



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:15 PM UTC

PDB ID : 6ZN9 / pdb_00006zn9
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

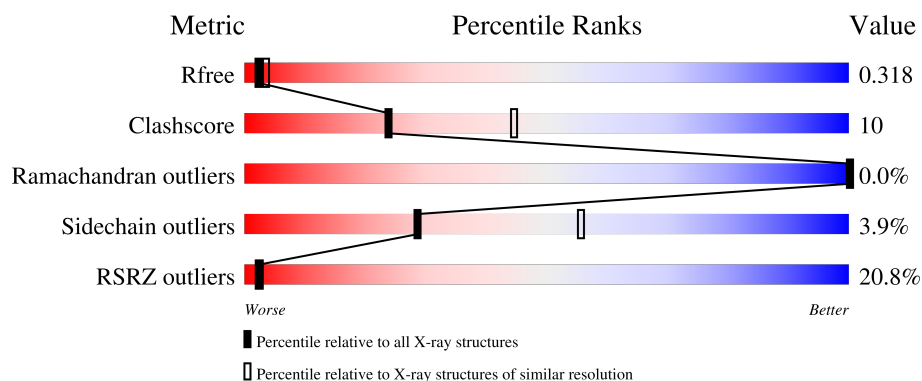
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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 $\leq 5\%$. 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	362	22% 75% 17% 6%
1	B	362	13% 69% 22% 6%
1	C	362	11% 73% 19% 7%
1	D	362	18% 69% 23% 6%
1	E	362	20% 75% 18% 6%

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Mol	Chain	Length	Quality of chain
1	F	362	
1	G	362	
1	H	362	
1	I	362	
1	J	362	
1	K	362	
1	L	362	

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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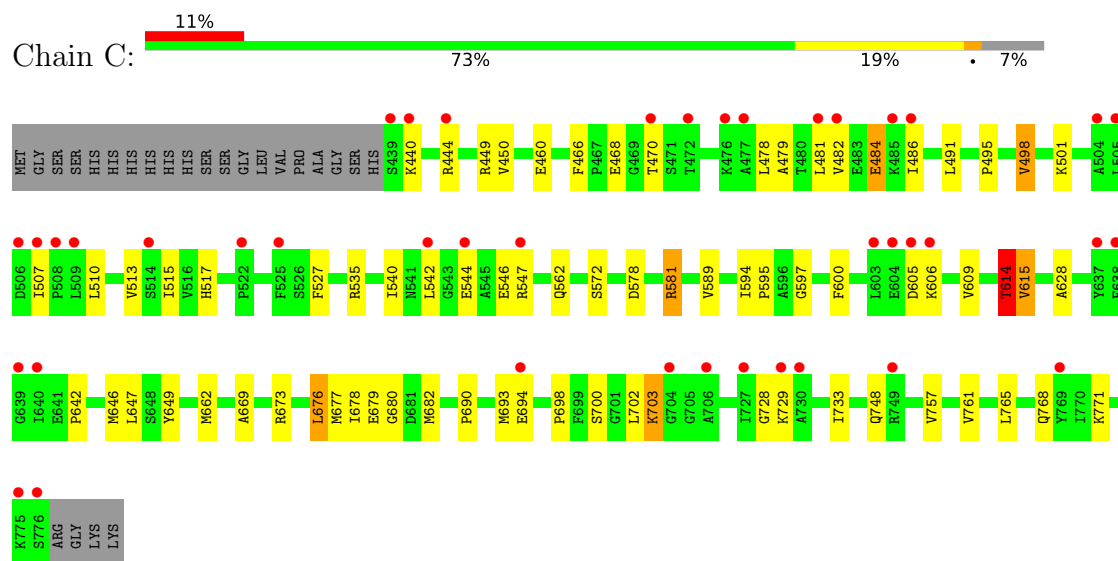
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Chain	Residue	Modelled	Actual	Comment	Reference
K	434	PRO	-	expression tag	UNP Q6MM15
K	435	ALA	-	expression tag	UNP Q6MM15
K	436	GLY	-	expression tag	UNP Q6MM15
K	437	SER	-	expression tag	UNP Q6MM15
K	438	HIS	-	expression tag	UNP Q6MM15
E	419	MET	-	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
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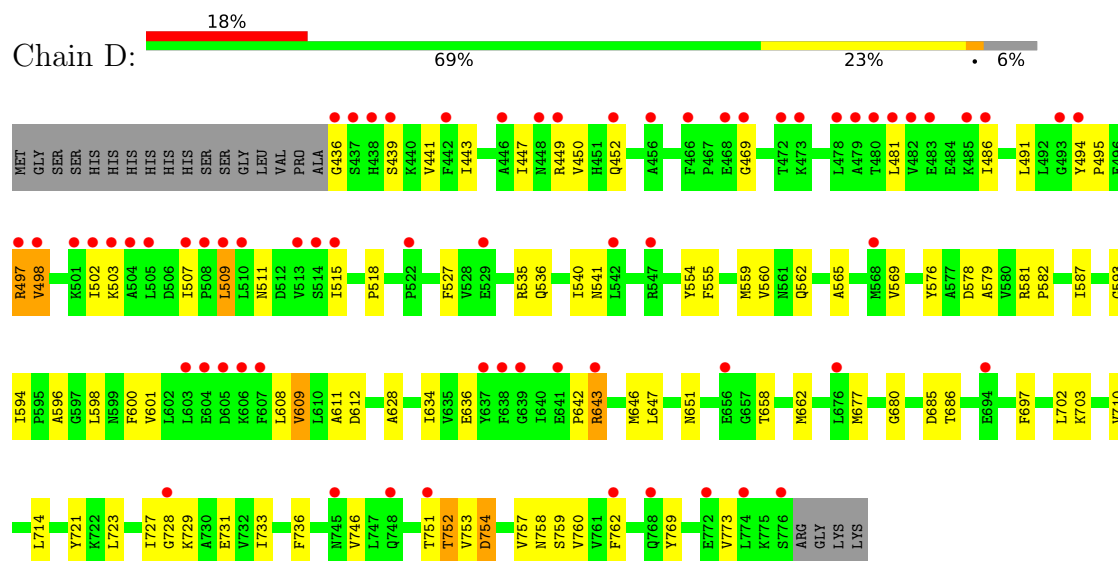
3 Residue-property plots [i](#)

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.

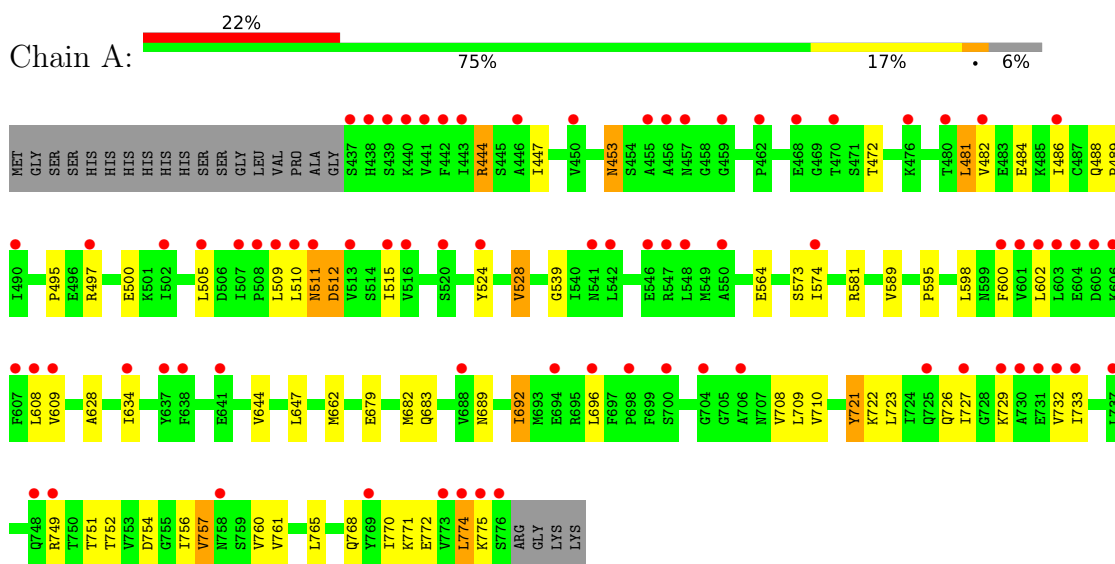
- Molecule 1: Malate dehydrogenase



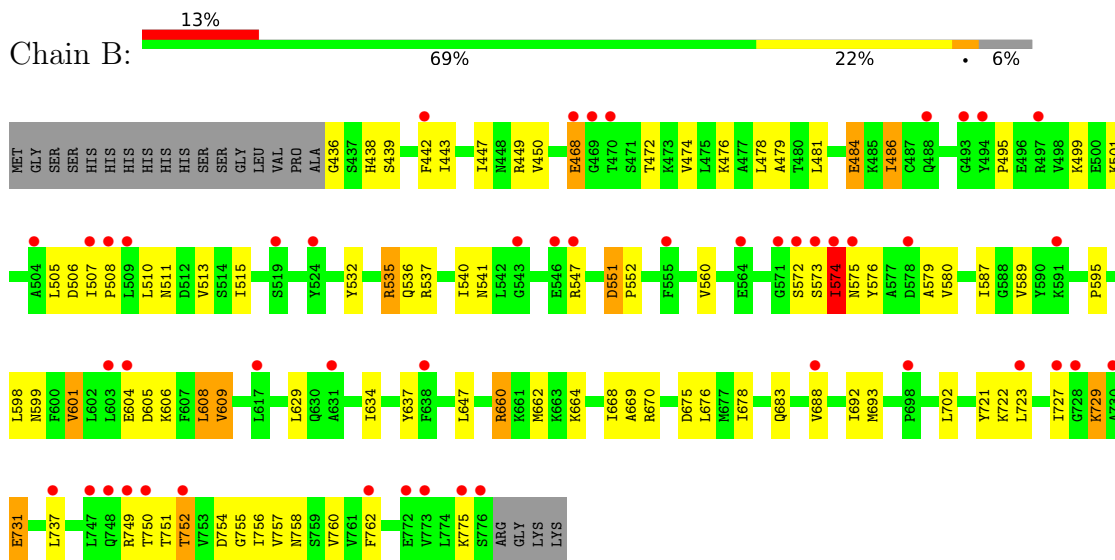
- Molecule 1: Malate dehydrogenase



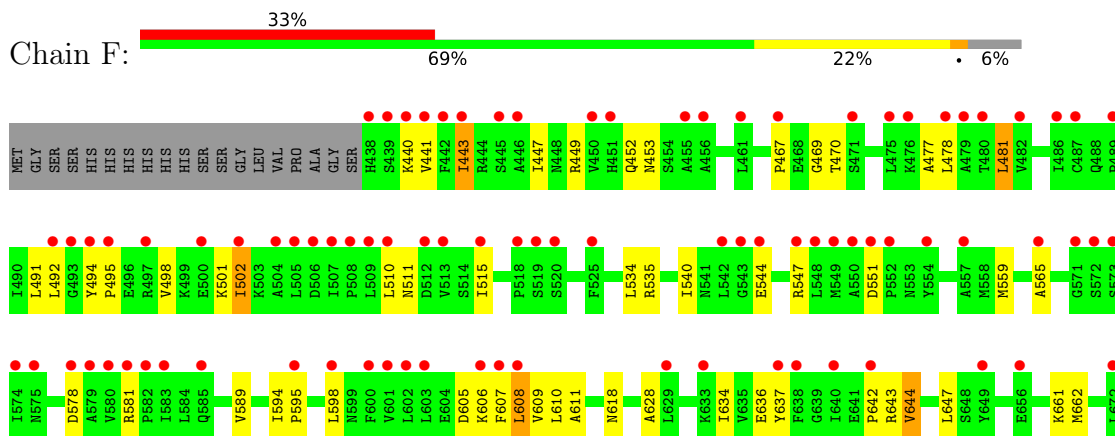
- Molecule 1: Malate dehydrogenase

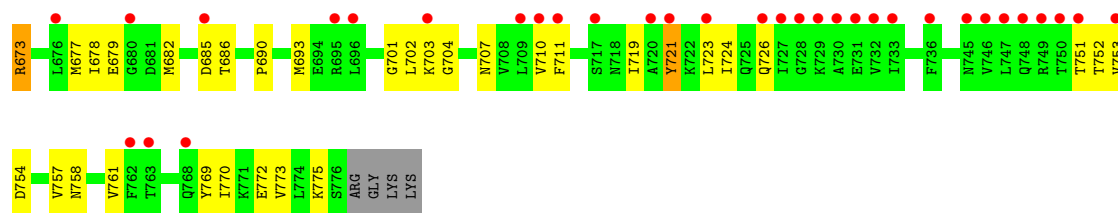


- Molecule 1: Malate dehydrogenase

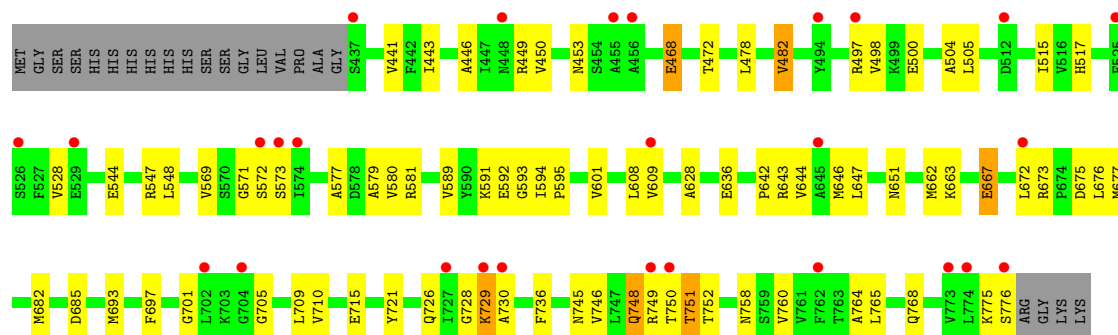


- Molecule 1: Malate dehydrogenase

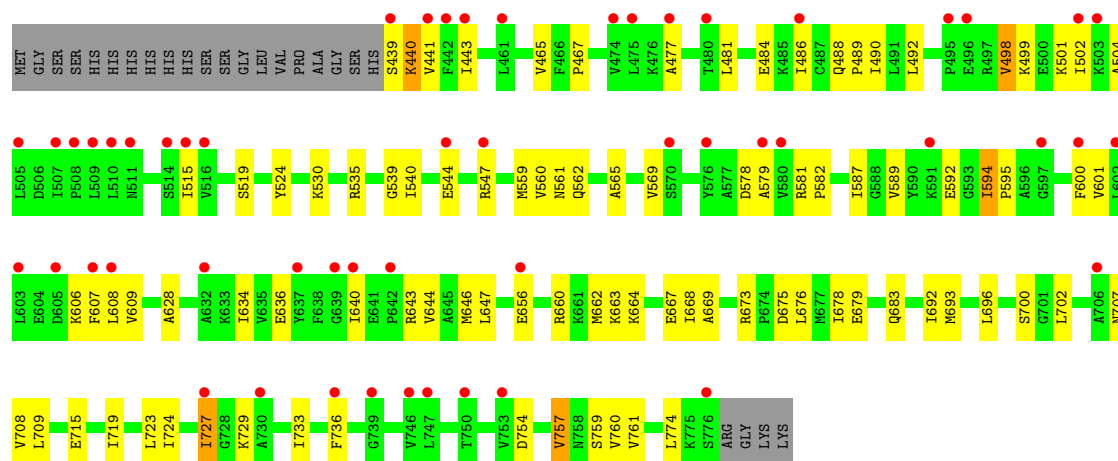




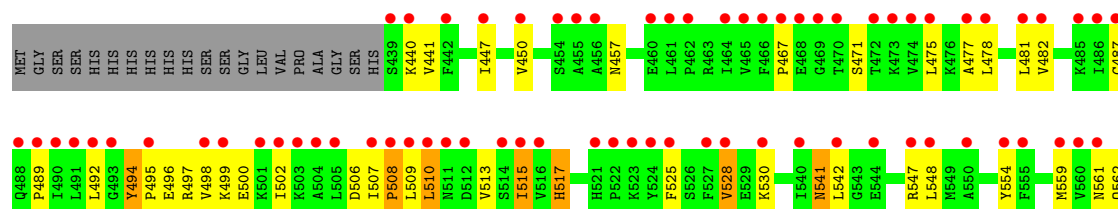
• Molecule 1: Malate dehydrogenase

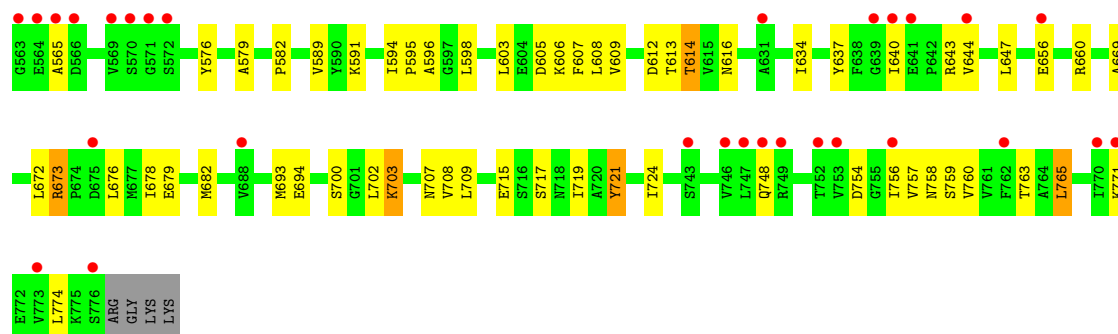


• Molecule 1: Malate dehydrogenase

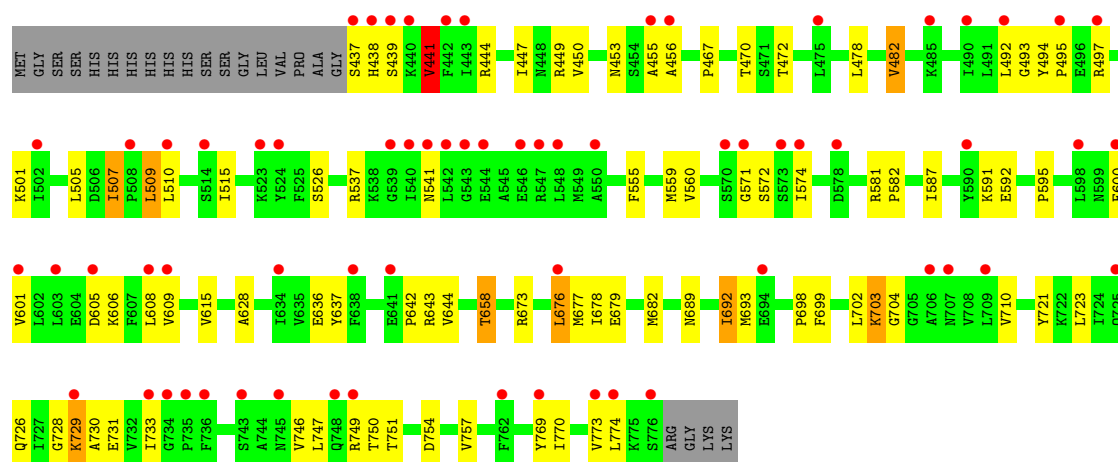


• Molecule 1: Malate dehydrogenase

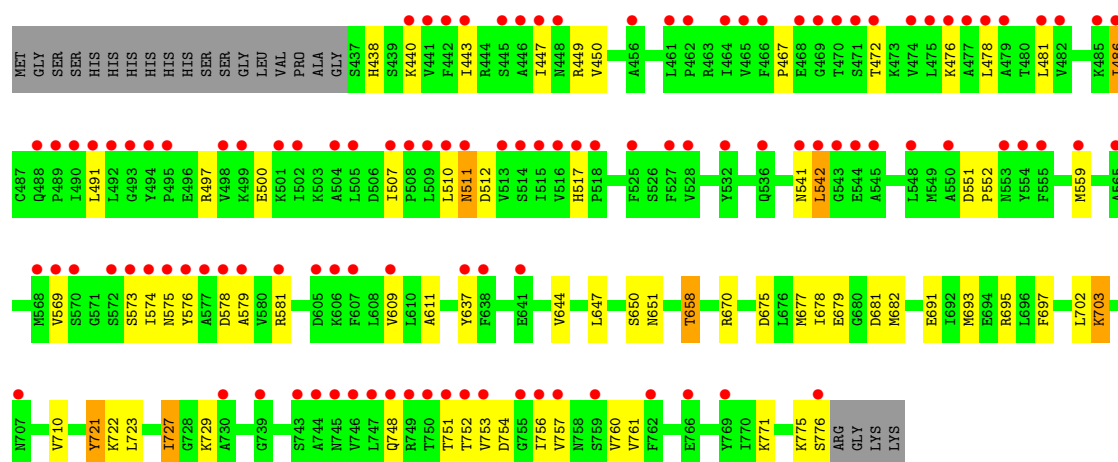
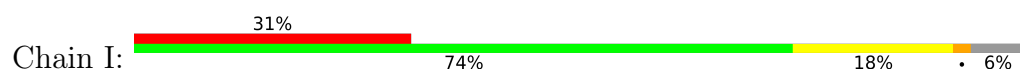




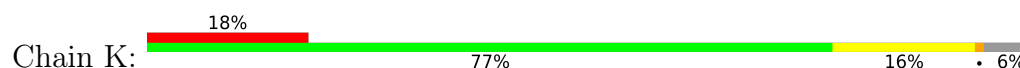
• Molecule 1: Malate dehydrogenase

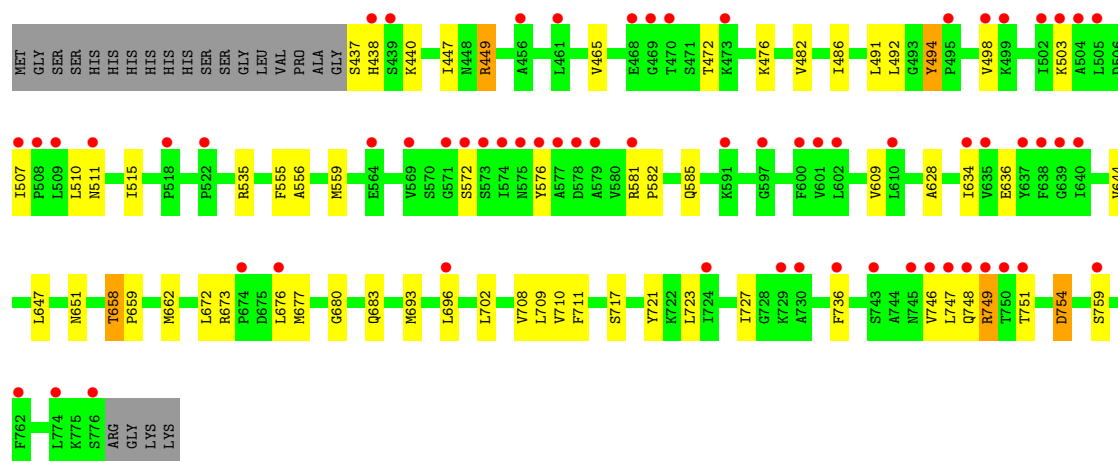


• Molecule 1: Malate dehydrogenase

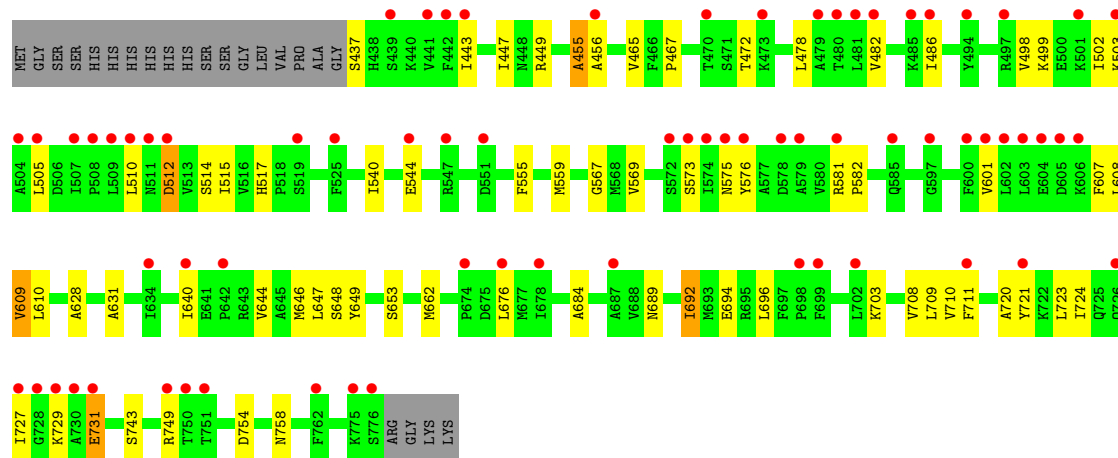
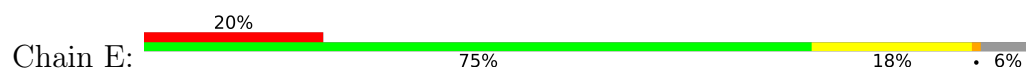


• Molecule 1: Malate dehydrogenase





• Molecule 1: Malate dehydrogenase



4 Data and refinement statistics

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 99.64 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.64-2.72) 96.0 (99.64-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.73Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.252 , 0.299 0.281 , 0.318	Depositor DCC
R_{free} test set	7795 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)	0.32 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.65	0/2650	1.04	4/3587 (0.1%)
1	B	0.71	0/2654	1.06	5/3592 (0.1%)
1	C	0.76	0/2642	1.07	10/3576 (0.3%)
1	D	0.74	0/2655	1.08	6/3593 (0.2%)
1	E	0.64	0/2651	1.00	4/3588 (0.1%)
1	F	0.58	0/2646	1.03	9/3582 (0.3%)
1	G	0.70	1/2651 (0.0%)	1.06	9/3588 (0.3%)
1	H	0.70	0/2651	1.03	8/3588 (0.2%)
1	I	0.75	1/2651 (0.0%)	1.11	7/3588 (0.2%)
1	J	0.71	1/2642 (0.0%)	1.03	3/3576 (0.1%)
1	K	0.67	0/2651	1.07	9/3588 (0.3%)
1	L	0.72	0/2642	1.10	11/3576 (0.3%)
All	All	0.70	3/31786 (0.0%)	1.06	85/43022 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	440	LYS	C-O	5.21	1.30	1.24
1	G	594	ILE	CA-CB	5.20	1.60	1.54
1	I	438	HIS	CA-CB	5.15	1.61	1.53

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	576	TYR	N-CA-C	10.00	121.77	111.07
1	K	748	GLN	N-CA-C	-7.99	98.03	110.42
1	F	644	VAL	N-CA-C	7.30	118.40	108.17
1	C	748	GLN	N-CA-C	-7.04	100.10	110.52
1	D	511	ASN	N-CA-C	6.91	120.93	112.23
1	L	506	ASP	N-CA-C	6.90	119.64	111.02
1	G	673	ARG	CA-C-N	6.83	126.97	119.87
1	G	673	ARG	C-N-CA	6.83	126.97	119.87
1	H	438	HIS	N-CA-C	-6.81	103.86	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	729	LYS	N-CA-C	-6.67	105.14	113.20
1	E	512	ASP	CB-CA-C	6.50	120.58	111.86
1	B	574	ILE	N-CA-C	6.47	118.14	108.96
1	K	749	ARG	NE-CZ-NH1	-6.38	115.11	121.50
1	G	572	SER	N-CA-C	-6.38	105.48	113.20
1	H	493	GLY	N-CA-C	-6.37	101.89	110.56
1	D	436	GLY	CA-C-N	6.36	129.63	120.79
1	D	436	GLY	C-N-CA	6.36	129.63	120.79
1	K	494	TYR	CA-C-N	6.32	126.53	119.32
1	K	494	TYR	C-N-CA	6.32	126.53	119.32
1	G	517	HIS	CA-C-N	6.25	125.74	119.24
1	G	517	HIS	C-N-CA	6.25	125.74	119.24
1	C	517	HIS	CA-C-N	6.13	125.61	119.24
1	C	517	HIS	C-N-CA	6.13	125.61	119.24
1	K	511	ASN	N-CA-C	-6.12	101.43	110.48
1	L	616	ASN	N-CA-C	6.09	118.65	108.96
1	I	511	ASN	N-CA-C	-6.01	101.58	110.48
1	H	676	LEU	N-CA-C	5.99	119.58	109.76
1	C	615	VAL	CB-CA-C	-5.95	106.66	111.71
1	L	494	TYR	CA-C-N	5.90	125.37	119.24
1	L	494	TYR	C-N-CA	5.90	125.37	119.24
1	B	486	ILE	N-CA-C	5.88	116.86	111.81
1	E	517	HIS	CA-C-N	5.87	125.34	119.24
1	E	517	HIS	C-N-CA	5.87	125.34	119.24
1	I	507	ILE	CA-C-N	5.84	126.35	120.04
1	I	507	ILE	C-N-CA	5.84	126.35	120.04
1	B	751	THR	N-CA-C	5.82	118.89	110.28
1	F	494	TYR	CA-C-N	5.59	125.70	119.32
1	F	494	TYR	C-N-CA	5.59	125.70	119.32
1	A	581	ARG	CA-C-N	-5.58	113.15	119.28
1	A	581	ARG	C-N-CA	-5.58	113.15	119.28
1	H	572	SER	N-CA-C	-5.50	106.34	113.16
1	A	564	GLU	N-CA-C	-5.49	106.54	113.18
1	G	728	GLY	N-CA-C	5.47	121.01	112.31
1	G	581	ARG	CA-C-N	-5.45	113.28	119.28
1	G	581	ARG	C-N-CA	-5.45	113.28	119.28
1	D	658	THR	CA-C-N	-5.43	113.32	118.97
1	D	658	THR	C-N-CA	-5.43	113.32	118.97
1	K	438	HIS	N-CA-C	-5.41	104.78	111.33
1	A	481	LEU	N-CA-C	5.41	119.05	112.23
1	E	455	ALA	N-CA-C	-5.39	102.90	110.50
1	C	594	ILE	CA-C-N	-5.35	114.29	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	594	ILE	C-N-CA	-5.35	114.29	119.90
1	H	726	GLN	CA-C-N	-5.34	117.16	122.77
1	H	726	GLN	C-N-CA	-5.34	117.16	122.77
1	C	614	THR	N-CA-C	5.34	120.70	114.62
1	L	510	LEU	N-CA-C	5.33	119.34	112.41
1	F	481	LEU	N-CA-C	5.32	118.94	112.23
1	I	517	HIS	CA-C-N	5.31	124.76	119.24
1	I	517	HIS	C-N-CA	5.31	124.76	119.24
1	G	593	GLY	N-CA-C	5.29	120.12	112.82
1	L	513	VAL	N-CA-C	5.26	117.44	109.12
1	F	443	ILE	N-CA-C	-5.26	105.26	110.62
1	J	727	ILE	N-CA-C	-5.25	108.38	113.53
1	I	486	ILE	N-CA-C	5.22	116.30	111.81
1	K	749	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	B	551	ASP	CA-C-N	5.20	125.50	119.47
1	B	551	ASP	C-N-CA	5.20	125.50	119.47
1	L	700	SER	N-CA-C	5.20	117.77	110.23
1	F	673	ARG	CA-C-N	5.19	125.27	119.87
1	F	673	ARG	C-N-CA	5.19	125.27	119.87
1	H	441	VAL	CB-CA-C	-5.13	105.40	111.97
1	J	539	GLY	CA-C-N	-5.13	116.28	123.10
1	J	539	GLY	C-N-CA	-5.13	116.28	123.10
1	L	517	HIS	CA-C-N	5.11	124.56	119.24
1	L	517	HIS	C-N-CA	5.11	124.56	119.24
1	C	680	GLY	CA-C-O	-5.07	116.78	121.96
1	F	551	ASP	CA-C-N	5.07	125.10	119.32
1	F	551	ASP	C-N-CA	5.07	125.10	119.32
1	I	727	ILE	N-CA-C	-5.07	107.89	112.96
1	L	673	ARG	CA-C-N	5.06	125.13	119.87
1	L	673	ARG	C-N-CA	5.06	125.13	119.87
1	D	680	GLY	CA-C-O	-5.05	116.81	121.96
1	K	680	GLY	N-CA-C	-5.05	104.37	111.09
1	C	581	ARG	CA-C-N	-5.03	113.75	119.28
1	C	581	ARG	C-N-CA	-5.03	113.75	119.28

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	52	0
1	B	2610	0	2678	67	0
1	C	2598	0	2675	47	0
1	D	2611	0	2681	57	0
1	E	2607	0	2678	45	0
1	F	2602	0	2674	72	0
1	G	2607	0	2678	53	0
1	H	2607	0	2678	71	0
1	I	2607	0	2678	56	0
1	J	2598	0	2675	63	0
1	K	2607	0	2678	48	0
1	L	2598	0	2675	60	0
All	All	31258	0	32123	639	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 (639) 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	1.54
1:A:453:ASN:CG	1:A:768:GLN:NE2	1.75	1.45
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:693:MET:HE3	1:H:702:LEU:HD23	1.66	0.78
1:I:677:MET:HE3	1:I:702:LEU:HA	1.65	0.78
1:F:636:GLU:OE2	1:F:673:ARG:NH2	2.17	0.78
1:K:677:MET:HE3	1:K:702:LEU:HA	1.67	0.77
1:J:693:MET:HE3	1:J:702:LEU:HD23	1.66	0.76
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:774:LEU:C	1:A:774:LEU:HD22	2.13	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:F:559:MET:HE2	1:F:565:ALA:HB2	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:HD22	1:A:774:LEU:O	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:H:677:MET:HE3	1:H:702:LEU:HA	1.71	0.71
1:F:643:ARG:HH12	1:F:704:GLY:C	1.98	0.70
1:D:677:MET:HE3	1:D:702:LEU:HA	1.72	0.70
1:A:573:SER:O	1:A:749:ARG:NH2	2.24	0.70
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:643:ARG:HG2	1:D:677:MET:HE2	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:A:453:ASN:CG	1:A:768:GLN:HE21	1.98	0.62
1:B:547:ARG:NH2	1:G:573:SER:O	2.27	0.62
1:G:729:LYS:HZ3	1:H:729:LYS:HG2	1.65	0.61
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
1:F:449:ARG:HA	1:F:452:GLN:HG2	1.83	0.60
1:J:559:MET:HE2	1:J:565:ALA:HB2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:PHE:HB2	1:A:733:ILE:CG1	2.33	0.59
1:C:693:MET:HE3	1:C:702:LEU:HD23	1.85	0.59
1:D:541:ASN:CG	1:K:749:ARG:HH12	2.11	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:E:465:VAL:HG21	1:E:559:MET:HE1	1.85	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:B:547:ARG:HH12	1:G:573:SER:C	2.12	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:L:547:ARG:HH12	1:I:573:SER:C	2.12	0.57
1:G:628:ALA:HB1	1:G:644:VAL:HG11	1.87	0.57
1:K:693:MET:HE3	1:K:702:LEU:HD23	1.87	0.57
1:C:642:PRO:HG2	1:C:676:LEU:CD1	2.35	0.57
1:C:677:MET:HE1	1:H:698:PRO:HB2	1.86	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:K:555:PHE:CD2	1:K:559:MET:HE2	2.41	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:J:636:GLU:CD	1:J:673:ARG:HH22	2.13	0.56
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:I:693:MET:HE3	1:I:702:LEU:HD23	1.87	0.55
1:E:646:MET:HB3	1:E:662:MET:HE3	1.89	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: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:L:679:GLU:HB3	1:L:682:MET:HE1	1.89	0.54
1:E:555:PHE:CD2	1:E:559:MET:HE2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:D:646:MET:HB3	1:D:662:MET:HE3	1.91	0.52
1:A:608:LEU:HD23	1:A:709:LEU:HD21	1.90	0.52
1:G:729:LYS:NZ	1:H:729:LYS:HG2	2.24	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: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:C:628:ALA:HB2	1:C:646:MET:HE1	1.93	0.51
1:G:646:MET:HB3	1:G:662:MET:HE3	1.93	0.51
1:G:729:LYS:CD	1:H:729:LYS:H	2.23	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:F:693:MET:HE3	1:F:702:LEU:HD22	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:F:772:GLU:O	1:F:775:LYS:HG2	2.11	0.49
1:J:606:LYS:HZ1	1:J:640:ILE:HG21	1.77	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:A:453:ASN:OD1	1:A:768:GLN:CD	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:689:ASN:CG	1:H:692:ILE:HD12	2.38	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:G:749:ARG:C	1:G:751:THR:H	2.21	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:A:679:GLU:HB3	1:A:682:MET:HE1	1.95	0.48
1:C:700:SER:O	1:H:703:LYS:HE3	2.13	0.48
1:D:643:ARG:HG2	1:D:677:MET:CE	2.44	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:I:682:MET:SD	1:I:693:MET:HE1	2.53	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:K:465:VAL:HG21	1:K:559:MET:HE1	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:682:MET:SD	1:F:693:MET:HE1	2.55	0.47
1:E:692:ILE:HG23	1:E:696:LEU:HD12	1.97	0.47
1:F:636:GLU:CD	1:F:673:ARG:HH22	2.19	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:I:551:ASP:OD1	1:I:552:PRO:HD2	2.13	0.47
1:C:544:GLU:OE2	1:C:547:ARG:NH2	2.44	0.47
1:A:689:ASN:CG	1:A:692:ILE:HD12	2.39	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:L:693:MET:HE3	1:L:702:LEU:HD23	1.97	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:B:436:GLY:HA2	1:B:731:GLU:CD	2.41	0.46
1:G:571:GLY:C	1:G:573:SER:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:541:ASN:CG	1:K:749:ARG:NH1	2.73	0.46
1:A:600:PHE:HB2	1:A:733:ILE:HG13	1.98	0.46
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:J:646:MET:HB3	1:J:662:MET:HE3	1.98	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: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: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: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:643:ARG:HG2	1:H:677:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:555:PHE:CD2	1:H:559:MET:HE2	2.52	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:J:579:ALA:O	1:J:582:PRO:HD2	2.18	0.44
1:K:556:ALA:HA	1:K:559:MET:HE3	1.99	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: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:H:679:GLU:HB3	1:H:682:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:559:MET:HE2	1:I:559:MET:HB3	1.94	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
1:G:672:LEU:HD23	1:G:672:LEU:HA	1.70	0.44
1:L:559:MET:HE2	1:L:565:ALA:HB2	2.00	0.44
1:L:759:SER:O	1:L:763:THR:OG1	2.30	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:K:749:ARG:C	1:K:751:THR:H	2.24	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: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:G:497:ARG:NH1	1:G:500:GLU:OE1	2.52	0.43
1:I:679:GLU:HB3	1:I:682:MET:HE1	1.99	0.43
1:K:465:VAL:HG21	1:K:559:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:MET:HE2	1:D:565:ALA:HB2	2.00	0.43
1:I:775:LYS:O	1:I:776:SER:OG	2.32	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:J:683:GLN:CD	1:I:722:LYS:HE3	2.44	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:693:MET:CE	1:H:702:LEU:HD23	2.42	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:693:MET:HE3	1:B:702:LEU:HD23	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
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:H:728:GLY:C	1:H:730:ALA:H	2.26	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:F:690:PRO:HB3	1:F:704:GLY:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:642:PRO:C	1:F:643:ARG:HG3	2.45	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:679:GLU:HB3	1:C:682:MET:HE1	2.01	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:G:775:LYS:O	1:G:776:SER:OG	2.19	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:I:541:ASN:CG	1:I:542:LEU:H	2.27	0.41
1:I:677:MET:HE1	1:I:703:LYS:O	2.20	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: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
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: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:H:677:MET:HE1	1:H:703:LYS:O	2.21	0.41
1:E:676:LEU:HD23	1:E:676:LEU:HA	1.65	0.41
1:F:535:ARG:HB3	1:F:540:ILE:HD12	2.02	0.41
1:F:721:TYR:CD1	1:F:721:TYR:C	2.98	0.41
1:I:541:ASN:CG	1:I:542:LEU:N	2.78	0.41
1:A:488:GLN:HA	1:A:489:PRO:HD3	1.88	0.41
1:B:573:SER:C	1:B:749:ARG:HD3	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:650:SER:OG	1:I:681:ASP:OD2	2.34	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:K:492:LEU:HD21	1:K:559:MET:HE1	2.03	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
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:G:682:MET:SD	1:G:693:MET:HE1	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	59
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 ⓘ

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%)	262 (93%)	19 (7%)	14	33
1	B	281/301 (93%)	266 (95%)	15 (5%)	20	44
1	C	282/301 (94%)	273 (97%)	9 (3%)	34	62
1	D	282/301 (94%)	269 (95%)	13 (5%)	24	50
1	E	282/301 (94%)	272 (96%)	10 (4%)	32	59
1	F	281/301 (93%)	275 (98%)	6 (2%)	47	73
1	G	282/301 (94%)	268 (95%)	14 (5%)	22	46
1	H	282/301 (94%)	271 (96%)	11 (4%)	28	56
1	I	282/301 (94%)	276 (98%)	6 (2%)	47	73
1	J	282/301 (94%)	270 (96%)	12 (4%)	26	52
1	K	282/301 (94%)	275 (98%)	7 (2%)	42	69
1	L	282/301 (94%)	271 (96%)	11 (4%)	28	56
All	All	3381/3612 (94%)	3248 (96%)	133 (4%)	28	56

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	482	VAL
1	C	484	GLU
1	C	498	VAL
1	C	609	VAL
1	C	614	THR
1	C	676	LEU
1	C	703	LYS
1	C	729	LYS
1	C	757	VAL
1	D	441	VAL

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Mol	Chain	Res	Type
1	D	443	ILE
1	D	497	ARG
1	D	498	VAL
1	D	509	LEU
1	D	535	ARG
1	D	609	VAL
1	D	634	ILE
1	D	643	ARG
1	D	703	LYS
1	D	721	TYR
1	D	752	THR
1	D	754	ASP
1	A	444	ARG
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	634	ILE
1	A	692	ILE
1	A	721	TYR
1	A	726	GLN
1	A	757	VAL
1	A	770	ILE
1	A	771	LYS
1	A	772	GLU
1	A	774	LEU
1	A	775	LYS
1	B	468	GLU
1	B	484	GLU
1	B	506	ASP
1	B	535	ARG
1	B	574	ILE
1	B	601	VAL
1	B	608	LEU
1	B	609	VAL
1	B	634	ILE
1	B	660	ARG
1	B	692	ILE

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Mol	Chain	Res	Type
1	B	721	TYR
1	B	729	LYS
1	B	731	GLU
1	B	752	THR
1	F	441	VAL
1	F	453	ASN
1	F	502	ILE
1	F	608	LEU
1	F	634	ILE
1	F	721	TYR
1	G	441	VAL
1	G	468	GLU
1	G	482	VAL
1	G	528	VAL
1	G	609	VAL
1	G	667	GLU
1	G	709	LEU
1	G	721	TYR
1	G	726	GLN
1	G	729	LYS
1	G	748	GLN
1	G	750	THR
1	G	751	THR
1	G	752	THR
1	J	439	SER
1	J	441	VAL
1	J	484	GLU
1	J	498	VAL
1	J	515	ILE
1	J	569	VAL
1	J	592	GLU
1	J	594	ILE
1	J	634	ILE
1	J	727	ILE
1	J	757	VAL
1	J	774	LEU
1	L	441	VAL
1	L	457	ASN
1	L	515	ILE
1	L	528	VAL
1	L	541	ASN
1	L	591	LYS

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Mol	Chain	Res	Type
1	L	614	THR
1	L	634	ILE
1	L	703	LYS
1	L	721	TYR
1	L	765	LEU
1	H	441	VAL
1	H	444	ARG
1	H	482	VAL
1	H	507	ILE
1	H	509	LEU
1	H	526	SER
1	H	609	VAL
1	H	658	THR
1	H	692	ILE
1	H	703	LYS
1	H	721	TYR
1	I	542	LEU
1	I	609	VAL
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	634	ILE
1	K	658	THR
1	K	721	TYR
1	K	754	ASP
1	E	443	ILE
1	E	449	ARG
1	E	482	VAL
1	E	512	ASP
1	E	514	SER
1	E	609	VAL
1	E	692	ILE
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 (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	453	ASN
1	C	718	ASN
1	C	768	GLN
1	D	541	ASN
1	D	561	ASN
1	D	562	GLN
1	A	517	HIS
1	A	562	GLN
1	A	718	ASN
1	A	768	GLN
1	B	536	GLN
1	B	541	ASN
1	B	585	GLN
1	B	718	ASN
1	F	758	ASN
1	L	511	ASN
1	L	561	ASN
1	L	562	GLN
1	L	718	ASN
1	H	453	ASN
1	H	553	ASN
1	H	562	GLN
1	H	718	ASN
1	H	768	GLN
1	I	517	HIS
1	I	748	GLN
1	K	748	GLN
1	E	561	ASN
1	E	562	GLN
1	E	718	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/362 (93%)	1.30	78 (22%) 2 2	48, 81, 150, 174	0
1	B	341/362 (94%)	0.91	48 (14%) 6 5	42, 72, 131, 182	0
1	C	338/362 (93%)	0.88	41 (12%) 8 8	36, 63, 119, 183	0
1	D	341/362 (94%)	1.06	66 (19%) 3 3	33, 67, 123, 187	0
1	E	340/362 (93%)	1.36	71 (20%) 2 2	32, 89, 144, 202	0
1	F	339/362 (93%)	1.70	120 (35%) 1 1	61, 100, 154, 187	0
1	G	340/362 (93%)	0.78	27 (7%) 18 16	42, 69, 115, 178	0
1	H	340/362 (93%)	1.16	66 (19%) 3 3	32, 81, 139, 196	0
1	I	340/362 (93%)	1.53	112 (32%) 1 1	32, 87, 160, 241	0
1	J	338/362 (93%)	1.14	53 (15%) 5 4	32, 77, 121, 184	0
1	K	340/362 (93%)	1.11	64 (18%) 3 3	32, 75, 136, 222	0
1	L	338/362 (93%)	1.44	100 (29%) 1 1	36, 89, 171, 267	0
All	All	4075/4344 (93%)	1.20	846 (20%) 2 2	32, 79, 145, 267	0

All (846) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	438	HIS	7.9
1	A	605	ASP	6.9
1	I	574	ILE	6.3
1	F	572	SER	5.9
1	I	491	LEU	5.7
1	K	573	SER	5.7
1	C	694	GLU	5.5
1	B	546	GLU	5.5
1	L	491	LEU	5.5
1	H	439	SER	5.5
1	F	439	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	L	762	PHE	5.4
1	H	600	PHE	5.4
1	L	464	ILE	5.2
1	F	550	ALA	5.1
1	L	487	CYS	5.1
1	A	550	ALA	5.1
1	C	504	ALA	5.0
1	A	607	PHE	5.0
1	B	524	TYR	4.9
1	H	547	ARG	4.9
1	I	509	LEU	4.9
1	D	641	GLU	4.9
1	A	602	LEU	4.8
1	K	572	SER	4.8
1	K	578	ASP	4.8
1	L	489	PRO	4.8
1	E	547	ARG	4.8
1	L	478	LEU	4.8
1	E	504	ALA	4.7
1	L	515	ILE	4.7
1	H	574	ILE	4.7
1	I	579	ALA	4.7
1	J	509	LEU	4.7
1	A	547	ARG	4.7
1	C	507	ILE	4.6
1	G	750	THR	4.6
1	I	507	ILE	4.6
1	L	472	THR	4.6
1	A	437	SER	4.6
1	A	730	ALA	4.6
1	A	603	LEU	4.6
1	I	481	LEU	4.6
1	D	605	ASP	4.6
1	L	565	ALA	4.5
1	K	508	PRO	4.5
1	F	547	ARG	4.5
1	I	572	SER	4.5
1	A	773	VAL	4.5
1	A	776	SER	4.4
1	F	579	ALA	4.4
1	I	495	PRO	4.4
1	A	694	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	L	490	ILE	4.4
1	H	605	ASP	4.4
1	C	605	ASP	4.4
1	E	507	ILE	4.4
1	I	490	ILE	4.4
1	B	497	ARG	4.3
1	L	465	VAL	4.3
1	F	519	SER	4.3
1	H	440	LYS	4.3
1	D	603	LEU	4.2
1	I	776	SER	4.2
1	B	727	ILE	4.2
1	B	547	ARG	4.2
1	K	509	LEU	4.2
1	J	776	SER	4.2
1	C	509	LEU	4.2
1	A	438	HIS	4.2
1	E	606	LYS	4.1
1	L	502	ILE	4.1
1	A	440	LYS	4.1
1	E	730	ALA	4.1
1	D	509	LEU	4.1
1	K	439	SER	4.1
1	L	569	VAL	4.1
1	G	749	ARG	4.1
1	F	607	PHE	4.1
1	F	747	LEU	4.1
1	D	437	SER	4.0
1	I	498	VAL	4.0
1	I	515	ILE	4.0
1	H	776	SER	4.0
1	K	759	SER	4.0
1	K	776	SER	4.0
1	F	494	TYR	4.0
1	J	605	ASP	4.0
1	L	776	SER	3.9
1	L	510	LEU	3.9
1	A	606	LYS	3.9
1	A	638	PHE	3.9
1	J	443	ILE	3.9
1	H	443	ILE	3.9
1	E	494	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	439	SER	3.8
1	A	704	GLY	3.8
1	A	442	PHE	3.8
1	D	449	ARG	3.8
1	E	578	ASP	3.8
1	I	470	THR	3.8
1	F	762	PHE	3.8
1	J	656	GLU	3.8
1	I	751	THR	3.8
1	F	554	TYR	3.8
1	A	774	LEU	3.8
1	J	508	PRO	3.8
1	J	746	VAL	3.7
1	K	639	GLY	3.7
1	D	547	ARG	3.7
1	L	499	LYS	3.7
1	A	688	VAL	3.7
1	F	548	LEU	3.7
1	I	747	LEU	3.7
1	I	486	ILE	3.7
1	L	748	GLN	3.7
1	F	551	ASP	3.7
1	E	574	ILE	3.7
1	I	637	TYR	3.7
1	I	548	LEU	3.6
1	A	502	ILE	3.6
1	B	507	ILE	3.6
1	F	507	ILE	3.6
1	C	470	THR	3.6
1	E	749	ARG	3.6
1	I	762	PHE	3.6
1	L	473	LYS	3.6
1	E	579	ALA	3.6
1	I	641	GLU	3.6
1	I	492	LEU	3.6
1	E	581	ARG	3.6
1	C	638	PHE	3.6
1	A	641	GLU	3.6
1	I	510	LEU	3.6
1	I	743	SER	3.6
1	D	728	GLY	3.5
1	H	456	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	456	ALA	3.5
1	I	489	PRO	3.5
1	C	482	VAL	3.5
1	A	601	VAL	3.5
1	L	474	VAL	3.5
1	I	482	VAL	3.5
1	G	776	SER	3.5
1	A	507	ILE	3.5
1	I	502	ILE	3.5
1	I	578	ASP	3.5
1	E	551	ASP	3.5
1	I	555	PHE	3.5
1	I	475	LEU	3.5
1	I	505	LEU	3.5
1	E	603	LEU	3.5
1	D	438	HIS	3.5
1	B	494	TYR	3.5
1	C	776	SER	3.5
1	I	472	THR	3.5
1	A	609	VAL	3.5
1	B	573	SER	3.5
1	L	501	LYS	3.5
1	B	493	GLY	3.5
1	F	544	GLU	3.5
1	I	468	GLU	3.5
1	L	481	LEU	3.5
1	L	505	LEU	3.5
1	F	601	VAL	3.5
1	C	637	TYR	3.4
1	L	770	ILE	3.4
1	I	769	TYR	3.4
1	C	606	LYS	3.4
1	D	469	GLY	3.4
1	F	728	GLY	3.4
1	J	511	ASN	3.4
1	E	456	ALA	3.4
1	D	604	GLU	3.4
1	F	602	LEU	3.4
1	I	465	VAL	3.4
1	K	507	ILE	3.4
1	C	769	TYR	3.4
1	J	706	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	745	ASN	3.4
1	L	466	PHE	3.4
1	E	572	SER	3.4
1	I	749	ARG	3.4
1	L	486	ILE	3.4
1	J	480	THR	3.4
1	A	604	GLU	3.4
1	F	509	LEU	3.4
1	L	749	ARG	3.4
1	H	548	LEU	3.4
1	K	730	ALA	3.4
1	F	578	ASP	3.4
1	L	559	MET	3.4
1	L	439	SER	3.3
1	F	508	PRO	3.3
1	I	469	GLY	3.3
1	B	773	VAL	3.3
1	D	485	LYS	3.3
1	K	499	LYS	3.3
1	G	774	LEU	3.3
1	A	446	ALA	3.3
1	F	442	PHE	3.3
1	L	498	VAL	3.3
1	K	574	ILE	3.3
1	G	437	SER	3.3
1	L	524	TYR	3.3
1	H	638	PHE	3.3
1	I	575	ASN	3.3
1	F	506	ASP	3.3
1	E	441	VAL	3.3
1	C	508	PRO	3.3
1	F	505	LEU	3.3
1	E	505	LEU	3.3
1	D	473	LYS	3.3
1	I	748	GLN	3.3
1	B	470	THR	3.2
1	B	519	SER	3.2
1	F	441	VAL	3.2
1	F	513	VAL	3.2
1	I	464	ILE	3.2
1	K	762	PHE	3.2
1	E	762	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	745	ASN	3.2
1	J	544	GLU	3.2
1	L	475	LEU	3.2
1	H	603	LEU	3.2
1	K	564	GLU	3.2
1	D	504	ALA	3.2
1	I	569	VAL	3.2
1	F	750	THR	3.2
1	D	436	GLY	3.2
1	L	469	GLY	3.2
1	A	450	VAL	3.2
1	A	486	ILE	3.2
1	A	733	ILE	3.2
1	C	440	LYS	3.2
1	D	478	LEU	3.2
1	A	731	GLU	3.2
1	A	443	ILE	3.2
1	J	507	ILE	3.2
1	I	756	ILE	3.2
1	A	732	VAL	3.2
1	I	442	PHE	3.2
1	I	516	VAL	3.2
1	F	695	ARG	3.1
1	E	642	PRO	3.1
1	B	504	ALA	3.1
1	A	490	ILE	3.1
1	G	572	SER	3.1
1	D	542	LEU	3.1
1	A	608	LEU	3.1
1	J	510	LEU	3.1
1	K	469	GLY	3.1
1	F	479	ALA	3.1
1	I	446	ALA	3.1
1	D	498	VAL	3.1
1	B	688	VAL	3.1
1	E	729	LYS	3.1
1	F	672	LEU	3.1
1	L	509	LEU	3.1
1	E	510	LEU	3.1
1	L	508	PRO	3.1
1	E	508	PRO	3.1
1	J	502	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	501	LYS	3.1
1	L	516	VAL	3.1
1	L	560	VAL	3.1
1	D	656	GLU	3.1
1	L	462	PRO	3.1
1	B	752	THR	3.1
1	L	440	LYS	3.1
1	I	554	TYR	3.0
1	D	748	GLN	3.0
1	D	606	LYS	3.0
1	C	486	ILE	3.0
1	F	583	ILE	3.0
1	C	749	ARG	3.0
1	J	602	LEU	3.0
1	J	576	TYR	3.0
1	L	675	ASP	3.0
1	J	515	ILE	3.0
1	L	470	THR	3.0
1	G	773	VAL	3.0
1	I	441	VAL	3.0
1	K	638	PHE	3.0
1	I	478	LEU	3.0
1	F	731	GLU	3.0
1	L	521	HIS	3.0
1	F	502	ILE	3.0
1	K	470	THR	3.0
1	K	571	GLY	3.0
1	C	525	PHE	3.0
1	F	482	VAL	3.0
1	L	495	PRO	3.0
1	I	508	PRO	3.0
1	K	495	PRO	3.0
1	F	729	LYS	3.0
1	F	745	ASN	3.0
1	G	448	ASN	3.0
1	H	729	LYS	3.0
1	H	490	ILE	3.0
1	E	727	ILE	3.0
1	E	480	THR	3.0
1	D	513	VAL	3.0
1	F	711	PHE	3.0
1	J	600	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	603	LEU	2.9
1	I	766	GLU	2.9
1	A	729	LYS	2.9
1	A	511	ASN	2.9
1	A	480	THR	2.9
1	E	470	THR	2.9
1	D	442	PHE	2.9
1	E	674	PRO	2.9
1	B	776	SER	2.9
1	B	748	GLN	2.9
1	H	749	ARG	2.9
1	L	640	ILE	2.9
1	H	706	ALA	2.9
1	F	696	LEU	2.9
1	L	548	LEU	2.9
1	K	468	GLU	2.9
1	K	750	THR	2.9
1	F	455	ALA	2.9
1	I	479	ALA	2.9
1	F	723	LEU	2.9
1	J	442	PHE	2.9
1	I	525	PHE	2.9
1	I	527	PHE	2.9
1	K	746	VAL	2.9
1	J	514	SER	2.9
1	E	575	ASN	2.9
1	F	571	GLY	2.9
1	F	440	LYS	2.9
1	D	762	PHE	2.9
1	J	736	PHE	2.9
1	F	549	MET	2.8
1	F	581	ARG	2.8
1	F	585	GLN	2.8
1	A	439	SER	2.8
1	F	487	CYS	2.8
1	L	554	TYR	2.8
1	I	532	TYR	2.8
1	D	505	LEU	2.8
1	B	603	LEU	2.8
1	F	478	LEU	2.8
1	F	510	LEU	2.8
1	H	608	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	607	PHE	2.8
1	L	746	VAL	2.8
1	F	497	ARG	2.8
1	H	725	GLN	2.8
1	J	503	LYS	2.8
1	F	598	LEU	2.8
1	I	545	ALA	2.8
1	K	579	ALA	2.8
1	B	762	PHE	2.8
1	L	641	GLU	2.8
1	B	749	ARG	2.8
1	H	508	PRO	2.8
1	C	476	LYS	2.8
1	L	493	GLY	2.8
1	I	461	LEU	2.8
1	D	529	GLU	2.8
1	F	638	PHE	2.8
1	H	609	VAL	2.8
1	K	635	VAL	2.8
1	K	724	ILE	2.8
1	H	437	SER	2.8
1	J	747	LEU	2.8
1	L	566	ASP	2.8
1	D	482	VAL	2.8
1	D	751	THR	2.8
1	A	441	VAL	2.8
1	F	730	ALA	2.8
1	L	504	ALA	2.8
1	L	564	GLU	2.8
1	H	455	ALA	2.8
1	I	752	THR	2.8
1	I	466	PHE	2.8
1	K	749	ARG	2.8
1	B	698	PRO	2.7
1	L	488	GLN	2.7
1	F	608	LEU	2.7
1	J	461	LEU	2.7
1	I	542	LEU	2.7
1	K	610	LEU	2.7
1	E	509	LEU	2.7
1	K	456	ALA	2.7
1	D	607	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	751	THR	2.7
1	H	769	TYR	2.7
1	H	502	ILE	2.7
1	A	520	SER	2.7
1	C	444	ARG	2.7
1	L	544	GLU	2.7
1	C	730	ALA	2.7
1	F	446	ALA	2.7
1	F	504	ALA	2.7
1	F	557	ALA	2.7
1	G	455	ALA	2.7
1	I	638	PHE	2.7
1	D	452	GLN	2.7
1	A	476	LYS	2.7
1	E	678	ILE	2.7
1	L	492	LEU	2.7
1	H	598	LEU	2.7
1	J	739	GLY	2.7
1	L	514	SER	2.7
1	A	456	ALA	2.7
1	F	751	THR	2.7
1	I	744	ALA	2.7
1	C	729	LYS	2.7
1	K	522	PRO	2.7
1	E	721	TYR	2.7
1	J	640	ILE	2.7
1	L	540	ILE	2.7
1	G	702	LEU	2.7
1	J	439	SER	2.7
1	H	641	GLU	2.7
1	I	544	GLU	2.7
1	J	477	ALA	2.7
1	H	523	LYS	2.7
1	E	485	LYS	2.7
1	F	574	ILE	2.6
1	K	640	ILE	2.6
1	E	486	ILE	2.6
1	I	499	LYS	2.6
1	E	699	PHE	2.6
1	F	676	LEU	2.6
1	H	676	LEU	2.6
1	E	702	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	511	ASN	2.6
1	H	573	SER	2.6
1	A	515	ILE	2.6
1	A	510	LEU	2.6
1	I	476	LYS	2.6
1	E	544	GLU	2.6
1	C	639	GLY	2.6
1	D	479	ALA	2.6
1	A	455	ALA	2.6
1	F	525	PHE	2.6
1	L	511	ASN	2.6
1	E	573	SER	2.6
1	G	512	ASP	2.6
1	A	634	ILE	2.6
1	F	486	ILE	2.6
1	B	775	LYS	2.6
1	D	483	GLU	2.6
1	E	731	GLU	2.6
1	B	469	GLY	2.6
1	J	753	VAL	2.6
1	I	474	VAL	2.6
1	I	607	PHE	2.6
1	K	600	PHE	2.6
1	E	519	SER	2.5
1	C	481	LEU	2.5
1	D	774	LEU	2.5
1	A	509	LEU	2.5
1	K	505	LEU	2.5
1	C	547	ARG	2.5
1	G	497	ARG	2.5
1	I	494	TYR	2.5
1	K	637	TYR	2.5
1	E	601	VAL	2.5
1	A	600	PHE	2.5
1	F	726	GLN	2.5
1	J	632	ALA	2.5
1	L	555	PHE	2.5
1	I	570	SER	2.5
1	I	759	SER	2.5
1	F	515	ILE	2.5
1	A	775	LYS	2.5
1	E	698	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	688	VAL	2.5
1	B	730	ALA	2.5
1	L	743	SER	2.5
1	L	542	LEU	2.5
1	I	581	ARG	2.5
1	H	694	GLU	2.5
1	L	450	VAL	2.5
1	D	638	PHE	2.5
1	H	748	GLN	2.5
1	I	746	VAL	2.5
1	I	565	ALA	2.5
1	D	510	LEU	2.5
1	F	443	ILE	2.5
1	G	727	ILE	2.5
1	C	604	GLU	2.5
1	L	460	GLU	2.5
1	J	597	GLY	2.5
1	L	571	GLY	2.5
1	D	508	PRO	2.5
1	J	495	PRO	2.5
1	F	720	ALA	2.5
1	I	477	ALA	2.5
1	C	485	LYS	2.4
1	F	703	LYS	2.4
1	E	473	LYS	2.4
1	D	745	ASN	2.4
1	D	507	ILE	2.4
1	D	515	ILE	2.4
1	D	676	LEU	2.4
1	L	507	ILE	2.4
1	H	634	ILE	2.4
1	F	445	SER	2.4
1	H	546	GLU	2.4
1	A	508	PRO	2.4
1	B	543	GLY	2.4
1	F	552	PRO	2.4
1	L	522	PRO	2.4
1	L	563	GLY	2.4
1	H	543	GLY	2.4
1	K	576	TYR	2.4
1	F	606	LYS	2.4
1	I	750	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	502	ILE	2.4
1	F	629	LEU	2.4
1	J	608	LEU	2.4
1	H	540	ILE	2.4
1	C	544	GLU	2.4
1	C	704	GLY	2.4
1	I	493	GLY	2.4
1	D	503	LYS	2.4
1	F	476	LYS	2.4
1	L	523	LYS	2.4
1	L	771	LYS	2.4
1	I	504	ALA	2.4
1	B	509	LEU	2.4
1	B	574	ILE	2.4
1	B	750	THR	2.4
1	F	475	LEU	2.4
1	L	752	THR	2.4
1	I	443	ILE	2.4
1	C	506	ASP	2.4
1	B	468	GLU	2.4
1	F	495	PRO	2.4
1	K	473	LYS	2.4
1	L	639	GLY	2.4
1	A	725	GLN	2.4
1	I	536	GLN	2.4
1	L	773	VAL	2.4
1	D	637	TYR	2.4
1	A	706	ALA	2.4
1	F	456	ALA	2.4
1	G	494	TYR	2.4
1	L	456	ALA	2.4
1	I	550	ALA	2.4
1	I	730	ALA	2.4
1	F	492	LEU	2.4
1	I	511	ASN	2.4
1	F	500	GLU	2.4
1	H	570	SER	2.4
1	I	568	MET	2.4
1	I	440	LYS	2.4
1	A	513	VAL	2.4
1	F	746	VAL	2.4
1	J	441	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	609	VAL	2.4
1	K	498	VAL	2.4
1	D	446	ALA	2.4
1	G	730	ALA	2.4
1	K	774	LEU	2.3
1	L	756	ILE	2.3
1	G	529	GLU	2.3
1	D	568	MET	2.3
1	K	729	LYS	2.3
1	K	743	SER	2.3
1	H	495	PRO	2.3
1	B	728	GLY	2.3
1	D	497	ARG	2.3
1	J	547	ARG	2.3
1	L	547	ARG	2.3
1	B	442	PHE	2.3
1	C	505	LEU	2.3
1	A	696	LEU	2.3
1	J	505	LEU	2.3
1	J	579	ALA	2.3
1	I	577	ALA	2.3
1	E	525	PHE	2.3
1	I	447	ILE	2.3
1	H	438	HIS	2.3
1	L	561	ASN	2.3
1	E	511	ASN	2.3
1	H	544	GLU	2.3
1	I	485	LYS	2.3
1	K	503	LYS	2.3
1	K	591	LYS	2.3
1	L	570	SER	2.3
1	H	578	ASP	2.3
1	E	512	ASP	2.3
1	A	462	PRO	2.3
1	D	493	GLY	2.3
1	D	639	GLY	2.3
1	A	749	ARG	2.3
1	F	749	ARG	2.3
1	G	704	GLY	2.3
1	I	739	GLY	2.3
1	E	728	GLY	2.3
1	E	482	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	634	ILE	2.3
1	C	472	THR	2.3
1	D	480	THR	2.3
1	J	637	TYR	2.3
1	D	501	LYS	2.3
1	A	468	GLU	2.3
1	B	564	GLU	2.3
1	B	575	ASN	2.3
1	L	468	GLU	2.3
1	L	503	LYS	2.3
1	E	503	LYS	2.3
1	K	575	ASN	2.3
1	I	605	ASP	2.3
1	A	497	ARG	2.3
1	E	497	ARG	2.3
1	F	732	VAL	2.3
1	H	601	VAL	2.3
1	C	542	LEU	2.3
1	A	548	LEU	2.3
1	B	737	LEU	2.3
1	J	603	LEU	2.3
1	L	442	PHE	2.3
1	F	565	ALA	2.3
1	J	486	ILE	2.3
1	F	480	THR	2.3
1	A	546	GLU	2.3
1	E	604	GLU	2.3
1	D	439	SER	2.3
1	D	522	PRO	2.3
1	D	776	SER	2.3
1	A	698	PRO	2.3
1	H	497	ARG	2.3
1	I	445	SER	2.3
1	L	461	LEU	2.3
1	L	482	VAL	2.3
1	H	709	LEU	2.3
1	E	602	LEU	2.3
1	E	711	PHE	2.3
1	C	477	ALA	2.2
1	C	727	ILE	2.2
1	D	486	ILE	2.2
1	K	577	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	634	ILE	2.2
1	E	640	ILE	2.2
1	B	591	LYS	2.2
1	G	729	LYS	2.2
1	F	763	THR	2.2
1	A	524	TYR	2.2
1	L	467	PRO	2.2
1	B	578	ASP	2.2
1	F	768	GLN	2.2
1	E	439	SER	2.2
1	B	571	GLY	2.2
1	F	493	GLY	2.2
1	F	680	GLY	2.2
1	B	723	LEU	2.2
1	H	475	LEU	2.2
1	H	542	LEU	2.2
1	I	757	VAL	2.2
1	K	461	LEU	2.2
1	C	775	LYS	2.2
1	F	451	HIS	2.2
1	F	633	LYS	2.2
1	L	477	ALA	2.2
1	L	485	LYS	2.2
1	K	736	PHE	2.2
1	I	559	MET	2.2
1	K	438	HIS	2.2
1	B	604	GLU	2.2
1	B	772	GLU	2.2
1	A	769	TYR	2.2
1	F	721	TYR	2.2
1	K	581	ARG	2.2
1	I	518	PRO	2.2
1	A	748	GLN	2.2
1	F	520	SER	2.2
1	J	570	SER	2.2
1	L	572	SER	2.2
1	I	514	SER	2.2
1	E	776	SER	2.2
1	A	737	LEU	2.2
1	I	513	VAL	2.2
1	A	574	ILE	2.2
1	A	727	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	600	PHE	2.2
1	H	550	ALA	2.2
1	E	751	THR	2.2
1	H	524	TYR	2.2
1	H	541	ASN	2.2
1	I	448	ASN	2.2
1	B	508	PRO	2.2
1	F	748	GLN	2.2
1	E	585	GLN	2.2
1	A	505	LEU	2.2
1	J	639	GLY	2.2
1	L	747	LEU	2.2
1	K	602	LEU	2.2
1	A	516	VAL	2.2
1	J	516	VAL	2.2
1	B	555	PHE	2.2
1	F	733	ILE	2.2
1	L	525	PHE	2.2
1	E	600	PHE	2.2
1	L	656	GLU	2.2
1	F	642	PRO	2.2
1	I	606	LYS	2.2
1	F	709	LEU	2.2
1	F	450	VAL	2.2
1	L	447	ILE	2.2
1	H	773	VAL	2.2
1	I	753	VAL	2.2
1	E	443	ILE	2.2
1	G	645	ALA	2.1
1	D	468	GLU	2.1
1	D	694	GLU	2.1
1	F	575	ASN	2.1
1	A	637	TYR	2.1
1	F	637	TYR	2.1
1	K	748	GLN	2.1
1	K	676	LEU	2.1
1	I	543	GLY	2.1
1	I	755	GLY	2.1
1	C	514	SER	2.1
1	F	471	SER	2.1
1	F	710	VAL	2.1
1	G	609	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	474	VAL	2.1
1	K	502	ILE	2.1
1	K	569	VAL	2.1
1	F	736	PHE	2.1
1	E	442	PHE	2.1
1	C	706	ALA	2.1
1	J	730	ALA	2.1
1	K	504	ALA	2.1
1	J	496	GLU	2.1
1	D	643	ARG	2.1
1	D	472	THR	2.1
1	F	489	PRO	2.1
1	F	582	PRO	2.1
1	H	735	PRO	2.1
1	D	448	ASN	2.1
1	I	488	GLN	2.1
1	A	542	LEU	2.1
1	F	461	LEU	2.1
1	H	510	LEU	2.1
1	H	590	TYR	2.1
1	E	481	LEU	2.1
1	K	597	GLY	2.1
1	E	597	GLY	2.1
1	F	512	ASP	2.1
1	F	685	ASP	2.1
1	F	753	VAL	2.1
1	J	580	VAL	2.1
1	D	466	PHE	2.1
1	D	514	SER	2.1
1	G	762	PHE	2.1
1	H	442	PHE	2.1
1	H	743	SER	2.1
1	I	471	SER	2.1
1	I	573	SER	2.1
1	L	550	ALA	2.1
1	E	687	ALA	2.1
1	E	775	LYS	2.1
1	F	595	PRO	2.1
1	J	642	PRO	2.1
1	B	617	LEU	2.1
1	G	672	LEU	2.1
1	H	492	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	774	LEU	2.1
1	I	541	ASN	2.1
1	F	649	TYR	2.1
1	I	576	TYR	2.1
1	E	576	TYR	2.1
1	C	640	ILE	2.1
1	H	762	PHE	2.1
1	B	572	SER	2.1
1	L	454	SER	2.1
1	D	772	GLU	2.1
1	G	456	ALA	2.1
1	H	485	LYS	2.1
1	E	501	LYS	2.1
1	J	750	THR	2.1
1	F	467	PRO	2.1
1	K	674	PRO	2.1
1	D	481	LEU	2.1
1	F	542	LEU	2.1
1	K	696	LEU	2.1
1	A	457	ASN	2.1
1	A	541	ASN	2.1
1	H	707	ASN	2.1
1	H	745	ASN	2.1
1	A	459	GLY	2.1
1	H	734	GLY	2.1
1	F	580	VAL	2.1
1	L	753	VAL	2.1
1	B	638	PHE	2.1
1	G	525	PHE	2.1
1	L	512	ASP	2.0
1	D	456	ALA	2.0
1	F	573	SER	2.0
1	F	717	SER	2.0
1	G	573	SER	2.0
1	L	631	ALA	2.0
1	E	479	ALA	2.0
1	J	591	LYS	2.0
1	I	462	PRO	2.0
1	D	768	GLN	2.0
1	B	488	GLN	2.0
1	J	475	LEU	2.0
1	E	676	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	726	GLN	2.0
1	A	758	ASN	2.0
1	I	517	HIS	2.0
1	I	553	ASN	2.0
1	F	543	GLY	2.0
1	F	640	ILE	2.0
1	F	656	GLU	2.0
1	L	527	PHE	2.0
1	H	736	PHE	2.0
1	B	631	ALA	2.0
1	L	455	ALA	2.0
1	E	605	ASP	2.0
1	L	530	LYS	2.0
1	A	700	SER	2.0
1	G	526	SER	2.0
1	H	514	SER	2.0
1	C	522	PRO	2.0
1	A	470	THR	2.0
1	F	518	PRO	2.0
1	K	518	PRO	2.0
1	E	750	THR	2.0
1	C	603	LEU	2.0
1	B	747	LEU	2.0
1	K	747	LEU	2.0
1	F	727	ILE	2.0
1	G	574	ILE	2.0
1	J	727	ILE	2.0
1	H	539	GLY	2.0
1	H	571	GLY	2.0
1	H	733	ILE	2.0
1	I	707	ASN	2.0
1	A	482	VAL	2.0
1	L	528	VAL	2.0
1	L	644	VAL	2.0
1	I	528	VAL	2.0
1	K	601	VAL	2.0
1	D	494	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.