



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:03 PM GMT

PDB ID : 4E4G  
Title : Crystal structure of putative Methylmalonate-semialdehyde dehydrogenase from *Sinorhizobium meliloti* 1021  
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2012-03-12  
Resolution : 2.90 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

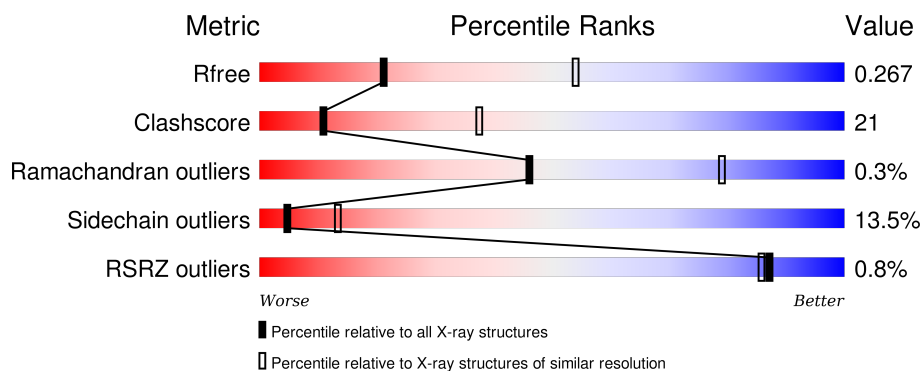
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	521	
1	B	521	
1	C	521	
1	D	521	
1	E	521	

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Mol	Chain	Length	Quality of chain
1	F	521	<div><div></div><div>2%</div><div>47%</div><div>38%</div><div>8%</div><div>7%</div></div>
1	G	521	<div><div></div><div>58%</div><div>30%</div><div>5%</div><div>7%</div></div>
1	H	521	<div><div></div><div>56%</div><div>33%</div><div>•</div><div>7%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29653 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 Methylmalonate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	Se	0	0	0
			3681	2325	640	693	5	18			
1	B	486	Total	C	N	O	S	Se	0	0	0
			3665	2316	638	689	5	17			
1	C	486	Total	C	N	O	S	Se	0	0	0
			3664	2315	637	689	5	18			
1	D	488	Total	C	N	O	S	Se	0	0	0
			3681	2325	640	693	5	18			
1	E	486	Total	C	N	O	S	Se	0	0	0
			3665	2316	638	689	5	17			
1	F	484	Total	C	N	O	S	Se	0	0	0
			3644	2301	635	686	5	17			
1	G	485	Total	C	N	O	S	Se	0	0	0
			3660	2312	636	688	5	19			
1	H	485	Total	C	N	O	S	Se	0	0	0
			3653	2307	637	687	5	17			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4
A	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
A	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
A	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
A	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4
A	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
A	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
A	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
A	-16	SER	-	EXPRESSION TAG	UNP Q92RW4
A	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
A	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
A	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
A	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
A	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
A	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
A	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
A	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
A	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
A	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4
A	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
A	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
A	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4
B	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4
B	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
B	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
B	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
B	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4
B	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
B	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
B	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
B	-16	SER	-	EXPRESSION TAG	UNP Q92RW4
B	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
B	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
B	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
B	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4
B	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
B	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
B	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
B	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
B	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
B	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
B	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4
B	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
B	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
B	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4
C	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4
C	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
C	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
C	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
C	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4
C	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
C	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
C	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
C	-16	SER	-	EXPRESSION TAG	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
C	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
C	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
C	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4
C	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
C	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
C	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
C	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
C	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
C	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
C	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4
C	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
C	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
C	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4
D	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4
D	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
D	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
D	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
D	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4
D	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
D	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
D	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
D	-16	SER	-	EXPRESSION TAG	UNP Q92RW4
D	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
D	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
D	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
D	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4
D	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
D	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
D	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
D	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
D	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
D	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
D	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4
D	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
D	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
D	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4
E	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4
E	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
E	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
E	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
E	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
E	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
E	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
E	-16	SER	-	EXPRESSION TAG	UNP Q92RW4
E	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
E	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
E	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
E	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4
E	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
E	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
E	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
E	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
E	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
E	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
E	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4
E	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
E	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
E	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4
F	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4
F	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
F	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
F	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
F	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4
F	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
F	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
F	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
F	-16	SER	-	EXPRESSION TAG	UNP Q92RW4
F	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
F	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
F	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
F	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4
F	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
F	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
F	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
F	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
F	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
F	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
F	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4
F	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
F	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
F	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4
G	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
G	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
G	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
G	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4
G	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
G	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
G	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
G	-16	SER	-	EXPRESSION TAG	UNP Q92RW4
G	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
G	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
G	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
G	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4
G	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
G	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
G	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
G	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
G	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
G	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
G	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4
G	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
G	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
G	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4
H	-24	MSE	-	EXPRESSION TAG	UNP Q92RW4
H	-23	HIS	-	EXPRESSION TAG	UNP Q92RW4
H	-22	HIS	-	EXPRESSION TAG	UNP Q92RW4
H	-21	HIS	-	EXPRESSION TAG	UNP Q92RW4
H	-20	HIS	-	EXPRESSION TAG	UNP Q92RW4
H	-19	HIS	-	EXPRESSION TAG	UNP Q92RW4
H	-18	HIS	-	EXPRESSION TAG	UNP Q92RW4
H	-17	SER	-	EXPRESSION TAG	UNP Q92RW4
H	-16	SER	-	EXPRESSION TAG	UNP Q92RW4
H	-15	GLY	-	EXPRESSION TAG	UNP Q92RW4
H	-14	VAL	-	EXPRESSION TAG	UNP Q92RW4
H	-13	ASP	-	EXPRESSION TAG	UNP Q92RW4
H	-12	LEU	-	EXPRESSION TAG	UNP Q92RW4
H	-11	GLY	-	EXPRESSION TAG	UNP Q92RW4
H	-10	THR	-	EXPRESSION TAG	UNP Q92RW4
H	-9	GLU	-	EXPRESSION TAG	UNP Q92RW4
H	-8	ASN	-	EXPRESSION TAG	UNP Q92RW4
H	-7	LEU	-	EXPRESSION TAG	UNP Q92RW4
H	-6	TYR	-	EXPRESSION TAG	UNP Q92RW4
H	-5	PHE	-	EXPRESSION TAG	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	GLN	-	EXPRESSION TAG	UNP Q92RW4
H	-3	SER	-	EXPRESSION TAG	UNP Q92RW4
H	-2	MSE	-	EXPRESSION TAG	UNP Q92RW4

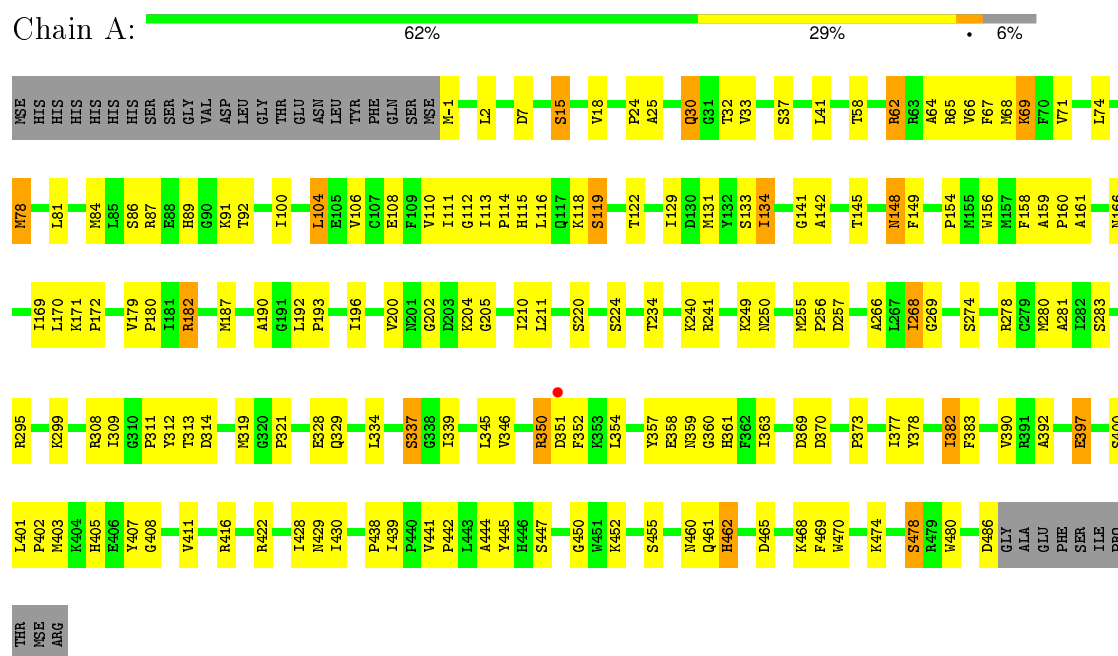
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	44	Total	O	0	0
			44	44		
2	C	51	Total	O	0	0
			51	51		
2	D	35	Total	O	0	0
			35	35		
2	E	33	Total	O	0	0
			33	33		
2	F	35	Total	O	0	0
			35	35		
2	G	42	Total	O	0	0
			42	42		
2	H	42	Total	O	0	0
			42	42		

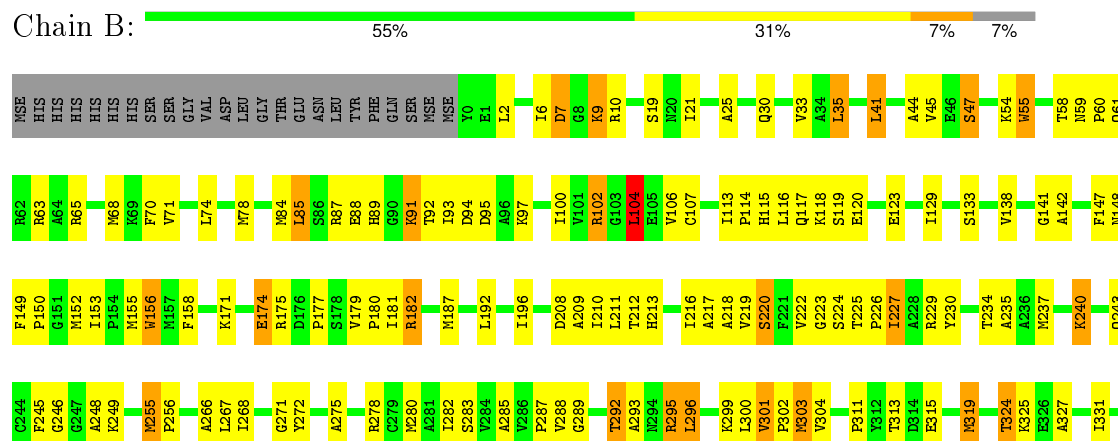
### 3 Residue-property plots

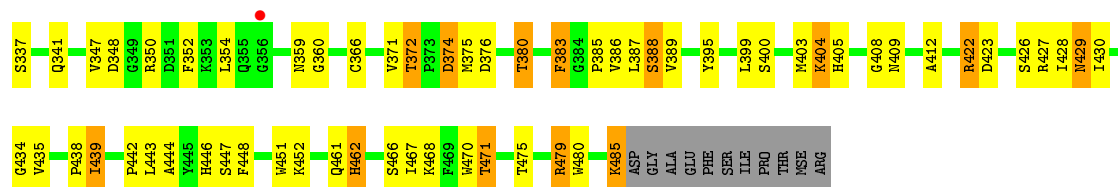
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Methylmalonate-semialdehyde dehydrogenase

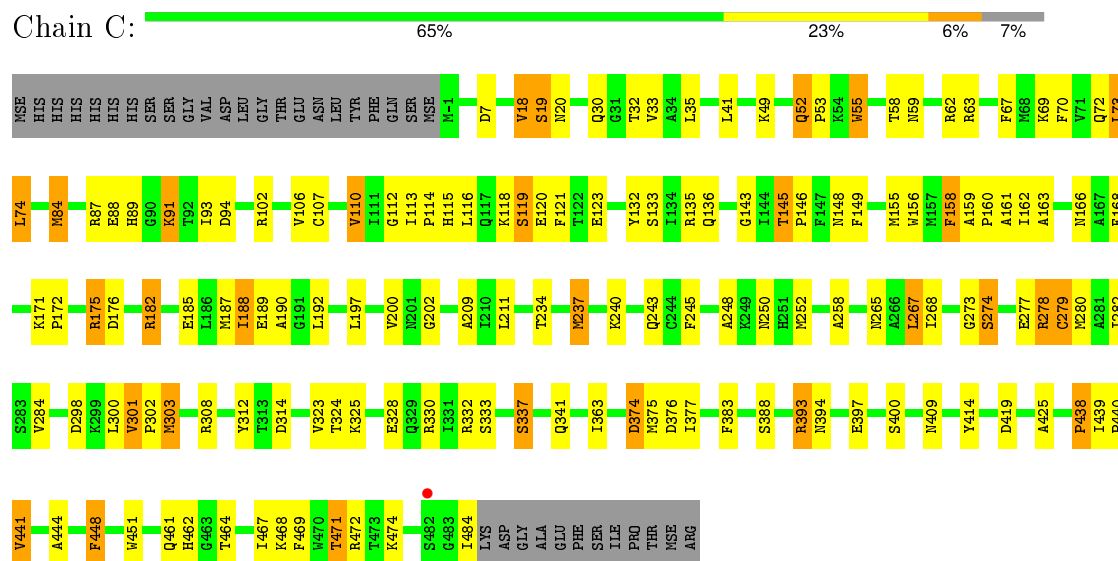


- Molecule 1: Methylmalonate-semialdehyde dehydrogenase

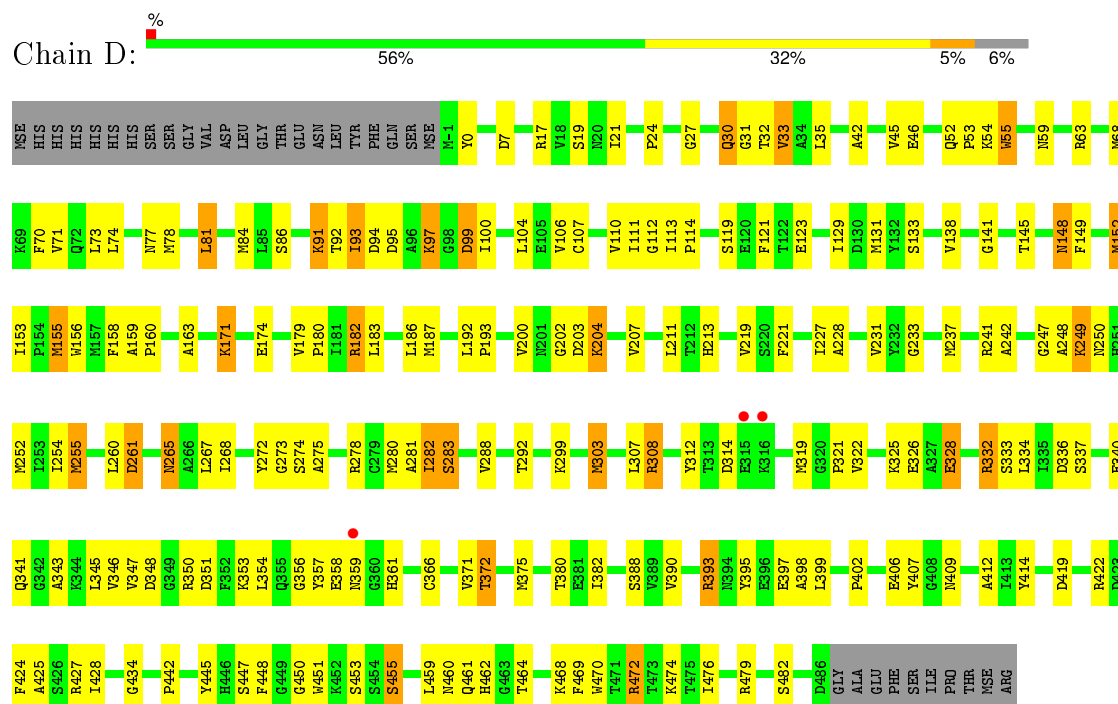




- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



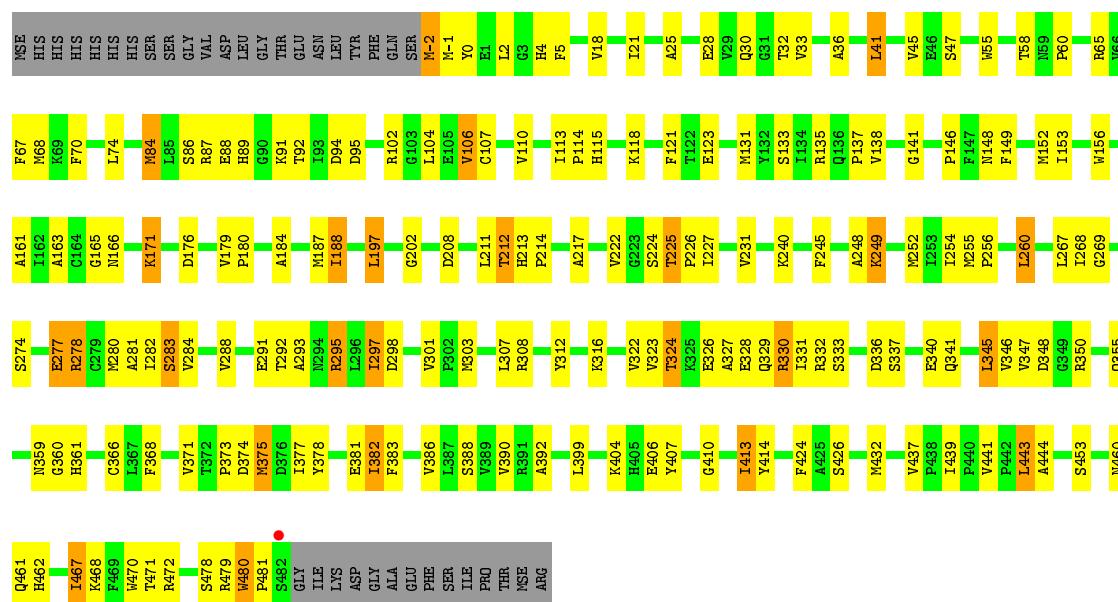
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



- Molecule 1: Methylmalonate-semialdehyde dehydrogenase

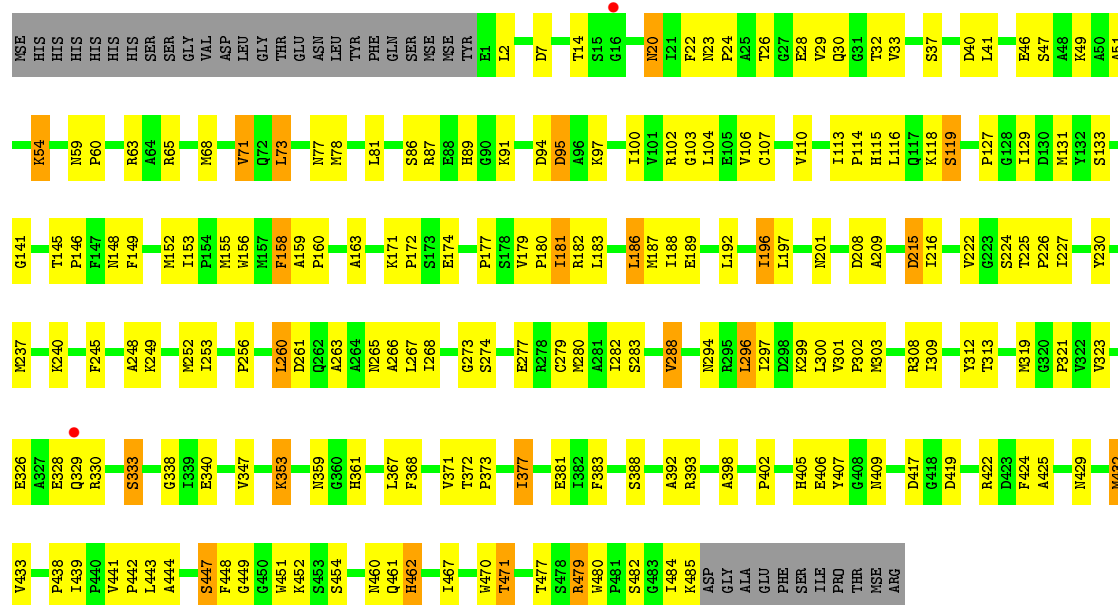






• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain H: 56% 33% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.44Å 171.28Å 159.69Å 90.00° 124.03° 90.00°	Depositor
Resolution (Å)	19.97 – 2.90 19.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.97-2.90) 98.9 (19.97-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.188 , 0.269 0.188 , 0.267	Depositor DCC
$R_{free}$ test set	4795 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 95963 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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 38.02 % 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 3.9244e-04. 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.60	1/3742 (0.0%)	0.72	1/5043 (0.0%)
1	B	0.60	2/3726 (0.1%)	0.74	4/5022 (0.1%)
1	C	0.61	1/3725 (0.0%)	0.75	2/5021 (0.0%)
1	D	0.63	1/3742 (0.0%)	0.73	3/5043 (0.1%)
1	E	0.60	1/3726 (0.0%)	0.77	7/5022 (0.1%)
1	F	0.75	8/3704 (0.2%)	0.77	5/4993 (0.1%)
1	G	0.61	2/3720 (0.1%)	0.75	1/5012 (0.0%)
1	H	0.62	2/3713 (0.1%)	0.73	1/5004 (0.0%)
All	All	0.63	18/29798 (0.1%)	0.75	24/40160 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	357	TYR	CG-CD2	13.39	1.56	1.39
1	F	357	TYR	CE1-CZ	9.63	1.51	1.38
1	F	451	TRP	CD2-CE2	6.00	1.48	1.41
1	C	55	TRP	CD2-CE2	5.79	1.48	1.41
1	A	312	TYR	CE1-CZ	-5.69	1.31	1.38
1	F	156	TRP	CD2-CE2	5.43	1.47	1.41
1	F	55	TRP	CD2-CE2	5.39	1.47	1.41
1	G	480	TRP	CD2-CE2	5.30	1.47	1.41
1	E	156	TRP	CD2-CE2	5.27	1.47	1.41
1	F	31	GLY	C-N	5.27	1.46	1.34
1	G	55	TRP	CD2-CE2	5.21	1.47	1.41
1	D	55	TRP	CD2-CE2	5.21	1.47	1.41
1	F	357	TYR	CD2-CE2	5.16	1.47	1.39
1	H	451	TRP	CD2-CE2	5.15	1.47	1.41
1	B	55	TRP	CD2-CE2	5.11	1.47	1.41
1	H	480	TRP	CD2-CE2	5.11	1.47	1.41
1	F	470	TRP	CD2-CE2	5.10	1.47	1.41
1	B	156	TRP	CD2-CE2	5.02	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	84	MSE	N-CA-CB	-6.81	98.34	110.60
1	E	259	ASP	CB-CG-OD1	-6.46	112.49	118.30
1	F	349	GLY	N-CA-C	6.34	128.95	113.10
1	F	332	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	F	273	GLY	N-CA-C	-5.84	98.50	113.10
1	B	319	MSE	N-CA-CB	-5.62	100.47	110.60
1	D	255	MSE	N-CA-CB	-5.55	100.61	110.60
1	E	229	ARG	N-CA-C	-5.48	96.20	111.00
1	B	104	LEU	CA-CB-CG	5.37	127.65	115.30
1	E	267	LEU	CA-CB-CG	5.37	127.64	115.30
1	E	296	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	74	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	D	81	LEU	CA-CB-CG	5.25	127.37	115.30
1	G	-1	MSE	N-CA-CB	-5.24	101.16	110.60
1	E	432	MSE	CA-CB-CG	-5.22	104.43	113.30
1	F	13	GLY	N-CA-C	-5.22	100.06	113.10
1	B	255	MSE	N-CA-CB	-5.21	101.23	110.60
1	D	152	MSE	CB-CA-C	-5.17	100.05	110.40
1	E	259	ASP	CB-CG-OD2	5.15	122.94	118.30
1	H	432	MSE	CA-CB-CG	-5.09	104.66	113.30
1	F	267	LEU	CA-CB-CG	5.06	126.94	115.30
1	C	303	MSE	CA-CB-CG	-5.03	104.75	113.30
1	B	429	ASN	CB-CA-C	-5.00	100.39	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3681	0	3652	107	0
1	B	3665	0	3639	161	0
1	C	3664	0	3635	117	0
1	D	3681	0	3652	140	0
1	E	3665	0	3639	225	1
1	F	3644	0	3617	253	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3660	0	3630	128	0
1	H	3653	0	3630	148	0
2	A	58	0	0	2	0
2	B	44	0	0	2	0
2	C	51	0	0	3	0
2	D	35	0	0	1	0
2	E	33	0	0	1	0
2	F	35	0	0	2	0
2	G	42	0	0	2	0
2	H	42	0	0	5	0
All	All	29653	0	29094	1224	1

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 21.

All (1224) 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:F:70:PHE:CE1	1:F:187:MSE:SE	2.30	1.33
1:H:110:VAL:CG1	1:H:163:ALA:HB2	1.78	1.13
1:F:126:GLY:HA3	1:F:129:ILE:HB	1.28	1.12
1:F:68:MSE:HE1	1:H:71:VAL:HG11	1.14	1.11
1:F:152:MSE:HE2	1:F:153:ILE:HD11	1.29	1.09
1:B:74:LEU:CD2	1:B:155:MSE:HE1	1.83	1.09
1:C:74:LEU:HD11	1:C:155:MSE:HE1	1.33	1.09
1:F:350:ARG:CG	1:F:351:ASP:H	1.64	1.08
1:F:174:GLU:HG3	1:F:203:ASP:OD2	1.54	1.08
1:G:324:THR:HG22	1:G:327:ALA:H	1.17	1.06
1:F:70:PHE:CD1	1:F:187:MSE:SE	2.60	1.05
1:E:432:MSE:HE3	1:E:442:PRO:HD2	1.38	1.04
1:E:131:MSE:HE2	1:F:446:HIS:CD2	1.93	1.04
1:E:131:MSE:HE1	1:F:443:LEU:H	1.22	1.03
1:H:110:VAL:HG13	1:H:163:ALA:CB	1.90	1.02
1:F:99:ASP:O	1:F:152:MSE:HB2	1.60	1.01
1:D:372:THR:HG22	1:D:375:MSE:HE3	1.45	0.98
1:E:138:VAL:HA	1:E:472:ARG:HD2	1.45	0.98
1:F:187:MSE:HB3	1:F:192:LEU:HD12	1.43	0.98
1:G:324:THR:CG2	1:G:327:ALA:H	1.76	0.98
1:D:372:THR:CG2	1:D:375:MSE:HE3	1.93	0.98
1:F:350:ARG:HG2	1:F:351:ASP:H	1.29	0.98
1:B:74:LEU:HD21	1:B:155:MSE:HE1	1.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:GLU:HB2	1:F:175:ARG:NH1	1.79	0.96
1:F:227:ILE:O	1:F:231:VAL:HG23	1.65	0.96
1:F:152:MSE:CE	1:F:153:ILE:HD11	1.96	0.95
1:G:322:VAL:CG1	1:G:323:VAL:N	2.30	0.95
1:F:148:ASN:ND2	1:F:383:PHE:HZ	1.65	0.94
1:B:70:PHE:HE2	1:B:155:MSE:HE3	1.31	0.94
1:H:338:GLY:HA3	1:H:377:ILE:HD12	1.50	0.93
1:D:280:MSE:HE1	1:D:409:ASN:HB3	1.50	0.93
1:F:148:ASN:HD21	1:F:383:PHE:HZ	1.05	0.93
1:B:78:MSE:HE2	1:B:97:LYS:HG3	1.50	0.92
1:F:360:GLY:HA3	1:F:362:PHE:HE1	1.33	0.92
1:D:393:ARG:HH22	1:D:397:GLU:HG3	1.33	0.92
1:H:51:ALA:HB1	1:H:196:ILE:HD12	1.49	0.92
1:E:429:ASN:HB3	1:E:452:LYS:HE2	1.49	0.91
1:F:350:ARG:CG	1:F:351:ASP:N	2.30	0.91
1:D:280:MSE:CE	1:D:409:ASN:HB3	2.00	0.91
1:F:324:THR:C	1:F:361:HIS:CD2	2.44	0.91
1:F:350:ARG:HG2	1:F:351:ASP:N	1.81	0.90
1:D:70:PHE:HE2	1:D:155:MSE:HE3	1.36	0.90
1:E:308:ARG:NH1	1:E:316:LYS:HB2	1.87	0.90
1:D:255:MSE:HE1	1:D:395:TYR:HB2	1.54	0.90
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.37	0.90
1:C:474:LYS:HE2	1:D:425:ALA:O	1.73	0.88
1:A:41:LEU:HD11	1:A:210:ILE:HG13	1.56	0.88
1:E:259:ASP:OD1	1:E:260:LEU:N	2.06	0.88
1:G:322:VAL:HG12	1:G:323:VAL:N	1.84	0.88
1:F:362:PHE:CD1	1:F:362:PHE:N	2.41	0.88
1:F:153:ILE:CD1	1:F:153:ILE:N	2.36	0.88
1:F:362:PHE:N	1:F:362:PHE:HD1	1.72	0.88
1:H:110:VAL:HG11	1:H:163:ALA:HB2	1.53	0.87
1:E:156:TRP:CE3	1:E:461:GLN:HG2	2.08	0.87
1:F:26:THR:OG1	1:F:28:GLU:HG2	1.75	0.87
1:C:341:GLN:HE22	1:C:376:ASP:H	1.22	0.87
1:B:116:LEU:HB3	1:B:467:ILE:HD13	1.55	0.87
1:F:325:LYS:N	1:F:361:HIS:CD2	2.42	0.87
1:F:70:PHE:HE1	1:F:187:MSE:SE	2.01	0.86
1:H:110:VAL:HG13	1:H:163:ALA:HB2	1.53	0.86
1:E:308:ARG:HH12	1:E:316:LYS:HB2	1.41	0.86
1:F:152:MSE:HE2	1:F:153:ILE:CD1	2.05	0.86
1:G:4:HIS:CE1	1:G:36:ALA:HB2	2.10	0.86
1:C:89:HIS:ND1	1:C:91:LYS:HG2	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:ARG:N	1:G:295:ARG:HD2	1.91	0.85
1:E:300:LEU:HD23	1:E:367:LEU:HD11	1.57	0.85
1:H:110:VAL:CG1	1:H:163:ALA:CB	2.51	0.85
1:B:268:ILE:HG13	1:B:303:MSE:HG2	1.58	0.85
1:F:126:GLY:CA	1:F:129:ILE:HB	2.08	0.84
1:F:350:ARG:HG3	1:F:351:ASP:H	1.43	0.84
1:G:323:VAL:HG22	1:G:323:VAL:O	1.76	0.84
1:C:74:LEU:HD11	1:C:155:MSE:CE	2.07	0.84
1:E:131:MSE:HE2	1:F:446:HIS:HD2	1.39	0.84
1:B:275:ALA:HA	1:B:319:MSE:HE2	1.58	0.84
1:E:102:ARG:HG2	1:E:102:ARG:HH21	1.43	0.84
1:E:131:MSE:HE1	1:F:443:LEU:N	1.91	0.84
1:D:250:ASN:HD21	1:D:280:MSE:HE2	1.42	0.84
1:C:156:TRP:CE3	1:C:461:GLN:HG2	2.13	0.83
1:C:148:ASN:ND2	1:C:149:PHE:CE2	2.46	0.83
1:G:293:ALA:O	1:G:297:ILE:HG12	1.79	0.83
1:G:188:ILE:HD11	2:G:502:HOH:O	1.77	0.83
1:F:127:PRO:HG3	2:G:531:HOH:O	1.77	0.82
1:B:41:LEU:HD11	1:B:210:ILE:HG13	1.60	0.82
1:F:148:ASN:ND2	1:F:383:PHE:CZ	2.48	0.82
1:F:347:VAL:HG11	1:F:366:CYS:HA	1.62	0.81
1:A:405:HIS:HD2	1:A:407:TYR:H	1.29	0.81
1:F:256:PRO:HD3	1:F:288:VAL:CG2	2.10	0.81
1:E:255:MSE:CB	1:E:257:ASP:OD1	2.28	0.81
1:C:148:ASN:ND2	1:C:149:PHE:CD2	2.48	0.81
1:G:324:THR:HG22	1:G:327:ALA:N	1.96	0.80
1:E:131:MSE:HE3	1:F:446:HIS:HB2	1.63	0.80
1:B:319:MSE:HE2	1:B:385:PRO:HB3	1.61	0.80
1:H:103:GLY:O	1:H:106:VAL:HG12	1.82	0.80
1:F:68:MSE:CE	1:H:71:VAL:HG11	2.05	0.80
1:A:403:MSE:SE	1:A:429:ASN:ND2	2.65	0.80
1:D:70:PHE:CE2	1:D:155:MSE:HE3	2.16	0.80
1:G:255:MSE:HE1	1:G:413:ILE:HD11	1.61	0.80
1:E:431:GLY:HA2	1:E:451:TRP:NE1	1.96	0.79
1:D:207:VAL:O	1:D:211:LEU:HD23	1.79	0.79
1:E:131:MSE:CE	1:F:443:LEU:H	1.96	0.79
1:G:323:VAL:O	1:G:323:VAL:CG2	2.30	0.79
1:C:74:LEU:CD1	1:C:155:MSE:HE1	2.12	0.79
1:G:0:TYR:CE1	1:G:30:GLN:HG3	2.16	0.79
1:H:248:ALA:O	1:H:381:GLU:HG3	1.83	0.79
1:H:280:MSE:CE	1:H:409:ASN:ND2	2.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:THR:HG23	1:B:327:ALA:H	1.48	0.79
1:F:135:ARG:HH12	1:F:467:ILE:CG2	1.96	0.79
1:D:203:ASP:CG	1:D:204:LYS:H	1.84	0.79
1:E:295:ARG:HH11	1:E:295:ARG:HG3	1.45	0.79
1:G:252:MSE:HE2	1:G:254:ILE:HG12	1.63	0.78
1:F:35:LEU:HD13	1:F:203:ASP:H	1.46	0.78
1:E:187:MSE:HE3	1:E:192:LEU:HD22	1.65	0.78
1:F:171:LYS:HE2	1:F:207:VAL:HG22	1.66	0.78
1:E:131:MSE:CE	1:F:446:HIS:HB2	2.14	0.78
1:B:115:HIS:CD2	1:B:118:LYS:HE3	2.18	0.78
1:F:175:ARG:HH21	1:F:175:ARG:HG3	1.49	0.77
1:F:308:ARG:HB3	1:F:317:ALA:HA	1.65	0.77
1:G:322:VAL:HG13	1:G:323:VAL:H	1.49	0.77
1:G:248:ALA:O	1:G:381:GLU:HG3	1.85	0.77
1:E:227:ILE:O	1:E:230:TYR:HB3	1.84	0.77
1:B:65:ARG:HA	1:B:68:MSE:HE3	1.64	0.76
1:D:393:ARG:HH22	1:D:397:GLU:CG	1.96	0.76
1:B:319:MSE:CE	1:B:385:PRO:HB3	2.14	0.76
1:H:115:HIS:HA	1:H:118:LYS:HE3	1.67	0.76
1:E:159:ALA:HB3	1:E:160:PRO:HD3	1.68	0.76
1:A:78:MSE:HE3	1:A:100:ILE:HG21	1.67	0.76
1:G:179:VAL:HB	1:G:180:PRO:HD3	1.67	0.76
1:H:30:GLN:OE1	1:H:87:ARG:HD2	1.85	0.76
1:E:451:TRP:O	1:E:452:LYS:HB2	1.86	0.75
1:H:187:MSE:HE3	1:H:192:LEU:HD22	1.66	0.75
1:G:225:THR:HG21	1:G:407:TYR:HE1	1.52	0.75
1:F:153:ILE:HD13	1:F:153:ILE:N	2.02	0.75
1:G:327:ALA:O	1:G:331:ILE:HD12	1.86	0.75
1:E:371:VAL:HG21	1:E:388:SER:HB3	1.67	0.75
1:B:89:HIS:ND1	1:B:91:LYS:HB3	2.02	0.74
1:F:192:LEU:HD22	1:F:196:ILE:HD11	1.67	0.74
1:E:207:VAL:O	1:E:211:LEU:CD2	2.35	0.74
1:E:153:ILE:HG13	1:E:157:MSE:HE2	1.67	0.74
1:D:207:VAL:O	1:D:211:LEU:CD2	2.35	0.74
1:D:249:LYS:HD3	1:D:283:SER:OG	1.88	0.74
1:F:174:GLU:CG	1:F:203:ASP:OD2	2.34	0.74
1:F:442:PRO:HG2	1:F:447:SER:O	1.88	0.74
1:F:311:PRO:HG2	1:F:357:TYR:CZ	2.23	0.73
1:A:62:ARG:NH1	2:A:553:HOH:O	2.21	0.73
1:G:225:THR:HG21	1:G:407:TYR:CE1	2.22	0.73
1:A:65:ARG:HA	1:A:68:MSE:HE3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:GLU:OE2	1:C:332:ARG:NH1	2.21	0.73
1:B:376:ASP:O	1:B:380:THR:HG23	1.87	0.73
1:D:156:TRP:CE3	1:D:461:GLN:HG2	2.24	0.73
1:A:350:ARG:CG	1:A:350:ARG:HH11	2.01	0.73
1:F:68:MSE:HE1	1:H:71:VAL:CG1	2.08	0.72
1:C:274:SER:HA	2:C:511:HOH:O	1.90	0.72
1:E:192:LEU:HD11	1:E:196:ILE:HG21	1.69	0.72
1:F:369:ASP:O	1:F:370:ASP:HB2	1.87	0.72
1:C:280:MSE:CE	1:C:409:ASN:ND2	2.52	0.72
1:E:484:ILE:O	1:E:485:LYS:HG2	1.89	0.72
1:B:84:MSE:HE1	1:B:182:ARG:HG2	1.70	0.72
1:H:467:ILE:O	1:H:471:THR:HB	1.89	0.72
1:E:451:TRP:CH2	1:F:472:ARG:HD3	2.24	0.72
1:B:289:GLY:HA3	1:B:292:THR:HG23	1.72	0.72
1:B:70:PHE:CE2	1:B:155:MSE:HE3	2.21	0.71
1:B:116:LEU:HD13	1:B:467:ILE:CD1	2.20	0.71
1:C:265:ASN:OD1	1:C:303:MSE:HE1	1.90	0.71
1:H:78:MSE:HE2	1:H:97:LYS:HA	1.72	0.71
1:B:280:MSE:O	1:B:439:ILE:HG22	1.91	0.71
1:E:71:VAL:HG13	1:E:104:LEU:HG	1.72	0.71
1:B:372:THR:HG22	1:B:375:MSE:HG3	1.71	0.71
1:B:92:THR:HG22	1:B:94:ASP:N	2.04	0.71
1:F:328:GLU:HG3	1:F:363:ILE:HD11	1.73	0.71
1:C:472:ARG:NH1	1:D:451:TRP:CE3	2.58	0.71
1:F:322:VAL:HG12	1:F:323:VAL:H	1.55	0.70
1:F:350:ARG:O	1:F:351:ASP:CG	2.28	0.70
1:G:92:THR:HG22	1:G:94:ASP:H	1.56	0.70
1:G:41:LEU:O	1:G:45:VAL:HG23	1.91	0.70
1:F:362:PHE:HD1	1:F:362:PHE:H	1.38	0.70
1:E:255:MSE:HB2	1:E:257:ASP:OD1	1.92	0.70
1:G:0:TYR:HE1	1:G:30:GLN:HG3	1.54	0.70
1:B:324:THR:CG2	1:B:327:ALA:H	2.04	0.70
1:E:255:MSE:HB3	1:E:257:ASP:OD1	1.90	0.70
1:D:356:GLY:C	1:D:358:GLU:OE1	2.30	0.70
1:F:350:ARG:C	1:F:351:ASP:OD2	2.30	0.70
1:G:322:VAL:CG1	1:G:323:VAL:H	1.98	0.69
1:F:171:LYS:HE2	1:F:207:VAL:CG2	2.21	0.69
1:H:22:PHE:O	1:H:30:GLN:NE2	2.25	0.69
1:E:309:ILE:HG12	1:E:319:MSE:HE3	1.73	0.69
1:H:78:MSE:HE2	1:H:97:LYS:HG2	1.73	0.69
1:D:110:VAL:HG13	1:D:163:ALA:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:THR:HB	1:E:172:PRO:HA	1.75	0.69
1:B:311:PRO:HG2	1:B:313:THR:HG22	1.73	0.69
1:B:211:LEU:HD13	1:B:234:THR:HB	1.73	0.69
1:H:301:VAL:HG12	1:H:347:VAL:HG23	1.75	0.69
1:G:153:ILE:O	1:G:156:TRP:HB2	1.93	0.69
1:C:84:MSE:HE1	1:C:182:ARG:HG3	1.75	0.69
1:B:74:LEU:HD21	1:B:155:MSE:CE	2.20	0.69
1:E:268:ILE:HD12	1:E:300:LEU:HD12	1.74	0.69
1:G:252:MSE:HB2	1:G:282:ILE:HD12	1.74	0.68
1:A:78:MSE:HE2	1:A:78:MSE:HA	1.75	0.68
1:F:153:ILE:HD12	1:F:153:ILE:N	2.07	0.68
1:G:30:GLN:NE2	1:G:87:ARG:HE	1.90	0.68
1:A:115:HIS:HD2	1:A:118:LYS:NZ	1.91	0.68
1:H:129:ILE:HG13	1:H:479:ARG:HG3	1.76	0.68
1:C:280:MSE:HE1	1:C:409:ASN:CG	2.13	0.68
1:H:78:MSE:HE1	1:H:100:ILE:HB	1.75	0.68
1:D:393:ARG:NH2	1:D:397:GLU:HG3	2.07	0.68
1:G:274:SER:O	1:G:277:GLU:HG3	1.94	0.68
1:C:341:GLN:HB2	1:C:375:MSE:HE3	1.76	0.68
1:F:361:HIS:N	1:F:361:HIS:ND1	2.41	0.68
1:B:372:THR:HB	1:B:375:MSE:HE3	1.76	0.68
1:B:7:ASP:O	1:B:9:LYS:HE3	1.94	0.68
1:F:325:LYS:N	1:F:361:HIS:HD2	1.90	0.67
1:F:371:VAL:HG12	1:F:372:THR:N	2.09	0.67
1:E:168:PHE:HE1	1:E:470:TRP:CH2	2.12	0.67
1:C:107:CYS:SG	1:C:155:MSE:HE2	2.35	0.67
1:E:448:PHE:C	1:E:448:PHE:CD1	2.66	0.67
1:G:255:MSE:CE	1:G:413:ILE:HD11	2.23	0.67
1:F:272:TYR:HE1	1:F:385:PRO:O	1.76	0.67
1:B:116:LEU:HD13	1:B:467:ILE:HD11	1.75	0.67
1:F:113:ILE:HG22	1:F:114:PRO:HD3	1.77	0.67
1:A:81:LEU:HD21	1:A:182:ARG:HG2	1.77	0.67
1:E:131:MSE:CE	1:F:446:HIS:CD2	2.76	0.66
1:E:259:ASP:C	1:E:259:ASP:OD1	2.30	0.66
1:F:26:THR:OG1	1:F:28:GLU:CG	2.43	0.66
1:G:371:VAL:HG23	1:G:390:VAL:HG22	1.76	0.66
1:C:171:LYS:HE3	1:C:202:GLY:O	1.95	0.66
1:E:127:PRO:C	1:E:129:ILE:HD12	2.15	0.66
1:E:149:PHE:O	1:E:153:ILE:HG22	1.94	0.66
1:F:324:THR:C	1:F:361:HIS:HD2	1.96	0.66
1:E:127:PRO:O	1:E:129:ILE:HD12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:MSE:HE2	1:B:97:LYS:CG	2.24	0.66
1:B:403:MSE:O	1:B:429:ASN:ND2	2.29	0.66
1:H:37:SER:H	1:H:40:ASP:HB2	1.61	0.66
1:H:266:ALA:HB1	1:H:438:PRO:HG3	1.77	0.66
1:B:372:THR:HG23	1:B:374:ASP:H	1.59	0.66
1:G:324:THR:HG23	1:G:326:GLU:OE1	1.96	0.66
1:A:358:GLU:O	1:A:359:ASN:HB2	1.95	0.66
1:E:467:ILE:O	1:E:471:THR:HB	1.96	0.66
1:A:309:ILE:HG12	1:A:319:MSE:HE3	1.78	0.66
1:F:256:PRO:HD3	1:F:288:VAL:HG23	1.78	0.65
1:E:432:MSE:HE3	1:E:441:VAL:HA	1.77	0.65
1:B:372:THR:CG2	1:B:374:ASP:H	2.09	0.65
1:F:113:ILE:CG2	1:F:114:PRO:HD3	2.26	0.65
1:B:220:SER:HB3	1:B:243:GLN:HG3	1.77	0.65
1:F:153:ILE:H	1:F:153:ILE:HD13	1.61	0.65
1:B:296:LEU:HD13	1:B:300:LEU:HD12	1.78	0.65
1:F:135:ARG:NH1	1:F:467:ILE:CG2	2.59	0.65
1:H:148:ASN:ND2	1:H:149:PHE:CE1	2.65	0.65
1:B:400:SER:O	1:B:404:LYS:HB2	1.98	0.65
1:F:252:MSE:SE	1:F:267:LEU:HD13	2.47	0.65
1:B:89:HIS:CE1	1:B:91:LYS:HB3	2.33	0.64
1:C:113:ILE:N	1:C:114:PRO:HD2	2.13	0.64
1:F:70:PHE:HE2	1:F:155:MSE:HE1	1.61	0.64
1:D:358:GLU:OE1	1:D:358:GLU:N	2.30	0.64
1:A:161:ALA:O	1:A:166:ASN:HB2	1.98	0.64
1:E:55:TRP:CZ2	1:E:63:ARG:HG2	2.32	0.64
1:E:432:MSE:HE1	1:E:441:VAL:HG23	1.80	0.64
1:E:228:ALA:O	1:E:229:ARG:C	2.36	0.64
1:C:148:ASN:HD21	1:C:149:PHE:HE2	1.44	0.64
1:D:332:ARG:HH12	1:D:350:ARG:HB2	1.61	0.64
1:F:369:ASP:OD1	1:F:370:ASP:N	2.29	0.64
1:B:45:VAL:HG11	1:B:213:HIS:CE1	2.33	0.64
1:G:366:CYS:HB2	1:G:386:VAL:HG22	1.80	0.64
1:F:70:PHE:HE1	1:F:187:MSE:CG	2.11	0.64
1:F:224:SER:HB2	1:F:227:ILE:HG12	1.79	0.64
1:A:486:ASP:OD1	1:C:394:ASN:HB2	1.98	0.64
1:E:207:VAL:O	1:E:211:LEU:HD22	1.98	0.64
1:H:159:ALA:HB3	1:H:160:PRO:CD	2.28	0.64
1:C:70:PHE:HE2	1:C:155:MSE:HE3	1.62	0.64
1:E:129:ILE:N	1:E:129:ILE:HD12	2.13	0.64
1:E:131:MSE:HE3	1:F:446:HIS:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:CD1	1:C:132:TYR:HB3	2.33	0.63
1:G:260:LEU:HD11	1:G:292:THR:HG23	1.81	0.63
1:F:88:GLU:CD	1:F:178:SER:OG	2.36	0.63
1:E:462:HIS:HA	1:E:466:SER:OG	1.98	0.63
1:B:78:MSE:HE2	1:B:97:LYS:HA	1.81	0.63
1:E:157:MSE:SE	1:E:220:SER:HB3	2.48	0.63
1:G:371:VAL:CG2	1:G:390:VAL:HG22	2.29	0.63
1:A:266:ALA:HB1	1:A:438:PRO:HB3	1.79	0.63
1:E:102:ARG:CG	1:E:102:ARG:HH21	2.11	0.63
1:H:22:PHE:C	1:H:30:GLN:HE21	2.02	0.63
1:B:485:LYS:NZ	1:D:419:ASP:OD2	2.31	0.63
1:B:366:CYS:HB2	1:B:386:VAL:HG22	1.80	0.63
1:G:225:THR:HG23	1:G:226:PRO:HD3	1.81	0.63
1:E:478:SER:HB2	1:F:435:VAL:HB	1.81	0.63
1:E:211:LEU:HD11	1:E:231:VAL:HG13	1.81	0.63
1:B:119:SER:CB	1:B:133:SER:O	2.47	0.63
1:C:30:GLN:HE22	1:C:87:ARG:HE	1.47	0.63
1:F:446:HIS:O	1:F:462:HIS:ND1	2.32	0.62
1:F:90:GLY:O	1:F:321:PRO:HD2	1.99	0.62
1:D:45:VAL:HG11	1:D:213:HIS:CE1	2.34	0.62
1:H:2:LEU:HD22	1:H:181:ILE:HD12	1.80	0.62
1:B:91:LYS:NZ	1:B:148:ASN:O	2.33	0.62
1:H:78:MSE:CE	1:H:97:LYS:HA	2.29	0.62
1:B:92:THR:HG22	1:B:94:ASP:H	1.64	0.62
1:H:156:TRP:CE3	1:H:461:GLN:HG2	2.35	0.62
1:D:203:ASP:CG	1:D:204:LYS:N	2.53	0.62
1:C:374:ASP:N	1:C:374:ASP:OD1	2.31	0.62
1:E:268:ILE:HD13	1:E:303:MSE:SE	2.49	0.62
1:A:179:VAL:HB	1:A:180:PRO:HD3	1.82	0.62
1:B:71:VAL:HG13	1:B:104:LEU:HD21	1.81	0.62
1:H:106:VAL:HA	1:H:444:ALA:HB1	1.81	0.62
1:C:248:ALA:HB1	1:C:250:ASN:OD1	1.99	0.62
1:E:268:ILE:CD1	1:E:300:LEU:HD12	2.29	0.61
1:H:115:HIS:O	1:H:118:LYS:HG3	2.00	0.61
1:E:171:LYS:NZ	1:E:171:LYS:O	2.30	0.61
1:H:33:VAL:HG11	1:H:174:GLU:HB2	1.82	0.61
1:B:55:TRP:CZ2	1:B:63:ARG:HG2	2.35	0.61
1:H:77:ASN:O	1:H:81:LEU:HB2	2.00	0.61
1:B:301:VAL:HG12	1:B:302:PRO:HD3	1.82	0.61
1:H:224:SER:OG	1:H:227:ILE:HD12	2.00	0.61
1:E:127:PRO:O	1:E:129:ILE:CD1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLY:HA2	1:A:430:ILE:HG13	1.83	0.61
1:A:159:ALA:HB3	1:A:160:PRO:HD3	1.81	0.61
1:B:119:SER:HB2	1:C:121:PHE:HB3	1.83	0.61
1:E:372:THR:HB	1:E:375:MSE:HG3	1.83	0.61
1:F:183:LEU:HA	1:F:186:LEU:HD12	1.81	0.61
1:E:211:LEU:H	1:E:211:LEU:HD22	1.66	0.61
1:F:152:MSE:CE	1:F:153:ILE:CD1	2.73	0.60
1:G:348:ASP:OD1	1:G:350:ARG:HB2	2.00	0.60
1:C:211:LEU:O	1:C:240:LYS:HE2	2.02	0.60
1:F:59:ASN:HD22	1:F:59:ASN:C	2.03	0.60
1:C:135:ARG:HD3	1:C:471:THR:HG21	1.83	0.60
1:F:192:LEU:HD13	1:F:196:ILE:HD11	1.82	0.60
1:B:78:MSE:HE1	1:B:100:ILE:HB	1.84	0.60
1:H:280:MSE:CE	1:H:409:ASN:CG	2.69	0.60
1:C:273:GLY:O	1:C:278:ARG:NH2	2.34	0.60
1:F:175:ARG:NH2	1:F:175:ARG:HG3	2.17	0.60
1:H:280:MSE:HE3	1:H:409:ASN:ND2	2.17	0.60
1:F:179:VAL:HB	1:F:180:PRO:HD3	1.83	0.60
1:F:302:PRO:O	1:F:306:SER:OG	2.20	0.60
1:B:447:SER:HA	1:B:462:HIS:CD2	2.37	0.60
1:H:225:THR:HB	1:H:226:PRO:HD3	1.83	0.60
1:H:353:LYS:HA	1:H:353:LYS:HE3	1.84	0.60
1:B:113:ILE:HD11	1:B:117:GLN:HG3	1.84	0.60
1:D:227:ILE:O	1:D:231:VAL:HG23	2.02	0.60
1:D:0:TYR:O	1:D:31:GLY:HA2	2.02	0.60
1:E:257:ASP:N	1:E:257:ASP:OD1	2.34	0.60
1:F:35:LEU:HD12	1:F:36:ALA:N	2.16	0.60
1:B:115:HIS:HD2	1:B:118:LYS:HE3	1.62	0.59
1:C:268:ILE:HG13	1:C:303:MSE:HB3	1.84	0.59
1:F:446:HIS:O	1:F:462:HIS:CE1	2.55	0.59
1:F:439:ILE:O	1:F:439:ILE:CG2	2.49	0.59
1:B:74:LEU:HD22	1:B:155:MSE:HE1	1.77	0.59
1:B:467:ILE:O	1:B:471:THR:HB	2.01	0.59
1:D:354:LEU:O	1:D:357:TYR:HB2	2.02	0.59
1:B:222:VAL:HG13	1:B:245:PHE:HB2	1.84	0.59
1:C:337:SER:O	1:C:341:GLN:HG3	2.02	0.59
1:C:279:CYS:O	1:C:280:MSE:HE2	2.02	0.59
1:E:474:LYS:HD2	1:F:430:ILE:O	2.02	0.59
1:B:187:MSE:HG2	1:B:192:LEU:HD22	1.84	0.59
1:C:252:MSE:SE	1:C:267:LEU:HD13	2.53	0.59
1:E:432:MSE:CE	1:E:441:VAL:HG23	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NH1	1:A:469:PHE:O	2.35	0.59
1:G:65:ARG:HA	1:G:68:MSE:HE3	1.85	0.59
1:H:65:ARG:HA	1:H:68:MSE:HG2	1.84	0.59
1:C:467:ILE:O	1:C:471:THR:HB	2.03	0.59
1:F:334:LEU:HD13	1:F:382:ILE:HG12	1.85	0.59
1:D:110:VAL:HG13	1:D:163:ALA:CB	2.32	0.59
1:C:425:ALA:O	1:D:474:LYS:HE2	2.03	0.59
1:F:446:HIS:ND1	2:F:506:HOH:O	2.23	0.58
1:G:332:ARG:NH2	1:G:350:ARG:O	2.36	0.58
1:G:171:LYS:NZ	1:G:202:GLY:O	2.36	0.58
1:C:19:SER:HB2	1:C:35:LEU:HD21	1.85	0.58
1:D:171:LYS:HE3	1:D:202:GLY:O	2.03	0.58
1:C:308:ARG:NH1	1:C:314:ASP:OD2	2.35	0.58
1:D:158:PHE:CE1	1:D:187:MSE:HE3	2.38	0.58
1:B:119:SER:HB3	1:B:133:SER:O	2.04	0.58
1:G:222:VAL:HG22	1:G:245:PHE:HB2	1.83	0.58
1:F:252:MSE:HE2	1:F:254:ILE:CG1	2.33	0.58
1:D:371:VAL:HB	1:D:390:VAL:HG22	1.85	0.58
1:A:249:LYS:HE3	1:A:283:SER:CB	2.34	0.58
1:F:187:MSE:HB3	1:F:192:LEU:CD1	2.27	0.58
1:C:119:SER:HB2	1:C:133:SER:O	2.03	0.58
1:D:52:GLN:HG3	1:D:53:PRO:HD3	1.85	0.58
1:A:145:THR:OG1	1:A:172:PRO:HA	2.03	0.58
1:B:423:ASP:O	1:B:427:ARG:HG3	2.04	0.58
1:H:179:VAL:HB	1:H:180:PRO:HD3	1.85	0.58
1:D:33:VAL:HG21	1:D:174:GLU:HB2	1.86	0.58
1:A:78:MSE:HE1	1:A:100:ILE:HG13	1.86	0.58
1:D:92:THR:OG1	1:D:95:ASP:OD2	2.21	0.58
1:F:249:LYS:HG3	1:F:405:HIS:HE2	1.67	0.58
1:G:179:VAL:HB	1:G:180:PRO:CD	2.34	0.58
1:D:110:VAL:CG1	1:D:163:ALA:HB2	2.33	0.58
1:B:7:ASP:OD1	1:B:47:SER:HB3	2.03	0.58
1:C:171:LYS:HE2	1:C:172:PRO:O	2.03	0.58
1:H:372:THR:HB	1:H:373:PRO:HD2	1.85	0.58
1:F:350:ARG:C	1:F:351:ASP:CG	2.63	0.57
1:G:146:PRO:HD3	1:G:222:VAL:O	2.04	0.57
1:A:-1:MSE:HA	1:A:30:GLN:O	2.04	0.57
1:F:369:ASP:OD1	1:F:370:ASP:CG	2.42	0.57
1:E:252:MSE:HB2	1:E:282:ILE:HD13	1.85	0.57
1:C:162:ILE:HD11	1:C:197:LEU:HB2	1.85	0.57
1:G:252:MSE:SE	1:G:267:LEU:HD13	2.55	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:HB2	1:A:133:SER:O	2.04	0.57
1:G:84:MSE:O	1:G:88:GLU:HG3	2.03	0.57
1:H:37:SER:HG	1:H:40:ASP:CG	2.07	0.57
1:B:446:HIS:O	1:B:462:HIS:HD2	1.87	0.57
1:E:115:HIS:HA	1:E:118:LYS:HD2	1.87	0.57
1:B:92:THR:CG2	1:B:93:ILE:N	2.67	0.57
1:F:88:GLU:OE2	1:F:178:SER:OG	2.23	0.57
1:B:408:GLY:HA2	1:B:430:ILE:HG12	1.87	0.57
1:E:249:LYS:HD3	1:E:283:SER:OG	2.04	0.57
1:E:258:ALA:HB2	1:E:414:TYR:O	2.05	0.57
1:B:158:PHE:CE1	1:B:187:MSE:HE3	2.40	0.57
1:B:25:ALA:O	1:B:360:GLY:HA3	2.05	0.57
1:E:345:LEU:HD22	1:E:347:VAL:O	2.05	0.57
1:G:437:VAL:HG21	1:H:477:THR:HG22	1.87	0.57
1:D:241:ARG:NH1	1:D:469:PHE:O	2.38	0.57
1:B:256:PRO:HA	1:B:292:THR:HG21	1.84	0.57
1:E:372:THR:HG22	1:E:374:ASP:H	1.69	0.57
1:C:41:LEU:HD22	1:C:209:ALA:HB1	1.87	0.57
1:D:357:TYR:N	1:D:358:GLU:OE1	2.38	0.57
1:B:461:GLN:NE2	2:B:532:HOH:O	2.38	0.57
1:C:41:LEU:HD22	1:C:209:ALA:CB	2.34	0.57
1:B:267:LEU:HD22	1:B:387:LEU:HD21	1.87	0.57
1:G:330:ARG:NH2	1:G:382:ILE:O	2.38	0.57
1:A:78:MSE:CE	1:A:78:MSE:HA	2.34	0.56
1:B:220:SER:HB3	1:B:243:GLN:CG	2.35	0.56
1:F:92:THR:HG22	1:F:93:ILE:N	2.19	0.56
1:E:327:ALA:O	1:E:331:ILE:HD12	2.05	0.56
1:B:289:GLY:CA	1:B:292:THR:HG23	2.35	0.56
1:D:158:PHE:HE1	1:D:187:MSE:HE3	1.70	0.56
1:E:171:LYS:HE2	1:E:172:PRO:O	2.05	0.56
1:A:442:PRO:HG2	1:A:447:SER:O	2.05	0.56
1:F:121:PHE:CD2	1:F:132:TYR:HB3	2.40	0.56
1:H:51:ALA:HB1	1:H:196:ILE:CD1	2.28	0.56
1:H:110:VAL:HG13	1:H:163:ALA:HB1	1.85	0.56
1:F:174:GLU:HB2	1:F:175:ARG:HH12	1.69	0.56
1:C:55:TRP:CZ2	1:C:63:ARG:HG2	2.41	0.56
1:A:268:ILE:HG22	1:A:269:GLY:N	2.20	0.56
1:C:185:GLU:O	1:C:188:ILE:HG13	2.05	0.56
1:E:149:PHE:O	1:E:153:ILE:CG2	2.53	0.56
1:E:257:ASP:O	1:E:416:ARG:NH2	2.38	0.56
1:E:252:MSE:SE	1:E:254:ILE:HD11	2.56	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:VAL:HG11	1:F:213:HIS:CE1	2.40	0.56
1:E:431:GLY:CA	1:E:451:TRP:CD1	2.88	0.56
1:F:325:LYS:CA	1:F:361:HIS:HD2	2.17	0.56
1:G:148:ASN:HB3	1:G:149:PHE:HD1	1.71	0.56
1:D:254:ILE:HD12	1:D:254:ILE:N	2.21	0.56
1:B:480:TRP:HB3	1:D:419:ASP:HB2	1.88	0.56
1:G:65:ARG:HG3	1:G:68:MSE:HE3	1.87	0.56
1:F:93:ILE:HD12	1:F:94:ASP:N	2.21	0.56
1:B:113:ILE:N	1:B:114:PRO:HD2	2.21	0.56
1:E:295:ARG:NH1	1:E:295:ARG:HG3	2.16	0.56
1:E:78:MSE:HE2	1:E:97:LYS:HG2	1.88	0.56
1:G:137:PRO:HG3	1:G:165:GLY:HA3	1.86	0.56
1:G:89:HIS:ND1	1:G:91:LYS:HD2	2.21	0.56
1:E:431:GLY:HA2	1:E:451:TRP:CD1	2.39	0.55
1:E:451:TRP:CZ3	1:F:472:ARG:HD3	2.40	0.55
1:H:141:GLY:HA3	1:H:470:TRP:HZ3	1.71	0.55
1:B:41:LEU:HD13	1:B:209:ALA:HB3	1.88	0.55
1:H:37:SER:OG	1:H:40:ASP:CG	2.44	0.55
1:D:74:LEU:HD11	1:D:155:MSE:CE	2.35	0.55
1:F:147:PHE:CE1	1:F:323:VAL:HG11	2.40	0.55
1:H:68:MSE:O	1:H:71:VAL:HG12	2.05	0.55
1:F:59:ASN:ND2	1:F:59:ASN:C	2.60	0.55
1:B:192:LEU:HD11	1:B:196:ILE:HG21	1.87	0.55
1:F:395:TYR:HB3	1:H:485:LYS:HD2	1.88	0.55
1:E:140:ILE:HD12	1:E:140:ILE:N	2.21	0.55
1:D:325:LYS:HA	1:D:328:GLU:HG2	1.88	0.55
1:F:270:ALA:O	1:F:281:ALA:HB1	2.07	0.55
1:E:148:ASN:HD22	1:E:383:PHE:HZ	1.53	0.55
1:A:295:ARG:O	1:A:299:LYS:HG3	2.07	0.55
1:E:248:ALA:O	1:E:381:GLU:HG3	2.07	0.55
1:C:325:LYS:HG3	1:E:16:GLY:HA3	1.88	0.55
1:A:115:HIS:HD2	1:A:118:LYS:HZ2	1.52	0.55
1:C:119:SER:CB	1:C:133:SER:O	2.55	0.55
1:E:37:SER:OG	1:E:40:ASP:OD2	2.22	0.55
1:F:252:MSE:HE1	1:F:263:ALA:HB1	1.89	0.55
1:A:24:PRO:HB2	1:A:321:PRO:HG2	1.89	0.55
1:A:334:LEU:O	1:A:337:SER:HB3	2.07	0.55
1:F:26:THR:CB	1:F:28:GLU:HG2	2.37	0.55
1:E:78:MSE:HE1	1:E:100:ILE:HD13	1.88	0.55
1:C:115:HIS:O	1:C:118:LYS:HG2	2.07	0.55
1:C:280:MSE:CE	1:C:409:ASN:CG	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ILE:HG22	1:A:382:ILE:HD11	1.89	0.55
1:D:207:VAL:C	1:D:211:LEU:HD23	2.28	0.54
1:A:81:LEU:CD2	1:A:182:ARG:HG2	2.37	0.54
1:D:141:GLY:HA3	1:D:470:TRP:HZ3	1.72	0.54
1:E:133:SER:HB3	2:F:506:HOH:O	2.07	0.54
1:D:280:MSE:HE2	1:D:280:MSE:HA	1.90	0.54
1:H:145:THR:HG22	1:H:153:ILE:HG22	1.89	0.54
1:B:218:ALA:HB3	1:B:470:TRP:CZ3	2.42	0.54
1:H:102:ARG:HH12	1:H:443:LEU:HD23	1.70	0.54
1:F:480:TRP:HB3	1:H:419:ASP:HB2	1.88	0.54
1:C:439:ILE:HG22	1:C:441:VAL:HG12	1.90	0.54
1:E:127:PRO:N	1:E:129:ILE:HD13	2.23	0.54
1:G:443:LEU:HD13	1:H:131:MSE:HE1	1.90	0.54
1:D:179:VAL:HB	1:D:180:PRO:HD3	1.88	0.54
1:F:252:MSE:HE2	1:F:254:ILE:HG13	1.90	0.54
1:A:268:ILE:CG2	1:A:269:GLY:N	2.70	0.54
1:D:247:GLY:O	1:D:407:TYR:CD1	2.60	0.54
1:F:360:GLY:CA	1:F:362:PHE:HE1	2.13	0.54
1:G:5:PHE:CE1	1:G:188:ILE:HD13	2.43	0.54
1:F:304:VAL:CG1	1:F:347:VAL:HG23	2.38	0.54
1:D:192:LEU:HD12	1:D:193:PRO:HD2	1.90	0.54
1:E:247:GLY:O	1:E:454:SER:OG	2.21	0.54
1:H:280:MSE:HE2	1:H:409:ASN:ND2	2.22	0.53
1:F:88:GLU:OE1	1:F:178:SER:OG	2.26	0.53
1:A:149:PHE:HZ	1:A:278:ARG:HG2	1.74	0.53
1:B:177:PRO:O	1:B:181:ILE:HD12	2.08	0.53
1:F:99:ASP:OD2	1:F:149:PHE:HA	2.08	0.53
1:A:350:ARG:NH1	1:A:350:ARG:HG3	2.11	0.53
1:D:158:PHE:HE1	1:D:187:MSE:CE	2.19	0.53
1:C:110:VAL:HG13	1:C:163:ALA:CB	2.38	0.53
1:H:253:ILE:HD12	1:H:424:PHE:CE1	2.42	0.53
1:F:417:ASP:OD2	1:F:419:ASP:HB3	2.08	0.53
1:B:19:SER:HB2	1:B:35:LEU:HD11	1.90	0.53
1:H:301:VAL:HG23	1:H:302:PRO:HD3	1.89	0.53
1:C:69:LYS:HD3	1:C:190:ALA:HA	1.89	0.53
1:B:337:SER:O	1:B:341:GLN:HG3	2.09	0.53
1:C:323:VAL:HG22	1:C:324:THR:HG23	1.91	0.53
1:G:5:PHE:HE1	1:G:188:ILE:HD13	1.73	0.53
1:E:459:LEU:HD21	1:F:459:LEU:HD21	1.90	0.53
1:F:325:LYS:N	1:F:361:HIS:NE2	2.57	0.53
1:E:308:ARG:HH11	1:E:316:LYS:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:PHE:HB3	1:E:244:CYS:SG	2.49	0.53
1:G:278:ARG:HG3	1:G:281:ALA:HB2	1.90	0.53
1:C:448:PHE:C	1:C:448:PHE:CD1	2.82	0.53
1:F:347:VAL:HB	1:F:367:LEU:HB3	1.91	0.53
1:H:148:ASN:ND2	1:H:149:PHE:HE1	2.07	0.53
1:H:159:ALA:HB3	1:H:160:PRO:HD3	1.91	0.53
1:F:78:MSE:HE2	1:F:97:LYS:HG2	1.91	0.53
1:A:257:ASP:O	1:A:416:ARG:HG3	2.08	0.53
1:H:288:VAL:HA	1:H:392:ALA:O	2.08	0.53
1:E:168:PHE:CE1	1:E:470:TRP:CH2	2.94	0.53
1:H:148:ASN:HD22	1:H:149:PHE:HD1	1.52	0.53
1:E:373:PRO:HA	1:E:378:TYR:CD2	2.43	0.53
1:F:176:ASP:N	1:F:177:PRO:HD3	2.24	0.53
1:C:70:PHE:CE2	1:C:155:MSE:HE3	2.42	0.53
1:F:19:SER:HB3	1:F:174:GLU:OE2	2.09	0.53
1:C:30:GLN:NE2	1:C:87:ARG:HE	2.07	0.53
1:H:328:GLU:OE1	1:H:361:HIS:HA	2.09	0.53
1:G:328:GLU:O	1:G:332:ARG:HG3	2.09	0.52
1:B:248:ALA:HB2	1:B:409:ASN:HD22	1.74	0.52
1:H:429:ASN:O	1:H:452:LYS:HE2	2.10	0.52
1:H:26:THR:HG22	1:H:28:GLU:H	1.74	0.52
1:D:337:SER:O	1:D:341:GLN:HB2	2.10	0.52
1:E:253:ILE:HD12	1:E:424:PHE:CE1	2.44	0.52
1:D:250:ASN:HD21	1:D:280:MSE:CE	2.18	0.52
1:G:0:TYR:OH	1:G:30:GLN:NE2	2.43	0.52
1:F:309:ILE:HB	1:F:352:PHE:CZ	2.45	0.52
1:F:49:LYS:HG3	1:F:140:ILE:HD11	1.91	0.52
1:E:419:ASP:HB2	1:G:480:TRP:HB3	1.92	0.52
1:D:345:LEU:HD23	1:D:345:LEU:C	2.30	0.52
1:F:328:GLU:OE1	1:F:361:HIS:HB3	2.09	0.52
1:A:369:ASP:OD1	1:A:370:ASP:N	2.42	0.52
1:H:296:LEU:HD13	1:H:300:LEU:HD22	1.91	0.52
1:H:417:ASP:O	1:H:419:ASP:N	2.40	0.52
1:A:171:LYS:O	1:A:171:LYS:HG3	2.09	0.52
1:D:268:ILE:HD13	1:D:303:MSE:HE3	1.92	0.52
1:G:341:GLN:HB2	1:G:375:MSE:HE3	1.91	0.52
1:F:126:GLY:HA3	1:F:129:ILE:CB	2.20	0.52
1:G:156:TRP:CE3	1:G:461:GLN:HG2	2.45	0.52
1:D:288:VAL:HG22	1:D:398:ALA:HB2	1.92	0.52
1:F:115:HIS:HD2	1:F:118:LYS:NZ	2.07	0.52
1:D:399:LEU:HD13	1:D:424:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLN:O	1:B:65:ARG:HG3	2.10	0.52
1:A:411:VAL:HG12	1:A:430:ILE:HG21	1.92	0.52
1:D:91:LYS:NZ	1:D:148:ASN:O	2.42	0.52
1:D:24:PRO:HB2	1:D:321:PRO:HB2	1.92	0.52
1:H:23:ASN:HB3	1:H:26:THR:HB	1.92	0.52
1:E:329:GLN:O	1:E:332:ARG:HB2	2.10	0.52
1:E:432:MSE:CE	1:E:441:VAL:HA	2.39	0.52
1:G:87:ARG:HG3	1:G:312:TYR:OH	2.09	0.52
1:C:110:VAL:HG13	1:C:163:ALA:HB2	1.92	0.52
1:E:280:MSE:HE2	1:E:409:ASN:OD1	2.10	0.52
1:G:115:HIS:HD2	1:G:118:LYS:NZ	2.07	0.52
1:A:439:ILE:O	1:A:439:ILE:HG22	2.10	0.52
1:E:137:PRO:O	1:E:472:ARG:HD2	2.10	0.51
1:D:74:LEU:CD1	1:D:155:MSE:HE1	2.39	0.51
1:F:304:VAL:HG12	1:F:347:VAL:HG23	1.90	0.51
1:B:115:HIS:O	1:B:118:LYS:HG3	2.10	0.51
1:E:67:PHE:O	1:E:71:VAL:HG23	2.09	0.51
1:B:429:ASN:ND2	1:B:452:LYS:HD3	2.24	0.51
1:H:447:SER:HB3	1:H:460:ASN:HD22	1.76	0.51
1:B:179:VAL:HB	1:B:180:PRO:HD3	1.90	0.51
1:F:206:ALA:O	1:F:210:ILE:HG13	2.10	0.51
1:E:255:MSE:HE1	1:E:395:TYR:HD2	1.75	0.51
1:E:256:PRO:HA	1:E:292:THR:HG21	1.91	0.51
1:A:74:LEU:HD23	1:A:104:LEU:HB2	1.92	0.51
1:G:268:ILE:HD13	1:G:303:MSE:HB3	1.91	0.51
1:H:153:ILE:O	1:H:156:TRP:HB2	2.10	0.51
1:H:261:ASP:O	1:H:265:ASN:OD1	2.28	0.51
1:F:325:LYS:HA	1:F:361:HIS:HD2	1.76	0.51
1:G:135:ARG:HH12	1:G:467:ILE:HG22	1.75	0.51
1:G:92:THR:HG22	1:G:94:ASP:N	2.26	0.51
1:H:37:SER:OG	1:H:40:ASP:OD2	2.29	0.51
1:F:424:PHE:O	1:F:428:ILE:HG13	2.11	0.51
1:B:423:ASP:OD2	1:B:427:ARG:NH1	2.44	0.51
1:H:141:GLY:HA3	1:H:470:TRP:CZ3	2.45	0.51
1:B:285:ALA:HB3	1:B:389:VAL:HG22	1.93	0.51
1:B:74:LEU:CD2	1:B:155:MSE:CE	2.72	0.51
1:E:428:ILE:HG12	1:E:429:ASN:H	1.76	0.51
1:F:314:ASP:OD2	1:F:317:ALA:HB2	2.09	0.51
1:A:78:MSE:HE2	1:A:78:MSE:O	2.11	0.51
1:A:192:LEU:HD11	1:A:196:ILE:HG21	1.92	0.51
1:D:17:ARG:HB3	1:D:35:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:GLY:O	1:F:246:GLY:HA2	2.11	0.51
1:E:444:ALA:O	1:E:462:HIS:HB2	2.11	0.51
1:E:309:ILE:HG23	1:E:319:MSE:O	2.10	0.51
1:H:294:ASN:O	1:H:297:ILE:HG13	2.11	0.51
1:D:74:LEU:HD11	1:D:155:MSE:HE1	1.92	0.51
1:A:480:TRP:HB3	1:C:419:ASP:HB2	1.93	0.51
1:A:249:LYS:HE3	1:A:283:SER:HB3	1.91	0.51
1:A:119:SER:CB	1:A:133:SER:O	2.59	0.51
1:H:484:ILE:O	1:H:484:ILE:HG23	2.11	0.51
1:E:382:ILE:HG22	1:E:384:GLY:H	1.75	0.51
1:A:64:ALA:HB1	1:A:111:ILE:O	2.11	0.51
1:B:129:ILE:HG12	1:B:479:ARG:HG3	1.92	0.51
1:B:78:MSE:CE	1:B:97:LYS:HA	2.41	0.50
1:D:153:ILE:O	1:D:156:TRP:HB2	2.11	0.50
1:F:371:VAL:HG13	1:F:375:MSE:CE	2.42	0.50
1:F:266:ALA:HB1	1:F:438:PRO:HB3	1.93	0.50
1:A:250:ASN:HB2	1:A:281:ALA:O	2.10	0.50
1:A:134:ILE:HD13	1:D:121:PHE:CE2	2.47	0.50
1:E:204:LYS:O	1:E:208:ASP:OD1	2.29	0.50
1:F:142:ALA:O	1:F:219:VAL:HA	2.11	0.50
1:G:60:PRO:HB2	1:G:114:PRO:HG3	1.92	0.50
1:F:192:LEU:CD2	1:F:196:ILE:HD11	2.39	0.50
1:B:348:ASP:OD1	1:B:350:ARG:HD3	2.11	0.50
1:H:208:ASP:OD1	1:H:230:TYR:OH	2.29	0.50
1:D:248:ALA:HB2	1:D:409:ASN:HB2	1.93	0.50
1:H:49:LYS:HD3	2:H:541:HOH:O	2.11	0.50
1:A:392:ALA:HB1	1:A:397:GLU:HG2	1.93	0.50
1:C:330:ARG:HB3	1:C:330:ARG:HH11	1.77	0.50
1:A:405:HIS:CD2	1:A:407:TYR:H	2.18	0.50
1:B:148:ASN:OD1	1:B:149:PHE:CD1	2.65	0.50
1:C:114:PRO:HG2	2:C:502:HOH:O	2.11	0.50
1:C:284:VAL:HA	1:C:388:SER:O	2.11	0.50
1:A:450:GLY:O	1:A:455:SER:OG	2.22	0.50
1:F:70:PHE:CE1	1:F:187:MSE:HA	2.47	0.50
1:B:141:GLY:HA3	1:B:470:TRP:CZ3	2.46	0.50
1:A:255:MSE:HE3	1:A:256:PRO:HD2	1.94	0.50
1:D:347:VAL:O	1:D:366:CYS:HA	2.11	0.50
1:G:252:MSE:HE3	1:G:414:TYR:CD1	2.46	0.50
1:F:371:VAL:CG1	1:F:372:THR:N	2.74	0.50
1:B:428:ILE:HD12	1:B:429:ASN:H	1.77	0.50
1:E:331:ILE:HG21	1:E:363:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:HG3	1:A:363:ILE:HD11	1.92	0.50
1:D:273:GLY:O	1:D:274:SER:HB2	2.11	0.50
1:F:70:PHE:CE2	1:F:155:MSE:HE1	2.44	0.50
1:F:369:ASP:OD1	1:F:370:ASP:OD1	2.29	0.50
1:H:309:ILE:HG12	1:H:319:MSE:HE2	1.94	0.50
1:F:135:ARG:HH12	1:F:467:ILE:HG22	1.73	0.50
1:F:274:SER:OG	1:F:274:SER:O	2.30	0.50
1:B:213:HIS:HB3	1:B:216:ILE:HD12	1.94	0.50
1:F:80:GLU:O	1:F:84:MSE:HB2	2.12	0.50
1:A:159:ALA:HB3	1:A:160:PRO:CD	2.42	0.49
1:B:245:PHE:CE2	1:B:461:GLN:HG2	2.47	0.49
1:H:372:THR:HB	1:H:373:PRO:CD	2.42	0.49
1:G:110:VAL:HG13	1:G:163:ALA:HB2	1.93	0.49
1:A:142:ALA:HA	1:A:169:ILE:O	2.12	0.49
1:E:314:ASP:OD1	1:E:315:GLU:N	2.45	0.49
1:C:52:GLN:HG3	1:C:53:PRO:HD3	1.93	0.49
1:H:299:LYS:O	1:H:303:MSE:HG3	2.12	0.49
1:C:107:CYS:SG	1:C:155:MSE:CE	2.99	0.49
1:E:432:MSE:HG2	1:E:442:PRO:HD3	1.94	0.49
1:D:399:LEU:O	1:D:402:PRO:HD2	2.12	0.49
1:E:127:PRO:HG3	2:H:528:HOH:O	2.11	0.49
1:G:171:LYS:O	1:G:171:LYS:HE3	2.12	0.49
1:F:161:ALA:HB2	1:F:470:TRP:CE2	2.47	0.49
1:G:373:PRO:HA	1:G:378:TYR:CD2	2.47	0.49
1:H:119:SER:HB2	1:H:133:SER:HB2	1.93	0.49
1:D:265:ASN:HD22	1:D:265:ASN:N	2.10	0.49
1:F:332:ARG:HA	1:F:335:ILE:HD12	1.95	0.49
1:F:224:SER:HB3	1:F:226:PRO:HD2	1.94	0.49
1:F:252:MSE:CE	1:F:263:ALA:HB1	2.42	0.49
1:C:330:ARG:HB3	1:C:330:ARG:NH1	2.27	0.49
1:D:27:GLY:HA3	1:D:359:ASN:O	2.13	0.49
1:C:237:MSE:HE3	1:D:233:GLY:HA3	1.95	0.49
1:D:93:ILE:O	1:D:97:LYS:HB3	2.11	0.49
1:A:7:ASP:O	1:A:7:ASP:OD2	2.30	0.49
1:E:265:ASN:OD1	1:E:303:MSE:HE1	2.12	0.49
1:E:225:THR:CG2	1:E:229:ARG:HH12	2.25	0.49
1:G:375:MSE:HE2	1:G:377:ILE:HG12	1.93	0.49
1:G:439:ILE:HG22	1:G:441:VAL:HG13	1.94	0.49
1:E:68:MSE:HE2	1:E:111:ILE:HG23	1.94	0.49
1:E:131:MSE:CE	1:F:446:HIS:CB	2.88	0.49
1:G:284:VAL:HG13	1:G:390:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:VAL:O	1:D:361:HIS:HB2	2.12	0.49
1:H:361:HIS:NE2	2:H:540:HOH:O	2.22	0.49
1:C:393:ARG:HB2	1:C:397:GLU:OE2	2.12	0.49
1:F:484:ILE:HD11	2:H:522:HOH:O	2.11	0.49
1:B:6:ILE:HD12	1:B:44:ALA:HB2	1.95	0.49
1:E:453:SER:OG	1:E:453:SER:O	2.30	0.49
1:C:341:GLN:HE22	1:C:376:ASP:N	2.02	0.49
1:F:371:VAL:HG21	1:F:388:SER:HB3	1.94	0.49
1:H:216:ILE:O	1:H:240:LYS:HE3	2.13	0.49
1:A:354:LEU:HD23	1:A:357:TYR:CD2	2.48	0.49
1:E:393:ARG:NH1	1:E:397:GLU:OE1	2.46	0.49
1:D:336:ASP:O	1:D:340:GLU:HG2	2.12	0.49
1:C:84:MSE:CE	1:C:182:ARG:HG3	2.42	0.49
1:D:180:PRO:HA	1:D:183:LEU:HD12	1.95	0.49
1:D:55:TRP:CZ2	1:D:63:ARG:HG2	2.47	0.49
1:F:350:ARG:O	1:F:351:ASP:OD2	2.30	0.49
1:F:325:LYS:CA	1:F:361:HIS:CD2	2.93	0.49
1:C:84:MSE:O	1:C:88:GLU:HG3	2.12	0.49
1:H:148:ASN:ND2	1:H:149:PHE:CD1	2.78	0.49
1:E:409:ASN:HD22	1:E:450:GLY:HA3	1.77	0.49
1:A:280:MSE:HG3	1:A:441:VAL:CG2	2.43	0.49
1:H:252:MSE:HE3	1:H:282:ILE:HG13	1.93	0.49
1:C:110:VAL:CG1	1:C:163:ALA:HB2	2.43	0.49
1:B:59:ASN:HB2	1:B:60:PRO:HD2	1.95	0.49
1:G:217:ALA:O	1:G:240:LYS:HB2	2.13	0.49
1:H:405:HIS:HE1	1:H:407:TYR:HD2	1.61	0.49
1:E:160:PRO:HB3	1:E:466:SER:HB3	1.95	0.49
1:A:24:PRO:HA	1:A:361:HIS:CE1	2.48	0.49
1:C:115:HIS:HD2	1:C:118:LYS:NZ	2.11	0.49
1:H:249:LYS:HB3	1:H:405:HIS:CE1	2.48	0.49
1:D:450:GLY:O	1:D:455:SER:HB2	2.13	0.49
1:H:280:MSE:HE1	1:H:409:ASN:CG	2.32	0.48
1:F:272:TYR:O	1:F:273:GLY:C	2.49	0.48
1:H:86:SER:HB3	1:H:312:TYR:CB	2.43	0.48
1:A:211:LEU:O	1:A:240:LYS:HE2	2.12	0.48
1:G:280:MSE:HG3	1:G:441:VAL:HG12	1.95	0.48
1:G:322:VAL:HG12	1:G:324:THR:H	1.78	0.48
1:F:360:GLY:HA3	1:F:362:PHE:CE1	2.26	0.48
1:D:249:LYS:HZ1	1:D:382:ILE:HD12	1.79	0.48
1:D:345:LEU:HD23	1:D:346:VAL:N	2.28	0.48
1:G:166:ASN:HD21	1:G:470:TRP:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:ILE:HA	1:H:116:LEU:HB2	1.95	0.48
1:B:107:CYS:SG	1:B:155:MSE:HE2	2.53	0.48
1:E:447:SER:HB3	1:E:460:ASN:CB	2.44	0.48
1:F:135:ARG:NH1	1:F:467:ILE:HG23	2.26	0.48
1:G:375:MSE:HE2	1:G:375:MSE:HB3	1.81	0.48
1:D:261:ASP:O	1:D:265:ASN:ND2	2.46	0.48
1:F:244:CYS:O	1:F:456:PHE:N	2.45	0.48
1:E:95:ASP:OD2	1:E:274:SER:OG	2.24	0.48
1:A:308:ARG:NH1	1:A:314:ASP:OD2	2.42	0.48
1:C:474:LYS:NZ	1:D:428:ILE:O	2.42	0.48
1:E:93:ILE:HG12	1:E:315:GLU:HG2	1.95	0.48
1:H:187:MSE:HG3	1:H:197:LEU:HD23	1.96	0.48
1:E:127:PRO:C	1:E:129:ILE:CD1	2.82	0.48
1:E:474:LYS:HE2	1:F:425:ALA:O	2.14	0.48
1:F:192:LEU:HD22	1:F:196:ILE:CD1	2.39	0.48
1:F:176:ASP:N	1:F:176:ASP:OD1	2.46	0.48
1:B:227:ILE:HD13	1:B:227:ILE:N	2.29	0.48
1:F:304:VAL:CG1	1:F:347:VAL:CG2	2.92	0.48
1:B:462:HIS:HA	1:B:466:SER:HB3	1.95	0.48
1:F:411:VAL:HG22	1:F:430:ILE:HG21	1.96	0.48
1:H:104:LEU:O	1:H:107:CYS:HB2	2.14	0.48
1:B:371:VAL:HG21	1:B:388:SER:HB3	1.95	0.48
1:E:131:MSE:CE	1:F:446:HIS:CG	2.96	0.48
1:C:106:VAL:HA	1:C:444:ALA:HB1	1.96	0.48
1:F:375:MSE:O	1:F:379:LYS:HG3	2.14	0.48
1:G:328:GLU:OE2	1:G:361:HIS:HA	2.14	0.48
1:G:18:VAL:HG13	1:G:32:THR:HB	1.95	0.48
1:D:78:MSE:HE1	1:D:100:ILE:HB	1.96	0.48
1:F:448:PHE:O	1:F:460:ASN:HB3	2.14	0.48
1:B:287:PRO:HB2	1:B:293:ALA:HB2	1.95	0.48
1:F:415:THR:HG21	1:F:420:ALA:HB3	1.96	0.48
1:E:228:ALA:HB1	1:E:244:CYS:HB3	1.95	0.47
1:H:51:ALA:CB	1:H:196:ILE:HD12	2.34	0.47
1:F:322:VAL:HG12	1:F:323:VAL:N	2.25	0.47
1:H:439:ILE:HG22	1:H:441:VAL:HG22	1.97	0.47
1:D:356:GLY:CA	1:D:358:GLU:OE1	2.62	0.47
1:F:161:ALA:HB2	1:F:470:TRP:CD2	2.49	0.47
1:D:307:LEU:HD13	1:D:319:MSE:HE2	1.95	0.47
1:H:59:ASN:O	1:H:63:ARG:HG3	2.14	0.47
1:A:69:LYS:HG2	1:A:190:ALA:HA	1.96	0.47
1:F:241:ARG:NH1	1:F:469:PHE:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ILE:N	1:E:114:PRO:CD	2.78	0.47
1:E:138:VAL:CA	1:E:472:ARG:HD2	2.32	0.47
1:B:301:VAL:HG12	1:B:302:PRO:CD	2.45	0.47
1:B:158:PHE:CE1	1:B:187:MSE:CE	2.97	0.47
1:E:119:SER:HB2	1:E:133:SER:O	2.14	0.47
1:C:258:ALA:HB2	1:C:414:TYR:O	2.14	0.47
1:F:260:LEU:H	1:F:260:LEU:HG	1.52	0.47
1:F:156:TRP:CE3	1:F:461:GLN:HG2	2.49	0.47
1:B:116:LEU:HB3	1:B:467:ILE:CD1	2.38	0.47
1:B:272:TYR:HD1	1:B:319:MSE:HE1	1.79	0.47
1:G:371:VAL:HG21	1:G:388:SER:HB3	1.97	0.47
1:F:88:GLU:OE2	1:F:177:PRO:HD2	2.15	0.47
1:F:249:LYS:HE3	1:F:381:GLU:HA	1.97	0.47
1:D:106:VAL:HG12	1:D:159:ALA:HB3	1.96	0.47
1:F:230:TYR:O	1:F:234:THR:HB	2.13	0.47
1:C:18:VAL:HG13	1:C:32:THR:HB	1.97	0.47
1:D:442:PRO:HG2	1:D:447:SER:O	2.14	0.47
1:A:390:VAL:HG11	1:A:401:LEU:HD21	1.96	0.47
1:B:324:THR:HG22	1:B:327:ALA:CB	2.45	0.47
1:A:354:LEU:HD23	1:A:357:TYR:HD2	1.80	0.47
1:E:11:VAL:HG12	1:E:12:ALA:O	2.15	0.47
1:E:309:ILE:HD12	1:E:352:PHE:CE1	2.50	0.47
1:C:375:MSE:HE2	1:C:377:ILE:HG12	1.96	0.47
1:E:255:MSE:CE	1:E:395:TYR:HD2	2.28	0.47
1:A:445:TYR:O	1:C:118:LYS:NZ	2.48	0.46
1:B:21:ILE:HG21	1:B:88:GLU:OE2	2.15	0.46
1:E:18:VAL:HG13	1:E:32:THR:HB	1.97	0.46
1:C:301:VAL:N	1:C:302:PRO:HD2	2.30	0.46
1:A:113:ILE:HA	1:A:116:LEU:HB2	1.96	0.46
1:E:432:MSE:HE1	1:E:448:PHE:CD2	2.50	0.46
1:E:131:MSE:HE2	1:F:446:HIS:CG	2.46	0.46
1:C:136:GLN:OE1	1:C:474:LYS:NZ	2.44	0.46
1:E:228:ALA:C	1:E:230:TYR:N	2.62	0.46
1:B:255:MSE:HE1	1:B:395:TYR:HB2	1.96	0.46
1:H:260:LEU:HD23	1:H:260:LEU:HA	1.77	0.46
1:B:448:PHE:C	1:B:448:PHE:CD1	2.89	0.46
1:F:371:VAL:HB	1:F:390:VAL:HG22	1.96	0.46
1:F:272:TYR:CE1	1:F:385:PRO:O	2.64	0.46
1:F:335:ILE:O	1:F:339:ILE:HG13	2.14	0.46
1:A:402:PRO:HB2	1:A:428:ILE:HD11	1.97	0.46
1:D:393:ARG:HH12	1:D:397:GLU:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:HIS:CE1	1:C:91:LYS:HG2	2.49	0.46
1:D:148:ASN:HB2	1:D:149:PHE:CD1	2.50	0.46
1:G:141:GLY:HA3	1:G:470:TRP:HZ3	1.80	0.46
1:H:371:VAL:HG21	1:H:388:SER:HB3	1.97	0.46
1:E:423:ASP:OD2	1:E:427:ARG:NH2	2.49	0.46
1:E:283:SER:O	1:E:387:LEU:HD12	2.15	0.46
1:G:301:VAL:HG22	1:G:346:VAL:HG12	1.97	0.46
1:E:263:ALA:O	1:E:267:LEU:HD22	2.15	0.46
1:F:171:LYS:HG3	1:F:200:VAL:O	2.16	0.46
1:B:348:ASP:OD1	1:B:350:ARG:CD	2.64	0.46
1:G:255:MSE:HG3	1:G:256:PRO:HD2	1.97	0.46
1:D:207:VAL:HG12	1:D:211:LEU:HD21	1.98	0.46
1:B:292:THR:O	1:B:296:LEU:HB2	2.16	0.46
1:A:408:GLY:CA	1:A:430:ILE:HG13	2.46	0.46
1:B:30:GLN:HE22	1:B:87:ARG:HD2	1.80	0.46
1:E:451:TRP:CE3	1:F:472:ARG:NE	2.84	0.46
1:H:301:VAL:HG12	1:H:367:LEU:HD23	1.96	0.46
1:B:85:LEU:HB2	1:B:179:VAL:HG21	1.98	0.46
1:D:267:LEU:HD23	1:D:282:ILE:HG21	1.98	0.46
1:G:106:VAL:HA	1:G:444:ALA:HB1	1.97	0.46
1:G:288:VAL:O	1:G:392:ALA:O	2.33	0.46
1:F:135:ARG:HD3	1:F:471:THR:HG21	1.98	0.46
1:A:30:GLN:HE22	1:A:87:ARG:HH11	1.64	0.46
1:G:278:ARG:HB3	1:G:278:ARG:HE	1.54	0.46
1:E:113:ILE:HA	1:E:116:LEU:HB2	1.97	0.46
1:G:2:LEU:HD12	1:G:21:ILE:HD11	1.97	0.46
1:C:158:PHE:CD1	1:C:158:PHE:C	2.90	0.46
1:E:131:MSE:HE1	1:F:443:LEU:HB2	1.97	0.46
1:H:447:SER:OG	1:H:460:ASN:HB2	2.16	0.46
1:A:141:GLY:HA3	1:A:470:TRP:HZ3	1.80	0.46
1:D:112:GLY:HA3	2:D:505:HOH:O	2.15	0.46
1:F:192:LEU:CD1	1:F:196:ILE:HD11	2.45	0.45
1:C:375:MSE:HB3	1:C:375:MSE:HE2	1.60	0.45
1:D:91:LYS:HG3	1:D:95:ASP:HB2	1.97	0.45
1:H:49:LYS:NZ	1:H:215:ASP:OD1	2.41	0.45
1:F:85:LEU:HD11	1:F:150:PRO:HD2	1.98	0.45
1:D:138:VAL:HA	1:D:472:ARG:HD3	1.97	0.45
1:F:399:LEU:O	1:F:402:PRO:HD2	2.15	0.45
1:A:112:GLY:HA2	2:C:514:HOH:O	2.16	0.45
1:E:153:ILE:HG23	1:E:154:PRO:HD3	1.98	0.45
1:G:87:ARG:HA	1:G:312:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:LYS:CD	1:E:283:SER:OG	2.65	0.45
1:F:257:ASP:HB3	1:H:484:ILE:HD13	1.99	0.45
1:H:222:VAL:HG22	1:H:245:PHE:HB2	1.98	0.45
1:E:255:MSE:HG3	1:E:415:THR:HB	1.97	0.45
1:E:78:MSE:O	1:E:78:MSE:HE3	2.16	0.45
1:D:129:ILE:HD11	1:D:479:ARG:NH2	2.30	0.45
1:H:432:MSE:HE2	1:H:449:GLY:O	2.16	0.45
1:E:305:GLU:HG3	2:E:528:HOH:O	2.15	0.45
1:G:-2:MSE:HE2	1:G:-2:MSE:HB3	1.73	0.45
1:E:411:VAL:HG21	1:E:428:ILE:CD1	2.46	0.45
1:G:131:MSE:HE1	1:H:443:LEU:HG	1.98	0.45
1:D:200:VAL:O	1:D:200:VAL:HG12	2.16	0.45
1:E:461:GLN:O	1:E:462:HIS:ND1	2.50	0.45
1:F:70:PHE:CE1	1:F:187:MSE:CG	2.91	0.45
1:F:207:VAL:HG12	1:F:211:LEU:HD12	1.99	0.45
1:F:252:MSE:CE	1:F:254:ILE:HG13	2.46	0.45
1:B:71:VAL:CG1	1:D:68:MSE:HE1	2.46	0.45
1:C:211:LEU:HD13	1:C:234:THR:HB	1.98	0.45
1:A:192:LEU:HD12	1:A:193:PRO:HD2	1.97	0.45
1:D:84:MSE:HE1	1:D:182:ARG:HG3	1.99	0.45
1:A:373:PRO:HA	1:A:378:TYR:CD2	2.51	0.45
1:H:73:LEU:HD12	1:H:186:LEU:HG	1.97	0.45
1:F:347:VAL:HG21	1:F:365:GLY:O	2.17	0.45
1:H:103:GLY:HA3	1:H:152:MSE:HA	1.99	0.45
1:D:174:GLU:N	1:D:174:GLU:OE2	2.44	0.45
1:G:115:HIS:HD2	1:G:118:LYS:HZ1	1.64	0.45
1:F:134:ILE:HG12	1:G:121:PHE:CE2	2.52	0.45
1:D:308:ARG:HA	1:D:308:ARG:HD2	1.66	0.45
1:G:406:GLU:HG2	1:G:453:SER:OG	2.17	0.45
1:G:252:MSE:HE3	1:G:414:TYR:CG	2.51	0.45
1:A:154:PRO:HB3	1:A:170:LEU:HD21	1.98	0.45
1:H:274:SER:O	1:H:277:GLU:HG3	2.17	0.45
1:B:174:GLU:CD	1:B:174:GLU:H	2.20	0.45
1:G:208:ASP:O	1:G:212:THR:HB	2.17	0.45
1:F:324:THR:O	1:F:361:HIS:CD2	2.70	0.45
1:B:331:ILE:HD12	1:B:385:PRO:HD2	1.98	0.45
1:C:148:ASN:HD22	1:C:149:PHE:HD2	1.65	0.45
1:F:256:PRO:HD3	1:F:288:VAL:HG22	1.96	0.45
1:E:192:LEU:HD11	1:E:196:ILE:CG2	2.44	0.45
1:E:207:VAL:O	1:E:211:LEU:HD23	2.15	0.45
1:D:348:ASP:OD1	1:D:350:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:LYS:CB	1:E:405:HIS:CE1	3.00	0.45
1:F:479:ARG:HG2	1:F:480:TRP:H	1.81	0.45
1:H:46:GLU:OE2	1:H:49:LYS:NZ	2.49	0.45
1:H:181:ILE:HD11	1:H:201:ASN:ND2	2.32	0.45
1:A:411:VAL:HG12	1:A:430:ILE:CG2	2.47	0.45
1:H:49:LYS:HB2	1:H:49:LYS:HE3	1.59	0.45
1:G:249:LYS:HD2	1:G:378:TYR:O	2.17	0.45
1:E:68:MSE:HA	1:E:111:ILE:HD11	1.99	0.45
1:E:458:ASP:HB3	1:F:241:ARG:HD3	1.98	0.45
1:C:112:GLY:O	1:C:116:LEU:HG	2.17	0.45
1:G:308:ARG:CZ	1:G:316:LYS:HD2	2.46	0.45
1:E:23:ASN:HA	1:E:24:PRO:HD3	1.85	0.45
1:E:122:THR:HG23	1:E:131:MSE:HB3	1.99	0.44
1:H:368:PHE:CE2	1:H:377:ILE:HD11	2.53	0.44
1:H:127:PRO:O	1:H:129:ILE:HD12	2.17	0.44
1:A:171:LYS:HA	1:A:200:VAL:O	2.18	0.44
1:G:113:ILE:N	1:G:114:PRO:CD	2.80	0.44
1:H:86:SER:HB3	1:H:312:TYR:HB2	1.99	0.44
1:D:0:TYR:CE1	1:D:30:GLN:HG3	2.52	0.44
1:F:106:VAL:HA	1:F:444:ALA:HB1	1.99	0.44
1:C:161:ALA:O	1:C:166:ASN:HB2	2.17	0.44
1:E:225:THR:O	1:E:229:ARG:HB2	2.17	0.44
1:H:256:PRO:HD3	1:H:288:VAL:HG13	1.99	0.44
1:E:253:ILE:HD11	1:E:402:PRO:HG3	2.00	0.44
1:C:145:THR:HA	1:C:146:PRO:HD3	1.82	0.44
1:H:41:LEU:HD22	1:H:209:ALA:HB1	1.99	0.44
1:C:175:ARG:HG2	1:C:175:ARG:H	1.57	0.44
1:D:354:LEU:HG	1:D:357:TYR:HD2	1.80	0.44
1:E:307:LEU:HD23	1:E:319:MSE:HE2	1.99	0.44
1:B:319:MSE:CE	1:B:385:PRO:CB	2.91	0.44
1:E:211:LEU:H	1:E:211:LEU:CD2	2.31	0.44
1:F:272:TYR:O	1:F:273:GLY:O	2.35	0.44
1:C:278:ARG:HB2	1:C:278:ARG:HE	1.25	0.44
1:G:330:ARG:HB3	1:G:330:ARG:HE	1.46	0.44
1:H:253:ILE:HD12	1:H:424:PHE:HE1	1.82	0.44
1:G:211:LEU:HD21	1:G:231:VAL:HG13	1.98	0.44
1:D:77:ASN:O	1:D:81:LEU:HB2	2.17	0.44
1:H:54:LYS:O	1:H:54:LYS:HE2	2.16	0.44
1:D:152:MSE:HE3	1:D:156:TRP:CZ2	2.53	0.44
1:B:120:GLU:HB3	1:C:118:LYS:HD3	2.00	0.44
1:D:42:ALA:O	1:D:46:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:O	1:A:360:GLY:HA3	2.18	0.44
1:H:263:ALA:O	1:H:267:LEU:HD12	2.18	0.44
1:G:184:ALA:HA	1:G:197:LEU:HD13	1.99	0.44
1:A:474:LYS:HB2	1:B:451:TRP:CZ2	2.52	0.44
1:A:91:LYS:NZ	1:A:148:ASN:O	2.50	0.44
1:H:461:GLN:O	1:H:462:HIS:O	2.35	0.44
1:E:225:THR:CG2	1:E:229:ARG:NH1	2.81	0.44
1:B:148:ASN:OD1	1:B:149:PHE:HD1	2.01	0.44
1:A:58:THR:HG22	1:A:62:ARG:HB3	1.99	0.44
1:F:411:VAL:HG21	1:F:428:ILE:HD13	1.98	0.44
1:F:213:HIS:HA	1:F:214:PRO:HD3	1.84	0.44
1:D:24:PRO:HA	1:D:361:HIS:CE1	2.52	0.44
1:E:301:VAL:N	1:E:302:PRO:HD2	2.33	0.44
1:D:131:MSE:HA	1:D:476:ILE:O	2.18	0.44
1:C:243:GLN:HG2	1:C:469:PHE:CE1	2.53	0.44
1:E:86:SER:OG	1:E:96:ALA:HB2	2.18	0.44
1:C:438:PRO:O	1:C:440:PRO:HD3	2.17	0.44
1:B:295:ARG:O	1:B:299:LYS:HG2	2.18	0.44
1:E:441:VAL:O	1:E:441:VAL:CG1	2.65	0.44
1:E:122:THR:HG22	1:F:446:HIS:NE2	2.33	0.44
1:F:170:LEU:HD23	1:F:199:VAL:HG22	1.99	0.44
1:H:308:ARG:HB3	1:H:308:ARG:HH11	1.83	0.44
1:B:319:MSE:HE1	1:B:385:PRO:CB	2.48	0.44
1:H:330:ARG:NH1	1:H:381:GLU:O	2.51	0.44
1:E:171:LYS:CE	1:E:172:PRO:O	2.65	0.44
1:F:273:GLY:O	1:F:274:SER:HB3	2.18	0.44
1:H:177:PRO:O	1:H:181:ILE:HG13	2.18	0.44
1:A:249:LYS:HE3	1:A:283:SER:HB2	1.98	0.44
1:F:92:THR:HG22	1:F:94:ASP:H	1.83	0.44
1:F:309:ILE:HB	1:F:352:PHE:CE2	2.53	0.44
1:E:280:MSE:HE2	1:E:409:ASN:CG	2.38	0.44
1:F:232:TYR:HB2	1:F:244:CYS:SG	2.58	0.44
1:F:253:ILE:HA	1:F:286:VAL:O	2.18	0.44
1:D:70:PHE:HE2	1:D:155:MSE:CE	2.17	0.43
1:A:78:MSE:HE1	1:A:100:ILE:CG1	2.49	0.43
1:B:462:HIS:CA	1:B:466:SER:HB3	2.48	0.43
1:G:2:LEU:HD12	1:G:21:ILE:CD1	2.48	0.43
1:C:451:TRP:CE2	1:D:472:ARG:HG3	2.53	0.43
1:B:412:ALA:HA	1:B:434:GLY:O	2.18	0.43
1:G:152:MSE:HB3	1:G:152:MSE:HE2	1.97	0.43
1:E:168:PHE:HE1	1:E:470:TRP:HH2	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:MSE:HE2	1:F:97:LYS:HA	2.00	0.43
1:E:253:ILE:HD12	1:E:424:PHE:CZ	2.52	0.43
1:B:208:ASP:O	1:B:212:THR:HG22	2.19	0.43
1:B:223:GLY:O	1:B:246:GLY:HA2	2.18	0.43
1:H:156:TRP:CE3	1:H:461:GLN:CG	3.01	0.43
1:F:311:PRO:HG2	1:F:357:TYR:CE1	2.53	0.43
1:E:86:SER:HB3	1:E:312:TYR:HB2	2.01	0.43
1:C:58:THR:HG22	1:C:62:ARG:HB2	2.00	0.43
1:C:73:LEU:HD21	1:C:189:GLU:HG2	2.01	0.43
1:E:337:SER:O	1:E:341:GLN:HB2	2.18	0.43
1:H:145:THR:OG1	1:H:172:PRO:HA	2.18	0.43
1:B:92:THR:HG22	1:B:93:ILE:N	2.31	0.43
1:C:171:LYS:HA	1:C:200:VAL:O	2.18	0.43
1:E:379:LYS:HA	1:E:405:HIS:NE2	2.33	0.43
1:E:82:ALA:HA	1:E:85:LEU:HD23	2.00	0.43
1:G:4:HIS:NE2	1:G:36:ALA:HB2	2.31	0.43
1:F:369:ASP:O	1:F:370:ASP:O	2.35	0.43
1:H:398:ALA:O	1:H:402:PRO:HD2	2.19	0.43
1:G:25:ALA:O	1:G:360:GLY:HA3	2.17	0.43
1:E:296:LEU:HD12	1:E:296:LEU:C	2.39	0.43
1:F:282:ILE:HD12	1:F:282:ILE:O	2.18	0.43
1:F:153:ILE:O	1:F:156:TRP:HB2	2.19	0.43
1:F:268:ILE:HD11	1:F:304:VAL:CG2	2.48	0.43
1:B:324:THR:HG22	1:B:327:ALA:HB2	2.00	0.43
1:E:171:LYS:HD3	1:E:207:VAL:HG23	1.99	0.43
1:D:30:GLN:O	1:D:30:GLN:HG2	2.16	0.43
1:E:248:ALA:CB	1:E:279:CYS:O	2.66	0.43
1:A:113:ILE:HG23	1:A:114:PRO:HD3	2.00	0.43
1:H:91:LYS:HD3	1:H:95:ASP:HB3	2.01	0.43
1:B:266:ALA:HB1	1:B:438:PRO:HB3	2.00	0.43
1:A:460:ASN:HB3	1:A:461:GLN:H	1.68	0.43
1:G:70:PHE:CE2	1:G:74:LEU:HD11	2.53	0.43
1:F:347:VAL:CG1	1:F:367:LEU:H	2.32	0.43
1:C:113:ILE:N	1:C:114:PRO:CD	2.81	0.43
1:E:249:LYS:HB2	1:E:405:HIS:HE1	1.84	0.43
1:B:2:LEU:HD22	1:B:181:ILE:HD13	2.01	0.43
1:A:339:ILE:HD11	1:A:345:LEU:HD22	2.01	0.43
1:B:422:ARG:O	1:B:426:SER:HB2	2.19	0.43
1:A:156:TRP:CE3	1:A:461:GLN:HG2	2.54	0.43
1:B:225:THR:HB	1:B:226:PRO:HD3	2.01	0.43
1:A:444:ALA:HA	1:A:462:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLY:HA3	1:C:168:PHE:HZ	1.84	0.43
1:G:104:LEU:O	1:G:107:CYS:HB2	2.19	0.43
1:E:122:THR:CG2	1:F:446:HIS:NE2	2.82	0.43
1:E:300:LEU:CD2	1:E:367:LEU:HD11	2.38	0.43
1:B:92:THR:HG22	1:B:95:ASP:H	1.84	0.43
1:H:301:VAL:CG2	1:H:302:PRO:HD3	2.49	0.43
1:D:332:ARG:NH1	1:D:350:ARG:HB2	2.31	0.43
1:D:86:SER:HB3	1:D:312:TYR:CB	2.48	0.43
1:D:221:PHE:CE1	1:D:228:ALA:HB2	2.54	0.43
1:E:213:HIS:ND1	1:E:214:PRO:HD2	2.34	0.43
1:E:224:SER:HB3	1:E:226:PRO:HD2	2.01	0.43
1:D:99:ASP:OD2	1:D:99:ASP:C	2.57	0.43
1:G:410:GLY:HA2	1:G:432:MSE:O	2.19	0.43
1:D:248:ALA:HB1	1:D:250:ASN:OD1	2.19	0.43
1:F:304:VAL:HG12	1:F:347:VAL:CG2	2.49	0.43
1:H:442:PRO:HG2	1:H:447:SER:O	2.19	0.43
1:G:161:ALA:O	1:G:166:ASN:ND2	2.52	0.43
1:H:59:ASN:HB2	1:H:60:PRO:CD	2.49	0.43
1:F:187:MSE:HE3	1:F:192:LEU:HD11	2.01	0.42
1:D:71:VAL:HA	1:D:74:LEU:HD12	2.01	0.42
1:E:462:HIS:HB2	1:E:463:GLY:H	1.70	0.42
1:A:78:MSE:HE2	1:A:78:MSE:CA	2.44	0.42
1:B:301:VAL:HG23	1:B:347:VAL:HG23	2.00	0.42
1:G:148:ASN:ND2	1:G:149:PHE:HE1	2.17	0.42
1:F:61:GLN:OE1	1:H:443:LEU:HD13	2.19	0.42
1:A:171:LYS:HE2	1:A:202:GLY:O	2.19	0.42
1:B:138:VAL:HG13	1:B:217:ALA:HB3	2.01	0.42
1:G:295:ARG:H	1:G:295:ARG:HD2	1.76	0.42
1:B:272:TYR:CE2	1:B:304:VAL:HG22	2.54	0.42
1:C:245:PHE:CD1	1:C:245:PHE:N	2.87	0.42
1:B:92:THR:CG2	1:B:94:ASP:H	2.29	0.42
1:B:442:PRO:HG2	1:B:447:SER:O	2.19	0.42
1:C:63:ARG:NH2	1:C:163:ALA:O	2.52	0.42
1:F:255:MSE:HE1	1:F:395:TYR:HA	2.01	0.42
1:G:249:LYS:HE2	1:G:283:SER:CB	2.49	0.42
1:E:108:GLU:HA	1:E:111:ILE:HD12	2.01	0.42
1:E:18:VAL:HA	1:E:33:VAL:O	2.19	0.42
1:F:373:PRO:HA	1:F:378:TYR:CD2	2.55	0.42
1:F:145:THR:HG21	1:F:154:PRO:HG3	2.01	0.42
1:A:67:PHE:O	1:A:71:VAL:HG23	2.19	0.42
1:E:255:MSE:HE3	1:E:413:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:LEU:O	1:E:240:LYS:HE2	2.19	0.42
1:B:289:GLY:HA3	1:B:292:THR:CG2	2.46	0.42
1:G:91:LYS:HG3	1:G:95:ASP:HB2	2.00	0.42
1:F:110:VAL:HG21	1:F:160:PRO:HA	2.01	0.42
1:B:319:MSE:HE1	1:B:385:PRO:HB3	2.00	0.42
1:E:99:ASP:OD1	1:E:152:MSE:HB2	2.20	0.42
1:H:280:MSE:HE1	1:H:409:ASN:CB	2.49	0.42
1:D:145:THR:HG22	1:D:153:ILE:HG22	2.02	0.42
1:G:382:ILE:HG12	1:G:382:ILE:H	1.73	0.42
1:F:401:LEU:HB2	1:F:402:PRO:HD3	2.00	0.42
1:B:153:ILE:O	1:B:156:TRP:HB2	2.19	0.42
1:D:459:LEU:HA	1:D:459:LEU:HD23	1.90	0.42
1:H:359:ASN:N	1:H:359:ASN:OD1	2.52	0.42
1:G:291:GLU:HA	1:G:295:ARG:HH11	1.85	0.42
1:B:275:ALA:HA	1:B:319:MSE:CE	2.40	0.42
1:F:249:LYS:HB2	1:F:405:HIS:CE1	2.55	0.42
1:D:159:ALA:N	1:D:160:PRO:HD2	2.34	0.42
1:E:24:PRO:HA	1:E:361:HIS:CE1	2.55	0.42
1:F:23:ASN:HD22	1:F:24:PRO:HD2	1.84	0.42
1:F:52:GLN:HB2	1:F:167:ALA:HB2	2.01	0.42
1:A:129:ILE:HA	1:A:478:SER:O	2.20	0.42
1:G:324:THR:HG22	1:G:327:ALA:CB	2.50	0.42
1:E:137:PRO:O	1:E:472:ARG:CD	2.68	0.42
1:E:462:HIS:N	1:E:466:SER:OG	2.52	0.42
1:H:152:MSE:HE2	1:H:153:ILE:HG13	2.00	0.42
1:B:211:LEU:HD13	1:B:234:THR:CB	2.48	0.42
1:E:141:GLY:HA3	1:E:470:TRP:HZ3	1.84	0.42
1:B:405:HIS:O	1:B:452:LYS:NZ	2.52	0.42
1:E:474:LYS:HA	1:F:431:GLY:O	2.18	0.42
1:A:106:VAL:HG21	1:A:156:TRP:CD1	2.55	0.42
1:C:93:ILE:HD11	1:C:312:TYR:HD2	1.85	0.42
1:C:187:MSE:HG3	1:C:192:LEU:HD22	2.02	0.42
1:E:428:ILE:HG12	1:E:429:ASN:N	2.34	0.42
1:F:369:ASP:O	1:F:370:ASP:C	2.54	0.42
1:E:302:PRO:O	1:E:305:GLU:HB2	2.20	0.42
1:H:24:PRO:HB2	1:H:321:PRO:HG2	2.00	0.42
1:G:345:LEU:HD22	1:G:347:VAL:O	2.20	0.42
1:G:345:LEU:HG	1:G:368:PHE:CE1	2.54	0.42
1:E:102:ARG:HB3	1:E:152:MSE:CG	2.50	0.42
1:A:25:ALA:HB1	1:A:311:PRO:HB3	2.01	0.42
1:A:18:VAL:HG13	1:A:32:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:MSE:HG2	1:H:158:PHE:CZ	2.55	0.42
1:F:70:PHE:HE1	1:F:187:MSE:HA	1.84	0.42
1:G:297:ILE:H	1:G:297:ILE:HG12	1.61	0.42
1:E:485:LYS:HE3	1:E:485:LYS:HA	2.02	0.42
1:A:211:LEU:HD13	1:A:234:THR:HB	2.02	0.42
1:G:213:HIS:HA	1:G:214:PRO:HD2	1.84	0.42
1:C:159:ALA:HB3	1:C:160:PRO:HD3	2.01	0.42
1:D:402:PRO:HB2	1:D:428:ILE:HD11	2.02	0.42
1:F:211:LEU:O	1:F:238:ASN:ND2	2.52	0.42
1:B:158:PHE:HE1	1:B:187:MSE:CE	2.33	0.42
1:D:322:VAL:N	1:D:361:HIS:O	2.47	0.42
1:E:81:LEU:O	1:E:85:LEU:HD22	2.19	0.42
1:E:299:LYS:H	1:E:299:LYS:HG2	1.68	0.42
1:H:192:LEU:HD21	1:H:196:ILE:HG22	2.01	0.41
1:E:192:LEU:HD12	1:E:193:PRO:HD2	2.02	0.41
1:A:115:HIS:HD2	1:A:118:LYS:HZ3	1.64	0.41
1:A:486:ASP:HA	2:A:548:HOH:O	2.20	0.41
1:D:94:ASP:O	1:D:97:LYS:HD3	2.20	0.41
1:E:251:HIS:HA	1:E:284:VAL:O	2.20	0.41
1:E:5:PHE:CE2	1:E:8:GLY:HA2	2.55	0.41
1:D:448:PHE:CD1	1:D:448:PHE:C	2.94	0.41
1:C:59:ASN:OD1	1:C:59:ASN:C	2.58	0.41
1:E:153:ILE:O	1:E:156:TRP:HB2	2.20	0.41
1:F:26:THR:O	1:F:359:ASN:HB2	2.20	0.41
1:C:341:GLN:NE2	1:C:375:MSE:HA	2.35	0.41
1:D:92:THR:O	1:D:95:ASP:N	2.49	0.41
1:A:108:GLU:HA	1:A:111:ILE:HD12	2.02	0.41
1:G:249:LYS:HE2	1:G:283:SER:HB2	2.02	0.41
1:D:113:ILE:HG22	1:D:114:PRO:HD3	2.01	0.41
1:H:20:ASN:HB2	1:H:29:VAL:HG13	2.01	0.41
1:B:104:LEU:C	1:B:104:LEU:HD13	2.41	0.41
1:E:115:HIS:CD2	1:E:118:LYS:HD3	2.56	0.41
1:D:278:ARG:HB2	1:D:281:ALA:HB2	2.01	0.41
1:H:329:GLN:O	1:H:333:SER:HB2	2.21	0.41
1:D:412:ALA:HA	1:D:434:GLY:O	2.20	0.41
1:F:74:LEU:HD11	1:F:155:MSE:HE1	2.02	0.41
1:G:326:GLU:H	1:G:326:GLU:CD	2.22	0.41
1:E:102:ARG:CB	1:E:152:MSE:HG3	2.51	0.41
1:D:211:LEU:HD22	1:D:211:LEU:N	2.36	0.41
1:F:484:ILE:CD1	2:H:522:HOH:O	2.68	0.41
1:B:147:PHE:CZ	1:B:383:PHE:HE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:HE1	1:B:354:LEU:HB2	1.85	0.41
1:C:148:ASN:OD1	1:C:277:GLU:O	2.37	0.41
1:B:85:LEU:HD22	1:B:150:PRO:HG2	2.03	0.41
1:F:35:LEU:HD12	1:F:36:ALA:H	1.85	0.41
1:E:447:SER:HB3	1:E:460:ASN:HB3	2.01	0.41
1:E:411:VAL:HB	1:E:430:ILE:HG21	2.02	0.41
1:F:304:VAL:HG11	1:F:347:VAL:CG2	2.51	0.41
1:C:252:MSE:HB2	1:C:282:ILE:HG12	2.02	0.41
1:A:89:HIS:HD2	1:A:91:LYS:H	1.67	0.41
1:E:213:HIS:HB3	1:E:216:ILE:HG13	2.02	0.41
1:C:176:ASP:N	1:C:176:ASP:OD1	2.52	0.41
1:D:272:TYR:O	1:D:275:ALA:N	2.54	0.41
1:E:411:VAL:HG22	1:E:412:ALA:H	1.84	0.41
1:E:462:HIS:CA	1:E:466:SER:OG	2.66	0.41
1:B:272:TYR:O	1:B:319:MSE:HE3	2.19	0.41
1:G:268:ILE:HG13	1:G:269:GLY:N	2.36	0.41
1:C:52:GLN:HB2	1:C:52:GLN:HE21	1.65	0.41
1:B:33:VAL:HG11	1:B:174:GLU:HB3	2.03	0.41
1:E:82:ALA:HA	1:E:85:LEU:CD2	2.50	0.41
1:F:297:ILE:HD11	1:F:389:VAL:HG21	2.03	0.41
1:B:106:VAL:HA	1:B:444:ALA:HB1	2.01	0.41
1:F:326:GLU:H	1:F:326:GLU:HG2	1.63	0.41
1:G:176:ASP:OD1	1:G:176:ASP:N	2.54	0.41
1:F:70:PHE:CE2	1:F:155:MSE:CE	3.04	0.41
1:E:448:PHE:HD1	1:E:448:PHE:O	2.02	0.41
1:D:255:MSE:HB2	1:D:414:TYR:O	2.21	0.41
1:F:310:GLY:HA2	1:F:311:PRO:HD3	1.78	0.41
1:G:460:ASN:HB3	1:G:461:GLN:H	1.68	0.41
1:F:309:ILE:HD12	1:F:352:PHE:CD2	2.56	0.41
1:F:115:HIS:HD2	1:F:118:LYS:HZ2	1.67	0.41
1:H:113:ILE:CG2	1:H:114:PRO:HD3	2.50	0.41
1:D:221:PHE:HE1	1:D:228:ALA:HB2	1.85	0.41
1:F:412:ALA:HA	1:F:434:GLY:O	2.21	0.41
1:B:235:ALA:HB1	1:B:240:LYS:HG3	2.02	0.41
1:C:245:PHE:CE1	1:C:461:GLN:NE2	2.89	0.41
1:F:369:ASP:OD1	1:F:369:ASP:C	2.59	0.41
1:E:126:GLY:HA3	1:E:129:ILE:HB	2.02	0.41
1:C:30:GLN:HE22	1:C:87:ARG:NE	2.14	0.41
1:E:36:ALA:HB1	1:E:40:ASP:HB2	2.02	0.41
1:D:141:GLY:HA3	1:D:470:TRP:CZ3	2.54	0.41
1:G:249:LYS:HE2	1:G:283:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:LEU:HD13	1:H:189:GLU:HG2	2.03	0.41
1:E:85:LEU:HD12	1:E:150:PRO:HG2	2.02	0.41
1:C:67:PHE:CE1	1:C:187:MSE:HE1	2.56	0.41
1:F:368:PHE:O	1:F:389:VAL:N	2.51	0.41
1:E:480:TRP:HA	1:E:481:PRO:HD2	1.78	0.41
1:G:67:PHE:CE1	1:G:187:MSE:HE1	2.56	0.41
1:D:219:VAL:O	1:D:242:ALA:HA	2.21	0.41
1:B:102:ARG:HB3	1:B:152:MSE:SE	2.71	0.41
1:A:15:SER:HB2	1:A:37:SER:HB3	2.02	0.41
1:D:343:ALA:HB2	1:D:375:MSE:SE	2.71	0.41
1:A:405:HIS:O	1:A:452:LYS:NZ	2.41	0.41
1:C:472:ARG:NH1	1:D:451:TRP:CZ3	2.89	0.41
1:H:37:SER:O	1:H:40:ASP:N	2.54	0.41
1:H:159:ALA:CB	1:H:160:PRO:CD	2.98	0.41
1:F:439:ILE:HG22	1:F:439:ILE:O	2.20	0.41
1:E:379:LYS:HG3	1:E:379:LYS:H	1.54	0.41
1:F:78:MSE:CE	1:F:97:LYS:HA	2.51	0.41
1:B:113:ILE:HA	1:B:116:LEU:HB2	2.02	0.40
1:C:106:VAL:HG11	1:C:156:TRP:HA	2.01	0.40
1:B:311:PRO:C	1:B:313:THR:N	2.74	0.40
1:B:71:VAL:HG13	1:B:104:LEU:CD2	2.51	0.40
1:D:21:ILE:O	1:D:30:GLN:O	2.39	0.40
1:D:325:LYS:HG2	1:D:361:HIS:CD2	2.56	0.40
1:E:88:GLU:HB3	1:E:176:ASP:HB3	2.03	0.40
1:E:155:MSE:HG2	1:E:158:PHE:CE2	2.56	0.40
1:H:448:PHE:CD1	1:H:448:PHE:C	2.94	0.40
1:E:403:MSE:O	1:E:429:ASN:ND2	2.52	0.40
1:E:308:ARG:NH1	1:E:316:LYS:O	2.54	0.40
1:B:256:PRO:HD3	1:B:288:VAL:HB	2.02	0.40
1:B:311:PRO:O	1:B:313:THR:N	2.54	0.40
1:C:267:LEU:HB3	1:C:300:LEU:HD11	2.03	0.40
1:F:85:LEU:HD22	1:F:91:LYS:HD3	2.03	0.40
1:B:142:ALA:HB3	1:B:219:VAL:HG22	2.03	0.40
1:H:425:ALA:HA	1:H:433:VAL:HG11	2.02	0.40
1:A:66:VAL:HG12	1:A:187:MSE:CE	2.50	0.40
1:B:271:GLY:HA2	1:B:282:ILE:O	2.21	0.40
1:A:131:MSE:HE1	1:B:443:LEU:HG	2.02	0.40
1:F:149:PHE:HB3	1:F:152:MSE:HB3	2.04	0.40
1:E:442:PRO:HG3	1:E:447:SER:O	2.21	0.40
1:E:137:PRO:HB3	1:E:166:ASN:OD1	2.21	0.40
1:E:211:LEU:HD12	1:E:235:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ILE:N	1:D:114:PRO:CD	2.84	0.40
1:D:107:CYS:O	1:D:111:ILE:HG13	2.22	0.40
1:E:102:ARG:HB3	1:E:152:MSE:HG3	2.02	0.40
1:H:20:ASN:HB3	1:H:32:THR:HG22	2.03	0.40
1:G:399:LEU:HD13	1:G:424:PHE:CD2	2.56	0.40
2:B:525:HOH:O	1:D:123:GLU:HG3	2.22	0.40
1:A:204:LYS:HG2	1:A:205:GLY:N	2.35	0.40
1:C:268:ILE:HA	1:C:268:ILE:HD13	1.93	0.40
1:H:308:ARG:HB3	1:H:308:ARG:NH1	2.35	0.40
1:F:293:ALA:O	1:F:297:ILE:HG12	2.22	0.40
1:H:89:HIS:C	1:H:89:HIS:ND1	2.75	0.40
1:H:326:GLU:H	1:H:326:GLU:CD	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ASP:O	1:F:299:LYS:NZ[4_446]	2.14	0.06

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/521 (93%)	457 (94%)	28 (6%)	1 (0%)	52	84
1	B	484/521 (93%)	455 (94%)	28 (6%)	1 (0%)	52	84
1	C	484/521 (93%)	457 (94%)	25 (5%)	2 (0%)	39	74
1	D	486/521 (93%)	457 (94%)	28 (6%)	1 (0%)	52	84
1	E	484/521 (93%)	451 (93%)	31 (6%)	2 (0%)	39	74
1	F	482/521 (92%)	450 (93%)	31 (6%)	1 (0%)	52	84
1	G	483/521 (93%)	456 (94%)	25 (5%)	2 (0%)	39	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	483/521 (93%)	452 (94%)	28 (6%)	3 (1%)	30	67
All	All	3872/4168 (93%)	3635 (94%)	224 (6%)	13 (0%)	46	79

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	462	HIS
1	A	462	HIS
1	C	462	HIS
1	D	462	HIS
1	E	462	HIS
1	F	462	HIS
1	B	462	HIS
1	C	438	PRO
1	G	462	HIS
1	H	146	PRO
1	H	273	GLY
1	E	177	PRO
1	G	481	PRO

### 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	383/391 (98%)	347 (91%)	36 (9%)	11	32
1	B	381/391 (97%)	330 (87%)	51 (13%)	5	13
1	C	381/391 (97%)	339 (89%)	42 (11%)	8	23
1	D	383/391 (98%)	327 (85%)	56 (15%)	4	12
1	E	381/391 (97%)	318 (84%)	63 (16%)	3	8
1	F	379/391 (97%)	310 (82%)	69 (18%)	2	6
1	G	381/391 (97%)	328 (86%)	53 (14%)	4	12
1	H	380/391 (97%)	339 (89%)	41 (11%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3049/3128 (98%)	2638 (86%)	411 (14%)	5 13

All (411) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	15	SER
1	A	30	GLN
1	A	33	VAL
1	A	62	ARG
1	A	69	LYS
1	A	78	MSE
1	A	86	SER
1	A	92	THR
1	A	104	LEU
1	A	110	VAL
1	A	119	SER
1	A	122	THR
1	A	134	ILE
1	A	148	ASN
1	A	158	PHE
1	A	182	ARG
1	A	220	SER
1	A	224	SER
1	A	268	ILE
1	A	274	SER
1	A	313	THR
1	A	329	GLN
1	A	337	SER
1	A	346	VAL
1	A	350	ARG
1	A	351	ASP
1	A	352	PHE
1	A	382	ILE
1	A	383	PHE
1	A	397	GLU
1	A	400	SER
1	A	422	ARG
1	A	465	ASP
1	A	468	LYS
1	A	478	SER
1	B	7	ASP

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Mol	Chain	Res	Type
1	B	9	LYS
1	B	10	ARG
1	B	35	LEU
1	B	41	LEU
1	B	47	SER
1	B	54	LYS
1	B	58	THR
1	B	85	LEU
1	B	91	LYS
1	B	102	ARG
1	B	104	LEU
1	B	123	GLU
1	B	171	LYS
1	B	174	GLU
1	B	175	ARG
1	B	182	ARG
1	B	220	SER
1	B	224	SER
1	B	227	ILE
1	B	229	ARG
1	B	230	TYR
1	B	237	MSE
1	B	240	LYS
1	B	249	LYS
1	B	278	ARG
1	B	283	SER
1	B	292	THR
1	B	295	ARG
1	B	296	LEU
1	B	301	VAL
1	B	303	MSE
1	B	315	GLU
1	B	324	THR
1	B	325	LYS
1	B	359	ASN
1	B	372	THR
1	B	374	ASP
1	B	380	THR
1	B	383	PHE
1	B	388	SER
1	B	399	LEU
1	B	404	LYS

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Mol	Chain	Res	Type
1	B	422	ARG
1	B	435	VAL
1	B	439	ILE
1	B	468	LYS
1	B	471	THR
1	B	475	THR
1	B	479	ARG
1	B	485	LYS
1	C	7	ASP
1	C	18	VAL
1	C	19	SER
1	C	20	ASN
1	C	33	VAL
1	C	49	LYS
1	C	52	GLN
1	C	72	GLN
1	C	73	LEU
1	C	84	MSE
1	C	91	LYS
1	C	94	ASP
1	C	102	ARG
1	C	110	VAL
1	C	119	SER
1	C	120	GLU
1	C	123	GLU
1	C	145	THR
1	C	158	PHE
1	C	175	ARG
1	C	182	ARG
1	C	188	ILE
1	C	237	MSE
1	C	267	LEU
1	C	274	SER
1	C	278	ARG
1	C	279	CYS
1	C	298	ASP
1	C	301	VAL
1	C	333	SER
1	C	337	SER
1	C	363	ILE
1	C	374	ASP
1	C	383	PHE

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Mol	Chain	Res	Type
1	C	393	ARG
1	C	400	SER
1	C	441	VAL
1	C	448	PHE
1	C	464	THR
1	C	468	LYS
1	C	471	THR
1	C	484	ILE
1	D	7	ASP
1	D	19	SER
1	D	30	GLN
1	D	32	THR
1	D	33	VAL
1	D	54	LYS
1	D	59	ASN
1	D	73	LEU
1	D	91	LYS
1	D	93	ILE
1	D	97	LYS
1	D	99	ASP
1	D	104	LEU
1	D	119	SER
1	D	133	SER
1	D	148	ASN
1	D	155	MSE
1	D	171	LYS
1	D	182	ARG
1	D	186	LEU
1	D	204	LYS
1	D	237	MSE
1	D	249	LYS
1	D	252	MSE
1	D	260	LEU
1	D	261	ASP
1	D	265	ASN
1	D	282	ILE
1	D	283	SER
1	D	292	THR
1	D	299	LYS
1	D	303	MSE
1	D	308	ARG
1	D	314	ASP

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Mol	Chain	Res	Type
1	D	326	GLU
1	D	328	GLU
1	D	332	ARG
1	D	333	SER
1	D	334	LEU
1	D	351	ASP
1	D	353	LYS
1	D	372	THR
1	D	380	THR
1	D	388	SER
1	D	393	ARG
1	D	406	GLU
1	D	422	ARG
1	D	427	ARG
1	D	445	TYR
1	D	453	SER
1	D	455	SER
1	D	460	ASN
1	D	464	THR
1	D	468	LYS
1	D	472	ARG
1	D	482	SER
1	E	14	THR
1	E	17	ARG
1	E	30	GLN
1	E	33	VAL
1	E	35	LEU
1	E	66	VAL
1	E	73	LEU
1	E	92	THR
1	E	93	ILE
1	E	94	ASP
1	E	102	ARG
1	E	113	ILE
1	E	119	SER
1	E	152	MSE
1	E	153	ILE
1	E	158	PHE
1	E	171	LYS
1	E	175	ARG
1	E	176	ASP
1	E	182	ARG

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Mol	Chain	Res	Type
1	E	200	VAL
1	E	201	ASN
1	E	204	LYS
1	E	211	LEU
1	E	220	SER
1	E	229	ARG
1	E	234	THR
1	E	237	MSE
1	E	249	LYS
1	E	251	HIS
1	E	267	LEU
1	E	268	ILE
1	E	295	ARG
1	E	296	LEU
1	E	297	ILE
1	E	298	ASP
1	E	307	LEU
1	E	313	THR
1	E	316	LYS
1	E	319	MSE
1	E	334	LEU
1	E	336	ASP
1	E	345	LEU
1	E	346	VAL
1	E	355	GLN
1	E	361	HIS
1	E	367	LEU
1	E	379	LYS
1	E	380	THR
1	E	383	PHE
1	E	393	ARG
1	E	406	GLU
1	E	409	ASN
1	E	415	THR
1	E	441	VAL
1	E	448	PHE
1	E	453	SER
1	E	460	ASN
1	E	471	THR
1	E	474	LYS
1	E	478	SER
1	E	484	ILE

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Mol	Chain	Res	Type
1	E	485	LYS
1	F	1	GLU
1	F	14	THR
1	F	23	ASN
1	F	29	VAL
1	F	30	GLN
1	F	38	ASP
1	F	47	SER
1	F	54	LYS
1	F	59	ASN
1	F	76	ASP
1	F	94	ASP
1	F	104	LEU
1	F	110	VAL
1	F	119	SER
1	F	136	GLN
1	F	148	ASN
1	F	153	ILE
1	F	158	PHE
1	F	175	ARG
1	F	178	SER
1	F	186	LEU
1	F	188	ILE
1	F	203	ASP
1	F	234	THR
1	F	237	MSE
1	F	249	LYS
1	F	251	HIS
1	F	260	LEU
1	F	261	ASP
1	F	267	LEU
1	F	279	CYS
1	F	283	SER
1	F	295	ARG
1	F	298	ASP
1	F	299	LYS
1	F	305	GLU
1	F	306	SER
1	F	307	LEU
1	F	308	ARG
1	F	326	GLU
1	F	336	ASP

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Mol	Chain	Res	Type
1	F	340	GLU
1	F	348	ASP
1	F	351	ASP
1	F	359	ASN
1	F	361	HIS
1	F	362	PHE
1	F	363	ILE
1	F	375	MSE
1	F	377	ILE
1	F	383	PHE
1	F	404	LYS
1	F	411	VAL
1	F	413	ILE
1	F	415	THR
1	F	422	ARG
1	F	428	ILE
1	F	437	VAL
1	F	439	ILE
1	F	441	VAL
1	F	443	LEU
1	F	447	SER
1	F	454	SER
1	F	458	ASP
1	F	459	LEU
1	F	467	ILE
1	F	472	ARG
1	F	475	THR
1	F	484	ILE
1	G	-2	MSE
1	G	28	GLU
1	G	33	VAL
1	G	41	LEU
1	G	47	SER
1	G	58	THR
1	G	84	MSE
1	G	86	SER
1	G	102	ARG
1	G	106	VAL
1	G	123	GLU
1	G	133	SER
1	G	138	VAL
1	G	171	LYS

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Mol	Chain	Res	Type
1	G	188	ILE
1	G	197	LEU
1	G	212	THR
1	G	224	SER
1	G	225	THR
1	G	227	ILE
1	G	249	LYS
1	G	260	LEU
1	G	277	GLU
1	G	278	ARG
1	G	283	SER
1	G	295	ARG
1	G	297	ILE
1	G	298	ASP
1	G	307	LEU
1	G	324	THR
1	G	329	GLN
1	G	330	ARG
1	G	333	SER
1	G	336	ASP
1	G	337	SER
1	G	340	GLU
1	G	345	LEU
1	G	355	GLN
1	G	359	ASN
1	G	374	ASP
1	G	375	MSE
1	G	382	ILE
1	G	383	PHE
1	G	404	LYS
1	G	413	ILE
1	G	426	SER
1	G	443	LEU
1	G	467	ILE
1	G	468	LYS
1	G	471	THR
1	G	472	ARG
1	G	478	SER
1	G	479	ARG
1	H	7	ASP
1	H	14	THR
1	H	20	ASN

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Mol	Chain	Res	Type
1	H	47	SER
1	H	54	LYS
1	H	71	VAL
1	H	73	LEU
1	H	94	ASP
1	H	95	ASP
1	H	119	SER
1	H	158	PHE
1	H	171	LYS
1	H	181	ILE
1	H	182	ARG
1	H	183	LEU
1	H	186	LEU
1	H	188	ILE
1	H	196	ILE
1	H	215	ASP
1	H	237	MSE
1	H	260	LEU
1	H	268	ILE
1	H	279	CYS
1	H	283	SER
1	H	288	VAL
1	H	296	LEU
1	H	313	THR
1	H	323	VAL
1	H	333	SER
1	H	340	GLU
1	H	353	LYS
1	H	377	ILE
1	H	383	PHE
1	H	393	ARG
1	H	406	GLU
1	H	422	ARG
1	H	447	SER
1	H	454	SER
1	H	471	THR
1	H	479	ARG
1	H	482	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	75	ASN
1	A	89	HIS
1	A	115	HIS
1	A	359	ASN
1	A	405	HIS
1	A	429	ASN
1	B	30	GLN
1	B	77	ASN
1	B	115	HIS
1	B	265	ASN
1	B	429	ASN
1	B	461	GLN
1	B	462	HIS
1	C	20	ASN
1	C	30	GLN
1	C	52	GLN
1	C	61	GLN
1	C	115	HIS
1	C	148	ASN
1	C	243	GLN
1	C	341	GLN
1	C	446	HIS
1	C	460	ASN
1	C	461	GLN
1	D	250	ASN
1	D	265	ASN
1	D	361	HIS
1	E	115	HIS
1	E	243	GLN
1	E	409	ASN
1	E	436	ASN
1	F	23	ASN
1	F	59	ASN
1	F	115	HIS
1	F	238	ASN
1	F	243	GLN
1	F	329	GLN
1	G	30	GLN
1	G	115	HIS
1	G	148	ASN
1	G	243	GLN
1	G	359	ASN

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Mol	Chain	Res	Type
1	H	201	ASN
1	H	394	ASN
1	H	405	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	470/521 (90%)	-0.61	1 (0%) 95 95	17, 36, 55, 71	0
1	B	469/521 (90%)	-0.54	1 (0%) 95 95	19, 38, 58, 76	0
1	C	468/521 (89%)	-0.70	1 (0%) 95 95	15, 28, 49, 79	0
1	D	470/521 (90%)	-0.47	3 (0%) 90 89	15, 43, 75, 93	0
1	E	469/521 (90%)	-0.09	10 (2%) 67 62	21, 57, 81, 97	0
1	F	467/521 (89%)	-0.04	12 (2%) 59 54	29, 59, 87, 107	0
1	G	466/521 (89%)	-0.63	1 (0%) 95 95	18, 35, 53, 70	0
1	H	468/521 (89%)	-0.53	2 (0%) 93 92	18, 38, 57, 74	0
All	All	3747/4168 (89%)	-0.45	31 (0%) 87 86	15, 40, 73, 107	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	359	ASN	3.7
1	F	29	VAL	3.3
1	E	226	PRO	3.1
1	D	359	ASN	2.9
1	H	16	GLY	2.9
1	F	348	ASP	2.8
1	E	336	ASP	2.7
1	F	17	ARG	2.7
1	E	351	ASP	2.7
1	F	16	GLY	2.7
1	C	482	SER	2.6
1	E	355	GLN	2.6
1	E	14	THR	2.6
1	E	388	SER	2.4
1	F	14	THR	2.4
1	B	356	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	315	GLU	2.3
1	F	15	SER	2.3
1	A	351	ASP	2.3
1	F	174	GLU	2.3
1	E	15	SER	2.3
1	G	482	SER	2.3
1	F	349	GLY	2.2
1	E	393	ARG	2.2
1	E	26	THR	2.2
1	F	31	GLY	2.1
1	F	28	GLU	2.1
1	F	355	GLN	2.1
1	H	329	GLN	2.1
1	D	316	LYS	2.0
1	E	329	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.