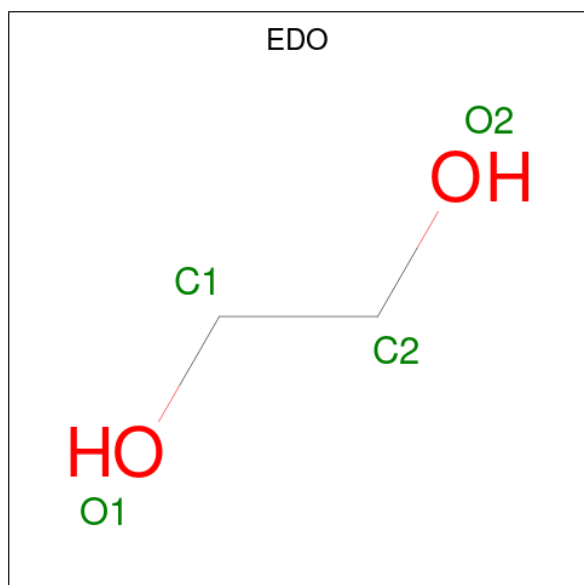
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	expression tag	UNP P49189
E	-13	MET	-	initiating methionine	UNP P49189
E	-12	GLY	-	expression tag	UNP P49189
E	-11	SER	-	expression tag	UNP P49189
E	-10	SER	-	expression tag	UNP P49189
E	-9	HIS	-	expression tag	UNP P49189
E	-8	HIS	-	expression tag	UNP P49189
E	-7	HIS	-	expression tag	UNP P49189
E	-6	HIS	-	expression tag	UNP P49189
E	-5	HIS	-	expression tag	UNP P49189
E	-4	HIS	-	expression tag	UNP P49189
E	-3	SER	-	expression tag	UNP P49189
E	-2	GLN	-	expression tag	UNP P49189
E	-1	ASP	-	expression tag	UNP P49189
E	0	PRO	-	expression tag	UNP P49189
F	-13	MET	-	initiating methionine	UNP P49189
F	-12	GLY	-	expression tag	UNP P49189
F	-11	SER	-	expression tag	UNP P49189
F	-10	SER	-	expression tag	UNP P49189
F	-9	HIS	-	expression tag	UNP P49189
F	-8	HIS	-	expression tag	UNP P49189
F	-7	HIS	-	expression tag	UNP P49189
F	-6	HIS	-	expression tag	UNP P49189
F	-5	HIS	-	expression tag	UNP P49189
F	-4	HIS	-	expression tag	UNP P49189
F	-3	SER	-	expression tag	UNP P49189
F	-2	GLN	-	expression tag	UNP P49189
F	-1	ASP	-	expression tag	UNP P49189
F	0	PRO	-	expression tag	UNP P49189
G	-13	MET	-	initiating methionine	UNP P49189
G	-12	GLY	-	expression tag	UNP P49189
G	-11	SER	-	expression tag	UNP P49189
G	-10	SER	-	expression tag	UNP P49189
G	-9	HIS	-	expression tag	UNP P49189
G	-8	HIS	-	expression tag	UNP P49189
G	-7	HIS	-	expression tag	UNP P49189
G	-6	HIS	-	expression tag	UNP P49189
G	-5	HIS	-	expression tag	UNP P49189
G	-4	HIS	-	expression tag	UNP P49189
G	-3	SER	-	expression tag	UNP P49189
G	-2	GLN	-	expression tag	UNP P49189
G	-1	ASP	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	PRO	-	expression tag	UNP P49189
H	-13	MET	-	initiating methionine	UNP P49189
H	-12	GLY	-	expression tag	UNP P49189
H	-11	SER	-	expression tag	UNP P49189
H	-10	SER	-	expression tag	UNP P49189
H	-9	HIS	-	expression tag	UNP P49189
H	-8	HIS	-	expression tag	UNP P49189
H	-7	HIS	-	expression tag	UNP P49189
H	-6	HIS	-	expression tag	UNP P49189
H	-5	HIS	-	expression tag	UNP P49189
H	-4	HIS	-	expression tag	UNP P49189
H	-3	SER	-	expression tag	UNP P49189
H	-2	GLN	-	expression tag	UNP P49189
H	-1	ASP	-	expression tag	UNP P49189
H	0	PRO	-	expression tag	UNP P49189

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		

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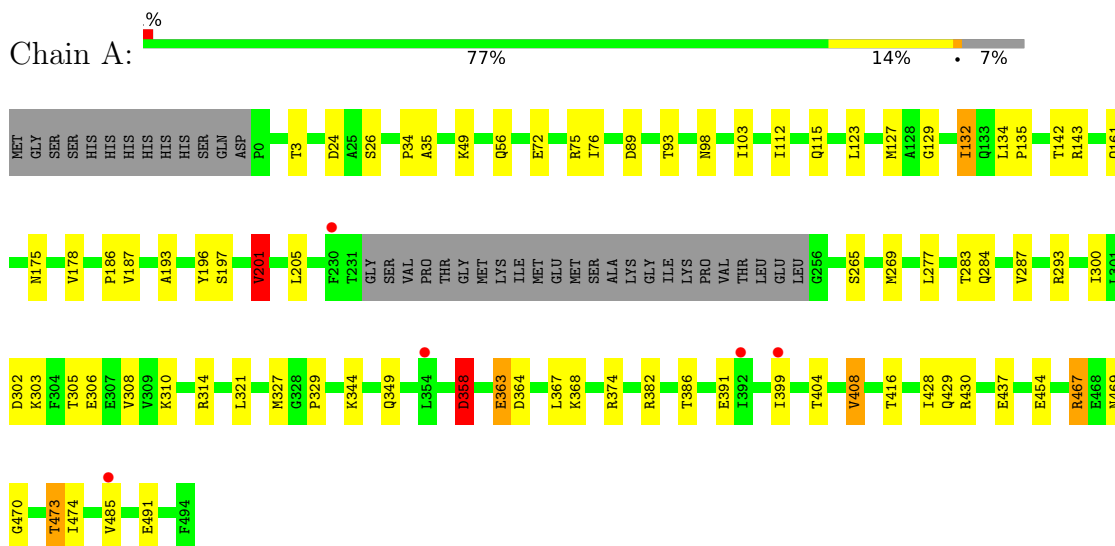
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	16	Total 16	O 16	0	0
3	C	7	Total 7	O 7	0	0
3	D	9	Total 9	O 9	0	0
3	E	5	Total 5	O 5	0	0
3	F	12	Total 12	O 12	0	0
3	G	8	Total 8	O 8	0	0
3	H	9	Total 9	O 9	0	0

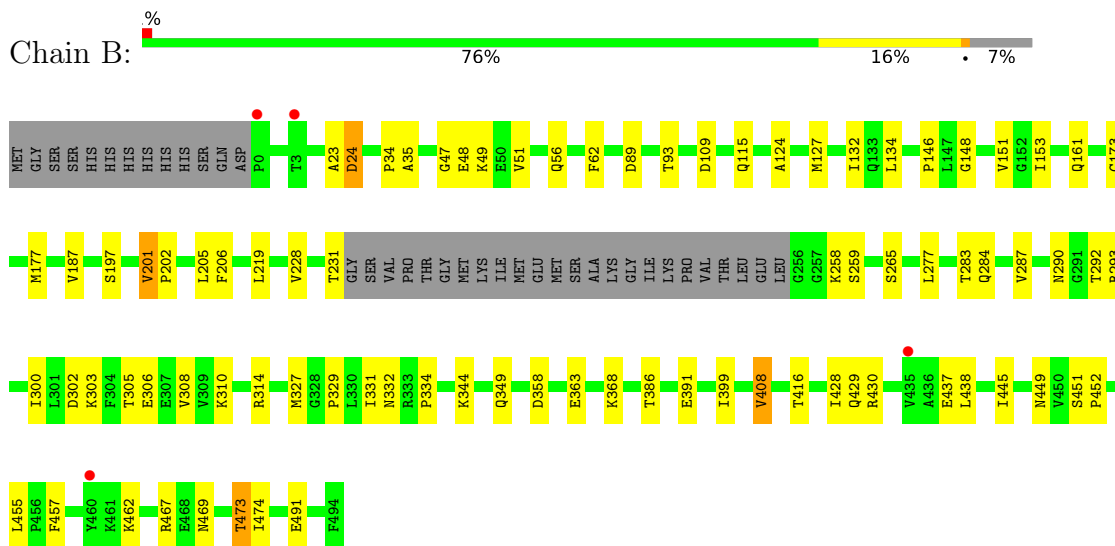
3 Residue-property plots [i](#)

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.

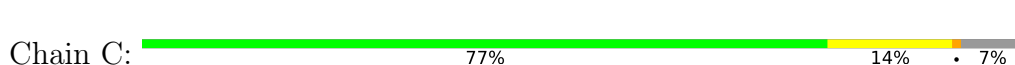
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

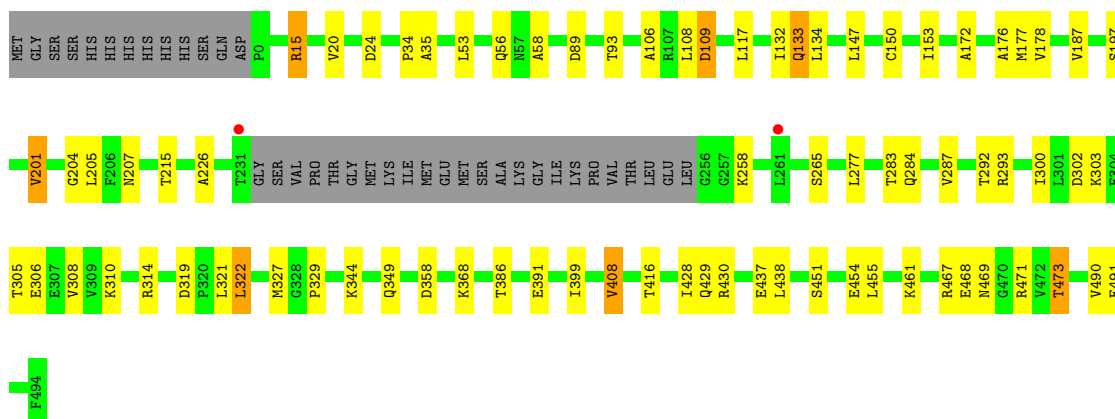


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

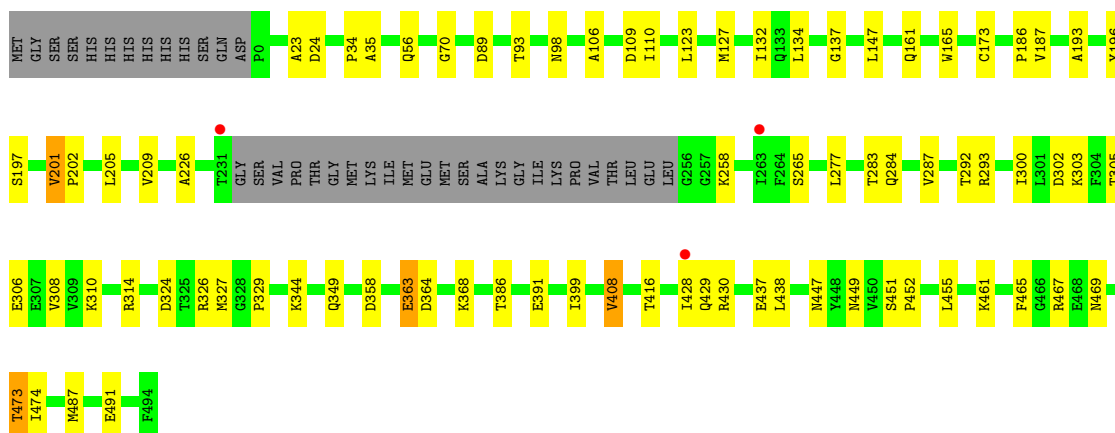
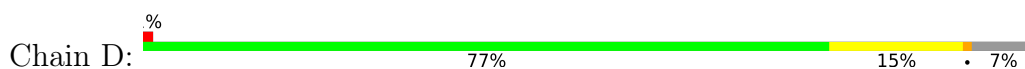


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

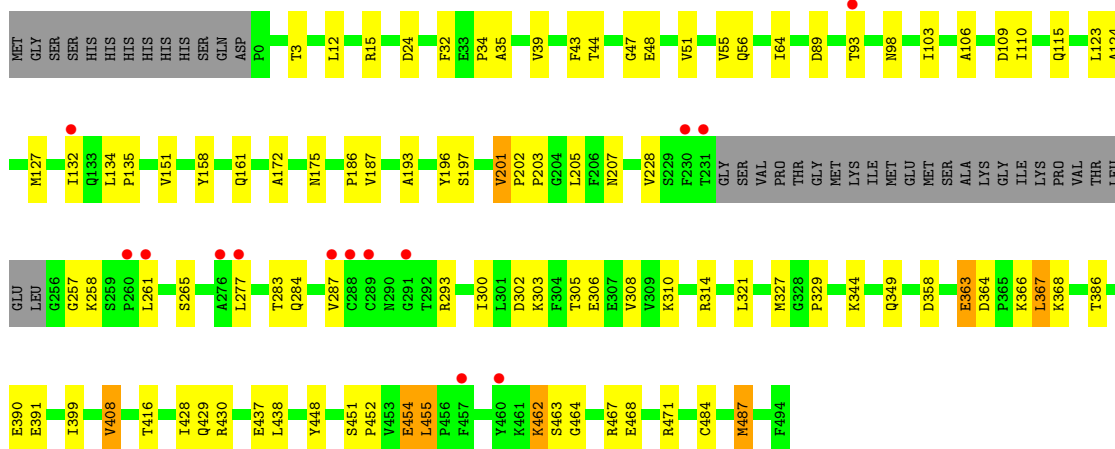
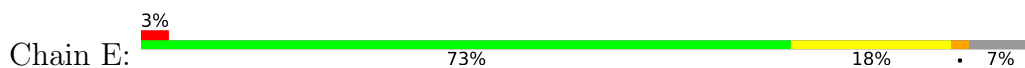




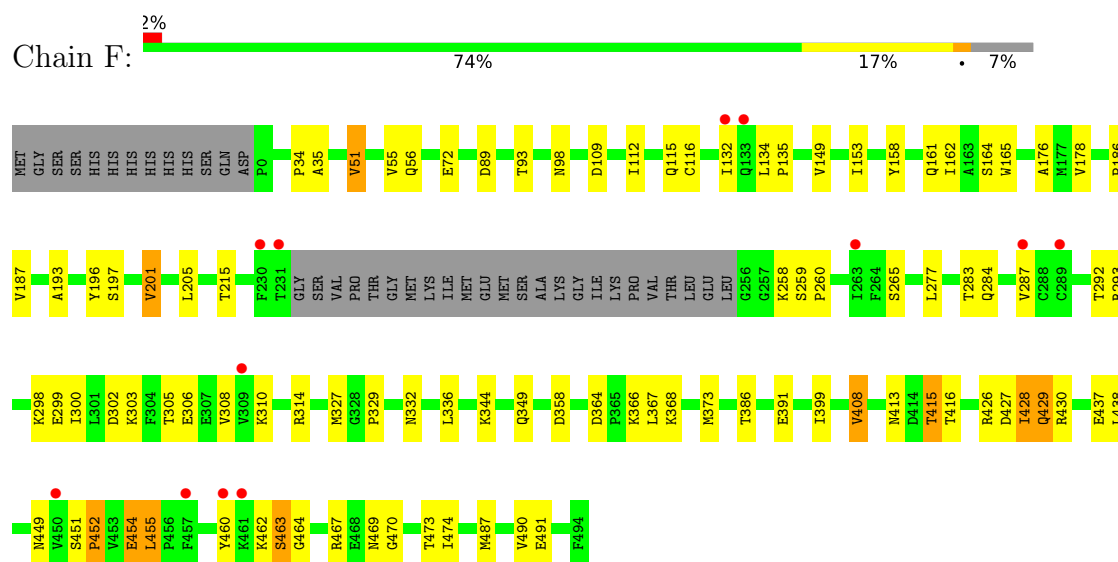
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



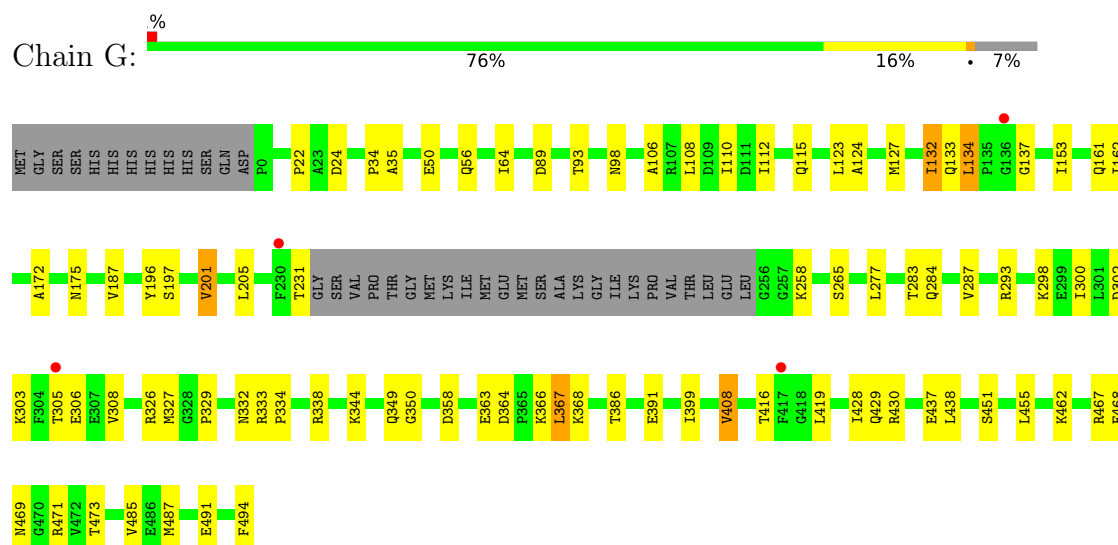
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



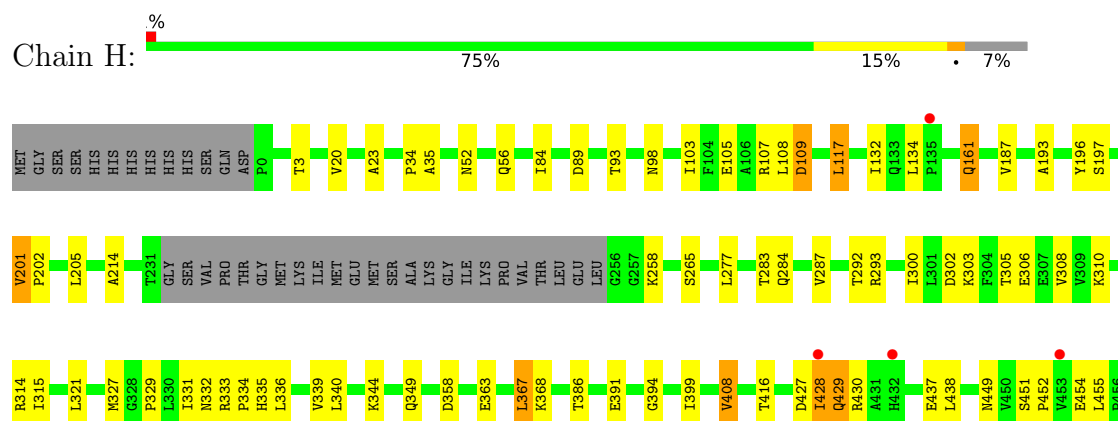
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

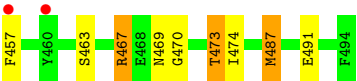


• Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



• Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	160.38Å 159.59Å 160.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.90 – 2.50 35.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.90-2.50) 99.9 (35.90-2.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.191 , 0.220 0.206 , 0.236	Depositor DCC
R_{free} test set	7140 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h 0.000 for -h,-l,-k 0.000 for k,h,-l 0.000 for l,h,k 0.000 for k,l,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28938	wwPDB-VP
Average B, all atoms (Å ²)	80.0	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 36.70 % 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 4.8021e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0.87	1/3676 (0.0%)	1.38	22/4971 (0.4%)
1	B	0.88	0/3676	1.37	15/4971 (0.3%)
1	C	0.86	0/3693	1.39	18/4994 (0.4%)
1	D	0.84	0/3676	1.37	24/4971 (0.5%)
1	E	0.84	0/3687	1.40	32/4986 (0.6%)
1	F	0.86	2/3676 (0.1%)	1.40	34/4971 (0.7%)
1	G	0.87	0/3676	1.39	22/4971 (0.4%)
1	H	0.86	0/3676	1.41	29/4971 (0.6%)
All	All	0.86	3/29436 (0.0%)	1.39	196/39806 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	VAL	CA-C	5.65	1.58	1.52
1	F	428	ILE	CA-CB	5.37	1.59	1.54
1	F	153	ILE	CG1-CD1	-5.14	1.31	1.51

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	427	ASP	CA-C-N	8.75	132.23	120.77
1	F	427	ASP	C-N-CA	8.75	132.23	120.77
1	G	187	VAL	N-CA-C	8.13	118.06	110.42
1	B	187	VAL	N-CA-C	8.11	118.05	110.42
1	H	187	VAL	N-CA-C	8.03	117.97	110.42
1	G	24	ASP	CA-CB-CG	7.95	120.55	112.60
1	H	109	ASP	CA-CB-CG	7.86	120.46	112.60
1	D	187	VAL	N-CA-C	7.80	117.87	110.30
1	E	187	VAL	N-CA-C	7.77	117.73	110.42
1	G	358	ASP	CA-CB-CG	7.71	120.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	115	GLN	CA-C-N	7.50	130.34	120.28
1	G	115	GLN	C-N-CA	7.50	130.34	120.28
1	F	187	VAL	N-CA-C	7.32	117.30	110.42
1	E	464	GLY	N-CA-C	-7.29	103.66	112.48
1	H	427	ASP	CA-C-N	7.20	129.70	120.70
1	H	427	ASP	C-N-CA	7.20	129.70	120.70
1	E	257	GLY	CA-C-N	7.05	132.78	120.87
1	E	257	GLY	C-N-CA	7.05	132.78	120.87
1	G	408	VAL	N-CA-CB	7.01	118.75	110.55
1	A	187	VAL	N-CA-C	6.80	116.81	110.42
1	C	358	ASP	CA-CB-CG	6.80	119.40	112.60
1	F	428	ILE	CA-C-N	6.75	129.32	120.28
1	F	428	ILE	C-N-CA	6.75	129.32	120.28
1	C	24	ASP	CA-CB-CG	6.73	119.33	112.60
1	D	364	ASP	CA-CB-CG	6.71	119.31	112.60
1	G	172	ALA	CA-C-N	6.66	129.87	120.28
1	G	172	ALA	C-N-CA	6.66	129.87	120.28
1	C	187	VAL	N-CA-C	6.64	116.66	110.42
1	E	64	ILE	CA-C-N	6.62	129.04	120.44
1	E	64	ILE	C-N-CA	6.62	129.04	120.44
1	D	408	VAL	N-CA-CB	6.59	118.26	110.55
1	B	408	VAL	N-CA-CB	6.56	118.23	110.55
1	A	115	GLN	CA-C-N	6.52	129.02	120.28
1	A	115	GLN	C-N-CA	6.52	129.02	120.28
1	D	358	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	408	VAL	N-CA-CB	6.51	118.16	110.55
1	F	463	SER	CA-C-N	6.51	131.60	121.32
1	F	463	SER	C-N-CA	6.51	131.60	121.32
1	F	413	ASN	CA-CB-CG	6.50	119.10	112.60
1	F	358	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	358	ASP	CA-CB-CG	6.49	119.09	112.60
1	H	103	ILE	CA-C-N	6.48	129.29	120.54
1	H	103	ILE	C-N-CA	6.48	129.29	120.54
1	C	408	VAL	N-CA-CB	6.46	118.11	110.55
1	E	115	GLN	CA-C-N	6.43	128.81	120.44
1	E	115	GLN	C-N-CA	6.43	128.81	120.44
1	B	197	SER	CA-C-N	6.40	128.86	120.28
1	B	197	SER	C-N-CA	6.40	128.86	120.28
1	E	358	ASP	CA-CB-CG	6.38	118.98	112.60
1	F	408	VAL	N-CA-CB	6.36	117.99	110.55
1	E	197	SER	CA-C-N	6.36	128.80	120.28
1	E	197	SER	C-N-CA	6.36	128.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	408	VAL	N-CA-CB	6.33	117.96	110.55
1	H	358	ASP	CA-CB-CG	6.32	118.92	112.60
1	E	408	VAL	N-CA-CB	6.31	117.94	110.55
1	D	109	ASP	CA-CB-CG	6.29	118.89	112.60
1	G	175	ASN	CA-CB-CG	6.23	118.83	112.60
1	F	197	SER	CA-C-N	6.20	128.58	120.28
1	F	197	SER	C-N-CA	6.20	128.58	120.28
1	C	197	SER	CA-C-N	6.14	128.51	120.28
1	C	197	SER	C-N-CA	6.14	128.51	120.28
1	B	109	ASP	CA-CB-CG	6.12	118.72	112.60
1	D	197	SER	CA-C-N	6.10	128.45	120.28
1	D	197	SER	C-N-CA	6.10	128.45	120.28
1	D	186	PRO	CA-C-N	6.09	128.32	120.70
1	D	186	PRO	C-N-CA	6.09	128.32	120.70
1	D	209	VAL	N-CA-CB	6.07	119.53	111.64
1	A	358	ASP	CA-CB-CG	6.02	118.62	112.60
1	E	172	ALA	CA-C-N	5.94	128.51	120.44
1	E	172	ALA	C-N-CA	5.94	128.51	120.44
1	A	197	SER	CA-C-N	5.85	128.12	120.28
1	A	197	SER	C-N-CA	5.85	128.12	120.28
1	F	115	GLN	CA-C-N	5.84	128.04	120.44
1	F	115	GLN	C-N-CA	5.84	128.04	120.44
1	A	193	ALA	CA-C-N	5.83	128.09	120.28
1	A	193	ALA	C-N-CA	5.83	128.09	120.28
1	E	462	LYS	CA-C-N	5.81	132.64	121.54
1	E	462	LYS	C-N-CA	5.81	132.64	121.54
1	E	98	ASN	CA-CB-CG	5.79	118.39	112.60
1	G	64	ILE	CA-C-N	5.79	127.96	120.44
1	G	64	ILE	C-N-CA	5.79	127.96	120.44
1	D	98	ASN	CA-CB-CG	5.78	118.38	112.60
1	H	331	ILE	N-CA-C	5.75	116.48	110.62
1	G	108	LEU	CA-C-N	5.73	128.43	120.29
1	G	108	LEU	C-N-CA	5.73	128.43	120.29
1	F	491	GLU	CB-CG-CD	5.71	122.31	112.60
1	F	176	ALA	N-CA-C	-5.70	101.59	110.42
1	F	109	ASP	CA-CB-CG	5.69	118.29	112.60
1	G	419	LEU	CD1-CG-CD2	5.69	123.31	110.80
1	G	112	ILE	CA-C-N	5.68	127.83	120.44
1	G	112	ILE	C-N-CA	5.68	127.83	120.44
1	F	460	TYR	CA-C-N	5.68	128.68	120.79
1	F	460	TYR	C-N-CA	5.68	128.68	120.79
1	E	47	GLY	CA-C-N	5.66	127.86	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	GLY	C-N-CA	5.66	127.86	120.28
1	F	464	GLY	N-CA-C	-5.64	103.58	111.09
1	E	103	ILE	CA-C-N	5.64	128.63	120.79
1	E	103	ILE	C-N-CA	5.64	128.63	120.79
1	B	429	GLN	CA-C-N	5.63	127.76	120.44
1	B	429	GLN	C-N-CA	5.63	127.76	120.44
1	E	429	GLN	CA-C-N	5.62	127.75	120.44
1	E	429	GLN	C-N-CA	5.62	127.75	120.44
1	H	197	SER	CA-C-N	5.57	127.75	120.28
1	H	197	SER	C-N-CA	5.57	127.75	120.28
1	G	197	SER	CA-C-N	5.55	127.72	120.28
1	G	197	SER	C-N-CA	5.55	127.72	120.28
1	D	429	GLN	CA-C-N	5.55	127.65	120.44
1	D	429	GLN	C-N-CA	5.55	127.65	120.44
1	C	429	GLN	CA-C-N	5.49	127.57	120.44
1	C	429	GLN	C-N-CA	5.49	127.57	120.44
1	F	98	ASN	CA-CB-CG	5.47	118.07	112.60
1	G	429	GLN	CA-C-N	5.45	127.52	120.44
1	G	429	GLN	C-N-CA	5.45	127.52	120.44
1	A	103	ILE	CA-C-N	5.44	127.88	120.54
1	A	103	ILE	C-N-CA	5.44	127.88	120.54
1	F	178	VAL	N-CA-CB	5.41	117.53	111.21
1	G	98	ASN	CA-CB-CG	5.40	118.00	112.60
1	F	186	PRO	CA-C-N	5.39	127.29	120.72
1	F	186	PRO	C-N-CA	5.39	127.29	120.72
1	H	193	ALA	CA-C-N	5.38	127.50	120.28
1	H	193	ALA	C-N-CA	5.38	127.50	120.28
1	C	172	ALA	CA-C-N	5.38	128.49	120.31
1	C	172	ALA	C-N-CA	5.38	128.49	120.31
1	B	115	GLN	CA-C-N	5.37	127.79	120.54
1	B	115	GLN	C-N-CA	5.37	127.79	120.54
1	F	193	ALA	CA-C-N	5.37	127.47	120.28
1	F	193	ALA	C-N-CA	5.37	127.47	120.28
1	D	24	ASP	CA-CB-CG	5.33	117.93	112.60
1	E	109	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	429	GLN	CA-C-N	5.30	127.34	120.44
1	A	429	GLN	C-N-CA	5.30	127.34	120.44
1	E	24	ASP	CA-CB-CG	5.29	117.89	112.60
1	H	333	ARG	N-CA-C	-5.29	105.26	112.35
1	H	107	ARG	CA-C-N	5.29	127.31	120.44
1	H	107	ARG	C-N-CA	5.29	127.31	120.44
1	F	454	GLU	CB-CG-CD	5.27	121.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	ALA	CA-C-N	5.26	127.33	120.28
1	D	193	ALA	C-N-CA	5.26	127.33	120.28
1	F	332	ASN	CA-CB-CG	5.25	117.85	112.60
1	E	48	GLU	CA-C-N	5.24	127.73	120.29
1	E	48	GLU	C-N-CA	5.24	127.73	120.29
1	C	109	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	98	ASN	CA-CB-CG	5.23	117.83	112.60
1	H	98	ASN	CA-CB-CG	5.22	117.83	112.60
1	C	178	VAL	N-CA-CB	5.21	117.31	111.21
1	H	23	ALA	CA-C-N	5.20	130.74	122.62
1	H	23	ALA	C-N-CA	5.20	130.74	122.62
1	B	452	PRO	CA-C-N	5.20	127.86	120.53
1	B	452	PRO	C-N-CA	5.20	127.86	120.53
1	F	215	THR	CA-C-N	5.20	125.71	119.94
1	F	215	THR	C-N-CA	5.20	125.71	119.94
1	A	175	ASN	CA-CB-CG	5.19	117.79	112.60
1	G	333	ARG	N-CA-C	-5.18	105.70	112.75
1	D	23	ALA	CA-C-N	5.18	130.71	122.62
1	D	23	ALA	C-N-CA	5.18	130.71	122.62
1	A	186	PRO	CA-C-N	5.17	127.03	120.72
1	A	186	PRO	C-N-CA	5.17	127.03	120.72
1	H	214	ALA	CA-C-N	5.17	127.21	120.28
1	H	214	ALA	C-N-CA	5.17	127.21	120.28
1	H	340	LEU	CA-C-N	5.14	125.69	119.98
1	H	340	LEU	C-N-CA	5.14	125.69	119.98
1	F	452	PRO	CA-C-N	5.13	127.21	120.60
1	F	452	PRO	C-N-CA	5.13	127.21	120.60
1	C	215	THR	CA-C-N	5.12	125.62	119.94
1	C	215	THR	C-N-CA	5.12	125.62	119.94
1	H	452	PRO	CA-C-N	5.11	127.74	120.53
1	H	452	PRO	C-N-CA	5.11	127.74	120.53
1	D	70	GLY	CA-C-N	5.10	127.54	120.29
1	D	70	GLY	C-N-CA	5.10	127.54	120.29
1	A	404	THR	CA-C-N	5.09	127.09	120.28
1	A	404	THR	C-N-CA	5.09	127.09	120.28
1	E	175	ASN	CA-CB-CG	5.08	117.68	112.60
1	C	461	LYS	CA-C-N	5.08	131.24	121.54
1	C	461	LYS	C-N-CA	5.08	131.24	121.54
1	E	186	PRO	CA-C-N	5.07	126.90	120.72
1	E	186	PRO	C-N-CA	5.07	126.90	120.72
1	H	429	GLN	CA-C-N	5.07	127.02	120.44
1	H	429	GLN	C-N-CA	5.07	127.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	VAL	N-CA-CB	5.05	117.12	111.21
1	H	428	ILE	CA-C-N	5.05	127.01	120.44
1	H	428	ILE	C-N-CA	5.05	127.01	120.44
1	F	429	GLN	CA-C-N	5.05	127.00	120.44
1	F	429	GLN	C-N-CA	5.05	127.00	120.44
1	E	193	ALA	CA-C-N	5.05	127.04	120.28
1	E	193	ALA	C-N-CA	5.05	127.04	120.28
1	A	112	ILE	CA-C-N	5.04	127.30	120.44
1	A	112	ILE	C-N-CA	5.04	127.30	120.44
1	B	48	GLU	CA-C-N	5.04	126.99	120.44
1	B	48	GLU	C-N-CA	5.04	126.99	120.44
1	C	108	LEU	CA-C-N	5.04	127.44	120.29
1	C	108	LEU	C-N-CA	5.04	127.44	120.29
1	B	331	ILE	N-CA-C	5.03	115.75	110.62
1	D	363	GLU	CB-CG-CD	5.02	121.13	112.60
1	D	452	PRO	CA-C-N	5.01	127.60	120.53
1	D	452	PRO	C-N-CA	5.01	127.60	120.53
1	D	324	ASP	CA-CB-CG	5.01	117.61	112.60

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	3604	0	3577	31	0
1	B	3604	0	3577	29	0
1	C	3614	0	3589	29	0
1	D	3604	0	3577	26	0
1	E	3611	0	3584	42	0
1	F	3604	0	3577	37	0
1	G	3604	0	3577	35	0
1	H	3604	0	3577	35	0
2	B	4	0	6	0	0
3	A	19	0	0	0	0
3	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	7	0	0	0	0
3	D	9	0	0	0	0
3	E	5	0	0	0	0
3	F	12	0	0	0	0
3	G	8	0	0	1	0
3	H	9	0	0	0	0
All	All	28938	0	28641	238	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 (238) 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:332:ASN:HB3	1:B:334:PRO:HD2	1.63	0.80
1:F:452:PRO:HD2	1:F:455:LEU:HD11	1.62	0.80
1:A:143:ARG:HD2	1:C:133:GLN:HG3	1.69	0.71
1:E:462:LYS:HB2	1:F:135:PRO:HD3	1.73	0.71
1:E:451:SER:HB2	1:E:455:LEU:HD11	1.72	0.70
1:E:467:ARG:HE	1:G:467:ARG:HH22	1.39	0.69
1:F:428:ILE:HB	1:H:428:ILE:HB	1.74	0.68
1:A:467:ARG:HH21	1:C:467:ARG:HH12	1.42	0.68
1:A:364:ASP:HB3	1:A:367:LEU:HD12	1.76	0.67
1:E:258:LYS:HE3	1:E:390:GLU:O	1.95	0.66
1:C:284:GLN:HA	1:C:327:MET:HE2	1.76	0.66
1:F:284:GLN:HA	1:F:327:MET:HE2	1.77	0.65
1:G:284:GLN:HA	1:G:327:MET:HE2	1.78	0.65
1:G:162:ILE:CD1	1:G:231:THR:HG21	2.26	0.65
1:B:284:GLN:HA	1:B:327:MET:HE2	1.79	0.65
1:F:469:ASN:O	1:F:473:THR:HG23	1.97	0.64
1:E:284:GLN:HA	1:E:327:MET:HE2	1.78	0.64
1:E:452:PRO:HB2	1:E:454:GLU:OE1	1.98	0.64
1:E:428:ILE:HG22	1:H:487:MET:SD	2.38	0.63
1:H:284:GLN:HA	1:H:327:MET:HE2	1.80	0.63
1:A:469:ASN:O	1:A:473:THR:HG23	1.98	0.63
1:A:284:GLN:HA	1:A:327:MET:HE2	1.80	0.62
1:D:201:VAL:HG13	1:D:205:LEU:HB3	1.80	0.62
1:C:469:ASN:O	1:C:473:THR:HG23	2.00	0.62
1:D:284:GLN:HA	1:D:327:MET:HE2	1.81	0.61
1:H:105:GLU:HA	1:H:108:LEU:HD12	1.82	0.61
1:G:162:ILE:HD11	1:G:231:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:ASN:O	1:H:56:GLN:HG2	2.01	0.61
1:B:469:ASN:O	1:B:473:THR:HG23	2.01	0.61
1:E:364:ASP:HB3	1:E:367:LEU:HD22	1.81	0.60
1:D:89:ASP:O	1:D:93:THR:HG23	2.02	0.60
1:G:469:ASN:O	1:G:473:THR:HG23	2.02	0.59
1:A:89:ASP:O	1:A:93:THR:HG23	2.03	0.59
1:C:89:ASP:O	1:C:93:THR:HG23	2.02	0.59
1:F:89:ASP:O	1:F:93:THR:HG23	2.04	0.58
1:H:89:ASP:O	1:H:93:THR:HG23	2.03	0.57
1:G:364:ASP:HB3	1:G:367:LEU:HD22	1.86	0.57
1:E:34:PRO:HB2	1:E:329:PRO:HG2	1.85	0.57
1:G:332:ASN:HB3	1:G:334:PRO:HD2	1.86	0.57
1:B:173:CYS:SG	1:B:474:ILE:HD12	2.45	0.56
1:E:468:GLU:HG3	1:E:471:ARG:NH2	2.21	0.56
1:H:469:ASN:O	1:H:473:THR:HG23	2.04	0.56
1:E:89:ASP:O	1:E:93:THR:HG23	2.06	0.56
1:F:428:ILE:HG23	1:F:429:GLN:H	1.71	0.56
1:E:201:VAL:HG13	1:E:205:LEU:HB3	1.88	0.55
1:G:89:ASP:O	1:G:93:THR:HG23	2.05	0.55
1:B:89:ASP:O	1:B:93:THR:HG23	2.07	0.55
1:D:201:VAL:HG22	1:D:205:LEU:HD23	1.89	0.55
1:F:201:VAL:HG13	1:F:205:LEU:HB3	1.87	0.55
1:A:24:ASP:HB2	1:A:49:LYS:HB2	1.87	0.55
1:A:467:ARG:HH21	1:C:467:ARG:NH1	2.03	0.55
1:A:467:ARG:HE	1:C:467:ARG:HH22	1.53	0.55
1:E:462:LYS:HD2	1:F:135:PRO:HB3	1.89	0.55
1:F:452:PRO:HB2	1:F:454:GLU:OE2	2.06	0.55
1:B:34:PRO:HB2	1:B:329:PRO:HG2	1.88	0.55
1:C:34:PRO:HB2	1:C:329:PRO:HG2	1.89	0.54
1:D:34:PRO:HB2	1:D:329:PRO:HG2	1.88	0.54
1:F:34:PRO:HB2	1:F:329:PRO:HG2	1.89	0.54
1:G:494:PHE:CD1	1:H:315:ILE:HG12	2.43	0.54
1:E:467:ARG:HE	1:G:467:ARG:NH2	2.04	0.54
1:D:202:PRO:HD2	1:D:205:LEU:HD22	1.90	0.53
1:G:35:ALA:HA	1:G:329:PRO:HG3	1.90	0.53
1:B:35:ALA:HA	1:B:329:PRO:HG3	1.90	0.53
1:F:364:ASP:HB3	1:F:367:LEU:HD22	1.91	0.53
1:H:35:ALA:HA	1:H:329:PRO:HG3	1.90	0.53
1:D:469:ASN:O	1:D:473:THR:HG23	2.09	0.53
1:F:366:LYS:HG3	1:F:367:LEU:HD13	1.90	0.52
1:F:35:ALA:HA	1:F:329:PRO:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:485:VAL:HG12	1:G:487:MET:HE2	1.90	0.52
1:A:35:ALA:HA	1:A:329:PRO:HG3	1.91	0.52
1:A:201:VAL:HG13	1:A:205:LEU:HB3	1.90	0.52
1:E:35:ALA:HA	1:E:329:PRO:HG3	1.90	0.52
1:G:134:LEU:HD12	1:H:463:SER:HA	1.91	0.52
1:H:196:TYR:O	1:H:201:VAL:HB	2.09	0.52
1:E:467:ARG:HH21	1:G:467:ARG:HH12	1.58	0.52
1:H:3:THR:OG1	1:H:321:LEU:HD13	2.10	0.52
1:H:34:PRO:HB2	1:H:329:PRO:HG2	1.91	0.52
1:A:75:ARG:HH11	1:A:76:ILE:HD13	1.75	0.52
1:B:151:VAL:HB	1:B:228:VAL:HG22	1.91	0.52
1:C:35:ALA:HA	1:C:329:PRO:HG3	1.91	0.52
1:E:12:LEU:HD12	1:E:43:PHE:HB3	1.91	0.52
1:D:35:ALA:HA	1:D:329:PRO:HG3	1.91	0.51
1:F:165:TRP:CD1	1:F:454:GLU:HG3	2.45	0.51
1:B:451:SER:HB2	1:B:455:LEU:HD12	1.92	0.51
1:F:258:LYS:HE2	1:F:292:THR:OG1	2.10	0.51
1:E:135:PRO:HD3	1:F:462:LYS:O	2.11	0.51
1:D:258:LYS:HE2	1:D:292:THR:OG1	2.10	0.51
1:E:32:PHE:CE1	1:E:39:VAL:HG22	2.46	0.51
1:D:305:THR:HG22	1:D:399:ILE:HD13	1.93	0.50
1:A:382:ARG:NH1	1:G:350:GLY:HA3	2.25	0.50
1:G:34:PRO:HB2	1:G:329:PRO:HG2	1.93	0.50
1:H:332:ASN:HB3	1:H:334:PRO:HD2	1.92	0.50
1:C:451:SER:HB2	1:C:455:LEU:HD12	1.93	0.50
1:A:135:PRO:HG3	1:B:462:LYS:HD2	1.94	0.50
1:E:310:LYS:HE2	1:E:314:ARG:HH22	1.77	0.50
1:A:305:THR:HG22	1:A:399:ILE:HD13	1.94	0.49
1:E:202:PRO:HD2	1:E:205:LEU:HD22	1.95	0.49
1:A:265:SER:HA	1:A:300:ILE:HG12	1.95	0.49
1:B:310:LYS:HE2	1:B:314:ARG:HH22	1.77	0.49
1:D:106:ALA:O	1:D:110:ILE:HG12	2.12	0.49
1:D:310:LYS:HE2	1:D:314:ARG:HH22	1.78	0.49
1:B:349:GLN:HE22	1:B:386:THR:HG23	1.78	0.49
1:B:124:ALA:HA	1:B:127:MET:HE2	1.95	0.49
1:E:158:TYR:CE2	1:E:452:PRO:HG3	2.48	0.49
1:G:265:SER:HA	1:G:300:ILE:HG12	1.95	0.49
1:B:305:THR:HG22	1:B:399:ILE:HD13	1.95	0.48
1:B:23:ALA:HB1	1:B:49:LYS:HE2	1.93	0.48
1:A:358:ASP:OD1	1:A:374:ARG:HD2	2.13	0.48
1:H:451:SER:HB2	1:H:455:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PRO:HB2	1:A:329:PRO:HG2	1.94	0.48
1:D:265:SER:HA	1:D:300:ILE:HG12	1.96	0.48
1:C:319:ASP:HB3	1:C:322:LEU:HD22	1.96	0.48
1:F:310:LYS:HE2	1:F:314:ARG:HH22	1.79	0.48
1:B:201:VAL:HG13	1:B:205:LEU:HB3	1.95	0.48
1:D:137:GLY:O	1:D:487:MET:HG3	2.14	0.47
1:E:124:ALA:HA	1:E:127:MET:HE2	1.96	0.47
1:G:305:THR:HG22	1:G:399:ILE:HD13	1.96	0.47
1:E:305:THR:HG22	1:E:399:ILE:HD13	1.95	0.47
1:F:260:PRO:HD3	1:F:415:THR:HG21	1.97	0.47
1:C:305:THR:HG22	1:C:399:ILE:HD13	1.95	0.47
1:D:173:CYS:SG	1:D:474:ILE:HD12	2.54	0.47
1:H:305:THR:HG22	1:H:399:ILE:HD13	1.97	0.47
1:H:310:LYS:HE2	1:H:314:ARG:HH22	1.78	0.47
1:B:24:ASP:HB3	1:B:47:GLY:HA3	1.97	0.47
1:B:265:SER:HA	1:B:300:ILE:HG12	1.97	0.47
1:C:490:VAL:HG12	1:D:447:ASN:OD1	2.14	0.47
1:G:201:VAL:HG13	1:G:205:LEU:HB3	1.96	0.47
1:A:310:LYS:HE2	1:A:314:ARG:HH22	1.79	0.47
1:G:137:GLY:O	1:G:487:MET:HG3	2.15	0.47
1:C:310:LYS:HE2	1:C:314:ARG:HH22	1.80	0.46
1:H:109:ASP:HB2	1:H:161:GLN:HB2	1.96	0.46
1:B:258:LYS:HE2	1:B:292:THR:OG1	2.15	0.46
1:E:265:SER:HA	1:E:300:ILE:HG12	1.96	0.46
1:F:298:LYS:HG3	1:F:299:GLU:OE1	2.16	0.46
1:G:468:GLU:HG3	1:G:471:ARG:NH2	2.31	0.46
1:C:265:SER:HA	1:C:300:ILE:HG12	1.97	0.46
1:C:106:ALA:O	1:C:109:ASP:HB2	2.16	0.46
1:C:204:GLY:HA2	1:C:207:ASN:OD1	2.16	0.46
1:C:150:CYS:O	1:C:177:MET:HA	2.16	0.45
1:D:165:TRP:HH2	1:D:465:PHE:HE1	1.64	0.45
1:D:300:ILE:HA	1:D:303:LYS:HE2	1.98	0.45
1:E:123:LEU:O	1:E:127:MET:HG3	2.16	0.45
1:E:366:LYS:HG3	1:E:367:LEU:HD13	1.98	0.45
1:E:467:ARG:HH21	1:G:467:ARG:NH1	2.13	0.45
1:F:336:LEU:HD11	1:F:373:MET:HB3	1.98	0.45
1:F:428:ILE:HG23	1:F:429:GLN:N	2.31	0.45
1:H:300:ILE:HA	1:H:303:LYS:HE2	1.99	0.45
1:H:35:ALA:O	1:H:367:LEU:HD12	2.16	0.45
1:H:265:SER:HA	1:H:300:ILE:HG12	1.99	0.45
1:A:349:GLN:HE22	1:A:386:THR:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:MET:HE2	1:H:429:GLN:HA	1.99	0.45
1:F:349:GLN:HE22	1:F:386:THR:HG23	1.82	0.45
1:G:300:ILE:HA	1:G:303:LYS:HE2	1.98	0.45
1:F:158:TYR:O	1:F:162:ILE:HG22	2.17	0.45
1:H:258:LYS:HE2	1:H:292:THR:OG1	2.16	0.45
1:F:426:ARG:O	1:H:428:ILE:HG22	2.16	0.45
1:A:300:ILE:HA	1:A:303:LYS:HE2	1.99	0.45
1:D:349:GLN:HE22	1:D:386:THR:HG23	1.82	0.45
1:F:51:VAL:O	1:F:55:VAL:HG23	2.17	0.45
1:E:106:ALA:O	1:E:110:ILE:HG12	2.17	0.44
1:C:300:ILE:HA	1:C:303:LYS:HE2	1.99	0.44
1:B:202:PRO:HD2	1:B:205:LEU:HD22	1.98	0.44
1:F:55:VAL:HG13	1:F:149:VAL:HG11	1.99	0.44
1:F:265:SER:HA	1:F:300:ILE:HG12	2.00	0.44
1:F:305:THR:HG22	1:F:399:ILE:HD13	1.98	0.44
1:A:3:THR:OG1	1:A:321:LEU:HD13	2.18	0.44
1:E:300:ILE:HA	1:E:303:LYS:HE2	2.00	0.44
1:E:487:MET:HE1	1:H:428:ILE:HG12	1.99	0.44
1:C:147:LEU:HB3	1:C:226:ALA:HB1	1.99	0.44
1:F:300:ILE:HA	1:F:303:LYS:HE2	1.99	0.44
1:H:470:GLY:O	1:H:474:ILE:HG12	2.17	0.44
1:D:165:TRP:HH2	1:D:465:PHE:CE1	2.36	0.44
1:B:24:ASP:HB3	1:B:47:GLY:CA	2.48	0.44
1:C:201:VAL:HG13	1:C:205:LEU:HB3	2.00	0.44
1:C:15:ARG:HE	1:C:20:VAL:HG21	1.82	0.43
1:A:132:ILE:HD13	1:B:457:PHE:CZ	2.53	0.43
1:C:15:ARG:HE	1:C:15:ARG:HB2	1.65	0.43
1:F:451:SER:HB2	1:F:455:LEU:HD12	2.00	0.43
1:C:468:GLU:HG3	1:C:471:ARG:NH2	2.33	0.43
1:E:349:GLN:HE22	1:E:386:THR:HG23	1.83	0.43
1:C:349:GLN:HE22	1:C:386:THR:HG23	1.83	0.43
1:H:84:ILE:HD12	1:H:117:LEU:HD13	2.01	0.43
1:G:22:PRO:HB3	1:G:50:GLU:HG2	1.99	0.43
1:H:349:GLN:HE22	1:H:386:THR:HG23	1.84	0.43
1:D:196:TYR:O	1:D:201:VAL:HB	2.19	0.43
1:G:366:LYS:HG3	1:G:367:LEU:HD13	2.01	0.43
1:H:202:PRO:HD2	1:H:205:LEU:HD22	2.01	0.43
1:D:165:TRP:CH2	1:D:465:PHE:HE1	2.37	0.43
1:G:124:ALA:HA	1:G:127:MET:HE2	2.01	0.43
1:A:129:GLY:HA3	1:A:142:THR:O	2.19	0.43
1:A:123:LEU:O	1:A:127:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:VAL:HG22	1:B:445:ILE:HD12	2.00	0.42
1:F:470:GLY:O	1:F:474:ILE:HG12	2.19	0.42
1:G:451:SER:HB2	1:G:455:LEU:HD12	2.01	0.42
1:A:75:ARG:NH1	1:A:76:ILE:HD13	2.34	0.42
1:F:196:TYR:O	1:F:201:VAL:HB	2.19	0.42
1:H:3:THR:HG21	1:H:367:LEU:HD11	2.00	0.42
1:D:451:SER:HB2	1:D:455:LEU:HD12	2.01	0.42
1:E:202:PRO:HA	1:E:203:PRO:HD3	1.91	0.42
1:G:349:GLN:HE22	1:G:386:THR:HG23	1.83	0.42
1:H:339:VAL:HG11	1:H:394:GLY:HA3	2.00	0.42
1:B:51:VAL:HG13	1:B:219:LEU:HD23	2.01	0.42
1:C:58:ALA:HB1	1:C:176:ALA:HB1	2.01	0.42
1:E:3:THR:OG1	1:E:321:LEU:HD13	2.18	0.42
1:E:51:VAL:O	1:E:55:VAL:HG23	2.20	0.42
1:C:258:LYS:HE2	1:C:292:THR:OG1	2.19	0.42
1:G:123:LEU:O	1:G:127:MET:HG3	2.19	0.42
1:F:201:VAL:HG13	1:F:205:LEU:CB	2.50	0.42
1:B:300:ILE:HA	1:B:303:LYS:HE2	2.01	0.41
1:A:363:GLU:H	1:A:363:GLU:CD	2.28	0.41
1:B:177:MET:HE2	1:B:206:PHE:HE1	1.86	0.41
1:G:132:ILE:HD13	1:H:457:PHE:CZ	2.55	0.41
1:D:326:ARG:HD3	1:D:326:ARG:HA	1.93	0.41
1:E:15:ARG:HA	1:E:207:ASN:OD1	2.20	0.41
1:G:162:ILE:HD13	1:G:231:THR:HG21	2.02	0.41
1:A:196:TYR:O	1:A:201:VAL:HB	2.20	0.41
1:C:15:ARG:HH12	1:C:53:LEU:CD1	2.34	0.41
1:D:147:LEU:HB3	1:D:226:ALA:HB1	2.03	0.41
1:F:116:CYS:HB2	1:F:165:TRP:CZ3	2.54	0.41
1:G:326:ARG:HD3	1:G:326:ARG:HA	1.94	0.41
1:H:332:ASN:HB2	1:H:335:HIS:HB2	2.03	0.41
1:E:363:GLU:CD	1:E:363:GLU:H	2.28	0.41
1:F:428:ILE:CB	1:H:428:ILE:HB	2.48	0.41
1:B:62:PHE:HE1	1:B:146:PRO:HB2	1.84	0.40
1:C:15:ARG:HH12	1:C:53:LEU:HD13	1.87	0.40
1:E:151:VAL:HB	1:E:228:VAL:HG22	2.02	0.40
1:G:106:ALA:O	1:G:110:ILE:HG12	2.21	0.40
1:B:259:SER:HB2	1:B:290:ASN:O	2.21	0.40
1:D:123:LEU:O	1:D:127:MET:HG3	2.21	0.40
1:A:269:MET:HE1	1:A:300:ILE:HB	2.03	0.40
1:B:62:PHE:CE1	1:B:148:GLY:HA2	2.56	0.40
1:E:261:LEU:HD13	1:E:448:TYR:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:ARG:HH22	1:H:467:ARG:NH1	2.20	0.40
1:G:196:TYR:O	1:G:201:VAL:HB	2.22	0.40
1:A:470:GLY:O	1:A:474:ILE:HG12	2.21	0.40
1:E:196:TYR:O	1:E:201:VAL:HB	2.21	0.40
1:F:366:LYS:HG3	1:F:367:LEU:CD1	2.51	0.40
1:G:34:PRO:HG3	3:G:503:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	467/508 (92%)	457 (98%)	10 (2%)	0	100	100
1	B	467/508 (92%)	458 (98%)	9 (2%)	0	100	100
1	C	469/508 (92%)	463 (99%)	6 (1%)	0	100	100
1	D	467/508 (92%)	461 (99%)	6 (1%)	0	100	100
1	E	468/508 (92%)	456 (97%)	11 (2%)	1 (0%)	43	63
1	F	467/508 (92%)	455 (97%)	11 (2%)	1 (0%)	43	63
1	G	467/508 (92%)	460 (98%)	6 (1%)	1 (0%)	43	63
1	H	467/508 (92%)	461 (99%)	6 (1%)	0	100	100
All	All	3739/4064 (92%)	3671 (98%)	65 (2%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	463	SER
1	F	463	SER
1	G	298	LYS

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	384/416 (92%)	356 (93%)	28 (7%)	13	27
1	B	384/416 (92%)	355 (92%)	29 (8%)	12	26
1	C	386/416 (93%)	357 (92%)	29 (8%)	12	26
1	D	384/416 (92%)	357 (93%)	27 (7%)	14	29
1	E	385/416 (92%)	358 (93%)	27 (7%)	14	29
1	F	384/416 (92%)	353 (92%)	31 (8%)	11	23
1	G	384/416 (92%)	355 (92%)	29 (8%)	12	26
1	H	384/416 (92%)	354 (92%)	30 (8%)	11	24
All	All	3075/3328 (92%)	2845 (92%)	230 (8%)	12	26

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	56	GLN
1	A	72	GLU
1	A	132	ILE
1	A	134	LEU
1	A	161	GLN
1	A	201	VAL
1	A	277	LEU
1	A	283	THR
1	A	287	VAL
1	A	293	ARG
1	A	302	ASP
1	A	306	GLU
1	A	308	VAL
1	A	344	LYS
1	A	358	ASP
1	A	363	GLU
1	A	368	LYS
1	A	391	GLU

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Mol	Chain	Res	Type
1	A	408	VAL
1	A	416	THR
1	A	428	ILE
1	A	430	ARG
1	A	437	GLU
1	A	454	GLU
1	A	467	ARG
1	A	473	THR
1	A	491	GLU
1	B	24	ASP
1	B	56	GLN
1	B	132	ILE
1	B	134	LEU
1	B	153	ILE
1	B	161	GLN
1	B	201	VAL
1	B	231	THR
1	B	277	LEU
1	B	283	THR
1	B	287	VAL
1	B	293	ARG
1	B	302	ASP
1	B	306	GLU
1	B	308	VAL
1	B	344	LYS
1	B	363	GLU
1	B	368	LYS
1	B	391	GLU
1	B	408	VAL
1	B	416	THR
1	B	428	ILE
1	B	430	ARG
1	B	437	GLU
1	B	438	LEU
1	B	449	ASN
1	B	467	ARG
1	B	473	THR
1	B	491	GLU
1	C	15	ARG
1	C	56	GLN
1	C	117	LEU
1	C	132	ILE

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Mol	Chain	Res	Type
1	C	133	GLN
1	C	134	LEU
1	C	153	ILE
1	C	201	VAL
1	C	277	LEU
1	C	283	THR
1	C	287	VAL
1	C	293	ARG
1	C	302	ASP
1	C	306	GLU
1	C	308	VAL
1	C	321	LEU
1	C	322	LEU
1	C	344	LYS
1	C	368	LYS
1	C	391	GLU
1	C	408	VAL
1	C	416	THR
1	C	428	ILE
1	C	430	ARG
1	C	437	GLU
1	C	438	LEU
1	C	454	GLU
1	C	473	THR
1	C	491	GLU
1	D	56	GLN
1	D	132	ILE
1	D	134	LEU
1	D	161	GLN
1	D	201	VAL
1	D	277	LEU
1	D	283	THR
1	D	287	VAL
1	D	293	ARG
1	D	302	ASP
1	D	306	GLU
1	D	308	VAL
1	D	344	LYS
1	D	363	GLU
1	D	368	LYS
1	D	391	GLU
1	D	408	VAL

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Mol	Chain	Res	Type
1	D	416	THR
1	D	428	ILE
1	D	430	ARG
1	D	437	GLU
1	D	438	LEU
1	D	449	ASN
1	D	461	LYS
1	D	467	ARG
1	D	473	THR
1	D	491	GLU
1	E	44	THR
1	E	56	GLN
1	E	132	ILE
1	E	134	LEU
1	E	161	GLN
1	E	201	VAL
1	E	277	LEU
1	E	283	THR
1	E	287	VAL
1	E	293	ARG
1	E	302	ASP
1	E	306	GLU
1	E	308	VAL
1	E	344	LYS
1	E	363	GLU
1	E	367	LEU
1	E	368	LYS
1	E	391	GLU
1	E	408	VAL
1	E	416	THR
1	E	430	ARG
1	E	437	GLU
1	E	438	LEU
1	E	454	GLU
1	E	455	LEU
1	E	484	CYS
1	E	487	MET
1	F	51	VAL
1	F	56	GLN
1	F	72	GLU
1	F	112	ILE
1	F	132	ILE

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Mol	Chain	Res	Type
1	F	134	LEU
1	F	161	GLN
1	F	164	SER
1	F	201	VAL
1	F	259	SER
1	F	277	LEU
1	F	283	THR
1	F	287	VAL
1	F	293	ARG
1	F	302	ASP
1	F	306	GLU
1	F	308	VAL
1	F	344	LYS
1	F	368	LYS
1	F	391	GLU
1	F	408	VAL
1	F	415	THR
1	F	416	THR
1	F	430	ARG
1	F	437	GLU
1	F	438	LEU
1	F	449	ASN
1	F	455	LEU
1	F	467	ARG
1	F	487	MET
1	F	490	VAL
1	G	56	GLN
1	G	132	ILE
1	G	133	GLN
1	G	134	LEU
1	G	153	ILE
1	G	161	GLN
1	G	201	VAL
1	G	258	LYS
1	G	277	LEU
1	G	283	THR
1	G	287	VAL
1	G	293	ARG
1	G	302	ASP
1	G	306	GLU
1	G	308	VAL
1	G	338	ARG

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Mol	Chain	Res	Type
1	G	344	LYS
1	G	363	GLU
1	G	367	LEU
1	G	368	LYS
1	G	391	GLU
1	G	408	VAL
1	G	416	THR
1	G	428	ILE
1	G	430	ARG
1	G	437	GLU
1	G	438	LEU
1	G	462	LYS
1	G	491	GLU
1	H	20	VAL
1	H	117	LEU
1	H	132	ILE
1	H	134	LEU
1	H	161	GLN
1	H	201	VAL
1	H	277	LEU
1	H	283	THR
1	H	287	VAL
1	H	293	ARG
1	H	302	ASP
1	H	306	GLU
1	H	308	VAL
1	H	336	LEU
1	H	344	LYS
1	H	363	GLU
1	H	367	LEU
1	H	368	LYS
1	H	391	GLU
1	H	408	VAL
1	H	416	THR
1	H	430	ARG
1	H	437	GLU
1	H	438	LEU
1	H	449	ASN
1	H	454	GLU
1	H	467	ARG
1	H	473	THR
1	H	487	MET

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Mol	Chain	Res	Type
1	H	491	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	221	GLN
1	A	270	ASN
1	A	380	ASN
1	A	439	GLN
1	B	221	GLN
1	B	270	ASN
1	B	380	ASN
1	B	439	GLN
1	C	67	GLN
1	C	221	GLN
1	C	270	ASN
1	C	380	ASN
1	C	439	GLN
1	D	56	GLN
1	D	210	GLN
1	D	270	ASN
1	D	380	ASN
1	D	439	GLN
1	E	270	ASN
1	E	380	ASN
1	E	432	HIS
1	E	439	GLN
1	E	449	ASN
1	F	131	HIS
1	F	221	GLN
1	F	270	ASN
1	F	380	ASN
1	F	439	GLN
1	G	56	GLN
1	G	270	ASN
1	G	335	HIS
1	G	380	ASN
1	G	439	GLN
1	H	67	GLN
1	H	221	GLN
1	H	270	ASN

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Mol	Chain	Res	Type
1	H	380	ASN
1	H	439	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	B	501	-	3,3,3	0.69	0	2,2,2	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	471/508 (92%)	0.03	5 (1%) 78 75	44, 71, 106, 128	0
1	B	471/508 (92%)	-0.06	4 (0%) 82 80	46, 69, 102, 125	0
1	C	471/508 (92%)	0.12	2 (0%) 88 86	40, 77, 126, 146	2 (0%)
1	D	471/508 (92%)	0.07	3 (0%) 85 83	50, 76, 125, 146	0
1	E	471/508 (92%)	0.30	14 (2%) 52 48	41, 86, 139, 164	1 (0%)
1	F	471/508 (92%)	0.13	12 (2%) 58 54	51, 77, 121, 143	0
1	G	471/508 (92%)	-0.01	4 (0%) 82 80	44, 68, 105, 125	0
1	H	471/508 (92%)	0.18	6 (1%) 75 71	45, 84, 126, 148	0
All	All	3768/4064 (92%)	0.10	50 (1%) 75 71	40, 75, 123, 164	3 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	457	PHE	4.7
1	F	457	PHE	4.1
1	E	291	GLY	4.0
1	F	263	ILE	3.6
1	B	435	VAL	3.2
1	H	428	ILE	3.1
1	H	457	PHE	3.1
1	D	263	ILE	3.1
1	H	460	TYR	3.0
1	F	289	CYS	3.0
1	F	287	VAL	2.9
1	F	231	THR	2.9
1	A	399	ILE	2.9
1	H	432	HIS	2.8
1	A	485	VAL	2.8
1	E	231	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	231	THR	2.8
1	E	289	CYS	2.7
1	F	132	ILE	2.6
1	F	450	VAL	2.6
1	C	231	THR	2.5
1	F	460	TYR	2.5
1	G	230	PHE	2.4
1	E	132	ILE	2.4
1	A	354	LEU	2.4
1	H	453	VAL	2.3
1	E	277	LEU	2.3
1	E	287	VAL	2.3
1	E	288	CYS	2.3
1	E	261	LEU	2.3
1	B	460	TYR	2.3
1	G	136	GLY	2.2
1	C	261	LEU	2.2
1	E	230	PHE	2.2
1	F	230	PHE	2.2
1	F	309	VAL	2.2
1	E	460	TYR	2.2
1	A	230	PHE	2.2
1	F	133	GLN	2.1
1	E	276	ALA	2.1
1	E	260	PRO	2.1
1	G	305	THR	2.1
1	B	3	THR	2.1
1	E	93	THR	2.1
1	H	135	PRO	2.1
1	B	0	PRO	2.0
1	G	417	PHE	2.0
1	F	461	LYS	2.0
1	A	392	ILE	2.0
1	D	428	ILE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	501	4/4	0.81	0.16	79,81,81,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.