



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:57 AM UTC

PDB ID : 4E4G / pdb_00004e4g
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 (NYSGRC)
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

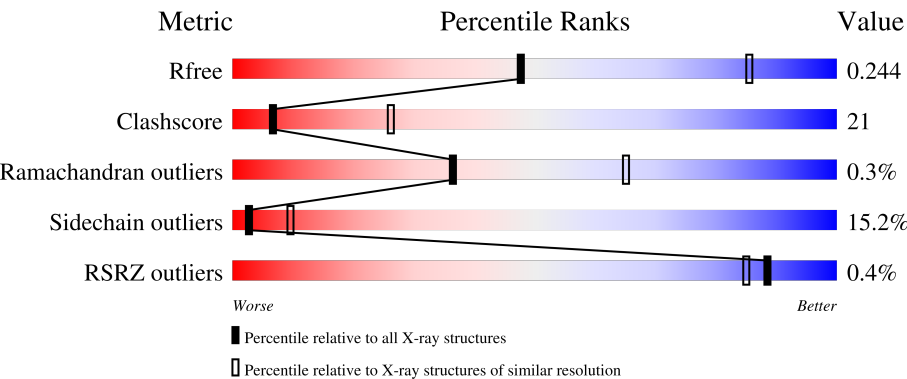
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	59%30%6%
1	B	521	53%33%7%7%
1	C	521	63%25%5%7%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	521	55%31%8%6%
1	E	521	% 47%35%11%7%
1	F	521	2% 46%37%9%7%
1	G	521	57%29%6%7%
1	H	521	55%32%6%7%

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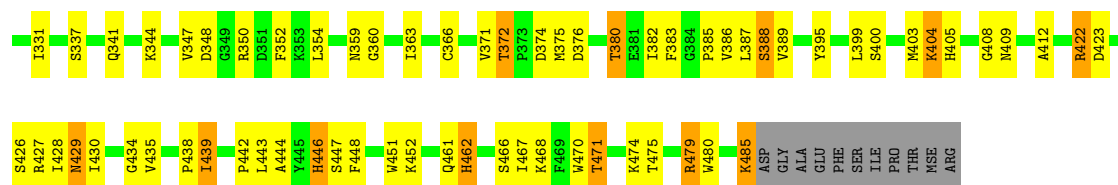
Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	GLN	-	expression tag	UNP Q92RW4
H	-3	SER	-	expression tag	UNP Q92RW4
H	-2	MSE	-	expression tag	UNP Q92RW4

- 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		

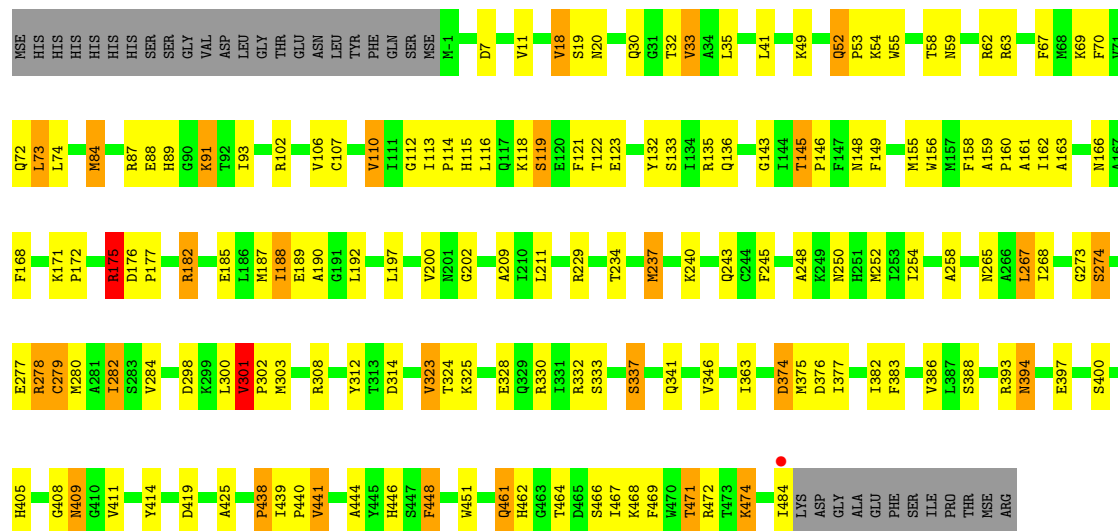
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase





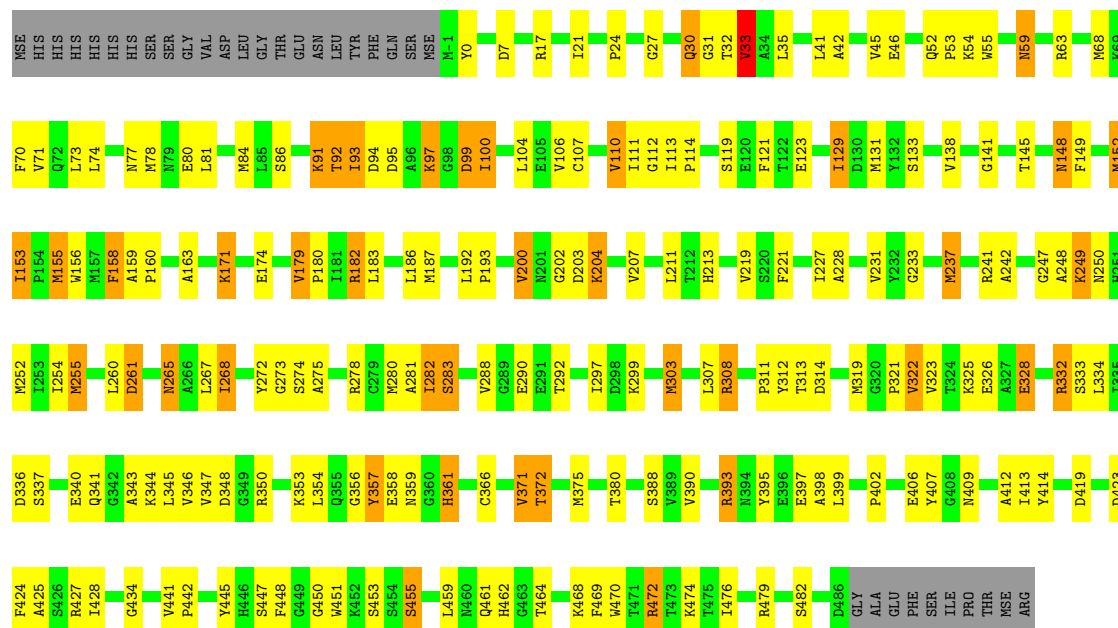
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain C: 63% 25% 5% 7%

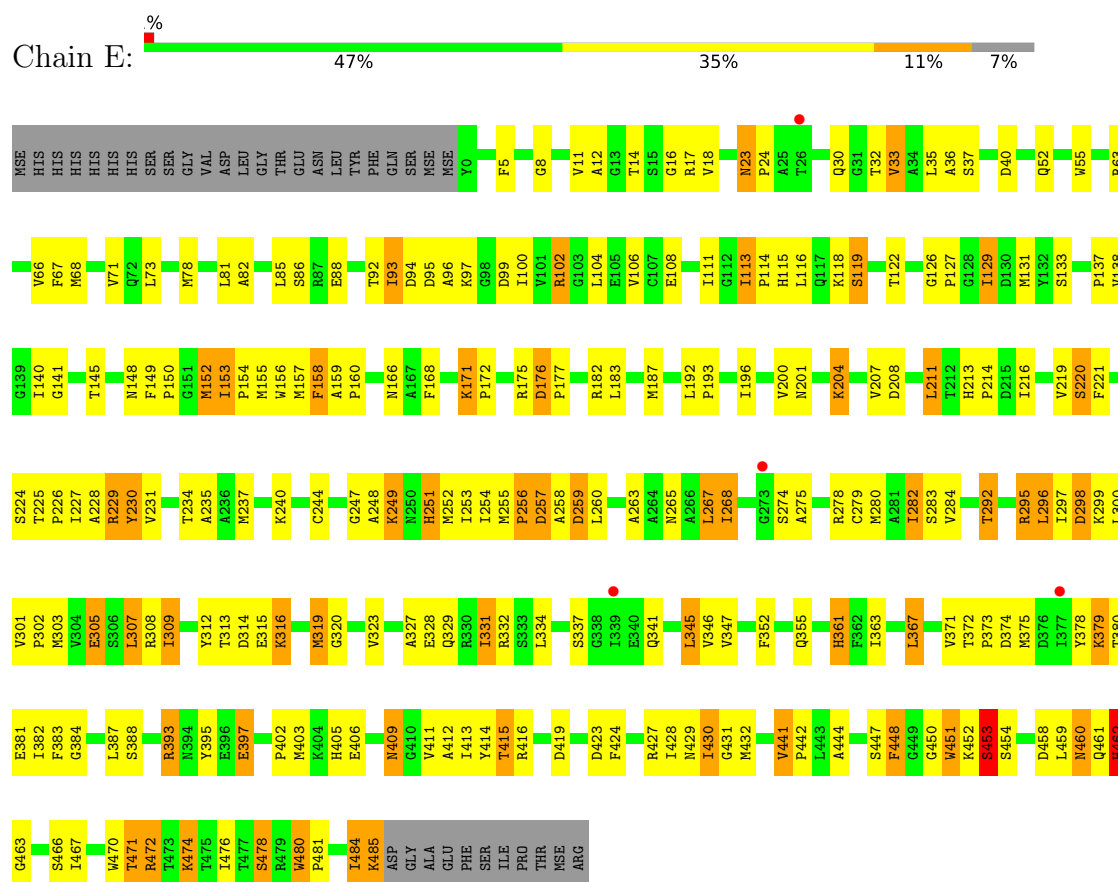


• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

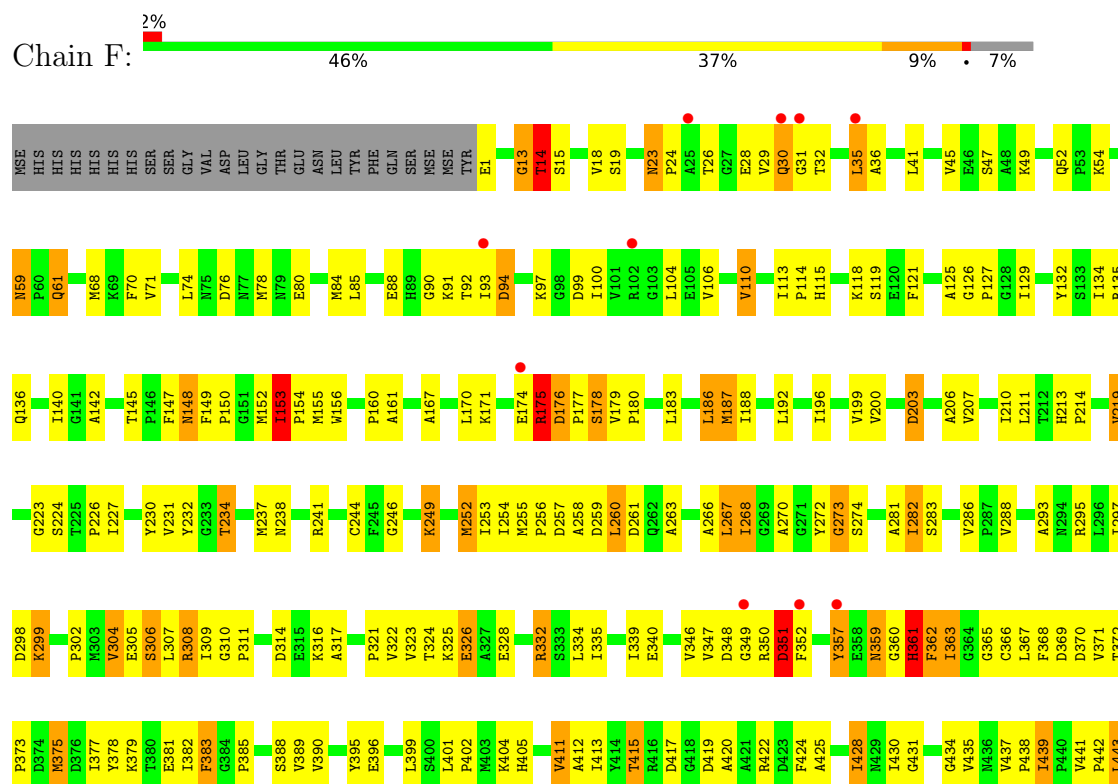
Chain D: 55% 31% 8% 6%



• Molecule 1: Methylmalonate-semialdehyde dehydrogenase



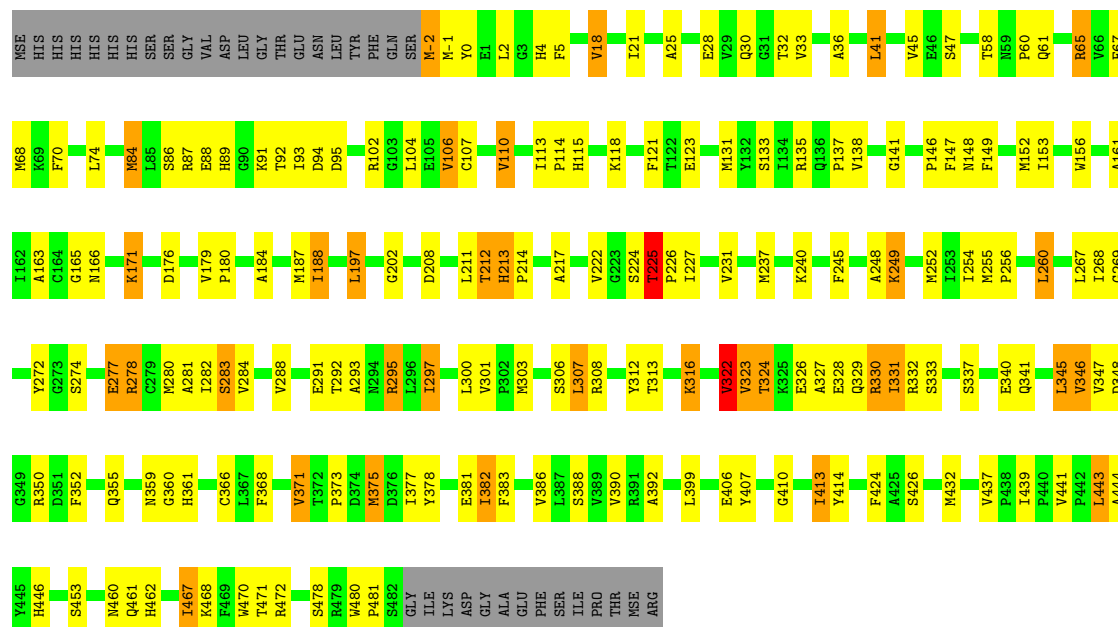
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase





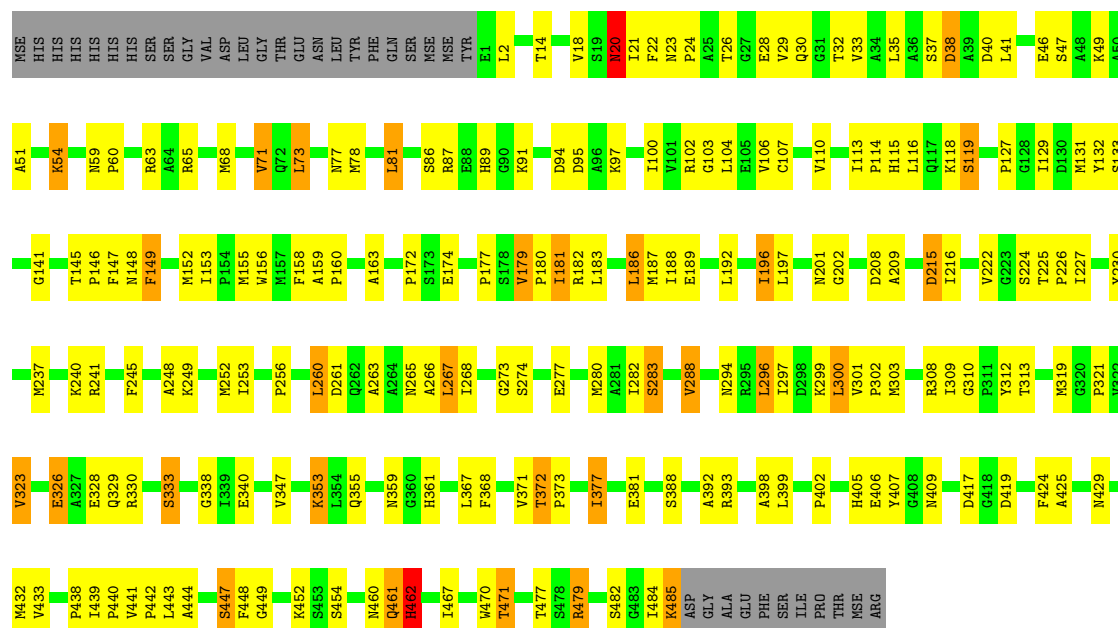
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain G: 57% 29% 6% 7%



• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain H: 55% 32% 6% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.6 (19.97-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.88Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.269 (Not available) , 0.244	Depositor DCC
R_{free} test set	4795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtrriage
Anisotropy	0.059	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29653	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	1/3742 (0.0%)	1.07	9/5043 (0.2%)
1	B	0.83	3/3726 (0.1%)	1.07	7/5022 (0.1%)
1	C	0.83	6/3725 (0.2%)	1.08	6/5021 (0.1%)
1	D	0.86	5/3742 (0.1%)	1.05	10/5043 (0.2%)
1	E	0.84	4/3726 (0.1%)	1.14	18/5022 (0.4%)
1	F	0.96	9/3704 (0.2%)	1.14	13/4993 (0.3%)
1	G	0.84	4/3720 (0.1%)	1.06	9/5012 (0.2%)
1	H	0.88	6/3713 (0.2%)	1.10	11/5004 (0.2%)
All	All	0.85	38/29798 (0.1%)	1.09	83/40160 (0.2%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	31	GLY	C-N	8.97	1.46	1.33
1	B	446	HIS	CG-ND1	-8.24	1.29	1.38
1	F	357	TYR	CG-CD2	8.20	1.56	1.39
1	G	446	HIS	CG-ND1	-7.78	1.29	1.38
1	F	30	GLN	CA-C	-7.53	1.42	1.52
1	H	462	HIS	CG-ND1	-7.32	1.30	1.38
1	G	446	HIS	CD2-NE2	-7.19	1.29	1.37
1	E	462	HIS	CG-ND1	-6.88	1.30	1.38
1	F	30	GLN	CA-CB	6.83	1.64	1.53
1	F	30	GLN	C-O	6.30	1.32	1.24
1	H	149	PHE	C-O	-6.24	1.18	1.24
1	A	6	ILE	C-O	-6.11	1.17	1.24
1	D	129	ILE	C-O	-6.10	1.17	1.24
1	H	462	HIS	CD2-NE2	-5.97	1.31	1.37
1	E	229	ARG	N-CA	-5.84	1.39	1.46
1	E	462	HIS	CD2-NE2	-5.81	1.31	1.37
1	B	446	HIS	CD2-NE2	-5.64	1.31	1.37
1	F	332	ARG	NE-CZ	5.64	1.39	1.33
1	D	152	MSE	CA-C	-5.62	1.45	1.52
1	D	361	HIS	CE1-NE2	5.62	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	322	VAL	C-O	-5.61	1.17	1.24
1	C	409	ASN	C-O	-5.50	1.17	1.23
1	D	361	HIS	CG-CD2	5.50	1.41	1.35
1	D	153	ILE	C-O	-5.44	1.17	1.24
1	F	357	TYR	CE1-CZ	5.34	1.51	1.38
1	C	408	GLY	C-O	-5.31	1.16	1.23
1	F	175	ARG	C-O	-5.31	1.18	1.24
1	H	21	ILE	C-O	-5.30	1.17	1.24
1	F	361	HIS	CA-C	-5.20	1.47	1.53
1	H	461	GLN	C-O	-5.17	1.17	1.23
1	C	177	PRO	C-O	-5.11	1.17	1.24
1	H	440	PRO	N-CA	-5.10	1.43	1.47
1	G	322	VAL	CA-CB	-5.09	1.47	1.54
1	E	451	TRP	NE1-CE2	-5.09	1.31	1.37
1	C	301	VAL	CA-CB	5.03	1.57	1.53
1	C	405	HIS	CA-C	-5.03	1.46	1.52
1	B	446	HIS	C-O	-5.03	1.18	1.23
1	C	446	HIS	CA-C	-5.01	1.46	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	229	ARG	N-CA-C	-13.83	96.20	111.28
1	F	349	GLY	N-CA-C	12.64	128.95	112.77
1	F	273	GLY	N-CA-C	-11.67	98.50	111.93
1	F	125	ALA	N-CA-C	-9.89	100.50	111.28
1	E	323	VAL	N-CA-C	8.44	119.22	110.36
1	A	84	MSE	N-CA-CB	-8.02	98.34	110.12
1	F	13	GLY	N-CA-C	-7.84	100.06	111.03
1	E	230	TYR	N-CA-C	7.74	119.35	111.07
1	C	301	VAL	N-CA-CB	7.51	115.23	110.50
1	B	255	MSE	N-CA-CB	-7.34	101.23	109.74
1	D	80	GLU	N-CA-C	-7.24	104.71	113.97
1	D	357	TYR	N-CA-C	-7.14	104.50	112.57
1	E	257	ASP	N-CA-C	7.11	119.10	111.36
1	E	52	GLN	CA-C-N	-7.04	111.24	119.05
1	E	52	GLN	C-N-CA	-7.04	111.24	119.05
1	G	323	VAL	N-CA-C	7.00	119.76	112.83
1	D	255	MSE	N-CA-CB	-6.99	100.61	110.04
1	D	152	MSE	CB-CA-C	-6.87	100.05	110.90
1	F	32	THR	N-CA-C	6.77	120.01	109.52
1	C	175	ARG	N-CA-C	6.70	118.66	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	323	VAL	N-CA-C	6.60	116.76	110.42
1	H	202	GLY	N-CA-C	6.55	121.32	111.42
1	H	38	ASP	N-CA-C	-6.51	104.19	111.28
1	B	319	MSE	N-CA-CB	-6.49	100.47	111.31
1	D	323	VAL	N-CA-C	6.41	116.55	110.53
1	H	20	ASN	N-CA-C	6.33	120.02	109.95
1	F	153	ILE	N-CA-CB	6.31	114.47	110.50
1	G	-1	MSE	N-CA-CB	-6.12	101.16	110.77
1	A	33	VAL	CB-CA-C	-6.09	102.86	111.21
1	F	351	ASP	N-CA-C	-6.08	103.54	111.74
1	E	259	ASP	N-CA-C	-5.99	101.42	110.28
1	D	129	ILE	N-CA-C	5.97	116.47	108.11
1	D	152	MSE	N-CA-C	5.96	117.58	111.14
1	E	453	SER	N-CA-C	-5.96	105.93	112.72
1	H	132	TYR	N-CA-C	5.88	118.05	108.76
1	G	213	HIS	CA-C-N	5.86	125.53	119.56
1	G	213	HIS	C-N-CA	5.86	125.53	119.56
1	B	176	ASP	CA-C-N	5.83	126.34	120.04
1	B	176	ASP	C-N-CA	5.83	126.34	120.04
1	A	148	ASN	N-CA-C	5.73	117.53	111.28
1	H	283	SER	N-CA-C	-5.72	105.97	113.12
1	A	59	ASN	CA-C-N	5.70	125.82	119.32
1	A	59	ASN	C-N-CA	5.70	125.82	119.32
1	G	225	THR	CA-C-N	-5.60	112.83	119.05
1	G	225	THR	C-N-CA	-5.60	112.83	119.05
1	F	258	ALA	N-CA-C	5.55	117.49	110.33
1	C	33	VAL	CB-CA-C	-5.53	102.92	110.77
1	G	147	PHE	N-CA-C	-5.47	105.34	112.23
1	H	310	GLY	CA-C-N	5.46	125.45	120.21
1	H	310	GLY	C-N-CA	5.46	125.45	120.21
1	F	282	ILE	N-CA-C	5.41	115.98	108.84
1	A	20	ASN	N-CA-C	5.32	118.61	110.20
1	D	158	PHE	N-CA-C	5.32	117.99	111.82
1	A	300	LEU	CA-C-N	5.29	124.56	120.33
1	A	300	LEU	C-N-CA	5.29	124.56	120.33
1	B	429	ASN	CB-CA-C	-5.27	100.39	110.57
1	D	237	MSE	N-CA-C	-5.25	105.63	111.36
1	B	140	ILE	N-CA-C	5.25	115.54	107.77
1	F	14	THR	N-CA-C	-5.23	102.31	110.10
1	F	15	SER	N-CA-C	5.23	116.94	108.26
1	G	346	VAL	N-CA-C	5.23	115.95	110.62
1	A	17	ARG	N-CA-C	5.22	117.80	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	386	VAL	N-CA-C	5.18	115.95	107.24
1	E	430	ILE	N-CA-C	5.15	115.39	107.77
1	H	323	VAL	N-CA-C	5.15	116.61	111.00
1	B	177	PRO	N-CA-C	5.12	121.18	114.27
1	H	372	THR	CA-C-N	5.11	125.40	119.47
1	H	372	THR	C-N-CA	5.11	125.40	119.47
1	E	275	ALA	N-CA-C	-5.11	104.59	111.54
1	E	23	ASN	CA-C-N	5.09	124.70	119.05
1	E	23	ASN	C-N-CA	5.09	124.70	119.05
1	E	480	TRP	CA-C-N	5.08	125.01	119.78
1	E	480	TRP	C-N-CA	5.08	125.01	119.78
1	C	394	ASN	N-CA-C	5.06	115.21	108.38
1	G	237	MSE	N-CA-CB	-5.04	102.46	110.22
1	D	33	VAL	CB-CA-C	-5.03	103.33	110.83
1	E	256	PRO	CA-C-N	5.03	127.43	120.29
1	E	256	PRO	C-N-CA	5.03	127.43	120.29
1	H	241	ARG	N-CA-C	-5.03	103.08	110.52
1	F	176	ASP	N-CA-C	5.03	116.79	109.30
1	E	320	GLY	CA-C-N	5.00	126.09	119.84
1	E	320	GLY	C-N-CA	5.00	126.09	119.84
1	F	100	ILE	N-CA-C	5.00	117.70	112.90

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	3681	0	3652	113	0
1	B	3665	0	3639	167	0
1	C	3664	0	3635	117	0
1	D	3681	0	3652	143	0
1	E	3665	0	3639	226	1
1	F	3644	0	3617	258	1
1	G	3660	0	3630	132	0
1	H	3653	0	3630	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1253	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 (1253) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:THR:C	1:F:361:HIS:CD2	2.44	0.95
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:D:280:MSE:HE1	1:D:409:ASN:HB3	1.50	0.93
1:H:338:GLY:HA3	1:H:377:ILE:HD12	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:D:280:MSE:CE	1:D:409:ASN:HB3	2.00	0.91
1:F:350:ARG:CG	1:F:351:ASP:N	2.30	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:HG3	1:A:350:ARG:HH11	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:F:362:PHE:CD1	1:F:362:PHE:N	2.41	0.88
1:G:322:VAL:HG12	1:G:323:VAL:N	1.84	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:E:156:TRP:CE3	1:E:461:GLN:HG2	2.08	0.87
1:H:110:VAL:HG11	1:H:163:ALA:HB2	1.53	0.87
1:C:341:GLN:HE22	1:C:376:ASP:H	1.22	0.87
1:F:26:THR:OG1	1:F:28:GLU:HG2	1.75	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:E:308:ARG:HH12	1:E:316:LYS:HB2	1.41	0.86
1:H:110:VAL:HG13	1:H:163:ALA:HB2	1.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:HG13	1:B:303:MSE:HG2	1.58	0.85
1:H:110:VAL:CG1	1:H:163:ALA:CB	2.51	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:O	1:G:323:VAL:HG22	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:D:250:ASN:HD21	1:D:280:MSE:HE2	1.42	0.84
1:E:131:MSE:HE1	1:F:443:LEU:N	1.91	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:D:203:ASP:CG	1:D:204:LYS:H	1.84	0.83
1:G:188:ILE:HD11	2:G:502:HOH:O	1.77	0.83
1:G:293:ALA:O	1:G:297:ILE:HG12	1.79	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:A:405:HIS:HD2	1:A:407:TYR:H	1.29	0.81
1:F:347:VAL:HG11	1:F:366:CYS:HA	1.62	0.81
1:E:255:MSE:CB	1:E:257:ASP:OD1	2.28	0.81
1:F:256:PRO:HD3	1:F:288:VAL:CG2	2.10	0.81
1:C:148:ASN:ND2	1:C:149:PHE:CD2	2.48	0.81
1:B:319:MSE:HE2	1:B:385:PRO:HB3	1.61	0.80
1:E:131:MSE:HE3	1:F:446:HIS:HB2	1.63	0.80
1:G:324:THR:HG22	1:G:327:ALA:N	1.96	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
1:B:324:THR:HG23	1:B:327:ALA:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ARG:HH12	1:F:467:ILE:CG2	1.96	0.79
1:E:295:ARG:HG3	1:E:295:ARG:HH11	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:HG3	1:F:175:ARG:HH21	1.49	0.77
1:F:308:ARG:HB3	1:F:317:ALA:HA	1.65	0.77
1:G:248:ALA:O	1:G:381:GLU:HG3	1.85	0.77
1:G:322:VAL:HG13	1:G:323:VAL:H	1.49	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:B:319:MSE:CE	1:B:385:PRO:HB3	2.14	0.76
1:D:393:ARG:HH22	1:D:397:GLU:CG	1.96	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:F:350:ARG:O	1:F:351:ASP:CG	2.28	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:E:371:VAL:HG21	1:E:388:SER:HB3	1.67	0.75
1:F:153:ILE:N	1:F:153:ILE:HD13	2.02	0.75
1:G:327:ALA:O	1:G:331:ILE:HD12	1.86	0.75
1:B:89:HIS:ND1	1:B:91:LYS:HB3	2.02	0.74
1:D:356:GLY:C	1:D:358:GLU:OE1	2.30	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: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:E:153:ILE:HG13	1:E:157:MSE:HE2	1.67	0.74
1:F:350:ARG:C	1:F:351:ASP:OD2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HA	1:A:68:MSE:HE3	1.68	0.73
1:B:376:ASP:O	1:B:380:THR:HG23	1.87	0.73
1:C:328:GLU:OE2	1:C:332:ARG:NH1	2.21	0.73
1:D:156:TRP:CE3	1:D:461:GLN:HG2	2.24	0.73
1:A:350:ARG:HH11	1:A:350:ARG:CG	2.01	0.73
1:C:280:MSE:HE1	1:C:409:ASN:CG	2.13	0.73
1:C:274:SER:HA	2:C:511:HOH:O	1.90	0.72
1:F:68:MSE:HE1	1:H:71:VAL:CG1	2.08	0.72
1:C:280:MSE:CE	1:C:409:ASN:ND2	2.52	0.72
1:E:192:LEU:HD11	1:E:196:ILE:HG21	1.69	0.72
1:E:484:ILE:O	1:E:485:LYS:HG2	1.89	0.72
1:F:369:ASP:O	1:F:370:ASP:HB2	1.87	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:E:448:PHE:CD1	1:E:448:PHE:C	2.66	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:B:372:THR:HG22	1:B:375:MSE:HG3	1.71	0.71
1:E:71:VAL:HG13	1:E:104:LEU:HG	1.72	0.71
1:E:127:PRO:C	1:E:129:ILE:HD12	2.15	0.71
1:B:92:THR:HG22	1:B:94:ASP:N	2.04	0.71
1:C:472:ARG:NH1	1:D:451:TRP:CE3	2.58	0.71
1:F:328:GLU:HG3	1:F:363:ILE:HD11	1.73	0.71
1:F:322:VAL:HG12	1:F:323:VAL:H	1.55	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:E:255:MSE:HB2	1:E:257:ASP:OD1	1.92	0.70
1:F:324:THR:C	1:F:361:HIS:HD2	1.96	0.70
1:F:362:PHE:HD1	1:F:362:PHE:H	1.38	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:259:ASP:OD1	1:E:259:ASP:C	2.30	0.70
1:E:255:MSE:HB3	1:E:257:ASP:OD1	1.90	0.70
1:F:171:LYS:HE2	1:F:207:VAL:CG2	2.21	0.69
1:G:322:VAL:CG1	1:G:323:VAL:H	1.98	0.69
1:H:22:PHE:O	1:H:30:GLN:NE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:ILE:HG12	1:E:319:MSE:HE3	1.73	0.69
1:D:110:VAL:HG13	1:D:163:ALA:HB2	1.75	0.69
1:H:78:MSE:HE2	1:H:97:LYS:HG2	1.73	0.69
1:B:311:PRO:HG2	1:B:313:THR:HG22	1.73	0.69
1:E:145:THR:HB	1:E:172:PRO:HA	1.75	0.69
1:E:228:ALA:O	1:E:229:ARG:C	2.36	0.69
1:B:211:LEU:HD13	1:B:234:THR:HB	1.73	0.69
1:G:153:ILE:O	1:G:156:TRP:HB2	1.93	0.69
1:H:301:VAL:HG12	1:H:347:VAL:HG23	1.75	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:A:78:MSE:HE2	1:A:78:MSE:HA	1.75	0.68
1:G:252:MSE:HB2	1:G:282:ILE:HD12	1.74	0.68
1:F:153:ILE:N	1:F:153:ILE:HD12	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:F:88:GLU:CD	1:F:178:SER:OG	2.36	0.68
1:H:129:ILE:HG13	1:H:479:ARG:HG3	1.76	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:B:372:THR:HB	1:B:375:MSE:HE3	1.76	0.68
1:F:361:HIS:ND1	1:F:361:HIS:N	2.41	0.68
1:H:22:PHE:C	1:H:30:GLN:HE21	2.02	0.68
1:B:7:ASP:O	1:B:9:LYS:HE3	1.94	0.68
1:E:168:PHE:HE1	1:E:470:TRP:CH2	2.12	0.67
1:F:371:VAL:HG12	1:F:372:THR:N	2.09	0.67
1:C:107:CYS:SG	1:C:155:MSE:HE2	2.35	0.67
1:F:272:TYR:HE1	1:F:385:PRO:O	1.76	0.67
1:F:350:ARG:C	1:F:351:ASP:CG	2.63	0.67
1:G:255:MSE:CE	1:G:413:ILE:HD11	2.23	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: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:149:PHE:O	1:E:153:ILE:HG22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:PRO:O	1:E:129:ILE:HD12	1.96	0.66
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:H:37:SER:HG	1:H:40:ASP:CG	2.03	0.66
1:A:358:GLU:O	1:A:359:ASN:HB2	1.95	0.66
1:G:324:THR:HG23	1:G:326:GLU:OE1	1.96	0.66
1:A:309:ILE:HG12	1:A:319:MSE:HE3	1.78	0.66
1:E:467:ILE:O	1:E:471:THR:HB	1.96	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:H:280:MSE:CE	1:H:409:ASN:CG	2.69	0.65
1:B:220:SER:HB3	1:B:243:GLN:HG3	1.77	0.65
1:F:113:ILE:CG2	1:F:114:PRO:HD3	2.26	0.65
1:B:296:LEU:HD13	1:B:300:LEU:HD12	1.78	0.65
1:F:153:ILE:HD13	1:F:153:ILE:H	1.61	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:59:ASN:C	1:F:59:ASN:HD22	2.03	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:A:161:ALA:O	1:A:166:ASN:HB2	1.98	0.64
1:D:358:GLU:OE1	1:D:358:GLU:N	2.30	0.64
1:E:55:TRP:CZ2	1:E:63:ARG:HG2	2.32	0.64
1:F:70:PHE:HE2	1:F:155:MSE:HE1	1.61	0.64
1:E:432:MSE:HE1	1:E:441:VAL:HG23	1.80	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:B:45:VAL:HG11	1:B:213:HIS:CE1	2.33	0.64
1:F:369:ASP:OD1	1:F:370:ASP:N	2.29	0.64
1:G:366:CYS:HB2	1:G:386:VAL:HG22	1.80	0.64
1:A:486:ASP:OD1	1:C:394:ASN:HB2	1.98	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:F:325:LYS:N	1:F:361:HIS:HD2	1.90	0.64
1:E:207:VAL:O	1:E:211:LEU:HD22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:E:129:ILE:N	2.13	0.64
1:C:121:PHE:CD1	1:C:132:TYR:HB3	2.33	0.63
1:E:131:MSE:HE3	1:F:446:HIS:CB	2.28	0.63
1:G:260:LEU:HD11	1:G:292:THR:HG23	1.81	0.63
1:D:203:ASP:CG	1:D:204:LYS:N	2.53	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:B:366:CYS:HB2	1:B:386:VAL:HG22	1.80	0.63
1:B:485:LYS:NZ	1:D:419:ASP:OD2	2.31	0.63
1:E:102:ARG:HH21	1:E:102:ARG:CG	2.11	0.63
1:E:478:SER:HB2	1:F:435:VAL:HB	1.81	0.63
1:G:225:THR:HG23	1:G:226:PRO:HD3	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:E:211:LEU:HD11	1:E:231:VAL:HG13	1.81	0.63
1:F:446:HIS:O	1:F:462:HIS:ND1	2.32	0.62
1:D:45:VAL:HG11	1:D:213:HIS:CE1	2.34	0.62
1:F:90:GLY:O	1:F:321:PRO:HD2	1.99	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:B:92:THR:HG22	1:B:94:ASP:H	1.64	0.62
1:H:78:MSE:CE	1:H:97:LYS:HA	2.29	0.62
1:H:156:TRP:CE3	1:H:461:GLN:HG2	2.35	0.62
1:C:374:ASP:OD1	1:C:374:ASP:N	2.31	0.62
1:F:369:ASP:OD1	1:F:370:ASP:CG	2.42	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:E:268:ILE:HD13	1:E:303:MSE:SE	2.49	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:B:55:TRP:CZ2	1:B:63:ARG:HG2	2.35	0.61
1:E:171:LYS:O	1:E:171:LYS:NZ	2.30	0.61
1:E:268:ILE:CD1	1:E:300:LEU:HD12	2.29	0.61
1:H:33:VAL:HG11	1:H:174:GLU:HB2	1.82	0.61
1:H:77:ASN:O	1:H:81:LEU:HB2	2.00	0.61
1:H:115:HIS:O	1:H:118:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:159:ALA:HB3	1:A:160:PRO:HD3	1.81	0.61
1:A:408:GLY:HA2	1:A:430:ILE:HG13	1.83	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:H:37:SER:OG	1:H:40:ASP:CG	2.44	0.61
1:E:211:LEU:HD22	1:E:211:LEU:H	1.66	0.61
1:F:152:MSE:CE	1:F:153:ILE:CD1	2.73	0.60
1:C:135:ARG:HD3	1:C:471:THR:HG21	1.83	0.60
1:C:211:LEU:O	1:C:240:LYS:HE2	2.02	0.60
1:G:348:ASP:OD1	1:G:350:ARG:HB2	2.00	0.60
1:B:78:MSE:HE1	1:B:100:ILE:HB	1.84	0.60
1:C:273:GLY:O	1:C:278:ARG:NH2	2.34	0.60
1:F:192:LEU:HD13	1:F:196:ILE:HD11	1.82	0.60
1:B:447:SER:HA	1:B:462:HIS:CD2	2.37	0.60
1:F:175:ARG:HG3	1:F:175:ARG:NH2	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:H:280:MSE:HE3	1:H:409:ASN:ND2	2.17	0.60
1:H:225:THR:HB	1:H:226:PRO:HD3	1.83	0.60
1:H:353:LYS:HE3	1:H:353:LYS:HA	1.84	0.60
1:B:113:ILE:HD11	1:B:117:GLN:HG3	1.84	0.60
1:D:0:TYR:O	1:D:31:GLY:HA2	2.02	0.60
1:D:227:ILE:O	1:D:231:VAL:HG23	2.02	0.60
1:E:257:ASP:OD1	1:E:257:ASP:N	2.34	0.60
1:F:59:ASN:C	1:F:59:ASN:ND2	2.60	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:439:ILE:O	1:F:439:ILE:CG2	2.49	0.59
1:F:446:HIS:O	1:F:462:HIS:CE1	2.55	0.59
1:B:74:LEU:HD22	1:B:155:MSE:HE1	1.77	0.59
1:B:222:VAL:HG13	1:B:245:PHE:HB2	1.84	0.59
1:B:467:ILE:O	1:B:471:THR:HB	2.01	0.59
1:C:280:MSE:CE	1:C:409:ASN:CG	2.74	0.59
1:D:354:LEU:O	1:D:357:TYR:HB2	2.02	0.59
1:B:187:MSE:HG2	1:B:192:LEU:HD22	1.84	0.59
1:C:279:CYS:O	1:C:280:MSE:HE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:SER:O	1:C:341:GLN:HG3	2.02	0.59
1:D:207:VAL:C	1:D:211:LEU:HD23	2.28	0.59
1:E:474:LYS:HD2	1:F:430:ILE:O	2.02	0.59
1:C:252:MSE:SE	1:C:267:LEU:HD13	2.53	0.59
1:A:241:ARG:NH1	1:A:469:PHE:O	2.35	0.59
1:E:432:MSE:CE	1:E:441:VAL:HG23	2.33	0.59
1:G:65:ARG:HA	1:G:68:MSE:HE3	1.85	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:H:65:ARG:HA	1:H:68:MSE:HG2	1.84	0.59
1:C:425:ALA:O	1:D:474:LYS:HE2	2.03	0.59
1:D:110:VAL:HG13	1:D:163:ALA:CB	2.32	0.59
1:F:446:HIS:ND1	2:F:506:HOH:O	2.23	0.58
1:G:171:LYS:NZ	1:G:202:GLY:O	2.36	0.58
1:G:332:ARG:NH2	1:G:350:ARG:O	2.36	0.58
1:C:19:SER:HB2	1:C:35:LEU:HD21	1.85	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:D:171:LYS:HE3	1:D:202:GLY:O	2.03	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:A:249:LYS:HE3	1:A:283:SER:CB	2.34	0.58
1:D:371:VAL:HB	1:D:390:VAL:HG22	1.85	0.58
1:F:252:MSE:HE2	1:F:254:ILE:CG1	2.33	0.58
1:A:145:THR:OG1	1:A:172:PRO:HA	2.03	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:F:187:MSE:HB3	1:F:192:LEU:CD1	2.27	0.58
1:B:423:ASP:O	1:B:427:ARG:HG3	2.04	0.58
1:D:33:VAL:HG21	1:D:174:GLU:HB2	1.86	0.58
1:H:179:VAL:HB	1:H:180:PRO:HD3	1.85	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: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:C:448:PHE:CD1	1:C:448:PHE:C	2.82	0.58
1:D:110:VAL:CG1	1:D:163:ALA:HB2	2.33	0.58
1:G:179:VAL:HB	1:G:180:PRO:CD	2.34	0.58
1:H:372:THR:HB	1:H:373:PRO:HD2	1.85	0.58
1:A:-1:MSE:HA	1:A:30:GLN:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:PRO:HD3	1:G:222:VAL:O	2.04	0.57
1:C:162:ILE:HD11	1:C:197:LEU:HB2	1.85	0.57
1:E:252:MSE:HB2	1:E:282:ILE:HD13	1.85	0.57
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:G:252:MSE:SE	1:G:267:LEU:HD13	2.55	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:B:408:GLY:HA2	1:B:430:ILE:HG12	1.87	0.57
1:F:88:GLU:OE2	1:F:178:SER:OG	2.23	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:D:345:LEU:HD23	1:D:345:LEU:C	2.30	0.57
1:B:25:ALA:O	1:B:360:GLY:HA3	2.05	0.57
1:D:241:ARG:NH1	1:D:469:PHE:O	2.38	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:B:256:PRO:HA	1:B:292:THR:HG21	1.84	0.57
1:C:41:LEU:HD22	1:C:209:ALA:HB1	1.87	0.57
1:E:372:THR:HG22	1:E:374:ASP:H	1.69	0.57
1:B:267:LEU:HD22	1:B:387:LEU:HD21	1.87	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:D:357:TYR:N	1:D:358:GLU:OE1	2.38	0.57
1:G:330:ARG:NH2	1:G:382:ILE:O	2.38	0.57
1:A:78:MSE:HA	1:A:78:MSE:CE	2.34	0.56
1:B:220:SER:HB3	1:B:243:GLN:CG	2.35	0.56
1:E:327:ALA:O	1:E:331:ILE:HD12	2.05	0.56
1:F:92:THR:HG22	1:F:93:ILE:N	2.19	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:A:442:PRO:HG2	1:A:447:SER:O	2.05	0.56
1:E:171:LYS:HE2	1:E:172:PRO: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:A:268:ILE:HG22	1:A:269:GLY:N	2.20	0.56
1:C:55:TRP:CZ2	1:C:63:ARG:HG2	2.41	0.56
1:C:185:GLU:O	1:C:188:ILE:HG13	2.05	0.56
1:F:174:GLU:HB2	1:F:175:ARG:HH12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:VAL:HG13	1:H:163:ALA:HB1	1.85	0.56
1:E:149:PHE:O	1:E:153:ILE:CG2	2.53	0.56
1:E:252:MSE:SE	1:E:254:ILE:HD11	2.56	0.56
1:E:257:ASP:O	1:E:416:ARG:NH2	2.38	0.56
1:F:45:VAL:HG11	1:F:213:HIS:CE1	2.40	0.56
1:D:254:ILE:HD12	1:D:254:ILE:N	2.21	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:B:480:TRP:HB3	1:D:419:ASP:HB2	1.88	0.56
1:F:93:ILE:HD12	1:F:94:ASP:N	2.21	0.56
1:G:65:ARG:HG3	1:G:68:MSE:HE3	1.87	0.56
1:B:113:ILE:N	1:B:114:PRO:HD2	2.21	0.56
1:E:78:MSE:HE2	1:E:97:LYS:HG2	1.88	0.56
1:E:295:ARG:HG3	1:E:295:ARG:NH1	2.16	0.56
1:G:89:HIS:ND1	1:G:91:LYS:HD2	2.21	0.56
1:G:137:PRO:HG3	1:G:165:GLY:HA3	1.86	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: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:B:192:LEU:HD11	1:B:196:ILE:HG21	1.87	0.55
1:D:325:LYS:HA	1:D:328:GLU:HG2	1.88	0.55
1:E:140:ILE:HD12	1:E:140:ILE:N	2.21	0.55
1:F:395:TYR:HB3	1:H:485:LYS:HD2	1.88	0.55
1:H:68:MSE:O	1:H:71:VAL:HG12	2.05	0.55
1:A:295:ARG:O	1:A:299:LYS:HG3	2.07	0.55
1:C:325:LYS:HG3	1:E:16:GLY:HA3	1.88	0.55
1:E:148:ASN:HD22	1:E:383:PHE:HZ	1.53	0.55
1:E:248:ALA:O	1:E:381:GLU:HG3	2.07	0.55
1:F:270:ALA:O	1:F:281:ALA:HB1	2.07	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: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:252:MSE:HE1	1:F:263:ALA:HB1	1.89	0.55
1:C:115:HIS:O	1:C:118:LYS:HG2	2.07	0.55
1:E:78:MSE:HE1	1:E:100:ILE:HD13	1.88	0.55
1:F:26:THR:CB	1:F:28:GLU:HG2	2.37	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: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:B:218:ALA:HB3	1:B:470:TRP:CZ3	2.42	0.54
1:D:280:MSE:HE2	1:D:280:MSE:HA	1.90	0.54
1:E:133:SER:HB3	2:F:506:HOH:O	2.07	0.54
1:H:102:ARG:HH12	1:H:443:LEU:HD23	1.70	0.54
1:H:145:THR:HG22	1:H:153:ILE:HG22	1.89	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:D:179:VAL:HB	1:D:180:PRO:HD3	1.88	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: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:252:MSE:HE2	1:F:254:ILE:HG13	1.90	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: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:88:GLU:OE1	1:F:178:SER:OG	2.26	0.53
1:H:280:MSE:HE2	1:H:409:ASN:ND2	2.22	0.53
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.11	0.53
1:B:19:SER:HB2	1:B:35:LEU:HD11	1.90	0.53
1:C:110:VAL:HG13	1:C:163:ALA:CB	2.38	0.53
1:D:158:PHE:HE1	1:D:187:MSE:CE	2.19	0.53
1:F:99:ASP:OD2	1:F:149:PHE:HA	2.08	0.53
1:F:417:ASP:OD2	1:F:419:ASP:HB3	2.08	0.53
1:H:253:ILE:HD12	1:H:424:PHE:CE1	2.42	0.53
1:B:337:SER:O	1:B:341:GLN:HG3	2.09	0.53
1:C:69:LYS:HD3	1:C:190:ALA:HA	1.89	0.53
1:F:272:TYR:O	1:F:273:GLY:C	2.49	0.53
1:H:280:MSE:HE1	1:H:409:ASN:CG	2.32	0.53
1:H:301:VAL:HG23	1:H:302:PRO:HD3	1.89	0.53
1:C:323:VAL:HG22	1:C:324:THR:HG23	1.91	0.53
1:E:459:LEU:HD21	1:F:459:LEU:HD21	1.90	0.53
1:G:5:PHE:HE1	1:G:188:ILE:HD13	1.73	0.53
1:E:221:PHE:HB3	1:E:244:CYS:SG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:ARG:HH11	1:E:316:LYS:HE2	1.73	0.53
1:F:325:LYS:N	1:F:361:HIS:NE2	2.57	0.53
1:G:278:ARG:HG3	1:G:281:ALA:HB2	1.90	0.53
1:A:257:ASP:O	1:A:416:ARG:HG3	2.08	0.53
1:F:78:MSE:HE2	1:F:97:LYS:HG2	1.91	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: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:E:373:PRO:HA	1:E:378:TYR:CD2	2.43	0.53
1:H:148:ASN:HD22	1:H:149:PHE:HD1	1.52	0.53
1:E:127:PRO:C	1:E:129:ILE:CD1	2.82	0.53
1:F:176:ASP:N	1:F:177:PRO:HD3	2.24	0.53
1:A:115:HIS:HD2	1:A:118:LYS:HZ1	1.55	0.53
1:C:30:GLN:NE2	1:C:87:ARG:HE	2.07	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:H:328:GLU:OE1	1:H:361:HIS:HA	2.09	0.53
1:B:248:ALA:HB2	1:B:409:ASN:HD22	1.74	0.52
1:G:328:GLU:O	1:G:332:ARG:HG3	2.09	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:H:26:THR:HG22	1:H:28:GLU:H	1.74	0.52
1:H:429:ASN:O	1:H:452:LYS:HE2	2.10	0.52
1:D:250:ASN:HD21	1:D:280:MSE:CE	2.18	0.52
1:E:419:ASP:HB2	1:G:480:TRP:HB3	1.92	0.52
1:F:49:LYS:HG3	1:F:140:ILE:HD11	1.91	0.52
1:F:309:ILE:HB	1:F:352:PHE:CZ	2.45	0.52
1:G:0:TYR:OH	1:G:30:GLN:NE2	2.43	0.52
1:A:369:ASP:OD1	1:A:370:ASP:N	2.42	0.52
1:F:328:GLU:OE1	1:F:361:HIS:HB3	2.09	0.52
1:H:296:LEU:HD13	1:H:300:LEU:HD22	1.91	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:H:417:ASP:O	1:H:419:ASP:N	2.40	0.52
1:D:288:VAL:HG22	1:D:398:ALA:HB2	1.92	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:F:115:HIS:HD2	1:F:118:LYS:NZ	2.07	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:D:399:LEU:HD13	1:D:424:PHE:CD2	2.45	0.52
1:A:411:VAL:HG12	1:A:430:ILE:HG21	1.92	0.52
1:D:24:PRO:HB2	1:D:321:PRO:HB2	1.92	0.52
1:D:91:LYS:NZ	1:D:148:ASN:O	2.42	0.52
1:E:329:GLN:O	1:E:332:ARG:HB2	2.10	0.52
1:H:23:ASN:HB3	1:H:26:THR:HB	1.92	0.52
1:A:439:ILE:O	1:A:439:ILE:HG22	2.10	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: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:G:115:HIS:HD2	1:G:118:LYS:NZ	2.07	0.52
1:B:115:HIS:O	1:B:118:LYS:HG3	2.10	0.51
1:B:179:VAL:HB	1:B:180:PRO:HD3	1.90	0.51
1:B:429:ASN:ND2	1:B:452:LYS:HD3	2.24	0.51
1:D:74:LEU:CD1	1:D:155:MSE:HE1	2.39	0.51
1:E:67:PHE:O	1:E:71:VAL:HG23	2.09	0.51
1:E:137:PRO:O	1:E:472:ARG:HD2	2.10	0.51
1:F:206:ALA:O	1:F:210:ILE:HG13	2.10	0.51
1:F:304:VAL:HG12	1:F:347:VAL:HG23	1.90	0.51
1:H:447:SER:HB3	1:H:460:ASN:HD22	1.76	0.51
1:A:74:LEU:HD23	1:A:104:LEU:HB2	1.92	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: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:B:448:PHE:CD1	1:B:448:PHE:C	2.89	0.51
1:E:228:ALA:C	1:E:230:TYR:N	2.62	0.51
1:B:285:ALA:HB3	1:B:389:VAL:HG22	1.93	0.51
1:B:423:ASP:OD2	1:B:427:ARG:NH1	2.44	0.51
1:F:424:PHE:O	1:F:428:ILE:HG13	2.11	0.51
1:G:92:THR:HG22	1:G:94:ASP:N	2.26	0.51
1:H:141:GLY:HA3	1:H:470:TRP:CZ3	2.45	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:B:74:LEU:CD2	1:B:155:MSE:CE	2.72	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:E:428:ILE:HG12	1:E:429:ASN:H	1.76	0.51
1:F:223:GLY:O	1:F:246:GLY:HA2	2.11	0.51
1:F:314:ASP:OD2	1:F:317:ALA:HB2	2.09	0.51
1:A:395:TYR:OH	1:A:423:ASP:OD2	2.22	0.51
1:D:395:TYR:OH	1:D:423:ASP:OD2	2.26	0.51
1:E:309:ILE:HG23	1:E:319:MSE:O	2.10	0.51
1:E:444:ALA:O	1:E:462:HIS:HB2	2.11	0.51
1:H:294:ASN:O	1:H:297:ILE:HG13	2.11	0.51
1:A:480:TRP:HB3	1:C:419:ASP:HB2	1.93	0.51
1:D:74:LEU:HD11	1:D:155:MSE:HE1	1.92	0.51
1:A:64:ALA:HB1	1:A:111:ILE:O	2.11	0.51
1:A:119:SER:CB	1:A:133:SER:O	2.59	0.51
1:A:249:LYS:HE3	1:A:283:SER:HB3	1.91	0.51
1:B:129:ILE:HG12	1:B:479:ARG:HG3	1.92	0.51
1:E:382:ILE:HG22	1:E:384:GLY:H	1.75	0.51
1:H:484:ILE:HG23	1:H:484:ILE:O	2.11	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:A:134:ILE:HD13	1:D:121:PHE:CE2	2.47	0.50
1:A:250:ASN:HB2	1:A:281:ALA:O	2.10	0.50
1:C:158:PHE:CD1	1:C:158:PHE:C	2.90	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:F:266:ALA:HB1	1:F:438:PRO:HB3	1.93	0.50
1:F:371:VAL:HG13	1:F:375:MSE:CE	2.42	0.50
1:G:60:PRO:HB2	1:G:114:PRO:HG3	1.92	0.50
1:B:348:ASP:OD1	1:B:350:ARG:HD3	2.11	0.50
1:F:192:LEU:CD2	1:F:196:ILE:HD11	2.39	0.50
1:H:208:ASP:OD1	1:H:230:TYR:OH	2.29	0.50
1:A:392:ALA:HB1	1:A:397:GLU:HG2	1.93	0.50
1:C:330:ARG:HH11	1:C:330:ARG:HB3	1.77	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:405:HIS:CD2	1:A:407:TYR:H	2.18	0.50
1:A:450:GLY:O	1:A:455:SER:OG	2.22	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:255:MSE:HE3	1:A:256:PRO:HD2	1.94	0.50
1:B:141:GLY:HA3	1:B:470:TRP:CZ3	2.46	0.50
1:D:347:VAL:O	1:D:366:CYS:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:PHE:CE1	1:F:187:MSE:HA	2.47	0.50
1:A:328:GLU:HG3	1:A:363:ILE:HD11	1.92	0.50
1:B:428:ILE:HD12	1:B:429:ASN:H	1.77	0.50
1:D:273:GLY:O	1:D:274:SER:HB2	2.11	0.50
1:E:331:ILE:HG21	1:E:363:ILE:HD13	1.92	0.50
1:F:371:VAL:CG1	1:F:372:THR:N	2.74	0.50
1:G:252:MSE:HE3	1:G:414:TYR:CD1	2.46	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: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:F:135:ARG:HH12	1:F:467:ILE:HG22	1.73	0.50
1:F:274:SER:O	1:F:274:SER:OG	2.30	0.50
1:A:142:ALA:HA	1:A:169:ILE:O	2.12	0.49
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:C:52:GLN:HG3	1:C:53:PRO:HD3	1.93	0.49
1:E:314:ASP:OD1	1:E:315:GLU:N	2.45	0.49
1:G:110:VAL:HG13	1:G:163:ALA:HB2	1.93	0.49
1:H:299:LYS:O	1:H:303:MSE:HG3	2.12	0.49
1:H:372:THR:HB	1:H:373:PRO:CD	2.42	0.49
1:B:174:GLU:CD	1:B:174:GLU:H	2.20	0.49
1:C:107:CYS:SG	1:C:155:MSE:CE	2.99	0.49
1:D:265:ASN:N	1:D:265:ASN:HD22	2.10	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:E:432:MSE:HG2	1:E:442:PRO:HD3	1.94	0.49
1:F:161:ALA:HB2	1:F:470:TRP:CE2	2.47	0.49
1:F:332:ARG:HA	1:F:335:ILE:HD12	1.95	0.49
1:G:171:LYS:HE3	1:G:171:LYS:O	2.12	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:A:7:ASP:O	1:A:7:ASP:OD2	2.30	0.49
1:C:237:MSE:HE3	1:D:233:GLY:HA3	1.95	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:D:93:ILE:O	1:D:97:LYS:HB3	2.11	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:E:68:MSE:HE2	1:E:111:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:THR:CG2	1:E:229:ARG:HH12	2.25	0.49
1:E:265:ASN:OD1	1:E:303:MSE:HE1	2.12	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:B:6:ILE:HD12	1:B:44:ALA:HB2	1.95	0.49
1:C:393:ARG:HB2	1:C:397:GLU:OE2	2.12	0.49
1:D:322:VAL:O	1:D:361:HIS:HB2	2.12	0.49
1:E:131:MSE:CE	1:F:446:HIS:CB	2.88	0.49
1:F:484:ILE:HD11	2:H:522:HOH:O	2.11	0.49
1:G:284:VAL:HG13	1:G:390:VAL:HG23	1.93	0.49
1:H:361:HIS:NE2	2:H:540:HOH:O	2.22	0.49
1:A:354:LEU:HD23	1:A:357:TYR:CD2	2.48	0.49
1:C:341:GLN:HE22	1:C:376:ASP:N	2.02	0.49
1:D:336:ASP:O	1:D:340:GLU:HG2	2.12	0.49
1:E:393:ARG:NH1	1:E:397:GLU:OE1	2.46	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:C:84:MSE:CE	1:C:182:ARG:HG3	2.42	0.49
1:D:55:TRP:CZ2	1:D:63:ARG:HG2	2.47	0.49
1:D:180:PRO:HA	1:D:183:LEU:HD12	1.95	0.49
1:A:280:MSE:HG3	1:A:441:VAL:CG2	2.43	0.49
1:C:84:MSE:O	1:C:88:GLU:HG3	2.12	0.49
1:E:409:ASN:HD22	1:E:450:GLY:HA3	1.77	0.49
1:F:325:LYS:CA	1:F:361:HIS:CD2	2.93	0.49
1:F:350:ARG:O	1:F:351:ASP:OD2	2.30	0.49
1:H:148:ASN:ND2	1:H:149:PHE:CD1	2.78	0.49
1:H:252:MSE:HE3	1:H:282:ILE:HG13	1.93	0.49
1:B:59:ASN:HB2	1:B:60:PRO:HD2	1.95	0.49
1:C:110:VAL:CG1	1:C:163:ALA:HB2	2.43	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: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:D:450:GLY:O	1:D:455:SER:HB2	2.13	0.49
1:E:160:PRO:HB3	1:E:466:SER:HB3	1.95	0.49
1:H:249:LYS:HB3	1:H:405:HIS:CE1	2.48	0.49
1:A:211:LEU:O	1:A:240:LYS:HE2	2.12	0.48
1:H:86:SER:HB3	1:H:312:TYR:CB	2.43	0.48
1:G:280:MSE:HG3	1:G:441:VAL:HG12	1.95	0.48
1:D:345:LEU:HD23	1:D:346:VAL:N	2.28	0.48
1:E:280:MSE:HE2	1:E:409:ASN:CG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:GLY:HA3	1:F:362:PHE:CE1	2.26	0.48
1:G:166:ASN:HD21	1:G:470:TRP:HB3	1.78	0.48
1:G:322:VAL:HG12	1:G:324:THR:H	1.78	0.48
1:H:113:ILE:HA	1:H:116:LEU:HB2	1.95	0.48
1:A:308:ARG:NH1	1:A:314:ASP:OD2	2.42	0.48
1:B:107:CYS:SG	1:B:155:MSE:HE2	2.53	0.48
1:C:136:GLN:OE1	1:C:474:LYS:NZ	2.44	0.48
1:D:261:ASP:O	1:D:265:ASN:ND2	2.46	0.48
1:E:95:ASP:OD2	1:E:274:SER:OG	2.24	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:F:244:CYS:O	1:F:456:PHE:N	2.45	0.48
1:G:375:MSE:HE2	1:G:375:MSE:HB3	1.81	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:E:474:LYS:HE2	1:F:425:ALA:O	2.14	0.48
1:H:187:MSE:HG3	1:H:197:LEU:HD23	1.96	0.48
1:B:227:ILE:N	1:B:227:ILE:HD13	2.29	0.48
1:F:176:ASP:N	1:F:176:ASP:OD1	2.46	0.48
1:F:192:LEU:HD22	1:F:196:ILE:CD1	2.39	0.48
1:B:462:HIS:HA	1:B:466:SER:HB3	1.95	0.48
1:E:296:LEU:C	1:E:296:LEU:HD12	2.39	0.48
1:F:304:VAL:CG1	1:F:347:VAL:CG2	2.92	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:B:287:PRO:HB2	1:B:293:ALA:HB2	1.95	0.48
1:C:106:VAL:HA	1:C:444:ALA:HB1	1.96	0.48
1:D:78:MSE:HE1	1:D:100:ILE:HB	1.96	0.48
1:E:131:MSE:CE	1:F:446:HIS:CG	2.96	0.48
1:F:375:MSE:O	1:F:379:LYS:HG3	2.14	0.48
1:F:415:THR:HG21	1:F:420:ALA:HB3	1.96	0.48
1:F:448:PHE:O	1:F:460:ASN:HB3	2.14	0.48
1:G:18:VAL:HG13	1:G:32:THR:HB	1.95	0.48
1:G:328:GLU:OE2	1:G:361:HIS:HA	2.14	0.48
1:E:228:ALA:HB1	1:E:244:CYS:HB3	1.95	0.47
1:D:99:ASP:OD2	1:D:99:ASP:C	2.57	0.47
1:F:322:VAL:HG12	1:F:323:VAL:N	2.25	0.47
1:H:51:ALA:CB	1:H:196:ILE:HD12	2.34	0.47
1:H:439:ILE:HG22	1:H:441:VAL:HG22	1.97	0.47
1:A:69:LYS:HG2	1:A:190:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LEU:HD13	1:D:319:MSE:HE2	1.95	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:H:59:ASN:O	1:H:63:ARG:HG3	2.14	0.47
1:E:113:ILE:N	1:E:114:PRO:CD	2.78	0.47
1:F:241:ARG:NH1	1:F:469:PHE:O	2.45	0.47
1:B:158:PHE:CE1	1:B:187:MSE:CE	2.97	0.47
1:B:301:VAL:HG12	1:B:302:PRO:CD	2.45	0.47
1:E:138:VAL:CA	1:E:472:ARG:HD2	2.32	0.47
1:C:258:ALA:HB2	1:C:414:TYR:O	2.14	0.47
1:E:119:SER:HB2	1:E:133:SER:O	2.14	0.47
1:F:260:LEU:H	1:F:260:LEU:HG	1.52	0.47
1:A:390:VAL:HG11	1:A:401:LEU:HD21	1.96	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:C:18:VAL:HG13	1:C:32:THR:HB	1.97	0.47
1:D:106:VAL:HG12	1:D:159:ALA:HB3	1.96	0.47
1:D:442:PRO:HG2	1:D:447:SER:O	2.14	0.47
1:F:88:GLU:OE2	1:F:177:PRO:HD2	2.15	0.47
1:F:156:TRP:CE3	1:F:461:GLN:HG2	2.49	0.47
1:F:230:TYR:O	1:F:234:THR:HB	2.13	0.47
1:F:249:LYS:HE3	1:F:381:GLU:HA	1.97	0.47
1:G:371:VAL:HG21	1:G:388:SER:HB3	1.97	0.47
1:A:354:LEU:HD23	1:A:357:TYR:HD2	1.80	0.47
1:B:324:THR:HG22	1:B:327:ALA:CB	2.45	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:F:369:ASP:O	1:F:370:ASP:C	2.54	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:113:ILE:HA	1:A:116:LEU:HB2	1.96	0.46
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:C:301:VAL:N	1:C:302:PRO:HD2	2.30	0.46
1:E:18:VAL:HG13	1:E:32:THR:HB	1.97	0.46
1:F:272:TYR:OH	1:F:366:CYS:O	2.31	0.46
1:B:255:MSE:HE1	1:B:395:TYR:HB2	1.96	0.46
1:E:131:MSE:HE2	1:F:446:HIS:CG	2.46	0.46
1:E:432:MSE:HE1	1:E:448:PHE:CD2	2.50	0.46
1:H:260:LEU:HD23	1:H:260:LEU:HA	1.77	0.46
1:A:402:PRO:HB2	1:A:428:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASN:OD1	1:C:59:ASN:C	2.58	0.46
1:D:448:PHE:CD1	1:D:448:PHE:C	2.94	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:F:371:VAL:HB	1:F:390:VAL:HG22	1.96	0.46
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:D:393:ARG:HH12	1:D:397:GLU:HG3	1.80	0.46
1:E:423:ASP:OD2	1:E:427:ARG:NH2	2.49	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:263:ALA:O	1:E:267:LEU:HD22	2.15	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:B:348:ASP:OD1	1:B:350:ARG:CD	2.64	0.46
1:F:171:LYS:HG3	1:F:200:VAL:O	2.16	0.46
1:F:272:TYR:C	1:F:273:GLY:O	2.53	0.46
1:G:326:GLU:H	1:G:326:GLU:CD	2.22	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:B:292:THR:O	1:B:296:LEU:HB2	2.16	0.46
1:D:207:VAL:HG12	1:D:211:LEU:HD21	1.98	0.46
1:G:255:MSE:HG3	1:G:256:PRO:HD2	1.97	0.46
1:B:85:LEU:HB2	1:B:179:VAL:HG21	1.98	0.46
1:B:104:LEU:C	1:B:104:LEU:HD13	2.41	0.46
1:D:267:LEU:HD23	1:D:282:ILE:HG21	1.98	0.46
1:E:451:TRP:CE3	1:F:472:ARG:NE	2.84	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:H:301:VAL:HG12	1:H:367:LEU:HD23	1.96	0.46
1:A:30:GLN:HE22	1:A:87:ARG:HH11	1.64	0.46
1:E:113:ILE:HA	1:E:116:LEU:HB2	1.97	0.46
1:F:135:ARG:HD3	1:F:471:THR:HG21	1.98	0.46
1:G:2:LEU:HD12	1:G:21:ILE:HD11	1.97	0.46
1:G:278:ARG:HE	1:G:278:ARG:HB3	1.54	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: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:112:GLY:HA2	2:C:514:HOH:O	2.16	0.45
1:C:375:MSE:HE2	1:C:375:MSE:HB3	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LYS:HG3	1:D:95:ASP:HB2	1.97	0.45
1:D:138:VAL:HA	1:D:472:ARG:HD3	1.97	0.45
1:F:85:LEU:HD11	1:F:150:PRO:HD2	1.98	0.45
1:F:192:LEU:CD1	1:F:196:ILE:HD11	2.45	0.45
1:F:369:ASP:OD1	1:F:369:ASP:C	2.59	0.45
1:F:399:LEU:O	1:F:402:PRO:HD2	2.15	0.45
1:H:49:LYS:NZ	1:H:215:ASP:OD1	2.41	0.45
1:E:153:ILE:HG23	1:E:154:PRO:HD3	1.98	0.45
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:G:87:ARG:HA	1:G:312:TYR:CE1	2.52	0.45
1:H:222:VAL:HG22	1:H:245:PHE:HB2	1.98	0.45
1:D:129:ILE:HD11	1:D:479:ARG:NH2	2.30	0.45
1:E:78:MSE:HE3	1:E:78:MSE:O	2.16	0.45
1:E:255:MSE:HG3	1:E:415:THR:HB	1.97	0.45
1:E:305:GLU:HG3	2:E:528:HOH:O	2.15	0.45
1:G:-2:MSE:HB3	1:G:-2:MSE:HE2	1.73	0.45
1:H:326:GLU:CD	1:H:326:GLU:H	2.24	0.45
1:H:432:MSE:HE2	1:H:449:GLY:O	2.16	0.45
1:H:448:PHE:CD1	1:H:448:PHE:C	2.94	0.45
1:D:200:VAL:O	1:D:200:VAL:HG12	2.16	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:A:86:SER:OG	1:A:91:LYS:O	2.32	0.45
1:E:461:GLN:O	1:E:462:HIS:ND1	2.50	0.45
1:A:192:LEU:HD12	1:A:193:PRO:HD2	1.97	0.45
1:A:373:PRO:HA	1:A:378:TYR:CD2	2.51	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:D:84:MSE:HE1	1:D:182:ARG:HG3	1.99	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:H:73:LEU:HD12	1:H:186:LEU:HG	1.97	0.45
1:D:174:GLU:OE2	1:D:174:GLU:N	2.44	0.45
1:D:308:ARG:HD2	1:D:308:ARG:HA	1.66	0.45
1:F:134:ILE:HG12	1:G:121:PHE:CE2	2.52	0.45
1:F:347:VAL:HG21	1:F:365:GLY:O	2.17	0.45
1:G:115:HIS:HD2	1:G:118:LYS:HZ1	1.64	0.45
1:G:406:GLU:HG2	1:G:453:SER:OG	2.17	0.45
1:H:103:GLY:HA3	1:H:152:MSE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HB3	1:A:170:LEU:HD21	1.98	0.45
1:G:208:ASP:O	1:G:212:THR:HB	2.17	0.45
1:G:252:MSE:HE3	1:G:414:TYR:CG	2.51	0.45
1:H:89:HIS:ND1	1:H:89:HIS:C	2.75	0.45
1:H:274:SER:O	1:H:277:GLU:HG3	2.17	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:D:348:ASP:OD1	1:D:350:ARG:HG2	2.17	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:E:249:LYS:CB	1:E:405:HIS:CE1	3.00	0.45
1:F:256:PRO:HD3	1:F:288:VAL:HG22	1.96	0.45
1:F:324:THR:O	1:F:361:HIS:CD2	2.70	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:A:411:VAL:HG12	1:A:430:ILE:CG2	2.47	0.45
1:C:112:GLY:O	1:C:116:LEU:HG	2.17	0.45
1:E:23:ASN:HA	1:E:24:PRO:HD3	1.85	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:G:249:LYS:HD2	1:G:378:TYR:O	2.17	0.45
1:G:308:ARG:CZ	1:G:316:LYS:HD2	2.46	0.45
1:H:49:LYS:HB2	1:H:49:LYS:HE3	1.59	0.45
1:H:181:ILE:HD11	1:H:201:ASN:ND2	2.32	0.45
1:A:171:LYS:HA	1:A:200:VAL:O	2.18	0.44
1:A:432:MSE:HE2	1:A:449:GLY:C	2.42	0.44
1:E:122:THR:HG23	1:E:131:MSE:HB3	1.99	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:H:127:PRO:O	1:H:129:ILE:HD12	2.17	0.44
1:H:368:PHE:CE2	1:H:377:ILE:HD11	2.53	0.44
1:C:161:ALA:O	1:C:166:ASN:HB2	2.17	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:145:THR:HA	1:C:146:PRO:HD3	1.82	0.44
1:C:175:ARG:H	1:C:175:ARG:HG2	1.57	0.44
1:E:225:THR:O	1:E:229:ARG:HB2	2.17	0.44
1:E:253:ILE:HD11	1:E:402:PRO:HG3	2.00	0.44
1:H:41:LEU:HD22	1:H:209:ALA:HB1	1.99	0.44
1:H:256:PRO:HD3	1:H:288:VAL:HG13	1.99	0.44
1:D:354:LEU:HG	1:D:357:TYR:HD2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LEU:HD23	1:E:319:MSE:HE2	1.99	0.44
1:H:147:PHE:CD1	1:H:147:PHE:C	2.95	0.44
1:B:319:MSE:CE	1:B:385:PRO:CB	2.91	0.44
1:C:278:ARG:HE	1:C:278:ARG:HB2	1.25	0.44
1:D:77:ASN:O	1:D:81:LEU:HB2	2.17	0.44
1:E:211:LEU:CD2	1:E:211:LEU:H	2.31	0.44
1:F:272:TYR:O	1:F:273:GLY:O	2.35	0.44
1:G:211:LEU:HD21	1:G:231:VAL:HG13	1.98	0.44
1:G:330:ARG:HE	1:G:330:ARG:HB3	1.46	0.44
1:H:54:LYS:HE2	1:H:54:LYS:O	2.16	0.44
1:H:253:ILE:HD12	1:H:424:PHE:HE1	1.82	0.44
1:A:25:ALA:O	1:A:360:GLY:HA3	2.18	0.44
1:A:91:LYS:NZ	1:A:148:ASN:O	2.50	0.44
1:A:474:LYS:HB2	1:B:451:TRP:CZ2	2.52	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
1:D:152:MSE:HE3	1:D:156:TRP:CZ2	2.53	0.44
1:G:184:ALA:HA	1:G:197:LEU:HD13	1.99	0.44
1:H:263:ALA:O	1:H:267:LEU:HD12	2.18	0.44
1:A:58:THR:HG22	1:A:62:ARG:HB3	1.99	0.44
1:A:115:HIS:HD2	1:A:118:LYS:HZ2	1.62	0.44
1:B:148:ASN:OD1	1:B:149:PHE:HD1	2.01	0.44
1:B:295:ARG:O	1:B:299:LYS:HG2	2.18	0.44
1:B:311:PRO:C	1:B:313:THR:N	2.74	0.44
1:C:243:GLN:HG2	1:C:469:PHE:CE1	2.53	0.44
1:C:438:PRO:O	1:C:440:PRO:HD3	2.17	0.44
1:D:24:PRO:HA	1:D:361:HIS:CE1	2.52	0.44
1:D:131:MSE:HA	1:D:476:ILE:O	2.18	0.44
1:E:86:SER:OG	1:E:96:ALA:HB2	2.18	0.44
1:E:225:THR:CG2	1:E:229:ARG:NH1	2.81	0.44
1:E:301:VAL:N	1:E:302:PRO:HD2	2.33	0.44
1:F:213:HIS:HA	1:F:214:PRO:HD3	1.84	0.44
1:F:411:VAL:HG21	1:F:428:ILE:HD13	1.98	0.44
1:H:461:GLN:O	1:H:462:HIS:O	2.35	0.44
1:E:122:THR:HG22	1:F:446:HIS:NE2	2.33	0.44
1:E:441:VAL:O	1:E:441:VAL:CG1	2.65	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:A:249:LYS:HE3	1:A:283:SER:HB2	1.98	0.44
1:B:77:ASN:O	1:B:78:MSE:C	2.59	0.44
1:B:319:MSE:HE1	1:B:385:PRO:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:LYS:CE	1:E:172:PRO:O	2.65	0.44
1:F:92:THR:HG22	1:F:94:ASP:H	1.83	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:F:273:GLY:O	1:F:274:SER:HB3	2.18	0.44
1:F:309:ILE:HB	1:F:352:PHE:CE2	2.53	0.44
1:H:177:PRO:O	1:H:181:ILE:HG13	2.18	0.44
1:H:330:ARG:NH1	1:H:381:GLU:O	2.51	0.44
1:A:78:MSE:HE1	1:A:100:ILE:CG1	2.49	0.43
1:B:412:ALA:HA	1:B:434:GLY:O	2.18	0.43
1:B:462:HIS:CA	1:B:466:SER:HB3	2.48	0.43
1:C:451:TRP:CE2	1:D:472:ARG:HG3	2.53	0.43
1:D:70:PHE:HE2	1:D:155:MSE:CE	2.17	0.43
1:G:2:LEU:HD12	1:G:21:ILE:CD1	2.48	0.43
1:G:152:MSE:HE2	1:G:152:MSE:HB3	1.97	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:D:311:PRO:C	1:D:313:THR:H	2.26	0.43
1:D:311:PRO:C	1:D:313:THR:N	2.75	0.43
1:E:168:PHE:HE1	1:E:470:TRP:HH2	1.62	0.43
1:E:253:ILE:HD12	1:E:424:PHE:CZ	2.52	0.43
1:F:13:GLY:O	1:F:14:THR:C	2.59	0.43
1:F:78:MSE:HE2	1:F:97:LYS:HA	2.00	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:86:SER:HB3	1:E:312:TYR:HB2	2.01	0.43
1:E:337:SER:O	1:E:341:GLN:HB2	2.18	0.43
1:F:311:PRO:HG2	1:F:357:TYR:CE1	2.53	0.43
1:H:156:TRP:CE3	1:H:461:GLN:CG	3.01	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:82:ALA:HA	1:E:85:LEU:HD23	2.00	0.43
1:E:379:LYS:HA	1:E:405:HIS:NE2	2.33	0.43
1:F:259:ASP:C	1:F:259:ASP:OD1	2.60	0.43
1:H:145:THR:OG1	1:H:172:PRO:HA	2.18	0.43
1:A:448:PHE:CD1	1:A:448:PHE:C	2.97	0.43
1:F:282:ILE:HD12	1:F:282:ILE:O	2.18	0.43
1:F:369:ASP:O	1:F:370:ASP:O	2.35	0.43
1:G:4:HIS:NE2	1:G:36:ALA:HB2	2.31	0.43
1:G:25:ALA:O	1:G:360:GLY:HA3	2.17	0.43
1:H:398:ALA:O	1:H:402:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ILE:HG23	1:A:114:PRO:HD3	2.00	0.43
1:A:460:ASN:HB3	1:A:461:GLN:H	1.68	0.43
1:B:266:ALA:HB1	1:B:438:PRO:HB3	2.00	0.43
1:B:324:THR:HG22	1:B:327:ALA:HB2	2.00	0.43
1:D:30:GLN:O	1:D:30:GLN:HG2	2.16	0.43
1:E:171:LYS:HD3	1:E:207:VAL:HG23	1.99	0.43
1:E:248:ALA:CB	1:E:279:CYS:O	2.66	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:G:70:PHE:CE2	1:G:74:LEU:HD11	2.53	0.43
1:H:91:LYS:HD3	1:H:95:ASP:HB3	2.01	0.43
1:A:339:ILE:HD11	1:A:345:LEU:HD22	2.01	0.43
1:B:2:LEU:HD22	1:B:181:ILE:HD13	2.01	0.43
1:B:422:ARG:O	1:B:426:SER:HB2	2.19	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:F:347:VAL:CG1	1:F:367:LEU:H	2.32	0.43
1:H:37:SER:OG	1:H:40:ASP:OD2	2.29	0.43
1:A:89:HIS:CD2	1:A:89:HIS:C	2.97	0.43
1:A:156:TRP:CE3	1:A:461:GLN:HG2	2.54	0.43
1:A:444:ALA:HA	1:A:462:HIS:ND1	2.33	0.43
1:B:158:PHE:CD1	1:B:158:PHE:C	2.97	0.43
1:B:225:THR:HB	1:B:226:PRO:HD3	2.01	0.43
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:B:92:THR:HG22	1:B:95:ASP:H	1.84	0.43
1:B:230:TYR:CD1	1:B:230:TYR:C	2.97	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:D:332:ARG:NH1	1:D:350:ARG:HB2	2.31	0.43
1:E:122:THR:CG2	1:F:446:HIS:NE2	2.82	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:E:300:LEU:CD2	1:E:367:LEU:HD11	2.38	0.43
1:G:410:GLY:HA2	1:G:432:MSE:O	2.19	0.43
1:H:301:VAL:CG2	1:H:302:PRO:HD3	2.49	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: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:H:442:PRO:HG2	1:H:447:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MSE:HE2	1:A:78:MSE:CA	2.44	0.42
1:A:171:LYS:HE2	1:A:202:GLY:O	2.19	0.42
1:A:272:TYR:O	1:A:273:GLY:C	2.61	0.42
1:B:138:VAL:HG13	1:B:217:ALA:HB3	2.01	0.42
1:B:301:VAL:HG23	1:B:347:VAL:HG23	2.00	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:F:61:GLN:OE1	1:H:443:LEU:HD13	2.19	0.42
1:F:187:MSE:HE3	1:F:192:LEU:HD11	2.01	0.42
1:G:148:ASN:ND2	1:G:149:PHE:HE1	2.17	0.42
1:G:306:SER:O	1:G:307:LEU:C	2.62	0.42
1:A:67:PHE:O	1:A:71:VAL:HG23	2.19	0.42
1:B:92:THR:CG2	1:B:94:ASP:H	2.29	0.42
1:B:272:TYR:CE2	1:B:304:VAL:HG22	2.54	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:C:245:PHE:CD1	1:C:245:PHE:N	2.87	0.42
1:E:18:VAL:HA	1:E:33:VAL:O	2.19	0.42
1:E:108:GLU:HA	1:E:111:ILE:HD12	2.01	0.42
1:F:145:THR:HG21	1:F:154:PRO:HG3	2.01	0.42
1:F:255:MSE:HE1	1:F:395:TYR:HA	2.01	0.42
1:F:373:PRO:HA	1:F:378:TYR:CD2	2.55	0.42
1:G:249:LYS:HE2	1:G:283:SER:CB	2.49	0.42
1:G:295:ARG:HD2	1:G:295:ARG:H	1.76	0.42
1:B:289:GLY:HA3	1:B:292:THR:CG2	2.46	0.42
1:B:405:HIS:O	1:B:452:LYS:NZ	2.52	0.42
1:E:211:LEU:O	1:E:240:LYS:HE2	2.19	0.42
1:E:255:MSE:HE3	1:E:413:ILE:HD11	2.01	0.42
1:F:110:VAL:HG21	1:F:160:PRO:HA	2.01	0.42
1:G:91:LYS:HG3	1:G:95:ASP:HB2	2.00	0.42
1:B:153:ILE:O	1:B:156:TRP:HB2	2.19	0.42
1:B:319:MSE:HE1	1:B:385:PRO:HB3	2.00	0.42
1:D:145:THR:HG22	1:D:153:ILE:HG22	2.02	0.42
1:D:459:LEU:HD23	1:D:459:LEU:HA	1.90	0.42
1:E:99:ASP:OD1	1:E:152:MSE:HB2	2.20	0.42
1:F:401:LEU:HB2	1:F:402:PRO:HD3	2.00	0.42
1:G:277:GLU:C	1:G:278:ARG:HG2	2.44	0.42
1:G:382:ILE:H	1:G:382:ILE:HG12	1.73	0.42
1:H:280:MSE:HE1	1:H:409:ASN:CB	2.49	0.42
1:H:359:ASN:OD1	1:H:359:ASN:N	2.52	0.42
1:A:129:ILE:HA	1:A:478:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ALA:HA	1:B:319:MSE:CE	2.40	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:F:249:LYS:HB2	1:F:405:HIS:CE1	2.55	0.42
1:G:291:GLU:HA	1:G:295:ARG:HH11	1.85	0.42
1:A:106:VAL:HG21	1:A:156:TRP:CD1	2.55	0.42
1:B:211:LEU:HD13	1:B:234:THR:CB	2.48	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:137:PRO:O	1:E:472:ARG:CD	2.68	0.42
1:E:141:GLY:HA3	1:E:470:TRP:HZ3	1.84	0.42
1:E:462:HIS:N	1:E:466:SER:OG	2.52	0.42
1:E:474:LYS:HA	1:F:431:GLY:O	2.18	0.42
1:G:324:THR:HG22	1:G:327:ALA:CB	2.50	0.42
1:H:152:MSE:HE2	1:H:153:ILE:HG13	2.00	0.42
1:B:171:LYS:C	1:B:171:LYS:HE2	2.45	0.42
1:E:302:PRO:O	1:E:305:GLU:HB2	2.20	0.42
1:E:428:ILE:HG12	1:E:429:ASN:N	2.34	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:H:24:PRO:HB2	1:H:321:PRO:HG2	2.00	0.42
1:A:18:VAL:HG13	1:A:32:THR:HB	2.02	0.42
1:A:25:ALA:HB1	1:A:311:PRO:HB3	2.01	0.42
1:B:266:ALA:O	1:B:267:LEU:C	2.62	0.42
1:E:102:ARG:HB3	1:E:152:MSE:CG	2.50	0.42
1:G:272:TYR:OH	1:G:366:CYS:O	2.31	0.42
1:H:155:MSE:HG2	1:H:158:PHE:CZ	2.55	0.42
1:A:211:LEU:HD13	1:A:234:THR:HB	2.02	0.42
1:C:159:ALA:HB3	1:C:160:PRO:HD3	2.01	0.42
1:E:485:LYS:HE3	1:E:485:LYS:HA	2.02	0.42
1:F:70:PHE:HE1	1:F:187:MSE:HA	1.84	0.42
1:G:213:HIS:HA	1:G:214:PRO:HD2	1.84	0.42
1:G:297:ILE:HG12	1:G:297:ILE:H	1.61	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:D:402:PRO:HB2	1:D:428:ILE:HD11	2.02	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:F:211:LEU:O	1:F:238:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:SER:O	1:H:38:ASP:C	2.61	0.42
1:A:486:ASP:HA	2:A:548:HOH:O	2.20	0.41
1:B:311:PRO:C	1:B:313:THR:H	2.28	0.41
1:D:94:ASP:O	1:D:97:LYS:HD3	2.20	0.41
1:E:5:PHE:CE2	1:E:8:GLY:HA2	2.55	0.41
1:E:192:LEU:HD12	1:E:193:PRO:HD2	2.02	0.41
1:E:251:HIS:HA	1:E:284:VAL:O	2.20	0.41
1:E:453:SER:O	1:E:453:SER:OG	2.30	0.41
1:H:192:LEU:HD21	1:H:196:ILE:HG22	2.01	0.41
1:A:108:GLU:HA	1:A:111:ILE:HD12	2.02	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:D:113:ILE:HG22	1:D:114:PRO:HD3	2.01	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:G:249:LYS:HE2	1:G:283:SER:HB2	2.02	0.41
1:H:20:ASN:HB2	1:H:29:VAL:HG13	2.01	0.41
1:D:278:ARG:HB2	1:D:281:ALA:HB2	2.01	0.41
1:D:412:ALA:HA	1:D:434:GLY:O	2.20	0.41
1:E:115:HIS:CD2	1:E:118:LYS:HD3	2.56	0.41
1:H:329:GLN:O	1:H:333:SER:HB2	2.21	0.41
1:B:147:PHE:CZ	1:B:383:PHE:HE2	2.38	0.41
1:B:352:PHE:HE1	1:B:354:LEU:HB2	1.85	0.41
1:D:211:LEU:N	1:D:211:LEU:HD22	2.36	0.41
1:E:102:ARG:CB	1:E:152:MSE:HG3	2.51	0.41
1:F:74:LEU:HD11	1:F:155:MSE:HE1	2.02	0.41
1:F:484:ILE:CD1	2:H:522:HOH:O	2.68	0.41
1:B:85:LEU:HD22	1:B:150:PRO:HG2	2.03	0.41
1:C:148:ASN:OD1	1:C:277:GLU:O	2.37	0.41
1:A:89:HIS:HD2	1:A:91:LYS:H	1.67	0.41
1:C:176:ASP:N	1:C:176:ASP:OD1	2.52	0.41
1:C:252:MSE:HB2	1:C:282:ILE:HG12	2.02	0.41
1:D:272:TYR:O	1:D:275:ALA:N	2.54	0.41
1:E:213:HIS:HB3	1:E:216:ILE:HG13	2.02	0.41
1:E:411:VAL:HB	1:E:430:ILE:HG21	2.02	0.41
1:E:447:SER:HB3	1:E:460:ASN:HB3	2.01	0.41
1:F:35:LEU:HD12	1:F:36:ALA:H	1.85	0.41
1:F:304:VAL:HG11	1:F:347:VAL:CG2	2.51	0.41
1:B:33:VAL:HG11	1:B:174:GLU:HB3	2.03	0.41
1:B:106:VAL:HA	1:B:444:ALA:HB1	2.01	0.41
1:B:272:TYR:O	1:B:319:MSE:HE3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:GLN:HE21	1:C:52:GLN:HB2	1.65	0.41
1:E:82:ALA:HA	1:E:85:LEU:CD2	2.50	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:F:297:ILE:HD11	1:F:389:VAL:HG21	2.03	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:G:268:ILE:HG13	1:G:269:GLY:N	2.36	0.41
1:B:235:ALA:HB1	1:B:240:LYS:HG3	2.02	0.41
1:D:221:PHE:HE1	1:D:228:ALA:HB2	1.85	0.41
1:D:255:MSE:HB2	1:D:414:TYR:O	2.21	0.41
1:E:448:PHE:O	1:E:448:PHE:HD1	2.02	0.41
1:F:70:PHE:CE2	1:F:155:MSE:CE	3.04	0.41
1:F:115:HIS:HD2	1:F:118:LYS:HZ2	1.67	0.41
1:F:309:ILE:HD12	1:F:352:PHE:CD2	2.56	0.41
1:F:310:GLY:HA2	1:F:311:PRO:HD3	1.78	0.41
1:F:324:THR:C	1:F:361:HIS:NE2	2.76	0.41
1:F:412:ALA:HA	1:F:434:GLY:O	2.21	0.41
1:G:460:ASN:HB3	1:G:461:GLN:H	1.68	0.41
1:H:113:ILE:CG2	1:H:114:PRO:HD3	2.50	0.41
1:A:15:SER:HB2	1:A:37:SER:HB3	2.02	0.41
1:B:102:ARG:HB3	1:B:152:MSE:SE	2.71	0.41
1:C:30:GLN:HE22	1:C:87:ARG:NE	2.14	0.41
1:C:67:PHE:CE1	1:C:187:MSE:HE1	2.56	0.41
1:C:245:PHE:CE1	1:C:461:GLN:NE2	2.89	0.41
1:D:141:GLY:HA3	1:D:470:TRP:CZ3	2.54	0.41
1:D:219:VAL:O	1:D:242:ALA:HA	2.21	0.41
1:E:36:ALA:HB1	1:E:40:ASP:HB2	2.02	0.41
1:E:85:LEU:HD12	1:E:150:PRO:HG2	2.02	0.41
1:E:126:GLY:HA3	1:E:129:ILE:HB	2.02	0.41
1:E:480:TRP:HA	1:E:481:PRO:HD2	1.78	0.41
1:F:368:PHE:O	1:F:389:VAL:N	2.51	0.41
1:G:67:PHE:CE1	1:G:187:MSE:HE1	2.56	0.41
1:G:249:LYS:HE2	1:G:283:SER:OG	2.20	0.41
1:H:73:LEU:HD13	1:H:189:GLU:HG2	2.03	0.41
1:C:472:ARG:NH1	1:D:451:TRP:CZ3	2.89	0.41
1:D:343:ALA:HB2	1:D:375:MSE:SE	2.71	0.41
1:E:158:PHE:CD1	1:E:158:PHE:C	2.98	0.41
1:E:379:LYS:H	1:E:379:LYS:HG3	1.54	0.41
1:F:78:MSE:CE	1:F:97:LYS:HA	2.51	0.41
1:F:439:ILE:O	1:F:439:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:71:VAL:HG13	1:B:104:LEU:CD2	2.51	0.40
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: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:A:66:VAL:HG12	1:A:187:MSE:CE	2.50	0.40
1:A:131:MSE:HE1	1:B:443:LEU:HG	2.02	0.40
1:B:142:ALA:HB3	1:B:219:VAL:HG22	2.03	0.40
1:B:256:PRO:HD3	1:B:288:VAL:HB	2.02	0.40
1:B:271:GLY:HA2	1:B:282:ILE:O	2.21	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:E:308:ARG:NH1	1:E:316:LYS:O	2.54	0.40
1:E:403:MSE:O	1:E:429:ASN:ND2	2.52	0.40
1:F:85:LEU:HD22	1:F:91:LYS:HD3	2.03	0.40
1:H:425:ALA:HA	1:H:433:VAL:HG11	2.02	0.40
1:D:107:CYS:O	1:D:111:ILE:HG13	2.22	0.40
1:D:113:ILE:N	1:D:114:PRO:CD	2.84	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
1:E:442:PRO:HG3	1:E:447:SER:O	2.21	0.40
1:F:149:PHE:HB3	1:F:152:MSE:HB3	2.04	0.40
1:G:352:PHE:CD1	1:G:352:PHE:C	2.99	0.40
1:A:204:LYS:HG2	1:A:205:GLY:N	2.35	0.40
2:B:525:HOH:O	1:D:123:GLU:HG3	2.22	0.40
1:D:59:ASN:OD1	1:D:59:ASN:C	2.63	0.40
1:E:102:ARG:HB3	1:E:152:MSE:HG3	2.02	0.40
1:G:399:LEU:HD13	1:G:424:PHE:CD2	2.56	0.40
1:H:20:ASN:HB3	1:H:32:THR:HG22	2.03	0.40
1:H:158:PHE:C	1:H:158:PHE:CD1	3.00	0.40
1:H:432:MSE:HE2	1:H:449:GLY:C	2.46	0.40
1:A:52:GLN:O	1:A:53:PRO:C	2.63	0.40
1:C:268:ILE:HD13	1:C:268:ILE:HA	1.93	0.40
1:F:293:ALA:O	1:F:297:ILE:HG12	2.22	0.40
1:H:308:ARG:HB3	1:H:308:ARG:NH1	2.35	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 [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	486/521 (93%)	457 (94%)	28 (6%)	1 (0%)	43	72
1	B	484/521 (93%)	455 (94%)	28 (6%)	1 (0%)	43	72
1	C	484/521 (93%)	457 (94%)	25 (5%)	2 (0%)	30	59
1	D	486/521 (93%)	457 (94%)	28 (6%)	1 (0%)	43	72
1	E	484/521 (93%)	451 (93%)	31 (6%)	2 (0%)	30	59
1	F	482/521 (92%)	450 (93%)	31 (6%)	1 (0%)	43	72
1	G	483/521 (93%)	456 (94%)	25 (5%)	2 (0%)	30	59
1	H	483/521 (93%)	452 (94%)	28 (6%)	3 (1%)	21	51
All	All	3872/4168 (93%)	3635 (94%)	224 (6%)	13 (0%)	36	65

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

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Mol	Chain	Res	Type
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%)	343 (90%)	40 (10%)	7	23
1	B	381/391 (97%)	326 (86%)	55 (14%)	3	11
1	C	381/391 (97%)	332 (87%)	49 (13%)	4	13
1	D	383/391 (98%)	317 (83%)	66 (17%)	2	7
1	E	381/391 (97%)	307 (81%)	74 (19%)	1	5
1	F	379/391 (97%)	303 (80%)	76 (20%)	1	4
1	G	381/391 (97%)	322 (84%)	59 (16%)	2	9
1	H	380/391 (97%)	336 (88%)	44 (12%)	5	18
All	All	3049/3128 (98%)	2586 (85%)	463 (15%)	3	9

All (463) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	11	VAL
1	A	15	SER
1	A	18	VAL
1	A	30	GLN
1	A	33	VAL
1	A	62	ARG
1	A	69	LYS
1	A	74	LEU
1	A	78	MSE
1	A	86	SER
1	A	92	THR
1	A	104	LEU
1	A	110	VAL

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Mol	Chain	Res	Type
1	A	119	SER
1	A	122	THR
1	A	134	ILE
1	A	138	VAL
1	A	148	ASN
1	A	182	ARG
1	A	220	SER
1	A	224	SER
1	A	268	ILE
1	A	274	SER
1	A	278	ARG
1	A	313	THR
1	A	326	GLU
1	A	329	GLN
1	A	346	VAL
1	A	350	ARG
1	A	351	ASP
1	A	352	PHE
1	A	354	LEU
1	A	358	GLU
1	A	382	ILE
1	A	397	GLU
1	A	400	SER
1	A	465	ASP
1	A	468	LYS
1	A	478	SER
1	B	7	ASP
1	B	9	LYS
1	B	10	ARG
1	B	35	LEU
1	B	47	SER
1	B	54	LYS
1	B	58	THR
1	B	85	LEU
1	B	91	LYS
1	B	92	THR
1	B	102	ARG
1	B	104	LEU
1	B	123	GLU
1	B	138	VAL
1	B	171	LYS
1	B	174	GLU

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Mol	Chain	Res	Type
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	291	GLU
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	344	LYS
1	B	359	ASN
1	B	363	ILE
1	B	372	THR
1	B	380	THR
1	B	382	ILE
1	B	388	SER
1	B	399	LEU
1	B	404	LYS
1	B	422	ARG
1	B	435	VAL
1	B	439	ILE
1	B	468	LYS
1	B	471	THR
1	B	474	LYS
1	B	475	THR
1	B	479	ARG
1	B	485	LYS
1	C	7	ASP
1	C	11	VAL
1	C	18	VAL

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Mol	Chain	Res	Type
1	C	20	ASN
1	C	33	VAL
1	C	49	LYS
1	C	52	GLN
1	C	54	LYS
1	C	72	GLN
1	C	73	LEU
1	C	84	MSE
1	C	91	LYS
1	C	102	ARG
1	C	110	VAL
1	C	119	SER
1	C	122	THR
1	C	123	GLU
1	C	145	THR
1	C	175	ARG
1	C	182	ARG
1	C	188	ILE
1	C	229	ARG
1	C	237	MSE
1	C	254	ILE
1	C	267	LEU
1	C	274	SER
1	C	278	ARG
1	C	279	CYS
1	C	282	ILE
1	C	298	ASP
1	C	301	VAL
1	C	333	SER
1	C	337	SER
1	C	346	VAL
1	C	363	ILE
1	C	374	ASP
1	C	382	ILE
1	C	383	PHE
1	C	400	SER
1	C	411	VAL
1	C	441	VAL
1	C	448	PHE
1	C	461	GLN
1	C	464	THR
1	C	466	SER

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Mol	Chain	Res	Type
1	C	468	LYS
1	C	471	THR
1	C	474	LYS
1	C	484	ILE
1	D	7	ASP
1	D	30	GLN
1	D	32	THR
1	D	33	VAL
1	D	41	LEU
1	D	54	LYS
1	D	59	ASN
1	D	73	LEU
1	D	91	LYS
1	D	92	THR
1	D	93	ILE
1	D	97	LYS
1	D	99	ASP
1	D	100	ILE
1	D	104	LEU
1	D	110	VAL
1	D	119	SER
1	D	133	SER
1	D	148	ASN
1	D	155	MSE
1	D	171	LYS
1	D	179	VAL
1	D	182	ARG
1	D	186	LEU
1	D	200	VAL
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	268	ILE
1	D	282	ILE
1	D	283	SER
1	D	290	GLU
1	D	292	THR
1	D	297	ILE

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Mol	Chain	Res	Type
1	D	299	LYS
1	D	303	MSE
1	D	308	ARG
1	D	314	ASP
1	D	322	VAL
1	D	326	GLU
1	D	328	GLU
1	D	332	ARG
1	D	333	SER
1	D	334	LEU
1	D	344	LYS
1	D	353	LYS
1	D	371	VAL
1	D	372	THR
1	D	380	THR
1	D	388	SER
1	D	393	ARG
1	D	406	GLU
1	D	413	ILE
1	D	427	ARG
1	D	441	VAL
1	D	445	TYR
1	D	453	SER
1	D	455	SER
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	106	VAL
1	E	113	ILE
1	E	119	SER

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Mol	Chain	Res	Type
1	E	129	ILE
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
1	E	183	LEU
1	E	200	VAL
1	E	201	ASN
1	E	204	LYS
1	E	211	LEU
1	E	219	VAL
1	E	220	SER
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	278	ARG
1	E	282	ILE
1	E	292	THR
1	E	295	ARG
1	E	296	LEU
1	E	297	ILE
1	E	298	ASP
1	E	305	GLU
1	E	307	LEU
1	E	309	ILE
1	E	313	THR
1	E	316	LYS
1	E	319	MSE
1	E	328	GLU
1	E	331	ILE
1	E	334	LEU
1	E	345	LEU
1	E	346	VAL
1	E	355	GLN
1	E	361	HIS
1	E	367	LEU

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Mol	Chain	Res	Type
1	E	379	LYS
1	E	380	THR
1	E	393	ARG
1	E	397	GLU
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	472	ARG
1	E	474	LYS
1	E	476	ILE
1	E	478	SER
1	E	484	ILE
1	E	485	LYS
1	F	1	GLU
1	F	14	THR
1	F	18	VAL
1	F	23	ASN
1	F	29	VAL
1	F	30	GLN
1	F	35	LEU
1	F	41	LEU
1	F	47	SER
1	F	54	LYS
1	F	59	ASN
1	F	61	GLN
1	F	71	VAL
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	175	ARG
1	F	178	SER
1	F	186	LEU

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Mol	Chain	Res	Type
1	F	187	MSE
1	F	188	ILE
1	F	203	ASP
1	F	219	VAL
1	F	234	THR
1	F	237	MSE
1	F	249	LYS
1	F	252	MSE
1	F	260	LEU
1	F	261	ASP
1	F	267	LEU
1	F	268	ILE
1	F	283	SER
1	F	295	ARG
1	F	298	ASP
1	F	299	LYS
1	F	304	VAL
1	F	305	GLU
1	F	306	SER
1	F	307	LEU
1	F	308	ARG
1	F	316	LYS
1	F	326	GLU
1	F	340	GLU
1	F	346	VAL
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	396	GLU
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

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Mol	Chain	Res	Type
1	F	439	ILE
1	F	441	VAL
1	F	443	LEU
1	F	447	SER
1	F	454	SER
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	18	VAL
1	G	28	GLU
1	G	33	VAL
1	G	41	LEU
1	G	47	SER
1	G	58	THR
1	G	61	GLN
1	G	65	ARG
1	G	84	MSE
1	G	86	SER
1	G	93	ILE
1	G	102	ARG
1	G	106	VAL
1	G	110	VAL
1	G	123	GLU
1	G	133	SER
1	G	138	VAL
1	G	171	LYS
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

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Mol	Chain	Res	Type
1	G	300	LEU
1	G	307	LEU
1	G	313	THR
1	G	316	LYS
1	G	322	VAL
1	G	324	THR
1	G	329	GLN
1	G	330	ARG
1	G	331	ILE
1	G	333	SER
1	G	337	SER
1	G	340	GLU
1	G	345	LEU
1	G	355	GLN
1	G	359	ASN
1	G	371	VAL
1	G	375	MSE
1	G	382	ILE
1	G	383	PHE
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	H	14	THR
1	H	18	VAL
1	H	20	ASN
1	H	35	LEU
1	H	47	SER
1	H	54	LYS
1	H	71	VAL
1	H	73	LEU
1	H	81	LEU
1	H	94	ASP
1	H	119	SER
1	H	179	VAL
1	H	181	ILE
1	H	182	ARG
1	H	183	LEU

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Mol	Chain	Res	Type
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	267	LEU
1	H	268	ILE
1	H	283	SER
1	H	288	VAL
1	H	296	LEU
1	H	300	LEU
1	H	313	THR
1	H	323	VAL
1	H	326	GLU
1	H	333	SER
1	H	340	GLU
1	H	353	LYS
1	H	355	GLN
1	H	377	ILE
1	H	393	ARG
1	H	399	LEU
1	H	406	GLU
1	H	447	SER
1	H	454	SER
1	H	471	THR
1	H	479	ARG
1	H	482	SER
1	H	485	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) 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	243	GLN
1	A	359	ASN
1	A	394	ASN
1	A	405	HIS
1	A	429	ASN

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Mol	Chain	Res	Type
1	A	461	GLN
1	B	30	GLN
1	B	77	ASN
1	B	79	ASN
1	B	115	HIS
1	B	265	ASN
1	B	361	HIS
1	B	409	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	77	ASN
1	C	115	HIS
1	C	341	GLN
1	C	361	HIS
1	C	409	ASN
1	C	446	HIS
1	C	460	ASN
1	C	461	GLN
1	D	201	ASN
1	D	250	ASN
1	D	265	ASN
1	D	361	HIS
1	E	115	HIS
1	E	243	GLN
1	E	262	GLN
1	E	409	ASN
1	E	436	ASN
1	F	23	ASN
1	F	30	GLN
1	F	59	ASN
1	F	77	ASN
1	F	115	HIS
1	F	117	GLN
1	F	238	ASN
1	F	243	GLN
1	F	329	GLN
1	G	30	GLN
1	G	79	ASN

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Mol	Chain	Res	Type
1	G	115	HIS
1	G	148	ASN
1	G	359	ASN
1	G	361	HIS
1	G	446	HIS
1	G	462	HIS
1	H	61	GLN
1	H	201	ASN
1	H	243	GLN
1	H	265	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/521 (90%)	-0.69	0 100 100	17, 36, 55, 71	0
1	B	469/521 (90%)	-0.58	0 100 100	19, 38, 58, 76	0
1	C	468/521 (89%)	-0.79	1 (0%) 91 89	15, 28, 49, 79	0
1	D	470/521 (90%)	-0.49	0 100 100	15, 43, 75, 93	0
1	E	469/521 (90%)	0.03	4 (0%) 81 75	21, 57, 81, 97	0
1	F	467/521 (89%)	0.17	10 (2%) 63 54	29, 59, 87, 107	0
1	G	466/521 (89%)	-0.69	0 100 100	18, 35, 53, 70	0
1	H	468/521 (89%)	-0.63	0 100 100	18, 38, 57, 74	0
All	All	3747/4168 (89%)	-0.46	15 (0%) 88 85	15, 40, 73, 107	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	31	GLY	2.9
1	E	377	ILE	2.8
1	F	35	LEU	2.8
1	F	174	GLU	2.8
1	F	349	GLY	2.6
1	F	93	ILE	2.5
1	F	25	ALA	2.5
1	C	484	ILE	2.4
1	E	273	GLY	2.2
1	E	339	ILE	2.2
1	F	30	GLN	2.1
1	F	102	ARG	2.1
1	F	357	TYR	2.1
1	E	26	THR	2.1
1	F	352	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.