Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2021 – 02:22 am GMT

PDB ID	:	6ZN9
Title	:	MaeB PTA domain apoprotein
Authors	:	Lovering, A.L.; Harding, C.J.
Deposited on	:	2020-07-06
Resolution	:	2.72 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 following versions of software and data (see references ①) were used in the production of this report:

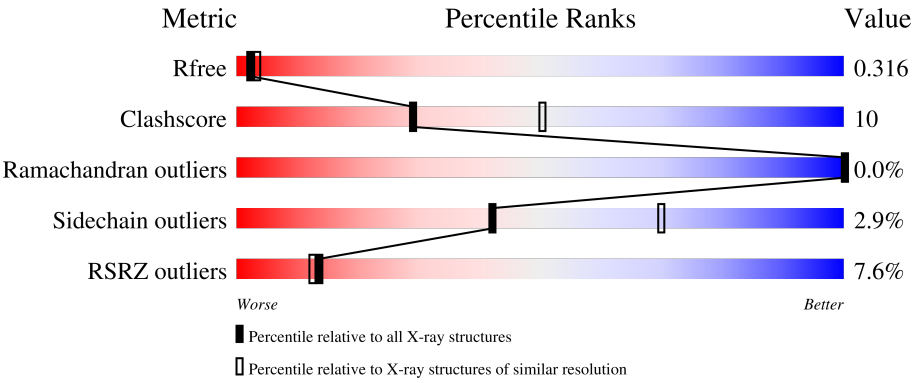
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

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 2.72 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 <=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	362	7% 77% 16% • 6%
1	B	362	4% 70% 22% • 6%
1	C	362	3% 75% 17% • 7%
1	D	362	3% 71% 21% • 6%
1	E	362	8% 76% 17% • 6%

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Mol	Chain	Length	Quality of chain
1	F	362	15% 71% 22% • 6%
1	G	362	% 74% 19% • 6%
1	H	362	8% 71% 22% • 6%
1	I	362	10% 77% 17% • 6%
1	J	362	7% 69% 24% • 7%
1	K	362	7% 79% 14% • 6%
1	L	362	13% 69% 22% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31258 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	338	Total	C	N	O	S	0	0	0
			2598	1658	444	485	11			
1	D	341	Total	C	N	O	S	0	0	0
			2611	1665	447	488	11			
1	A	340	Total	C	N	O	S	0	0	0
			2606	1663	446	486	11			
1	B	341	Total	C	N	O	S	0	0	0
			2610	1665	447	487	11			
1	F	339	Total	C	N	O	S	0	0	0
			2602	1661	445	485	11			
1	G	340	Total	C	N	O	S	0	0	0
			2607	1663	446	487	11			
1	J	338	Total	C	N	O	S	0	0	0
			2598	1658	444	485	11			
1	L	338	Total	C	N	O	S	0	0	0
			2598	1658	444	485	11			
1	H	340	Total	C	N	O	S	0	0	0
			2607	1663	446	487	11			
1	I	340	Total	C	N	O	S	0	0	0
			2607	1663	446	487	11			
1	K	340	Total	C	N	O	S	0	0	0
			2607	1663	446	487	11			
1	E	340	Total	C	N	O	S	0	0	0
			2607	1663	446	487	11			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	419	MET	-	initiating methionine	UNP Q6MM15
C	420	GLY	-	expression tag	UNP Q6MM15
C	421	SER	-	expression tag	UNP Q6MM15
C	422	SER	-	expression tag	UNP Q6MM15
C	423	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
C	424	HIS	-	expression tag	UNP Q6MM15
C	425	HIS	-	expression tag	UNP Q6MM15
C	426	HIS	-	expression tag	UNP Q6MM15
C	427	HIS	-	expression tag	UNP Q6MM15
C	428	HIS	-	expression tag	UNP Q6MM15
C	429	SER	-	expression tag	UNP Q6MM15
C	430	SER	-	expression tag	UNP Q6MM15
C	431	GLY	-	expression tag	UNP Q6MM15
C	432	LEU	-	expression tag	UNP Q6MM15
C	433	VAL	-	expression tag	UNP Q6MM15
C	434	PRO	-	expression tag	UNP Q6MM15
C	435	ALA	-	expression tag	UNP Q6MM15
C	436	GLY	-	expression tag	UNP Q6MM15
C	437	SER	-	expression tag	UNP Q6MM15
C	438	HIS	-	expression tag	UNP Q6MM15
D	419	MET	-	initiating methionine	UNP Q6MM15
D	420	GLY	-	expression tag	UNP Q6MM15
D	421	SER	-	expression tag	UNP Q6MM15
D	422	SER	-	expression tag	UNP Q6MM15
D	423	HIS	-	expression tag	UNP Q6MM15
D	424	HIS	-	expression tag	UNP Q6MM15
D	425	HIS	-	expression tag	UNP Q6MM15
D	426	HIS	-	expression tag	UNP Q6MM15
D	427	HIS	-	expression tag	UNP Q6MM15
D	428	HIS	-	expression tag	UNP Q6MM15
D	429	SER	-	expression tag	UNP Q6MM15
D	430	SER	-	expression tag	UNP Q6MM15
D	431	GLY	-	expression tag	UNP Q6MM15
D	432	LEU	-	expression tag	UNP Q6MM15
D	433	VAL	-	expression tag	UNP Q6MM15
D	434	PRO	-	expression tag	UNP Q6MM15
D	435	ALA	-	expression tag	UNP Q6MM15
D	436	GLY	-	expression tag	UNP Q6MM15
D	437	SER	-	expression tag	UNP Q6MM15
D	438	HIS	-	expression tag	UNP Q6MM15
A	419	MET	-	initiating methionine	UNP Q6MM15
A	420	GLY	-	expression tag	UNP Q6MM15
A	421	SER	-	expression tag	UNP Q6MM15
A	422	SER	-	expression tag	UNP Q6MM15
A	423	HIS	-	expression tag	UNP Q6MM15
A	424	HIS	-	expression tag	UNP Q6MM15
A	425	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
A	426	HIS	-	expression tag	UNP Q6MM15
A	427	HIS	-	expression tag	UNP Q6MM15
A	428	HIS	-	expression tag	UNP Q6MM15
A	429	SER	-	expression tag	UNP Q6MM15
A	430	SER	-	expression tag	UNP Q6MM15
A	431	GLY	-	expression tag	UNP Q6MM15
A	432	LEU	-	expression tag	UNP Q6MM15
A	433	VAL	-	expression tag	UNP Q6MM15
A	434	PRO	-	expression tag	UNP Q6MM15
A	435	ALA	-	expression tag	UNP Q6MM15
A	436	GLY	-	expression tag	UNP Q6MM15
A	437	SER	-	expression tag	UNP Q6MM15
A	438	HIS	-	expression tag	UNP Q6MM15
B	419	MET	-	initiating methionine	UNP Q6MM15
B	420	GLY	-	expression tag	UNP Q6MM15
B	421	SER	-	expression tag	UNP Q6MM15
B	422	SER	-	expression tag	UNP Q6MM15
B	423	HIS	-	expression tag	UNP Q6MM15
B	424	HIS	-	expression tag	UNP Q6MM15
B	425	HIS	-	expression tag	UNP Q6MM15
B	426	HIS	-	expression tag	UNP Q6MM15
B	427	HIS	-	expression tag	UNP Q6MM15
B	428	HIS	-	expression tag	UNP Q6MM15
B	429	SER	-	expression tag	UNP Q6MM15
B	430	SER	-	expression tag	UNP Q6MM15
B	431	GLY	-	expression tag	UNP Q6MM15
B	432	LEU	-	expression tag	UNP Q6MM15
B	433	VAL	-	expression tag	UNP Q6MM15
B	434	PRO	-	expression tag	UNP Q6MM15
B	435	ALA	-	expression tag	UNP Q6MM15
B	436	GLY	-	expression tag	UNP Q6MM15
B	437	SER	-	expression tag	UNP Q6MM15
B	438	HIS	-	expression tag	UNP Q6MM15
F	419	MET	-	initiating methionine	UNP Q6MM15
F	420	GLY	-	expression tag	UNP Q6MM15
F	421	SER	-	expression tag	UNP Q6MM15
F	422	SER	-	expression tag	UNP Q6MM15
F	423	HIS	-	expression tag	UNP Q6MM15
F	424	HIS	-	expression tag	UNP Q6MM15
F	425	HIS	-	expression tag	UNP Q6MM15
F	426	HIS	-	expression tag	UNP Q6MM15
F	427	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
F	428	HIS	-	expression tag	UNP Q6MM15
F	429	SER	-	expression tag	UNP Q6MM15
F	430	SER	-	expression tag	UNP Q6MM15
F	431	GLY	-	expression tag	UNP Q6MM15
F	432	LEU	-	expression tag	UNP Q6MM15
F	433	VAL	-	expression tag	UNP Q6MM15
F	434	PRO	-	expression tag	UNP Q6MM15
F	435	ALA	-	expression tag	UNP Q6MM15
F	436	GLY	-	expression tag	UNP Q6MM15
F	437	SER	-	expression tag	UNP Q6MM15
F	438	HIS	-	expression tag	UNP Q6MM15
G	419	MET	-	initiating methionine	UNP Q6MM15
G	420	GLY	-	expression tag	UNP Q6MM15
G	421	SER	-	expression tag	UNP Q6MM15
G	422	SER	-	expression tag	UNP Q6MM15
G	423	HIS	-	expression tag	UNP Q6MM15
G	424	HIS	-	expression tag	UNP Q6MM15
G	425	HIS	-	expression tag	UNP Q6MM15
G	426	HIS	-	expression tag	UNP Q6MM15
G	427	HIS	-	expression tag	UNP Q6MM15
G	428	HIS	-	expression tag	UNP Q6MM15
G	429	SER	-	expression tag	UNP Q6MM15
G	430	SER	-	expression tag	UNP Q6MM15
G	431	GLY	-	expression tag	UNP Q6MM15
G	432	LEU	-	expression tag	UNP Q6MM15
G	433	VAL	-	expression tag	UNP Q6MM15
G	434	PRO	-	expression tag	UNP Q6MM15
G	435	ALA	-	expression tag	UNP Q6MM15
G	436	GLY	-	expression tag	UNP Q6MM15
G	437	SER	-	expression tag	UNP Q6MM15
G	438	HIS	-	expression tag	UNP Q6MM15
J	419	MET	-	initiating methionine	UNP Q6MM15
J	420	GLY	-	expression tag	UNP Q6MM15
J	421	SER	-	expression tag	UNP Q6MM15
J	422	SER	-	expression tag	UNP Q6MM15
J	423	HIS	-	expression tag	UNP Q6MM15
J	424	HIS	-	expression tag	UNP Q6MM15
J	425	HIS	-	expression tag	UNP Q6MM15
J	426	HIS	-	expression tag	UNP Q6MM15
J	427	HIS	-	expression tag	UNP Q6MM15
J	428	HIS	-	expression tag	UNP Q6MM15
J	429	SER	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
J	430	SER	-	expression tag	UNP Q6MM15
J	431	GLY	-	expression tag	UNP Q6MM15
J	432	LEU	-	expression tag	UNP Q6MM15
J	433	VAL	-	expression tag	UNP Q6MM15
J	434	PRO	-	expression tag	UNP Q6MM15
J	435	ALA	-	expression tag	UNP Q6MM15
J	436	GLY	-	expression tag	UNP Q6MM15
J	437	SER	-	expression tag	UNP Q6MM15
J	438	HIS	-	expression tag	UNP Q6MM15
L	419	MET	-	initiating methionine	UNP Q6MM15
L	420	GLY	-	expression tag	UNP Q6MM15
L	421	SER	-	expression tag	UNP Q6MM15
L	422	SER	-	expression tag	UNP Q6MM15
L	423	HIS	-	expression tag	UNP Q6MM15
L	424	HIS	-	expression tag	UNP Q6MM15
L	425	HIS	-	expression tag	UNP Q6MM15
L	426	HIS	-	expression tag	UNP Q6MM15
L	427	HIS	-	expression tag	UNP Q6MM15
L	428	HIS	-	expression tag	UNP Q6MM15
L	429	SER	-	expression tag	UNP Q6MM15
L	430	SER	-	expression tag	UNP Q6MM15
L	431	GLY	-	expression tag	UNP Q6MM15
L	432	LEU	-	expression tag	UNP Q6MM15
L	433	VAL	-	expression tag	UNP Q6MM15
L	434	PRO	-	expression tag	UNP Q6MM15
L	435	ALA	-	expression tag	UNP Q6MM15
L	436	GLY	-	expression tag	UNP Q6MM15
L	437	SER	-	expression tag	UNP Q6MM15
L	438	HIS	-	expression tag	UNP Q6MM15
H	419	MET	-	initiating methionine	UNP Q6MM15
H	420	GLY	-	expression tag	UNP Q6MM15
H	421	SER	-	expression tag	UNP Q6MM15
H	422	SER	-	expression tag	UNP Q6MM15
H	423	HIS	-	expression tag	UNP Q6MM15
H	424	HIS	-	expression tag	UNP Q6MM15
H	425	HIS	-	expression tag	UNP Q6MM15
H	426	HIS	-	expression tag	UNP Q6MM15
H	427	HIS	-	expression tag	UNP Q6MM15
H	428	HIS	-	expression tag	UNP Q6MM15
H	429	SER	-	expression tag	UNP Q6MM15
H	430	SER	-	expression tag	UNP Q6MM15
H	431	GLY	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
H	432	LEU	-	expression tag	UNP Q6MM15
H	433	VAL	-	expression tag	UNP Q6MM15
H	434	PRO	-	expression tag	UNP Q6MM15
H	435	ALA	-	expression tag	UNP Q6MM15
H	436	GLY	-	expression tag	UNP Q6MM15
H	437	SER	-	expression tag	UNP Q6MM15
H	438	HIS	-	expression tag	UNP Q6MM15
I	419	MET	-	initiating methionine	UNP Q6MM15
I	420	GLY	-	expression tag	UNP Q6MM15
I	421	SER	-	expression tag	UNP Q6MM15
I	422	SER	-	expression tag	UNP Q6MM15
I	423	HIS	-	expression tag	UNP Q6MM15
I	424	HIS	-	expression tag	UNP Q6MM15
I	425	HIS	-	expression tag	UNP Q6MM15
I	426	HIS	-	expression tag	UNP Q6MM15
I	427	HIS	-	expression tag	UNP Q6MM15
I	428	HIS	-	expression tag	UNP Q6MM15
I	429	SER	-	expression tag	UNP Q6MM15
I	430	SER	-	expression tag	UNP Q6MM15
I	431	GLY	-	expression tag	UNP Q6MM15
I	432	LEU	-	expression tag	UNP Q6MM15
I	433	VAL	-	expression tag	UNP Q6MM15
I	434	PRO	-	expression tag	UNP Q6MM15
I	435	ALA	-	expression tag	UNP Q6MM15
I	436	GLY	-	expression tag	UNP Q6MM15
I	437	SER	-	expression tag	UNP Q6MM15
I	438	HIS	-	expression tag	UNP Q6MM15
K	419	MET	-	initiating methionine	UNP Q6MM15
K	420	GLY	-	expression tag	UNP Q6MM15
K	421	SER	-	expression tag	UNP Q6MM15
K	422	SER	-	expression tag	UNP Q6MM15
K	423	HIS	-	expression tag	UNP Q6MM15
K	424	HIS	-	expression tag	UNP Q6MM15
K	425	HIS	-	expression tag	UNP Q6MM15
K	426	HIS	-	expression tag	UNP Q6MM15
K	427	HIS	-	expression tag	UNP Q6MM15
K	428	HIS	-	expression tag	UNP Q6MM15
K	429	SER	-	expression tag	UNP Q6MM15
K	430	SER	-	expression tag	UNP Q6MM15
K	431	GLY	-	expression tag	UNP Q6MM15
K	432	LEU	-	expression tag	UNP Q6MM15
K	433	VAL	-	expression tag	UNP Q6MM15

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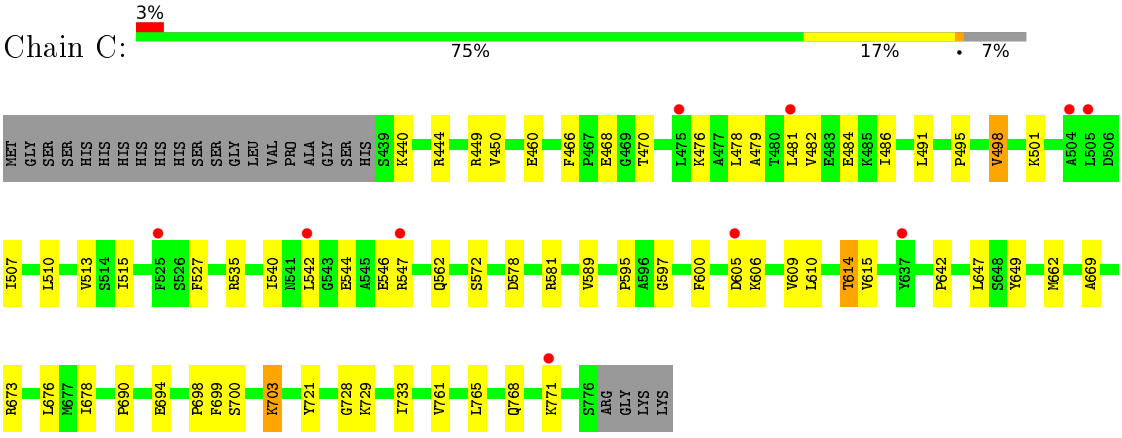
Chain	Residue	Modelled	Actual	Comment	Reference
K	434	PRO	-	expression tag	UNP Q6MM15
K	435	ALA	-	expression tag	UNP Q6MM15
K	436	GLY	-	expression tag	UNP Q6MM15
K	437	SER	-	expression tag	UNP Q6MM15
K	438	HIS	-	expression tag	UNP Q6MM15
E	419	MET	-	initiating methionine	UNP Q6MM15
E	420	GLY	-	expression tag	UNP Q6MM15
E	421	SER	-	expression tag	UNP Q6MM15
E	422	SER	-	expression tag	UNP Q6MM15
E	423	HIS	-	expression tag	UNP Q6MM15
E	424	HIS	-	expression tag	UNP Q6MM15
E	425	HIS	-	expression tag	UNP Q6MM15
E	426	HIS	-	expression tag	UNP Q6MM15
E	427	HIS	-	expression tag	UNP Q6MM15
E	428	HIS	-	expression tag	UNP Q6MM15
E	429	SER	-	expression tag	UNP Q6MM15
E	430	SER	-	expression tag	UNP Q6MM15
E	431	GLY	-	expression tag	UNP Q6MM15
E	432	LEU	-	expression tag	UNP Q6MM15
E	433	VAL	-	expression tag	UNP Q6MM15
E	434	PRO	-	expression tag	UNP Q6MM15
E	435	ALA	-	expression tag	UNP Q6MM15
E	436	GLY	-	expression tag	UNP Q6MM15
E	437	SER	-	expression tag	UNP Q6MM15
E	438	HIS	-	expression tag	UNP Q6MM15

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

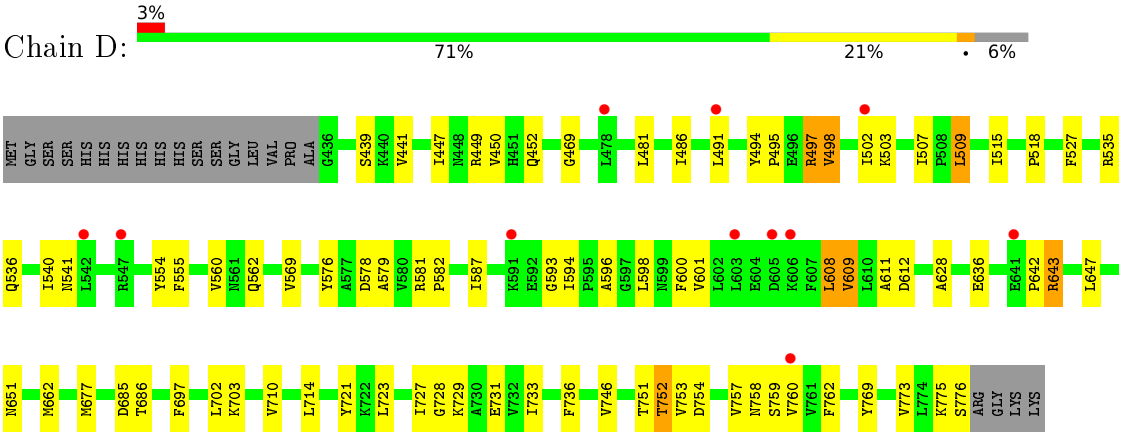
- Molecule 1: Malate dehydrogenase

Chain C:



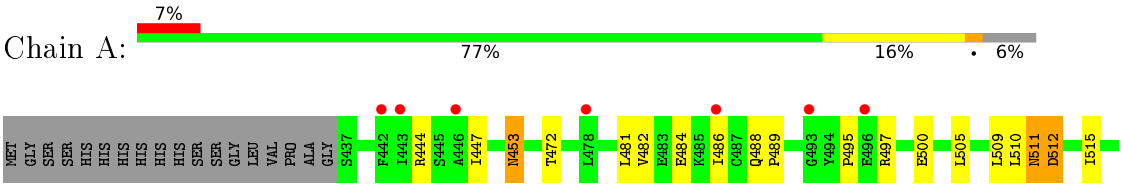
- Molecule 1: Malate dehydrogenase

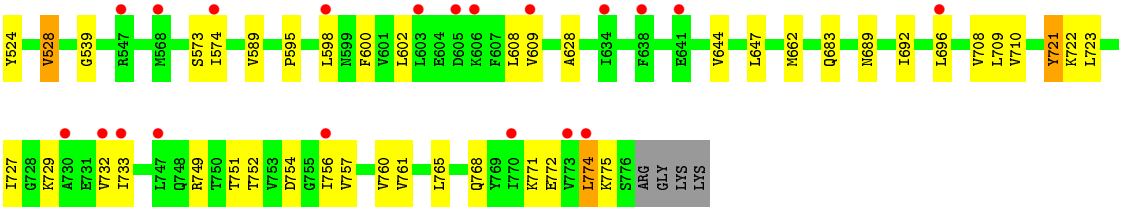
Chain D:



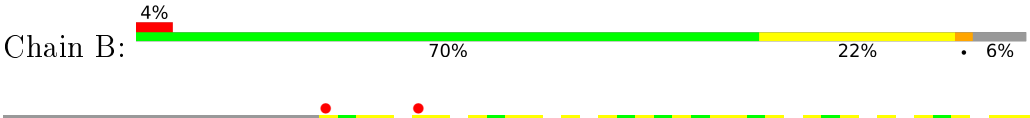
- Molecule 1: Malate dehydrogenase

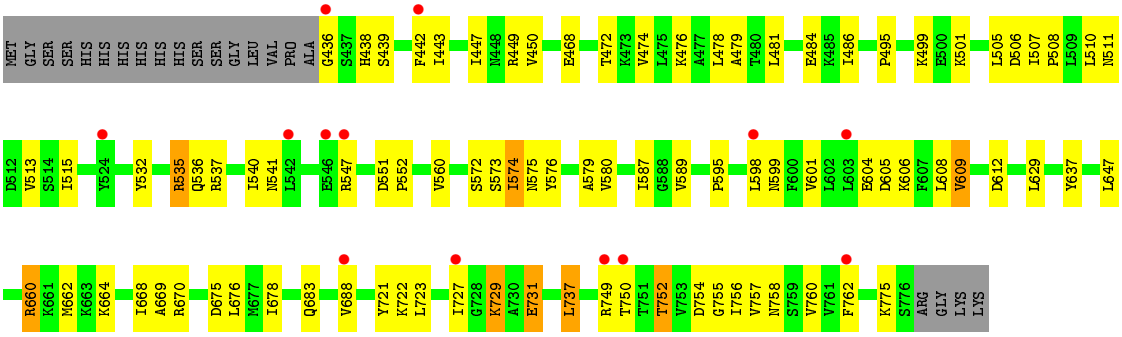
Chain A:



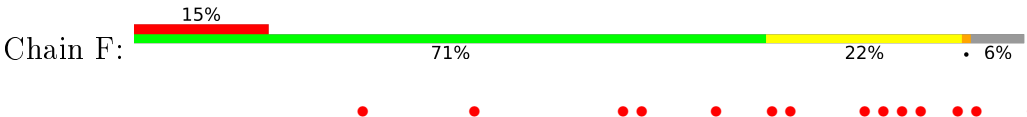


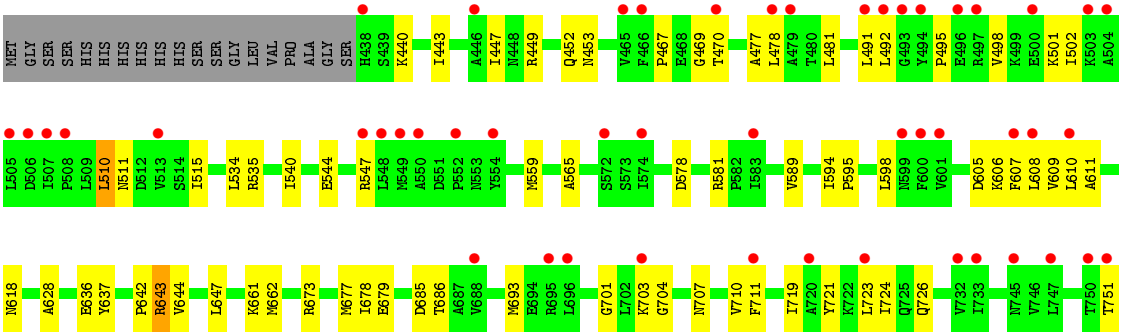
• Molecule 1: Malate dehydrogenase



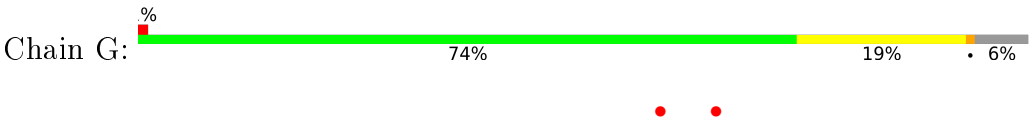


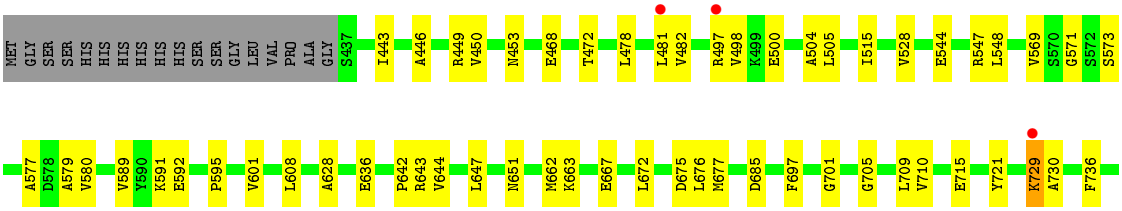
• Molecule 1: Malate dehydrogenase

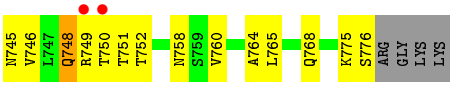




• Molecule 1: Malate dehydrogenase

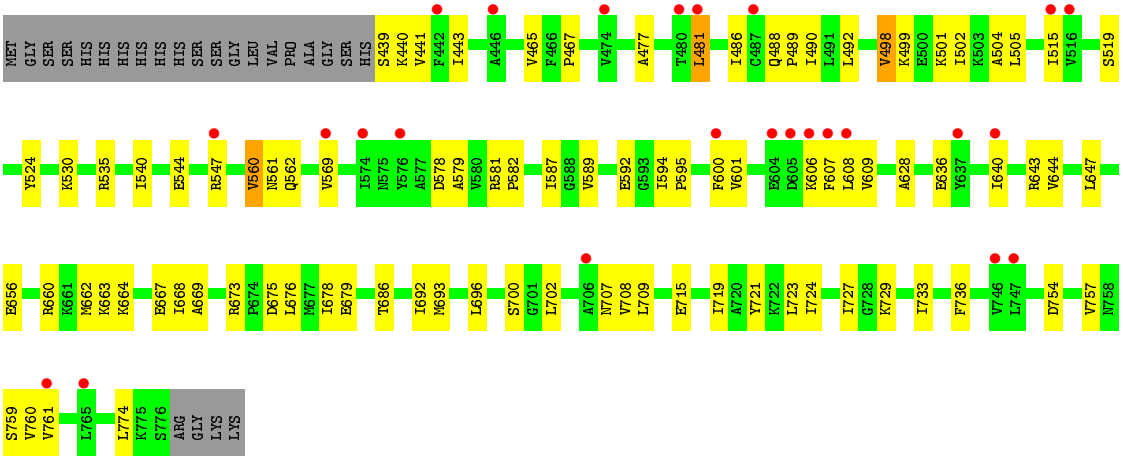






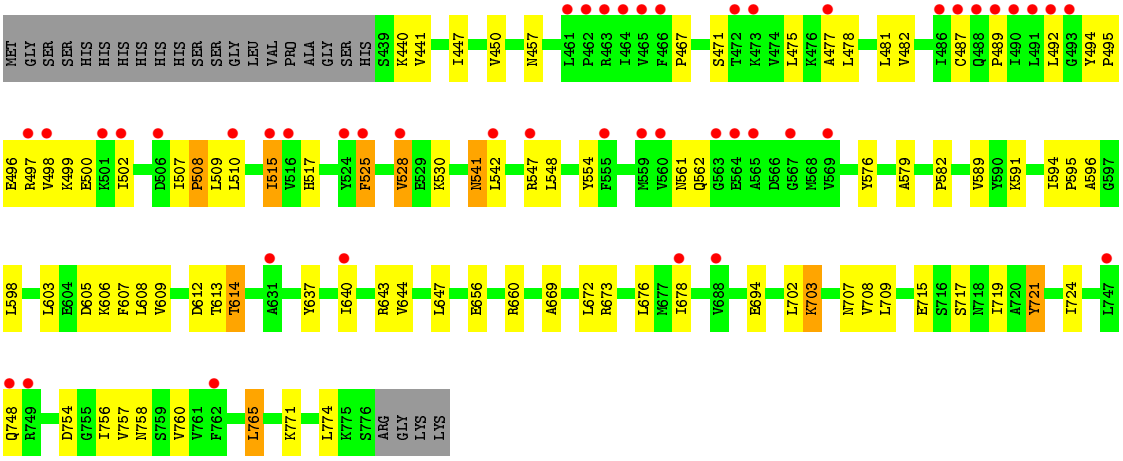
- Molecule 1: Malate dehydrogenase

Chain J:



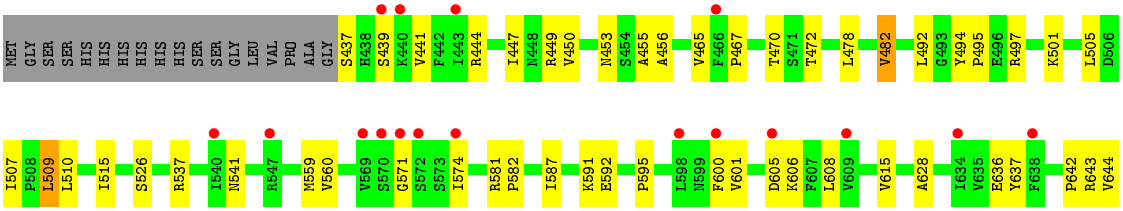
- Molecule 1: Malate dehydrogenase

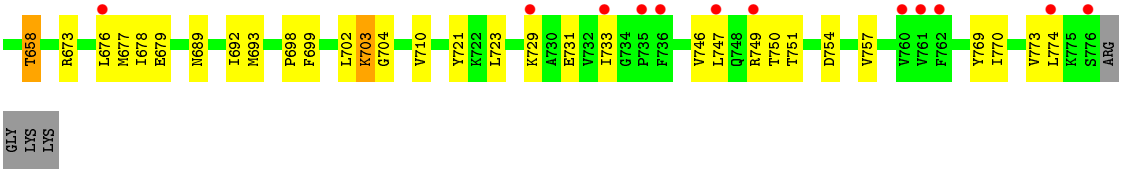
Chain L:



- Molecule 1: Malate dehydrogenase

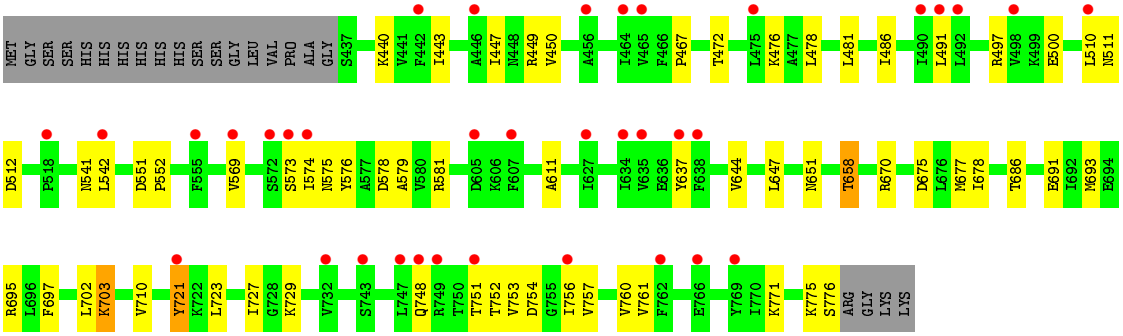
Chain H:





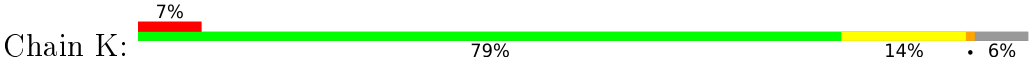
• Molecule 1: Malate dehydrogenase

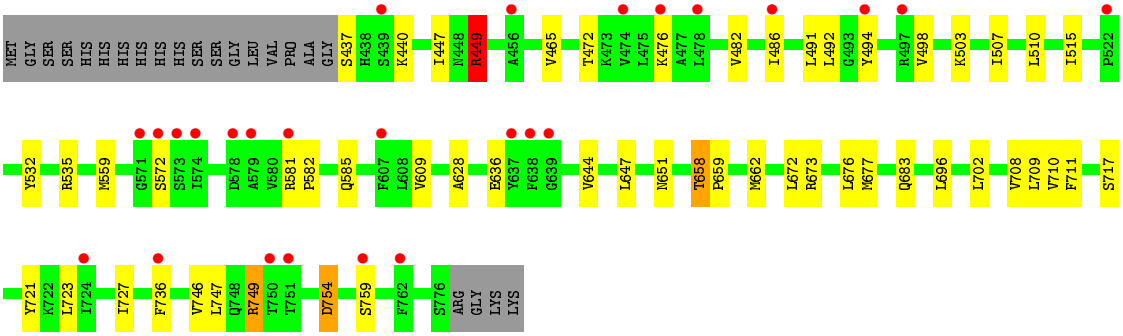
Chain I:



• Molecule 1: Malate dehydrogenase

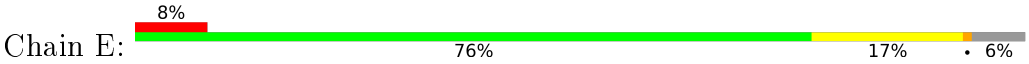
Chain K:

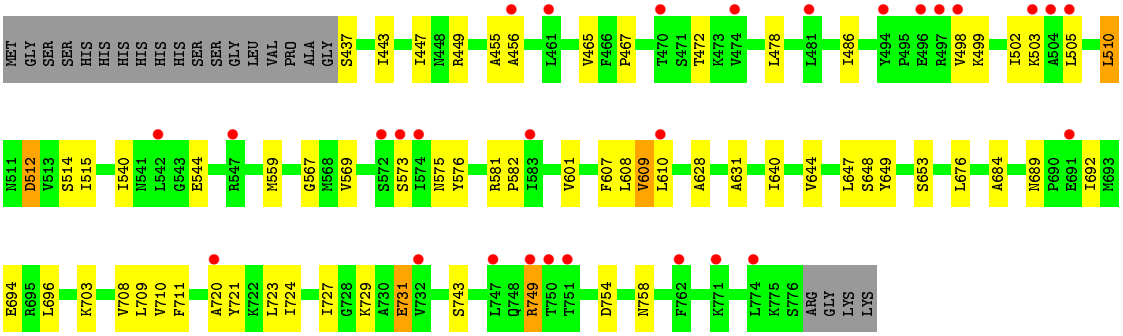




• Molecule 1: Malate dehydrogenase

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.22Å 151.28Å 285.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.64 – 2.72 125.12 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.64-2.72) 95.9 (125.12-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.73Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.252 , 0.299 0.278 , 0.316	Depositor DCC
R_{free} test set	7485 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	31258	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/2650	0.71	0/3587
1	B	0.56	0/2654	0.74	3/3592 (0.1%)
1	C	0.58	0/2642	0.73	1/3576 (0.0%)
1	D	0.58	0/2655	0.73	1/3593 (0.0%)
1	E	0.48	0/2651	0.66	2/3588 (0.1%)
1	F	0.44	0/2646	0.69	1/3582 (0.0%)
1	G	0.56	0/2651	0.73	1/3588 (0.0%)
1	H	0.55	0/2651	0.70	0/3588
1	I	0.57	0/2651	0.72	0/3588
1	J	0.57	1/2642 (0.0%)	0.71	1/3576 (0.0%)
1	K	0.52	0/2651	0.74	3/3588 (0.1%)
1	L	0.56	0/2642	0.72	0/3576
All	All	0.54	1/31786 (0.0%)	0.72	13/43022 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	560	VAL	CB-CG2	-5.10	1.42	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	749	ARG	NE-CZ-NH1	-10.37	115.11	120.30
1	B	737	LEU	CB-CG-CD1	-7.42	98.39	111.00
1	K	749	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	G	481	LEU	CA-CB-CG	6.85	131.05	115.30
1	F	643	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	K	449	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	737	LEU	CA-CB-CG	5.58	128.13	115.30
1	B	612	ASP	CB-CG-OD1	5.25	123.03	118.30
1	E	512	ASP	CB-CA-C	5.09	120.58	110.40
1	J	481	LEU	CA-CB-CG	5.07	126.96	115.30
1	D	608	LEU	CA-CB-CG	5.06	126.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	749	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	C	610	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2606	0	2675	51	0
1	B	2610	0	2678	64	0
1	C	2598	0	2675	44	0
1	D	2611	0	2681	56	0
1	E	2607	0	2678	43	0
1	F	2602	0	2674	68	0
1	G	2607	0	2678	52	0
1	H	2607	0	2678	70	0
1	I	2607	0	2678	49	0
1	J	2598	0	2675	61	0
1	K	2607	0	2678	45	0
1	L	2598	0	2675	56	0
All	All	31258	0	32123	607	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 10.

All (607) 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:A:453:ASN:CG	1:A:768:GLN:HE22	1.07	1.49
1:A:453:ASN:CG	1:A:768:GLN:NE2	1.75	1.38
1:A:453:ASN:ND2	1:A:768:GLN:NE2	2.05	1.05
1:A:453:ASN:OD1	1:A:768:GLN:NE2	1.80	0.98
1:B:439:SER:CB	1:B:731:GLU:OE1	2.13	0.97
1:L:598:LEU:HD11	1:L:609:VAL:HB	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:544:GLU:HG2	1:G:547:ARG:HH12	1.34	0.91
1:L:530:LYS:HD3	1:L:562:GLN:HE22	1.37	0.89
1:C:450:VAL:HA	1:C:768:GLN:HE22	1.36	0.87
1:B:547:ARG:NH1	1:G:573:SER:OG	2.10	0.85
1:I:450:VAL:HG11	1:I:486:ILE:HG12	1.57	0.84
1:F:598:LEU:HD11	1:F:609:VAL:HB	1.58	0.84
1:B:436:GLY:HA2	1:B:731:GLU:OE2	1.79	0.82
1:E:437:SER:N	1:E:731:GLU:OE1	2.12	0.82
1:H:507:ILE:HG21	1:H:510:LEU:CD1	2.12	0.80
1:G:573:SER:O	1:G:749:ARG:NH2	2.14	0.80
1:K:465:VAL:HG21	1:K:559:MET:HE3	1.64	0.79
1:G:715:GLU:OE2	1:H:658:THR:HG21	1.82	0.79
1:L:507:ILE:HG12	1:L:510:LEU:HD13	1.64	0.79
1:I:721:TYR:OH	1:I:748:GLN:NE2	2.16	0.78
1:F:636:GLU:OE2	1:F:673:ARG:NH2	2.17	0.78
1:J:715:GLU:OE2	1:I:658:THR:HG21	1.86	0.76
1:L:715:GLU:OE2	1:K:658:THR:HG21	1.86	0.75
1:D:752:THR:OG1	1:D:754:ASP:OD1	2.04	0.74
1:D:541:ASN:ND2	1:K:749:ARG:HH12	1.83	0.74
1:A:512:ASP:OD1	1:A:512:ASP:N	2.20	0.74
1:D:601:VAL:HG22	1:D:608:LEU:HB2	1.70	0.74
1:L:724:ILE:HD13	1:K:727:ILE:HD11	1.68	0.73
1:I:677:MET:HE3	1:I:702:LEU:HA	1.70	0.73
1:A:481:LEU:HD21	1:A:757:VAL:HG23	1.69	0.73
1:K:449:ARG:HH11	1:K:449:ARG:HG2	1.53	0.73
1:H:541:ASN:ND2	1:E:749:ARG:HH21	1.87	0.73
1:A:774:LEU:O	1:A:774:LEU:HD22	1.87	0.72
1:H:449:ARG:O	1:H:453:ASN:ND2	2.21	0.72
1:H:439:SER:N	1:H:731:GLU:OE1	2.23	0.72
1:B:598:LEU:HD11	1:B:609:VAL:HG13	1.70	0.72
1:H:507:ILE:HG21	1:H:510:LEU:HD13	1.72	0.72
1:J:440:LYS:HA	1:J:443:ILE:HD12	1.72	0.71
1:A:511:ASN:N	1:A:511:ASN:OD1	2.23	0.71
1:B:574:ILE:HG13	1:B:579:ALA:HB2	1.71	0.71
1:A:573:SER:O	1:A:749:ARG:NH2	2.24	0.70
1:A:774:LEU:HD22	1:A:774:LEU:C	2.13	0.69
1:D:677:MET:HE3	1:D:702:LEU:HA	1.73	0.69
1:H:472:THR:HG23	1:H:505:LEU:HD21	1.75	0.69
1:H:507:ILE:CG2	1:H:510:LEU:HD13	2.21	0.69
1:E:499:LYS:HA	1:E:502:ILE:HG12	1.74	0.68
1:C:535:ARG:HB3	1:C:540:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:677:MET:HE3	1:H:702:LEU:HA	1.74	0.68
1:F:643:ARG:NH1	1:F:703:LYS:O	2.27	0.68
1:B:495:PRO:HA	1:B:515:ILE:HG21	1.73	0.68
1:D:643:ARG:HG2	1:D:677:MET:HE2	1.75	0.67
1:C:703:LYS:NZ	1:H:698:PRO:O	2.25	0.67
1:H:507:ILE:CG2	1:H:510:LEU:CD1	2.73	0.67
1:D:578:ASP:OD1	1:D:581:ARG:NH2	2.27	0.67
1:A:453:ASN:ND2	1:A:768:GLN:HE21	1.91	0.67
1:A:723:LEU:HD22	1:A:727:ILE:HD12	1.76	0.67
1:B:575:ASN:OD1	1:B:576:TYR:N	2.29	0.66
1:L:495:PRO:HD3	1:L:517:HIS:HB2	1.77	0.66
1:K:498:VAL:HG11	1:K:515:ILE:HG21	1.78	0.66
1:F:643:ARG:HH12	1:F:704:GLY:C	1.98	0.65
1:A:749:ARG:HH22	1:F:544:GLU:HG2	1.61	0.65
1:E:575:ASN:OD1	1:E:576:TYR:N	2.29	0.65
1:I:476:LYS:HD3	1:I:753:VAL:HG21	1.77	0.65
1:K:677:MET:HE3	1:K:702:LEU:HA	1.79	0.64
1:E:720:ALA:O	1:E:724:ILE:HG12	1.98	0.64
1:K:636:GLU:OE2	1:K:673:ARG:NH2	2.30	0.64
1:C:486:ILE:HD13	1:C:761:VAL:HG22	1.78	0.63
1:C:578:ASP:OD1	1:C:581:ARG:NH2	2.30	0.63
1:I:574:ILE:HG23	1:I:579:ALA:HB2	1.80	0.63
1:D:481:LEU:HD22	1:D:486:ILE:HD11	1.80	0.63
1:B:560:VAL:HG21	1:B:587:ILE:HD11	1.80	0.63
1:J:535:ARG:HB3	1:J:540:ILE:HD12	1.81	0.63
1:F:605:ASP:OD1	1:F:606:LYS:N	2.32	0.63
1:J:486:ILE:HD13	1:J:761:VAL:HG22	1.81	0.62
1:A:628:ALA:HB2	1:A:710:VAL:HG21	1.80	0.62
1:I:754:ASP:HA	1:I:757:VAL:HG22	1.79	0.62
1:F:610:LEU:HD22	1:F:711:PHE:HE1	1.65	0.62
1:F:502:ILE:HG23	1:F:510:LEU:HD11	1.81	0.62
1:B:752:THR:HG23	1:B:755:GLY:H	1.65	0.62
1:H:449:ARG:NH1	1:H:637:TYR:OH	2.33	0.62
1:E:502:ILE:HG13	1:E:503:LYS:N	2.15	0.62
1:D:498:VAL:HG21	1:D:515:ILE:HD13	1.82	0.62
1:B:547:ARG:NH2	1:G:573:SER:O	2.27	0.62
1:C:440:LYS:HD2	1:C:440:LYS:N	2.16	0.61
1:J:544:GLU:OE1	1:J:547:ARG:NH2	2.33	0.61
1:C:450:VAL:HA	1:C:768:GLN:NE2	2.13	0.61
1:J:715:GLU:O	1:J:719:ILE:HG12	2.00	0.61
1:A:727:ILE:HD11	1:B:688:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:ARG:HA	1:F:452:GLN:HG2	1.83	0.60
1:L:496:GLU:O	1:L:500:GLU:HG3	2.02	0.60
1:E:498:VAL:O	1:E:502:ILE:HG23	2.01	0.60
1:D:439:SER:N	1:D:731:GLU:OE1	2.35	0.60
1:H:541:ASN:HD21	1:E:749:ARG:NH2	2.00	0.60
1:H:494:TYR:HB2	1:H:497:ARG:HG2	1.84	0.60
1:J:729:LYS:HG3	1:I:729:LYS:CB	2.31	0.59
1:K:647:LEU:HD11	1:K:709:LEU:HB3	1.83	0.59
1:A:600:PHE:HB2	1:A:733:ILE:CG1	2.33	0.59
1:D:598:LEU:HD11	1:D:609:VAL:HG13	1.84	0.59
1:H:541:ASN:HD21	1:E:749:ARG:HH21	1.50	0.59
1:E:502:ILE:HB	1:E:510:LEU:HD11	1.85	0.59
1:B:537:ARG:NH2	1:H:679:GLU:OE1	2.34	0.59
1:I:575:ASN:OD1	1:I:576:TYR:N	2.36	0.59
1:K:644:VAL:HG22	1:K:708:VAL:HB	1.83	0.59
1:H:509:LEU:HD12	1:H:509:LEU:O	2.03	0.58
1:I:486:ILE:HD13	1:I:761:VAL:HG22	1.85	0.58
1:L:637:TYR:HE1	1:L:765:LEU:HD21	1.68	0.58
1:B:664:LYS:HE3	1:B:668:ILE:HD11	1.83	0.58
1:B:447:ILE:O	1:B:450:VAL:HG12	2.03	0.58
1:B:536:GLN:HB2	1:H:699:PHE:CE2	2.39	0.58
1:H:505:LEU:HB2	1:H:507:ILE:HD11	1.85	0.58
1:F:610:LEU:HD22	1:F:711:PHE:CE1	2.38	0.58
1:B:580:VAL:HG23	1:B:737:LEU:HD11	1.86	0.57
1:C:468:GLU:OE1	1:C:572:SER:N	2.37	0.57
1:I:691:GLU:OE1	1:I:695:ARG:NH1	2.38	0.57
1:C:498:VAL:HG11	1:C:515:ILE:HD13	1.84	0.57
1:A:486:ILE:HD13	1:A:761:VAL:HG22	1.86	0.57
1:J:636:GLU:OE1	1:J:673:ARG:NH2	2.38	0.57
1:J:692:ILE:HG23	1:J:696:LEU:HD12	1.87	0.57
1:G:628:ALA:HB1	1:G:644:VAL:HG11	1.87	0.57
1:C:642:PRO:HG2	1:C:676:LEU:CD1	2.35	0.57
1:J:729:LYS:HG3	1:I:729:LYS:HB2	1.86	0.57
1:A:722:LYS:HE2	1:B:683:GLN:OE1	2.05	0.56
1:F:447:ILE:HD11	1:F:761:VAL:HG22	1.88	0.56
1:J:560:VAL:HG21	1:J:587:ILE:HD11	1.87	0.56
1:B:670:ARG:NH1	1:B:678:ILE:O	2.39	0.56
1:F:578:ASP:OD1	1:F:581:ARG:NH2	2.39	0.56
1:B:510:LEU:O	1:B:513:VAL:HG22	2.05	0.56
1:B:560:VAL:CG2	1:B:587:ILE:HD11	2.35	0.56
1:A:751:THR:HG22	1:A:752:THR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:601:VAL:HB	1:H:608:LEU:HB2	1.86	0.56
1:C:440:LYS:HD2	1:C:440:LYS:H	1.71	0.55
1:B:442:PHE:HE2	1:B:762:PHE:HZ	1.53	0.55
1:G:498:VAL:HG11	1:G:515:ILE:HG21	1.88	0.55
1:L:481:LEU:HD11	1:L:757:VAL:HG13	1.88	0.55
1:D:628:ALA:HB2	1:D:710:VAL:HG21	1.87	0.55
1:B:589:VAL:HG11	1:B:595:PRO:HD3	1.88	0.55
1:J:578:ASP:OD1	1:J:581:ARG:NH2	2.38	0.55
1:B:499:LYS:NZ	1:B:511:ASN:O	2.38	0.55
1:C:600:PHE:HB2	1:C:733:ILE:HG12	1.87	0.55
1:A:644:VAL:HG22	1:A:708:VAL:HB	1.89	0.55
1:B:468:GLU:OE2	1:B:572:SER:HB2	2.06	0.55
1:H:495:PRO:HA	1:H:515:ILE:HG21	1.89	0.55
1:D:560:VAL:HG21	1:D:587:ILE:HD11	1.89	0.55
1:D:736:PHE:HE1	1:D:759:SER:HA	1.71	0.55
1:B:601:VAL:HG22	1:B:608:LEU:HB3	1.88	0.55
1:D:752:THR:OG1	1:D:753:VAL:N	2.39	0.54
1:D:541:ASN:CG	1:K:749:ARG:HH12	2.11	0.54
1:G:579:ALA:HB3	1:G:746:VAL:HG11	1.87	0.54
1:G:642:PRO:HG2	1:G:676:LEU:HD21	1.89	0.54
1:H:643:ARG:HG2	1:H:677:MET:HE2	1.88	0.54
1:B:754:ASP:O	1:B:758:ASN:ND2	2.40	0.54
1:E:573:SER:HA	1:E:749:ARG:HH11	1.72	0.54
1:F:679:GLU:OE2	1:H:537:ARG:NH1	2.37	0.54
1:G:601:VAL:HB	1:G:608:LEU:HB2	1.88	0.54
1:F:723:LEU:HD13	1:E:684:ALA:HB1	1.89	0.54
1:J:663:LYS:NZ	1:J:667:GLU:OE2	2.33	0.54
1:H:449:ARG:HG2	1:H:453:ASN:HD21	1.73	0.54
1:K:754:ASP:OD1	1:K:754:ASP:N	2.28	0.54
1:D:495:PRO:HA	1:D:515:ILE:HG12	1.90	0.54
1:A:696:LEU:HD11	1:B:750:THR:HG22	1.90	0.54
1:G:729:LYS:HD3	1:H:729:LYS:HB3	1.89	0.54
1:E:502:ILE:HB	1:E:510:LEU:CD1	2.38	0.54
1:J:601:VAL:HB	1:J:608:LEU:HB2	1.91	0.53
1:C:642:PRO:HG2	1:C:676:LEU:HD11	1.89	0.53
1:D:569:VAL:HG21	1:D:760:VAL:HG22	1.91	0.53
1:L:447:ILE:O	1:L:450:VAL:HG12	2.08	0.53
1:H:447:ILE:O	1:H:450:VAL:HG12	2.09	0.53
1:D:449:ARG:HA	1:D:452:GLN:HG2	1.90	0.53
1:D:554:TYR:CE2	1:D:582:PRO:HG3	2.42	0.53
1:F:751:THR:HG22	1:F:752:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:754:ASP:HA	1:J:757:VAL:HG12	1.90	0.53
1:L:467:PRO:HA	1:L:492:LEU:HB2	1.91	0.53
1:L:475:LEU:HD13	1:L:502:ILE:HG22	1.90	0.53
1:K:449:ARG:HH11	1:K:449:ARG:CG	2.18	0.53
1:D:685:ASP:OD2	1:D:686:THR:N	2.42	0.53
1:L:721:TYR:OH	1:L:748:GLN:OE1	2.27	0.53
1:D:751:THR:HG22	1:D:752:THR:O	2.08	0.53
1:B:756:ILE:O	1:B:760:VAL:HG23	2.09	0.53
1:I:578:ASP:HA	1:I:581:ARG:NH1	2.24	0.53
1:B:481:LEU:HD21	1:B:757:VAL:HG13	1.89	0.53
1:F:440:LYS:HA	1:F:443:ILE:HG22	1.91	0.53
1:F:772:GLU:HG3	1:F:775:LYS:HE3	1.90	0.53
1:G:449:ARG:O	1:G:453:ASN:ND2	2.39	0.53
1:B:547:ARG:HH12	1:G:573:SER:C	2.12	0.53
1:K:491:LEU:HB2	1:K:515:ILE:HG12	1.90	0.53
1:F:724:ILE:HD13	1:E:727:ILE:HD11	1.91	0.52
1:G:729:LYS:NZ	1:H:729:LYS:HG2	2.24	0.52
1:L:547:ARG:HH12	1:I:573:SER:C	2.12	0.52
1:C:589:VAL:HG11	1:C:595:PRO:HD3	1.91	0.52
1:L:498:VAL:HG21	1:L:515:ILE:HG12	1.92	0.52
1:H:770:ILE:O	1:H:774:LEU:HG	2.09	0.52
1:D:596:ALA:HB1	1:D:612:ASP:HB2	1.91	0.52
1:L:603:LEU:HD12	1:L:606:LYS:HE3	1.92	0.52
1:A:608:LEU:HD23	1:A:709:LEU:HD21	1.90	0.52
1:G:729:LYS:HZ3	1:H:729:LYS:HG2	1.75	0.52
1:C:690:PRO:O	1:C:694:GLU:HG2	2.08	0.52
1:I:449:ARG:HD2	1:I:637:TYR:OH	2.10	0.52
1:I:771:LYS:O	1:I:775:LYS:HG2	2.09	0.52
1:E:465:VAL:HG21	1:E:559:MET:HE3	1.92	0.52
1:F:540:ILE:HG23	1:F:544:GLU:HB3	1.92	0.52
1:F:643:ARG:HH12	1:F:704:GLY:CA	2.23	0.52
1:G:544:GLU:HG2	1:G:547:ARG:NH1	2.16	0.52
1:A:472:THR:HG23	1:A:505:LEU:HD11	1.92	0.51
1:J:561:ASN:OD1	1:J:562:GLN:NE2	2.41	0.51
1:A:495:PRO:HA	1:A:515:ILE:HG21	1.91	0.51
1:E:609:VAL:HG21	1:E:631:ALA:HB1	1.90	0.51
1:B:507:ILE:HD12	1:B:508:PRO:HD2	1.92	0.51
1:D:502:ILE:HG13	1:D:503:LYS:N	2.25	0.51
1:B:605:ASP:OD1	1:B:606:LYS:N	2.37	0.51
1:B:449:ARG:NH1	1:B:637:TYR:OH	2.44	0.51
1:H:754:ASP:O	1:H:757:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:729:LYS:CD	1:H:729:LYS:H	2.23	0.51
1:J:636:GLU:CD	1:J:673:ARG:HH22	2.13	0.51
1:I:511:ASN:O	1:I:512:ASP:HB2	2.10	0.51
1:D:598:LEU:HD13	1:D:611:ALA:HB2	1.93	0.51
1:B:723:LEU:HD22	1:B:727:ILE:HD11	1.93	0.51
1:G:642:PRO:HG2	1:G:676:LEU:CD2	2.41	0.51
1:H:591:LYS:HG3	1:H:592:GLU:HG2	1.93	0.51
1:C:605:ASP:OD1	1:C:606:LYS:N	2.44	0.51
1:A:598:LEU:HG	1:A:609:VAL:HG13	1.93	0.51
1:J:656:GLU:OE2	1:J:660:ARG:NH2	2.44	0.51
1:I:478:LEU:HA	1:I:481:LEU:HG	1.93	0.50
1:F:772:GLU:HA	1:F:775:LYS:HE3	1.93	0.50
1:H:437:SER:O	1:H:441:VAL:HG23	2.12	0.50
1:I:447:ILE:O	1:I:450:VAL:HG12	2.11	0.50
1:J:686:THR:HG22	1:J:693:MET:HE1	1.93	0.50
1:I:670:ARG:NH1	1:I:678:ILE:O	2.41	0.50
1:G:577:ALA:O	1:G:580:VAL:HG12	2.12	0.50
1:K:494:TYR:O	1:K:498:VAL:HG12	2.11	0.50
1:F:628:ALA:HB2	1:F:710:VAL:HG21	1.94	0.50
1:A:683:GLN:OE1	1:B:722:LYS:NZ	2.45	0.50
1:G:677:MET:HG3	1:G:701:GLY:O	2.11	0.50
1:H:478:LEU:O	1:H:482:VAL:HG22	2.12	0.50
1:H:571:GLY:HA2	1:H:574:ILE:HG12	1.94	0.50
1:F:608:LEU:HD11	1:F:707:ASN:HA	1.94	0.49
1:E:567:GLY:HA2	1:E:743:SER:O	2.12	0.49
1:H:769:TYR:O	1:H:773:VAL:HG13	2.11	0.49
1:K:651:ASN:ND2	1:K:683:GLN:OE1	2.45	0.49
1:K:658:THR:HG23	1:K:659:PRO:HD3	1.93	0.49
1:J:465:VAL:HA	1:J:490:ILE:HB	1.93	0.49
1:L:647:LEU:HD11	1:L:709:LEU:HB3	1.94	0.49
1:K:447:ILE:HG23	1:K:486:ILE:HD11	1.94	0.49
1:L:771:LYS:HA	1:L:774:LEU:HD12	1.94	0.49
1:H:693:MET:CE	1:H:702:LEU:HD23	2.42	0.49
1:F:772:GLU:O	1:F:775:LYS:HG2	2.11	0.49
1:J:729:LYS:HE2	1:I:729:LYS:HD2	1.94	0.49
1:L:643:ARG:HB3	1:L:702:LEU:HD11	1.94	0.49
1:A:447:ILE:HG12	1:A:486:ILE:HD11	1.93	0.49
1:F:754:ASP:O	1:F:758:ASN:ND2	2.46	0.49
1:L:656:GLU:OE1	1:L:660:ARG:NH1	2.46	0.49
1:D:576:TYR:CE1	1:D:746:VAL:HG23	2.48	0.49
1:F:644:VAL:HB	1:F:678:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:507:ILE:HD12	1:L:508:PRO:HD2	1.95	0.49
1:E:601:VAL:HG22	1:E:608:LEU:HB2	1.95	0.49
1:F:502:ILE:HD13	1:F:510:LEU:HD13	1.95	0.48
1:H:746:VAL:HG12	1:H:747:LEU:O	2.12	0.48
1:J:499:LYS:O	1:J:502:ILE:HG13	2.12	0.48
1:J:719:ILE:HD12	1:I:647:LEU:HB3	1.95	0.48
1:C:649:TYR:CG	1:D:714:LEU:HD23	2.49	0.48
1:D:647:LEU:O	1:D:662:MET:HG3	2.13	0.48
1:J:481:LEU:HD11	1:J:757:VAL:HA	1.95	0.48
1:L:561:ASN:HD22	1:L:562:GLN:NE2	2.11	0.48
1:H:644:VAL:HB	1:H:678:ILE:HG23	1.95	0.48
1:K:572:SER:HB3	1:K:747:LEU:HD12	1.96	0.48
1:J:729:LYS:HE2	1:I:729:LYS:CD	2.43	0.48
1:A:729:LYS:HD3	1:B:729:LYS:HE2	1.96	0.48
1:H:560:VAL:CG2	1:H:587:ILE:HD11	2.44	0.48
1:A:444:ARG:HE	1:A:444:ARG:HA	1.77	0.48
1:J:729:LYS:HG3	1:I:729:LYS:HB3	1.95	0.48
1:L:596:ALA:HB1	1:L:612:ASP:HB2	1.96	0.48
1:H:605:ASP:OD1	1:H:606:LYS:N	2.40	0.48
1:D:494:TYR:O	1:D:498:VAL:HG13	2.13	0.48
1:C:700:SER:O	1:H:703:LYS:HE3	2.13	0.48
1:J:606:LYS:HZ1	1:J:640:ILE:HG21	1.79	0.48
1:G:468:GLU:H	1:G:468:GLU:HG2	1.41	0.47
1:L:594:ILE:HD12	1:L:595:PRO:HD2	1.96	0.47
1:E:601:VAL:CG2	1:E:608:LEU:HB2	2.44	0.47
1:G:775:LYS:O	1:G:776:SER:OG	2.19	0.47
1:G:579:ALA:HB3	1:G:746:VAL:CG1	2.43	0.47
1:I:478:LEU:HD23	1:I:481:LEU:HD21	1.97	0.47
1:G:663:LYS:O	1:G:667:GLU:HG2	2.15	0.47
1:J:530:LYS:HD3	1:J:562:GLN:NE2	2.29	0.47
1:L:613:THR:HA	1:L:717:SER:HB2	1.96	0.47
1:H:595:PRO:HB2	1:H:615:VAL:HG11	1.97	0.47
1:C:444:ARG:HG2	1:G:504:ALA:HA	1.95	0.47
1:F:502:ILE:HG12	1:F:510:LEU:HD22	1.95	0.47
1:H:723:LEU:HD23	1:H:723:LEU:HA	1.58	0.47
1:E:610:LEU:HD22	1:E:711:PHE:CE1	2.50	0.47
1:D:447:ILE:O	1:D:450:VAL:HG12	2.15	0.47
1:E:692:ILE:HG23	1:E:696:LEU:HD12	1.97	0.47
1:F:753:VAL:O	1:F:757:VAL:HG23	2.15	0.47
1:J:669:ALA:HB1	1:J:678:ILE:HD13	1.96	0.47
1:H:492:LEU:HD21	1:H:559:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:551:ASP:OD1	1:I:552:PRO:HD2	2.13	0.47
1:K:492:LEU:HD21	1:K:559:MET:HE1	1.95	0.47
1:C:544:GLU:OE2	1:C:547:ARG:NH2	2.44	0.47
1:J:673:ARG:HG2	1:J:675:ASP:OD1	2.15	0.47
1:L:548:LEU:HD22	1:L:554:TYR:CE1	2.50	0.47
1:K:723:LEU:O	1:K:727:ILE:HG12	2.15	0.47
1:E:472:THR:HG23	1:E:505:LEU:HD22	1.96	0.47
1:C:600:PHE:HB2	1:C:733:ILE:CG1	2.44	0.47
1:B:532:TYR:HE1	1:B:541:ASN:HA	1.80	0.47
1:F:647:LEU:O	1:F:662:MET:HG3	2.15	0.47
1:L:477:ALA:O	1:L:481:LEU:HD13	2.14	0.47
1:C:614:THR:HG23	1:C:615:VAL:HG23	1.97	0.47
1:A:602:LEU:HD11	1:A:733:ILE:HG12	1.96	0.47
1:H:494:TYR:HB2	1:H:497:ARG:CG	2.45	0.47
1:I:751:THR:HG22	1:I:752:THR:O	2.15	0.47
1:L:478:LEU:O	1:L:482:VAL:HG22	2.15	0.46
1:K:498:VAL:CG1	1:K:515:ILE:HD13	2.45	0.46
1:D:497:ARG:HD2	1:D:497:ARG:HA	1.69	0.46
1:C:647:LEU:O	1:C:662:MET:HG3	2.14	0.46
1:A:754:ASP:HA	1:A:757:VAL:CG1	2.45	0.46
1:B:436:GLY:CA	1:B:731:GLU:OE2	2.59	0.46
1:F:481:LEU:CD1	1:F:757:VAL:HG22	2.46	0.46
1:F:726:GLN:OE1	1:E:689:ASN:HB2	2.15	0.46
1:J:724:ILE:HD11	1:I:723:LEU:HD13	1.97	0.46
1:K:572:SER:HB3	1:K:747:LEU:CD1	2.45	0.46
1:C:597:GLY:HA3	1:C:614:THR:HG22	1.98	0.46
1:F:469:GLY:HA2	1:F:491:LEU:HD22	1.96	0.46
1:G:628:ALA:HB2	1:G:710:VAL:HG21	1.96	0.46
1:I:449:ARG:HD2	1:I:637:TYR:CZ	2.51	0.46
1:J:644:VAL:HB	1:J:678:ILE:HG23	1.98	0.46
1:H:560:VAL:HG21	1:H:587:ILE:HD11	1.97	0.46
1:H:600:PHE:HB2	1:H:733:ILE:CG1	2.46	0.46
1:E:573:SER:HA	1:E:749:ARG:NH1	2.30	0.46
1:B:598:LEU:HD12	1:B:599:ASN:N	2.31	0.46
1:J:676:LEU:HA	1:J:676:LEU:HD23	1.72	0.46
1:B:443:ILE:HG12	1:B:758:ASN:OD1	2.15	0.46
1:J:560:VAL:CG2	1:J:587:ILE:HD11	2.46	0.46
1:L:497:ARG:O	1:L:500:GLU:HB2	2.16	0.46
1:A:600:PHE:HB2	1:A:733:ILE:HG13	1.98	0.46
1:A:774:LEU:C	1:A:774:LEU:CD2	2.84	0.46
1:H:465:VAL:HG21	1:H:559:MET:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:PRO:O	1:H:703:LYS:HE2	2.16	0.46
1:B:572:SER:O	1:B:749:ARG:NH1	2.45	0.46
1:K:503:LYS:HE2	1:K:503:LYS:HB2	1.69	0.46
1:D:541:ASN:ND2	1:K:749:ARG:NH1	2.58	0.45
1:A:600:PHE:HB2	1:A:733:ILE:HG12	1.98	0.45
1:B:675:ASP:OD1	1:B:675:ASP:N	2.40	0.45
1:L:754:ASP:O	1:L:758:ASN:ND2	2.50	0.45
1:H:770:ILE:O	1:H:773:VAL:HG22	2.16	0.45
1:K:472:THR:HG22	1:K:476:LYS:HD2	1.99	0.45
1:C:460:GLU:OE2	1:C:771:LYS:NZ	2.49	0.45
1:A:754:ASP:HA	1:A:757:VAL:HG12	1.98	0.45
1:A:756:ILE:O	1:A:760:VAL:HG23	2.16	0.45
1:F:559:MET:HE1	1:F:565:ALA:HB2	1.98	0.45
1:F:770:ILE:HA	1:F:773:VAL:HG22	1.97	0.45
1:J:723:LEU:HD23	1:J:723:LEU:HA	1.68	0.45
1:E:455:ALA:O	1:E:456:ALA:HB3	2.16	0.45
1:B:676:LEU:HA	1:B:676:LEU:HD23	1.69	0.45
1:F:447:ILE:HD13	1:F:447:ILE:HA	1.75	0.45
1:C:542:LEU:O	1:C:546:GLU:HG3	2.15	0.45
1:D:481:LEU:HD21	1:D:757:VAL:HG13	1.97	0.45
1:D:527:PHE:CE1	1:D:562:GLN:HG3	2.51	0.45
1:B:723:LEU:HD23	1:B:723:LEU:HA	1.73	0.45
1:J:481:LEU:HD21	1:J:760:VAL:HG11	1.98	0.45
1:I:541:ASN:ND2	1:K:696:LEU:O	2.48	0.45
1:C:699:PHE:HD1	1:K:532:TYR:HH	1.64	0.45
1:D:507:ILE:HD11	1:D:509:LEU:HG	1.99	0.45
1:D:636:GLU:HG3	1:D:642:PRO:HG3	1.98	0.45
1:B:669:ALA:HB1	1:B:678:ILE:HD13	1.99	0.45
1:F:686:THR:HG22	1:F:693:MET:HE1	1.98	0.45
1:L:481:LEU:HD11	1:L:757:VAL:HA	1.99	0.45
1:H:467:PRO:HA	1:H:492:LEU:HB2	1.99	0.45
1:H:749:ARG:HG3	1:H:750:THR:HG23	1.99	0.45
1:K:437:SER:O	1:K:440:LYS:N	2.50	0.45
1:E:540:ILE:HG23	1:E:544:GLU:HB3	1.98	0.45
1:E:498:VAL:HG11	1:E:515:ILE:HG12	1.99	0.45
1:E:723:LEU:O	1:E:727:ILE:HG12	2.17	0.45
1:D:481:LEU:CD2	1:D:757:VAL:HG13	2.47	0.45
1:B:598:LEU:CD1	1:B:609:VAL:HG13	2.42	0.45
1:B:660:ARG:HG2	1:B:660:ARG:HH11	1.82	0.45
1:F:769:TYR:O	1:F:773:VAL:HG13	2.16	0.45
1:J:594:ILE:HD12	1:J:595:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:440:LYS:N	1:L:440:LYS:HD2	2.30	0.45
1:L:494:TYR:CE1	1:L:517:HIS:CE1	3.05	0.45
1:L:672:LEU:O	1:L:673:ARG:HG2	2.17	0.45
1:K:628:ALA:HB2	1:K:710:VAL:HG21	1.99	0.45
1:E:447:ILE:HG23	1:E:486:ILE:HD11	1.98	0.45
1:H:747:LEU:HB3	1:H:751:THR:HG21	1.99	0.45
1:I:440:LYS:HA	1:I:443:ILE:HG22	1.99	0.45
1:I:497:ARG:O	1:I:500:GLU:HB3	2.17	0.45
1:E:648:SER:OG	1:E:649:TYR:N	2.48	0.45
1:K:507:ILE:HG21	1:K:510:LEU:HD13	1.99	0.45
1:D:729:LYS:HD2	1:D:729:LYS:HA	1.80	0.45
1:J:477:ALA:O	1:J:481:LEU:HD13	2.17	0.45
1:L:724:ILE:CD1	1:K:727:ILE:HD11	2.43	0.45
1:K:647:LEU:O	1:K:662:MET:HG3	2.17	0.45
1:D:769:TYR:O	1:D:773:VAL:HG23	2.17	0.44
1:A:524:TYR:O	1:A:528:VAL:HG13	2.17	0.44
1:G:544:GLU:CG	1:G:547:ARG:HH12	2.17	0.44
1:J:467:PRO:HA	1:J:492:LEU:HD12	1.99	0.44
1:I:478:LEU:HD13	1:I:510:LEU:HD21	1.99	0.44
1:G:647:LEU:O	1:G:662:MET:HG3	2.17	0.44
1:G:749:ARG:C	1:G:751:THR:H	2.21	0.44
1:J:579:ALA:O	1:J:582:PRO:HD2	2.18	0.44
1:C:669:ALA:HB1	1:C:678:ILE:HD13	2.00	0.44
1:F:544:GLU:OE2	1:F:547:ARG:NE	2.43	0.44
1:J:589:VAL:HG11	1:J:595:PRO:HD3	2.00	0.44
1:J:643:ARG:HB3	1:J:702:LEU:CD1	2.47	0.44
1:H:628:ALA:HB2	1:H:710:VAL:HG21	1.99	0.44
1:I:756:ILE:O	1:I:760:VAL:HG23	2.18	0.44
1:A:453:ASN:OD1	1:A:768:GLN:CD	2.53	0.44
1:A:647:LEU:O	1:A:662:MET:HG3	2.17	0.44
1:A:723:LEU:HD23	1:A:723:LEU:HA	1.64	0.44
1:L:715:GLU:O	1:L:719:ILE:HG12	2.18	0.44
1:I:478:LEU:CD1	1:I:491:LEU:HD11	2.47	0.44
1:J:501:LYS:HA	1:J:504:ALA:HB3	1.99	0.44
1:L:756:ILE:O	1:L:760:VAL:HG23	2.18	0.44
1:E:478:LEU:HD23	1:E:478:LEU:HA	1.73	0.44
1:E:694:GLU:OE2	1:E:703:LYS:NZ	2.31	0.44
1:C:466:PHE:HB2	1:C:491:LEU:HD23	2.00	0.44
1:B:580:VAL:CG2	1:B:737:LEU:HD11	2.47	0.44
1:F:594:ILE:HD12	1:F:595:PRO:HD2	2.00	0.44
1:F:618:ASN:OD1	1:F:661:LYS:NZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:672:LEU:HD23	1:G:672:LEU:HA	1.70	0.44
1:H:689:ASN:CG	1:H:692:ILE:HD12	2.38	0.44
1:K:507:ILE:CG2	1:K:510:LEU:HD13	2.48	0.44
1:E:754:ASP:O	1:E:758:ASN:ND2	2.51	0.44
1:D:518:PRO:HB3	1:D:555:PHE:CG	2.53	0.44
1:F:608:LEU:CD1	1:F:707:ASN:HA	2.47	0.44
1:J:535:ARG:HD3	1:J:540:ILE:HD12	2.00	0.44
1:L:525:PHE:O	1:L:528:VAL:HG22	2.18	0.44
1:L:644:VAL:HG22	1:L:708:VAL:HB	2.00	0.44
1:H:642:PRO:HG2	1:H:676:LEU:HD21	1.99	0.44
1:D:758:ASN:O	1:D:762:PHE:HD2	2.01	0.44
1:G:685:ASP:OD1	1:G:685:ASP:N	2.50	0.44
1:D:481:LEU:HD22	1:D:486:ILE:CD1	2.45	0.43
1:G:764:ALA:O	1:G:768:GLN:HG2	2.17	0.43
1:D:593:GLY:O	1:D:594:ILE:HD12	2.18	0.43
1:A:444:ARG:NH1	1:A:484:GLU:OE1	2.51	0.43
1:F:498:VAL:CG1	1:F:515:ILE:HD13	2.48	0.43
1:F:589:VAL:HG11	1:F:595:PRO:HD3	1.99	0.43
1:F:598:LEU:HD13	1:F:611:ALA:HB2	2.00	0.43
1:G:591:LYS:HG2	1:G:592:GLU:HG3	2.01	0.43
1:L:576:TYR:OH	1:L:614:THR:HG21	2.18	0.43
1:B:478:LEU:HD23	1:B:478:LEU:HA	1.87	0.43
1:G:601:VAL:HG13	1:G:730:ALA:HB1	2.00	0.43
1:J:498:VAL:O	1:J:502:ILE:HG23	2.17	0.43
1:I:677:MET:HE1	1:I:703:LYS:O	2.18	0.43
1:K:746:VAL:HG12	1:K:747:LEU:O	2.18	0.43
1:D:536:GLN:HA	1:D:540:ILE:O	2.18	0.43
1:D:643:ARG:HG2	1:D:677:MET:CE	2.44	0.43
1:G:497:ARG:NH1	1:G:500:GLU:OE1	2.52	0.43
1:C:694:GLU:OE1	1:H:704:GLY:N	2.51	0.43
1:B:501:LYS:O	1:B:505:LEU:HD13	2.19	0.43
1:L:440:LYS:HD2	1:L:440:LYS:H	1.84	0.43
1:I:467:PRO:HD2	1:I:569:VAL:O	2.18	0.43
1:H:677:MET:HE1	1:H:703:LYS:O	2.19	0.43
1:I:675:ASP:OD1	1:I:675:ASP:N	2.49	0.43
1:C:478:LEU:HA	1:C:481:LEU:HG	1.99	0.43
1:B:472:THR:HG22	1:B:501:LYS:HE2	2.01	0.43
1:B:647:LEU:O	1:B:662:MET:HG3	2.19	0.43
1:F:719:ILE:O	1:F:723:LEU:HB2	2.19	0.43
1:L:547:ARG:NH1	1:I:573:SER:OG	2.52	0.43
1:D:579:ALA:O	1:D:582:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ILE:HD13	1:B:484:GLU:HG2	2.00	0.43
1:B:468:GLU:HG3	1:B:474:VAL:HG21	2.01	0.43
1:B:574:ILE:HG13	1:B:579:ALA:CB	2.45	0.43
1:J:647:LEU:O	1:J:662:MET:HG3	2.19	0.43
1:L:579:ALA:O	1:L:582:PRO:HD2	2.18	0.43
1:K:723:LEU:HD23	1:K:723:LEU:HA	1.83	0.43
1:E:610:LEU:HD22	1:E:711:PHE:HE1	1.83	0.43
1:J:664:LYS:O	1:J:668:ILE:HG13	2.19	0.42
1:E:607:PHE:CE2	1:E:640:ILE:HD12	2.54	0.42
1:A:589:VAL:HG11	1:A:595:PRO:HD3	2.00	0.42
1:F:481:LEU:HD11	1:F:757:VAL:HG22	2.02	0.42
1:F:636:GLU:HG3	1:F:642:PRO:HG3	2.01	0.42
1:J:647:LEU:HD11	1:J:709:LEU:HB3	2.01	0.42
1:H:470:THR:O	1:H:501:LYS:HD3	2.19	0.42
1:H:677:MET:CE	1:H:702:LEU:HD12	2.49	0.42
1:I:510:LEU:HD12	1:I:510:LEU:HA	1.90	0.42
1:E:581:ARG:HB3	1:E:582:PRO:HD3	2.01	0.42
1:D:491:LEU:O	1:D:515:ILE:HD12	2.20	0.42
1:B:484:GLU:HB3	1:B:486:ILE:HD12	2.02	0.42
1:G:446:ALA:O	1:G:450:VAL:HG23	2.19	0.42
1:G:589:VAL:HG11	1:G:595:PRO:HD3	2.00	0.42
1:H:455:ALA:O	1:H:456:ALA:HB3	2.18	0.42
1:H:600:PHE:HB2	1:H:733:ILE:HG12	2.01	0.42
1:H:754:ASP:HA	1:H:757:VAL:HG22	2.01	0.42
1:I:578:ASP:HA	1:I:581:ARG:HH12	1.83	0.42
1:E:467:PRO:HD2	1:E:569:VAL:O	2.19	0.42
1:E:647:LEU:HD11	1:E:709:LEU:HB3	2.00	0.42
1:C:673:ARG:HG2	1:C:676:LEU:HD23	2.00	0.42
1:A:689:ASN:CG	1:A:692:ILE:HD12	2.39	0.42
1:G:478:LEU:O	1:G:482:VAL:HB	2.19	0.42
1:G:569:VAL:HG21	1:G:760:VAL:HG22	2.01	0.42
1:C:495:PRO:HA	1:C:515:ILE:HG12	2.02	0.42
1:D:651:ASN:HB3	1:D:697:PHE:CZ	2.54	0.42
1:F:470:THR:O	1:F:501:LYS:HD3	2.19	0.42
1:F:502:ILE:HG12	1:F:510:LEU:CD2	2.50	0.42
1:F:636:GLU:CD	1:F:673:ARG:HH22	2.19	0.42
1:J:606:LYS:HG3	1:J:607:PHE:N	2.35	0.42
1:H:449:ARG:NH1	1:H:453:ASN:HD21	2.16	0.42
1:C:510:LEU:O	1:C:513:VAL:HG22	2.19	0.42
1:C:676:LEU:HA	1:C:676:LEU:HD13	1.78	0.42
1:A:721:TYR:OH	1:A:722:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:472:THR:HG22	1:G:505:LEU:HD11	2.01	0.42
1:L:499:LYS:HA	1:L:502:ILE:HG13	2.01	0.42
1:K:581:ARG:HB3	1:K:582:PRO:HD3	2.02	0.42
1:K:677:MET:HE3	1:K:677:MET:HB3	1.90	0.42
1:D:600:PHE:HB2	1:D:733:ILE:HG12	2.02	0.42
1:A:539:GLY:N	1:E:653:SER:HA	2.34	0.42
1:B:573:SER:HA	1:B:749:ARG:NH1	2.35	0.42
1:D:469:GLY:HA2	1:D:491:LEU:HD22	2.01	0.42
1:A:600:PHE:O	1:A:732:VAL:HA	2.20	0.42
1:L:694:GLU:OE2	1:L:703:LYS:HE2	2.20	0.42
1:H:581:ARG:HB3	1:H:582:PRO:HD3	2.02	0.42
1:I:644:VAL:HB	1:I:678:ILE:HG23	2.00	0.42
1:F:534:LEU:HD23	1:F:534:LEU:HA	1.90	0.42
1:F:685:ASP:OD2	1:F:686:THR:N	2.52	0.42
1:G:548:LEU:HA	1:G:548:LEU:HD23	1.87	0.42
1:G:748:GLN:O	1:G:751:THR:HB	2.20	0.42
1:L:607:PHE:CE2	1:L:640:ILE:HD12	2.55	0.42
1:L:669:ALA:HB1	1:L:678:ILE:HD13	2.02	0.42
1:D:775:LYS:O	1:D:776:SER:OG	2.26	0.41
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.72	0.41
1:B:535:ARG:HB3	1:B:540:ILE:HB	2.01	0.41
1:G:571:GLY:C	1:G:573:SER:H	2.22	0.41
1:J:729:LYS:CG	1:I:729:LYS:HB3	2.49	0.41
1:J:736:PHE:HE1	1:J:759:SER:HA	1.85	0.41
1:L:471:SER:O	1:L:475:LEU:HG	2.20	0.41
1:K:535:ARG:HD2	1:K:585:GLN:HB3	2.02	0.41
1:B:438:HIS:CB	1:B:604:GLU:OE2	2.68	0.41
1:J:628:ALA:HB1	1:J:644:VAL:HG11	2.01	0.41
1:C:614:THR:CG2	1:C:615:VAL:HG23	2.49	0.41
1:A:472:THR:HG23	1:A:505:LEU:CD1	2.50	0.41
1:F:606:LYS:HG3	1:F:607:PHE:N	2.35	0.41
1:G:643:ARG:HD3	1:G:705:GLY:O	2.21	0.41
1:J:609:VAL:CG2	1:J:708:VAL:HG22	2.50	0.41
1:L:487:CYS:O	1:L:489:PRO:HD3	2.21	0.41
1:K:736:PHE:HE1	1:K:759:SER:HA	1.86	0.41
1:C:527:PHE:CE1	1:C:562:GLN:HG3	2.55	0.41
1:F:477:ALA:O	1:F:481:LEU:HD13	2.20	0.41
1:F:772:GLU:HG3	1:F:775:LYS:CE	2.50	0.41
1:J:501:LYS:HZ3	1:J:505:LEU:HD11	1.86	0.41
1:E:628:ALA:HB2	1:E:710:VAL:HG21	2.02	0.41
1:F:495:PRO:HA	1:F:515:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:736:PHE:HD1	1:G:745:ASN:HD21	1.69	0.41
1:J:519:SER:HA	1:J:524:TYR:CD2	2.55	0.41
1:H:693:MET:HE3	1:H:702:LEU:HD23	2.03	0.41
1:K:672:LEU:HA	1:K:672:LEU:HD23	1.83	0.41
1:C:444:ARG:NH2	1:C:484:GLU:OE2	2.53	0.41
1:C:479:ALA:HB2	1:C:507:ILE:HG21	2.02	0.41
1:B:476:LYS:O	1:B:479:ALA:HB3	2.19	0.41
1:F:440:LYS:O	1:F:443:ILE:HG22	2.21	0.41
1:G:478:LEU:HD23	1:G:478:LEU:HA	1.62	0.41
1:G:675:ASP:OD1	1:G:675:ASP:N	2.50	0.41
1:J:608:LEU:CD2	1:J:707:ASN:HA	2.50	0.41
1:L:676:LEU:HD23	1:L:676:LEU:HA	1.90	0.41
1:E:676:LEU:HD23	1:E:676:LEU:HA	1.65	0.41
1:D:541:ASN:CG	1:K:749:ARG:NH1	2.73	0.41
1:F:535:ARG:HB3	1:F:540:ILE:HD12	2.02	0.41
1:A:488:GLN:HA	1:A:489:PRO:HD3	1.88	0.41
1:F:449:ARG:NH1	1:F:637:TYR:O	2.54	0.41
1:L:608:LEU:CD2	1:L:707:ASN:HA	2.51	0.41
1:H:676:LEU:HD23	1:H:676:LEU:HA	1.81	0.41
1:I:686:THR:HG22	1:I:693:MET:HE1	2.02	0.41
1:C:642:PRO:HG2	1:C:676:LEU:HD12	2.02	0.41
1:B:551:ASP:HA	1:B:552:PRO:HD2	1.83	0.41
1:B:629:LEU:HD23	1:B:629:LEU:HA	1.84	0.41
1:B:775:LYS:HE2	1:B:775:LYS:HB3	1.87	0.41
1:F:467:PRO:HA	1:F:492:LEU:HB2	2.03	0.41
1:F:478:LEU:HA	1:F:478:LEU:HD23	1.75	0.41
1:G:729:LYS:HZ3	1:H:729:LYS:H	1.68	0.41
1:J:481:LEU:HD21	1:J:760:VAL:CG1	2.51	0.41
1:L:482:VAL:HG23	1:L:509:LEU:HD23	2.03	0.41
1:L:589:VAL:HG11	1:L:595:PRO:HD3	2.03	0.41
1:L:605:ASP:OD1	1:L:606:LYS:N	2.51	0.41
1:H:636:GLU:OE2	1:H:673:ARG:NH2	2.41	0.41
1:I:775:LYS:O	1:I:776:SER:OG	2.32	0.41
1:E:644:VAL:HG22	1:E:708:VAL:HB	2.03	0.41
1:C:449:ARG:HB3	1:C:765:LEU:HD21	2.03	0.41
1:D:560:VAL:CG2	1:D:587:ILE:HD11	2.50	0.41
1:D:581:ARG:HB3	1:D:582:PRO:HD3	2.02	0.41
1:F:644:VAL:HB	1:F:678:ILE:HG12	2.03	0.41
1:I:472:THR:O	1:I:476:LYS:HG3	2.21	0.41
1:E:447:ILE:HG12	1:E:486:ILE:HD11	2.03	0.41
1:D:723:LEU:O	1:D:727:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:754:ASP:OD1	1:D:754:ASP:N	2.38	0.40
1:B:605:ASP:OD1	1:B:606:LYS:HG2	2.21	0.40
1:F:481:LEU:HD11	1:F:757:VAL:HA	2.03	0.40
1:F:677:MET:HG3	1:F:701:GLY:O	2.20	0.40
1:G:636:GLU:HG3	1:G:642:PRO:HG3	2.03	0.40
1:G:651:ASN:HB3	1:G:697:PHE:CZ	2.56	0.40
1:I:478:LEU:HD11	1:I:491:LEU:HD11	2.03	0.40
1:K:676:LEU:HD23	1:K:676:LEU:HA	1.75	0.40
1:F:775:LYS:O	1:F:775:LYS:HG3	2.21	0.40
1:J:679:GLU:HG2	1:J:700:SER:OG	2.21	0.40
1:F:511:ASN:OD1	1:F:511:ASN:N	2.53	0.40
1:G:765:LEU:HD23	1:G:765:LEU:HA	1.92	0.40
1:J:488:GLN:HA	1:J:489:PRO:HD3	1.85	0.40
1:K:711:PHE:CD2	1:K:717:SER:HA	2.57	0.40
1:F:598:LEU:HD12	1:F:610:LEU:O	2.21	0.40
1:G:443:ILE:HD12	1:G:758:ASN:OD1	2.21	0.40
1:J:600:PHE:HB2	1:J:733:ILE:CG1	2.51	0.40
1:J:606:LYS:HG3	1:J:607:PHE:H	1.86	0.40
1:K:498:VAL:HG13	1:K:515:ILE:HD13	2.02	0.40
1:C:470:THR:O	1:C:501:LYS:NZ	2.49	0.40
1:C:728:GLY:HA2	1:D:728:GLY:O	2.22	0.40
1:A:497:ARG:O	1:A:500:GLU:HB2	2.21	0.40
1:A:628:ALA:HB1	1:A:644:VAL:HG11	2.02	0.40
1:L:481:LEU:HD21	1:L:760:VAL:HB	2.04	0.40
1:L:541:ASN:OD1	1:L:542:LEU:N	2.54	0.40
1:I:611:ALA:O	1:I:710:VAL:HA	2.22	0.40
1:I:651:ASN:HB3	1:I:697:PHE:CZ	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	338/362 (93%)	332 (98%)	6 (2%)	0	100	100
1	B	339/362 (94%)	336 (99%)	3 (1%)	0	100	100
1	C	336/362 (93%)	332 (99%)	4 (1%)	0	100	100
1	D	339/362 (94%)	334 (98%)	5 (2%)	0	100	100
1	E	338/362 (93%)	333 (98%)	5 (2%)	0	100	100
1	F	337/362 (93%)	331 (98%)	6 (2%)	0	100	100
1	G	338/362 (93%)	333 (98%)	5 (2%)	0	100	100
1	H	338/362 (93%)	335 (99%)	3 (1%)	0	100	100
1	I	338/362 (93%)	334 (99%)	4 (1%)	0	100	100
1	J	336/362 (93%)	331 (98%)	5 (2%)	0	100	100
1	K	338/362 (93%)	333 (98%)	5 (2%)	0	100	100
1	L	336/362 (93%)	332 (99%)	3 (1%)	1 (0%)	41	65
All	All	4051/4344 (93%)	3996 (99%)	54 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	508	PRO

5.3.2 Protein sidechains (i)

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	281/301 (93%)	268 (95%)	13 (5%)	27	52
1	B	281/301 (93%)	272 (97%)	9 (3%)	39	67
1	C	282/301 (94%)	274 (97%)	8 (3%)	43	71
1	D	282/301 (94%)	272 (96%)	10 (4%)	36	63
1	E	282/301 (94%)	273 (97%)	9 (3%)	39	67
1	F	281/301 (93%)	278 (99%)	3 (1%)	73	89
1	G	282/301 (94%)	275 (98%)	7 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	282/301 (94%)	275 (98%)	7 (2%)	47 75
1	I	282/301 (94%)	277 (98%)	5 (2%)	59 82
1	J	282/301 (94%)	273 (97%)	9 (3%)	39 67
1	K	282/301 (94%)	276 (98%)	6 (2%)	53 79
1	L	282/301 (94%)	271 (96%)	11 (4%)	32 59
All	All	3381/3612 (94%)	3284 (97%)	97 (3%)	42 70

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	476	LYS
1	C	482	VAL
1	C	498	VAL
1	C	609	VAL
1	C	614	THR
1	C	703	LYS
1	C	721	TYR
1	C	729	LYS
1	D	441	VAL
1	D	497	ARG
1	D	498	VAL
1	D	509	LEU
1	D	535	ARG
1	D	609	VAL
1	D	643	ARG
1	D	703	LYS
1	D	721	TYR
1	D	752	THR
1	A	453	ASN
1	A	482	VAL
1	A	509	LEU
1	A	510	LEU
1	A	511	ASN
1	A	512	ASP
1	A	528	VAL
1	A	574	ILE
1	A	721	TYR
1	A	771	LYS
1	A	772	GLU
1	A	774	LEU

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Mol	Chain	Res	Type
1	A	775	LYS
1	B	506	ASP
1	B	535	ARG
1	B	574	ILE
1	B	609	VAL
1	B	660	ARG
1	B	721	TYR
1	B	729	LYS
1	B	731	GLU
1	B	752	THR
1	F	453	ASN
1	F	510	LEU
1	F	721	TYR
1	G	528	VAL
1	G	709	LEU
1	G	721	TYR
1	G	729	LYS
1	G	748	GLN
1	G	750	THR
1	G	752	THR
1	J	439	SER
1	J	441	VAL
1	J	498	VAL
1	J	515	ILE
1	J	569	VAL
1	J	592	GLU
1	J	721	TYR
1	J	727	ILE
1	J	774	LEU
1	L	441	VAL
1	L	457	ASN
1	L	515	ILE
1	L	525	PHE
1	L	528	VAL
1	L	541	ASN
1	L	591	LYS
1	L	614	THR
1	L	703	LYS
1	L	721	TYR
1	L	765	LEU
1	H	444	ARG
1	H	482	VAL

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Mol	Chain	Res	Type
1	H	509	LEU
1	H	526	SER
1	H	658	THR
1	H	703	LYS
1	H	721	TYR
1	I	542	LEU
1	I	658	THR
1	I	703	LYS
1	I	721	TYR
1	I	727	ILE
1	K	449	ARG
1	K	482	VAL
1	K	609	VAL
1	K	658	THR
1	K	721	TYR
1	K	754	ASP
1	E	443	ILE
1	E	449	ARG
1	E	510	LEU
1	E	512	ASP
1	E	514	SER
1	E	609	VAL
1	E	721	TYR
1	E	729	LYS
1	E	731	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	768	GLN
1	D	541	ASN
1	A	768	GLN
1	F	758	ASN
1	L	562	GLN
1	H	453	ASN
1	H	768	GLN
1	I	517	HIS
1	I	748	GLN
1	E	758	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	340/362 (93%)	0.55	27 (7%) 12 11	48, 81, 150, 174	0
1	B	341/362 (94%)	0.43	13 (3%) 40 40	42, 72, 131, 182	0
1	C	338/362 (93%)	0.40	10 (2%) 50 51	36, 63, 119, 183	0
1	D	341/362 (94%)	0.44	11 (3%) 47 48	33, 67, 123, 187	0
1	E	340/362 (93%)	0.68	29 (8%) 10 9	32, 89, 144, 202	0
1	F	339/362 (93%)	0.90	53 (15%) 2 1	61, 100, 154, 187	0
1	G	340/362 (93%)	0.43	5 (1%) 73 76	42, 69, 115, 178	0
1	H	340/362 (93%)	0.62	29 (8%) 10 9	32, 81, 139, 196	0
1	I	340/362 (93%)	0.83	36 (10%) 6 4	32, 87, 160, 241	0
1	J	338/362 (93%)	0.60	25 (7%) 14 13	32, 77, 121, 184	0
1	K	340/362 (93%)	0.60	26 (7%) 13 12	32, 75, 136, 222	0
1	L	338/362 (93%)	0.86	46 (13%) 3 2	36, 89, 171, 267	0
All	All	4075/4344 (93%)	0.61	310 (7%) 13 12	32, 79, 145, 267	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	572	SER	9.4
1	K	573	SER	7.3
1	A	774	LEU	6.6
1	E	749	ARG	6.5
1	F	601	VAL	6.2
1	L	472	THR	6.0
1	F	572	SER	5.5
1	J	442	PHE	5.5
1	E	572	SER	5.5
1	I	751	THR	5.5
1	I	574	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	I	492	LEU	5.4
1	F	500	GLU	5.4
1	F	494	TYR	5.0
1	E	496	GLU	4.9
1	L	565	ALA	4.8
1	G	729	LYS	4.8
1	A	605	ASP	4.7
1	E	504	ALA	4.6
1	F	503	LYS	4.6
1	J	761	VAL	4.5
1	G	750	THR	4.4
1	I	572	SER	4.4
1	L	490	ILE	4.4
1	I	510	LEU	4.4
1	J	474	VAL	4.4
1	I	490	ILE	4.3
1	H	729	LYS	4.3
1	J	640	ILE	4.3
1	L	473	LYS	4.3
1	F	607	PHE	4.3
1	D	605	ASP	4.2
1	F	497	ARG	4.1
1	L	487	CYS	4.1
1	A	733	ILE	4.1
1	J	605	ASP	4.0
1	L	489	PRO	3.9
1	E	547	ARG	3.9
1	H	600	PHE	3.9
1	B	750	THR	3.8
1	F	703	LYS	3.8
1	L	501	LYS	3.8
1	F	505	LEU	3.7
1	F	492	LEU	3.7
1	F	696	LEU	3.7
1	L	466	PHE	3.7
1	L	464	ILE	3.7
1	L	749	ARG	3.7
1	F	608	LEU	3.7
1	L	493	GLY	3.6
1	A	638	PHE	3.6
1	B	762	PHE	3.5
1	H	574	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	498	VAL	3.5
1	L	560	VAL	3.5
1	L	559	MET	3.5
1	J	746	VAL	3.5
1	K	759	SER	3.4
1	I	518	PRO	3.4
1	I	442	PHE	3.4
1	I	762	PHE	3.4
1	A	442	PHE	3.4
1	L	525	PHE	3.4
1	L	465	VAL	3.4
1	I	498	VAL	3.4
1	L	462	PRO	3.4
1	L	510	LEU	3.4
1	A	443	ILE	3.3
1	F	750	THR	3.3
1	K	456	ALA	3.3
1	E	494	TYR	3.3
1	C	481	LEU	3.3
1	L	502	ILE	3.3
1	I	465	VAL	3.3
1	I	749	ARG	3.3
1	F	720	ALA	3.3
1	H	443	ILE	3.2
1	D	547	ARG	3.2
1	F	504	ALA	3.2
1	B	547	ARG	3.2
1	G	749	ARG	3.2
1	I	637	TYR	3.2
1	H	598	LEU	3.2
1	H	605	ASP	3.1
1	L	762	PHE	3.1
1	H	762	PHE	3.1
1	K	750	THR	3.1
1	F	610	LEU	3.1
1	L	564	GLU	3.1
1	K	574	ILE	3.1
1	C	505	LEU	3.1
1	F	583	ILE	3.1
1	F	723	LEU	3.1
1	L	492	LEU	3.1
1	E	574	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	546	GLU	3.1
1	E	774	LEU	3.1
1	H	571	GLY	3.1
1	I	766	GLU	3.1
1	L	555	PHE	3.1
1	L	569	VAL	3.1
1	I	743	SER	3.0
1	I	573	SER	3.0
1	L	748	GLN	3.0
1	K	497	ARG	3.0
1	I	605	ASP	3.0
1	K	571	GLY	3.0
1	B	524	TYR	3.0
1	F	478	LEU	3.0
1	E	583	ILE	3.0
1	F	506	ASP	3.0
1	H	760	VAL	3.0
1	E	481	LEU	3.0
1	K	638	PHE	2.9
1	F	507	ILE	2.9
1	E	762	PHE	2.9
1	F	438	HIS	2.9
1	I	555	PHE	2.9
1	A	773	VAL	2.9
1	B	603	LEU	2.9
1	L	631	ALA	2.9
1	L	498	VAL	2.9
1	I	475	LEU	2.9
1	L	640	ILE	2.8
1	F	711	PHE	2.8
1	F	747	LEU	2.8
1	C	547	ARG	2.8
1	J	515	ILE	2.8
1	K	724	ILE	2.8
1	H	638	PHE	2.8
1	C	605	ASP	2.8
1	E	750	THR	2.8
1	F	732	VAL	2.8
1	D	478	LEU	2.8
1	E	747	LEU	2.8
1	J	569	VAL	2.8
1	L	547	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	481	LEU	2.8
1	H	774	LEU	2.8
1	F	493	GLY	2.8
1	A	446	ALA	2.8
1	I	747	LEU	2.8
1	H	570	SER	2.8
1	A	598	LEU	2.8
1	K	478	LEU	2.8
1	J	547	ARG	2.7
1	I	446	ALA	2.7
1	F	695	ARG	2.7
1	L	497	ARG	2.7
1	H	572	SER	2.7
1	B	749	ARG	2.7
1	A	486	ILE	2.7
1	H	733	ILE	2.7
1	I	635	VAL	2.7
1	L	524	TYR	2.7
1	K	607	PHE	2.7
1	F	751	THR	2.7
1	J	747	LEU	2.7
1	J	765	LEU	2.7
1	B	727	ILE	2.7
1	K	578	ASP	2.7
1	H	749	ARG	2.7
1	K	579	ALA	2.7
1	L	516	VAL	2.7
1	K	474	VAL	2.7
1	K	762	PHE	2.7
1	A	547	ARG	2.6
1	H	634	ILE	2.6
1	J	480	THR	2.6
1	E	461	LEU	2.6
1	E	503	LYS	2.6
1	F	554	TYR	2.6
1	F	774	LEU	2.6
1	I	607	PHE	2.6
1	F	547	ARG	2.6
1	H	609	VAL	2.6
1	A	603	LEU	2.6
1	L	563	GLY	2.6
1	D	760	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	491	LEU	2.6
1	C	771	LYS	2.5
1	I	464	ILE	2.5
1	I	627	ILE	2.5
1	E	720	ALA	2.5
1	H	466	PHE	2.5
1	A	730	ALA	2.5
1	F	550	ALA	2.5
1	I	569	VAL	2.5
1	F	768	GLN	2.5
1	H	735	PRO	2.5
1	I	769	TYR	2.5
1	J	606	LYS	2.5
1	L	506	ASP	2.5
1	A	634	ILE	2.5
1	E	505	LEU	2.5
1	F	549	MET	2.5
1	G	497	ARG	2.5
1	E	470	THR	2.5
1	L	486	ILE	2.5
1	H	569	VAL	2.5
1	J	706	ALA	2.4
1	K	751	THR	2.4
1	A	609	VAL	2.4
1	F	761	VAL	2.4
1	H	547	ARG	2.4
1	F	548	LEU	2.4
1	F	688	VAL	2.4
1	C	475	LEU	2.4
1	D	606	LYS	2.4
1	L	515	ILE	2.4
1	I	756	ILE	2.4
1	L	747	LEU	2.4
1	F	762	PHE	2.4
1	L	688	VAL	2.4
1	A	568	MET	2.4
1	L	542	LEU	2.4
1	K	486	ILE	2.4
1	E	691	GLU	2.4
1	J	446	ALA	2.3
1	H	676	LEU	2.3
1	H	440	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	756	ILE	2.3
1	H	747	LEU	2.3
1	D	641	GLU	2.3
1	A	747	LEU	2.3
1	F	479	ALA	2.3
1	H	776	SER	2.3
1	E	751	THR	2.3
1	D	502	ILE	2.3
1	D	603	LEU	2.3
1	A	493	GLY	2.3
1	I	721	TYR	2.3
1	K	439	SER	2.3
1	J	516	VAL	2.3
1	B	542	LEU	2.3
1	E	610	LEU	2.3
1	F	446	ALA	2.3
1	J	576	TYR	2.3
1	A	641	GLU	2.3
1	J	607	PHE	2.3
1	I	634	ILE	2.3
1	A	732	VAL	2.3
1	C	542	LEU	2.2
1	L	463	ARG	2.2
1	K	637	TYR	2.2
1	H	540	ILE	2.2
1	I	732	VAL	2.2
1	F	733	ILE	2.2
1	K	639	GLY	2.2
1	J	608	LEU	2.2
1	A	574	ILE	2.2
1	L	528	VAL	2.2
1	B	598	LEU	2.2
1	C	525	PHE	2.2
1	D	591	LYS	2.2
1	K	494	TYR	2.2
1	E	474	VAL	2.2
1	C	504	ALA	2.2
1	A	606	LYS	2.2
1	F	496	GLU	2.2
1	D	491	LEU	2.2
1	B	436	GLY	2.2
1	B	442	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	552	PRO	2.2
1	L	488	GLN	2.2
1	F	599	ASN	2.1
1	A	478	LEU	2.1
1	F	470	THR	2.1
1	F	513	VAL	2.1
1	J	574	ILE	2.1
1	K	522	PRO	2.1
1	I	638	PHE	2.1
1	F	574	ILE	2.1
1	E	542	LEU	2.1
1	E	456	ALA	2.1
1	F	745	ASN	2.1
1	C	637	TYR	2.1
1	D	542	LEU	2.1
1	A	696	LEU	2.1
1	G	481	LEU	2.1
1	K	736	PHE	2.1
1	E	732	VAL	2.1
1	K	581	ARG	2.1
1	F	465	VAL	2.1
1	F	491	LEU	2.1
1	L	461	LEU	2.1
1	H	761	VAL	2.1
1	H	439	SER	2.1
1	E	497	ARG	2.1
1	H	736	PHE	2.1
1	E	573	SER	2.1
1	J	604	GLU	2.1
1	L	477	ALA	2.1
1	F	466	PHE	2.1
1	L	567	GLY	2.1
1	L	491	LEU	2.0
1	L	678	ILE	2.0
1	A	496	GLU	2.0
1	J	600	PHE	2.0
1	E	771	LYS	2.0
1	I	748	GLN	2.0
1	B	688	VAL	2.0
1	A	770	ILE	2.0
1	F	508	PRO	2.0
1	J	637	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	456	ALA	2.0
1	F	600	PHE	2.0
1	J	487	CYS	2.0
1	I	542	LEU	2.0
1	K	476	LYS	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 monosaccharides 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.