



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:17 PM EST

PDB ID : 4QYJ
Title : Structure of Phenylacetaldehyde Dehydrogenase from *Pseudomonas putida* S12
Authors : Crabo, A.G.; Gassner, G.T.; Sazinsky, M.H.
Deposited on : 2014-07-24
Resolution : 2.83 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

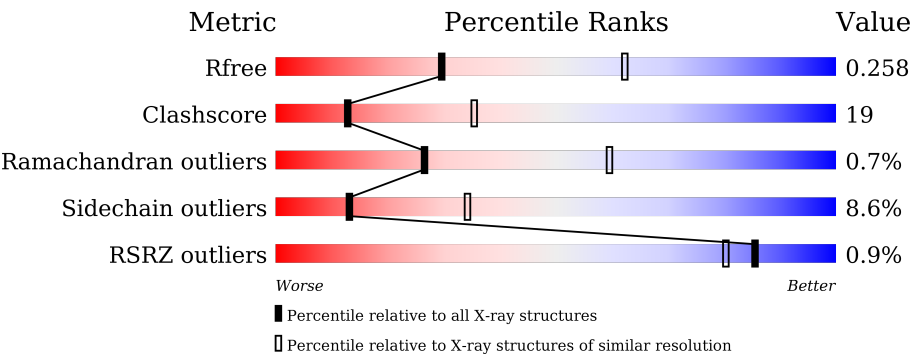
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 ≥ 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	516	
1	B	516	
1	C	516	
1	D	516	
1	E	516	
1	F	516	

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Mol	Chain	Length	Quality of chain
1	G	516	<div><div>%</div><div><div></div><div>63%</div><div>26%</div><div>•</div><div>7%</div></div></div>
1	H	516	<div><div>%</div><div><div></div><div>60%</div><div>28%</div><div>6%</div><div>7%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27306 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3416	2170	580	651	15			
1	B	481	Total	C	N	O	S	0	0	0
			3411	2169	579	648	15			
1	C	481	Total	C	N	O	S	0	0	0
			3409	2167	580	647	15			
1	D	481	Total	C	N	O	S	0	0	0
			3419	2173	584	647	15			
1	E	481	Total	C	N	O	S	0	0	0
			3408	2166	580	647	15			
1	F	481	Total	C	N	O	S	0	0	0
			3411	2169	579	648	15			
1	G	481	Total	C	N	O	S	0	0	0
			3419	2172	584	648	15			
1	H	481	Total	C	N	O	S	0	0	0
			3413	2170	581	647	15			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP V4GH04
A	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
A	-17	SER	-	EXPRESSION TAG	UNP V4GH04
A	-16	SER	-	EXPRESSION TAG	UNP V4GH04
A	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-9	SER	-	EXPRESSION TAG	UNP V4GH04
A	-8	SER	-	EXPRESSION TAG	UNP V4GH04
A	-7	GLY	-	EXPRESSION TAG	UNP V4GH04

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
A	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
A	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
A	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
A	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
A	-1	SER	-	EXPRESSION TAG	UNP V4GH04
A	0	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-19	MET	-	EXPRESSION TAG	UNP V4GH04
B	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
B	-17	SER	-	EXPRESSION TAG	UNP V4GH04
B	-16	SER	-	EXPRESSION TAG	UNP V4GH04
B	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-9	SER	-	EXPRESSION TAG	UNP V4GH04
B	-8	SER	-	EXPRESSION TAG	UNP V4GH04
B	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
B	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
B	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
B	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
B	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
B	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
B	-1	SER	-	EXPRESSION TAG	UNP V4GH04
B	0	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-19	MET	-	EXPRESSION TAG	UNP V4GH04
C	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
C	-17	SER	-	EXPRESSION TAG	UNP V4GH04
C	-16	SER	-	EXPRESSION TAG	UNP V4GH04
C	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-9	SER	-	EXPRESSION TAG	UNP V4GH04
C	-8	SER	-	EXPRESSION TAG	UNP V4GH04
C	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
C	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
C	-5	VAL	-	EXPRESSION TAG	UNP V4GH04

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
C	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
C	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
C	-1	SER	-	EXPRESSION TAG	UNP V4GH04
C	0	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-19	MET	-	EXPRESSION TAG	UNP V4GH04
D	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
D	-17	SER	-	EXPRESSION TAG	UNP V4GH04
D	-16	SER	-	EXPRESSION TAG	UNP V4GH04
D	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-9	SER	-	EXPRESSION TAG	UNP V4GH04
D	-8	SER	-	EXPRESSION TAG	UNP V4GH04
D	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
D	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
D	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
D	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
D	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
D	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
D	-1	SER	-	EXPRESSION TAG	UNP V4GH04
D	0	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-19	MET	-	EXPRESSION TAG	UNP V4GH04
E	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
E	-17	SER	-	EXPRESSION TAG	UNP V4GH04
E	-16	SER	-	EXPRESSION TAG	UNP V4GH04
E	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-9	SER	-	EXPRESSION TAG	UNP V4GH04
E	-8	SER	-	EXPRESSION TAG	UNP V4GH04
E	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
E	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
E	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
E	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
E	-3	ARG	-	EXPRESSION TAG	UNP V4GH04

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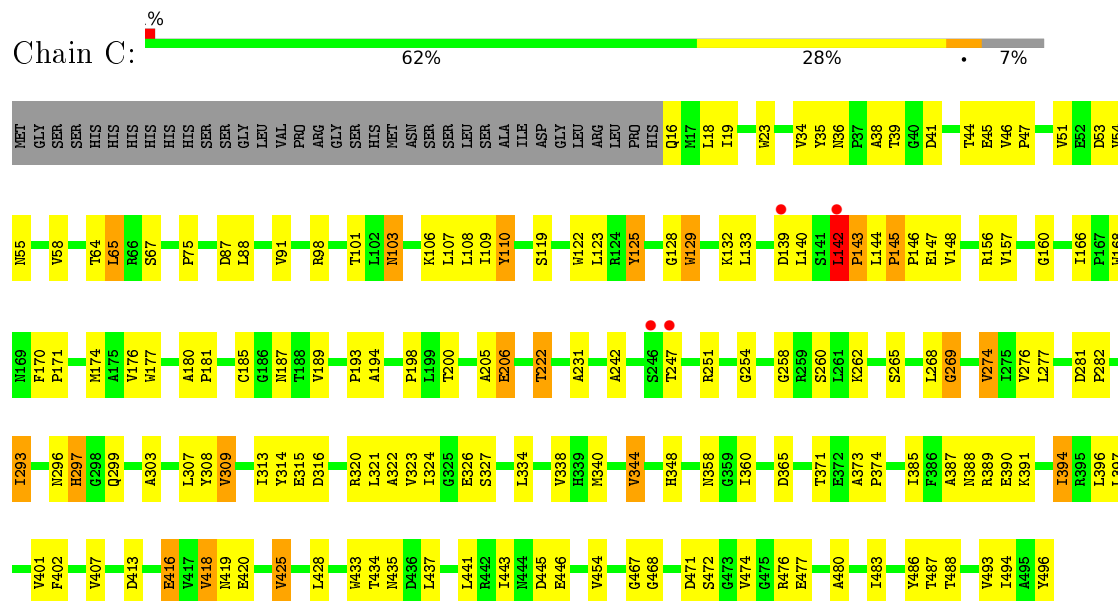
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
E	-1	SER	-	EXPRESSION TAG	UNP V4GH04
E	0	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-19	MET	-	EXPRESSION TAG	UNP V4GH04
F	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
F	-17	SER	-	EXPRESSION TAG	UNP V4GH04
F	-16	SER	-	EXPRESSION TAG	UNP V4GH04
F	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-9	SER	-	EXPRESSION TAG	UNP V4GH04
F	-8	SER	-	EXPRESSION TAG	UNP V4GH04
F	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
F	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
F	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
F	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
F	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
F	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
F	-1	SER	-	EXPRESSION TAG	UNP V4GH04
F	0	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-19	MET	-	EXPRESSION TAG	UNP V4GH04
G	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
G	-17	SER	-	EXPRESSION TAG	UNP V4GH04
G	-16	SER	-	EXPRESSION TAG	UNP V4GH04
G	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-9	SER	-	EXPRESSION TAG	UNP V4GH04
G	-8	SER	-	EXPRESSION TAG	UNP V4GH04
G	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
G	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
G	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
G	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
G	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
G	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
G	-1	SER	-	EXPRESSION TAG	UNP V4GH04

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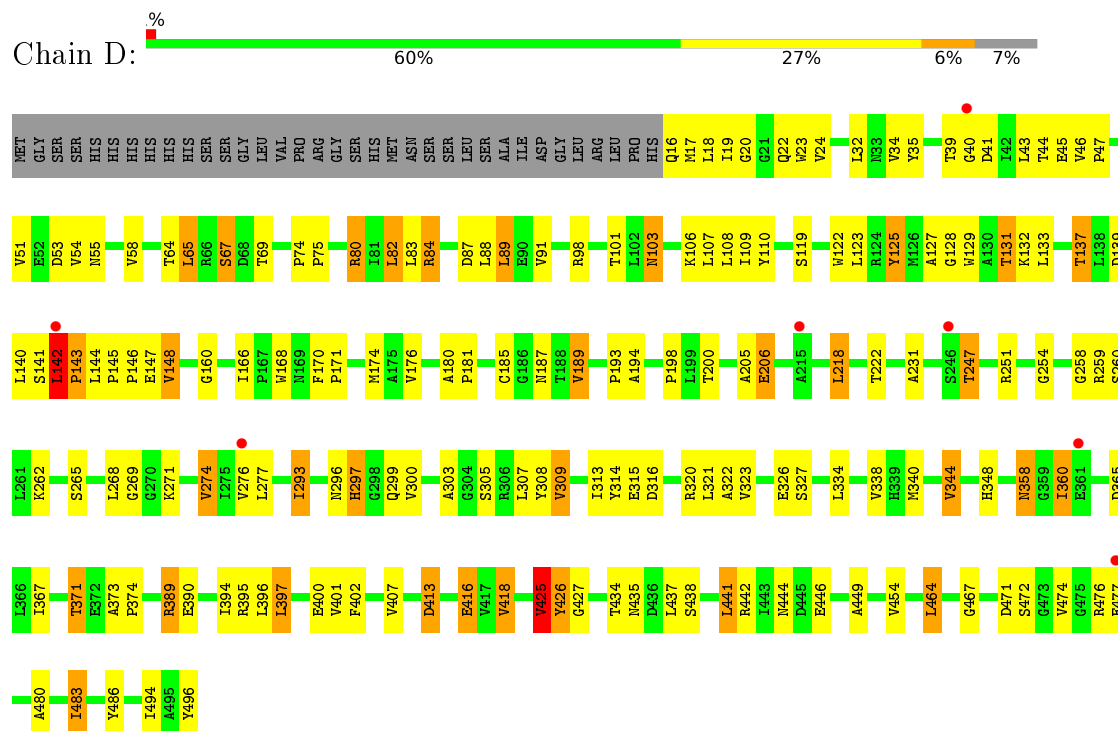
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-19	MET	-	EXPRESSION TAG	UNP V4GH04
H	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
H	-17	SER	-	EXPRESSION TAG	UNP V4GH04
H	-16	SER	-	EXPRESSION TAG	UNP V4GH04
H	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-9	SER	-	EXPRESSION TAG	UNP V4GH04
H	-8	SER	-	EXPRESSION TAG	UNP V4GH04
H	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
H	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
H	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
H	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
H	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
H	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
H	-1	SER	-	EXPRESSION TAG	UNP V4GH04
H	0	HIS	-	EXPRESSION TAG	UNP V4GH04

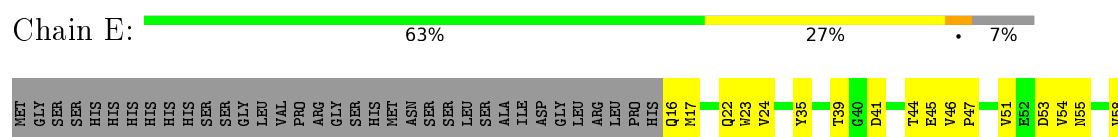
- Molecule 1: Aldehyde dehydrogenase

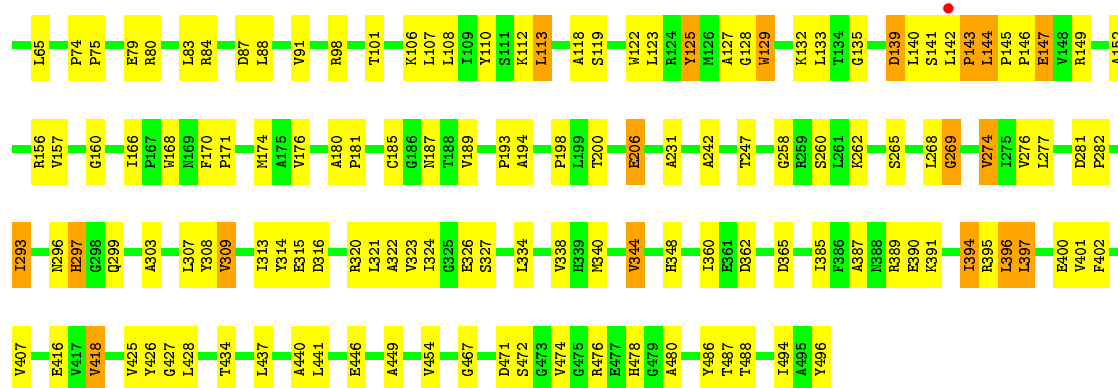


- Molecule 1: Aldehyde dehydrogenase

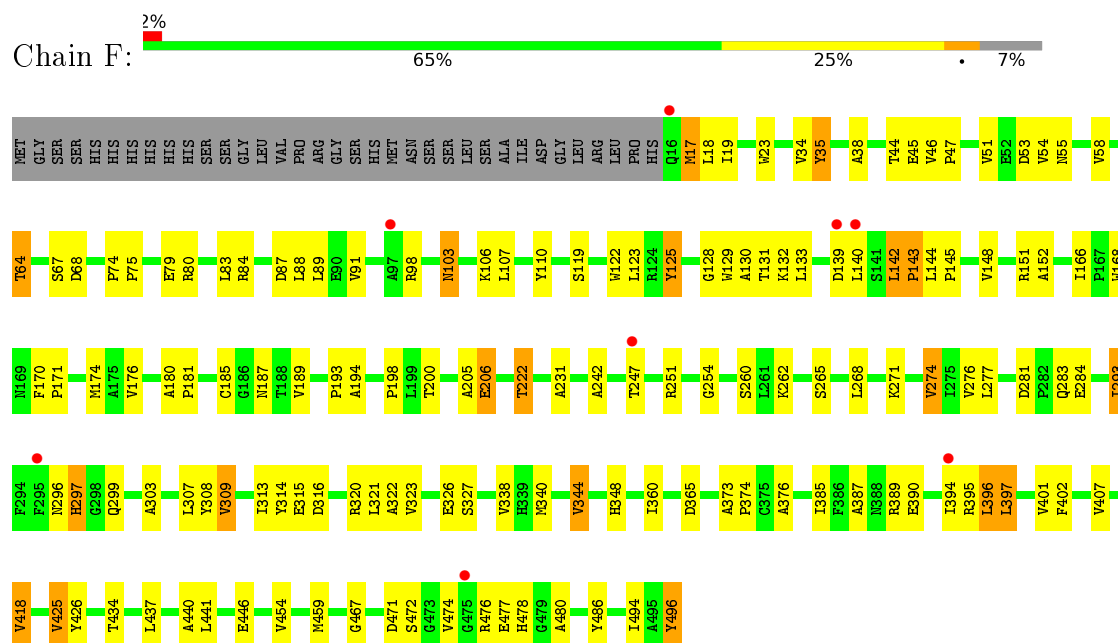


- Molecule 1: Aldehyde dehydrogenase

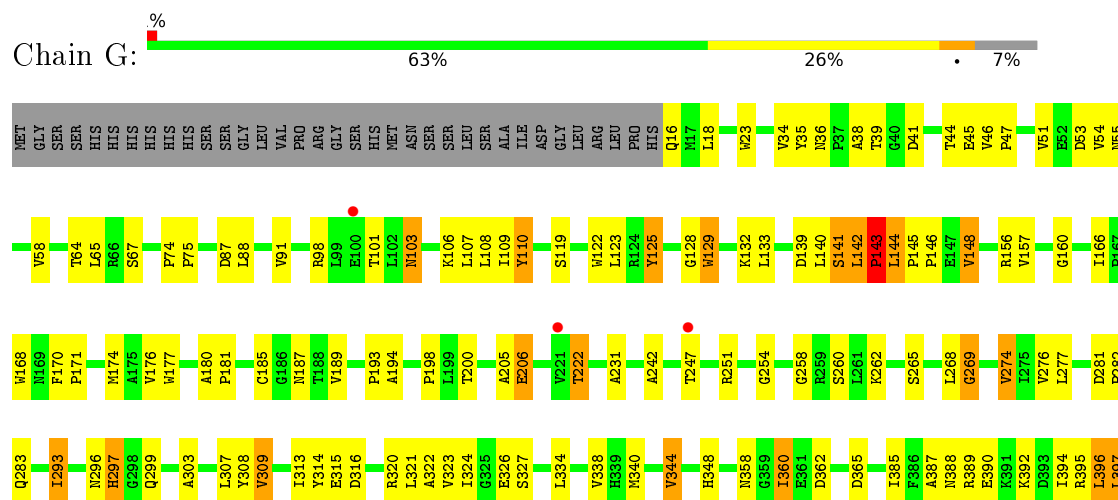




• Molecule 1: Aldehyde dehydrogenase

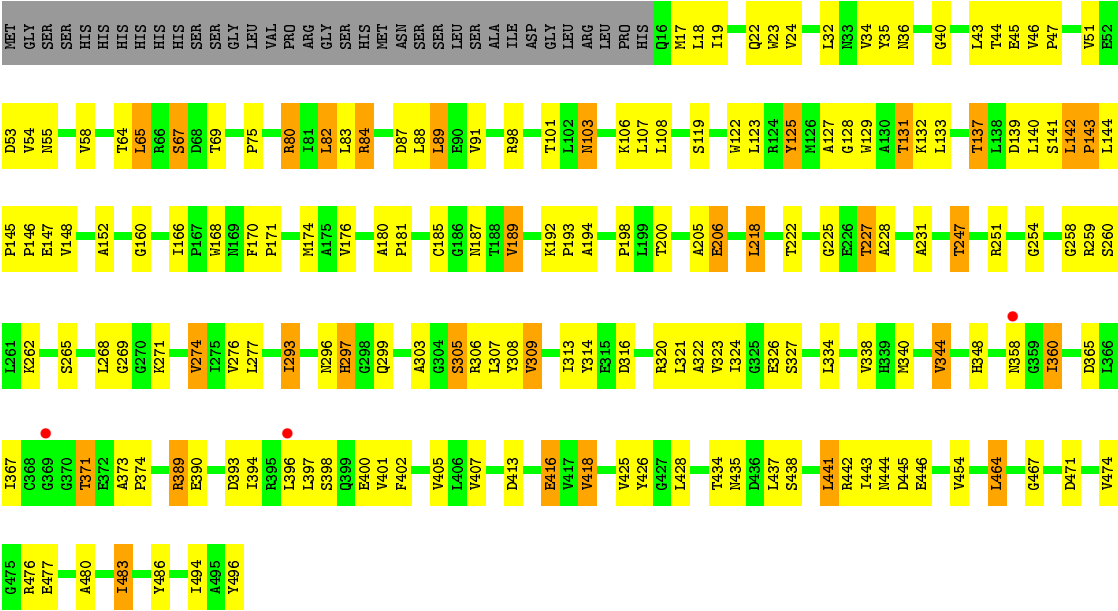


• Molecule 1: Aldehyde dehydrogenase





● Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.09Å 118.69Å 304.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.83 49.99 – 2.83	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.99-2.83) 81.4 (49.99-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.254 , 0.258 0.254 , 0.258	Depositor DCC
R_{free} test set	4660 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -2.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	27306	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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	1.70	20/3485 (0.6%)	1.09	16/4781 (0.3%)
1	B	1.70	18/3480 (0.5%)	1.11	23/4774 (0.5%)
1	C	1.70	23/3478 (0.7%)	1.08	16/4772 (0.3%)
1	D	1.69	21/3488 (0.6%)	1.10	15/4783 (0.3%)
1	E	1.68	23/3477 (0.7%)	1.08	16/4771 (0.3%)
1	F	1.70	17/3480 (0.5%)	1.09	15/4774 (0.3%)
1	G	1.73	23/3488 (0.7%)	1.11	16/4784 (0.3%)
1	H	1.71	19/3482 (0.5%)	1.11	15/4776 (0.3%)
All	All	1.70	164/27858 (0.6%)	1.10	132/38215 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	496	TYR	CD2-CE2	-5.97	1.30	1.39
1	C	496	TYR	CD2-CE2	-5.94	1.30	1.39
1	H	398	SER	CB-OG	-5.88	1.34	1.42
1	E	143	PRO	N-CD	5.80	1.55	1.47
1	G	146	PRO	N-CD	-5.80	1.39	1.47
1	H	496	TYR	CD1-CE1	-5.79	1.30	1.39
1	F	496	TYR	CD1-CE1	-5.79	1.30	1.39
1	B	496	TYR	CD1-CE1	-5.79	1.30	1.39
1	A	35	TYR	CD2-CE2	-5.78	1.30	1.39
1	E	35	TYR	CD2-CE2	-5.78	1.30	1.39
1	D	496	TYR	CD1-CE1	-5.77	1.30	1.39
1	A	496	TYR	CD1-CE1	-5.77	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	35	TYR	CD2-CE2	-5.73	1.30	1.39
1	D	35	TYR	CD2-CE2	-5.72	1.30	1.39
1	A	143	PRO	N-CD	5.72	1.55	1.47
1	E	496	TYR	CD1-CE1	-5.70	1.30	1.39
1	D	35	TYR	CE2-CZ	-5.58	1.31	1.38
1	C	35	TYR	CD2-CE2	-5.57	1.30	1.39
1	A	35	TYR	CE2-CZ	-5.56	1.31	1.38
1	E	35	TYR	CE2-CZ	-5.55	1.31	1.38
1	G	323	VAL	CB-CG2	-5.55	1.41	1.52
1	H	35	TYR	CE2-CZ	-5.54	1.31	1.38
1	E	125	TYR	CE2-CZ	-5.54	1.31	1.38
1	C	323	VAL	CB-CG2	-5.53	1.41	1.52
1	E	418	VAL	CB-CG1	-5.52	1.41	1.52
1	E	323	VAL	CB-CG2	-5.52	1.41	1.52
1	G	35	TYR	CD2-CE2	-5.51	1.31	1.39
1	D	418	VAL	CB-CG1	-5.51	1.41	1.52
1	A	323	VAL	CB-CG2	-5.51	1.41	1.52
1	A	418	VAL	CB-CG1	-5.51	1.41	1.52
1	C	418	VAL	CB-CG1	-5.51	1.41	1.52
1	H	418	VAL	CB-CG1	-5.50	1.41	1.52
1	B	323	VAL	CB-CG2	-5.50	1.41	1.52
1	B	418	VAL	CB-CG1	-5.50	1.41	1.52
1	D	125	TYR	CE2-CZ	-5.49	1.31	1.38
1	G	418	VAL	CB-CG1	-5.49	1.41	1.52
1	C	125	TYR	CE2-CZ	-5.48	1.31	1.38
1	A	125	TYR	CE2-CZ	-5.48	1.31	1.38
1	F	418	VAL	CB-CG1	-5.48	1.41	1.52
1	B	125	TYR	CE2-CZ	-5.47	1.31	1.38
1	F	323	VAL	CB-CG2	-5.47	1.41	1.52
1	D	323	VAL	CB-CG2	-5.47	1.41	1.52
1	H	323	VAL	CB-CG2	-5.47	1.41	1.52
1	F	309	VAL	CB-CG1	-5.46	1.41	1.52
1	G	125	TYR	CE2-CZ	-5.46	1.31	1.38
1	D	309	VAL	CB-CG1	-5.45	1.41	1.52
1	E	496	TYR	CE1-CZ	-5.45	1.31	1.38
1	H	308	TYR	CD1-CE1	-5.45	1.31	1.39
1	D	308	TYR	CD1-CE1	-5.45	1.31	1.39
1	H	125	TYR	CE2-CZ	-5.45	1.31	1.38
1	G	309	VAL	CB-CG1	-5.44	1.41	1.52
1	E	308	TYR	CD1-CE1	-5.44	1.31	1.39
1	E	486	TYR	CD2-CE2	-5.44	1.31	1.39
1	A	309	VAL	CB-CG1	-5.44	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	TYR	CD1-CE1	-5.42	1.31	1.39
1	A	486	TYR	CD2-CE2	-5.42	1.31	1.39
1	B	309	VAL	CB-CG1	-5.42	1.41	1.52
1	C	486	TYR	CD2-CE2	-5.42	1.31	1.39
1	F	125	TYR	CE2-CZ	-5.42	1.31	1.38
1	G	344	VAL	CB-CG2	-5.42	1.41	1.52
1	C	309	VAL	CB-CG1	-5.41	1.41	1.52
1	F	496	TYR	CE1-CZ	-5.41	1.31	1.38
1	D	344	VAL	CB-CG2	-5.41	1.41	1.52
1	F	344	VAL	CB-CG2	-5.41	1.41	1.52
1	G	486	TYR	CD2-CE2	-5.41	1.31	1.39
1	D	486	TYR	CD2-CE2	-5.41	1.31	1.39
1	E	309	VAL	CB-CG1	-5.41	1.41	1.52
1	G	496	TYR	CD1-CE1	-5.40	1.31	1.39
1	H	309	VAL	CB-CG1	-5.40	1.41	1.52
1	B	344	VAL	CB-CG2	-5.40	1.41	1.52
1	A	344	VAL	CB-CG2	-5.40	1.41	1.52
1	A	496	TYR	CE1-CZ	-5.40	1.31	1.38
1	B	496	TYR	CE1-CZ	-5.40	1.31	1.38
1	G	308	TYR	CD1-CE1	-5.40	1.31	1.39
1	H	344	VAL	CB-CG2	-5.40	1.41	1.52
1	C	308	TYR	CD1-CE1	-5.40	1.31	1.39
1	B	308	TYR	CD1-CE1	-5.39	1.31	1.39
1	B	314	TYR	CE2-CZ	-5.39	1.31	1.38
1	C	344	VAL	CB-CG2	-5.39	1.41	1.52
1	H	486	TYR	CD2-CE2	-5.38	1.31	1.39
1	C	425	VAL	CB-CG1	-5.38	1.41	1.52
1	C	496	TYR	CD1-CE1	-5.38	1.31	1.39
1	B	486	TYR	CD2-CE2	-5.37	1.31	1.39
1	D	496	TYR	CE1-CZ	-5.37	1.31	1.38
1	B	425	VAL	CB-CG1	-5.37	1.41	1.52
1	F	35	TYR	CD1-CE1	-5.37	1.31	1.39
1	A	314	TYR	CE2-CZ	-5.37	1.31	1.38
1	D	425	VAL	CB-CG1	-5.37	1.41	1.52
1	G	425	VAL	CB-CG1	-5.36	1.41	1.52
1	E	344	VAL	CB-CG2	-5.36	1.41	1.52
1	B	35	TYR	CD1-CE1	-5.36	1.31	1.39
1	F	308	TYR	CD1-CE1	-5.35	1.31	1.39
1	C	314	TYR	CE2-CZ	-5.35	1.31	1.38
1	E	314	TYR	CE2-CZ	-5.34	1.31	1.38
1	H	496	TYR	CE1-CZ	-5.34	1.31	1.38
1	F	425	VAL	CB-CG1	-5.34	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	314	TYR	CE2-CZ	-5.33	1.31	1.38
1	F	314	TYR	CE2-CZ	-5.33	1.31	1.38
1	H	416	GLU	CD-OE1	-5.31	1.19	1.25
1	E	416	GLU	CD-OE1	-5.31	1.19	1.25
1	A	400	GLU	CG-CD	-5.31	1.44	1.51
1	F	486	TYR	CD2-CE2	-5.30	1.31	1.39
1	H	314	TYR	CE2-CZ	-5.30	1.31	1.38
1	E	400	GLU	CG-CD	-5.29	1.44	1.51
1	H	480	ALA	CA-CB	-5.29	1.41	1.52
1	G	314	TYR	CE2-CZ	-5.28	1.31	1.38
1	D	480	ALA	CA-CB	-5.27	1.41	1.52
1	D	416	GLU	CD-OE1	-5.27	1.19	1.25
1	F	480	ALA	CA-CB	-5.26	1.41	1.52
1	G	480	ALA	CA-CB	-5.25	1.41	1.52
1	C	480	ALA	CA-CB	-5.25	1.41	1.52
1	A	480	ALA	CA-CB	-5.24	1.41	1.52
1	B	480	ALA	CA-CB	-5.24	1.41	1.52
1	E	480	ALA	CA-CB	-5.23	1.41	1.52
1	G	35	TYR	CD1-CE1	-5.20	1.31	1.39
1	C	54	VAL	CB-CG1	-5.20	1.42	1.52
1	A	54	VAL	CB-CG1	-5.18	1.42	1.52
1	C	177	TRP	CG-CD1	-5.17	1.29	1.36
1	G	54	VAL	CB-CG1	-5.17	1.42	1.52
1	E	54	VAL	CB-CG1	-5.17	1.42	1.52
1	C	35	TYR	CD1-CE1	-5.16	1.31	1.39
1	B	54	VAL	CB-CG1	-5.15	1.42	1.52
1	D	54	VAL	CB-CG1	-5.15	1.42	1.52
1	C	358	ASN	CB-CG	-5.14	1.39	1.51
1	G	177	TRP	CG-CD1	-5.14	1.29	1.36
1	H	54	VAL	CB-CG1	-5.14	1.42	1.52
1	F	54	VAL	CB-CG1	-5.14	1.42	1.52
1	H	54	VAL	CB-CG2	-5.13	1.42	1.52
1	B	315	GLU	CD-OE2	-5.13	1.20	1.25
1	G	358	ASN	CB-CG	-5.13	1.39	1.51
1	C	54	VAL	CB-CG2	-5.12	1.42	1.52
1	G	54	VAL	CB-CG2	-5.12	1.42	1.52
1	F	315	GLU	CD-OE2	-5.12	1.20	1.25
1	E	54	VAL	CB-CG2	-5.12	1.42	1.52
1	F	54	VAL	CB-CG2	-5.12	1.42	1.52
1	G	148	VAL	CB-CG1	-5.12	1.42	1.52
1	D	54	VAL	CB-CG2	-5.11	1.42	1.52
1	A	54	VAL	CB-CG2	-5.11	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	VAL	CB-CG2	-5.11	1.42	1.52
1	B	148	VAL	CB-CG1	-5.09	1.42	1.52
1	C	38	ALA	CA-CB	-5.09	1.41	1.52
1	G	38	ALA	CA-CB	-5.09	1.41	1.52
1	D	148	VAL	CB-CG1	-5.08	1.42	1.52
1	H	148	VAL	CB-CG1	-5.07	1.42	1.52
1	G	110	TYR	CE2-CZ	-5.07	1.31	1.38
1	H	496	TYR	CE2-CZ	-5.06	1.31	1.38
1	A	35	TYR	CD1-CE1	-5.06	1.31	1.39
1	C	371	THR	CA-CB	-5.06	1.40	1.53
1	A	315	GLU	CD-OE2	-5.05	1.20	1.25
1	E	496	TYR	CE2-CZ	-5.04	1.31	1.38
1	C	315	GLU	CD-OE2	-5.04	1.20	1.25
1	E	110	TYR	CE2-CZ	-5.04	1.32	1.38
1	D	496	TYR	CE2-CZ	-5.03	1.32	1.38
1	E	35	TYR	CD1-CE1	-5.03	1.31	1.39
1	C	110	TYR	CE2-CZ	-5.03	1.32	1.38
1	E	308	TYR	CD2-CE2	-5.03	1.31	1.39
1	E	315	GLU	CD-OE2	-5.02	1.20	1.25
1	F	110	TYR	CE2-CZ	-5.02	1.32	1.38
1	B	496	TYR	CE2-CZ	-5.02	1.32	1.38
1	D	315	GLU	CD-OE2	-5.02	1.20	1.25
1	D	35	TYR	CD1-CE1	-5.02	1.31	1.39
1	G	315	GLU	CD-OE2	-5.01	1.20	1.25
1	A	496	TYR	CE2-CZ	-5.01	1.32	1.38
1	C	308	TYR	CD2-CE2	-5.00	1.31	1.39

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	LEU	C-N-CD	-8.38	102.15	120.60
1	G	142	LEU	N-CA-C	6.28	127.95	111.00
1	E	428	LEU	N-CA-C	5.96	127.08	111.00
1	E	360	ILE	CG1-CB-CG2	-5.95	98.32	111.40
1	C	360	ILE	CG1-CB-CG2	-5.94	98.33	111.40
1	A	360	ILE	CG1-CB-CG2	-5.94	98.34	111.40
1	D	360	ILE	CG1-CB-CG2	-5.93	98.35	111.40
1	H	360	ILE	CG1-CB-CG2	-5.93	98.36	111.40
1	B	360	ILE	CG1-CB-CG2	-5.92	98.36	111.40
1	G	360	ILE	CG1-CB-CG2	-5.92	98.37	111.40
1	F	360	ILE	CG1-CB-CG2	-5.92	98.38	111.40
1	C	394	ILE	N-CA-C	-5.91	95.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	391	LYS	N-CA-CB	-5.87	100.04	110.60
1	E	139	ASP	C-N-CA	-5.83	107.14	121.70
1	B	148	VAL	N-CA-CB	5.79	124.25	111.50
1	E	147	GLU	CB-CA-C	-5.76	98.87	110.40
1	C	142	LEU	N-CA-C	5.73	126.48	111.00
1	F	38	ALA	CB-CA-C	5.73	118.69	110.10
1	B	40	GLY	N-CA-C	-5.72	98.81	113.10
1	B	395	ARG	N-CA-C	5.71	126.41	111.00
1	D	123	LEU	CB-CA-C	5.70	121.03	110.20
1	H	123	LEU	CB-CA-C	5.70	121.02	110.20
1	E	123	LEU	CB-CA-C	5.68	120.99	110.20
1	A	123	LEU	CB-CA-C	5.67	120.97	110.20
1	B	123	LEU	CB-CA-C	5.67	120.97	110.20
1	F	123	LEU	CB-CA-C	5.66	120.96	110.20
1	C	123	LEU	CB-CA-C	5.66	120.96	110.20
1	B	141	SER	N-CA-C	-5.64	95.77	111.00
1	G	123	LEU	CB-CA-C	5.64	120.92	110.20
1	F	129	TRP	CB-CA-C	-5.59	99.22	110.40
1	H	393	ASP	N-CA-C	-5.58	95.92	111.00
1	A	16	GLN	N-CA-C	-5.58	95.93	111.00
1	B	129	TRP	CB-CA-C	-5.58	99.24	110.40
1	F	53	ASP	CB-CA-C	-5.57	99.25	110.40
1	B	148	VAL	N-CA-C	-5.57	95.96	111.00
1	E	16	GLN	N-CA-C	-5.57	95.97	111.00
1	B	53	ASP	CB-CA-C	-5.56	99.28	110.40
1	A	53	ASP	CB-CA-C	-5.55	99.29	110.40
1	G	53	ASP	CB-CA-C	-5.55	99.29	110.40
1	D	53	ASP	CB-CA-C	-5.55	99.30	110.40
1	C	53	ASP	CB-CA-C	-5.54	99.31	110.40
1	E	53	ASP	CB-CA-C	-5.54	99.31	110.40
1	H	133	LEU	CA-CB-CG	5.52	128.00	115.30
1	H	53	ASP	CB-CA-C	-5.52	99.36	110.40
1	D	133	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	133	LEU	CA-CB-CG	5.50	127.95	115.30
1	E	133	LEU	CA-CB-CG	5.50	127.95	115.30
1	G	133	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	133	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	133	LEU	CA-CB-CG	5.50	127.94	115.30
1	F	133	LEU	CA-CB-CG	5.49	127.92	115.30
1	G	395	ARG	CB-CA-C	-5.48	99.43	110.40
1	H	269	GLY	N-CA-C	5.47	126.79	113.10
1	D	269	GLY	N-CA-C	5.47	126.78	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	GLY	N-CA-C	5.46	126.75	113.10
1	A	269	GLY	N-CA-C	5.46	126.75	113.10
1	C	269	GLY	N-CA-C	5.46	126.75	113.10
1	G	269	GLY	N-CA-C	5.46	126.75	113.10
1	B	16	GLN	N-CA-C	-5.43	96.33	111.00
1	G	87	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	395	ARG	N-CA-CB	-5.37	100.94	110.60
1	G	194	ALA	CB-CA-C	5.37	118.15	110.10
1	C	87	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	194	ALA	CB-CA-C	5.35	118.12	110.10
1	E	194	ALA	CB-CA-C	5.35	118.12	110.10
1	A	194	ALA	CB-CA-C	5.34	118.12	110.10
1	A	394	ILE	N-CA-C	-5.34	96.58	111.00
1	D	194	ALA	CB-CA-C	5.34	118.11	110.10
1	A	87	ASP	CB-CG-OD2	5.34	123.10	118.30
1	E	87	ASP	CB-CG-OD2	5.34	123.10	118.30
1	H	194	ALA	CB-CA-C	5.32	118.08	110.10
1	B	194	ALA	CB-CA-C	5.31	118.07	110.10
1	F	194	ALA	CB-CA-C	5.30	118.05	110.10
1	H	87	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	480	ALA	CB-CA-C	-5.28	102.18	110.10
1	A	480	ALA	CB-CA-C	-5.28	102.18	110.10
1	G	480	ALA	CB-CA-C	-5.27	102.19	110.10
1	E	480	ALA	CB-CA-C	-5.27	102.20	110.10
1	B	87	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	480	ALA	CB-CA-C	-5.26	102.20	110.10
1	F	87	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	87	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	480	ALA	CB-CA-C	-5.25	102.22	110.10
1	D	480	ALA	CB-CA-C	-5.25	102.22	110.10
1	H	480	ALA	CB-CA-C	-5.25	102.22	110.10
1	F	88	LEU	CB-CA-C	-5.24	100.25	110.20
1	B	88	LEU	CB-CA-C	-5.24	100.25	110.20
1	H	483	ILE	CB-CA-C	-5.24	101.13	111.60
1	E	88	LEU	CB-CA-C	-5.23	100.25	110.20
1	A	88	LEU	CB-CA-C	-5.22	100.27	110.20
1	D	483	ILE	CB-CA-C	-5.22	101.16	111.60
1	D	88	LEU	CB-CA-C	-5.22	100.29	110.20
1	G	88	LEU	CB-CA-C	-5.21	100.30	110.20
1	C	88	LEU	CB-CA-C	-5.21	100.31	110.20
1	H	88	LEU	CB-CA-C	-5.20	100.31	110.20
1	G	142	LEU	C-N-CD	5.18	139.29	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	GLY	N-CA-C	5.18	126.05	113.10
1	H	428	LEU	N-CA-C	5.18	124.99	111.00
1	B	394	ILE	CB-CA-C	-5.17	101.26	111.60
1	G	293	ILE	CB-CA-C	-5.16	101.27	111.60
1	C	293	ILE	CB-CA-C	-5.15	101.30	111.60
1	A	428	LEU	N-CA-C	5.15	124.90	111.00
1	F	293	ILE	CB-CA-C	-5.15	101.30	111.60
1	B	293	ILE	CB-CA-C	-5.14	101.32	111.60
1	G	98	ARG	CB-CA-C	5.14	120.67	110.40
1	A	293	ILE	CB-CA-C	-5.13	101.33	111.60
1	E	293	ILE	CB-CA-C	-5.12	101.35	111.60
1	H	293	ILE	CB-CA-C	-5.12	101.35	111.60
1	C	98	ARG	CB-CA-C	5.12	120.64	110.40
1	D	293	ILE	CB-CA-C	-5.12	101.35	111.60
1	A	394	ILE	CB-CA-C	-5.12	101.36	111.60
1	A	98	ARG	CB-CA-C	5.10	120.61	110.40
1	D	98	ARG	CB-CA-C	5.10	120.59	110.40
1	B	98	ARG	CB-CA-C	5.09	120.58	110.40
1	G	143	PRO	CA-N-CD	-5.09	104.38	111.50
1	H	98	ARG	CB-CA-C	5.08	120.57	110.40
1	B	64	THR	CB-CA-C	-5.08	97.88	111.60
1	F	64	THR	CB-CA-C	-5.08	97.88	111.60
1	F	303	ALA	CB-CA-C	-5.08	102.48	110.10
1	E	98	ARG	CB-CA-C	5.08	120.56	110.40
1	F	98	ARG	CB-CA-C	5.08	120.56	110.40
1	C	303	ALA	CB-CA-C	-5.07	102.49	110.10
1	G	303	ALA	CB-CA-C	-5.07	102.50	110.10
1	B	303	ALA	CB-CA-C	-5.06	102.50	110.10
1	B	130	ALA	CB-CA-C	5.06	117.69	110.10
1	A	303	ALA	CB-CA-C	-5.05	102.52	110.10
1	H	303	ALA	CB-CA-C	-5.05	102.53	110.10
1	F	130	ALA	CB-CA-C	5.04	117.67	110.10
1	E	303	ALA	CB-CA-C	-5.04	102.54	110.10
1	C	391	LYS	N-CA-C	5.04	124.60	111.00
1	D	303	ALA	CB-CA-C	-5.04	102.55	110.10
1	D	413	ASP	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	141	SER	Peptide

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	3416	0	3298	161	0
1	B	3411	0	3298	134	0
1	C	3409	0	3292	138	0
1	D	3419	0	3314	132	0
1	E	3408	0	3290	146	0
1	F	3411	0	3298	121	0
1	G	3419	0	3309	120	0
1	H	3413	0	3303	140	0
All	All	27306	0	26402	1033	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1033) 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:C:156:ARG:CG	1:C:487:THR:HG21	1.58	1.34
1:B:397:LEU:CD1	1:B:407:VAL:HG11	1.57	1.34
1:E:156:ARG:CG	1:E:487:THR:HG21	1.58	1.33
1:B:156:ARG:CG	1:B:487:THR:HG21	1.58	1.33
1:G:156:ARG:CG	1:G:487:THR:HG21	1.58	1.32
1:A:156:ARG:CG	1:A:487:THR:HG21	1.58	1.30
1:A:241:VAL:HG11	1:A:257:CYS:SG	1.73	1.28
1:G:139:ASP:O	1:G:140:LEU:HD23	1.28	1.28
1:C:156:ARG:HG3	1:C:487:THR:CG2	1.76	1.16
1:A:156:ARG:HG3	1:A:487:THR:CG2	1.76	1.16
1:H:271:LYS:HE3	1:H:306:ARG:CG	1.75	1.15
1:B:142:LEU:HB2	1:B:143:PRO:CA	1.77	1.15
1:G:156:ARG:HG3	1:G:487:THR:CG2	1.76	1.14
1:E:156:ARG:HG3	1:E:487:THR:CG2	1.76	1.14
1:B:142:LEU:CB	1:B:143:PRO:HA	1.69	1.14
1:B:156:ARG:HG3	1:B:487:THR:CG2	1.76	1.14
1:D:139:ASP:O	1:D:140:LEU:CD1	1.96	1.13
1:A:79:GLU:O	1:A:83:LEU:HD13	1.48	1.13
1:H:142:LEU:HB2	1:H:143:PRO:HA	1.13	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:CD1	1:A:407:VAL:HG11	1.80	1.12
1:E:79:GLU:O	1:E:83:LEU:HD13	1.48	1.11
1:A:142:LEU:HB2	1:A:143:PRO:HA	1.34	1.10
1:A:394:ILE:HD13	1:A:394:ILE:N	1.52	1.10
1:D:139:ASP:O	1:D:140:LEU:HD12	1.53	1.08
1:F:139:ASP:O	1:F:140:LEU:HG	1.52	1.08
1:A:397:LEU:HD12	1:A:407:VAL:HG11	1.33	1.07
1:F:140:LEU:HD11	1:F:152:ALA:HB2	1.16	1.07
1:B:397:LEU:HD12	1:B:407:VAL:HG11	1.16	1.07
1:D:142:LEU:HB2	1:D:143:PRO:HA	1.11	1.07
1:H:396:LEU:HD23	1:H:407:VAL:HB	1.33	1.06
1:C:142:LEU:CB	1:C:143:PRO:HA	1.84	1.06
1:H:271:LYS:HE3	1:H:306:ARG:HG3	1.09	1.06
1:B:283:GLN:OE1	1:B:320:ARG:HD3	1.54	1.04
1:B:139:ASP:O	1:B:140:LEU:HD13	1.57	1.04
1:F:283:GLN:HG2	1:F:320:ARG:HD3	1.39	1.03
1:A:362:ASP:HB3	1:A:394:ILE:HG23	1.41	1.02
1:A:394:ILE:HD13	1:A:394:ILE:H	0.88	1.02
1:A:156:ARG:HG3	1:A:487:THR:HG21	1.02	1.01
1:E:156:ARG:HG3	1:E:487:THR:HG21	1.02	1.01
1:A:241:VAL:CG1	1:A:257:CYS:SG	2.48	1.01
1:C:156:ARG:HG3	1:C:487:THR:HG21	1.02	1.01
1:C:142:LEU:HB2	1:C:143:PRO:HA	1.02	1.00
1:E:139:ASP:O	1:E:140:LEU:HD23	1.60	0.99
1:H:142:LEU:HB2	1:H:143:PRO:CA	1.91	0.99
1:G:156:ARG:HG3	1:G:487:THR:HG21	1.02	0.99
1:E:144:LEU:HB3	1:E:145:PRO:HD2	1.45	0.99
1:A:139:ASP:HB2	1:D:75:PRO:HG2	1.45	0.99
1:F:140:LEU:HD11	1:F:152:ALA:CB	1.92	0.99
1:F:142:LEU:HB2	1:F:143:PRO:HA	1.46	0.98
1:C:144:LEU:HB3	1:C:148:VAL:HG11	1.45	0.98
1:E:139:ASP:HB2	1:H:75:PRO:HG2	1.46	0.98
1:B:156:ARG:HG3	1:B:487:THR:HG21	1.02	0.97
1:C:142:LEU:HB2	1:C:143:PRO:CA	1.94	0.97
1:B:397:LEU:CD1	1:B:407:VAL:CG1	2.42	0.97
1:H:425:VAL:O	1:H:471:ASP:HB2	1.66	0.96
1:C:413:ASP:OD1	1:C:416:GLU:HG2	1.65	0.95
1:B:139:ASP:HB2	1:C:75:PRO:HG2	1.48	0.95
1:D:142:LEU:HB2	1:D:143:PRO:CA	1.98	0.94
1:E:118:ALA:O	1:E:122:TRP:HD1	1.50	0.93
1:B:139:ASP:O	1:B:140:LEU:CD1	2.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:O	1:A:122:TRP:HD1	1.50	0.92
1:E:122:TRP:HZ3	1:E:478:HIS:ND1	1.67	0.92
1:F:139:ASP:O	1:F:140:LEU:CG	2.18	0.92
1:E:397:LEU:HD12	1:E:407:VAL:HG11	1.50	0.92
1:E:144:LEU:HB3	1:E:145:PRO:CD	1.98	0.90
1:A:139:ASP:O	1:A:140:LEU:HD12	1.71	0.90
1:A:122:TRP:HZ3	1:A:478:HIS:ND1	1.67	0.89
1:D:142:LEU:CB	1:D:143:PRO:HA	1.93	0.89
1:H:396:LEU:CD2	1:H:407:VAL:HB	2.02	0.89
1:C:144:LEU:HD13	1:C:148:VAL:CG1	2.00	0.89
1:A:394:ILE:CD1	1:A:394:ILE:H	1.73	0.88
1:D:139:ASP:O	1:D:140:LEU:HD13	1.71	0.88
1:E:140:LEU:HD11	1:E:152:ALA:CB	2.02	0.88
1:H:271:LYS:CE	1:H:306:ARG:HG3	2.01	0.88
1:B:397:LEU:HD12	1:B:407:VAL:CG1	2.04	0.88
1:A:75:PRO:HG2	1:D:139:ASP:HB2	1.53	0.88
1:B:75:PRO:HG2	1:C:139:ASP:HB3	1.57	0.86
1:A:139:ASP:O	1:A:140:LEU:CD1	2.22	0.86
1:H:142:LEU:CB	1:H:143:PRO:HA	1.94	0.86
1:C:139:ASP:O	1:C:140:LEU:HD12	1.76	0.85
1:E:397:LEU:CD1	1:E:407:VAL:HG11	2.06	0.85
1:H:271:LYS:HG3	1:H:306:ARG:HE	1.40	0.85
1:A:362:ASP:CB	1:A:394:ILE:HG23	2.06	0.85
1:E:75:PRO:HG2	1:H:139:ASP:HB2	1.59	0.84
1:F:283:GLN:HG2	1:F:320:ARG:CD	2.07	0.84
1:H:140:LEU:HD11	1:H:152:ALA:HB2	1.59	0.84
1:B:142:LEU:HB2	1:B:143:PRO:HA	0.86	0.84
1:E:58:VAL:HG12	1:E:58:VAL:O	1.77	0.84
1:C:58:VAL:O	1:C:58:VAL:HG12	1.77	0.84
1:D:58:VAL:HG12	1:D:58:VAL:O	1.77	0.84
1:F:58:VAL:HG12	1:F:58:VAL:O	1.77	0.84
1:B:58:VAL:O	1:B:58:VAL:HG12	1.77	0.84
1:E:139:ASP:OD1	1:E:139:ASP:O	1.96	0.83
1:A:394:ILE:CD1	1:A:394:ILE:N	2.30	0.83
1:H:58:VAL:O	1:H:58:VAL:HG12	1.77	0.83
1:E:389:ARG:O	1:E:390:GLU:CB	2.27	0.83
1:A:389:ARG:O	1:A:390:GLU:CB	2.27	0.83
1:A:142:LEU:HB2	1:A:143:PRO:CA	2.09	0.82
1:C:144:LEU:CD1	1:C:148:VAL:HG12	2.08	0.82
1:F:389:ARG:O	1:F:390:GLU:CB	2.27	0.82
1:A:58:VAL:O	1:A:58:VAL:HG12	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ARG:HG2	1:E:487:THR:HG21	1.61	0.82
1:A:122:TRP:CZ3	1:A:478:HIS:ND1	2.48	0.82
1:E:122:TRP:CZ3	1:E:478:HIS:ND1	2.48	0.81
1:E:142:LEU:HD22	1:F:459:MET:HB3	1.61	0.81
1:C:144:LEU:CD1	1:C:148:VAL:CG1	2.57	0.81
1:H:271:LYS:HE2	1:H:397:LEU:O	1.81	0.81
1:C:156:ARG:HG2	1:C:487:THR:HG21	1.61	0.81
1:G:58:VAL:HG12	1:G:58:VAL:O	1.77	0.81
1:B:371:THR:O	1:B:371:THR:HG23	1.78	0.81
1:H:166:ILE:HG12	1:H:193:PRO:HA	1.63	0.81
1:D:166:ILE:HG12	1:D:193:PRO:HA	1.63	0.81
1:D:40:GLY:O	1:D:41:ASP:OD1	1.97	0.81
1:B:51:VAL:HG22	1:B:231:ALA:HB2	1.63	0.81
1:E:166:ILE:HG12	1:E:193:PRO:HA	1.63	0.81
1:E:51:VAL:HG22	1:E:231:ALA:HB2	1.63	0.81
1:F:166:ILE:HG12	1:F:193:PRO:HA	1.63	0.81
1:F:51:VAL:HG22	1:F:231:ALA:HB2	1.63	0.80
1:G:166:ILE:HG12	1:G:193:PRO:HA	1.63	0.80
1:F:139:ASP:HB2	1:G:75:PRO:HG2	1.61	0.80
1:A:51:VAL:HG22	1:A:231:ALA:HB2	1.63	0.80
1:A:241:VAL:HG22	1:A:264:VAL:HG23	1.64	0.80
1:C:166:ILE:HG12	1:C:193:PRO:HA	1.63	0.80
1:E:65:LEU:HD21	1:E:160:GLY:HA2	1.64	0.80
1:B:166:ILE:HG12	1:B:193:PRO:HA	1.63	0.80
1:B:293:ILE:HG13	1:B:293:ILE:O	1.81	0.80
1:B:156:ARG:HG2	1:B:487:THR:HG21	1.61	0.80
1:H:293:ILE:HG13	1:H:293:ILE:O	1.81	0.80
1:C:51:VAL:HG22	1:C:231:ALA:HB2	1.63	0.80
1:D:51:VAL:HG22	1:D:231:ALA:HB2	1.63	0.80
1:D:293:ILE:O	1:D:293:ILE:HG13	1.81	0.80
1:G:51:VAL:HG22	1:G:231:ALA:HB2	1.63	0.80
1:E:139:ASP:O	1:E:140:LEU:CD2	2.30	0.79
1:D:65:LEU:HD11	1:D:160:GLY:HA2	1.65	0.79
1:E:140:LEU:CD1	1:E:152:ALA:CB	2.60	0.79
1:C:293:ILE:O	1:C:293:ILE:HG13	1.81	0.79
1:C:396:LEU:HD13	1:C:396:LEU:O	1.83	0.79
1:A:293:ILE:HG13	1:A:293:ILE:O	1.81	0.78
1:F:293:ILE:O	1:F:293:ILE:HG13	1.81	0.78
1:H:142:LEU:CB	1:H:143:PRO:CA	2.58	0.78
1:H:51:VAL:HG22	1:H:231:ALA:HB2	1.63	0.78
1:A:166:ILE:HG12	1:A:193:PRO:HA	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:VAL:O	1:B:471:ASP:HB2	1.84	0.78
1:E:293:ILE:HG13	1:E:293:ILE:O	1.81	0.78
1:G:139:ASP:O	1:G:140:LEU:CD2	2.23	0.78
1:C:65:LEU:HD11	1:C:160:GLY:HA2	1.66	0.78
1:C:425:VAL:O	1:C:471:ASP:HB2	1.84	0.77
1:B:397:LEU:HD11	1:B:407:VAL:HG11	1.60	0.77
1:G:293:ILE:HG13	1:G:293:ILE:O	1.82	0.77
1:G:425:VAL:O	1:G:471:ASP:HB2	1.83	0.77
1:G:65:LEU:HD21	1:G:160:GLY:HA2	1.67	0.77
1:D:425:VAL:O	1:D:471:ASP:HB2	1.84	0.77
1:F:425:VAL:O	1:F:471:ASP:HB2	1.84	0.77
1:E:80:ARG:HE	1:E:84:ARG:HE	1.33	0.77
1:A:156:ARG:HG2	1:A:487:THR:HG21	1.61	0.76
1:C:144:LEU:HD12	1:C:148:VAL:HG12	1.66	0.76
1:A:425:VAL:O	1:A:471:ASP:HB2	1.85	0.76
1:E:128:GLY:O	1:E:132:LYS:HD2	1.86	0.76
1:D:394:ILE:CD1	1:D:396:LEU:HB3	2.15	0.76
1:C:394:ILE:O	1:C:394:ILE:HG13	1.86	0.76
1:G:156:ARG:HG2	1:G:487:THR:HG21	1.61	0.76
1:B:142:LEU:CB	1:B:143:PRO:CA	2.45	0.76
1:D:128:GLY:O	1:D:132:LYS:HD2	1.86	0.76
1:D:64:THR:O	1:D:67:SER:HB2	1.86	0.76
1:G:128:GLY:O	1:G:132:LYS:HD2	1.86	0.75
1:F:394:ILE:O	1:F:395:ARG:CB	2.34	0.75
1:A:128:GLY:O	1:A:132:LYS:HD2	1.86	0.75
1:A:80:ARG:HE	1:A:84:ARG:HE	1.33	0.75
1:H:128:GLY:O	1:H:132:LYS:HD2	1.86	0.75
1:F:144:LEU:HD13	1:F:148:VAL:CG1	2.16	0.75
1:E:425:VAL:O	1:E:471:ASP:HB2	1.85	0.74
1:C:128:GLY:O	1:C:132:LYS:HD2	1.86	0.74
1:C:139:ASP:O	1:C:140:LEU:CD1	2.36	0.74
1:F:64:THR:HG22	1:F:64:THR:O	1.87	0.74
1:H:64:THR:O	1:H:67:SER:HB2	1.86	0.74
1:B:64:THR:O	1:B:64:THR:HG22	1.87	0.73
1:B:397:LEU:HD11	1:B:407:VAL:CG1	2.13	0.73
1:F:296:ASN:ND2	1:F:299:GLN:O	2.20	0.72
1:D:483:ILE:HG22	1:D:483:ILE:O	1.89	0.72
1:D:394:ILE:HD11	1:D:396:LEU:HB3	1.71	0.72
1:H:483:ILE:HG22	1:H:483:ILE:O	1.89	0.72
1:E:296:ASN:ND2	1:E:299:GLN:O	2.23	0.71
1:H:142:LEU:HD13	1:H:144:LEU:HG	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:CB	1:C:148:VAL:HG11	2.20	0.71
1:F:144:LEU:CD1	1:F:148:VAL:HG12	2.21	0.70
1:H:65:LEU:HD11	1:H:160:GLY:HA2	1.73	0.70
1:H:389:ARG:O	1:H:390:GLU:CB	2.40	0.70
1:A:58:VAL:CG1	1:A:58:VAL:O	2.40	0.70
1:H:144:LEU:HB3	1:H:145:PRO:HD2	1.74	0.70
1:D:58:VAL:O	1:D:58:VAL:CG1	2.40	0.69
1:A:139:ASP:C	1:A:139:ASP:OD1	2.28	0.69
1:C:58:VAL:O	1:C:58:VAL:CG1	2.40	0.69
1:G:58:VAL:O	1:G:58:VAL:CG1	2.40	0.69
1:B:58:VAL:O	1:B:58:VAL:CG1	2.40	0.69
1:A:428:LEU:HD12	1:A:468:GLY:HA3	1.74	0.69
1:C:144:LEU:HB3	1:C:148:VAL:CG1	2.22	0.69
1:D:389:ARG:O	1:D:390:GLU:CB	2.40	0.69
1:E:146:PRO:O	1:E:147:GLU:CB	2.41	0.69
1:F:144:LEU:HD13	1:F:148:VAL:HG12	1.74	0.69
1:E:142:LEU:HB2	1:E:143:PRO:CA	2.22	0.68
1:E:122:TRP:CZ3	1:E:478:HIS:CE1	2.81	0.68
1:H:58:VAL:O	1:H:58:VAL:CG1	2.40	0.68
1:F:58:VAL:CG1	1:F:58:VAL:O	2.40	0.68
1:H:80:ARG:HH11	1:H:80:ARG:HG3	1.59	0.68
1:E:142:LEU:HB2	1:E:143:PRO:HA	1.75	0.68
1:D:441:LEU:O	1:D:444:ASN:HB3	1.93	0.68
1:B:157:VAL:O	1:B:487:THR:HG23	1.94	0.68
1:A:122:TRP:CZ3	1:A:478:HIS:CE1	2.81	0.68
1:D:80:ARG:HH11	1:D:80:ARG:HG3	1.58	0.68
1:E:140:LEU:CD1	1:E:152:ALA:HB2	2.24	0.68
1:C:157:VAL:O	1:C:487:THR:HG23	1.94	0.68
1:F:247:THR:HA	1:F:268:LEU:HB3	1.76	0.68
1:G:170:PHE:CE1	1:G:296:ASN:ND2	2.62	0.68
1:C:140:LEU:HD23	1:C:142:LEU:HD21	1.74	0.68
1:C:156:ARG:CG	1:C:487:THR:CG2	2.50	0.68
1:F:397:LEU:CD1	1:F:407:VAL:HG11	2.24	0.68
1:A:247:THR:HA	1:A:268:LEU:HB3	1.76	0.67
1:C:247:THR:HA	1:C:268:LEU:HB3	1.76	0.67
1:H:441:LEU:O	1:H:444:ASN:HB3	1.93	0.67
1:A:157:VAL:O	1:A:487:THR:HG23	1.94	0.67
1:G:247:THR:HA	1:G:268:LEU:HB3	1.76	0.67
1:G:157:VAL:O	1:G:487:THR:HG23	1.94	0.67
1:E:157:VAL:O	1:E:487:THR:HG23	1.94	0.67
1:F:144:LEU:HB3	1:F:145:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:THR:HA	1:E:268:LEU:HB3	1.76	0.67
1:B:437:LEU:HD11	1:B:441:LEU:HD11	1.77	0.66
1:B:496:TYR:CD2	1:D:441:LEU:HD23	2.30	0.66
1:E:58:VAL:CG1	1:E:58:VAL:O	2.40	0.66
1:F:496:TYR:CD2	1:H:441:LEU:HD23	2.30	0.66
1:E:79:GLU:O	1:E:83:LEU:CD1	2.38	0.66
1:E:80:ARG:NE	1:E:84:ARG:HE	1.93	0.66
1:G:389:ARG:O	1:G:390:GLU:CB	2.44	0.66
1:H:247:THR:HA	1:H:268:LEU:HB3	1.76	0.66
1:G:170:PHE:HB2	1:G:174:MET:HG2	1.78	0.66
1:A:357:ARG:O	1:A:361:GLU:HG3	1.94	0.66
1:E:118:ALA:O	1:E:122:TRP:CD1	2.42	0.66
1:A:118:ALA:O	1:A:122:TRP:CD1	2.42	0.66
1:D:247:THR:HA	1:D:268:LEU:HB3	1.76	0.66
1:E:140:LEU:HD11	1:E:152:ALA:HB3	1.78	0.66
1:B:156:ARG:CG	1:B:487:THR:CG2	2.50	0.66
1:E:437:LEU:HD11	1:E:441:LEU:HD11	1.77	0.66
1:A:487:THR:HG22	1:A:488:THR:N	2.12	0.66
1:F:142:LEU:HB2	1:F:143:PRO:CA	2.21	0.66
1:G:64:THR:O	1:G:67:SER:HB3	1.96	0.66
1:H:474:VAL:O	1:H:474:VAL:HG23	1.96	0.66
1:A:80:ARG:NE	1:A:84:ARG:HE	1.93	0.65
1:C:64:THR:O	1:C:67:SER:HB3	1.96	0.65
1:A:397:LEU:CD1	1:A:407:VAL:CG1	2.65	0.65
1:G:474:VAL:HG23	1:G:474:VAL:O	1.97	0.65
1:C:487:THR:HG22	1:C:488:THR:N	2.12	0.65
1:D:170:PHE:CE1	1:D:296:ASN:ND2	2.64	0.65
1:E:140:LEU:HD12	1:E:152:ALA:HB2	1.78	0.65
1:H:271:LYS:HG3	1:H:306:ARG:NE	2.10	0.65
1:H:84:ARG:HG3	1:H:84:ARG:HH11	1.62	0.65
1:D:144:LEU:HB3	1:D:145:PRO:HD2	1.79	0.64
1:D:140:LEU:HD23	1:D:142:LEU:HD21	1.79	0.64
1:A:428:LEU:HD12	1:A:468:GLY:CA	2.26	0.64
1:F:139:ASP:O	1:F:140:LEU:CD2	2.45	0.64
1:B:474:VAL:O	1:B:474:VAL:HG23	1.97	0.64
1:C:144:LEU:CB	1:C:148:VAL:CG1	2.75	0.64
1:C:493:VAL:HG21	1:D:464:LEU:HD11	1.79	0.64
1:G:487:THR:HG22	1:G:488:THR:N	2.12	0.64
1:D:474:VAL:HG23	1:D:474:VAL:O	1.96	0.64
1:E:467:GLY:HA3	1:E:476:ARG:HD3	1.78	0.64
1:G:493:VAL:HG21	1:H:464:LEU:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLY:O	1:B:132:LYS:HD2	1.97	0.64
1:C:413:ASP:OD1	1:C:416:GLU:CG	2.44	0.64
1:D:84:ARG:HG3	1:D:84:ARG:HH11	1.62	0.64
1:F:128:GLY:O	1:F:132:LYS:HD2	1.97	0.64
1:A:467:GLY:HA3	1:A:476:ARG:HD3	1.78	0.64
1:E:474:VAL:HG23	1:E:474:VAL:O	1.97	0.64
1:B:467:GLY:HA3	1:B:476:ARG:HD3	1.80	0.63
1:E:487:THR:HG22	1:E:488:THR:N	2.11	0.63
1:H:271:LYS:NZ	1:H:305:SER:HB2	2.13	0.63
1:D:467:GLY:HA3	1:D:476:ARG:HD3	1.80	0.63
1:E:277:LEU:HD12	1:E:434:THR:OG1	1.98	0.63
1:A:277:LEU:HD12	1:A:434:THR:OG1	1.98	0.63
1:B:426:TYR:HB3	1:B:472:SER:OG	1.98	0.63
1:A:474:VAL:HG23	1:A:474:VAL:O	1.97	0.63
1:F:139:ASP:C	1:F:140:LEU:HG	2.19	0.63
1:A:142:LEU:HD13	1:A:144:LEU:HG	1.80	0.63
1:C:365:ASP:HB3	1:C:387:ALA:HB3	1.80	0.63
1:B:487:THR:HG22	1:B:488:THR:N	2.12	0.63
1:G:365:ASP:HB3	1:G:387:ALA:HB3	1.80	0.63
1:F:474:VAL:HG23	1:F:474:VAL:O	1.97	0.63
1:B:277:LEU:HD12	1:B:434:THR:OG1	1.98	0.63
1:B:39:THR:O	1:B:41:ASP:N	2.31	0.62
1:F:277:LEU:HD12	1:F:434:THR:OG1	1.98	0.62
1:H:467:GLY:HA3	1:H:476:ARG:HD3	1.81	0.62
1:H:396:LEU:HD23	1:H:407:VAL:CB	2.21	0.62
1:C:467:GLY:HA3	1:C:476:ARG:HD3	1.81	0.62
1:E:394:ILE:CG2	1:E:394:ILE:O	2.47	0.62
1:F:467:GLY:HA3	1:F:476:ARG:HD3	1.80	0.62
1:E:139:ASP:O	1:E:140:LEU:CG	2.47	0.62
1:A:397:LEU:HD11	1:A:407:VAL:HG11	1.78	0.62
1:B:396:LEU:HD13	1:B:396:LEU:O	1.99	0.62
1:A:139:ASP:OD1	1:A:139:ASP:O	2.17	0.62
1:A:142:LEU:CB	1:A:143:PRO:HA	2.11	0.62
1:A:241:VAL:HG22	1:A:241:VAL:O	1.98	0.62
1:A:459:MET:HE3	1:B:144:LEU:HD21	1.82	0.62
1:D:65:LEU:CD1	1:D:160:GLY:HA2	2.30	0.62
1:G:467:GLY:HA3	1:G:476:ARG:HD3	1.80	0.62
1:H:389:ARG:HG2	1:H:389:ARG:HH11	1.65	0.62
1:A:139:ASP:O	1:A:140:LEU:HD13	2.00	0.61
1:A:114:MET:CE	1:A:295:PHE:CE1	2.82	0.61
1:B:247:THR:HA	1:B:268:LEU:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ARG:HH11	1:D:389:ARG:HG2	1.65	0.61
1:A:393:ASP:C	1:A:394:ILE:O	2.28	0.61
1:C:474:VAL:HG13	1:C:474:VAL:O	1.99	0.61
1:E:394:ILE:O	1:E:395:ARG:CB	2.46	0.61
1:B:125:TYR:CD1	1:D:131:THR:CG2	2.84	0.61
1:C:65:LEU:CD1	1:C:160:GLY:HA2	2.30	0.61
1:B:125:TYR:CD1	1:D:131:THR:HG23	2.36	0.61
1:F:142:LEU:CB	1:F:143:PRO:HA	2.25	0.61
1:F:125:TYR:CD1	1:H:131:THR:CG2	2.84	0.60
1:A:79:GLU:O	1:A:83:LEU:CD1	2.38	0.60
1:D:137:THR:O	1:D:137:THR:HG22	2.01	0.60
1:E:180:ALA:HB3	1:E:181:PRO:CD	2.32	0.60
1:H:442:ARG:HA	1:H:445:ASP:HB2	1.83	0.60
1:A:114:MET:CE	1:A:295:PHE:HE1	2.14	0.60
1:A:368:CYS:O	1:A:384:THR:HA	2.02	0.60
1:A:397:LEU:HD12	1:A:407:VAL:CG1	2.22	0.60
1:D:142:LEU:HD13	1:D:144:LEU:HG	1.83	0.60
1:H:192:LYS:HE3	1:H:225:GLY:HA2	1.84	0.60
1:H:271:LYS:HZ2	1:H:305:SER:HB2	1.66	0.60
1:A:180:ALA:HB3	1:A:181:PRO:CD	2.32	0.60
1:A:242:ALA:HA	1:A:265:SER:HB3	1.84	0.60
1:C:180:ALA:HB3	1:C:181:PRO:CD	2.32	0.60
1:D:180:ALA:HB3	1:D:181:PRO:CD	2.32	0.60
1:E:156:ARG:CG	1:E:487:THR:CG2	2.50	0.60
1:B:180:ALA:HB3	1:B:181:PRO:CD	2.32	0.60
1:H:65:LEU:CD1	1:H:160:GLY:HA2	2.32	0.60
1:B:297:HIS:CD2	1:B:297:HIS:N	2.69	0.60
1:D:426:TYR:HB3	1:D:472:SER:OG	2.01	0.59
1:H:146:PRO:O	1:H:147:GLU:CB	2.50	0.59
1:H:137:THR:HG22	1:H:137:THR:O	2.01	0.59
1:C:242:ALA:HA	1:C:265:SER:HB3	1.84	0.59
1:F:180:ALA:HB3	1:F:181:PRO:CD	2.32	0.59
1:E:242:ALA:HA	1:E:265:SER:HB3	1.84	0.59
1:F:125:TYR:CD1	1:H:131:THR:HG23	2.36	0.59
1:D:146:PRO:O	1:D:147:GLU:CB	2.50	0.59
1:G:242:ALA:HA	1:G:265:SER:HB3	1.84	0.59
1:A:241:VAL:HG21	1:A:253:ILE:CG2	2.33	0.59
1:F:151:ARG:HG2	1:F:496:TYR:HE2	1.68	0.59
1:G:156:ARG:CG	1:G:487:THR:CG2	2.50	0.59
1:E:142:LEU:N	1:E:143:PRO:HA	2.16	0.59
1:G:180:ALA:HB3	1:G:181:PRO:CD	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:ALA:HB3	1:H:181:PRO:CD	2.32	0.59
1:F:297:HIS:CD2	1:F:297:HIS:N	2.69	0.59
1:F:80:ARG:O	1:F:84:ARG:HG3	2.03	0.59
1:H:142:LEU:CD1	1:H:144:LEU:HG	2.31	0.59
1:D:139:ASP:C	1:D:139:ASP:OD1	2.41	0.59
1:A:139:ASP:CB	1:D:75:PRO:HG2	2.27	0.58
1:B:151:ARG:HG2	1:B:496:TYR:HE2	1.68	0.58
1:F:242:ALA:HA	1:F:265:SER:HB3	1.84	0.58
1:G:454:VAL:HB	1:H:494:ILE:HG23	1.84	0.58
1:B:242:ALA:HA	1:B:265:SER:HB3	1.84	0.58
1:B:80:ARG:O	1:B:84:ARG:HG3	2.03	0.58
1:G:277:LEU:HD12	1:G:434:THR:OG1	2.03	0.58
1:C:454:VAL:HB	1:D:494:ILE:HG23	1.84	0.58
1:E:142:LEU:HB3	1:F:459:MET:SD	2.43	0.58
1:C:142:LEU:HD13	1:C:144:LEU:HG	1.86	0.58
1:C:144:LEU:HB3	1:C:145:PRO:HD2	1.86	0.58
1:C:277:LEU:HD12	1:C:434:THR:OG1	2.03	0.58
1:F:140:LEU:CD1	1:F:152:ALA:HB2	2.11	0.58
1:E:113:LEU:N	1:E:113:LEU:HD23	2.18	0.57
1:D:142:LEU:CB	1:D:143:PRO:CA	2.66	0.57
1:F:144:LEU:HB3	1:F:145:PRO:CD	2.34	0.57
1:A:140:LEU:HG	1:B:461:ASP:HB2	1.87	0.57
1:A:477:GLU:HG3	1:A:478:HIS:CE1	2.38	0.57
1:E:101:THR:HG21	1:E:334:LEU:HG	1.86	0.57
1:B:101:THR:HG21	1:B:334:LEU:HG	1.86	0.57
1:C:101:THR:HG21	1:C:334:LEU:HG	1.86	0.57
1:C:146:PRO:O	1:C:147:GLU:C	2.37	0.57
1:D:397:LEU:HD23	1:D:407:VAL:HG11	1.86	0.57
1:H:396:LEU:CG	1:H:407:VAL:HB	2.34	0.57
1:H:144:LEU:HB3	1:H:145:PRO:CD	2.35	0.57
1:E:365:ASP:HB3	1:E:387:ALA:HB3	1.86	0.57
1:F:64:THR:O	1:F:64:THR:CG2	2.51	0.57
1:H:247:THR:HG21	1:H:426:TYR:OH	2.05	0.56
1:B:151:ARG:HG2	1:B:496:TYR:CE2	2.41	0.56
1:C:296:ASN:ND2	1:C:299:GLN:O	2.34	0.56
1:F:281:ASP:HB3	1:F:284:GLU:HB2	1.87	0.56
1:A:142:LEU:CB	1:A:143:PRO:CA	2.77	0.56
1:A:365:ASP:HB3	1:A:387:ALA:HB3	1.86	0.56
1:E:247:THR:HG21	1:E:426:TYR:OH	2.06	0.56
1:C:146:PRO:O	1:C:147:GLU:CB	2.50	0.56
1:F:365:ASP:HB2	1:F:387:ALA:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:395:ARG:C	1:F:397:LEU:H	2.08	0.56
1:H:101:THR:HG21	1:H:334:LEU:HG	1.87	0.56
1:C:277:LEU:HD12	1:C:434:THR:CB	2.36	0.56
1:G:260:SER:HB3	1:G:262:LYS:HE3	1.88	0.56
1:D:296:ASN:ND2	1:D:299:GLN:O	2.39	0.56
1:D:427:GLY:O	1:D:449:ALA:HA	2.06	0.56
1:E:260:SER:HB3	1:E:262:LYS:HE3	1.88	0.56
1:A:241:VAL:CG2	1:A:241:VAL:O	2.53	0.56
1:A:75:PRO:HG2	1:D:139:ASP:CB	2.31	0.56
1:D:389:ARG:HG2	1:D:389:ARG:NH1	2.21	0.56
1:G:277:LEU:HD12	1:G:434:THR:CB	2.36	0.56
1:H:260:SER:HB3	1:H:262:LYS:HE3	1.88	0.56
1:B:18:LEU:HD22	1:B:205:ALA:HB1	1.88	0.56
1:B:64:THR:O	1:B:64:THR:CG2	2.51	0.56
1:C:260:SER:HB3	1:C:262:LYS:HE3	1.88	0.56
1:D:101:THR:HG21	1:D:334:LEU:HG	1.86	0.56
1:F:151:ARG:HG2	1:F:496:TYR:CE2	2.40	0.56
1:G:101:THR:HG21	1:G:334:LEU:HG	1.86	0.56
1:H:84:ARG:HG3	1:H:84:ARG:NH1	2.21	0.56
1:A:149:ARG:NH1	1:C:445:ASP:OD1	2.39	0.55
1:E:140:LEU:CD1	1:E:152:ALA:HB3	2.34	0.55
1:F:260:SER:HB3	1:F:262:LYS:HE3	1.88	0.55
1:C:18:LEU:HD22	1:C:205:ALA:HB1	1.88	0.55
1:D:260:SER:HB3	1:D:262:LYS:HE3	1.88	0.55
1:D:84:ARG:HG3	1:D:84:ARG:NH1	2.21	0.55
1:A:397:LEU:HD11	1:A:407:VAL:CG1	2.35	0.55
1:A:144:LEU:HB3	1:A:145:PRO:HD2	1.88	0.55
1:B:369:GLY:HA3	1:B:384:THR:HA	1.88	0.55
1:F:18:LEU:HD22	1:F:205:ALA:HB1	1.88	0.55
1:G:18:LEU:HD22	1:G:205:ALA:HB1	1.88	0.55
1:F:494:ILE:HG21	1:H:437:LEU:HD21	1.87	0.55
1:H:271:LYS:HE3	1:H:306:ARG:HG2	1.79	0.55
1:B:365:ASP:HB2	1:B:387:ALA:HB3	1.88	0.55
1:E:135:GLY:H	1:H:137:THR:HG22	1.71	0.55
1:E:144:LEU:CB	1:E:145:PRO:CD	2.73	0.55
1:H:140:LEU:HD11	1:H:152:ALA:CB	2.35	0.55
1:B:140:LEU:HD23	1:B:142:LEU:HD21	1.89	0.55
1:D:18:LEU:HD22	1:D:205:ALA:HB1	1.88	0.55
1:D:394:ILE:HD12	1:D:396:LEU:HB3	1.87	0.55
1:H:18:LEU:HD22	1:H:205:ALA:HB1	1.88	0.55
1:B:40:GLY:O	1:B:41:ASP:OD1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:PRO:O	1:C:148:VAL:HB	2.07	0.55
1:A:135:GLY:H	1:D:137:THR:HG22	1.71	0.54
1:E:65:LEU:CD2	1:E:160:GLY:HA2	2.35	0.54
1:A:260:SER:HB3	1:A:262:LYS:HE3	1.88	0.54
1:A:459:MET:CE	1:B:144:LEU:HD21	2.38	0.54
1:A:114:MET:HE3	1:A:295:PHE:CE1	2.42	0.54
1:B:260:SER:HB3	1:B:262:LYS:HE3	1.88	0.54
1:G:65:LEU:CD2	1:G:160:GLY:HA2	2.37	0.54
1:C:142:LEU:CB	1:C:143:PRO:CA	2.61	0.54
1:E:39:THR:OG1	1:E:41:ASP:OD1	2.25	0.54
1:H:389:ARG:HG2	1:H:389:ARG:NH1	2.21	0.54
1:B:281:ASP:OD2	1:B:284:GLU:HG3	2.08	0.53
1:E:394:ILE:O	1:E:394:ILE:HG22	2.08	0.53
1:F:17:MET:HG2	1:F:47:PRO:HG2	1.88	0.53
1:C:389:ARG:O	1:C:390:GLU:CB	2.56	0.53
1:C:413:ASP:OD1	1:C:416:GLU:HB3	2.09	0.53
1:F:139:ASP:OD1	1:F:139:ASP:C	2.46	0.53
1:G:396:LEU:O	1:G:396:LEU:HD13	2.09	0.53
1:D:131:THR:HG22	1:D:132:LYS:NZ	2.24	0.53
1:F:23:TRP:HZ2	1:F:206:GLU:HB3	1.74	0.53
1:B:348:HIS:HE1	1:B:402:PHE:HB3	1.74	0.53
1:B:125:TYR:CE1	1:D:131:THR:HG23	2.44	0.53
1:F:348:HIS:HE1	1:F:402:PHE:HB3	1.74	0.53
1:G:348:HIS:HE1	1:G:402:PHE:HB3	1.74	0.53
1:H:271:LYS:HG2	1:H:397:LEU:O	2.08	0.53
1:H:277:LEU:HD12	1:H:434:THR:OG1	2.09	0.53
1:C:146:PRO:O	1:C:148:VAL:HG23	2.08	0.52
1:C:494:ILE:HG23	1:D:454:VAL:HB	1.92	0.52
1:D:23:TRP:HZ2	1:D:206:GLU:HB3	1.74	0.52
1:G:23:TRP:HZ2	1:G:206:GLU:HB3	1.74	0.52
1:H:131:THR:HG22	1:H:132:LYS:NZ	2.24	0.52
1:B:394:ILE:HG13	1:B:396:LEU:H	1.74	0.52
1:A:156:ARG:CG	1:A:487:THR:CG2	2.50	0.52
1:A:316:ASP:O	1:A:320:ARG:HG3	2.10	0.52
1:D:20:GLY:O	1:F:376:ALA:HB2	2.10	0.52
1:G:283:GLN:OE1	1:G:320:ARG:HD3	2.09	0.52
1:H:483:ILE:CG2	1:H:483:ILE:O	2.57	0.52
1:C:316:ASP:O	1:C:320:ARG:HG3	2.10	0.52
1:E:23:TRP:HZ2	1:E:206:GLU:HB3	1.74	0.52
1:F:125:TYR:CE1	1:H:131:THR:HG23	2.44	0.52
1:H:316:ASP:O	1:H:320:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:TRP:HZ2	1:B:206:GLU:HB3	1.74	0.52
1:D:277:LEU:HD12	1:D:434:THR:OG1	2.09	0.52
1:F:316:ASP:O	1:F:320:ARG:HG3	2.10	0.52
1:F:394:ILE:HG22	1:F:394:ILE:O	2.10	0.52
1:G:297:HIS:N	1:G:297:HIS:CD2	2.78	0.52
1:G:494:ILE:HG23	1:H:454:VAL:HB	1.91	0.52
1:H:277:LEU:HD12	1:H:434:THR:CB	2.40	0.52
1:B:119:SER:HB3	1:B:176:VAL:HG21	1.92	0.52
1:C:297:HIS:N	1:C:297:HIS:CD2	2.78	0.52
1:H:23:TRP:HZ2	1:H:206:GLU:HB3	1.74	0.52
1:A:23:TRP:HZ2	1:A:206:GLU:HB3	1.74	0.52
1:B:316:ASP:O	1:B:320:ARG:HG3	2.10	0.52
1:D:144:LEU:HB3	1:D:145:PRO:CD	2.40	0.52
1:A:168:TRP:CE3	1:A:344:VAL:HG21	2.45	0.52
1:B:140:LEU:HG	1:B:142:LEU:HD21	1.90	0.52
1:D:297:HIS:CD2	1:D:297:HIS:N	2.78	0.52
1:E:296:ASN:O	1:E:299:GLN:HB2	2.10	0.52
1:E:316:ASP:O	1:E:320:ARG:HG3	2.10	0.52
1:F:348:HIS:CE1	1:F:402:PHE:HB3	2.45	0.52
1:H:348:HIS:CE1	1:H:402:PHE:HB3	2.45	0.52
1:B:348:HIS:CE1	1:B:402:PHE:HB3	2.45	0.52
1:C:51:VAL:HG12	1:C:51:VAL:O	2.10	0.52
1:D:348:HIS:HE1	1:D:402:PHE:HB3	1.74	0.52
1:C:168:TRP:CE3	1:C:344:VAL:HG21	2.45	0.52
1:C:23:TRP:HZ2	1:C:206:GLU:HB3	1.74	0.52
1:E:348:HIS:HE1	1:E:402:PHE:HB3	1.74	0.52
1:G:296:ASN:O	1:G:299:GLN:HB2	2.10	0.52
1:H:348:HIS:HE1	1:H:402:PHE:HB3	1.74	0.52
1:B:51:VAL:HG12	1:B:51:VAL:O	2.10	0.51
1:F:168:TRP:CE3	1:F:344:VAL:HG21	2.45	0.51
1:G:316:ASP:O	1:G:320:ARG:HG3	2.10	0.51
1:A:348:HIS:HE1	1:A:402:PHE:HB3	1.74	0.51
1:C:39:THR:O	1:C:41:ASP:N	2.44	0.51
1:D:348:HIS:CE1	1:D:402:PHE:HB3	2.45	0.51
1:B:168:TRP:CE3	1:B:344:VAL:HG21	2.45	0.51
1:G:168:TRP:CE3	1:G:344:VAL:HG21	2.45	0.51
1:H:227:THR:OG1	1:H:228:ALA:N	2.43	0.51
1:A:297:HIS:N	1:A:297:HIS:CD2	2.78	0.51
1:E:168:TRP:CE3	1:E:344:VAL:HG21	2.45	0.51
1:F:46:VAL:CG1	1:F:47:PRO:HD2	2.41	0.51
1:A:348:HIS:CE1	1:A:402:PHE:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:VAL:CG1	1:B:47:PRO:HD2	2.41	0.51
1:C:348:HIS:CE1	1:C:402:PHE:HB3	2.45	0.51
1:C:296:ASN:O	1:C:299:GLN:HB2	2.10	0.51
1:C:394:ILE:O	1:C:394:ILE:CG1	2.58	0.51
1:D:316:ASP:O	1:D:320:ARG:HG3	2.10	0.51
1:E:426:TYR:CE1	1:E:471:ASP:HB3	2.46	0.51
1:D:168:TRP:CE3	1:D:344:VAL:HG21	2.45	0.51
1:G:348:HIS:CE1	1:G:402:PHE:HB3	2.45	0.51
1:G:46:VAL:CG1	1:G:47:PRO:HD2	2.40	0.51
1:C:348:HIS:HE1	1:C:402:PHE:HB3	1.74	0.51
1:D:296:ASN:O	1:D:299:GLN:HB2	2.10	0.51
1:E:321:LEU:HG	1:E:385:ILE:HD13	1.93	0.51
1:H:168:TRP:CE3	1:H:344:VAL:HG21	2.45	0.51
1:C:46:VAL:CG1	1:C:47:PRO:HD2	2.41	0.51
1:D:277:LEU:HD12	1:D:434:THR:CB	2.40	0.51
1:F:293:ILE:O	1:F:293:ILE:CG1	2.56	0.51
1:E:140:LEU:HD12	1:E:152:ALA:CB	2.37	0.51
1:F:119:SER:HB3	1:F:176:VAL:HG21	1.92	0.51
1:H:297:HIS:N	1:H:297:HIS:CD2	2.78	0.51
1:A:146:PRO:C	1:A:148:VAL:H	2.14	0.50
1:A:51:VAL:O	1:A:51:VAL:HG12	2.10	0.50
1:C:435:ASN:OD1	1:C:435:ASN:O	2.29	0.50
1:C:254:GLY:HA3	1:D:258:GLY:O	2.11	0.50
1:D:51:VAL:HG12	1:D:51:VAL:O	2.10	0.50
1:E:434:THR:HG21	1:E:440:ALA:HB2	1.93	0.50
1:F:321:LEU:HG	1:F:385:ILE:HD13	1.93	0.50
1:E:149:ARG:NH1	1:G:445:ASP:OD1	2.44	0.50
1:H:435:ASN:OD1	1:H:435:ASN:O	2.30	0.50
1:H:51:VAL:O	1:H:51:VAL:HG12	2.10	0.50
1:B:474:VAL:O	1:B:474:VAL:CG2	2.60	0.50
1:D:67:SER:OG	1:D:69:THR:HG22	2.12	0.50
1:E:139:ASP:OD1	1:E:139:ASP:C	2.48	0.50
1:C:397:LEU:HD23	1:C:407:VAL:HG11	1.92	0.50
1:E:348:HIS:CE1	1:E:402:PHE:HB3	2.45	0.50
1:A:321:LEU:HG	1:A:385:ILE:HD13	1.93	0.50
1:A:434:THR:HG21	1:A:440:ALA:HB2	1.94	0.50
1:B:293:ILE:CG1	1:B:293:ILE:O	2.56	0.50
1:C:293:ILE:O	1:C:293:ILE:CG1	2.56	0.50
1:D:435:ASN:O	1:D:435:ASN:OD1	2.30	0.50
1:F:434:THR:HG21	1:F:440:ALA:HB2	1.93	0.50
1:D:446:GLU:OE1	1:D:446:GLU:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ASP:O	1:F:140:LEU:HD23	2.10	0.50
1:B:79:GLU:O	1:B:83:LEU:HG	2.12	0.50
1:C:274:VAL:HG22	1:C:307:LEU:CD1	2.42	0.50
1:E:297:HIS:N	1:E:297:HIS:CD2	2.78	0.50
1:F:144:LEU:HD12	1:F:148:VAL:HG12	1.93	0.50
1:F:474:VAL:CG2	1:F:474:VAL:O	2.60	0.50
1:G:435:ASN:OD1	1:G:435:ASN:O	2.29	0.50
1:G:446:GLU:OE1	1:G:446:GLU:HA	2.12	0.50
1:A:274:VAL:HG22	1:A:307:LEU:CD1	2.42	0.50
1:A:393:ASP:O	1:A:393:ASP:CG	2.50	0.50
1:A:446:GLU:HA	1:A:446:GLU:OE1	2.12	0.50
1:B:107:LEU:HD21	1:B:338:VAL:HG12	1.94	0.50
1:B:283:GLN:OE1	1:B:320:ARG:NH1	2.36	0.50
1:B:274:VAL:HG22	1:B:307:LEU:CD1	2.42	0.50
1:B:321:LEU:HG	1:B:385:ILE:HD13	1.93	0.50
1:E:396:LEU:HD21	1:E:401:VAL:HG21	1.94	0.50
1:G:274:VAL:HG22	1:G:307:LEU:CD1	2.42	0.50
1:G:51:VAL:HG12	1:G:51:VAL:O	2.10	0.50
1:A:45:GLU:O	1:A:46:VAL:CG2	2.60	0.50
1:E:274:VAL:HG22	1:E:307:LEU:CD1	2.42	0.50
1:F:107:LEU:HD21	1:F:338:VAL:HG12	1.94	0.50
1:F:51:VAL:O	1:F:51:VAL:HG12	2.10	0.50
1:H:446:GLU:OE1	1:H:446:GLU:HA	2.12	0.50
1:A:393:ASP:O	1:A:393:ASP:OD1	2.29	0.49
1:B:446:GLU:OE1	1:B:446:GLU:HA	2.12	0.49
1:C:446:GLU:HA	1:C:446:GLU:OE1	2.12	0.49
1:D:425:VAL:HG12	1:D:426:TYR:CZ	2.47	0.49
1:F:274:VAL:HG22	1:F:307:LEU:CD1	2.42	0.49
1:A:22:GLN:O	1:A:24:VAL:HG23	2.12	0.49
1:B:140:LEU:CG	1:B:142:LEU:HD21	2.41	0.49
1:C:107:LEU:HD21	1:C:338:VAL:HG12	1.94	0.49
1:F:144:LEU:HD13	1:F:148:VAL:HG11	1.93	0.49
1:H:274:VAL:HG22	1:H:307:LEU:CD1	2.42	0.49
1:B:434:THR:HG21	1:B:440:ALA:HB2	1.94	0.49
1:D:23:TRP:CZ2	1:D:206:GLU:HB3	2.48	0.49
1:D:80:ARG:HH11	1:D:80:ARG:CG	2.24	0.49
1:G:321:LEU:HG	1:G:385:ILE:HD13	1.93	0.49
1:G:254:GLY:HA3	1:H:258:GLY:O	2.11	0.49
1:B:23:TRP:CZ2	1:B:206:GLU:HB3	2.48	0.49
1:C:321:LEU:HG	1:C:385:ILE:HD13	1.93	0.49
1:D:425:VAL:HG12	1:D:426:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:GLU:OE1	1:E:446:GLU:HA	2.12	0.49
1:F:446:GLU:OE1	1:F:446:GLU:HA	2.12	0.49
1:F:79:GLU:O	1:F:83:LEU:HG	2.12	0.49
1:G:107:LEU:HD21	1:G:338:VAL:HG12	1.94	0.49
1:D:274:VAL:HG22	1:D:307:LEU:CD1	2.42	0.49
1:C:493:VAL:CG2	1:D:464:LEU:HD11	2.43	0.49
1:E:293:ILE:CG1	1:E:293:ILE:O	2.56	0.49
1:E:51:VAL:HG12	1:E:51:VAL:O	2.10	0.49
1:G:16:GLN:OE1	1:G:23:TRP:HB3	2.13	0.49
1:A:107:LEU:HD21	1:A:338:VAL:HG12	1.94	0.49
1:E:142:LEU:H	1:E:143:PRO:HA	1.76	0.49
1:G:474:VAL:CG2	1:G:474:VAL:O	2.60	0.49
1:G:493:VAL:CG2	1:H:464:LEU:HD11	2.43	0.49
1:F:139:ASP:CB	1:G:75:PRO:HG2	2.38	0.49
1:A:474:VAL:CG2	1:A:474:VAL:O	2.60	0.49
1:B:144:LEU:HB3	1:B:145:PRO:HD2	1.94	0.49
1:C:23:TRP:CZ2	1:C:206:GLU:HB3	2.48	0.49
1:E:112:LYS:C	1:E:113:LEU:HD23	2.32	0.49
1:E:107:LEU:HD21	1:E:338:VAL:HG12	1.94	0.49
1:A:23:TRP:CZ2	1:A:206:GLU:HB3	2.48	0.49
1:B:140:LEU:CD2	1:B:142:LEU:HD21	2.43	0.49
1:F:23:TRP:CZ2	1:F:206:GLU:HB3	2.48	0.49
1:G:23:TRP:CZ2	1:G:206:GLU:HB3	2.48	0.49
1:D:474:VAL:CG2	1:D:474:VAL:O	2.59	0.48
1:E:397:LEU:HD11	1:E:407:VAL:HG21	1.94	0.48
1:E:487:THR:CG2	1:E:488:THR:N	2.76	0.48
1:E:122:TRP:HZ3	1:E:478:HIS:CG	2.31	0.48
1:E:45:GLU:O	1:E:46:VAL:CG2	2.60	0.48
1:H:23:TRP:CZ2	1:H:206:GLU:HB3	2.48	0.48
1:C:144:LEU:HD13	1:C:148:VAL:HG11	1.91	0.48
1:C:36:ASN:OD1	1:C:36:ASN:C	2.51	0.48
1:C:437:LEU:HD11	1:C:441:LEU:HD11	1.96	0.48
1:D:107:LEU:HD21	1:D:338:VAL:HG12	1.94	0.48
1:E:22:GLN:O	1:E:24:VAL:HG23	2.12	0.48
1:F:394:ILE:O	1:F:394:ILE:CG2	2.59	0.48
1:E:23:TRP:CZ2	1:E:206:GLU:HB3	2.48	0.48
1:E:474:VAL:O	1:E:474:VAL:CG2	2.60	0.48
1:G:36:ASN:C	1:G:36:ASN:OD1	2.51	0.48
1:H:107:LEU:HD21	1:H:338:VAL:HG12	1.94	0.48
1:A:114:MET:HE1	1:A:295:PHE:CE1	2.49	0.48
1:B:35:TYR:N	1:B:35:TYR:CD2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:THR:HG1	1:F:45:GLU:H	1.62	0.48
1:H:271:LYS:CE	1:H:397:LEU:O	2.59	0.48
1:H:271:LYS:O	1:H:271:LYS:HG3	2.12	0.48
1:A:296:ASN:O	1:A:299:GLN:HB2	2.14	0.48
1:C:144:LEU:HB3	1:C:145:PRO:CD	2.43	0.48
1:H:396:LEU:HD11	1:H:405:VAL:HG12	1.96	0.48
1:A:293:ILE:CG1	1:A:293:ILE:O	2.56	0.48
1:C:16:GLN:OE1	1:C:23:TRP:HB3	2.13	0.48
1:G:293:ILE:O	1:G:293:ILE:CG1	2.56	0.48
1:H:65:LEU:HD11	1:H:160:GLY:CA	2.41	0.48
1:D:293:ILE:O	1:D:293:ILE:CG1	2.56	0.48
1:D:296:ASN:HD22	1:D:300:VAL:HG22	1.79	0.48
1:B:125:TYR:CD2	1:B:125:TYR:C	2.87	0.47
1:C:269:GLY:O	1:C:472:SER:OG	2.25	0.47
1:F:125:TYR:C	1:F:125:TYR:CD2	2.87	0.47
1:H:474:VAL:O	1:H:474:VAL:CG2	2.59	0.47
1:A:125:TYR:C	1:A:125:TYR:CD2	2.87	0.47
1:F:396:LEU:HD13	1:F:407:VAL:HB	1.96	0.47
1:G:125:TYR:CD2	1:G:125:TYR:C	2.88	0.47
1:G:144:LEU:HB2	1:G:148:VAL:HG23	1.95	0.47
1:H:125:TYR:CD2	1:H:125:TYR:C	2.88	0.47
1:F:426:TYR:HB3	1:F:472:SER:OG	2.13	0.47
1:H:80:ARG:HH11	1:H:80:ARG:CG	2.25	0.47
1:H:89:LEU:HD12	1:H:89:LEU:HA	1.58	0.47
1:A:140:LEU:HG	1:B:461:ASP:CB	2.44	0.47
1:E:122:TRP:CZ3	1:E:478:HIS:CG	3.02	0.47
1:F:395:ARG:C	1:F:397:LEU:N	2.63	0.47
1:H:296:ASN:O	1:H:299:GLN:HB2	2.13	0.47
1:A:487:THR:CG2	1:A:488:THR:N	2.76	0.47
1:C:125:TYR:CD2	1:C:125:TYR:C	2.88	0.47
1:C:322:ALA:O	1:C:326:GLU:HB2	2.15	0.47
1:E:142:LEU:CB	1:E:143:PRO:HA	2.39	0.47
1:F:35:TYR:CD2	1:F:35:TYR:N	2.81	0.47
1:G:487:THR:CG2	1:G:488:THR:N	2.76	0.47
1:A:322:ALA:O	1:A:326:GLU:HB2	2.15	0.47
1:B:487:THR:CG2	1:B:488:THR:N	2.76	0.47
1:E:125:TYR:CD2	1:E:125:TYR:C	2.87	0.47
1:E:83:LEU:CD1	1:E:127:ALA:HB1	2.44	0.47
1:G:39:THR:O	1:G:41:ASP:N	2.47	0.47
1:H:322:ALA:O	1:H:326:GLU:HB2	2.15	0.47
1:A:83:LEU:CD1	1:A:127:ALA:HB1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:GLY:O	1:H:254:GLY:HA3	2.14	0.47
1:B:322:ALA:O	1:B:326:GLU:HB2	2.15	0.47
1:G:109:ILE:HG13	1:G:110:TYR:H	1.80	0.47
1:G:392:LYS:O	1:G:394:ILE:N	2.48	0.47
1:H:271:LYS:HE2	1:H:397:LEU:HA	1.97	0.47
1:B:166:ILE:O	1:B:166:ILE:HG13	2.15	0.47
1:D:185:CYS:HB2	1:D:187:ASN:ND2	2.30	0.47
1:E:185:CYS:HB2	1:E:187:ASN:ND2	2.30	0.47
1:B:185:CYS:HB2	1:B:187:ASN:ND2	2.30	0.47
1:B:371:THR:O	1:B:371:THR:CG2	2.43	0.47
1:F:166:ILE:O	1:F:166:ILE:HG13	2.15	0.47
1:A:372:GLU:O	1:A:374:PRO:HD3	2.15	0.46
1:A:17:MET:HE1	1:A:47:PRO:HB2	1.97	0.46
1:C:276:VAL:HB	1:C:309:VAL:HG13	1.97	0.46
1:C:46:VAL:CG1	1:C:47:PRO:CD	2.94	0.46
1:D:125:TYR:C	1:D:125:TYR:CD2	2.87	0.46
1:G:166:ILE:O	1:G:166:ILE:HG13	2.15	0.46
1:H:293:ILE:CG1	1:H:293:ILE:O	2.56	0.46
1:C:258:GLY:O	1:D:254:GLY:HA3	2.14	0.46
1:D:274:VAL:HG22	1:D:307:LEU:HD12	1.98	0.46
1:A:122:TRP:CZ3	1:A:478:HIS:CG	3.02	0.46
1:D:483:ILE:O	1:D:483:ILE:CG2	2.57	0.46
1:E:276:VAL:HB	1:E:309:VAL:HG13	1.97	0.46
1:F:44:THR:OG1	1:F:45:GLU:N	2.47	0.46
1:D:373:ALA:HA	1:D:374:PRO:HD3	1.80	0.46
1:E:166:ILE:HG13	1:E:166:ILE:O	2.15	0.46
1:E:44:THR:OG1	1:E:45:GLU:N	2.48	0.46
1:F:322:ALA:O	1:F:326:GLU:HB2	2.15	0.46
1:G:46:VAL:HG12	1:G:47:PRO:HD2	1.97	0.46
1:A:276:VAL:HB	1:A:309:VAL:HG13	1.97	0.46
1:A:75:PRO:CB	1:D:139:ASP:OD2	2.64	0.46
1:B:170:PHE:N	1:B:171:PRO:HD3	2.31	0.46
1:D:322:ALA:O	1:D:326:GLU:HB2	2.15	0.46
1:E:281:ASP:HA	1:E:282:PRO:HD2	1.78	0.46
1:E:322:ALA:O	1:E:326:GLU:HB2	2.15	0.46
1:G:362:ASP:HB3	1:G:394:ILE:HG22	1.97	0.46
1:A:148:VAL:HG12	1:A:149:ARG:N	2.30	0.46
1:A:170:PHE:N	1:A:171:PRO:HD3	2.31	0.46
1:A:392:LYS:O	1:A:394:ILE:HD13	2.15	0.46
1:B:274:VAL:HG22	1:B:307:LEU:HD12	1.98	0.46
1:E:17:MET:HE1	1:E:47:PRO:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:PHE:N	1:F:171:PRO:HD3	2.31	0.46
1:H:185:CYS:HB2	1:H:187:ASN:ND2	2.30	0.46
1:B:46:VAL:HG12	1:B:47:PRO:HD2	1.98	0.46
1:C:109:ILE:HG13	1:C:110:TYR:H	1.80	0.46
1:F:185:CYS:HB2	1:F:187:ASN:ND2	2.30	0.46
1:G:416:GLU:O	1:G:420:GLU:HG2	2.16	0.46
1:A:114:MET:HE1	1:A:295:PHE:CZ	2.51	0.46
1:B:170:PHE:HB2	1:B:174:MET:HG2	1.98	0.46
1:G:322:ALA:O	1:G:326:GLU:HB2	2.15	0.46
1:H:274:VAL:HG22	1:H:307:LEU:HD12	1.98	0.46
1:A:45:GLU:C	1:A:46:VAL:HG23	2.37	0.46
1:C:170:PHE:N	1:C:171:PRO:HD3	2.31	0.46
1:D:166:ILE:HG13	1:D:166:ILE:O	2.15	0.46
1:E:142:LEU:HD12	1:E:144:LEU:HG	1.97	0.46
1:E:170:PHE:N	1:E:171:PRO:HD3	2.31	0.46
1:G:276:VAL:HB	1:G:309:VAL:HG13	1.97	0.46
1:H:276:VAL:HB	1:H:309:VAL:HG13	1.98	0.46
1:H:443:ILE:HD13	1:H:443:ILE:HA	1.64	0.46
1:F:276:VAL:HB	1:F:309:VAL:HG13	1.97	0.46
1:F:46:VAL:CG1	1:F:47:PRO:CD	2.94	0.46
1:G:185:CYS:HB2	1:G:187:ASN:ND2	2.30	0.46
1:H:166:ILE:O	1:H:166:ILE:HG13	2.15	0.46
1:A:241:VAL:HG13	1:A:257:CYS:SG	2.47	0.45
1:B:276:VAL:HB	1:B:309:VAL:HG13	1.98	0.45
1:C:166:ILE:O	1:C:166:ILE:HG13	2.15	0.45
1:D:276:VAL:HB	1:D:309:VAL:HG13	1.98	0.45
1:E:139:ASP:C	1:E:140:LEU:HG	2.37	0.45
1:G:46:VAL:CG1	1:G:47:PRO:CD	2.93	0.45
1:A:129:TRP:HA	1:A:129:TRP:CE3	2.52	0.45
1:A:170:PHE:HB2	1:A:174:MET:HG2	1.98	0.45
1:C:487:THR:CG2	1:C:488:THR:N	2.76	0.45
1:H:170:PHE:HB2	1:H:174:MET:HG2	1.98	0.45
1:A:142:LEU:CD1	1:A:144:LEU:HG	2.47	0.45
1:B:46:VAL:CG1	1:B:47:PRO:CD	2.94	0.45
1:C:416:GLU:O	1:C:420:GLU:HG2	2.16	0.45
1:A:146:PRO:C	1:A:148:VAL:N	2.69	0.45
1:A:241:VAL:HG21	1:A:253:ILE:HG21	1.99	0.45
1:A:274:VAL:HG22	1:A:307:LEU:HD12	1.98	0.45
1:B:34:VAL:CG1	1:B:103:ASN:HD21	2.30	0.45
1:E:45:GLU:C	1:E:46:VAL:HG23	2.37	0.45
1:F:34:VAL:CG1	1:F:103:ASN:HD21	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:HA	1:A:282:PRO:HD2	1.78	0.45
1:A:296:ASN:ND2	1:A:299:GLN:O	2.48	0.45
1:D:34:VAL:CG1	1:D:103:ASN:HD21	2.30	0.45
1:A:75:PRO:CG	1:D:139:ASP:HB2	2.37	0.45
1:G:274:VAL:HG22	1:G:307:LEU:HD12	1.98	0.45
1:H:170:PHE:N	1:H:171:PRO:HD3	2.31	0.45
1:H:425:VAL:CG1	1:H:471:ASP:OD2	2.65	0.45
1:A:166:ILE:HG13	1:A:166:ILE:O	2.15	0.45
1:A:454:VAL:HB	1:B:494:ILE:HG23	1.99	0.45
1:B:44:THR:OG1	1:B:45:GLU:N	2.48	0.45
1:C:144:LEU:C	1:C:145:PRO:O	2.54	0.45
1:E:454:VAL:HB	1:F:494:ILE:HG23	1.99	0.45
1:A:427:GLY:O	1:A:449:ALA:HA	2.17	0.45
1:C:413:ASP:OD1	1:C:416:GLU:CB	2.64	0.45
1:C:46:VAL:HG12	1:C:47:PRO:HD2	1.97	0.45
1:D:170:PHE:N	1:D:171:PRO:HD3	2.31	0.45
1:F:274:VAL:HG22	1:F:307:LEU:HD12	1.98	0.45
1:G:44:THR:OG1	1:G:45:GLU:N	2.48	0.45
1:H:34:VAL:CG1	1:H:103:ASN:HD21	2.30	0.45
1:B:180:ALA:HB3	1:B:181:PRO:HD3	1.99	0.45
1:D:394:ILE:O	1:D:395:ARG:CB	2.65	0.45
1:E:437:LEU:HD21	1:G:494:ILE:HG21	1.98	0.45
1:A:122:TRP:CH2	1:A:478:HIS:CE1	3.05	0.45
1:C:274:VAL:HG22	1:C:307:LEU:HD12	1.98	0.45
1:D:189:VAL:HG22	1:D:218:LEU:HD23	1.99	0.45
1:F:373:ALA:HA	1:F:374:PRO:HD3	1.80	0.45
1:B:180:ALA:CB	1:B:181:PRO:CD	2.95	0.45
1:C:281:ASP:HA	1:C:282:PRO:HD2	1.78	0.45
1:G:360:ILE:HD13	1:G:360:ILE:HG21	1.66	0.45
1:H:44:THR:OG1	1:H:45:GLU:N	2.47	0.45
1:H:80:ARG:NH1	1:H:80:ARG:CG	2.80	0.45
1:D:89:LEU:HA	1:D:89:LEU:HD12	1.57	0.44
1:E:122:TRP:CH2	1:E:478:HIS:CE1	3.05	0.44
1:G:277:LEU:HD12	1:G:434:THR:HB	1.99	0.44
1:H:180:ALA:CB	1:H:181:PRO:CD	2.95	0.44
1:A:180:ALA:HB3	1:A:181:PRO:HD3	1.99	0.44
1:E:362:ASP:OD2	1:E:394:ILE:O	2.34	0.44
1:G:108:LEU:HD22	1:G:334:LEU:CD2	2.48	0.44
1:G:143:PRO:HD2	1:G:143:PRO:O	2.17	0.44
1:C:170:PHE:HB2	1:C:174:MET:HG2	1.98	0.44
1:E:108:LEU:HD22	1:E:334:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LEU:HB2	1:E:143:PRO:C	2.38	0.44
1:E:274:VAL:HG22	1:E:307:LEU:HD12	1.97	0.44
1:F:170:PHE:HB2	1:F:174:MET:HG2	1.98	0.44
1:F:180:ALA:CB	1:F:181:PRO:CD	2.95	0.44
1:F:46:VAL:HG12	1:F:47:PRO:HD2	1.98	0.44
1:G:64:THR:HA	1:G:67:SER:HB2	2.00	0.44
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.88	0.44
1:B:247:THR:HB	1:B:269:GLY:H	1.83	0.44
1:B:281:ASP:HB3	1:B:284:GLU:HB2	2.00	0.44
1:C:108:LEU:HD22	1:C:334:LEU:CD2	2.48	0.44
1:D:180:ALA:HB3	1:D:181:PRO:HD3	1.99	0.44
1:F:394:ILE:HG22	1:F:396:LEU:H	1.83	0.44
1:H:189:VAL:HG22	1:H:218:LEU:HD23	1.99	0.44
1:F:277:LEU:HD12	1:F:434:THR:CB	2.48	0.44
1:G:34:VAL:CG1	1:G:103:ASN:HD21	2.30	0.44
1:A:437:LEU:CD2	1:A:441:LEU:HD12	2.48	0.44
1:C:64:THR:HA	1:C:67:SER:HB2	1.99	0.44
1:B:139:ASP:O	1:B:140:LEU:HD12	2.09	0.44
1:B:108:LEU:HD22	1:B:334:LEU:CD2	2.47	0.44
1:G:64:THR:O	1:G:67:SER:CB	2.66	0.44
1:A:122:TRP:HZ3	1:A:478:HIS:CG	2.31	0.44
1:B:496:TYR:O	1:D:442:ARG:NH2	2.47	0.44
1:C:180:ALA:HB3	1:C:181:PRO:HD3	1.99	0.44
1:C:474:VAL:CG1	1:C:474:VAL:O	2.65	0.44
1:D:170:PHE:HB2	1:D:174:MET:HG2	1.98	0.44
1:D:108:LEU:HD22	1:D:334:LEU:CD2	2.47	0.44
1:E:129:TRP:HA	1:E:129:TRP:CE3	2.52	0.44
1:E:170:PHE:HB2	1:E:174:MET:HG2	1.98	0.44
1:G:144:LEU:C	1:G:145:PRO:O	2.54	0.44
1:D:82:LEU:HB3	1:D:127:ALA:HB2	2.00	0.44
1:D:180:ALA:HB3	1:D:181:PRO:HD2	2.00	0.44
1:D:401:VAL:O	1:D:402:PHE:CB	2.66	0.44
1:E:401:VAL:O	1:E:402:PHE:CB	2.66	0.44
1:H:17:MET:HG2	1:H:47:PRO:HG2	2.00	0.44
1:A:360:ILE:HD13	1:A:360:ILE:HG21	1.66	0.43
1:B:373:ALA:HA	1:B:374:PRO:HD3	1.80	0.43
1:C:34:VAL:CG1	1:C:103:ASN:HD21	2.30	0.43
1:C:146:PRO:C	1:C:148:VAL:N	2.67	0.43
1:C:44:THR:OG1	1:C:45:GLU:N	2.48	0.43
1:E:180:ALA:CB	1:E:181:PRO:CD	2.95	0.43
1:E:180:ALA:HB3	1:E:181:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:LEU:O	1:G:145:PRO:O	2.36	0.43
1:G:180:ALA:CB	1:G:181:PRO:CD	2.95	0.43
1:G:433:TRP:O	1:G:434:THR:HB	2.18	0.43
1:H:180:ALA:HB3	1:H:181:PRO:HD2	2.00	0.43
1:H:271:LYS:HE2	1:H:397:LEU:C	2.38	0.43
1:H:373:ALA:HA	1:H:374:PRO:HD3	1.81	0.43
1:A:324:ILE:HD13	1:A:324:ILE:HG21	1.60	0.43
1:D:17:MET:HG2	1:D:47:PRO:HG2	2.00	0.43
1:F:180:ALA:HB3	1:F:181:PRO:HD3	1.99	0.43
1:H:247:THR:CA	1:H:268:LEU:HB3	2.48	0.43
1:F:494:ILE:CG2	1:H:437:LEU:HD21	2.48	0.43
1:A:277:LEU:HD12	1:A:434:THR:CB	2.48	0.43
1:G:251:ARG:HG2	1:H:259:ARG:O	2.18	0.43
1:H:180:ALA:HB3	1:H:181:PRO:HD3	1.99	0.43
1:H:306:ARG:HD3	1:H:397:LEU:HD12	2.00	0.43
1:A:146:PRO:O	1:A:148:VAL:HG23	2.19	0.43
1:B:243:PHE:HE2	1:B:268:LEU:CD2	2.32	0.43
1:C:277:LEU:HD12	1:C:434:THR:HB	1.98	0.43
1:E:139:ASP:O	1:E:140:LEU:HG	2.17	0.43
1:E:394:ILE:HA	1:E:394:ILE:HD12	1.83	0.43
1:G:180:ALA:HB3	1:G:181:PRO:HD2	2.00	0.43
1:G:180:ALA:HB3	1:G:181:PRO:HD3	1.99	0.43
1:H:82:LEU:HB3	1:H:127:ALA:HB2	2.00	0.43
1:H:247:THR:HG21	1:H:426:TYR:CE1	2.54	0.43
1:B:108:LEU:HB2	1:B:334:LEU:HD23	2.00	0.43
1:D:108:LEU:HB2	1:D:334:LEU:HD23	2.00	0.43
1:A:145:PRO:O	1:A:148:VAL:HB	2.19	0.43
1:A:397:LEU:HD11	1:A:407:VAL:HG21	2.01	0.43
1:B:277:LEU:HD12	1:B:434:THR:CB	2.48	0.43
1:D:180:ALA:CB	1:D:181:PRO:CD	2.95	0.43
1:E:113:LEU:CD2	1:E:113:LEU:N	2.80	0.43
1:E:108:LEU:HB2	1:E:334:LEU:HD23	2.00	0.43
1:F:437:LEU:CD2	1:F:441:LEU:HD12	2.48	0.43
1:H:401:VAL:O	1:H:402:PHE:CB	2.66	0.43
1:B:180:ALA:HB3	1:B:181:PRO:HD2	2.00	0.43
1:B:247:THR:CA	1:B:268:LEU:HB3	2.49	0.43
1:E:277:LEU:HD12	1:E:434:THR:CB	2.48	0.43
1:F:142:LEU:CB	1:F:143:PRO:CA	2.88	0.43
1:F:477:GLU:HG3	1:F:478:HIS:CE1	2.54	0.43
1:H:324:ILE:HD13	1:H:324:ILE:HG21	1.60	0.43
1:H:108:LEU:HD22	1:H:334:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:MET:CE	1:A:295:PHE:CZ	3.02	0.43
1:A:397:LEU:CD1	1:A:407:VAL:HG21	2.49	0.43
1:B:360:ILE:HD13	1:B:360:ILE:HG21	1.66	0.43
1:B:401:VAL:O	1:B:402:PHE:CB	2.66	0.43
1:G:401:VAL:O	1:G:402:PHE:CB	2.66	0.43
1:E:437:LEU:HD21	1:G:494:ILE:CG2	2.49	0.43
1:D:371:THR:O	1:D:371:THR:HG23	2.19	0.43
1:E:180:ALA:HB3	1:E:181:PRO:HD3	1.99	0.43
1:E:269:GLY:O	1:E:472:SER:OG	2.25	0.43
1:G:269:GLY:O	1:G:472:SER:OG	2.25	0.43
1:G:74:PRO:HA	1:G:75:PRO:HD3	1.87	0.43
1:A:401:VAL:O	1:A:402:PHE:CB	2.66	0.42
1:E:426:TYR:CD1	1:E:471:ASP:HB3	2.54	0.42
1:F:74:PRO:HA	1:F:75:PRO:HD3	1.88	0.42
1:B:477:GLU:HG3	1:B:478:HIS:CE1	2.54	0.42
1:C:108:LEU:HB2	1:C:334:LEU:HD23	2.00	0.42
1:C:251:ARG:HG2	1:D:259:ARG:O	2.18	0.42
1:D:360:ILE:HG21	1:D:360:ILE:HD13	1.66	0.42
1:E:168:TRP:HE3	1:E:344:VAL:HG21	1.85	0.42
1:B:247:THR:HA	1:B:268:LEU:HD22	2.02	0.42
1:C:180:ALA:HB3	1:C:181:PRO:HD2	2.00	0.42
1:G:109:ILE:HG13	1:G:110:TYR:N	2.35	0.42
1:G:39:THR:O	1:G:39:THR:OG1	2.28	0.42
1:H:168:TRP:HE3	1:H:344:VAL:HG21	1.85	0.42
1:C:433:TRP:O	1:C:434:THR:HB	2.18	0.42
1:D:44:THR:OG1	1:D:45:GLU:N	2.48	0.42
1:E:185:CYS:HB2	1:E:187:ASN:HD22	1.85	0.42
1:F:168:TRP:HE3	1:F:344:VAL:HG21	1.85	0.42
1:B:393:ASP:C	1:B:394:ILE:O	2.56	0.42
1:E:17:MET:CE	1:E:47:PRO:HB2	2.50	0.42
1:E:74:PRO:HA	1:E:75:PRO:HD3	1.88	0.42
1:G:170:PHE:N	1:G:171:PRO:HD3	2.35	0.42
1:G:46:VAL:HG11	1:G:222:THR:HG21	2.02	0.42
1:H:371:THR:O	1:H:371:THR:HG23	2.19	0.42
1:B:168:TRP:HE3	1:B:344:VAL:HG21	1.85	0.42
1:C:180:ALA:CB	1:C:181:PRO:CD	2.95	0.42
1:D:131:THR:HG22	1:D:132:LYS:HZ2	1.84	0.42
1:D:74:PRO:HA	1:D:75:PRO:HD3	1.88	0.42
1:E:45:GLU:C	1:E:46:VAL:CG2	2.87	0.42
1:B:437:LEU:HD21	1:D:494:ILE:HG21	2.02	0.42
1:E:139:ASP:HB2	1:H:75:PRO:CG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ASN:O	1:E:55:ASN:OD1	2.37	0.42
1:F:180:ALA:HB3	1:F:181:PRO:HD2	2.00	0.42
1:G:108:LEU:HB2	1:G:334:LEU:HD23	2.00	0.42
1:A:17:MET:CE	1:A:47:PRO:HB2	2.50	0.42
1:A:241:VAL:CG2	1:A:264:VAL:HG23	2.43	0.42
1:A:55:ASN:O	1:A:55:ASN:OD1	2.38	0.42
1:F:79:GLU:OE2	1:F:131:THR:HG21	2.20	0.42
1:A:168:TRP:HE3	1:A:344:VAL:HG21	1.85	0.41
1:A:45:GLU:C	1:A:46:VAL:CG2	2.87	0.41
1:B:79:GLU:OE2	1:B:131:THR:HG21	2.20	0.41
1:C:428:LEU:HD12	1:C:468:GLY:HA3	2.02	0.41
1:C:437:LEU:CD1	1:C:441:LEU:HD11	2.50	0.41
1:D:80:ARG:CG	1:D:80:ARG:NH1	2.80	0.41
1:G:185:CYS:HB2	1:G:187:ASN:HD22	1.85	0.41
1:H:360:ILE:HD13	1:H:360:ILE:HG21	1.66	0.41
1:A:180:ALA:CB	1:A:181:PRO:CD	2.95	0.41
1:C:394:ILE:O	1:C:397:LEU:HD12	2.20	0.41
1:G:394:ILE:O	1:G:397:LEU:HD12	2.20	0.41
1:H:119:SER:HB3	1:H:176:VAL:HG21	2.02	0.41
1:A:119:SER:HB3	1:A:176:VAL:HG21	2.02	0.41
1:A:180:ALA:HB3	1:A:181:PRO:HD2	2.00	0.41
1:B:64:THR:HA	1:B:67:SER:HB2	2.02	0.41
1:C:324:ILE:HG21	1:C:324:ILE:HD13	1.60	0.41
1:D:394:ILE:HG13	1:D:395:ARG:N	2.34	0.41
1:E:390:GLU:O	1:E:391:LYS:C	2.59	0.41
1:E:83:LEU:HD12	1:E:127:ALA:HB1	2.02	0.41
1:G:247:THR:CA	1:G:268:LEU:HB3	2.48	0.41
1:C:119:SER:HB3	1:C:176:VAL:HG21	2.02	0.41
1:G:34:VAL:HG13	1:G:103:ASN:HD21	1.86	0.41
1:F:496:TYR:CE2	1:H:441:LEU:HD23	2.55	0.41
1:A:44:THR:OG1	1:A:45:GLU:N	2.48	0.41
1:G:119:SER:HB3	1:G:176:VAL:HG21	2.02	0.41
1:G:428:LEU:HD12	1:G:468:GLY:HA3	2.01	0.41
1:H:185:CYS:HB2	1:H:187:ASN:HD22	1.85	0.41
1:G:388:ASN:O	1:G:388:ASN:OD1	2.39	0.41
1:H:34:VAL:HG13	1:H:103:ASN:HD21	1.86	0.41
1:H:108:LEU:HB2	1:H:334:LEU:HD23	2.01	0.41
1:H:397:LEU:HD13	1:H:407:VAL:HG11	2.03	0.41
1:H:64:THR:C	1:H:67:SER:HB2	2.40	0.41
1:C:109:ILE:HG13	1:C:110:TYR:N	2.35	0.41
1:D:168:TRP:HE3	1:D:344:VAL:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:LEU:C	1:F:19:ILE:HG13	2.41	0.41
1:F:401:VAL:O	1:F:402:PHE:CB	2.66	0.41
1:F:397:LEU:HD13	1:F:407:VAL:HG11	2.02	0.41
1:F:75:PRO:HG2	1:G:139:ASP:HB3	2.03	0.41
1:H:36:ASN:O	1:H:40:GLY:N	2.52	0.41
1:B:46:VAL:HG11	1:B:222:THR:HG21	2.02	0.41
1:C:145:PRO:HB2	1:C:148:VAL:HG21	2.03	0.41
1:C:46:VAL:HG11	1:C:222:THR:HG21	2.02	0.41
1:B:496:TYR:CE2	1:D:441:LEU:HD23	2.55	0.41
1:E:427:GLY:O	1:E:449:ALA:HA	2.21	0.41
1:G:166:ILE:CG1	1:G:193:PRO:HA	2.44	0.41
1:G:324:ILE:HG21	1:G:324:ILE:HD13	1.60	0.41
1:A:83:LEU:HD12	1:A:127:ALA:CB	2.50	0.41
1:C:129:TRP:CG	1:C:483:ILE:HD11	2.55	0.41
1:D:18:LEU:C	1:D:19:ILE:HG13	2.41	0.41
1:D:277:LEU:HD12	1:D:434:THR:HB	2.02	0.41
1:D:65:LEU:HD11	1:D:160:GLY:CA	2.43	0.41
1:F:247:THR:CA	1:F:268:LEU:HB3	2.48	0.41
1:H:277:LEU:HD12	1:H:434:THR:HB	2.02	0.41
1:A:416:GLU:O	1:A:420:GLU:HG2	2.20	0.41
1:B:144:LEU:C	1:B:145:PRO:O	2.57	0.41
1:H:18:LEU:C	1:H:19:ILE:HG13	2.41	0.41
1:B:144:LEU:HB3	1:B:145:PRO:CD	2.51	0.41
1:B:144:LEU:HA	1:B:144:LEU:HD23	1.86	0.41
1:C:144:LEU:CB	1:C:148:VAL:HG12	2.50	0.41
1:C:18:LEU:C	1:C:19:ILE:HG13	2.41	0.41
1:C:34:VAL:HG13	1:C:103:ASN:HD21	1.86	0.41
1:C:46:VAL:HG12	1:C:47:PRO:CD	2.51	0.41
1:D:119:SER:HB3	1:D:176:VAL:HG21	2.02	0.41
1:E:324:ILE:HD13	1:E:324:ILE:HG21	1.60	0.41
1:G:143:PRO:CD	1:G:143:PRO:O	2.69	0.41
1:G:46:VAL:HG12	1:G:47:PRO:CD	2.51	0.41
1:H:306:ARG:CD	1:H:397:LEU:HD12	2.51	0.41
1:A:129:TRP:C	1:A:131:THR:H	2.25	0.40
1:A:142:LEU:HD13	1:A:144:LEU:CG	2.49	0.40
1:B:119:SER:OG	1:B:173:LEU:HD12	2.21	0.40
1:C:247:THR:CA	1:C:268:LEU:HB3	2.48	0.40
1:C:443:ILE:HD13	1:C:443:ILE:HG21	1.72	0.40
1:D:185:CYS:HB2	1:D:187:ASN:HD22	1.85	0.40
1:D:426:TYR:CD1	1:D:471:ASP:HB3	2.56	0.40
1:E:83:LEU:HD12	1:E:127:ALA:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD22	1:A:205:ALA:HB1	2.03	0.40
1:B:179:ILE:HG22	1:B:189:VAL:HG21	2.03	0.40
1:B:296:ASN:O	1:B:299:GLN:HB2	2.21	0.40
1:B:320:ARG:HH11	1:B:320:ARG:HD3	1.77	0.40
1:B:34:VAL:HG13	1:B:103:ASN:HD21	1.86	0.40
1:C:388:ASN:OD1	1:C:388:ASN:O	2.39	0.40
1:C:401:VAL:O	1:C:402:PHE:CB	2.66	0.40
1:D:358:ASN:C	1:D:358:ASN:HD22	2.24	0.40
1:F:34:VAL:HG13	1:F:103:ASN:HD21	1.86	0.40
1:F:64:THR:HA	1:F:67:SER:HB2	2.02	0.40
1:G:281:ASP:HA	1:G:282:PRO:HD2	1.78	0.40
1:H:139:ASP:OD1	1:H:139:ASP:C	2.57	0.40
1:A:247:THR:CA	1:A:268:LEU:HB3	2.48	0.40
1:A:45:GLU:O	1:A:46:VAL:HG22	2.22	0.40
1:B:46:VAL:HG12	1:B:47:PRO:CD	2.52	0.40
1:C:185:CYS:HB2	1:C:187:ASN:ND2	2.35	0.40
1:F:46:VAL:HG11	1:F:222:THR:HG21	2.02	0.40
1:A:83:LEU:HD12	1:A:127:ALA:HB1	2.02	0.40
1:A:51:VAL:CG1	1:A:51:VAL:O	2.70	0.40
1:E:494:ILE:HG23	1:F:454:VAL:HB	2.03	0.40
1:E:258:GLY:O	1:F:254:GLY:HA3	2.22	0.40
1:G:144:LEU:O	1:G:145:PRO:C	2.56	0.40
1:G:168:TRP:HE3	1:G:344:VAL:HG21	1.85	0.40
1:G:51:VAL:O	1:G:51:VAL:CG1	2.70	0.40
1:C:146:PRO:O	1:C:148:VAL:N	2.55	0.40
1:C:373:ALA:HA	1:C:374:PRO:HD3	1.80	0.40
1:D:109:ILE:HG13	1:D:110:TYR:N	2.37	0.40
1:D:64:THR:C	1:D:67:SER:HB2	2.40	0.40
1:E:119:SER:HB3	1:E:176:VAL:HG21	2.02	0.40
1:G:129:TRP:CE3	1:G:129:TRP:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/516 (93%)	440 (92%)	36 (8%)	3 (1%)	30	63
1	B	479/516 (93%)	429 (90%)	46 (10%)	4 (1%)	24	56
1	C	479/516 (93%)	439 (92%)	36 (8%)	4 (1%)	24	56
1	D	479/516 (93%)	434 (91%)	42 (9%)	3 (1%)	30	63
1	E	479/516 (93%)	439 (92%)	38 (8%)	2 (0%)	39	72
1	F	479/516 (93%)	433 (90%)	43 (9%)	3 (1%)	30	63
1	G	479/516 (93%)	439 (92%)	38 (8%)	2 (0%)	39	72
1	H	479/516 (93%)	436 (91%)	39 (8%)	4 (1%)	24	56
All	All	3832/4128 (93%)	3489 (91%)	318 (8%)	25 (1%)	26	59

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	C	143	PRO
1	D	143	PRO
1	F	143	PRO
1	A	394	ILE
1	B	297	HIS
1	C	142	LEU
1	E	144	LEU
1	B	142	LEU
1	H	142	LEU
1	C	145	PRO
1	D	142	LEU
1	A	198	PRO
1	B	198	PRO
1	C	198	PRO
1	D	198	PRO
1	E	198	PRO
1	F	142	LEU
1	F	198	PRO
1	G	198	PRO
1	H	198	PRO
1	H	394	ILE
1	B	143	PRO
1	H	143	PRO
1	G	143	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	338/408 (83%)	320 (95%)	18 (5%)	28	60
1	B	337/408 (83%)	315 (94%)	22 (6%)	21	49
1	C	336/408 (82%)	316 (94%)	20 (6%)	24	54
1	D	338/408 (83%)	281 (83%)	57 (17%)	2	7
1	E	336/408 (82%)	319 (95%)	17 (5%)	29	61
1	F	337/408 (83%)	315 (94%)	22 (6%)	21	49
1	G	338/408 (83%)	314 (93%)	24 (7%)	18	44
1	H	337/408 (83%)	286 (85%)	51 (15%)	3	9
All	All	2697/3264 (83%)	2466 (91%)	231 (9%)	13	34

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	A	106	LYS
1	A	129	TRP
1	A	141	SER
1	A	189	VAL
1	A	200	THR
1	A	206	GLU
1	A	241	VAL
1	A	274	VAL
1	A	297	HIS
1	A	313	ILE
1	A	327	SER
1	A	340	MET
1	A	361	GLU
1	A	368	CYS
1	A	394	ILE
1	A	397	LEU
1	A	418	VAL
1	B	55	ASN

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Mol	Chain	Res	Type
1	B	68	ASP
1	B	89	LEU
1	B	91	VAL
1	B	103	ASN
1	B	106	LYS
1	B	122	TRP
1	B	140	LEU
1	B	189	VAL
1	B	200	THR
1	B	206	GLU
1	B	222	THR
1	B	251	ARG
1	B	271	LYS
1	B	274	VAL
1	B	297	HIS
1	B	313	ILE
1	B	327	SER
1	B	340	MET
1	B	371	THR
1	B	418	VAL
1	B	426	TYR
1	C	55	ASN
1	C	65	LEU
1	C	91	VAL
1	C	103	ASN
1	C	106	LYS
1	C	122	TRP
1	C	129	TRP
1	C	189	VAL
1	C	200	THR
1	C	206	GLU
1	C	222	THR
1	C	274	VAL
1	C	297	HIS
1	C	313	ILE
1	C	327	SER
1	C	340	MET
1	C	416	GLU
1	C	418	VAL
1	C	419	ASN
1	C	477	GLU
1	D	16	GLN

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Mol	Chain	Res	Type
1	D	22	GLN
1	D	24	VAL
1	D	32	LEU
1	D	39	THR
1	D	43	LEU
1	D	46	VAL
1	D	55	ASN
1	D	65	LEU
1	D	67	SER
1	D	80	ARG
1	D	82	LEU
1	D	83	LEU
1	D	84	ARG
1	D	89	LEU
1	D	91	VAL
1	D	103	ASN
1	D	106	LYS
1	D	122	TRP
1	D	129	TRP
1	D	131	THR
1	D	137	THR
1	D	141	SER
1	D	148	VAL
1	D	189	VAL
1	D	200	THR
1	D	206	GLU
1	D	218	LEU
1	D	222	THR
1	D	247	THR
1	D	251	ARG
1	D	265	SER
1	D	271	LYS
1	D	274	VAL
1	D	297	HIS
1	D	305	SER
1	D	313	ILE
1	D	321	LEU
1	D	327	SER
1	D	340	MET
1	D	358	ASN
1	D	365	ASP
1	D	367	ILE

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Mol	Chain	Res	Type
1	D	371	THR
1	D	389	ARG
1	D	397	LEU
1	D	400	GLU
1	D	413	ASP
1	D	416	GLU
1	D	418	VAL
1	D	425	VAL
1	D	426	TYR
1	D	437	LEU
1	D	438	SER
1	D	441	LEU
1	D	464	LEU
1	D	477	GLU
1	E	91	VAL
1	E	106	LYS
1	E	113	LEU
1	E	129	TRP
1	E	141	SER
1	E	189	VAL
1	E	200	THR
1	E	206	GLU
1	E	274	VAL
1	E	297	HIS
1	E	313	ILE
1	E	327	SER
1	E	340	MET
1	E	394	ILE
1	E	396	LEU
1	E	397	LEU
1	E	418	VAL
1	F	17	MET
1	F	55	ASN
1	F	68	ASP
1	F	89	LEU
1	F	91	VAL
1	F	103	ASN
1	F	106	LYS
1	F	122	TRP
1	F	189	VAL
1	F	200	THR
1	F	206	GLU

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Mol	Chain	Res	Type
1	F	222	THR
1	F	251	ARG
1	F	271	LYS
1	F	274	VAL
1	F	297	HIS
1	F	313	ILE
1	F	327	SER
1	F	340	MET
1	F	396	LEU
1	F	397	LEU
1	F	418	VAL
1	G	55	ASN
1	G	91	VAL
1	G	103	ASN
1	G	106	LYS
1	G	122	TRP
1	G	129	TRP
1	G	141	SER
1	G	142	LEU
1	G	144	LEU
1	G	189	VAL
1	G	200	THR
1	G	206	GLU
1	G	222	THR
1	G	274	VAL
1	G	297	HIS
1	G	313	ILE
1	G	327	SER
1	G	340	MET
1	G	396	LEU
1	G	397	LEU
1	G	416	GLU
1	G	418	VAL
1	G	419	ASN
1	G	477	GLU
1	H	22	GLN
1	H	24	VAL
1	H	32	LEU
1	H	43	LEU
1	H	46	VAL
1	H	55	ASN
1	H	65	LEU

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Mol	Chain	Res	Type
1	H	67	SER
1	H	69	THR
1	H	80	ARG
1	H	82	LEU
1	H	83	LEU
1	H	84	ARG
1	H	89	LEU
1	H	91	VAL
1	H	103	ASN
1	H	106	LYS
1	H	122	TRP
1	H	129	TRP
1	H	131	THR
1	H	137	THR
1	H	141	SER
1	H	189	VAL
1	H	200	THR
1	H	206	GLU
1	H	218	LEU
1	H	222	THR
1	H	227	THR
1	H	247	THR
1	H	251	ARG
1	H	265	SER
1	H	274	VAL
1	H	297	HIS
1	H	305	SER
1	H	313	ILE
1	H	321	LEU
1	H	327	SER
1	H	340	MET
1	H	358	ASN
1	H	365	ASP
1	H	367	ILE
1	H	371	THR
1	H	389	ARG
1	H	400	GLU
1	H	413	ASP
1	H	416	GLU
1	H	418	VAL
1	H	438	SER
1	H	441	LEU

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Mol	Chain	Res	Type
1	H	464	LEU
1	H	477	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	319	GLN
1	B	103	ASN
1	B	121	GLN
1	B	319	GLN
1	B	358	ASN
1	C	103	ASN
1	C	319	GLN
1	C	478	HIS
1	D	103	ASN
1	D	121	GLN
1	D	296	ASN
1	D	319	GLN
1	E	121	GLN
1	E	319	GLN
1	F	103	ASN
1	F	121	GLN
1	F	319	GLN
1	F	358	ASN
1	G	103	ASN
1	G	296	ASN
1	G	319	GLN
1	G	478	HIS
1	H	103	ASN
1	H	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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, 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	481/516 (93%)	-0.05	4 (0%) 87 82	16, 27, 35, 41	0
1	B	481/516 (93%)	-0.04	4 (0%) 87 82	16, 25, 33, 45	0
1	C	481/516 (93%)	0.04	4 (0%) 87 82	17, 27, 37, 44	0
1	D	481/516 (93%)	0.04	7 (1%) 76 69	16, 28, 38, 44	0
1	E	481/516 (93%)	-0.00	1 (0%) 95 94	17, 26, 35, 43	0
1	F	481/516 (93%)	0.05	8 (1%) 73 65	17, 25, 33, 43	0
1	G	481/516 (93%)	0.01	3 (0%) 90 87	18, 28, 35, 46	0
1	H	481/516 (93%)	0.22	3 (0%) 90 87	18, 29, 37, 45	0
All	All	3848/4128 (93%)	0.03	34 (0%) 85 80	16, 27, 36, 46	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	396	LEU	4.8
1	E	142	LEU	3.6
1	B	140	LEU	3.2
1	D	246	SER	3.0
1	C	246	SER	2.9
1	F	475	GLY	2.8
1	F	16	GLN	2.8
1	A	142	LEU	2.7
1	G	247	THR	2.6
1	D	215	ALA	2.6
1	D	276	VAL	2.5
1	A	51	VAL	2.5
1	D	477	GLU	2.5
1	A	55	ASN	2.4
1	B	142	LEU	2.4
1	F	247	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	40	GLY	2.3
1	F	97	ALA	2.3
1	D	361	GLU	2.3
1	F	140	LEU	2.3
1	D	142	LEU	2.2
1	G	221	VAL	2.2
1	C	247	THR	2.2
1	B	31	THR	2.2
1	H	369	GLY	2.1
1	C	139	ASP	2.1
1	F	394	ILE	2.1
1	H	358	ASN	2.1
1	B	139	ASP	2.1
1	C	142	LEU	2.1
1	F	295	PHE	2.1
1	F	139	ASP	2.1
1	A	143	PRO	2.1
1	G	100	GLU	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.