



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:12 am BST

PDB ID : 4DAL  
Title : Crystal structure of Putative aldehyde dehydrogenase from Sinorhizobium meliloti 1021  
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Seidel, R.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2012-01-12  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

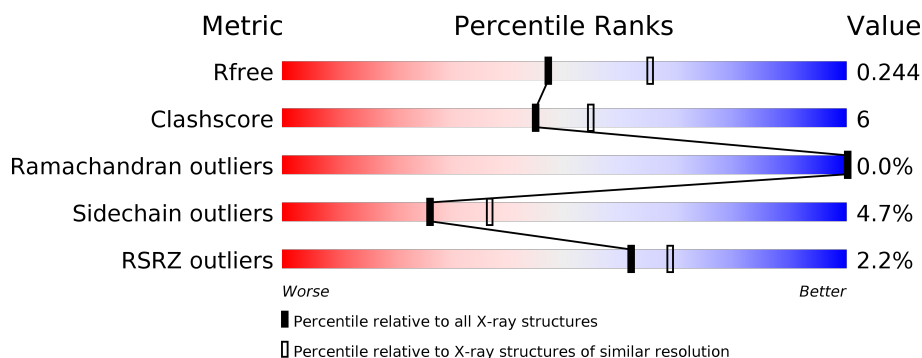
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	498	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	B	498	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
1	C	498	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	D	498	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	E	498	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• •</div> </div> </div>
1	F	498	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	498	 % 80% 13% • 5%
1	H	498	 4% 82% 13% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	600	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29632 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 Putative aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	Se	0	1	0
			3610	2272	633	689	5	11			
1	B	476	Total	C	N	O	S	Se	0	1	0
			3610	2269	633	690	6	12			
1	C	476	Total	C	N	O	S	Se	0	2	0
			3618	2274	636	690	6	12			
1	D	476	Total	C	N	O	S	Se	0	1	0
			3613	2271	633	692	5	12			
1	E	476	Total	C	N	O	S	Se	0	1	0
			3610	2269	633	690	6	12			
1	F	476	Total	C	N	O	S	Se	0	0	0
			3607	2267	633	690	5	12			
1	G	475	Total	C	N	O	S	Se	0	2	0
			3622	2280	636	689	5	12			
1	H	476	Total	C	N	O	S	Se	0	0	0
			3607	2267	633	690	5	12			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
A	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
A	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
A	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
A	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
A	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
A	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
A	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
A	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
A	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
A	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
A	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
A	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
A	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
A	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
A	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
B	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
B	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
B	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
B	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
B	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
B	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
B	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
B	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
B	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
B	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
B	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
B	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
B	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
B	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
B	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
B	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
B	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
C	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
C	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
C	-14	SER	-	EXPRESSION TAG	UNP Q92ND9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
C	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
C	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
C	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
C	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
C	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
C	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
C	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
C	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
C	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
C	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
C	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
C	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
C	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
D	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
D	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
D	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
D	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
D	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
D	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
D	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
D	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
D	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
D	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
D	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
D	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
D	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
D	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
D	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
D	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
D	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
E	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
E	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
E	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
E	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
E	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
E	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
E	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
E	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
E	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
E	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
E	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
E	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
E	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
E	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
E	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
E	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
E	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
E	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
E	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
E	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
E	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
E	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
F	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
F	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
F	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
F	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
F	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
F	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
F	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
F	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
F	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
F	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
F	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
F	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
F	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
F	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
F	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
F	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
F	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
F	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
F	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
F	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
F	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
F	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
F	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
G	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
G	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
G	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
G	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
G	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
G	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
G	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
G	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
G	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
G	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
G	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
G	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
G	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
G	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
G	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
G	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
G	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
G	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
G	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
G	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
G	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
G	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
H	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
H	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
H	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
H	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
H	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
H	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
H	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
H	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
H	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
H	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
H	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
H	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
H	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
H	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
H	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
H	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
H	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
H	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
H	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
H	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9

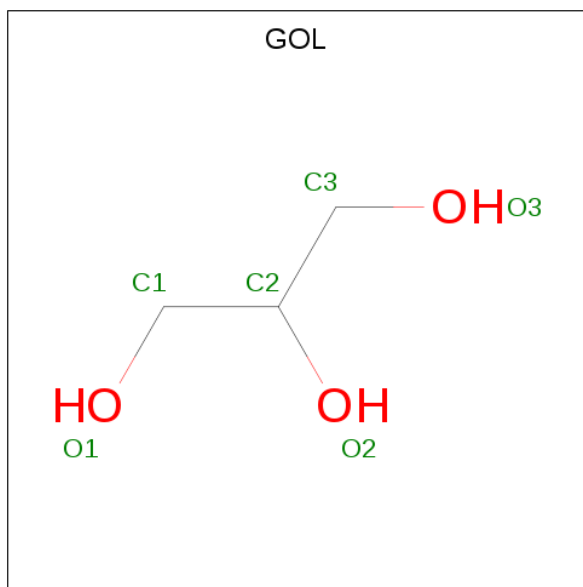
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
H	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
H	0	MSE	-	EXPRESSION TAG	UNP Q92ND9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	79	Total O 79 79	0	0
3	B	94	Total O 94 94	0	0
3	C	72	Total O 72 72	0	0
3	D	75	Total O 75 75	0	0
3	E	96	Total O 96 96	0	0
3	F	74	Total O 74 74	0	0

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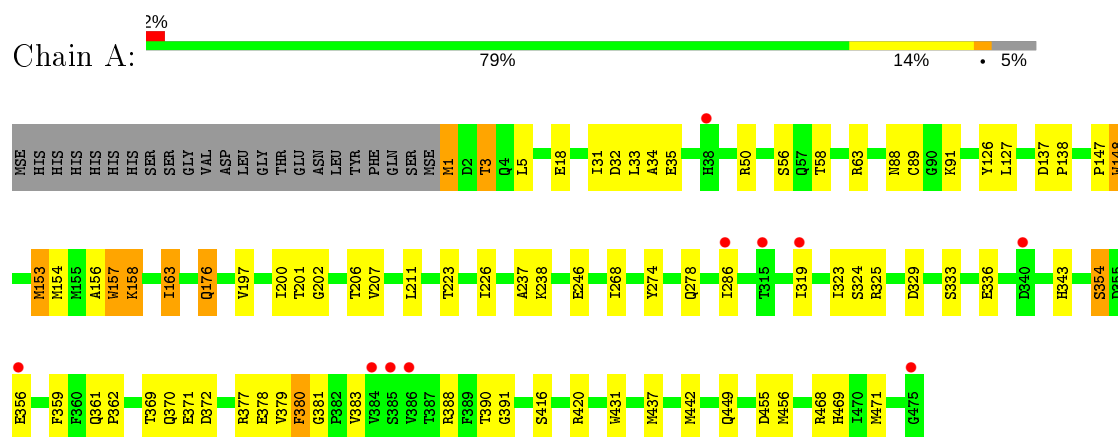
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	131	Total 131	O 131	0	0
3	H	102	Total 102	O 102	0	0

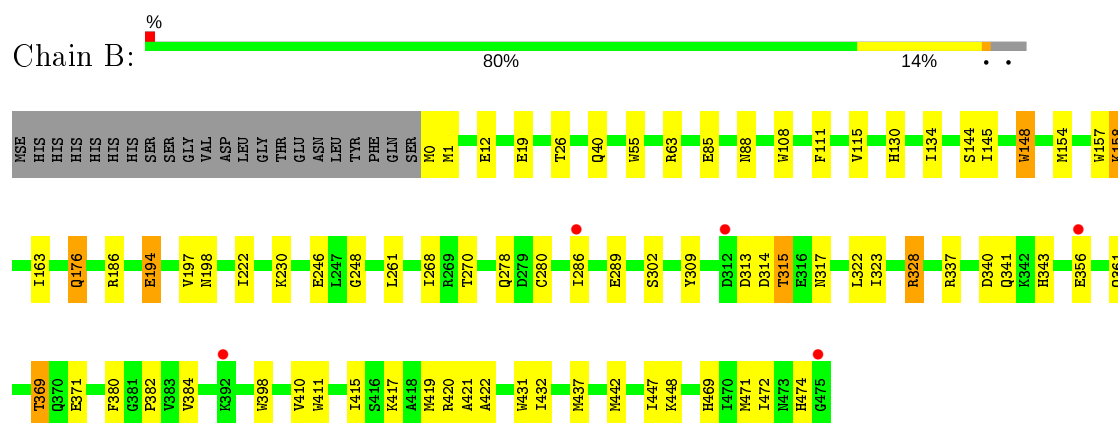
### 3 Residue-property plots [i](#)

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

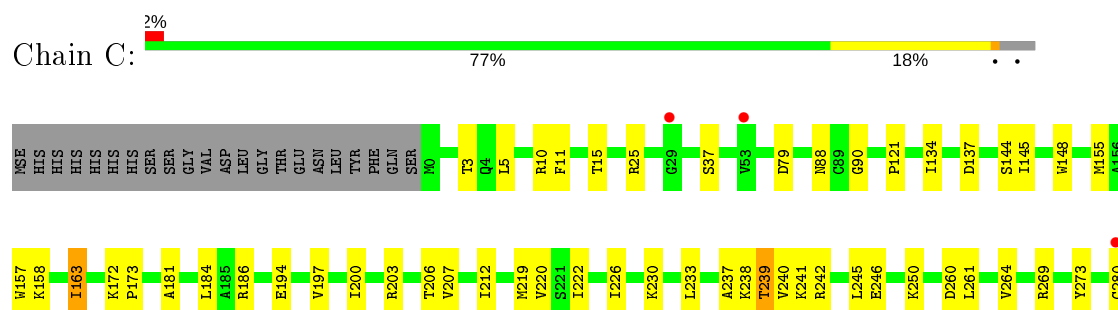
#### • Molecule 1: Putative aldehyde dehydrogenase

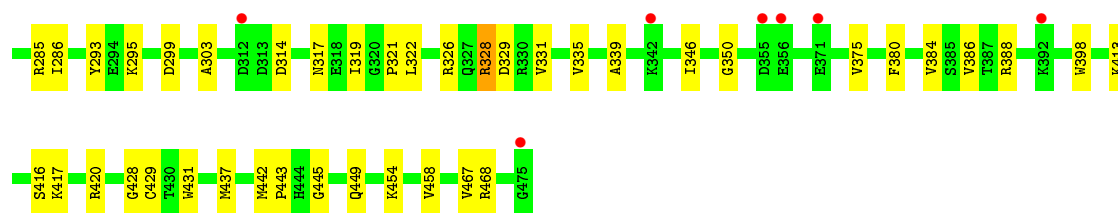


#### • Molecule 1: Putative aldehyde dehydrogenase

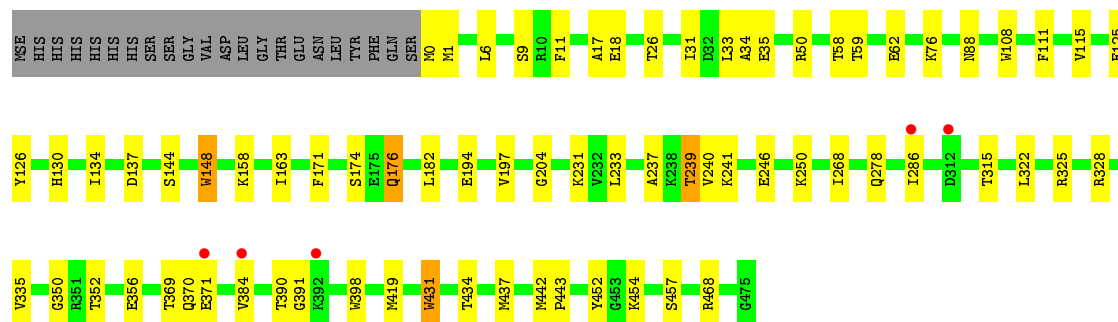
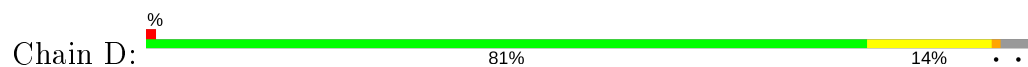


#### • Molecule 1: Putative aldehyde dehydrogenase

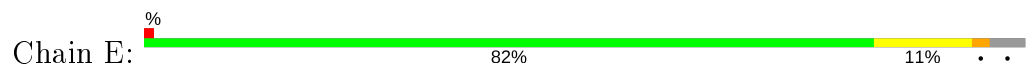




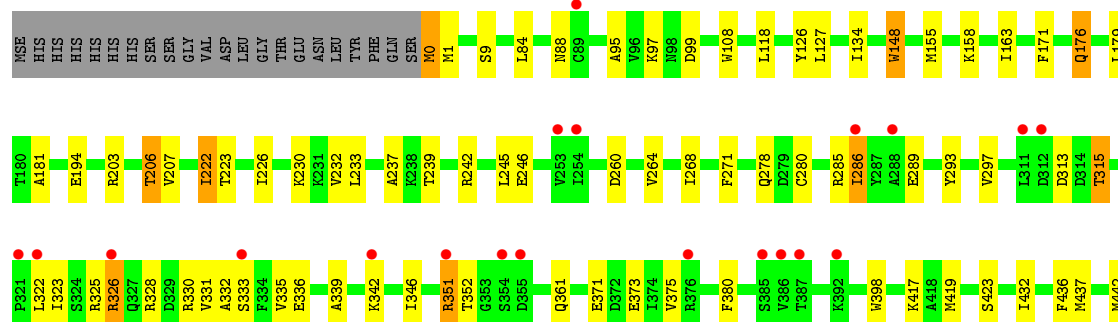
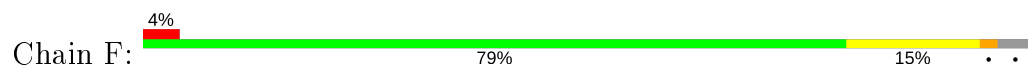
• Molecule 1: Putative aldehyde dehydrogenase

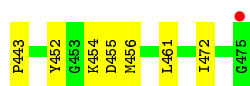


• Molecule 1: Putative aldehyde dehydrogenase

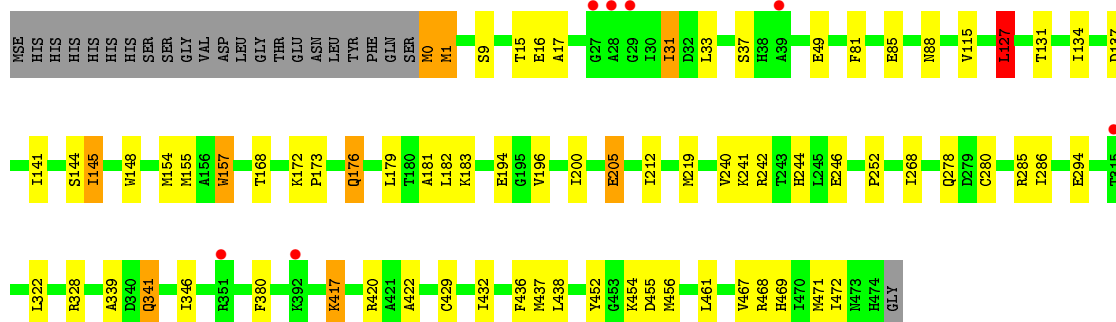
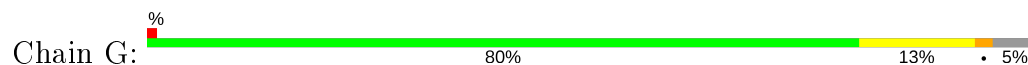


• Molecule 1: Putative aldehyde dehydrogenase

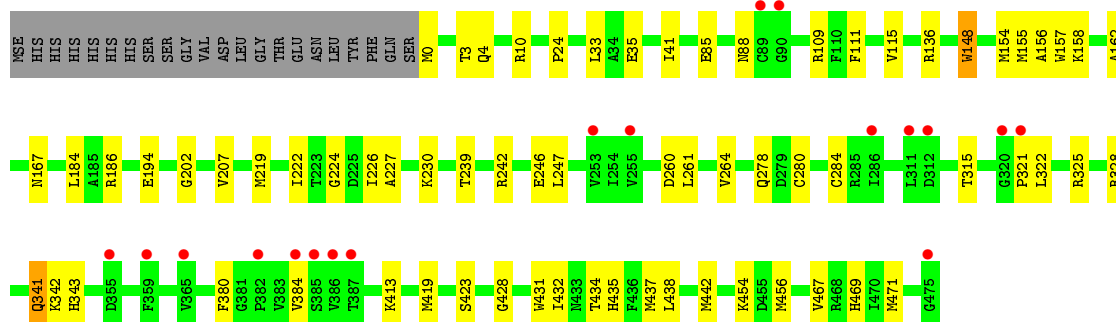
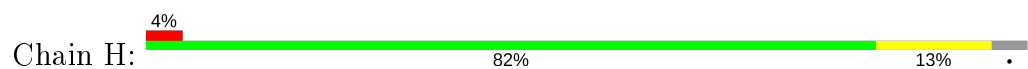




• Molecule 1: Putative aldehyde dehydrogenase



• Molecule 1: Putative aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.46Å 150.75Å 159.57Å 90.00° 102.13° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.98-2.30) 97.5 (19.98-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.184 , 0.237 0.200 , 0.244	Depositor DCC
$R_{free}$ test set	8581 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	29632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	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 22.61 % 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 5.5007e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

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

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	0.65	4/3675 (0.1%)	0.69	1/4977 (0.0%)
1	B	0.59	5/3672 (0.1%)	0.68	0/4969
1	C	0.58	4/3683 (0.1%)	0.67	0/4983
1	D	0.62	4/3675 (0.1%)	0.69	0/4973
1	E	0.61	3/3672 (0.1%)	0.69	0/4969
1	F	0.62	4/3666 (0.1%)	0.67	0/4961
1	G	0.64	1/3689 (0.0%)	0.71	1/4993 (0.0%)
1	H	0.64	2/3666 (0.1%)	0.71	3/4961 (0.1%)
All	All	0.62	27/29398 (0.1%)	0.69	5/39786 (0.0%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	326	ARG	CZ-NH2	8.83	1.44	1.33
1	D	148	TRP	CD2-CE2	6.60	1.49	1.41
1	B	148	TRP	CD2-CE2	6.53	1.49	1.41
1	H	148	TRP	CD2-CE2	6.42	1.49	1.41
1	C	148	TRP	CD2-CE2	5.97	1.48	1.41
1	F	148	TRP	CD2-CE2	5.90	1.48	1.41
1	E	148	TRP	CD2-CE2	5.70	1.48	1.41
1	A	148[A]	TRP	CD2-CE2	5.67	1.48	1.41
1	A	148[B]	TRP	CD2-CE2	5.67	1.48	1.41
1	D	431	TRP	CD2-CE2	5.62	1.48	1.41
1	D	108	TRP	CD2-CE2	5.59	1.48	1.41
1	C	157	TRP	CD2-CE2	5.55	1.48	1.41
1	D	398	TRP	CD2-CE2	5.47	1.48	1.41
1	G	157	TRP	CD2-CE2	5.43	1.47	1.41
1	B	398	TRP	CD2-CE2	5.42	1.47	1.41
1	C	398	TRP	CD2-CE2	5.33	1.47	1.41
1	E	157	TRP	CD2-CE2	5.30	1.47	1.41
1	B	411	TRP	CD2-CE2	5.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	TRP	CD2-CE2	5.21	1.47	1.41
1	B	108	TRP	CD2-CE2	5.21	1.47	1.41
1	B	431	TRP	CD2-CE2	5.21	1.47	1.41
1	F	108	TRP	CD2-CE2	5.15	1.47	1.41
1	F	398	TRP	CD2-CE2	5.10	1.47	1.41
1	E	431	TRP	CD2-CE2	5.09	1.47	1.41
1	H	431	TRP	CD2-CE2	5.05	1.47	1.41
1	C	431	TRP	CD2-CE2	5.04	1.47	1.41
1	A	431	TRP	CD2-CE2	5.02	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	109	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	G	127	LEU	CA-CB-CG	6.51	130.28	115.30
1	H	136	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	H	109	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	A	388	ARG	NE-CZ-NH1	-5.44	117.58	120.30

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	3610	0	3571	62	0
1	B	3610	0	3575	47	0
1	C	3618	0	3588	63	0
1	D	3613	0	3576	49	0
1	E	3610	0	3575	44	0
1	F	3607	0	3570	54	0
1	G	3622	0	3590	50	0
1	H	3607	0	3570	35	0
2	A	6	0	8	5	0
2	D	6	0	8	1	0
3	A	79	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	94	0	0	2	0
3	C	72	0	0	2	0
3	D	75	0	0	3	0
3	E	96	0	0	0	0
3	F	74	0	0	4	0
3	G	131	0	0	4	0
3	H	102	0	0	4	0
All	All	29632	0	28631	374	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 (374) 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:E:328:ARG:HH21	1:E:328:ARG:HG2	1.11	1.07
1:D:176:GLN:H	1:D:176:GLN:HE21	1.10	0.98
1:G:339:ALA:HB2	1:G:346:ILE:HD11	1.51	0.93
1:B:19:GLU:HG3	3:B:555:HOH:O	1.72	0.89
1:G:339:ALA:HB2	1:G:346:ILE:CD1	2.09	0.83
1:F:1:MSE:HE3	1:F:84:LEU:HD11	1.59	0.83
1:H:280:CYS:HB3	3:H:516:HOH:O	1.78	0.82
1:F:289:GLU:HG2	3:F:548:HOH:O	1.77	0.82
1:G:242:ARG:HD3	3:G:594:HOH:O	1.80	0.80
1:G:268:ILE:HD13	1:G:286:ILE:HD13	1.62	0.80
1:G:134:ILE:HD11	1:H:442:MSE:SE	2.32	0.80
1:A:442:MSE:SE	1:B:134:ILE:HD11	2.32	0.80
1:C:328:ARG:HG2	1:C:328:ARG:HH21	1.46	0.80
1:A:268:ILE:HD13	1:A:286:ILE:HD13	1.64	0.79
1:G:176:GLN:HE21	1:G:176:GLN:H	1.30	0.79
1:B:26:THR:O	1:B:356:GLU:HG3	1.83	0.79
1:E:328:ARG:NH2	1:E:328:ARG:HG2	1.91	0.78
1:A:268:ILE:HD13	1:A:286:ILE:CD1	2.14	0.78
1:E:328:ARG:HH21	1:E:328:ARG:CG	1.97	0.74
1:A:238:LYS:O	1:B:230:LYS:HE3	1.86	0.74
1:C:280[A]:CYS:SG	3:C:559:HOH:O	2.45	0.74
1:H:4:GLN:HG3	1:H:186:ARG:HH22	1.54	0.73
1:D:369:THR:HG22	1:D:371:GLU:H	1.52	0.73
1:F:332:ALA:O	1:F:336:GLU:HG2	1.88	0.73
1:C:203:ARG:HB2	1:C:206:THR:HG22	1.71	0.72
1:G:268:ILE:HD13	1:G:286:ILE:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ILE:HD11	1:C:197:VAL:HG22	1.73	0.71
1:C:206:THR:HG23	1:C:207:VAL:H	1.56	0.71
1:G:472:ILE:HG12	1:H:432:ILE:HD12	1.72	0.71
1:D:9:SER:HB3	1:D:194:GLU:HG3	1.72	0.70
1:H:35:GLU:HG2	1:H:202:GLY:HA2	1.74	0.69
1:E:390:THR:HG22	1:E:391:GLY:N	2.08	0.69
1:C:328:ARG:CG	1:C:328:ARG:HH21	2.05	0.69
1:F:206:THR:HG23	1:F:207:VAL:H	1.58	0.69
1:E:133:MSE:HE1	1:G:131:THR:HG21	1.75	0.69
1:B:286:ILE:HD12	1:B:384:VAL:CG1	2.23	0.68
1:D:148:TRP:HD1	1:D:174:SER:HG	1.42	0.68
1:D:268:ILE:HD13	1:D:286:ILE:HD13	1.76	0.67
1:G:137:ASP:OD2	1:G:468:ARG:HD3	1.95	0.67
1:B:148:TRP:HZ3	1:B:278:GLN:OE1	1.78	0.67
1:C:145:ILE:HB	1:C:222:ILE:HD13	1.77	0.67
1:C:286:ILE:HD11	1:C:384:VAL:HG11	1.77	0.66
1:C:442:MSE:SE	1:D:134:ILE:HD11	2.46	0.66
1:A:437:MSE:HE2	1:A:437:MSE:HA	1.76	0.66
1:G:145:ILE:HG23	1:G:172:LYS:HE3	1.78	0.66
1:H:41:ILE:HD11	1:H:207:VAL:HG13	1.77	0.66
1:C:328:ARG:HG2	1:C:328:ARG:NH2	2.11	0.65
1:C:137:ASP:OD2	1:C:468:ARG:HD3	1.97	0.65
1:F:1:MSE:HE1	1:F:179:LEU:HD22	1.78	0.65
1:B:369:THR:HG23	1:B:371:GLU:H	1.62	0.65
1:G:417:LYS:HG3	1:G:420[A]:ARG:HH11	1.62	0.64
1:A:237:ALA:O	1:B:230:LYS:HG2	1.97	0.64
1:B:313:ASP:OD1	1:B:315:THR:HB	1.98	0.64
1:F:203:ARG:HB2	1:F:206:THR:HG22	1.80	0.63
1:F:222:ILE:HG21	1:F:232:VAL:HG21	1.80	0.63
1:A:343:HIS:HE1	1:A:372:ASP:OD2	1.81	0.63
1:B:419:MSE:CE	1:B:432:ILE:HD12	2.28	0.63
1:E:233:LEU:HD23	1:F:237:ALA:HA	1.80	0.63
1:A:379:VAL:H	2:A:600:GOL:H11	1.64	0.63
1:A:148[B]:TRP:CD1	1:A:323:ILE:HB	2.33	0.63
1:C:226:ILE:HG22	1:C:230:LYS:HE3	1.81	0.62
1:E:328:ARG:NH2	1:E:329:ASP:OD1	2.33	0.62
1:C:443:PRO:HB2	1:C:454:LYS:HD2	1.82	0.62
1:D:390:THR:HG22	1:D:391:GLY:N	2.14	0.61
1:C:295:LYS:HE2	1:C:299:ASP:OD2	2.00	0.61
1:B:289:GLU:HG2	3:B:530:HOH:O	2.01	0.61
1:B:148:TRP:CZ3	1:B:278:GLN:OE1	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLN:HG3	1:B:323:ILE:HG12	1.83	0.61
1:D:176:GLN:H	1:D:176:GLN:NE2	1.90	0.61
1:G:455:ASP:O	1:G:456:MSE:HB2	2.01	0.61
1:A:18:GLU:HA	1:A:34:ALA:HA	1.82	0.61
1:D:239:THR:HG23	1:D:241:LYS:HG3	1.83	0.60
1:E:147:PRO:HD3	1:E:223:THR:HB	1.83	0.60
1:A:56:SER:HB2	1:A:138:PRO:HG2	1.84	0.60
1:C:212:ILE:O	1:C:241:LYS:HE3	2.02	0.60
1:A:148[A]:TRP:CD1	1:A:176:GLN:NE2	2.70	0.59
1:A:380:PHE:H	2:A:600:GOL:H11	1.68	0.59
1:D:148:TRP:HZ3	1:D:278:GLN:OE1	1.85	0.59
1:B:163:ILE:HD11	1:B:197:VAL:CG2	2.32	0.59
1:B:437:MSE:HA	1:B:437:MSE:HE2	1.85	0.59
1:F:313:ASP:OD1	1:F:315:THR:HB	2.03	0.59
1:C:237:ALA:HA	1:D:233:LEU:HD13	1.84	0.58
1:F:203:ARG:HB2	1:F:206:THR:CG2	2.33	0.58
1:B:341:GLN:HG2	1:B:343:HIS:CE1	2.38	0.58
1:D:0:MSE:HG3	1:D:1:MSE:H	1.69	0.58
1:C:233:LEU:HD23	1:D:237:ALA:HA	1.86	0.58
1:A:378:GLU:HG3	2:A:600:GOL:H32	1.86	0.57
1:B:248:GLY:HA2	1:B:280[B]:CYS:SG	2.44	0.57
1:D:443:PRO:HB2	1:D:454:LYS:HD2	1.86	0.57
1:G:212:ILE:O	1:G:241:LYS:HE3	2.04	0.57
1:C:163:ILE:HD11	1:C:197:VAL:CG2	2.34	0.57
1:D:26:THR:O	1:D:356:GLU:HG3	2.03	0.57
1:E:89:CYS:HB2	1:E:91:LYS:HG3	1.86	0.57
1:E:35:GLU:HG2	1:E:202:GLY:HA2	1.85	0.57
1:F:322:LEU:CD1	1:F:328:ARG:HA	2.35	0.56
1:G:417:LYS:HG3	1:G:420[A]:ARG:NH1	2.20	0.56
1:A:148[A]:TRP:HZ3	1:A:278:GLN:OE1	1.88	0.56
1:B:268:ILE:HD13	1:B:286:ILE:HD13	1.86	0.56
1:H:437:MSE:HA	1:H:437:MSE:HE2	1.88	0.56
1:E:219:MSE:HG3	1:E:242:ARG:HB3	1.88	0.55
1:G:173:PRO:HD2	1:G:200:ILE:O	2.06	0.55
1:D:268:ILE:HD13	1:D:286:ILE:CD1	2.37	0.55
1:C:339:ALA:HB2	1:C:346:ILE:CD1	2.37	0.55
1:C:134:ILE:HD11	1:D:442:MSE:SE	2.57	0.55
1:G:294:GLU:HG2	3:G:578:HOH:O	2.07	0.55
1:A:3:THR:HG23	1:A:3:THR:O	2.06	0.55
1:B:286:ILE:CD1	1:B:384:VAL:CG1	2.84	0.55
1:F:419:MSE:CE	1:F:432:ILE:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:LEU:HD13	1:D:328:ARG:HA	1.89	0.55
1:A:369:THR:HG22	1:A:370:GLN:N	2.22	0.55
1:D:17:ALA:O	1:D:35:GLU:HG3	2.07	0.55
1:G:15:THR:HB	1:G:37:SER:HB3	1.89	0.55
1:B:163:ILE:HD11	1:B:197:VAL:HG21	1.88	0.54
1:G:9:SER:HB3	1:G:194:GLU:HG3	1.89	0.54
1:A:126:TYR:CE1	1:B:442:MSE:HE3	2.42	0.54
1:A:50:ARG:HG3	3:A:751:HOH:O	2.08	0.54
1:F:322:LEU:HD13	1:F:328:ARG:HA	1.89	0.54
1:E:176:GLN:HG3	1:E:323:ILE:CG1	2.38	0.54
1:H:322:LEU:CD1	1:H:328:ARG:HA	2.37	0.54
1:F:455:ASP:O	1:F:456:MSE:HB2	2.08	0.54
1:H:322:LEU:HD13	1:H:328:ARG:HA	1.90	0.54
1:E:176:GLN:HG3	1:E:323:ILE:HG12	1.90	0.54
1:B:447:ILE:HG22	1:B:448:LYS:N	2.23	0.53
1:B:447:ILE:HG22	1:B:448:LYS:H	1.72	0.53
1:G:472:ILE:HD13	1:H:419:MSE:HE1	1.90	0.53
1:C:260:ASP:HB2	1:C:413:LYS:HE3	1.90	0.53
1:E:242:ARG:NH1	1:F:452:TYR:HB3	2.24	0.53
1:F:176:GLN:HG3	1:F:323:ILE:HG13	1.89	0.53
1:A:5:LEU:CD2	1:A:201:THR:HG23	2.38	0.53
1:E:407:ALA:HB1	1:E:431:TRP:CZ3	2.44	0.53
1:A:158:LYS:HE2	1:A:223:THR:OG1	2.09	0.52
1:E:322:LEU:HD13	1:E:328:ARG:HA	1.91	0.52
1:F:351:ARG:O	1:F:361:GLN:HB2	2.08	0.52
1:A:369:THR:HG22	1:A:371:GLU:H	1.73	0.52
1:A:379:VAL:N	2:A:600:GOL:H11	2.24	0.52
1:C:286:ILE:HD12	1:C:386:VAL:HG22	1.91	0.52
1:F:155:MSE:HG3	1:F:171:PHE:CZ	2.44	0.52
1:D:137:ASP:OD2	1:D:468:ARG:HD3	2.10	0.52
1:C:155:MSE:SE	1:C:181:ALA:HA	2.60	0.52
1:C:260:ASP:O	1:C:264:VAL:HG23	2.09	0.52
1:A:268:ILE:CD1	1:A:286:ILE:HD13	2.39	0.51
1:F:339:ALA:HB2	1:F:346:ILE:HD12	1.91	0.51
1:G:31:ILE:HD11	1:G:179:LEU:HD21	1.91	0.51
1:F:194:GLU:O	1:F:194:GLU:HG2	2.11	0.51
1:A:153:MSE:HG2	1:A:154:MSE:HE2	1.92	0.51
1:A:137:ASP:OD2	1:A:468:ARG:HD3	2.11	0.51
1:D:148:TRP:CZ3	1:D:278:GLN:OE1	2.64	0.51
1:H:341:GLN:HG3	1:H:343:HIS:CE1	2.45	0.51
1:B:55:TRP:CZ2	1:B:63:ARG:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:O	1:A:63:ARG:NH2	2.44	0.50
1:A:156:ALA:HB2	3:A:724:HOH:O	2.12	0.50
1:H:156:ALA:HB2	3:H:514:HOH:O	2.12	0.50
1:A:274:TYR:HA	1:A:319:ILE:HD11	1.92	0.50
1:H:438:LEU:HD22	1:H:456:MSE:HE1	1.93	0.50
1:F:331:VAL:O	1:F:335:VAL:HG23	2.11	0.50
1:G:436:PHE:HB3	1:G:437:MSE:HE3	1.93	0.50
1:C:155:MSE:SE	1:C:184:LEU:HD23	2.61	0.50
1:A:206:THR:HG23	1:A:207:VAL:N	2.27	0.50
1:A:163:ILE:HD11	1:A:197:VAL:CG2	2.42	0.50
1:F:148:TRP:HZ3	1:F:278:GLN:OE1	1.95	0.50
1:G:280:CYS:SG	3:G:525:HOH:O	2.60	0.49
1:A:390:THR:HG22	1:A:391:GLY:N	2.27	0.49
1:B:12:GLU:HG2	1:B:40:GLN:HE21	1.77	0.49
1:C:286:ILE:HD11	1:C:384:VAL:CG1	2.41	0.49
1:H:4:GLN:HG3	1:H:186:ARG:NH2	2.24	0.49
1:C:328:ARG:NH2	1:C:329:ASP:OD1	2.45	0.49
1:E:155:MSE:SE	1:E:184:LEU:HD23	2.61	0.49
1:H:24:PRO:HB2	1:H:321:PRO:HG2	1.94	0.49
1:H:148:TRP:HZ3	1:H:278:GLN:OE1	1.95	0.49
1:C:467:VAL:HB	1:D:454:LYS:HE3	1.94	0.49
1:E:442:MSE:SE	1:F:134:ILE:HD11	2.63	0.49
1:B:417:LYS:HG3	1:B:420:ARG:HH11	1.77	0.49
1:F:148:TRP:CZ3	1:F:278:GLN:OE1	2.66	0.49
1:A:154:MSE:HE1	1:A:157:TRP:CZ3	2.48	0.49
1:A:206:THR:HG23	1:A:207:VAL:HG23	1.94	0.49
1:F:452:TYR:CD2	3:F:546:HOH:O	2.55	0.49
1:A:268:ILE:HD13	1:A:286:ILE:HD11	1.95	0.49
1:A:379:VAL:H	2:A:600:GOL:C1	2.24	0.49
1:C:90:GLY:HA3	1:C:321:PRO:HD2	1.95	0.49
1:D:250:LYS:NZ	3:D:725:HOH:O	2.45	0.49
1:A:147:PRO:HD2	1:A:154:MSE:HG3	1.95	0.48
1:C:173:PRO:HD2	1:C:200:ILE:O	2.13	0.48
1:B:111:PHE:O	1:B:115:VAL:HG23	2.13	0.48
1:D:286:ILE:HD12	1:D:384:VAL:CG1	2.42	0.48
1:B:309:TYR:OH	1:B:361:GLN:HG2	2.14	0.48
1:E:174:SER:OG	1:E:176:GLN:NE2	2.46	0.48
1:A:35:GLU:HG2	1:A:202:GLY:HA2	1.95	0.48
1:B:286:ILE:CD1	1:B:384:VAL:HG11	2.43	0.48
1:E:3:THR:O	1:E:3:THR:HG23	2.13	0.48
1:F:118:LEU:HD21	1:F:461:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ILE:HG13	1:C:220:VAL:HG11	1.95	0.48
1:E:133:MSE:HE1	1:G:131:THR:CG2	2.44	0.48
1:G:339:ALA:HB2	1:G:346:ILE:HD12	1.95	0.48
1:H:227:ALA:CB	3:H:555:HOH:O	2.61	0.48
1:E:390:THR:HG22	1:E:391:GLY:H	1.78	0.48
1:B:419:MSE:HE2	1:B:432:ILE:HD12	1.94	0.47
1:C:121:PRO:HB2	1:D:442:MSE:HE1	1.96	0.47
1:D:240:VAL:O	1:D:240:VAL:HG12	2.14	0.47
1:H:148:TRP:CZ3	1:H:278:GLN:OE1	2.67	0.47
1:C:331:VAL:O	1:C:335:VAL:HG23	2.15	0.47
1:D:390:THR:CG2	1:D:391:GLY:N	2.77	0.47
1:F:226:ILE:HG22	1:F:230:LYS:HE2	1.96	0.47
1:A:354:SER:HB2	1:A:359:PHE:HB2	1.95	0.47
1:C:239:THR:HG21	1:C:241:LYS:HE2	1.96	0.47
1:A:226:ILE:HD13	1:A:449:GLN:HG2	1.97	0.47
1:D:58:THR:HB	1:D:62:GLU:HG3	1.97	0.47
1:C:11:PHE:CZ	1:C:186:ARG:HA	2.50	0.47
1:C:285:ARG:HD3	1:C:375:VAL:HG13	1.97	0.47
1:G:437:MSE:HE2	1:G:437:MSE:HA	1.96	0.47
1:C:203:ARG:HB2	1:C:206:THR:CG2	2.42	0.47
1:B:314:ASP:HA	1:B:317:ASN:ND2	2.31	0.47
1:C:442:MSE:HE3	1:D:126:TYR:CE2	2.50	0.47
1:E:223:THR:HG23	1:E:246:GLU:HB3	1.96	0.46
1:C:233:LEU:HD13	1:C:245:LEU:HD11	1.96	0.46
1:C:335:VAL:HG11	1:C:350:GLY:HA2	1.98	0.46
1:F:443:PRO:HB2	1:F:454:LYS:HD2	1.97	0.46
1:C:322:LEU:CD1	1:C:328:ARG:HA	2.44	0.46
1:H:41:ILE:CD1	1:H:207:VAL:HG13	2.45	0.46
1:B:415:ILE:O	1:B:419:MSE:HG2	2.16	0.46
1:C:437:MSE:HA	1:C:437:MSE:HE2	1.98	0.46
1:F:351:ARG:HG2	1:F:352:THR:H	1.81	0.46
1:H:226:ILE:HG22	1:H:230:LYS:HE3	1.97	0.46
1:C:250:LYS:HE2	1:C:375:VAL:O	2.16	0.46
1:C:11:PHE:HZ	1:C:186:ARG:HA	1.81	0.46
1:F:163:ILE:HG21	1:F:163:ILE:HD13	1.65	0.46
1:G:341:GLN:O	3:G:559:HOH:O	2.20	0.46
1:B:286:ILE:HD12	1:B:384:VAL:HG12	1.95	0.45
1:E:154:MSE:HE1	1:E:157:TRP:CZ3	2.50	0.45
1:E:273:TYR:O	1:E:319:ILE:CD1	2.64	0.45
1:E:3:THR:O	1:E:3:THR:CG2	2.63	0.45
1:E:442:MSE:HE3	1:F:126:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:0:MSE:HG2	1:F:1:MSE:HG3	1.96	0.45
1:F:222:ILE:HG13	1:F:223:THR:N	2.31	0.45
1:F:280:CYS:SG	3:F:557:HOH:O	2.60	0.45
1:H:111:PHE:O	1:H:115:VAL:HG23	2.16	0.45
1:E:134:ILE:HD11	1:F:442:MSE:SE	2.67	0.45
1:B:268:ILE:HD13	1:B:286:ILE:CD1	2.46	0.45
1:C:219:MSE:SE	1:C:242[B]:ARG:HD2	2.66	0.45
1:D:437:MSE:HE2	1:D:437:MSE:HA	1.98	0.45
1:B:422:ALA:HB2	1:B:432:ILE:HD11	1.99	0.45
1:D:390:THR:HG22	1:D:391:GLY:H	1.82	0.45
1:C:206:THR:HG23	1:C:207:VAL:N	2.25	0.45
1:C:339:ALA:HB2	1:C:346:ILE:HD12	1.97	0.45
1:A:148[A]:TRP:CZ3	1:A:278:GLN:OE1	2.70	0.45
1:B:145:ILE:HB	1:B:222:ILE:HD12	1.99	0.45
1:C:240:VAL:O	1:C:240:VAL:HG12	2.17	0.45
1:E:390:THR:CG2	1:E:391:GLY:N	2.75	0.45
1:F:260:ASP:O	1:F:264:VAL:HG23	2.16	0.44
1:E:432:ILE:HD12	1:F:472:ILE:HG12	1.98	0.44
1:G:219:MSE:HE2	1:G:244:HIS:HB2	1.99	0.44
1:D:111:PHE:O	1:D:115:VAL:HG23	2.17	0.44
1:F:280:CYS:HB3	3:F:519:HOH:O	2.18	0.44
1:G:322:LEU:HD13	1:G:328:ARG:HA	1.99	0.44
1:C:144:SER:OG	1:C:158:LYS:HD3	2.18	0.44
1:C:314:ASP:HA	1:C:317:ASN:HD22	1.82	0.44
1:E:254:ILE:HB	1:E:410:VAL:HG23	2.00	0.44
1:E:455:ASP:O	1:E:456:MSE:HB2	2.18	0.44
1:G:154:MSE:HE1	1:G:157:TRP:CZ3	2.53	0.44
1:G:115:VAL:HA	1:G:461:LEU:HD21	1.99	0.44
1:H:284:CYS:HA	1:H:384:VAL:HG22	1.98	0.44
1:A:469:HIS:HE1	1:A:471:MSE:HE3	1.82	0.44
1:E:155:MSE:SE	1:E:181:ALA:HA	2.67	0.44
1:H:219:MSE:HA	1:H:242:ARG:O	2.17	0.44
1:A:469:HIS:CE1	1:A:471:MSE:HE3	2.53	0.44
1:D:431:TRP:HB3	1:D:434:THR:HG23	1.99	0.44
1:A:381:GLY:O	1:A:383:VAL:N	2.50	0.44
1:G:155:MSE:SE	1:G:181:ALA:HA	2.68	0.44
1:G:268:ILE:HG21	1:G:286:ILE:HD11	2.00	0.44
1:A:3:THR:O	1:A:3:THR:CG2	2.65	0.43
1:C:242[A]:ARG:CZ	1:D:452:TYR:HB3	2.48	0.43
1:F:437:MSE:HA	1:F:437:MSE:HE2	1.99	0.43
1:G:454:LYS:HE3	1:H:467:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:ARG:NH2	3:H:595:HOH:O	2.51	0.43
1:H:155:MSE:SE	1:H:184:LEU:HD23	2.69	0.43
1:A:238:LYS:HB2	1:A:238:LYS:HE3	1.75	0.43
1:D:204:GLY:O	2:D:600:GOL:H2	2.17	0.43
1:G:81:PHE:CE1	1:G:183:LYS:HD3	2.54	0.43
1:A:1:MSE:HE3	3:A:757:HOH:O	2.18	0.43
1:F:268:ILE:HD13	1:F:286:ILE:HD12	2.01	0.43
1:E:73:ALA:HB1	1:E:187:LEU:HD13	2.01	0.43
1:G:33:LEU:HD21	1:G:182:LEU:HD11	2.00	0.43
1:H:434:THR:OG1	1:H:435:HIS:N	2.50	0.43
1:G:467:VAL:HB	1:H:454:LYS:HE3	2.00	0.43
1:A:390:THR:HG22	1:A:391:GLY:H	1.82	0.43
1:D:286:ILE:CD1	1:D:384:VAL:CG1	2.97	0.43
1:D:335:VAL:HG11	1:D:350:GLY:HA2	2.00	0.43
1:E:273:TYR:O	1:E:319:ILE:HD11	2.19	0.43
1:E:447:ILE:HG22	1:F:242:ARG:HH22	1.84	0.43
1:F:1:MSE:CE	1:F:179:LEU:HD22	2.46	0.43
1:D:148:TRP:HD1	1:D:174:SER:OG	2.01	0.43
1:D:163:ILE:HD11	1:D:197:VAL:CG2	2.49	0.43
1:G:469:HIS:CE1	1:G:471:MSE:HE3	2.54	0.43
1:E:118:LEU:HD21	1:E:461:LEU:HD23	2.00	0.42
1:C:339:ALA:HB2	1:C:346:ILE:HD11	1.99	0.42
1:E:242:ARG:CZ	1:F:452:TYR:HB3	2.49	0.42
1:F:95:ALA:O	1:F:99:ASP:HB2	2.19	0.42
1:A:455:ASP:O	1:A:456:MSE:HB2	2.19	0.42
1:C:15:THR:HB	1:C:37:SER:HB3	2.02	0.42
1:D:6:LEU:HD13	1:D:11:PHE:CZ	2.55	0.42
1:E:135:ARG:HD3	1:E:470:ILE:HD13	2.02	0.42
1:F:293:TYR:O	1:F:297:VAL:HG23	2.19	0.42
1:G:438:LEU:HD22	1:G:456:MSE:HE1	2.00	0.42
1:A:148[B]:TRP:CE2	1:A:323:ILE:HG21	2.55	0.42
1:A:31:ILE:HG22	1:A:32:ASP:N	2.34	0.42
1:D:144:SER:HB2	1:D:171:PHE:HD1	1.84	0.42
1:H:162:ALA:O	1:H:167:ASN:HB2	2.20	0.42
1:B:337:ARG:O	1:B:340:ASP:HB2	2.19	0.42
1:D:163:ILE:HD11	1:D:197:VAL:HG21	2.01	0.42
1:F:0:MSE:HB3	1:F:0:MSE:HE2	1.95	0.42
1:G:0:MSE:O	1:G:1:MSE:HB2	2.19	0.42
1:A:148[B]:TRP:CD1	1:A:323:ILE:CB	3.02	0.42
1:B:410:VAL:HG21	1:B:421:ALA:HB1	2.01	0.42
1:E:416:SER:OG	1:E:420:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:GLU:H	1:G:205:GLU:HG3	1.43	0.42
1:B:341:GLN:CG	1:B:343:HIS:CE1	3.02	0.42
1:C:314:ASP:HA	1:C:317:ASN:ND2	2.35	0.42
1:D:419:MSE:HE3	3:D:752:HOH:O	2.18	0.42
1:A:31:ILE:CG2	1:A:32:ASP:N	2.83	0.42
1:C:226:ILE:CG2	1:C:230:LYS:HE3	2.48	0.42
1:C:416:SER:HB3	1:C:420:ARG:HH22	1.85	0.41
1:D:50:ARG:NH2	3:D:767:HOH:O	2.52	0.41
1:G:148[B]:TRP:CZ3	1:G:278:GLN:OE1	2.73	0.41
1:A:416:SER:HB3	1:A:420:ARG:NH1	2.35	0.41
1:F:155:MSE:SE	1:F:181:ALA:HA	2.71	0.41
1:C:273:TYR:O	1:C:319:ILE:HG21	2.21	0.41
1:A:329:ASP:O	1:A:333:SER:HB2	2.19	0.41
1:B:154:MSE:HE1	1:B:157:TRP:CZ3	2.55	0.41
1:B:286:ILE:HD11	1:B:384:VAL:HG11	2.02	0.41
1:C:269:ARG:HD2	1:C:303:ALA:HB1	2.03	0.41
1:F:285:ARG:HD2	1:F:375:VAL:HG13	2.02	0.41
1:H:260:ASP:O	1:H:264:VAL:HG23	2.20	0.41
1:C:5:LEU:O	1:C:11:PHE:HA	2.20	0.41
1:A:89:CYS:HB2	1:A:91:LYS:HG3	2.03	0.41
1:A:200:ILE:HD11	1:A:211:LEU:HD22	2.03	0.41
1:B:469:HIS:CE1	1:B:471:MSE:HE3	2.55	0.41
1:F:233:LEU:HD13	1:F:245:LEU:HD11	2.01	0.41
1:E:467:VAL:HB	1:F:454:LYS:HE3	2.02	0.41
1:G:168:THR:HG22	1:G:196:VAL:HA	2.03	0.41
1:H:224:GLY:O	1:H:247:LEU:HA	2.21	0.41
1:A:361:GLN:HA	1:A:362:PRO:HD2	1.94	0.41
1:B:130:HIS:HA	1:B:472:ILE:O	2.21	0.41
1:D:18:GLU:HA	1:D:34:ALA:HA	2.03	0.41
1:D:59:THR:OG1	1:D:62:GLU:HG2	2.20	0.41
1:F:9:SER:HA	1:F:194:GLU:HB2	2.03	0.41
1:A:319:ILE:HD13	1:A:319:ILE:HA	1.82	0.41
1:B:144:SER:HB3	1:B:158:LYS:HG2	2.02	0.41
1:C:293:TYR:CD1	1:C:388:ARG:HB2	2.56	0.41
1:H:469:HIS:CE1	1:H:471:MSE:HE3	2.56	0.41
1:A:148[A]:TRP:HD1	1:A:176:GLN:HE21	1.66	0.41
1:C:172:LYS:NZ	1:C:173:PRO:O	2.51	0.41
1:C:458:VAL:HG12	3:C:522:HOH:O	2.20	0.41
1:F:271:PHE:HB3	1:F:436:PHE:HB2	2.03	0.41
1:G:468:ARG:HA	1:H:428:GLY:O	2.21	0.41
1:B:194:GLU:H	1:B:194:GLU:HG3	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:GLY:HA3	1:C:445:GLY:O	2.20	0.41
1:E:194:GLU:O	1:E:194:GLU:HG2	2.21	0.41
1:H:413:LYS:HA	1:H:413:LYS:HD2	1.84	0.41
1:A:148[B]:TRP:NE1	1:A:323:ILE:HB	2.36	0.40
1:A:323:ILE:HG23	1:A:324:SER:N	2.36	0.40
1:G:240:VAL:O	1:G:240:VAL:HG12	2.20	0.40
1:H:154:MSE:HE1	1:H:157:TRP:CZ3	2.56	0.40
1:B:322:LEU:HD21	1:B:382:PRO:HD3	2.04	0.40
1:D:125:GLU:HA	1:D:130:HIS:O	2.21	0.40
1:E:460:ALA:O	1:E:464:TYR:HD2	2.04	0.40
1:F:127:LEU:HA	1:F:127:LEU:HD12	1.93	0.40
1:F:1:MSE:CE	1:F:84:LEU:HD11	2.42	0.40
1:G:16:GLU:HB3	1:G:17:ALA:H	1.71	0.40
1:G:422:ALA:HB2	1:G:432:ILE:HD11	2.03	0.40
1:G:49:GLU:HA	1:G:141:ILE:HD11	2.03	0.40
1:B:322:LEU:HD12	1:B:328:ARG:HA	2.03	0.40
1:D:6:LEU:HB2	1:D:11:PHE:CE1	2.57	0.40
1:D:33:LEU:HD21	1:D:182:LEU:HD11	2.04	0.40
1:E:59:THR:HG21	1:G:127:LEU:HA	2.03	0.40
1:G:252:PRO:HA	1:G:285:ARG:O	2.22	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	474/498 (95%)	459 (97%)	15 (3%)	0	100	100
1	B	475/498 (95%)	454 (96%)	21 (4%)	0	100	100
1	C	476/498 (96%)	461 (97%)	15 (3%)	0	100	100
1	D	475/498 (95%)	456 (96%)	18 (4%)	1 (0%)	47	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	475/498 (95%)	452 (95%)	23 (5%)	0	100	100
1	F	474/498 (95%)	452 (95%)	22 (5%)	0	100	100
1	G	475/498 (95%)	457 (96%)	18 (4%)	0	100	100
1	H	474/498 (95%)	459 (97%)	15 (3%)	0	100	100
All	All	3798/3984 (95%)	3650 (96%)	147 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	370	GLN

### 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	370/377 (98%)	354 (96%)	16 (4%)	29	40
1	B	371/377 (98%)	353 (95%)	18 (5%)	25	35
1	C	372/377 (99%)	355 (95%)	17 (5%)	27	38
1	D	371/377 (98%)	359 (97%)	12 (3%)	39	54
1	E	371/377 (98%)	349 (94%)	22 (6%)	19	27
1	F	370/377 (98%)	348 (94%)	22 (6%)	19	27
1	G	372/377 (99%)	356 (96%)	16 (4%)	29	40
1	H	370/377 (98%)	353 (95%)	17 (5%)	27	38
All	All	2967/3016 (98%)	2827 (95%)	140 (5%)	26	37

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	3	THR
1	A	33	LEU

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Mol	Chain	Res	Type
1	A	88	ASN
1	A	127	LEU
1	A	153	MSE
1	A	158	LYS
1	A	163	ILE
1	A	176	GLN
1	A	246	GLU
1	A	325	ARG
1	A	336	GLU
1	A	354	SER
1	A	356	GLU
1	A	377	ARG
1	A	380	PHE
1	B	0	MSE
1	B	1	MSE
1	B	85	GLU
1	B	88	ASN
1	B	158	LYS
1	B	176	GLN
1	B	186	ARG
1	B	194	GLU
1	B	198	ASN
1	B	246	GLU
1	B	261	LEU
1	B	270	THR
1	B	302	SER
1	B	315	THR
1	B	328	ARG
1	B	369	THR
1	B	380	PHE
1	B	474	HIS
1	C	3	THR
1	C	10	ARG
1	C	25	ARG
1	C	79	ASP
1	C	88	ASN
1	C	163	ILE
1	C	194	GLU
1	C	238	LYS
1	C	239	THR
1	C	246	GLU
1	C	261	LEU

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Mol	Chain	Res	Type
1	C	326	ARG
1	C	328	ARG
1	C	380	PHE
1	C	417	LYS
1	C	429	CYS
1	C	449	GLN
1	D	31	ILE
1	D	76	LYS
1	D	88	ASN
1	D	158	LYS
1	D	176	GLN
1	D	231	LYS
1	D	239	THR
1	D	246	GLU
1	D	315	THR
1	D	325	ARG
1	D	352	THR
1	D	457	SER
1	E	3	THR
1	E	76	LYS
1	E	85	GLU
1	E	88	ASN
1	E	99	ASP
1	E	127	LEU
1	E	144	SER
1	E	158	LYS
1	E	176	GLN
1	E	194	GLU
1	E	231	LYS
1	E	239	THR
1	E	242	ARG
1	E	246	GLU
1	E	294	GLU
1	E	319	ILE
1	E	328	ARG
1	E	355	ASP
1	E	371	GLU
1	E	380	PHE
1	E	413	LYS
1	E	417	LYS
1	F	0	MSE
1	F	88	ASN

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Mol	Chain	Res	Type
1	F	97	LYS
1	F	158	LYS
1	F	176	GLN
1	F	206	THR
1	F	222	ILE
1	F	239	THR
1	F	246	GLU
1	F	286	ILE
1	F	315	THR
1	F	325	ARG
1	F	326	ARG
1	F	330	ARG
1	F	333	SER
1	F	342	LYS
1	F	351	ARG
1	F	371	GLU
1	F	373	GLU
1	F	380	PHE
1	F	417	LYS
1	F	423	SER
1	G	0	MSE
1	G	1	MSE
1	G	31	ILE
1	G	85	GLU
1	G	88	ASN
1	G	127	LEU
1	G	144	SER
1	G	145	ILE
1	G	176	GLN
1	G	205	GLU
1	G	246	GLU
1	G	341	GLN
1	G	380	PHE
1	G	417	LYS
1	G	429	CYS
1	G	452	TYR
1	H	0	MSE
1	H	3	THR
1	H	33	LEU
1	H	85	GLU
1	H	88	ASN
1	H	158	LYS

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Mol	Chain	Res	Type
1	H	194	GLU
1	H	222	ILE
1	H	239	THR
1	H	246	GLU
1	H	261	LEU
1	H	315	THR
1	H	325	ARG
1	H	341	GLN
1	H	342	LYS
1	H	380	PHE
1	H	423	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	HIS
1	B	176	GLN
1	B	244	HIS
1	C	341	GLN
1	D	94	ASN
1	D	176	GLN
1	E	176	GLN
1	E	341	GLN
1	F	176	GLN
1	G	176	GLN
1	H	94	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are 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	GOL	A	600	-	5,5,5	0.69	0	5,5,5	0.84	0
2	GOL	D	600	-	5,5,5	0.47	0	5,5,5	0.40	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	GOL	A	600	-	-	2/4/4/4	-
2	GOL	D	600	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	600	GOL	C1-C2-C3-O3
2	A	600	GOL	C1-C2-C3-O3
2	A	600	GOL	O2-C2-C3-O3
2	D	600	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	GOL	5	0
2	D	600	GOL	1	0



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	464/498 (93%)	-0.02	10 (2%) 62 69	32, 65, 100, 120	0
1	B	464/498 (93%)	-0.19	5 (1%) 80 85	34, 60, 90, 116	0
1	C	464/498 (93%)	-0.05	10 (2%) 62 69	30, 64, 96, 121	0
1	D	464/498 (93%)	-0.11	5 (1%) 80 85	37, 64, 96, 121	0
1	E	464/498 (93%)	-0.08	7 (1%) 73 79	32, 63, 94, 114	0
1	F	464/498 (93%)	0.05	21 (4%) 33 40	32, 66, 118, 156	0
1	G	463/498 (92%)	-0.21	7 (1%) 73 79	32, 56, 84, 110	0
1	H	464/498 (93%)	0.07	18 (3%) 39 46	38, 65, 99, 125	0
All	All	3711/3984 (93%)	-0.07	83 (2%) 62 69	30, 63, 100, 156	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	475	GLY	5.5
1	C	475	GLY	5.2
1	F	342	LYS	4.2
1	H	355	ASP	4.2
1	F	286	ILE	4.2
1	F	355	ASP	4.1
1	F	351	ARG	3.7
1	B	312	ASP	3.5
1	H	386	VAL	3.5
1	F	475	GLY	3.5
1	H	384	VAL	3.3
1	A	385	SER	3.3
1	E	475	GLY	3.2
1	E	286	ILE	3.1
1	A	384	VAL	3.1
1	E	320	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	386	VAL	3.0
1	C	342	LYS	3.0
1	F	312	ASP	3.0
1	H	321	PRO	3.0
1	C	312	ASP	2.9
1	A	386	VAL	2.9
1	A	286	ILE	2.9
1	H	385	SER	2.9
1	G	27	GLY	2.9
1	E	355	ASP	2.9
1	F	322	LEU	2.9
1	F	392	LYS	2.9
1	C	356	GLU	2.9
1	F	333	SER	2.8
1	B	286	ILE	2.8
1	E	386	VAL	2.8
1	A	38	HIS	2.8
1	F	387	THR	2.7
1	F	253	VAL	2.7
1	E	199	VAL	2.7
1	D	286	ILE	2.7
1	F	354	SER	2.7
1	F	376	ARG	2.7
1	C	29	GLY	2.7
1	D	312	ASP	2.6
1	H	286	ILE	2.6
1	B	392	LYS	2.5
1	H	475	GLY	2.5
1	F	385	SER	2.4
1	H	255	VAL	2.4
1	C	53	VAL	2.4
1	H	365	VAL	2.4
1	C	392	LYS	2.4
1	F	89	CYS	2.4
1	H	359	PHE	2.4
1	A	475	GLY	2.4
1	H	253	VAL	2.4
1	G	392	LYS	2.3
1	G	29	GLY	2.3
1	D	392	LYS	2.3
1	G	315	THR	2.3
1	A	319	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	356	GLU	2.3
1	A	315	THR	2.3
1	A	340	ASP	2.2
1	F	288	ALA	2.2
1	F	311	LEU	2.2
1	D	371	GLU	2.2
1	H	382	PRO	2.2
1	D	384	VAL	2.2
1	G	39	ALA	2.2
1	H	387	THR	2.2
1	H	320	GLY	2.2
1	F	326	ARG	2.1
1	A	356	GLU	2.1
1	F	254	ILE	2.1
1	H	311	LEU	2.1
1	C	355	ASP	2.1
1	G	351	ARG	2.1
1	E	384	VAL	2.1
1	H	90	GLY	2.1
1	C	371	GLU	2.0
1	F	321	PRO	2.0
1	H	312	ASP	2.0
1	G	28	ALA	2.0
1	C	280[A]	CYS	2.0
1	H	89	CYS	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	GOL	A	600	6/6	0.85	0.35	58,68,70,70	0
2	GOL	D	600	6/6	0.88	0.17	63,70,74,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.