



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:36 AM UTC

PDB ID : 4V6H / pdb_00004v6h
Title : Crystal structure of succinate-semialdehyde dehydrogenase from Burkholderia pseudomallei
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2009-07-24
Resolution : 2.70 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

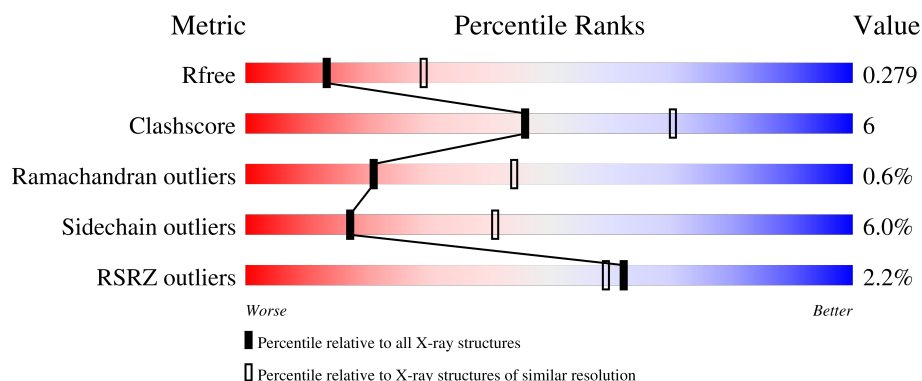
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1	484	11% 77% 21% .
1	2	484	2% 77% 20% .
1	3	484	2% 81% 18% .
1	4	484	% 82% 16% .
1	5	484	% 83% 15% .

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Mol	Chain	Length	Quality of chain
1	6	484	 88% 12%
1	A	484	 86% 12% .
1	B	484	 89% 10% .
1	C	484	 85% 13% .
1	D	484	 82% 17%
1	E	484	 85% 13% .
1	F	484	 86% 12% .
1	G	484	 85% 13% .
1	H	484	 86% 13% .
1	I	484	 79% 20% .
1	J	484	 82% 15% .
1	K	484	 86% 12% .
1	L	484	 86% 13% .
1	M	484	 83% 15% .
1	N	484	 87% 12% .
1	O	484	 86% 13% .
1	P	484	 86% 13% .
1	Q	484	 81% 18% .
1	R	484	 84% 14% .
1	S	484	 86% 13% .
1	T	484	 81% 18% .
1	U	484	 77% 21% .
1	V	484	 81% 17% .
1	W	484	 88% 11% .
1	X	484	 77% 20% .

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Mol	Chain	Length	Quality of chain
1	Y	484	6% 77% 21%
1	Z	484	9% 73% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 114732 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 Succinate-semialdehyde dehydrogenase (NADP+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	B	482	Total	C	N	O	S	0	0	0
			3553	2261	607	671	14			
1	C	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	D	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	E	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	F	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	G	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	H	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	I	482	Total	C	N	O	S	0	0	0
			3520	2242	597	667	14			
1	J	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	K	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	L	482	Total	C	N	O	S	0	0	0
			3543	2255	607	667	14			
1	M	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	N	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	O	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	P	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	R	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	S	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	T	482	Total	C	N	O	S	0	0	0
			3535	2248	606	667	14			
1	U	482	Total	C	N	O	S	0	0	0
			3521	2241	601	665	14			
1	V	482	Total	C	N	O	S	0	0	0
			3532	2248	603	667	14			
1	W	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	X	482	Total	C	N	O	S	0	0	0
			3515	2235	603	663	14			
1	Y	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	Z	482	Total	C	N	O	S	0	0	0
			3532	2248	603	667	14			
1	1	482	Total	C	N	O	S	0	0	0
			3510	2235	595	666	14			
1	2	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	3	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	4	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	5	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	6	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q3JS51
A	2	PRO	-	expression tag	UNP Q3JS51
A	3	GLY	-	expression tag	UNP Q3JS51
A	4	SER	-	expression tag	UNP Q3JS51
B	1	GLY	-	expression tag	UNP Q3JS51
B	2	PRO	-	expression tag	UNP Q3JS51
B	3	GLY	-	expression tag	UNP Q3JS51

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	expression tag	UNP Q3JS51
C	1	GLY	-	expression tag	UNP Q3JS51
C	2	PRO	-	expression tag	UNP Q3JS51
C	3	GLY	-	expression tag	UNP Q3JS51
C	4	SER	-	expression tag	UNP Q3JS51
D	1	GLY	-	expression tag	UNP Q3JS51
D	2	PRO	-	expression tag	UNP Q3JS51
D	3	GLY	-	expression tag	UNP Q3JS51
D	4	SER	-	expression tag	UNP Q3JS51
E	1	GLY	-	expression tag	UNP Q3JS51
E	2	PRO	-	expression tag	UNP Q3JS51
E	3	GLY	-	expression tag	UNP Q3JS51
E	4	SER	-	expression tag	UNP Q3JS51
F	1	GLY	-	expression tag	UNP Q3JS51
F	2	PRO	-	expression tag	UNP Q3JS51
F	3	GLY	-	expression tag	UNP Q3JS51
F	4	SER	-	expression tag	UNP Q3JS51
G	1	GLY	-	expression tag	UNP Q3JS51
G	2	PRO	-	expression tag	UNP Q3JS51
G	3	GLY	-	expression tag	UNP Q3JS51
G	4	SER	-	expression tag	UNP Q3JS51
H	1	GLY	-	expression tag	UNP Q3JS51
H	2	PRO	-	expression tag	UNP Q3JS51
H	3	GLY	-	expression tag	UNP Q3JS51
H	4	SER	-	expression tag	UNP Q3JS51
I	1	GLY	-	expression tag	UNP Q3JS51
I	2	PRO	-	expression tag	UNP Q3JS51
I	3	GLY	-	expression tag	UNP Q3JS51
I	4	SER	-	expression tag	UNP Q3JS51
J	1	GLY	-	expression tag	UNP Q3JS51
J	2	PRO	-	expression tag	UNP Q3JS51
J	3	GLY	-	expression tag	UNP Q3JS51
J	4	SER	-	expression tag	UNP Q3JS51
K	1	GLY	-	expression tag	UNP Q3JS51
K	2	PRO	-	expression tag	UNP Q3JS51
K	3	GLY	-	expression tag	UNP Q3JS51
K	4	SER	-	expression tag	UNP Q3JS51
L	1	GLY	-	expression tag	UNP Q3JS51
L	2	PRO	-	expression tag	UNP Q3JS51
L	3	GLY	-	expression tag	UNP Q3JS51
L	4	SER	-	expression tag	UNP Q3JS51
M	1	GLY	-	expression tag	UNP Q3JS51

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Chain	Residue	Modelled	Actual	Comment	Reference
M	2	PRO	-	expression tag	UNP Q3JS51
M	3	GLY	-	expression tag	UNP Q3JS51
M	4	SER	-	expression tag	UNP Q3JS51
N	1	GLY	-	expression tag	UNP Q3JS51
N	2	PRO	-	expression tag	UNP Q3JS51
N	3	GLY	-	expression tag	UNP Q3JS51
N	4	SER	-	expression tag	UNP Q3JS51
O	1	GLY	-	expression tag	UNP Q3JS51
O	2	PRO	-	expression tag	UNP Q3JS51
O	3	GLY	-	expression tag	UNP Q3JS51
O	4	SER	-	expression tag	UNP Q3JS51
P	1	GLY	-	expression tag	UNP Q3JS51
P	2	PRO	-	expression tag	UNP Q3JS51
P	3	GLY	-	expression tag	UNP Q3JS51
P	4	SER	-	expression tag	UNP Q3JS51
Q	1	GLY	-	expression tag	UNP Q3JS51
Q	2	PRO	-	expression tag	UNP Q3JS51
Q	3	GLY	-	expression tag	UNP Q3JS51
Q	4	SER	-	expression tag	UNP Q3JS51
R	1	GLY	-	expression tag	UNP Q3JS51
R	2	PRO	-	expression tag	UNP Q3JS51
R	3	GLY	-	expression tag	UNP Q3JS51
R	4	SER	-	expression tag	UNP Q3JS51
S	1	GLY	-	expression tag	UNP Q3JS51
S	2	PRO	-	expression tag	UNP Q3JS51
S	3	GLY	-	expression tag	UNP Q3JS51
S	4	SER	-	expression tag	UNP Q3JS51
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T	3	GLY	-	expression tag	UNP Q3JS51
T	4	SER	-	expression tag	UNP Q3JS51
U	1	GLY	-	expression tag	UNP Q3JS51
U	2	PRO	-	expression tag	UNP Q3JS51
U	3	GLY	-	expression tag	UNP Q3JS51
U	4	SER	-	expression tag	UNP Q3JS51
V	1	GLY	-	expression tag	UNP Q3JS51
V	2	PRO	-	expression tag	UNP Q3JS51
V	3	GLY	-	expression tag	UNP Q3JS51
V	4	SER	-	expression tag	UNP Q3JS51
W	1	GLY	-	expression tag	UNP Q3JS51
W	2	PRO	-	expression tag	UNP Q3JS51
W	3	GLY	-	expression tag	UNP Q3JS51

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Chain	Residue	Modelled	Actual	Comment	Reference
W	4	SER	-	expression tag	UNP Q3JS51
X	1	GLY	-	expression tag	UNP Q3JS51
X	2	PRO	-	expression tag	UNP Q3JS51
X	3	GLY	-	expression tag	UNP Q3JS51
X	4	SER	-	expression tag	UNP Q3JS51
Y	1	GLY	-	expression tag	UNP Q3JS51
Y	2	PRO	-	expression tag	UNP Q3JS51
Y	3	GLY	-	expression tag	UNP Q3JS51
Y	4	SER	-	expression tag	UNP Q3JS51
Z	1	GLY	-	expression tag	UNP Q3JS51
Z	2	PRO	-	expression tag	UNP Q3JS51
Z	3	GLY	-	expression tag	UNP Q3JS51
Z	4	SER	-	expression tag	UNP Q3JS51
1	1	GLY	-	expression tag	UNP Q3JS51
1	2	PRO	-	expression tag	UNP Q3JS51
1	3	GLY	-	expression tag	UNP Q3JS51
1	4	SER	-	expression tag	UNP Q3JS51
2	1	GLY	-	expression tag	UNP Q3JS51
2	2	PRO	-	expression tag	UNP Q3JS51
2	3	GLY	-	expression tag	UNP Q3JS51
2	4	SER	-	expression tag	UNP Q3JS51
3	1	GLY	-	expression tag	UNP Q3JS51
3	2	PRO	-	expression tag	UNP Q3JS51
3	3	GLY	-	expression tag	UNP Q3JS51
3	4	SER	-	expression tag	UNP Q3JS51
4	1	GLY	-	expression tag	UNP Q3JS51
4	2	PRO	-	expression tag	UNP Q3JS51
4	3	GLY	-	expression tag	UNP Q3JS51
4	4	SER	-	expression tag	UNP Q3JS51
5	1	GLY	-	expression tag	UNP Q3JS51
5	2	PRO	-	expression tag	UNP Q3JS51
5	3	GLY	-	expression tag	UNP Q3JS51
5	4	SER	-	expression tag	UNP Q3JS51
6	1	GLY	-	expression tag	UNP Q3JS51
6	2	PRO	-	expression tag	UNP Q3JS51
6	3	GLY	-	expression tag	UNP Q3JS51
6	4	SER	-	expression tag	UNP Q3JS51

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	46	Total O 46 46	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	59	Total O 59 59	0	0
2	C	56	Total O 56 56	0	0
2	D	60	Total O 60 60	0	0
2	E	72	Total O 72 72	0	0
2	F	75	Total O 75 75	0	0
2	G	66	Total O 66 66	0	0
2	H	58	Total O 58 58	0	0
2	I	24	Total O 24 24	0	0
2	J	35	Total O 35 35	0	0
2	K	55	Total O 55 55	0	0
2	L	57	Total O 57 57	0	0
2	M	40	Total O 40 40	0	0
2	N	46	Total O 46 46	0	0
2	O	39	Total O 39 39	0	0
2	P	74	Total O 74 74	0	0
2	Q	22	Total O 22 22	0	0
2	R	35	Total O 35 35	0	0
2	S	55	Total O 55 55	0	0
2	T	13	Total O 13 13	0	0
2	U	13	Total O 13 13	0	0
2	V	29	Total O 29 29	0	0

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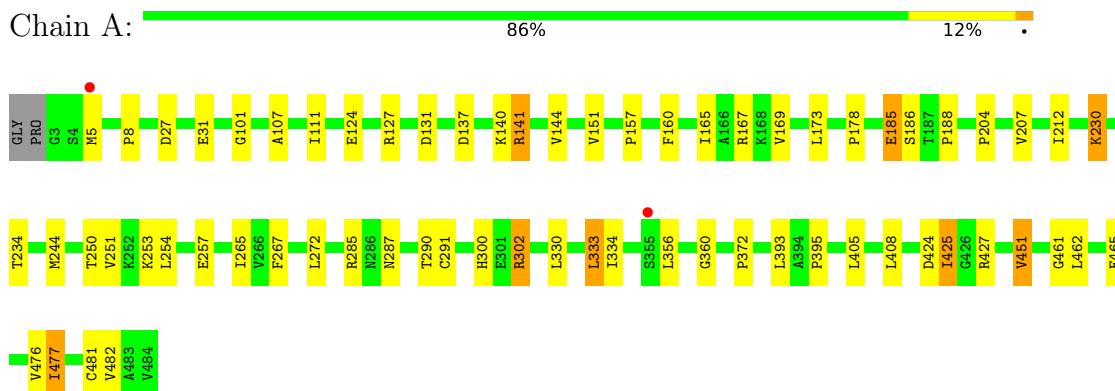
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	W	44	Total 44	O 44	0	0
2	X	8	Total 8	O 8	0	0
2	Y	36	Total 36	O 36	0	0
2	Z	20	Total 20	O 20	0	0
2	1	28	Total 28	O 28	0	0
2	2	37	Total 37	O 37	0	0
2	3	45	Total 45	O 45	0	0
2	4	46	Total 46	O 46	0	0
2	5	54	Total 54	O 54	0	0
2	6	57	Total 57	O 57	0	0

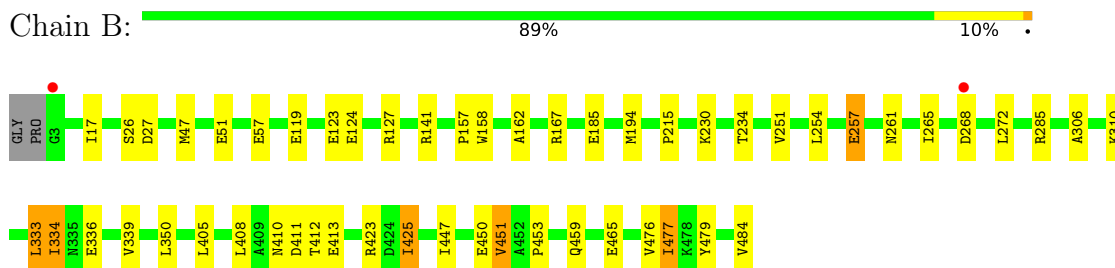
3 Residue-property plots

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.

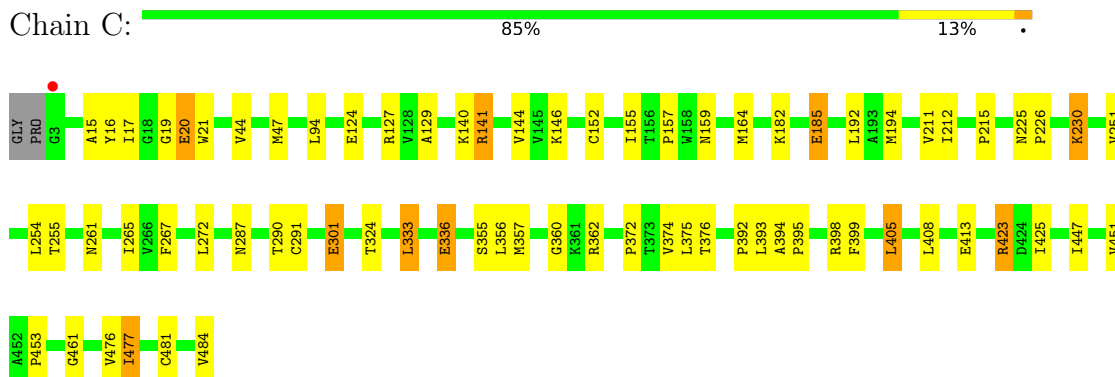
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



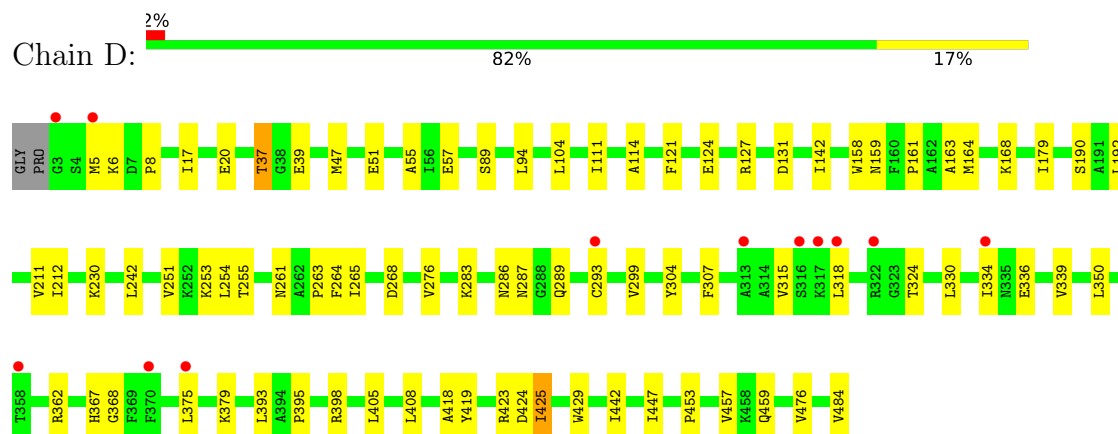
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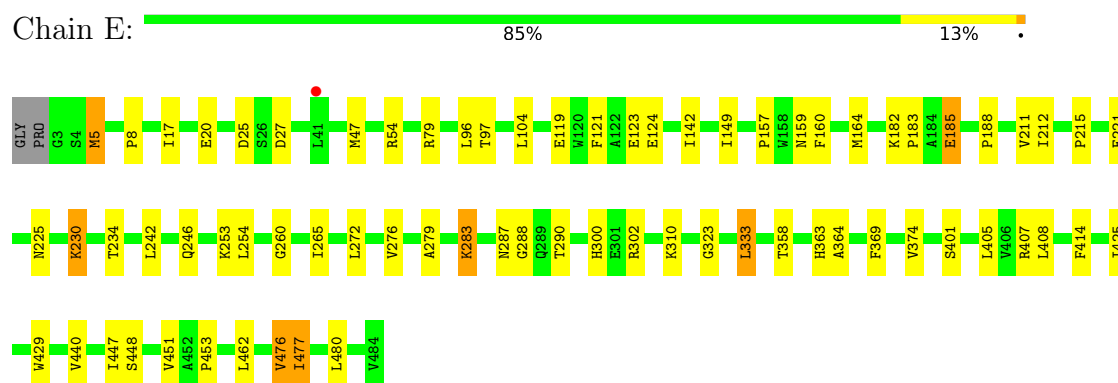
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



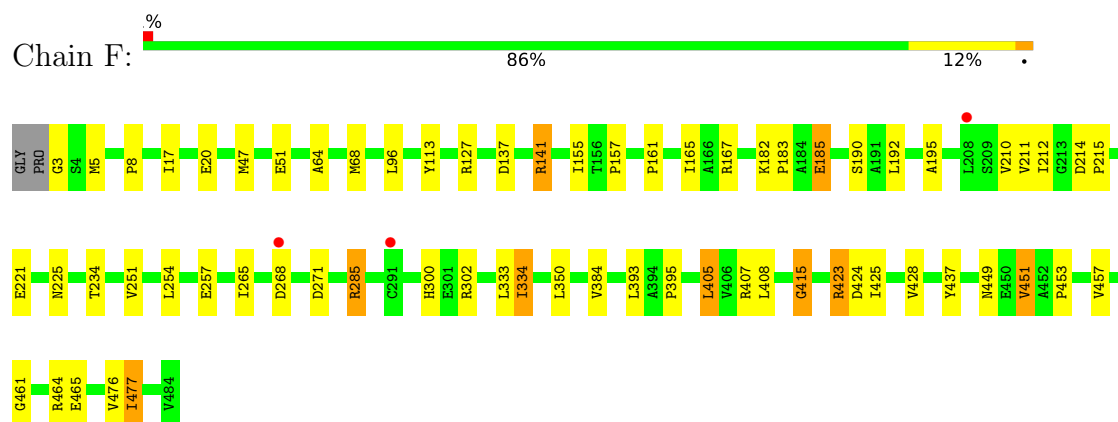
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



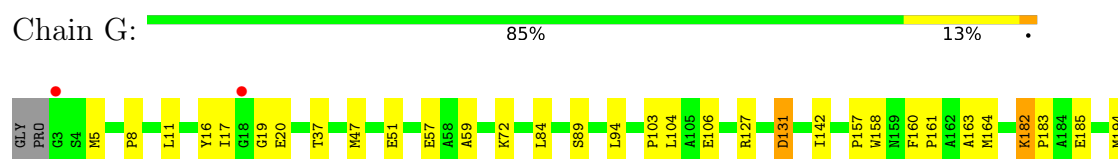
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

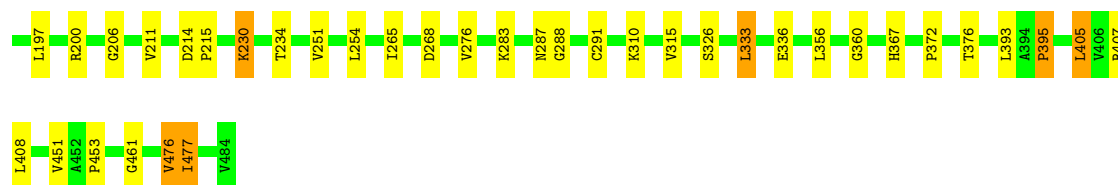


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

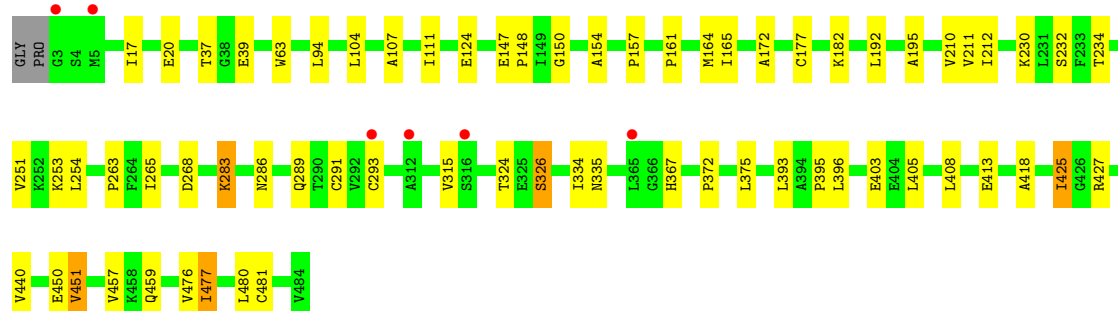
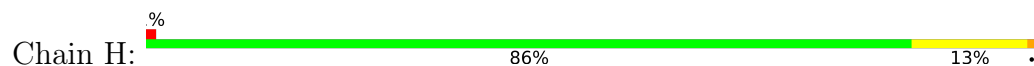


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

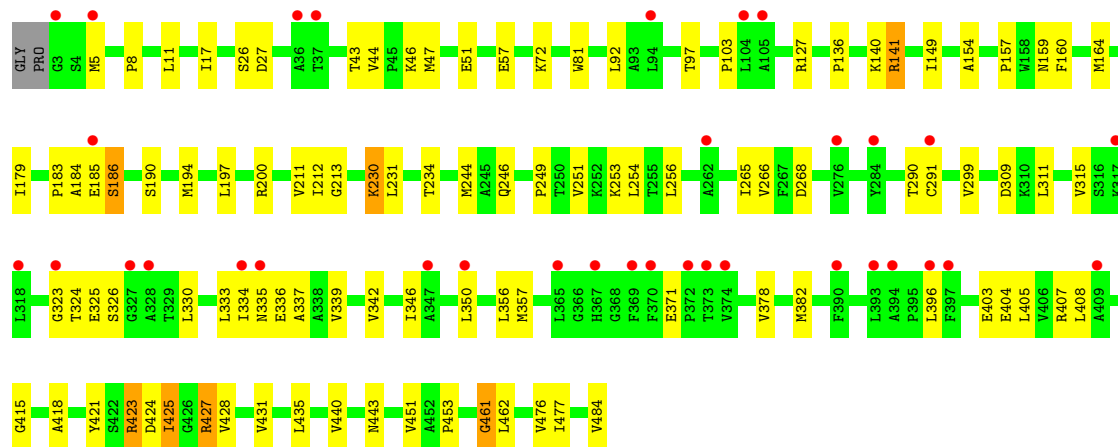
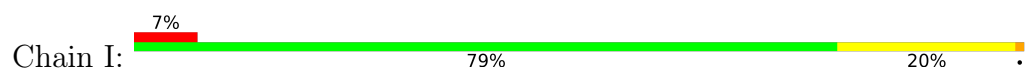




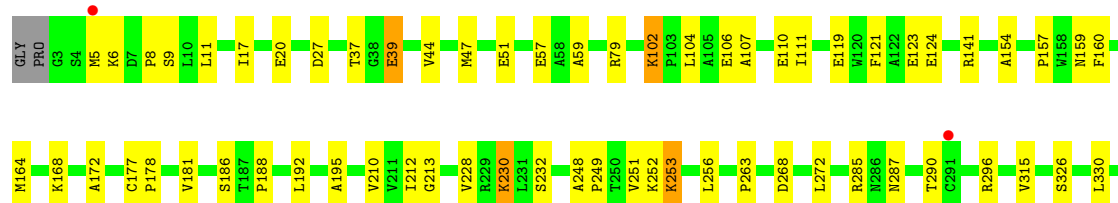
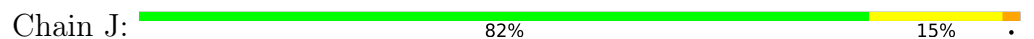
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

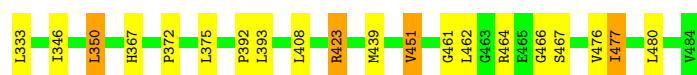


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

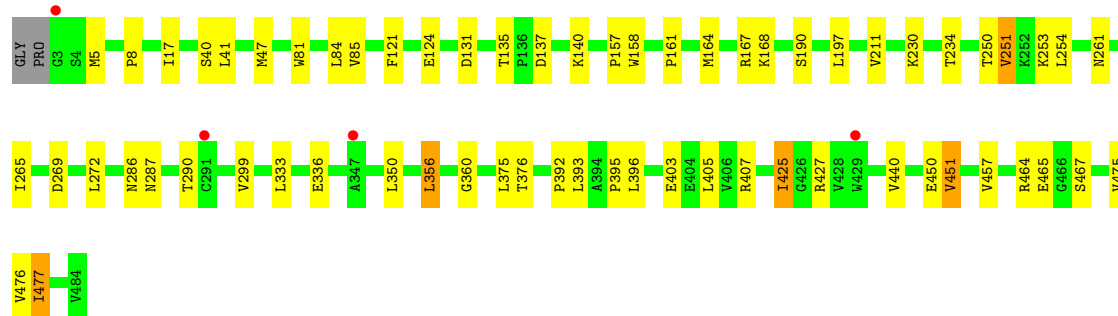
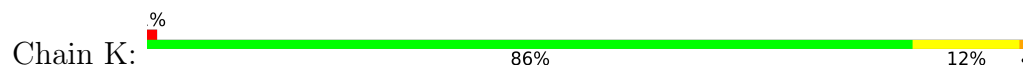


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

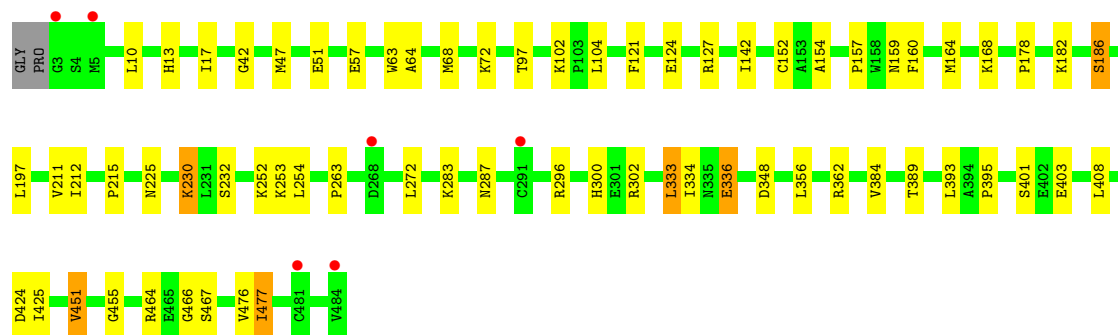
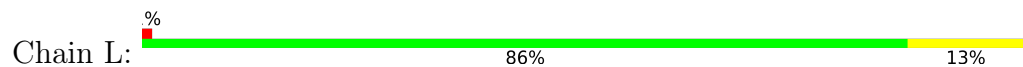




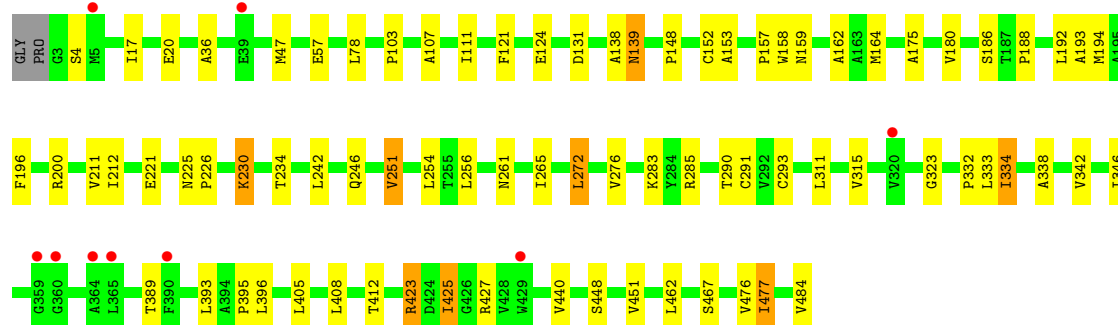
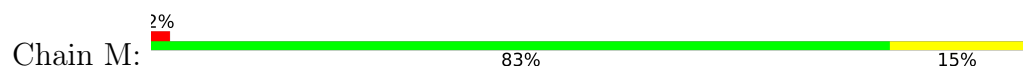
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



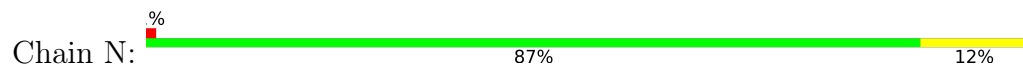
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

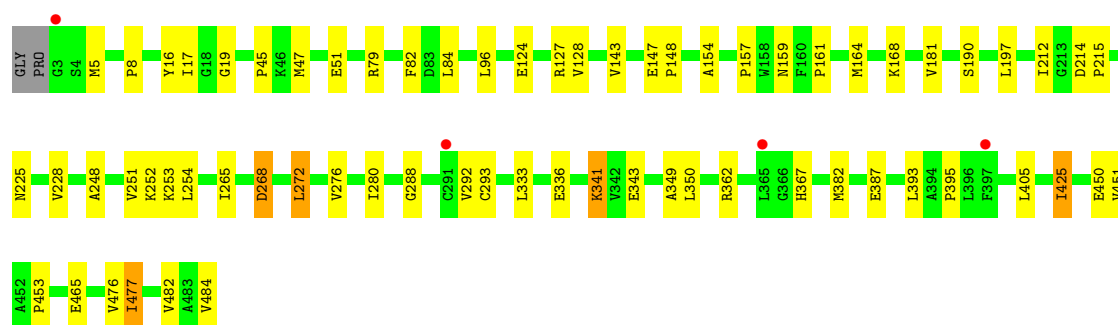
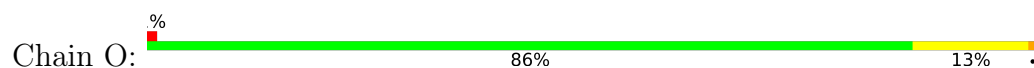


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

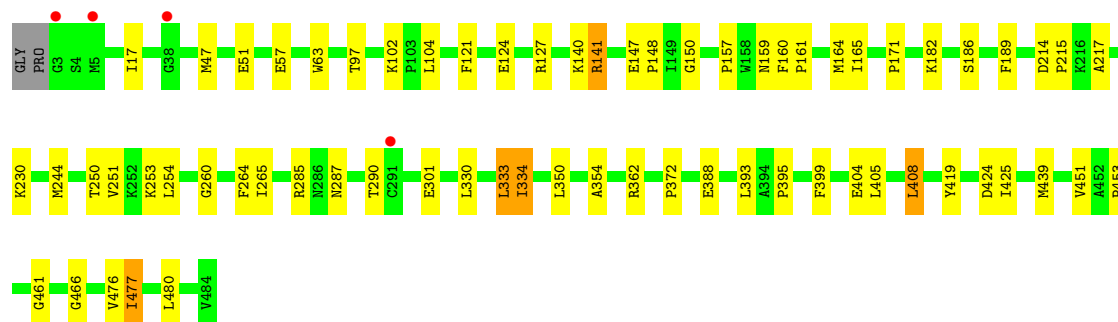
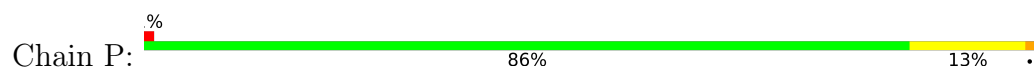




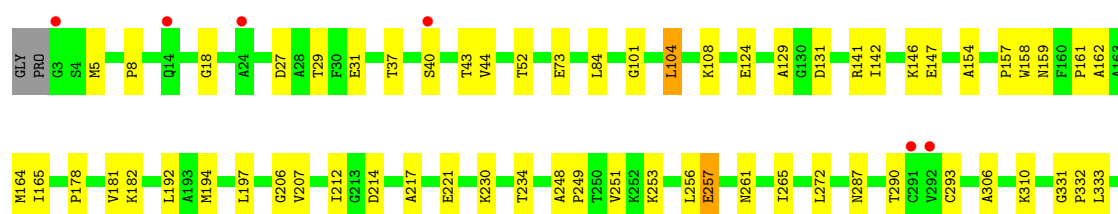
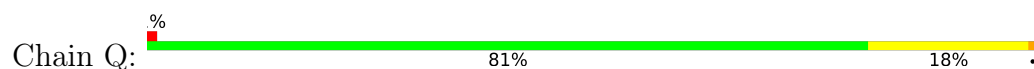
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP⁺)



• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP⁺)

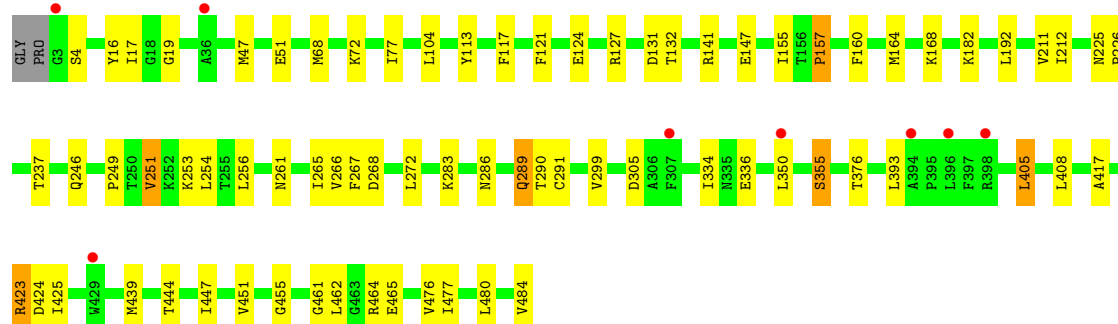
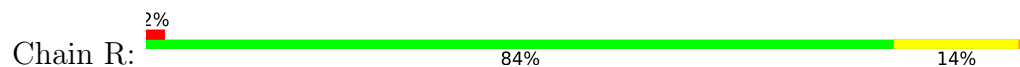


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP⁺)

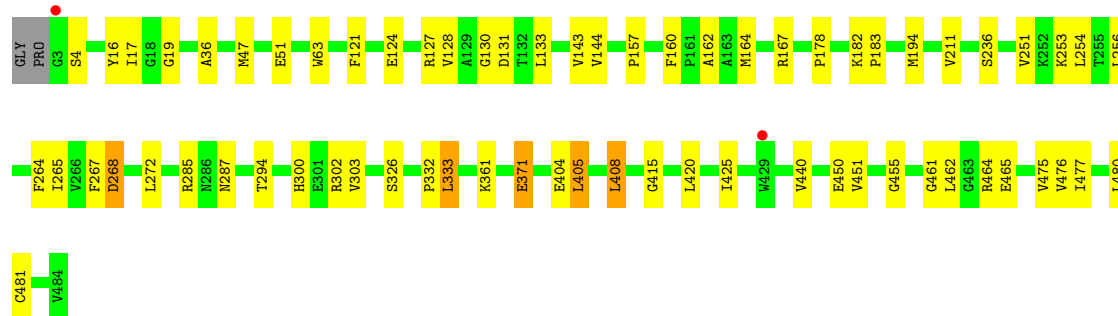
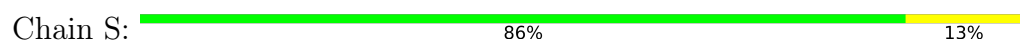




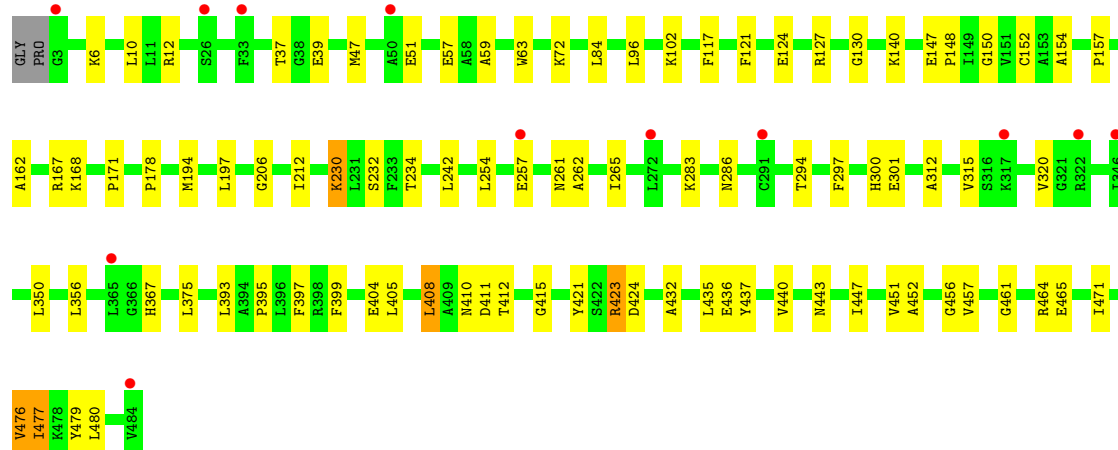
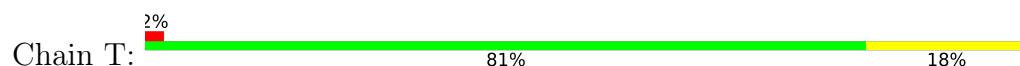
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



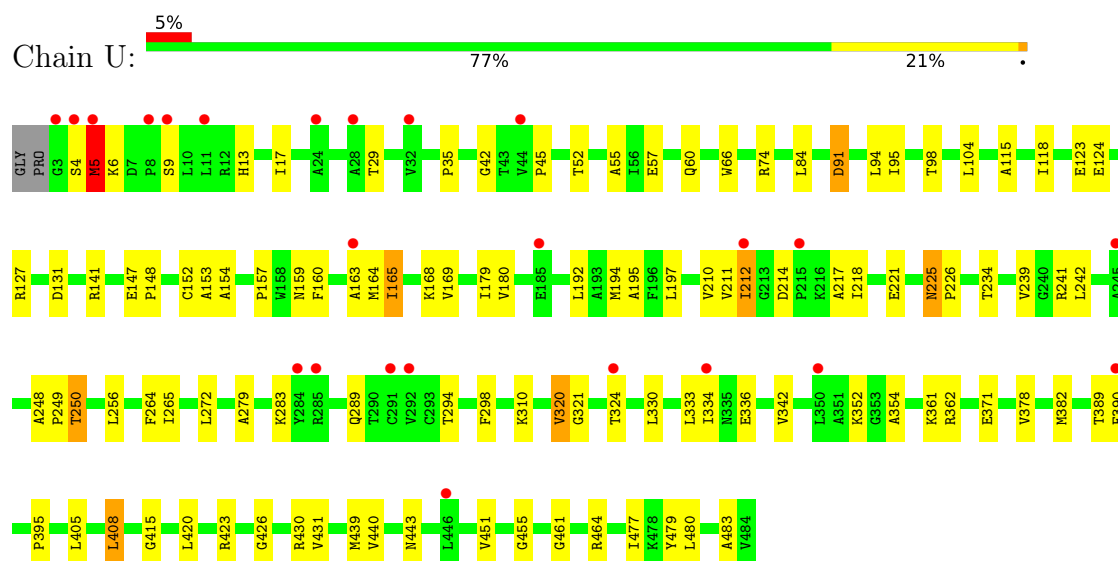
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



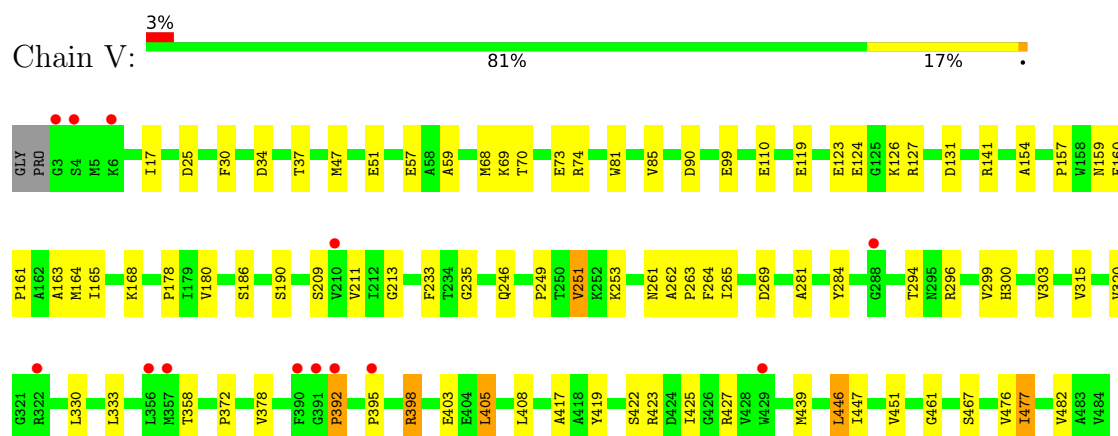
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



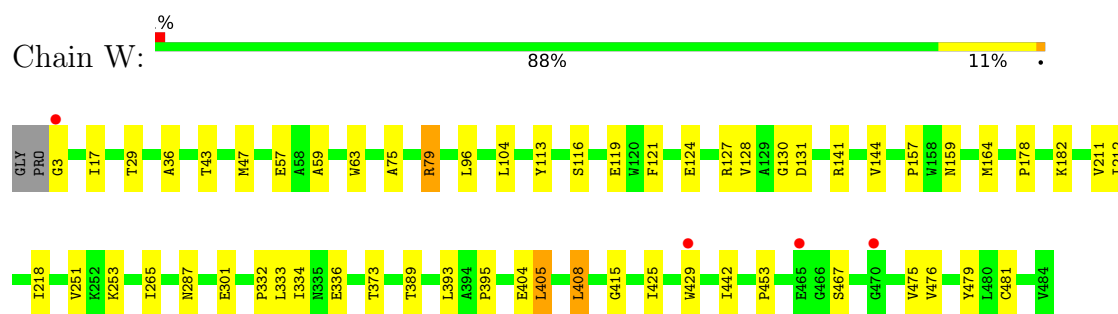
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



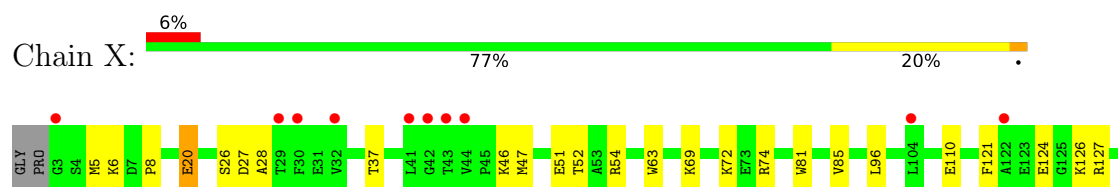
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

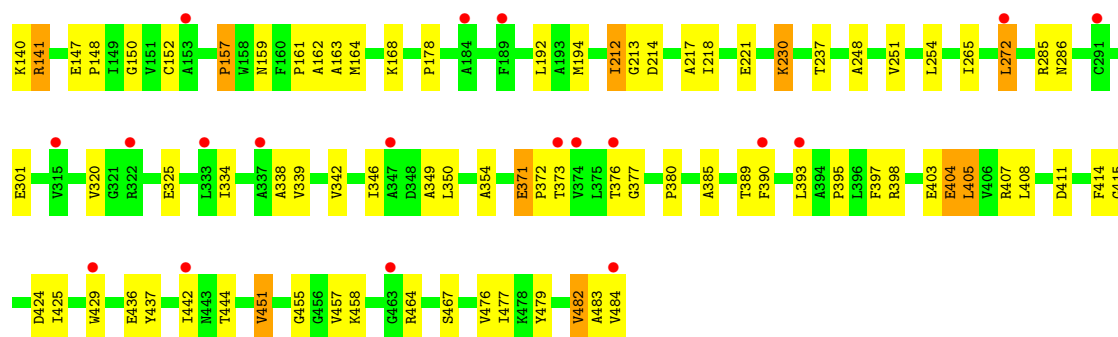


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

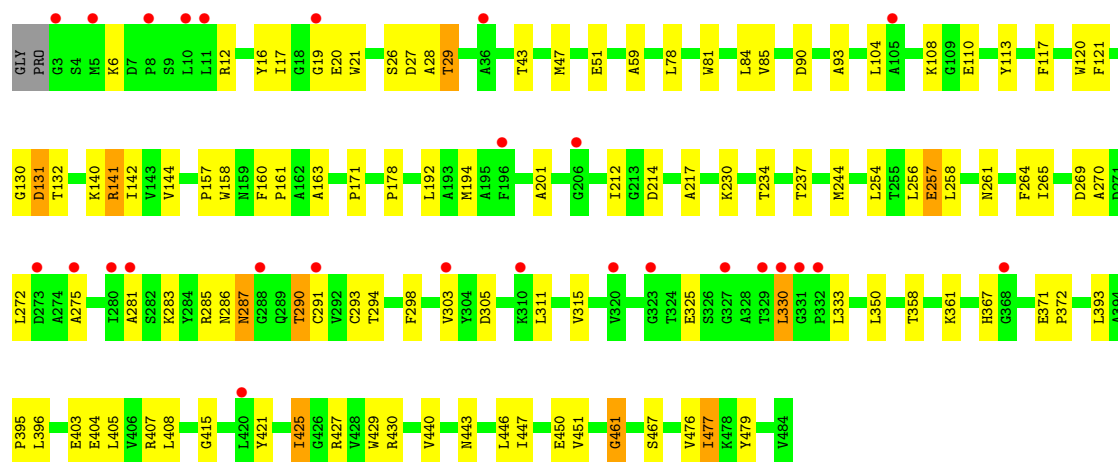
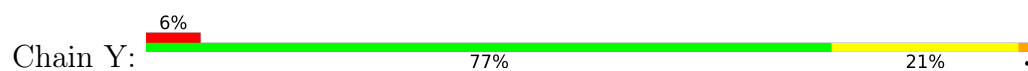


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

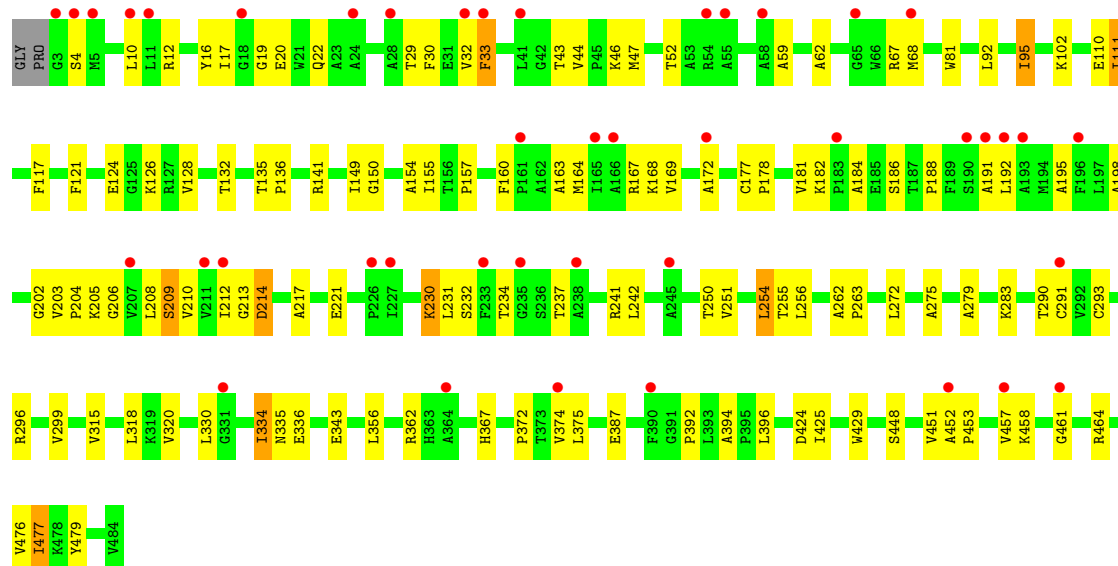
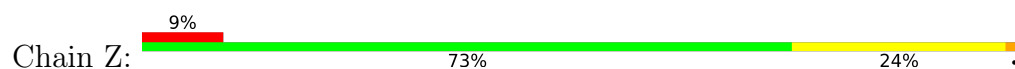




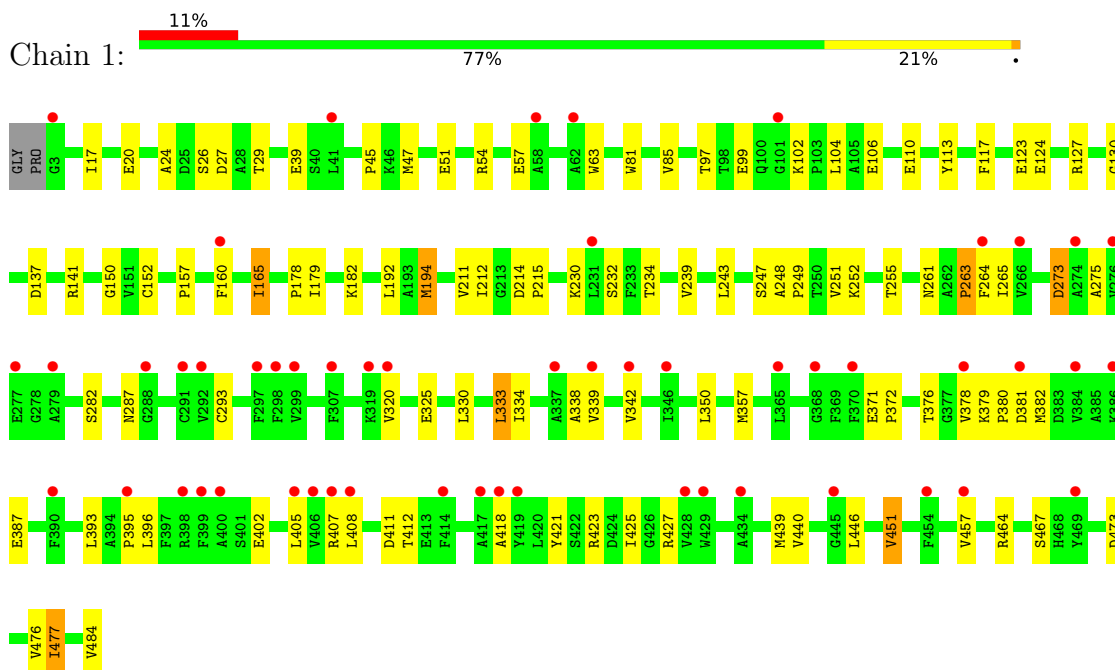
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



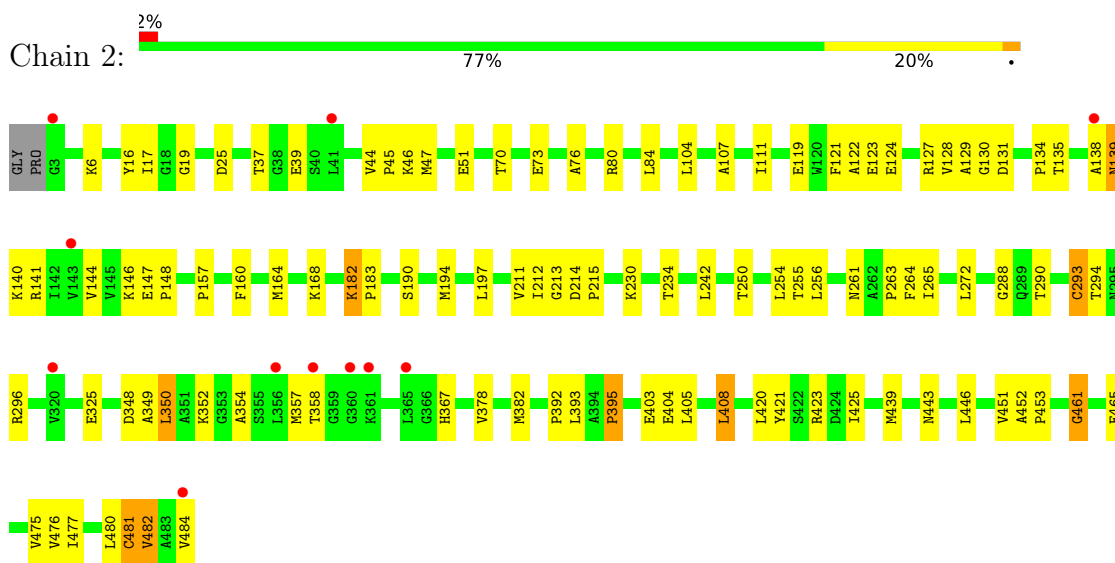
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



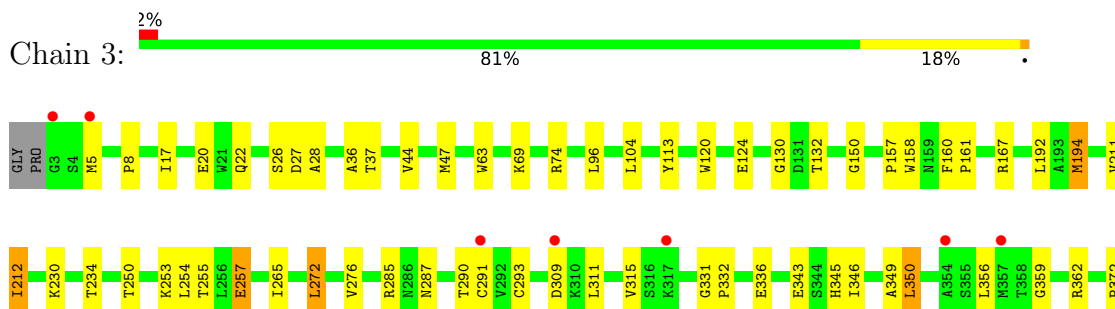
● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

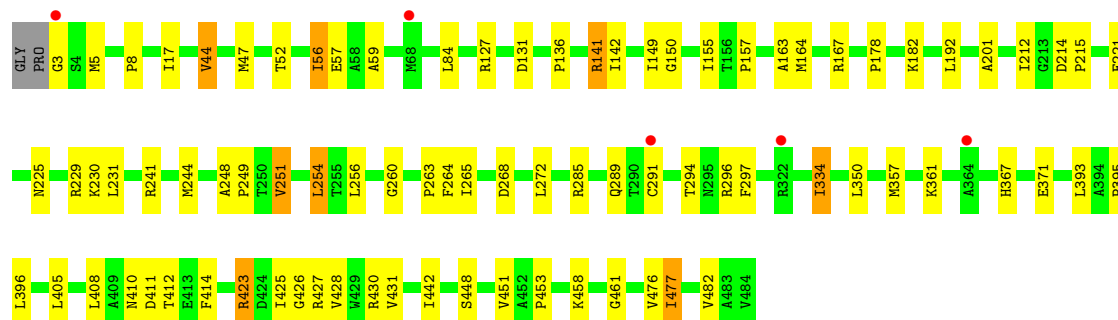
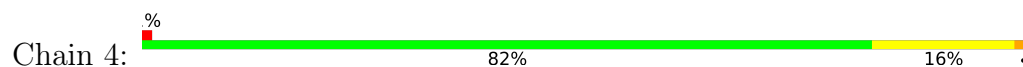


● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

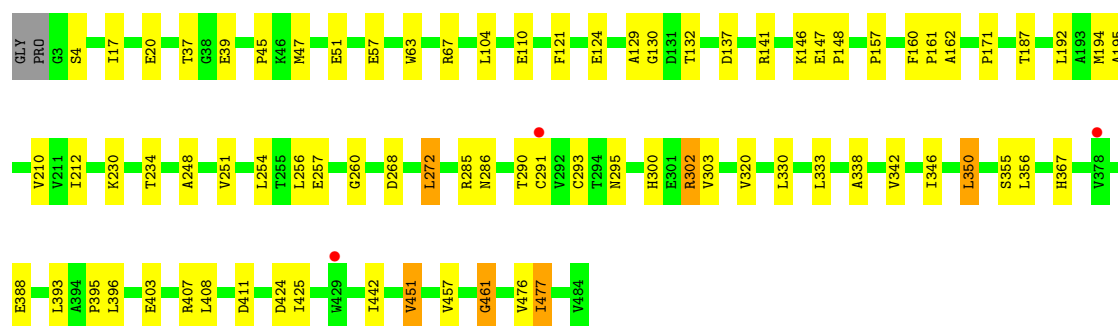
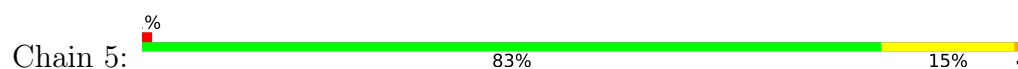




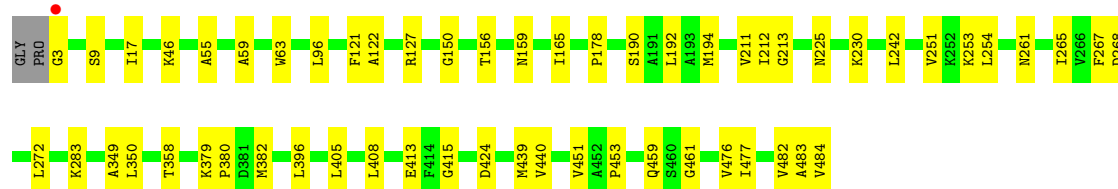
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.66Å 164.87Å 278.90Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	49.47 – 2.70 49.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.47-2.70) 98.5 (49.47-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.282 0.235 , 0.279	Depositor DCC
R_{free} test set	22748 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	114732	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8625e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.62	0/3584	0.90	1/4884 (0.0%)
1	2	0.53	0/3619	0.87	1/4925 (0.0%)
1	3	0.54	0/3619	0.90	0/4925
1	4	0.53	0/3619	0.90	4/4925 (0.1%)
1	5	0.53	0/3619	0.87	1/4925 (0.0%)
1	6	0.54	0/3619	0.89	5/4925 (0.1%)
1	A	0.52	0/3623	0.86	2/4930 (0.0%)
1	B	0.52	0/3627	0.85	0/4935
1	C	0.53	0/3623	0.88	1/4930 (0.0%)
1	D	0.54	0/3623	0.85	1/4930 (0.0%)
1	E	0.53	0/3623	0.84	0/4930
1	F	0.53	0/3623	0.86	1/4930 (0.0%)
1	G	0.52	0/3623	0.87	1/4930 (0.0%)
1	H	0.53	0/3623	0.87	1/4930 (0.0%)
1	I	0.55	0/3594	0.87	1/4896 (0.0%)
1	J	0.52	0/3623	0.86	2/4930 (0.0%)
1	K	0.52	0/3619	0.86	0/4925
1	L	0.54	0/3617	0.87	0/4922
1	M	0.53	0/3619	0.87	0/4925
1	N	0.51	0/3619	0.84	0/4925
1	O	0.53	0/3619	0.89	3/4925 (0.1%)
1	P	0.51	0/3619	0.86	2/4925 (0.0%)
1	Q	0.55	0/3619	0.88	1/4925 (0.0%)
1	R	0.54	0/3619	0.88	1/4925 (0.0%)
1	S	0.52	0/3619	0.87	2/4925 (0.0%)
1	T	0.55	0/3609	0.86	2/4913 (0.0%)
1	U	0.60	0/3594	0.90	5/4894 (0.1%)
1	V	0.56	0/3606	0.89	0/4910
1	W	0.54	0/3619	0.86	0/4925
1	X	0.62	0/3588	0.91	3/4885 (0.1%)
1	Y	0.55	0/3619	0.85	1/4925 (0.0%)
1	Z	0.59	0/3606	0.92	6/4910 (0.1%)
All	All	0.54	0/115694	0.87	48/157464 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	6	0	1
1	U	0	1
All	All	0	2

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	461	GLY	N-CA-C	10.40	122.03	111.21
1	6	461	GLY	N-CA-C	7.56	119.19	111.56
1	Z	461	GLY	N-CA-C	7.32	118.82	111.21
1	C	461	GLY	N-CA-C	7.01	119.90	110.43
1	T	461	GLY	N-CA-C	6.64	119.40	110.43
1	5	461	GLY	N-CA-C	6.36	119.89	110.60
1	U	159	ASN	N-CA-C	6.12	117.94	111.28
1	2	461	GLY	N-CA-C	6.07	119.46	110.60
1	G	461	GLY	N-CA-C	5.92	119.28	111.52
1	6	379	LYS	CA-C-N	5.90	127.21	119.84
1	6	379	LYS	C-N-CA	5.90	127.21	119.84
1	A	461	GLY	N-CA-C	5.88	117.50	111.56
1	X	371	GLU	CA-C-N	5.88	126.22	119.93
1	X	371	GLU	C-N-CA	5.88	126.22	119.93
1	U	5	MET	N-CA-C	-5.78	101.65	110.14
1	J	102	LYS	CA-C-N	5.72	126.99	119.84
1	J	102	LYS	C-N-CA	5.72	126.99	119.84
1	Y	461	GLY	N-CA-C	5.67	117.29	111.56
1	1	179	ILE	N-CA-C	5.54	115.67	108.35
1	Z	214	ASP	CA-C-N	5.49	125.32	119.28
1	Z	214	ASP	C-N-CA	5.49	125.32	119.28
1	R	334	ILE	N-CA-C	5.46	116.85	110.62
1	S	160	PHE	CA-C-N	5.40	125.22	119.28
1	S	160	PHE	C-N-CA	5.40	125.22	119.28
1	U	225	ASN	CA-C-N	5.39	125.10	119.82
1	U	225	ASN	C-N-CA	5.39	125.10	119.82
1	T	456	GLY	N-CA-C	5.36	118.96	111.14
1	U	334	ILE	N-CA-C	5.30	116.03	110.62
1	H	335	ASN	N-CA-C	5.29	115.52	108.38
1	P	189	PHE	N-CA-C	5.26	117.02	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	147	GLU	N-CA-C	5.20	114.29	108.25
1	F	461	GLY	N-CA-C	5.20	119.19	111.76
1	4	142	ILE	N-CA-C	5.16	115.28	107.80
1	4	44	VAL	N-CA-C	-5.16	104.96	109.19
1	A	101	GLY	N-CA-C	5.15	119.09	113.58
1	6	225	ASN	CA-C-N	5.15	124.81	119.56
1	6	225	ASN	C-N-CA	5.15	124.81	119.56
1	Z	262	ALA	N-CA-C	5.14	117.02	109.71
1	O	225	ASN	CA-C-N	5.11	124.77	119.56
1	O	225	ASN	C-N-CA	5.11	124.77	119.56
1	O	367	HIS	CB-CA-C	-5.10	110.29	117.23
1	I	461	GLY	N-CA-C	5.08	116.69	111.56
1	Z	102	LYS	CA-C-N	5.07	126.18	119.84
1	Z	102	LYS	C-N-CA	5.07	126.18	119.84
1	X	20	GLU	N-CA-C	5.04	117.46	109.50
1	4	477	ILE	N-CA-C	5.02	115.20	108.17
1	4	458	LYS	CB-CA-C	-5.02	110.77	116.54
1	D	179	ILE	N-CA-C	5.01	115.13	108.27

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	6	267	PHE	Peptide
1	U	4	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3510	0	3426	56	0
1	2	3545	0	3503	65	0
1	3	3545	0	3503	56	0
1	4	3545	0	3503	45	0
1	5	3545	0	3503	44	0
1	6	3545	0	3503	22	0
1	A	3549	0	3507	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3553	0	3511	36	0
1	C	3549	0	3507	43	0
1	D	3549	0	3507	51	0
1	E	3549	0	3507	47	0
1	F	3549	0	3507	50	0
1	G	3549	0	3507	40	0
1	H	3549	0	3507	38	0
1	I	3520	0	3450	55	0
1	J	3549	0	3507	52	0
1	K	3545	0	3503	38	0
1	L	3543	0	3496	36	0
1	M	3545	0	3503	46	0
1	N	3545	0	3503	26	0
1	O	3545	0	3503	31	0
1	P	3545	0	3503	42	0
1	Q	3545	0	3503	49	0
1	R	3545	0	3503	35	0
1	S	3545	0	3503	38	0
1	T	3535	0	3474	52	0
1	U	3521	0	3463	54	0
1	V	3532	0	3472	49	0
1	W	3545	0	3503	35	0
1	X	3515	0	3438	63	0
1	Y	3545	0	3503	69	0
1	Z	3532	0	3472	80	0
2	1	28	0	0	0	0
2	2	37	0	0	2	0
2	3	45	0	0	1	0
2	4	46	0	0	2	0
2	5	54	0	0	1	0
2	6	57	0	0	1	0
2	A	46	0	0	0	0
2	B	59	0	0	1	0
2	C	56	0	0	1	0
2	D	60	0	0	3	0
2	E	72	0	0	2	0
2	F	75	0	0	4	0
2	G	66	0	0	1	0
2	H	58	0	0	1	0
2	I	24	0	0	1	0
2	J	35	0	0	2	0
2	K	55	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	57	0	0	2	0
2	M	40	0	0	1	0
2	N	46	0	0	0	0
2	O	39	0	0	0	0
2	P	74	0	0	1	0
2	Q	22	0	0	0	0
2	R	35	0	0	0	0
2	S	55	0	0	1	0
2	T	13	0	0	0	0
2	U	13	0	0	1	0
2	V	29	0	0	1	0
2	W	44	0	0	1	0
2	X	8	0	0	0	0
2	Y	36	0	0	2	0
2	Z	20	0	0	5	0
All	All	114732	0	111803	1315	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 6.

All (1315) 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:D:242:LEU:HD22	1:1:26:SER:HA	1.18	1.18
1:S:17:ILE:HD11	1:S:47:MET:HE1	1.27	1.13
1:L:17:ILE:HD11	1:L:47:MET:HE1	1.34	1.07
1:D:47:MET:HE3	1:D:51:GLU:HB3	1.38	1.04
1:4:476:VAL:HG21	1:5:457:VAL:HG12	1.36	1.04
1:Z:192:LEU:HD11	1:Z:212:ILE:HD11	1.39	1.02
1:W:17:ILE:HD11	1:W:47:MET:HE1	1.43	0.99
1:F:17:ILE:HD11	1:F:47:MET:HE1	1.45	0.98
1:V:47:MET:HE3	1:V:51:GLU:HB3	1.44	0.94
1:R:47:MET:HE3	1:R:51:GLU:HB3	1.50	0.93
1:G:17:ILE:HD11	1:G:47:MET:HE1	1.50	0.93
1:H:265:ILE:HG21	1:H:405:LEU:HD21	1.51	0.91
1:B:47:MET:HE3	1:B:51:GLU:CB	2.00	0.91
1:R:192:LEU:HD21	1:R:212:ILE:HD11	1.53	0.90
1:C:17:ILE:HD11	1:C:47:MET:HE1	1.54	0.90
1:S:17:ILE:CD1	1:S:47:MET:HE1	2.00	0.90
1:P:47:MET:HE3	1:P:51:GLU:HB3	1.54	0.88
1:Y:265:ILE:HG21	1:Y:405:LEU:HD21	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:MET:HE3	1:B:51:GLU:HB3	1.56	0.86
1:V:47:MET:HE3	1:V:51:GLU:CB	2.03	0.86
1:4:17:ILE:HD11	1:4:47:MET:HE1	1.58	0.85
1:Y:26:SER:O	1:Y:28:ALA:N	2.09	0.85
1:J:160:PHE:HE2	1:J:290:THR:HG22	1.42	0.85
1:E:17:ILE:HD11	1:E:47:MET:HE1	1.58	0.84
1:C:375:LEU:HD12	1:C:393:LEU:HD11	1.58	0.84
1:R:47:MET:HE2	1:R:211:VAL:HG13	1.60	0.84
1:K:17:ILE:HD11	1:K:47:MET:HE1	1.60	0.84
1:I:17:ILE:HD11	1:I:47:MET:HE1	1.58	0.83
1:Z:192:LEU:HD11	1:Z:212:ILE:CD1	2.09	0.83
1:Y:192:LEU:HD21	1:Y:212:ILE:HD11	1.58	0.82
1:M:138:ALA:O	1:M:139:ASN:HB2	1.77	0.82
1:J:5:MET:HE3	1:J:8:PRO:HA	1.61	0.82
1:Y:265:ILE:CG2	1:Y:405:LEU:HD21	2.10	0.81
1:2:47:MET:HE3	1:2:51:GLU:HB3	1.61	0.81
1:F:47:MET:HE2	1:F:211:VAL:HG13	1.60	0.81
1:Y:477:ILE:HD11	1:2:453:PRO:HG2	1.62	0.81
1:R:17:ILE:HD11	1:R:47:MET:HE1	1.61	0.81
1:N:47:MET:HE2	1:N:51:GLU:HG2	1.63	0.79
1:G:47:MET:HE3	1:G:51:GLU:HB3	1.65	0.79
1:H:251:VAL:HG12	1:H:251:VAL:O	1.83	0.79
1:X:385:ALA:HB2	1:X:397:PHE:HZ	1.46	0.78
1:3:272:LEU:O	1:3:276:VAL:HG23	1.83	0.78
1:L:47:MET:HE3	1:L:51:GLU:HB3	1.65	0.78
1:4:476:VAL:CG2	1:5:457:VAL:HG12	2.14	0.78
1:Y:270:ALA:O	1:Y:272:LEU:HD12	1.83	0.78
1:L:17:ILE:CD1	1:L:47:MET:HE1	2.13	0.78
1:F:407:ARG:HD3	2:F:516:HOH:O	1.84	0.77
1:S:302:ARG:HD2	2:S:522:HOH:O	1.83	0.77
1:D:47:MET:HE3	1:D:51:GLU:CB	2.16	0.76
1:W:124:GLU:HG2	1:X:127:ARG:HH21	1.51	0.76
1:Z:334:ILE:HG23	1:Z:335:ASN:H	1.50	0.76
1:Z:110:GLU:HG3	1:Z:163:ALA:HB2	1.67	0.76
1:M:47:MET:HE3	1:M:212:ILE:H	1.51	0.75
1:1:265:ILE:HG21	1:1:405:LEU:HD21	1.68	0.75
1:G:47:MET:HE3	1:G:51:GLU:CB	2.17	0.75
1:S:47:MET:HE2	1:S:211:VAL:HG13	1.67	0.75
1:R:192:LEU:HD21	1:R:212:ILE:CD1	2.16	0.75
1:V:265:ILE:HG12	1:V:405:LEU:HD11	1.68	0.74
1:L:47:MET:HE3	1:L:51:GLU:CB	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:VAL:HG12	1:I:251:VAL:O	1.86	0.74
1:R:265:ILE:HG12	1:R:405:LEU:HD11	1.69	0.74
1:U:127:ARG:HH21	1:V:124:GLU:HG2	1.51	0.74
1:X:265:ILE:CG2	1:X:405:LEU:HD11	2.18	0.74
1:Q:375:LEU:HD12	1:Q:393:LEU:HD11	1.70	0.74
1:Q:265:ILE:HG23	1:Q:405:LEU:HD11	1.69	0.73
1:T:234:THR:HG23	1:T:257:GLU:HB2	1.69	0.73
1:J:480:LEU:HD23	1:K:440:VAL:HB	1.68	0.73
1:Z:17:ILE:HD11	1:Z:47:MET:HE1	1.71	0.72
1:2:17:ILE:HD11	1:2:47:MET:HE1	1.71	0.72
1:R:47:MET:HE3	1:R:51:GLU:CB	2.19	0.72
1:2:47:MET:HE3	1:2:51:GLU:CB	2.20	0.72
1:V:47:MET:HE2	1:V:211:VAL:HG13	1.70	0.72
1:J:17:ILE:HD11	1:J:47:MET:HE1	1.72	0.72
1:F:477:ILE:HD11	1:G:453:PRO:HB2	1.71	0.72
1:U:192:LEU:HD21	1:U:212:ILE:HD11	1.72	0.71
1:Y:265:ILE:HG12	1:Y:405:LEU:HD11	1.70	0.71
1:X:385:ALA:HB2	1:X:397:PHE:CZ	2.25	0.71
1:Z:62:ALA:HB2	1:Z:205:LYS:O	1.90	0.71
1:1:124:GLU:HG2	1:2:127:ARG:HH21	1.54	0.71
1:D:17:ILE:HD11	1:D:47:MET:HE1	1.72	0.71
1:2:157:PRO:HD2	1:2:164:MET:HG3	1.72	0.71
1:V:17:ILE:CD1	1:V:47:MET:HE1	2.20	0.71
1:I:418:ALA:HB3	1:I:440:VAL:HG22	1.73	0.71
1:S:47:MET:HE3	1:S:51:GLU:HB3	1.73	0.70
1:K:47:MET:HE3	1:K:211:VAL:HG13	1.72	0.70
1:C:127:ARG:HH21	1:D:124:GLU:HG2	1.56	0.70
1:3:26:SER:O	1:3:28:ALA:N	2.23	0.70
1:M:124:GLU:HG2	1:N:127:ARG:HH21	1.56	0.70
1:M:425:ILE:HG12	1:O:425:ILE:HG12	1.72	0.70
1:X:265:ILE:HG23	1:X:405:LEU:HD11	1.74	0.70
1:J:256:LEU:O	1:J:461:GLY:HA3	1.91	0.70
1:4:291:CYS:HB2	2:4:504:HOH:O	1.92	0.70
1:Q:332:PRO:HA	1:Q:368:GLY:O	1.92	0.69
1:I:47:MET:HE3	1:I:51:GLU:HB3	1.73	0.69
1:G:5:MET:HE3	1:G:8:PRO:HA	1.73	0.69
1:2:37:THR:OG1	1:2:39:GLU:HG2	1.92	0.69
1:D:37:THR:HB	1:D:39:GLU:HG2	1.75	0.69
1:F:47:MET:CE	1:F:211:VAL:HG13	2.23	0.69
1:Z:10:LEU:HA	2:Z:520:HOH:O	1.93	0.69
1:S:127:ARG:HH21	1:T:124:GLU:HG2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:265:ILE:HG23	1:M:405:LEU:HD11	1.75	0.68
1:3:124:GLU:HG2	1:4:127:ARG:HH21	1.57	0.68
1:M:251:VAL:HG12	1:M:251:VAL:O	1.91	0.68
1:1:378:VAL:HG13	1:1:382:MET:SD	2.32	0.68
1:3:120:TRP:CH2	1:3:451:VAL:HG23	2.28	0.68
1:Z:315:VAL:HG13	1:Z:372:PRO:HB2	1.75	0.68
1:B:413:GLU:HG2	1:B:459:GLN:HG3	1.75	0.68
1:I:200:ARG:HB2	2:I:514:HOH:O	1.94	0.68
1:T:265:ILE:HG23	1:T:405:LEU:HD11	1.75	0.68
1:V:17:ILE:HD11	1:V:47:MET:HE1	1.74	0.68
1:Y:90:ASP:HA	1:Y:108:LYS:NZ	2.09	0.68
1:W:63:TRP:CD1	1:W:178:PRO:HD3	2.29	0.68
1:Q:192:LEU:HD21	1:Q:212:ILE:HD11	1.76	0.67
1:O:124:GLU:HG2	1:P:127:ARG:HH21	1.59	0.67
1:F:47:MET:HE3	1:F:51:GLU:HB3	1.76	0.67
1:C:129:ALA:O	1:C:146:LYS:NZ	2.28	0.67
1:R:251:VAL:HG12	1:R:251:VAL:O	1.93	0.67
1:3:250:THR:C	1:6:459:GLN:HE22	2.02	0.67
1:F:192:LEU:HD11	1:F:212:ILE:HD11	1.76	0.67
1:Y:290:THR:OG1	1:Y:293:CYS:SG	2.47	0.67
1:W:429:TRP:CZ3	1:X:141:ARG:HG2	2.30	0.67
1:3:234:THR:HG23	1:3:257:GLU:HB2	1.77	0.66
1:6:192:LEU:HD21	1:6:212:ILE:HD11	1.77	0.66
1:A:300:HIS:CE1	1:A:302:ARG:HG3	2.30	0.66
1:U:157:PRO:HD2	1:U:164:MET:HG3	1.78	0.66
1:1:418:ALA:HB3	1:1:440:VAL:HG22	1.78	0.66
1:M:138:ALA:O	1:M:139:ASN:CB	2.42	0.66
1:B:423:ARG:HG3	1:D:424:ASP:OD1	1.96	0.66
1:G:200:ARG:HD2	2:G:518:HOH:O	1.96	0.66
1:Z:458:LYS:HA	2:Z:504:HOH:O	1.96	0.66
1:P:265:ILE:HG23	1:P:405:LEU:HD11	1.78	0.65
1:Y:120:TRP:CZ3	1:Y:451:VAL:HG12	2.31	0.65
1:5:110:GLU:HG3	1:5:160:PHE:HD1	1.61	0.65
1:F:47:MET:HE3	1:F:51:GLU:CB	2.26	0.65
1:N:22:GLN:OE1	1:N:54:ARG:NH2	2.29	0.65
1:P:466:GLY:HA3	2:P:525:HOH:O	1.96	0.65
1:B:47:MET:CE	1:B:51:GLU:HB3	2.25	0.65
1:G:251:VAL:HG12	1:G:251:VAL:O	1.95	0.65
1:S:265:ILE:HG12	1:S:405:LEU:HD11	1.76	0.65
1:5:302:ARG:HD2	2:5:545:HOH:O	1.96	0.65
1:F:5:MET:HE3	1:F:8:PRO:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4:SER:HA	2:M:525:HOH:O	1.96	0.65
1:Z:476:VAL:HG21	1:1:457:VAL:HG12	1.78	0.65
1:1:230:LYS:HE3	1:1:473:ASP:HB3	1.78	0.65
1:S:450:GLU:OE2	1:T:72:LYS:HE2	1.97	0.65
1:3:5:MET:HE3	1:3:8:PRO:HA	1.79	0.65
1:O:341:LYS:HE2	1:O:387:GLU:OE2	1.97	0.65
1:C:144:VAL:HG13	1:C:477:ILE:HD12	1.79	0.65
1:T:157:PRO:HD3	1:T:234:THR:HB	1.79	0.64
1:V:251:VAL:O	1:V:251:VAL:HG13	1.97	0.64
1:V:447:ILE:HG22	1:W:481:CYS:HB3	1.80	0.64
1:B:251:VAL:HG12	1:B:251:VAL:O	1.98	0.64
1:H:265:ILE:CG2	1:H:405:LEU:HD21	2.26	0.64
1:E:300:HIS:CE1	1:E:302:ARG:HG3	2.33	0.64
1:K:41:LEU:CB	2:K:514:HOH:O	2.45	0.64
1:A:424:ASP:OD1	1:C:423:ARG:HG3	1.98	0.64
1:T:265:ILE:CG2	1:T:405:LEU:HD11	2.27	0.64
1:2:138:ALA:O	1:2:139:ASN:HB2	1.98	0.64
1:C:251:VAL:HG12	1:C:251:VAL:O	1.96	0.64
1:G:47:MET:HE2	1:G:211:VAL:HG13	1.80	0.64
1:B:447:ILE:HG22	1:C:481:CYS:HB3	1.80	0.63
1:K:47:MET:CE	1:K:211:VAL:HG13	2.27	0.63
1:I:335:ASN:O	1:I:339:VAL:HG23	1.98	0.63
1:A:124:GLU:HG2	1:B:127:ARG:HH21	1.63	0.63
1:Q:478:LYS:NZ	1:T:432:ALA:O	2.29	0.63
1:F:192:LEU:HD11	1:F:212:ILE:CD1	2.28	0.63
1:K:393:LEU:O	1:K:395:PRO:HD3	1.99	0.63
1:M:157:PRO:HD2	1:M:164:MET:HG3	1.80	0.63
1:O:343:GLU:OE2	1:O:362:ARG:HD2	1.99	0.63
1:H:192:LEU:HD21	1:H:212:ILE:HD11	1.79	0.63
1:O:251:VAL:HG12	1:O:251:VAL:O	1.99	0.63
1:Z:52:THR:HB	1:Z:221:GLU:HG2	1.80	0.63
1:6:190:SER:O	1:6:194:MET:HG2	1.99	0.63
1:3:17:ILE:HD11	1:3:47:MET:HE1	1.80	0.63
1:L:300:HIS:CE1	1:L:302:ARG:HG3	2.34	0.63
1:J:47:MET:HE3	1:J:51:GLU:HB3	1.80	0.62
1:5:320:VAL:HG22	1:5:330:LEU:HD12	1.81	0.62
1:Y:16:TYR:CZ	1:Y:19:GLY:HA2	2.34	0.62
1:B:453:PRO:HG2	1:C:477:ILE:HD11	1.82	0.62
1:H:107:ALA:O	1:H:111:ILE:HG12	1.99	0.62
1:Y:234:THR:OG1	1:Y:257:GLU:HG3	2.00	0.62
1:W:47:MET:HE3	1:W:211:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:17:ILE:CD1	1:R:47:MET:HE1	2.29	0.62
1:M:251:VAL:O	1:M:251:VAL:CG1	2.47	0.62
1:Z:195:ALA:HA	1:Z:208:LEU:HD21	1.82	0.62
1:L:157:PRO:HD2	1:L:164:MET:HG3	1.82	0.62
1:U:195:ALA:HB2	1:U:210:VAL:HG21	1.80	0.62
1:Z:457:VAL:HG12	1:1:476:VAL:HG21	1.82	0.62
1:F:17:ILE:CD1	1:F:47:MET:HE1	2.26	0.62
1:K:5:MET:HE3	1:K:8:PRO:HA	1.82	0.62
1:Y:160:PHE:HE2	1:Y:290:THR:CG2	2.12	0.61
1:U:426:GLY:O	1:U:430:ARG:HG3	2.01	0.61
1:X:164:MET:O	1:X:168:LYS:HG2	2.00	0.61
1:5:110:GLU:HG3	1:5:160:PHE:CD1	2.35	0.61
1:C:124:GLU:HG2	1:D:127:ARG:HH21	1.65	0.61
1:I:26:SER:O	1:I:27:ASP:HB2	2.00	0.61
1:E:79:ARG:HH22	1:E:119:GLU:HG3	1.65	0.61
1:G:72:LYS:HE2	1:H:450:GLU:OE2	1.99	0.61
1:4:476:VAL:HG21	1:5:457:VAL:CG1	2.23	0.61
1:J:346:ILE:O	1:J:350:LEU:HB2	2.00	0.61
1:W:393:LEU:O	1:W:395:PRO:HD3	2.00	0.61
1:T:286:ASN:C	1:T:286:ASN:HD22	2.09	0.61
1:Q:476:VAL:HG21	1:T:457:VAL:HG12	1.82	0.61
1:Z:157:PRO:HD3	1:Z:234:THR:HB	1.82	0.61
1:V:477:ILE:HD11	1:W:453:PRO:HB2	1.82	0.61
1:J:160:PHE:CE2	1:J:290:THR:HG22	2.29	0.60
1:S:361:LYS:O	1:S:371:GLU:HB2	2.01	0.60
1:1:265:ILE:HG21	1:1:405:LEU:CD2	2.31	0.60
1:D:47:MET:HE2	1:D:211:VAL:HG13	1.83	0.60
1:I:311:LEU:O	1:I:315:VAL:HG23	2.01	0.60
1:O:157:PRO:HD2	1:O:164:MET:HG3	1.84	0.60
1:F:3:GLY:HA3	2:F:519:HOH:O	2.01	0.60
1:S:287:ASN:ND2	1:S:333:LEU:HD13	2.16	0.60
1:V:119:GLU:O	1:V:123:GLU:HG3	2.01	0.60
1:R:168:LYS:HE2	1:R:465:GLU:OE2	2.02	0.60
1:O:16:TYR:CZ	1:O:19:GLY:HA2	2.36	0.60
1:Z:315:VAL:CG1	1:Z:372:PRO:HB2	2.31	0.60
1:M:47:MET:CE	1:M:212:ILE:H	2.15	0.60
1:E:185:GLU:CD	1:E:215:PRO:HG3	2.26	0.60
1:P:157:PRO:HD2	1:P:164:MET:HG3	1.82	0.60
1:5:286:ASN:HB3	1:5:290:THR:HG23	1.82	0.60
1:R:157:PRO:HD2	1:R:164:MET:HG3	1.84	0.59
1:B:453:PRO:CG	1:C:477:ILE:HD11	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:GLU:CD	1:F:185:GLU:H	2.10	0.59
1:K:157:PRO:HD2	1:K:164:MET:HG3	1.85	0.59
1:Q:5:MET:HE3	1:Q:8:PRO:HA	1.83	0.59
1:2:265:ILE:HG12	1:2:405:LEU:HD11	1.84	0.59
1:5:346:ILE:O	1:5:350:LEU:HD22	2.02	0.59
1:F:453:PRO:HG2	1:G:477:ILE:HD11	1.85	0.59
1:U:17:ILE:HG23	1:U:55:ALA:HB2	1.84	0.59
1:6:265:ILE:HG21	1:6:405:LEU:HD21	1.84	0.59
1:B:17:ILE:HD11	1:B:47:MET:HE1	1.83	0.59
1:D:287:ASN:HD22	1:D:330:LEU:HD22	1.66	0.59
1:I:47:MET:HB2	1:I:212:ILE:O	2.03	0.59
1:3:311:LEU:O	1:3:315:VAL:HG23	2.02	0.59
1:P:265:ILE:HG23	1:P:405:LEU:CD1	2.32	0.59
1:Q:142:ILE:HD13	1:T:452:ALA:HB2	1.83	0.59
1:X:251:VAL:HG12	1:X:251:VAL:O	2.02	0.59
1:Q:157:PRO:HD2	1:Q:164:MET:HG3	1.83	0.59
1:1:393:LEU:O	1:1:395:PRO:HD3	2.03	0.59
1:3:349:ALA:HA	1:3:382:MET:HG2	1.84	0.59
1:K:121:PHE:HA	1:K:124:GLU:HB2	1.84	0.58
1:X:214:ASP:HB3	1:X:217:ALA:HB3	1.83	0.58
1:I:425:ILE:HG12	1:K:425:ILE:HG12	1.86	0.58
1:U:124:GLU:HG2	1:V:127:ARG:HH21	1.68	0.58
1:Z:149:ILE:HG23	1:Z:150:GLY:H	1.69	0.58
1:B:17:ILE:CD1	1:B:47:MET:HE1	2.33	0.58
1:J:251:VAL:HG12	1:J:251:VAL:O	2.03	0.58
1:X:6:LYS:H	1:X:6:LYS:HD2	1.68	0.58
1:Y:130:GLY:HA3	1:Y:144:VAL:O	2.04	0.58
1:1:192:LEU:HD21	1:1:212:ILE:HD11	1.86	0.58
1:X:415:GLY:HA2	1:X:437:TYR:CD1	2.38	0.58
1:Q:84:LEU:HB3	1:Q:197:LEU:HD22	1.85	0.58
1:2:47:MET:HE2	1:2:211:VAL:HG13	1.85	0.58
1:W:373:THR:HB	1:W:393:LEU:HD12	1.85	0.58
1:3:429:TRP:HZ3	1:4:141:ARG:HG2	1.69	0.58
1:3:192:LEU:HD21	1:3:212:ILE:HD11	1.85	0.58
1:T:393:LEU:O	1:T:395:PRO:HD3	2.04	0.57
1:4:453:PRO:HB2	1:5:477:ILE:HD11	1.86	0.57
1:H:251:VAL:O	1:H:251:VAL:CG1	2.52	0.57
1:S:157:PRO:HD2	1:S:164:MET:HG3	1.86	0.57
1:X:152:CYS:SG	1:X:230:LYS:HG2	2.44	0.57
1:P:244:MET:HA	1:P:254:LEU:HD21	1.85	0.57
1:Y:26:SER:C	1:Y:28:ALA:H	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:160:PHE:HB3	1:Z:163:ALA:HB3	1.85	0.57
1:Z:16:TYR:CZ	1:Z:19:GLY:HA2	2.38	0.57
1:R:256:LEU:HD12	1:S:251:VAL:HG13	1.84	0.57
1:E:260:GLY:HA2	1:E:414:PHE:HB3	1.85	0.57
1:I:184:ALA:C	1:I:186:SER:H	2.11	0.57
1:T:47:MET:HE2	1:T:51:GLU:HG2	1.87	0.57
1:1:113:TYR:CE1	1:1:117:PHE:HE2	2.22	0.57
1:N:330:LEU:HD13	1:N:372:PRO:HG3	1.87	0.57
1:5:147:GLU:HB2	1:5:148:PRO:HD2	1.85	0.57
1:A:140:LYS:O	1:A:141:ARG:HD3	2.04	0.56
1:L:47:MET:HB2	1:L:212:ILE:O	2.04	0.56
1:A:356:LEU:HD21	1:A:360:GLY:HA3	1.88	0.56
1:X:159:ASN:HB2	1:X:286:ASN:HD21	1.70	0.56
1:1:165:ILE:HG21	1:1:194:MET:HG2	1.87	0.56
1:M:283:LYS:HE2	1:M:393:LEU:O	2.05	0.56
1:M:477:ILE:HD11	1:P:453:PRO:HB2	1.87	0.56
1:Y:286:ASN:O	1:Y:287:ASN:HB2	2.05	0.56
1:4:5:MET:HE3	1:4:8:PRO:HA	1.86	0.56
1:E:182:LYS:HE2	1:E:215:PRO:HA	1.88	0.56
1:Y:81:TRP:O	1:Y:85:VAL:HG23	2.05	0.56
1:W:127:ARG:HH21	1:X:124:GLU:HG2	1.69	0.56
1:A:476:VAL:HG21	1:D:457:VAL:HG12	1.87	0.56
1:Z:374:VAL:HG22	1:Z:394:ALA:HB3	1.88	0.56
1:3:157:PRO:HD3	1:3:234:THR:HB	1.87	0.56
1:E:276:VAL:HG21	1:E:310:LYS:HB3	1.87	0.56
1:N:195:ALA:HB2	1:N:210:VAL:HG21	1.88	0.56
1:Y:12:ARG:HG3	1:Y:21:TRP:CH2	2.40	0.56
1:4:150:GLY:HA3	1:4:229:ARG:HD2	1.88	0.56
1:M:290:THR:HG1	1:M:293:CYS:HG	1.53	0.56
1:T:154:ALA:HA	1:T:232:SER:O	2.05	0.56
1:U:115:ALA:HA	1:U:118:ILE:HD12	1.88	0.56
1:J:375:LEU:HD12	1:J:393:LEU:HD11	1.87	0.56
1:2:350:LEU:HA	1:2:354:ALA:HB3	1.88	0.56
1:F:477:ILE:HD11	1:G:453:PRO:CB	2.35	0.55
1:I:265:ILE:HG12	1:I:405:LEU:HD11	1.88	0.55
1:Z:164:MET:O	1:Z:168:LYS:HG3	2.07	0.55
1:D:375:LEU:HD12	1:D:393:LEU:HD11	1.88	0.55
1:Q:104:LEU:HD22	1:Q:108:LYS:HE3	1.89	0.55
1:I:484:VAL:O	1:I:484:VAL:HG13	2.06	0.55
1:V:160:PHE:HB3	1:V:163:ALA:HB3	1.89	0.55
1:D:251:VAL:HG12	1:D:251:VAL:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:165:ILE:O	1:U:169:VAL:HB	2.07	0.55
1:X:272:LEU:HD13	1:X:272:LEU:H	1.72	0.55
1:Y:113:TYR:CE2	1:Y:117:PHE:HE2	2.25	0.55
1:1:379:LYS:CB	1:1:380:PRO:HD2	2.36	0.55
1:I:103:PRO:HA	1:I:323:GLY:HA2	1.89	0.55
1:Z:212:ILE:HG22	1:Z:213:GLY:N	2.22	0.55
1:1:407:ARG:O	1:1:411:ASP:HB2	2.07	0.55
1:Z:126:LYS:C	1:2:134:PRO:HG2	2.32	0.55
1:2:119:GLU:O	1:2:123:GLU:HG3	2.07	0.55
1:E:47:MET:HE3	1:E:211:VAL:HG13	1.88	0.55
1:H:427:ARG:CZ	2:H:532:HOH:O	2.54	0.55
1:P:47:MET:HE3	1:P:51:GLU:CB	2.33	0.55
1:U:160:PHE:HB3	1:U:163:ALA:HB3	1.87	0.55
1:1:63:TRP:CZ2	1:1:150:GLY:HA2	2.41	0.55
1:E:47:MET:CE	1:E:211:VAL:HG13	2.37	0.55
1:G:16:TYR:CZ	1:G:19:GLY:HA2	2.41	0.55
1:1:275:ALA:HA	1:1:421:TYR:CE1	2.42	0.55
1:5:286:ASN:HD22	1:5:290:THR:HG22	1.72	0.54
1:D:265:ILE:HG12	1:D:405:LEU:HD11	1.88	0.54
1:E:123:GLU:HB2	1:F:127:ARG:NH2	2.22	0.54
1:X:237:THR:OG1	1:X:414:PHE:HE1	1.90	0.54
1:3:343:GLU:OE1	1:3:362:ARG:NH1	2.40	0.54
1:B:265:ILE:HG12	1:B:405:LEU:HD11	1.88	0.54
1:H:192:LEU:HD21	1:H:212:ILE:CD1	2.37	0.54
1:A:477:ILE:HD11	1:D:453:PRO:HB2	1.89	0.54
1:F:251:VAL:O	1:F:251:VAL:HG12	2.07	0.54
1:Q:440:VAL:HB	1:T:480:LEU:HD23	1.89	0.54
1:W:59:ALA:HB1	1:W:178:PRO:HB2	1.89	0.54
1:B:447:ILE:HG22	1:C:481:CYS:CB	2.37	0.54
1:D:379:LYS:CB	2:D:522:HOH:O	2.55	0.54
1:E:364:ALA:HB3	1:J:9:SER:HB3	1.88	0.54
1:I:5:MET:HE3	1:I:8:PRO:HA	1.90	0.54
1:S:404:GLU:HG2	1:S:408:LEU:HD22	1.89	0.54
1:Z:184:ALA:C	1:Z:186:SER:H	2.14	0.54
1:L:455:GLY:HA3	1:L:464:ARG:HD3	1.89	0.54
1:M:148:PRO:HG3	1:M:175:ALA:O	2.08	0.54
1:N:157:PRO:HD2	1:N:164:MET:HG3	1.88	0.54
1:X:265:ILE:HG21	1:X:405:LEU:HD11	1.87	0.54
1:1:402:GLU:OE1	1:1:427:ARG:HG3	2.08	0.54
1:2:17:ILE:CD1	1:2:47:MET:HE1	2.37	0.54
1:A:167:ARG:NH2	1:A:465:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:VAL:O	1:I:251:VAL:CG1	2.56	0.54
1:R:113:TYR:CE1	1:R:117:PHE:HE2	2.26	0.54
1:Z:477:ILE:HG12	1:1:464:ARG:HE	1.72	0.54
1:F:161:PRO:O	1:F:165:ILE:HD13	2.08	0.54
1:Q:265:ILE:HG23	1:Q:405:LEU:CD1	2.38	0.54
1:S:124:GLU:HG2	1:T:127:ARG:HH21	1.72	0.54
1:U:354:ALA:HB2	1:U:382:MET:HE1	1.90	0.54
1:Y:214:ASP:HB3	1:Y:217:ALA:HB3	1.89	0.54
1:F:300:HIS:CE1	1:F:302:ARG:HG3	2.43	0.54
1:I:81:TRP:HZ2	1:I:194:MET:HG3	1.71	0.54
1:V:378:VAL:HG11	1:V:395:PRO:HB2	1.90	0.53
1:2:393:LEU:O	1:2:395:PRO:HD3	2.08	0.53
1:3:477:ILE:HG23	2:3:504:HOH:O	2.08	0.53
1:5:290:THR:OG1	1:5:293:CYS:SG	2.62	0.53
1:J:248:ALA:HB3	1:J:249:PRO:HD3	1.90	0.53
1:Y:256:LEU:O	1:Y:461:GLY:HA3	2.08	0.53
1:3:346:ILE:HG22	1:3:350:LEU:HD22	1.89	0.53
1:B:477:ILE:HD11	1:C:453:PRO:HB2	1.90	0.53
1:E:440:VAL:HB	1:H:480:LEU:HD23	1.89	0.53
1:P:214:ASP:HB3	1:P:217:ALA:HB3	1.91	0.53
1:I:342:VAL:O	1:I:346:ILE:HG13	2.09	0.53
1:Q:332:PRO:CA	1:Q:368:GLY:O	2.56	0.53
1:Q:450:GLU:OE2	1:R:72:LYS:HE2	2.08	0.53
1:R:286:ASN:O	1:R:289:GLN:HG3	2.08	0.53
1:Y:132:THR:OG1	1:1:130:GLY:HA3	2.08	0.53
1:4:265:ILE:HG12	1:4:405:LEU:HD11	1.90	0.53
1:D:393:LEU:O	1:D:395:PRO:HD3	2.08	0.53
1:F:415:GLY:HA2	1:F:437:TYR:CD1	2.42	0.53
1:J:160:PHE:HE2	1:J:290:THR:CG2	2.18	0.53
1:T:312:ALA:HA	1:T:315:VAL:HB	1.91	0.53
1:V:69:LYS:O	1:V:74:ARG:NH1	2.41	0.53
1:1:182:LYS:HE3	1:1:215:PRO:HA	1.91	0.53
1:4:264:PHE:HB2	1:4:294:THR:HG21	1.90	0.53
1:A:265:ILE:HG12	1:A:405:LEU:HD11	1.91	0.53
1:D:263:PRO:HD2	1:D:418:ALA:HA	1.91	0.53
1:I:431:VAL:O	1:I:435:LEU:HG	2.09	0.53
1:P:287:ASN:ND2	1:P:333:LEU:HD13	2.23	0.53
1:V:417:ALA:HB2	1:V:439:MET:HE3	1.91	0.53
1:Y:264:PHE:HB2	1:Y:294:THR:CG2	2.38	0.53
1:Z:160:PHE:CE2	1:Z:290:THR:HG22	2.43	0.53
1:5:260:GLY:O	1:5:388:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:CD1	1:A:372:PRO:HG3	2.39	0.53
1:B:158:TRP:CD2	1:B:334:ILE:HD12	2.44	0.53
1:Y:479:TYR:HD2	1:2:439:MET:HG2	1.73	0.53
1:E:429:TRP:CZ3	1:F:141:ARG:HG2	2.44	0.53
1:J:6:LYS:H	1:J:6:LYS:HD2	1.72	0.53
1:K:124:GLU:HG2	1:L:127:ARG:HH21	1.74	0.53
1:M:393:LEU:O	1:M:395:PRO:HD3	2.08	0.53
1:P:17:ILE:HG13	1:P:47:MET:HE1	1.91	0.53
1:Q:52:THR:HB	1:Q:221:GLU:HG2	1.91	0.53
1:X:28:ALA:O	1:X:46:LYS:HB3	2.08	0.53
1:X:52:THR:OG1	1:X:218:ILE:HG23	2.09	0.53
1:4:393:LEU:O	1:4:395:PRO:HD3	2.08	0.53
1:J:157:PRO:HD2	1:J:164:MET:HG3	1.90	0.53
1:K:269:ASP:CG	1:K:427:ARG:HH12	2.16	0.53
1:Q:481:CYS:HB3	1:T:447:ILE:HG22	1.90	0.53
1:Z:336:GLU:OE1	1:Z:362:ARG:NH2	2.42	0.53
1:G:265:ILE:HG12	1:G:405:LEU:HD11	1.91	0.53
1:H:315:VAL:HG13	1:H:372:PRO:HB2	1.91	0.53
1:V:281:ALA:HB1	1:V:446:LEU:HD12	1.91	0.53
1:Y:158:TRP:O	1:Y:161:PRO:HD3	2.08	0.53
1:G:17:ILE:CD1	1:G:47:MET:HE1	2.30	0.52
1:K:286:ASN:HD22	1:K:290:THR:HG22	1.74	0.52
1:Z:206:GLY:O	1:Z:208:LEU:N	2.40	0.52
1:2:140:LYS:HA	1:2:482:VAL:O	2.08	0.52
1:2:242:LEU:HD11	2:2:518:HOH:O	2.10	0.52
1:M:121:PHE:HA	1:M:124:GLU:HB2	1.92	0.52
1:X:96:LEU:HD11	1:X:161:PRO:HD2	1.90	0.52
1:J:154:ALA:HB1	1:J:168:LYS:HD3	1.91	0.52
1:E:17:ILE:CD1	1:E:47:MET:HE1	2.35	0.52
1:F:47:MET:HB2	1:F:212:ILE:O	2.09	0.52
1:3:399:PHE:CZ	1:3:405:LEU:HD22	2.44	0.52
1:G:356:LEU:HD21	1:G:360:GLY:HA3	1.90	0.52
1:O:5:MET:HE3	1:O:8:PRO:HA	1.92	0.52
1:2:157:PRO:HD3	1:2:234:THR:HB	1.92	0.52
1:4:289:GLN:HE22	1:4:334:ILE:H	1.57	0.52
1:K:167:ARG:NH2	1:K:465:GLU:OE1	2.41	0.52
1:V:461:GLY:HA2	1:W:251:VAL:HG11	1.92	0.52
1:1:287:ASN:HD22	1:1:333:LEU:HD13	1.74	0.52
1:C:140:LYS:O	1:C:141:ARG:HD3	2.10	0.52
1:X:26:SER:O	1:X:27:ASP:HB2	2.08	0.52
1:4:59:ALA:HB1	1:4:178:PRO:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:287:ASN:ND2	1:L:333:LEU:HD13	2.25	0.52
1:M:103:PRO:HA	1:M:323:GLY:HA2	1.92	0.52
1:T:152:CYS:SG	1:T:230:LYS:HG2	2.49	0.52
1:C:393:LEU:O	1:C:395:PRO:HD3	2.09	0.52
1:D:304:TYR:HE1	1:D:398:ARG:HB2	1.74	0.52
1:K:157:PRO:HD3	1:K:234:THR:HB	1.91	0.52
1:A:477:ILE:HD11	1:D:453:PRO:CB	2.40	0.52
1:I:149:ILE:HD13	1:I:230:LYS:HB3	1.92	0.52
1:J:154:ALA:HB3	1:J:181:VAL:HG22	1.92	0.52
1:P:265:ILE:CG2	1:P:405:LEU:HD11	2.40	0.52
1:U:320:VAL:HG12	1:U:321:GLY:H	1.75	0.52
1:3:265:ILE:CG2	1:3:405:LEU:HD21	2.39	0.52
1:F:424:ASP:O	1:F:428:VAL:HG23	2.10	0.51
1:Q:256:LEU:O	1:Q:461:GLY:HA3	2.09	0.51
1:Y:264:PHE:HB2	1:Y:294:THR:HG23	1.91	0.51
1:2:352:LYS:HD2	1:2:382:MET:HG2	1.92	0.51
1:3:477:ILE:HD11	1:6:453:PRO:HG3	1.92	0.51
1:P:160:PHE:HE2	1:P:290:THR:HG22	1.75	0.51
1:W:429:TRP:HB2	1:X:484:VAL:HG21	1.92	0.51
1:G:157:PRO:HD3	1:G:234:THR:HB	1.91	0.51
1:K:161:PRO:HB2	1:K:190:SER:HB2	1.91	0.51
1:U:265:ILE:HG12	1:U:405:LEU:HD11	1.91	0.51
1:X:63:TRP:CD1	1:X:178:PRO:HD3	2.46	0.51
1:1:338:ALA:O	1:1:342:VAL:HG23	2.11	0.51
1:5:256:LEU:O	1:5:461:GLY:HA3	2.10	0.51
1:T:37:THR:OG1	1:T:39:GLU:HG2	2.11	0.51
1:V:59:ALA:HB1	1:V:178:PRO:HB2	1.91	0.51
1:V:423:ARG:HG3	1:X:424:ASP:OD1	2.09	0.51
1:1:127:ARG:HH21	1:2:124:GLU:HG2	1.75	0.51
1:1:273:ASP:OD1	1:1:273:ASP:N	2.43	0.51
1:A:204:PRO:HG2	1:A:207:VAL:HG21	1.92	0.51
1:E:364:ALA:CB	1:J:9:SER:HB3	2.41	0.51
1:M:265:ILE:HG23	1:M:405:LEU:CD1	2.41	0.51
1:R:423:ARG:HG3	1:T:424:ASP:OD1	2.11	0.51
1:U:455:GLY:HA3	1:U:464:ARG:HD3	1.93	0.51
1:4:361:LYS:O	1:4:371:GLU:HB2	2.09	0.51
1:Q:464:ARG:HG3	1:T:477:ILE:HD11	1.93	0.51
1:Y:265:ILE:HG21	1:Y:405:LEU:CD2	2.36	0.51
1:1:17:ILE:CD1	1:1:211:VAL:HG12	2.40	0.51
1:2:84:LEU:HB3	1:2:197:LEU:HD22	1.93	0.51
1:4:221:GLU:O	1:4:225:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:VAL:CG2	1:D:457:VAL:HG12	2.40	0.51
1:B:234:THR:HG23	1:B:257:GLU:HB3	1.93	0.51
1:D:336:GLU:OE1	1:D:362:ARG:NH2	2.44	0.51
1:H:147:GLU:HB2	1:H:148:PRO:HD2	1.92	0.51
1:S:47:MET:HG2	1:S:51:GLU:HG2	1.92	0.51
1:X:162:ALA:HA	1:X:194:MET:HE1	1.92	0.51
1:Y:20:GLU:HG2	2:Y:519:HOH:O	2.10	0.51
1:O:84:LEU:HB3	1:O:197:LEU:HD22	1.92	0.51
1:U:214:ASP:HB3	1:U:217:ALA:HB3	1.92	0.51
1:2:190:SER:O	1:2:194:MET:HG2	2.10	0.51
1:T:96:LEU:HD21	1:T:102:LYS:HE3	1.91	0.51
1:X:5:MET:HE3	1:X:8:PRO:HA	1.93	0.51
1:Y:285:ARG:C	1:Y:287:ASN:H	2.19	0.51
1:Z:241:ARG:NE	1:1:249:PRO:O	2.42	0.51
1:Z:476:VAL:CG2	1:1:457:VAL:HG12	2.41	0.51
1:B:425:ILE:HG12	1:D:425:ILE:HG12	1.93	0.51
1:H:37:THR:HB	1:H:39:GLU:HG2	1.92	0.51
1:I:5:MET:HE1	1:I:11:LEU:HB2	1.93	0.51
1:M:311:LEU:O	1:M:315:VAL:HG23	2.11	0.51
1:V:157:PRO:HD2	1:V:164:MET:HG3	1.93	0.51
1:Y:283:LYS:HE2	1:Y:393:LEU:H	1.74	0.51
1:A:287:ASN:ND2	1:A:333:LEU:HD13	2.26	0.50
1:E:287:ASN:ND2	1:E:333:LEU:HD13	2.26	0.50
1:5:63:TRP:O	1:5:67:ARG:HG2	2.11	0.50
1:D:242:LEU:CD2	1:1:26:SER:HA	2.13	0.50
1:E:453:PRO:HB2	1:H:477:ILE:HD11	1.93	0.50
1:R:461:GLY:HA2	1:S:251:VAL:HG11	1.93	0.50
1:U:123:GLU:HG2	1:V:123:GLU:CD	2.37	0.50
1:V:263:PRO:HA	1:V:296:ARG:O	2.11	0.50
1:Y:47:MET:HE2	1:Y:51:GLU:HB3	1.93	0.50
1:Z:30:PHE:HD2	1:Z:46:LYS:HG3	1.76	0.50
1:6:349:ALA:HA	1:6:382:MET:HG2	1.93	0.50
1:A:230:LYS:HB2	1:A:253:LYS:HB3	1.93	0.50
1:O:147:GLU:HB2	1:O:148:PRO:HD2	1.93	0.50
1:U:310:LYS:HD2	2:U:513:HOH:O	2.11	0.50
1:C:17:ILE:CD1	1:C:211:VAL:HG12	2.42	0.50
1:E:79:ARG:NH2	1:E:119:GLU:HG3	2.26	0.50
1:L:336:GLU:OE1	1:L:362:ARG:NH1	2.30	0.50
1:M:186:SER:CB	1:M:334:ILE:HD11	2.42	0.50
1:2:76:ALA:O	1:2:80:ARG:HG3	2.11	0.50
1:4:482:VAL:HG22	1:5:442:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:266:VAL:HB	1:R:299:VAL:HG13	1.93	0.50
1:U:289:GLN:HG2	1:U:390:PHE:O	2.12	0.50
1:W:121:PHE:HA	1:W:124:GLU:HB2	1.93	0.50
1:Y:281:ALA:HB1	1:Y:446:LEU:HD21	1.94	0.50
1:3:113:TYR:OH	1:3:448:SER:HB3	2.12	0.50
1:B:306:ALA:O	1:B:310:LYS:HG3	2.12	0.50
1:G:5:MET:HE1	1:G:11:LEU:HB2	1.94	0.50
1:L:168:LYS:HD3	1:L:232:SER:OG	2.11	0.50
1:P:47:MET:CE	1:P:51:GLU:HB3	2.36	0.50
1:P:182:LYS:HE3	1:P:215:PRO:HA	1.93	0.50
1:Q:444:THR:OG1	1:T:140:LYS:NZ	2.44	0.50
1:T:262:ALA:HB3	1:T:294:THR:HA	1.94	0.50
1:U:361:LYS:O	1:U:371:GLU:HB2	2.11	0.50
1:V:269:ASP:O	1:V:423:ARG:HB2	2.12	0.50
1:C:336:GLU:OE1	1:C:362:ARG:NH2	2.45	0.50
1:I:47:MET:HE2	1:I:211:VAL:HG13	1.92	0.50
1:U:211:VAL:HG12	1:U:218:ILE:HD13	1.93	0.50
1:Y:90:ASP:HA	1:Y:108:LYS:HZ1	1.76	0.50
1:Z:424:ASP:OD1	1:2:423:ARG:HG3	2.12	0.50
1:3:26:SER:C	1:3:28:ALA:H	2.16	0.50
1:E:246:GLN:NE2	2:E:534:HOH:O	2.42	0.50
1:H:154:ALA:HA	1:H:232:SER:O	2.11	0.50
1:J:107:ALA:O	1:J:111:ILE:HG12	2.12	0.50
1:S:16:TYR:CZ	1:S:19:GLY:HA2	2.47	0.50
1:T:6:LYS:HD2	1:T:6:LYS:H	1.76	0.50
1:X:338:ALA:O	1:X:342:VAL:HG23	2.12	0.50
1:Y:141:ARG:HG3	1:Z:429:TRP:CZ3	2.47	0.50
1:2:45:PRO:O	1:2:212:ILE:HG22	2.11	0.50
1:3:290:THR:OG1	1:3:293:CYS:SG	2.67	0.50
1:4:453:PRO:CB	1:5:477:ILE:HD11	2.41	0.50
1:5:393:LEU:O	1:5:395:PRO:HD3	2.12	0.50
1:4:410:ASN:O	1:4:412:THR:N	2.43	0.50
1:I:136:PRO:HG3	1:L:451:VAL:CG1	2.42	0.49
1:O:154:ALA:HB3	1:O:181:VAL:HG22	1.94	0.49
1:S:162:ALA:O	1:S:194:MET:HE1	2.11	0.49
1:Y:311:LEU:O	1:Y:315:VAL:HG23	2.12	0.49
1:Z:192:LEU:CD1	1:Z:212:ILE:HD11	2.26	0.49
1:C:152:CYS:SG	1:C:230:LYS:HG2	2.53	0.49
1:M:192:LEU:HD11	1:M:212:ILE:HD12	1.94	0.49
1:1:17:ILE:HD11	1:1:211:VAL:HG12	1.94	0.49
1:2:160:PHE:HE2	1:2:290:THR:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:413:GLU:CB	1:6:459:GLN:HG3	2.42	0.49
1:A:169:VAL:HG13	1:A:173:LEU:HD13	1.93	0.49
1:A:330:LEU:HD13	1:A:372:PRO:HG3	1.93	0.49
1:B:119:GLU:O	1:B:123:GLU:HG3	2.11	0.49
1:E:123:GLU:HB2	1:F:127:ARG:HH22	1.77	0.49
1:K:168:LYS:HE2	1:K:465:GLU:OE2	2.13	0.49
1:U:152:CYS:HB2	1:U:179:ILE:HG13	1.94	0.49
1:4:263:PRO:HA	1:4:296:ARG:O	2.11	0.49
1:6:265:ILE:HG12	1:6:405:LEU:HD11	1.93	0.49
1:M:162:ALA:O	1:M:194:MET:HE1	2.11	0.49
1:O:288:GLY:HA2	1:O:293:CYS:SG	2.52	0.49
1:K:265:ILE:HG12	1:K:405:LEU:HD11	1.95	0.49
1:X:451:VAL:O	1:X:467:SER:HB3	2.13	0.49
1:Z:198:ALA:HB1	1:Z:203:VAL:HG21	1.93	0.49
1:2:230:LYS:NZ	1:2:255:THR:OG1	2.44	0.49
1:H:161:PRO:O	1:H:165:ILE:HD13	2.12	0.49
1:O:268:ASP:OD2	1:O:268:ASP:N	2.39	0.49
1:T:59:ALA:HA	1:T:206:GLY:O	2.12	0.49
1:T:404:GLU:HG2	1:T:408:LEU:HD22	1.94	0.49
1:K:17:ILE:CD1	1:K:211:VAL:HG22	2.42	0.49
1:O:276:VAL:O	1:O:280:ILE:HG12	2.13	0.49
1:Q:162:ALA:HA	1:Q:194:MET:HE1	1.94	0.49
1:S:63:TRP:CD1	1:S:178:PRO:HD3	2.47	0.49
1:X:342:VAL:O	1:X:346:ILE:HG13	2.13	0.49
1:2:138:ALA:O	1:2:139:ASN:CB	2.61	0.49
1:A:405:LEU:O	1:A:405:LEU:HG	2.09	0.49
1:F:451:VAL:HG22	1:G:142:ILE:HD13	1.95	0.49
1:N:348:ASP:OD1	1:N:352:LYS:NZ	2.38	0.49
1:Q:101:GLY:O	1:Q:332:PRO:HD2	2.13	0.49
1:W:429:TRP:CB	1:X:484:VAL:HG21	2.43	0.49
1:3:429:TRP:CZ3	1:4:141:ARG:HG2	2.48	0.49
1:F:161:PRO:HB2	1:F:190:SER:HB2	1.93	0.49
1:H:375:LEU:HD12	1:H:393:LEU:HD11	1.94	0.49
1:I:421:TYR:HA	1:I:443:ASN:OD1	2.13	0.49
1:J:17:ILE:CD1	1:J:47:MET:HE1	2.42	0.49
1:M:254:LEU:HD23	1:M:256:LEU:HD11	1.95	0.49
1:V:17:ILE:HD12	1:V:47:MET:HE1	1.95	0.49
1:4:334:ILE:HD13	1:4:334:ILE:O	2.12	0.49
1:B:157:PRO:HD3	1:B:234:THR:HB	1.95	0.48
1:G:276:VAL:HG21	1:G:310:LYS:HB3	1.94	0.48
1:M:477:ILE:HD11	1:P:453:PRO:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:161:PRO:O	1:P:165:ILE:HD13	2.12	0.48
1:Q:154:ALA:HB3	1:Q:181:VAL:HG22	1.95	0.48
1:V:422:SER:OG	1:V:427:ARG:HD2	2.13	0.48
1:Y:29:THR:OG1	1:Y:43:THR:HB	2.13	0.48
1:5:45:PRO:O	1:5:212:ILE:HG22	2.13	0.48
1:C:265:ILE:HG21	1:C:405:LEU:HD21	1.95	0.48
1:O:47:MET:HE2	1:O:51:GLU:HG2	1.94	0.48
1:O:477:ILE:C	1:O:477:ILE:HD12	2.38	0.48
1:R:447:ILE:HG22	1:S:481:CYS:HB3	1.95	0.48
1:V:110:GLU:HG3	1:V:163:ALA:HB2	1.93	0.48
1:X:380:PRO:HA	1:X:397:PHE:HE1	1.79	0.48
1:2:349:ALA:O	1:2:352:LYS:HB2	2.13	0.48
1:I:266:VAL:HB	1:I:299:VAL:HG13	1.95	0.48
1:M:342:VAL:O	1:M:346:ILE:HG13	2.13	0.48
1:N:182:LYS:NZ	1:N:183:PRO:O	2.44	0.48
1:N:375:LEU:HD12	1:N:393:LEU:HD11	1.95	0.48
1:Q:251:VAL:HG12	1:Q:251:VAL:O	2.12	0.48
1:Y:298:PHE:HE1	1:Y:408:LEU:HD23	1.77	0.48
1:2:47:MET:HB2	1:2:212:ILE:O	2.13	0.48
1:J:315:VAL:HG13	1:J:372:PRO:HB2	1.94	0.48
1:L:154:ALA:HB1	1:L:168:LYS:HD2	1.95	0.48
1:N:192:LEU:HD11	1:N:212:ILE:CD1	2.43	0.48
1:P:147:GLU:HB2	1:P:148:PRO:HD2	1.95	0.48
1:Q:480:LEU:HD23	1:T:440:VAL:HB	1.94	0.48
1:B:185:GLU:CD	1:B:215:PRO:HG3	2.39	0.48
1:F:265:ILE:HG12	1:F:405:LEU:HD11	1.94	0.48
1:M:36:ALA:HB2	1:M:332:PRO:HG3	1.96	0.48
1:S:128:VAL:HG11	1:S:475:VAL:HG11	1.96	0.48
1:V:372:PRO:HA	1:V:392:PRO:HB2	1.95	0.48
1:X:407:ARG:O	1:X:411:ASP:HB2	2.13	0.48
1:J:172:ALA:O	1:J:177:CYS:HB2	2.13	0.48
1:K:465:GLU:HG2	2:K:505:HOH:O	2.12	0.48
1:Z:149:ILE:HG23	1:Z:150:GLY:N	2.28	0.48
1:3:17:ILE:CD1	1:3:211:VAL:HG12	2.44	0.48
1:A:185:GLU:H	1:A:185:GLU:CD	2.22	0.48
1:D:304:TYR:CE1	1:D:398:ARG:HB2	2.49	0.48
1:X:415:GLY:HA2	1:X:437:TYR:CE1	2.49	0.48
1:J:102:LYS:NZ	1:J:110:GLU:OE1	2.37	0.48
1:Q:421:TYR:HA	1:Q:443:ASN:OD1	2.13	0.48
1:Z:160:PHE:HE2	1:Z:290:THR:HG22	1.79	0.48
1:5:37:THR:OG1	1:5:39:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:THR:HG23	1:I:323:GLY:HA3	1.96	0.48
1:J:47:MET:H	1:J:213:GLY:HA3	1.79	0.48
1:M:158:TRP:CD2	1:M:334:ILE:HD12	2.48	0.48
1:O:228:VAL:O	1:O:252:LYS:NZ	2.44	0.48
1:P:63:TRP:CZ2	1:P:150:GLY:HA2	2.49	0.48
1:X:52:THR:HB	1:X:221:GLU:HG2	1.95	0.48
1:2:256:LEU:O	1:2:461:GLY:HA3	2.13	0.48
1:4:248:ALA:HB3	1:4:249:PRO:HD3	1.96	0.48
1:F:3:GLY:N	2:F:536:HOH:O	2.46	0.48
1:I:47:MET:HG2	1:I:51:GLU:HG2	1.96	0.48
1:M:157:PRO:HD3	1:M:234:THR:HB	1.96	0.48
1:4:264:PHE:HB2	1:4:294:THR:CG2	2.43	0.48
1:H:37:THR:HG21	1:H:39:GLU:OE2	2.14	0.47
1:L:384:VAL:HG21	1:L:395:PRO:HG3	1.96	0.47
1:R:16:TYR:CZ	1:R:19:GLY:HA2	2.49	0.47
1:C:16:TYR:CZ	1:C:19:GLY:HA2	2.49	0.47
1:D:242:LEU:HB2	2:D:503:HOH:O	2.14	0.47
1:E:182:LYS:NZ	1:E:185:GLU:OE1	2.45	0.47
1:I:404:GLU:HA	1:I:407:ARG:HH12	1.79	0.47
1:K:287:ASN:ND2	1:K:333:LEU:HD12	2.29	0.47
1:U:439:MET:HG2	1:X:479:TYR:HD2	1.79	0.47
1:Y:142:ILE:HD13	1:2:452:ALA:HB2	1.96	0.47
1:3:444:THR:HB	1:6:483:ALA:HB2	1.95	0.47
1:4:163:ALA:O	1:4:167:ARG:HB2	2.14	0.47
1:J:5:MET:HE1	1:J:11:LEU:HB2	1.96	0.47
1:O:349:ALA:HA	1:O:382:MET:SD	2.55	0.47
1:U:483:ALA:HB2	1:X:444:THR:HB	1.96	0.47
1:V:70:THR:OG1	1:V:73:GLU:HB2	2.14	0.47
1:X:81:TRP:HZ2	1:X:194:MET:HB3	1.78	0.47
1:Y:429:TRP:CZ3	1:Z:141:ARG:HG2	2.49	0.47
1:1:123:GLU:HG2	1:2:123:GLU:CD	2.40	0.47
1:C:17:ILE:CD1	1:C:47:MET:HE1	2.37	0.47
1:F:425:ILE:HD12	1:H:425:ILE:HG12	1.97	0.47
1:H:157:PRO:HD3	1:H:234:THR:HB	1.96	0.47
1:J:37:THR:OG1	1:J:39:GLU:HG3	2.15	0.47
1:J:372:PRO:HA	1:J:392:PRO:HB2	1.97	0.47
1:Y:140:LYS:NZ	1:2:446:LEU:O	2.36	0.47
1:2:147:GLU:HB2	1:2:148:PRO:HD2	1.97	0.47
1:A:160:PHE:HE2	1:A:290:THR:HG22	1.80	0.47
1:A:300:HIS:ND1	1:A:302:ARG:HG3	2.29	0.47
1:D:114:ALA:HB2	1:D:163:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:ARG:HH21	1:H:124:GLU:HG2	1.79	0.47
1:O:393:LEU:O	1:O:395:PRO:HD3	2.15	0.47
1:B:167:ARG:NH2	1:B:465:GLU:OE1	2.48	0.47
1:E:25:ASP:CG	1:E:54:ARG:HH12	2.22	0.47
1:P:186:SER:HB3	1:P:334:ILE:HD11	1.97	0.47
1:R:283:LYS:HE2	1:R:393:LEU:O	2.14	0.47
1:R:424:ASP:OD1	1:T:423:ARG:HG3	2.15	0.47
1:4:251:VAL:O	1:4:251:VAL:HG13	2.14	0.47
1:F:183:PRO:HD2	1:F:211:VAL:O	2.15	0.47
1:G:103:PRO:HG2	1:G:106:GLU:HG3	1.96	0.47
1:J:121:PHE:HA	1:J:124:GLU:HB2	1.95	0.47
1:J:462:LEU:HD21	1:K:251:VAL:O	2.15	0.47
1:R:121:PHE:HA	1:R:124:GLU:HB2	1.97	0.47
1:S:167:ARG:NH2	1:S:465:GLU:OE1	2.48	0.47
1:U:91:ASP:OD2	1:U:91:ASP:N	2.46	0.47
1:V:161:PRO:O	1:V:165:ILE:HD13	2.14	0.47
1:W:3:GLY:N	2:W:501:HOH:O	2.47	0.47
1:X:81:TRP:O	1:X:85:VAL:HG23	2.15	0.47
1:Z:47:MET:HE2	1:Z:212:ILE:H	1.79	0.47
1:Z:334:ILE:HG23	1:Z:335:ASN:N	2.24	0.47
1:3:167:ARG:NH2	1:3:465:GLU:OE1	2.48	0.47
1:3:356:LEU:HD11	1:3:359:GLY:O	2.15	0.47
1:4:3:GLY:N	2:4:509:HOH:O	2.46	0.47
1:F:195:ALA:HB2	1:F:210:VAL:HG21	1.97	0.47
1:K:84:LEU:HB3	1:K:197:LEU:HD22	1.97	0.47
1:P:121:PHE:CD2	1:P:171:PRO:HD3	2.50	0.47
1:Q:415:GLY:HA2	1:Q:437:TYR:CD1	2.50	0.47
1:Z:254:LEU:HD23	1:Z:256:LEU:HD11	1.96	0.47
1:2:404:GLU:HG2	1:2:408:LEU:HD22	1.96	0.47
1:5:162:ALA:O	1:5:194:MET:HE1	2.15	0.47
1:A:127:ARG:HH21	1:B:124:GLU:HG2	1.80	0.47
1:D:5:MET:HE3	1:D:8:PRO:HA	1.97	0.47
1:P:17:ILE:HD11	1:P:47:MET:HE1	1.97	0.47
1:P:477:ILE:C	1:P:477:ILE:HD12	2.39	0.47
1:T:421:TYR:HA	1:T:443:ASN:OD1	2.13	0.47
1:W:265:ILE:HG12	1:W:405:LEU:HD11	1.95	0.47
1:2:358:THR:HA	1:3:309:ASP:OD1	2.15	0.47
1:3:423:ARG:HG3	1:5:424:ASP:OD1	2.15	0.47
1:3:477:ILE:HD11	1:6:453:PRO:CG	2.45	0.47
1:5:272:LEU:H	1:5:272:LEU:HD22	1.80	0.47
1:6:63:TRP:CZ2	1:6:150:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:O	1:B:27:ASP:HB2	2.15	0.47
1:H:413:GLU:CB	1:H:459:GLN:HG3	2.44	0.47
1:J:195:ALA:HB2	1:J:210:VAL:HG21	1.96	0.47
1:K:81:TRP:O	1:K:85:VAL:HG23	2.15	0.47
1:P:330:LEU:HD13	1:P:372:PRO:HG3	1.97	0.47
1:S:130:GLY:HA3	1:S:144:VAL:O	2.15	0.47
1:Y:93:ALA:CB	1:Y:108:LYS:HG2	2.45	0.47
1:Y:244:MET:HA	1:Y:254:LEU:HD21	1.97	0.47
1:C:356:LEU:HD21	1:C:360:GLY:HA3	1.97	0.46
1:E:97:THR:HG23	1:E:323:GLY:HA3	1.95	0.46
1:Y:110:GLU:HG3	1:Y:163:ALA:HB2	1.98	0.46
1:Y:427:ARG:HG3	1:Y:430:ARG:NH2	2.29	0.46
1:3:130:GLY:HA3	1:5:132:THR:OG1	2.16	0.46
1:D:158:TRP:CD2	1:D:334:ILE:HD12	2.50	0.46
1:L:186:SER:HB2	2:L:502:HOH:O	2.15	0.46
1:2:107:ALA:O	1:2:111:ILE:HG12	2.15	0.46
1:C:194:MET:HE3	1:C:194:MET:HB2	1.78	0.46
1:I:418:ALA:O	1:I:440:VAL:HA	2.15	0.46
1:L:466:GLY:HA3	2:L:513:HOH:O	2.16	0.46
1:M:107:ALA:O	1:M:111:ILE:HG12	2.16	0.46
1:Z:132:THR:OG1	1:2:130:GLY:HA3	2.14	0.46
1:F:234:THR:HG23	1:F:257:GLU:HB2	1.96	0.46
1:G:84:LEU:HB3	1:G:197:LEU:HD22	1.96	0.46
1:Q:265:ILE:CG2	1:Q:405:LEU:HD11	2.41	0.46
1:R:455:GLY:HA3	1:R:464:ARG:HD3	1.98	0.46
1:T:147:GLU:HB2	1:T:148:PRO:HD2	1.98	0.46
1:1:63:TRP:CD1	1:1:178:PRO:HD3	2.51	0.46
1:A:151:VAL:HA	1:A:178:PRO:HG2	1.96	0.46
1:I:335:ASN:HD21	1:I:337:ALA:HB3	1.81	0.46
1:L:152:CYS:SG	1:L:230:LYS:HG2	2.56	0.46
1:Q:146:LYS:HG2	1:Q:477:ILE:HG22	1.98	0.46
1:V:320:VAL:HG22	1:V:330:LEU:HB2	1.97	0.46
1:Y:17:ILE:HG13	1:Y:47:MET:HE1	1.96	0.46
1:2:288:GLY:HA2	1:2:293:CYS:SG	2.56	0.46
1:3:442:ILE:HD12	1:6:482:VAL:HG22	1.96	0.46
1:4:182:LYS:HE2	1:4:215:PRO:HA	1.96	0.46
1:I:157:PRO:HD3	1:I:234:THR:HB	1.97	0.46
1:J:476:VAL:HG21	1:K:457:VAL:HG12	1.97	0.46
1:R:47:MET:CE	1:R:211:VAL:HG13	2.39	0.46
1:W:429:TRP:HZ3	1:X:141:ARG:HG2	1.80	0.46
1:Y:477:ILE:HG23	2:Y:510:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:215:PRO:HG3	2:2:506:HOH:O	2.15	0.46
1:U:84:LEU:HB3	1:U:197:LEU:HD22	1.97	0.46
1:W:47:MET:HE2	1:W:212:ILE:H	1.81	0.46
1:X:455:GLY:HA3	1:X:464:ARG:HD3	1.97	0.46
1:Z:154:ALA:HB3	1:Z:181:VAL:HG22	1.98	0.46
1:B:47:MET:HE3	1:B:51:GLU:CG	2.46	0.46
1:I:404:GLU:HA	1:I:407:ARG:NH1	2.31	0.46
1:O:127:ARG:HH21	1:P:124:GLU:HG2	1.81	0.46
1:Y:131:ASP:OD1	1:Y:131:ASP:N	2.48	0.46
1:Z:387:GLU:HA	2:Z:519:HOH:O	2.15	0.46
1:D:89:SER:HB2	1:D:111:ILE:HG21	1.97	0.46
1:J:192:LEU:HD11	1:J:212:ILE:HD12	1.97	0.46
1:O:161:PRO:HB2	1:O:190:SER:HB2	1.96	0.46
1:P:160:PHE:CE2	1:P:290:THR:HG22	2.51	0.46
1:S:267:PHE:HE2	1:S:420:LEU:HD11	1.79	0.46
1:T:121:PHE:HA	1:T:124:GLU:HB2	1.98	0.46
1:W:131:ASP:HB2	1:W:144:VAL:HB	1.97	0.46
1:Y:361:LYS:O	1:Y:371:GLU:HB2	2.16	0.46
1:Z:155:ILE:HG23	1:Z:182:LYS:HD2	1.98	0.46
1:6:3:GLY:CA	2:6:550:HOH:O	2.63	0.46
1:G:158:TRP:O	1:G:161:PRO:HG3	2.16	0.46
1:H:172:ALA:O	1:H:177:CYS:HB2	2.16	0.46
1:R:480:LEU:HD23	1:S:440:VAL:HB	1.98	0.46
1:T:63:TRP:CD1	1:T:178:PRO:HD3	2.51	0.46
1:Z:214:ASP:HB3	1:Z:217:ALA:HB3	1.97	0.46
1:E:401:SER:HB3	1:N:357:MET:HG3	1.98	0.45
1:I:127:ARG:HH22	1:J:123:GLU:HB2	1.80	0.45
1:N:477:ILE:HD11	1:O:453:PRO:HB2	1.98	0.45
1:S:268:ASP:OD2	1:S:268:ASP:N	2.47	0.45
1:V:482:VAL:HA	1:W:442:ILE:HB	1.96	0.45
1:6:17:ILE:HG23	1:6:55:ALA:HB2	1.98	0.45
1:B:450:GLU:HG2	1:B:451:VAL:HG12	1.98	0.45
1:D:423:ARG:HA	1:D:423:ARG:HD2	1.76	0.45
1:I:378:VAL:HG13	1:I:382:MET:SD	2.56	0.45
1:N:356:LEU:HD11	1:N:360:GLY:HA3	1.98	0.45
1:S:36:ALA:HB2	1:S:332:PRO:HG3	1.97	0.45
1:X:301:GLU:HG2	1:X:398:ARG:HD3	1.98	0.45
1:5:234:THR:HA	1:5:257:GLU:O	2.15	0.45
1:G:283:LYS:O	1:G:288:GLY:HA2	2.15	0.45
1:W:404:GLU:HG2	1:W:408:LEU:HD22	1.97	0.45
1:Z:32:VAL:HG12	1:Z:33:PHE:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:HG23	1:A:257:GLU:HB2	1.98	0.45
1:C:17:ILE:O	1:C:20:GLU:N	2.45	0.45
1:E:476:VAL:CG2	1:H:457:VAL:HG12	2.47	0.45
1:I:157:PRO:HD2	1:I:164:MET:HG3	1.97	0.45
1:P:17:ILE:CD1	1:P:47:MET:HE1	2.47	0.45
1:T:10:LEU:O	1:T:12:ARG:HG2	2.16	0.45
1:U:336:GLU:OE1	1:U:362:ARG:NH2	2.47	0.45
1:U:443:ASN:HB2	1:X:483:ALA:HB3	1.98	0.45
1:2:157:PRO:CD	1:2:164:MET:HG3	2.45	0.45
1:R:155:ILE:HG12	1:R:182:LYS:HE3	1.98	0.45
1:U:420:LEU:HD13	1:U:431:VAL:HG11	1.98	0.45
1:X:72:LYS:HA	1:X:126:LYS:HD3	1.99	0.45
1:Y:275:ALA:HA	1:Y:421:TYR:CE1	2.52	0.45
1:2:129:ALA:O	1:2:146:LYS:HD2	2.17	0.45
1:D:17:ILE:CD1	1:D:47:MET:HE1	2.44	0.45
1:Q:287:ASN:ND2	1:Q:331:GLY:O	2.50	0.45
1:V:251:VAL:O	1:V:251:VAL:CG1	2.64	0.45
1:1:81:TRP:O	1:1:85:VAL:HG23	2.17	0.45
1:2:70:THR:OG1	1:2:73:GLU:HB2	2.16	0.45
1:2:182:LYS:NZ	1:2:183:PRO:O	2.50	0.45
1:F:415:GLY:HA2	1:F:437:TYR:CE1	2.51	0.45
1:I:46:LYS:HA	1:I:213:GLY:HA2	1.98	0.45
1:O:450:GLU:OE1	1:O:450:GLU:N	2.47	0.45
1:P:17:ILE:CG1	1:P:47:MET:HE1	2.47	0.45
1:P:97:THR:HG23	1:P:102:LYS:O	2.17	0.45
1:P:404:GLU:HG2	1:P:408:LEU:HD22	1.99	0.45
1:Y:234:THR:HA	1:Y:257:GLU:O	2.17	0.45
1:Y:440:VAL:HB	1:2:480:LEU:HD23	1.99	0.45
1:3:158:TRP:O	1:3:161:PRO:HD3	2.17	0.45
1:3:479:TYR:HD2	1:6:439:MET:HG2	1.81	0.45
1:4:155:ILE:HD12	1:4:231:LEU:HD11	1.99	0.45
1:4:426:GLY:O	1:4:430:ARG:HG3	2.16	0.45
1:E:157:PRO:HD3	1:E:234:THR:HB	1.99	0.45
1:N:423:ARG:HG3	1:P:424:ASP:OD1	2.15	0.45
1:O:168:LYS:HE2	1:O:465:GLU:OE2	2.15	0.45
1:V:300:HIS:HB3	1:V:303:VAL:HG22	1.99	0.45
1:Y:269:ASP:OD1	1:Y:269:ASP:N	2.49	0.45
1:Y:451:VAL:O	1:Y:467:SER:HB3	2.17	0.45
1:Z:20:GLU:HB3	1:Z:22:GLN:NE2	2.31	0.45
1:F:64:ALA:O	1:F:68:MET:HB2	2.17	0.45
1:G:194:MET:HE2	1:G:194:MET:HB2	1.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:263:PRO:HA	1:J:296:ARG:O	2.16	0.45
1:L:225:ASN:O	1:L:252:LYS:NZ	2.50	0.45
1:Q:290:THR:O	1:Q:293:CYS:HB2	2.16	0.45
1:Y:90:ASP:HA	1:Y:108:LYS:HZ3	1.81	0.45
1:1:287:ASN:ND2	1:1:333:LEU:HD13	2.32	0.45
1:H:157:PRO:HD2	1:H:164:MET:HG3	1.99	0.45
1:N:59:ALA:HB1	1:N:178:PRO:HB2	1.99	0.45
1:U:157:PRO:HD3	1:U:234:THR:HB	1.98	0.45
1:2:290:THR:HG1	1:2:293:CYS:HG	1.65	0.45
1:3:69:LYS:O	1:3:74:ARG:NH1	2.49	0.45
1:E:265:ILE:HG12	1:E:405:LEU:HD11	1.99	0.44
1:E:358:THR:HG22	1:E:374:VAL:HB	1.99	0.44
1:I:47:MET:HE3	1:I:51:GLU:CB	2.44	0.44
1:I:246:GLN:O	1:I:249:PRO:HD2	2.17	0.44
1:J:287:ASN:HD22	1:J:330:LEU:HD22	1.82	0.44
1:J:451:VAL:O	1:J:467:SER:HB3	2.18	0.44
1:Q:18:GLY:HA2	1:Q:206:GLY:HA2	1.99	0.44
1:4:428:VAL:HG13	1:4:442:ILE:HD13	1.99	0.44
1:M:153:ALA:HA	1:M:180:VAL:O	2.17	0.44
1:V:439:MET:HG2	1:W:479:TYR:HD2	1.82	0.44
1:X:157:PRO:HD2	1:X:164:MET:HG3	1.99	0.44
1:4:256:LEU:O	1:4:461:GLY:HA3	2.18	0.44
1:X:404:GLU:O	1:X:408:LEU:HB2	2.16	0.44
1:1:157:PRO:HD3	1:1:234:THR:HB	2.00	0.44
1:A:107:ALA:O	1:A:111:ILE:HG12	2.18	0.44
1:A:157:PRO:HD3	1:A:234:THR:HB	1.99	0.44
1:F:137:ASP:OD1	1:F:137:ASP:C	2.60	0.44
1:H:283:LYS:HD3	1:H:393:LEU:O	2.17	0.44
1:K:137:ASP:OD1	1:K:137:ASP:C	2.61	0.44
1:L:47:MET:HE3	1:L:51:GLU:HB2	1.97	0.44
1:L:121:PHE:HA	1:L:124:GLU:HB2	2.00	0.44
1:L:389:THR:HG21	1:L:393:LEU:HB3	2.00	0.44
1:U:154:ALA:HB1	1:U:168:LYS:HD3	2.00	0.44
1:Z:46:LYS:HA	1:Z:213:GLY:HA2	1.99	0.44
1:1:152:CYS:SG	1:1:230:LYS:HB3	2.58	0.44
1:I:190:SER:O	1:I:194:MET:HE2	2.18	0.44
1:T:415:GLY:HA2	1:T:437:TYR:CE1	2.53	0.44
1:Z:263:PRO:HA	1:Z:296:ARG:O	2.17	0.44
1:C:155:ILE:HG23	1:C:182:LYS:HD3	2.00	0.44
1:C:182:LYS:HD3	1:C:182:LYS:O	2.18	0.44
1:C:185:GLU:OE2	1:C:215:PRO:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:158:TRP:CG	1:M:334:ILE:HD12	2.53	0.44
1:Q:457:VAL:HG12	1:T:476:VAL:HG21	1.98	0.44
1:Q:477:ILE:HD11	1:T:464:ARG:HG3	1.98	0.44
1:W:128:VAL:HG11	1:W:475:VAL:HG11	2.00	0.44
1:2:46:LYS:HA	1:2:213:GLY:HA2	1.99	0.44
1:5:192:LEU:HD21	1:5:212:ILE:HD13	2.00	0.44
1:F:285:ARG:HE	1:F:285:ARG:HB2	1.49	0.44
1:I:160:PHE:HE2	1:I:290:THR:HG22	1.83	0.44
1:M:272:LEU:H	1:M:272:LEU:HD22	1.83	0.44
1:M:389:THR:HG21	1:M:393:LEU:HB3	1.98	0.44
1:N:90:ASP:OD1	1:N:108:LYS:HE2	2.18	0.44
1:U:5:MET:O	1:U:6:LYS:C	2.61	0.44
1:Z:356:LEU:HD12	1:Z:375:LEU:HD23	2.00	0.44
1:Z:479:TYR:HB3	1:1:439:MET:HG2	1.99	0.44
1:3:439:MET:HB3	1:3:447:ILE:HD12	2.00	0.44
1:4:136:PRO:HG3	1:5:451:VAL:HG13	2.00	0.44
1:4:260:GLY:HA2	1:4:414:PHE:HB3	2.00	0.44
1:5:137:ASP:OD1	1:5:137:ASP:C	2.60	0.44
1:G:47:MET:HE3	1:G:51:GLU:HB2	1.98	0.44
1:H:315:VAL:CG1	1:H:372:PRO:HB2	2.48	0.44
1:I:81:TRP:CZ2	1:I:194:MET:HG3	2.53	0.44
1:I:265:ILE:HD13	1:I:405:LEU:HD21	1.99	0.44
1:J:79:ARG:HH22	1:J:119:GLU:HG3	1.83	0.44
1:Q:439:MET:HG2	1:T:479:TYR:HD2	1.82	0.44
1:S:121:PHE:HA	1:S:124:GLU:HB2	2.00	0.44
1:S:254:LEU:HD12	1:S:256:LEU:HD21	2.00	0.44
1:T:168:LYS:HE2	1:T:465:GLU:OE2	2.18	0.44
1:U:153:ALA:HA	1:U:180:VAL:O	2.17	0.44
1:Y:405:LEU:O	1:Y:405:LEU:HG	2.18	0.44
1:Z:19:GLY:HA3	2:Z:510:HOH:O	2.18	0.44
1:Z:117:PHE:CE1	1:Z:167:ARG:HG3	2.52	0.44
1:D:121:PHE:HA	1:D:124:GLU:HB2	1.99	0.43
1:P:301:GLU:HG3	1:P:399:PHE:O	2.18	0.43
1:S:183:PRO:HD2	1:S:211:VAL:O	2.19	0.43
1:I:325:GLU:HG2	1:I:326:SER:N	2.32	0.43
1:I:453:PRO:HB2	1:L:477:ILE:HD11	2.00	0.43
1:J:423:ARG:HG3	1:L:424:ASP:OD1	2.17	0.43
1:O:79:ARG:O	1:O:82:PHE:HB3	2.17	0.43
1:T:162:ALA:HA	1:T:194:MET:HE1	1.99	0.43
1:Z:81:TRP:CH2	1:Z:169:VAL:HG11	2.52	0.43
1:3:345:HIS:CE1	1:3:387:GLU:HB3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:47:MET:HE2	1:5:51:GLU:HG2	2.00	0.43
1:D:299:VAL:HG21	1:D:307:PHE:CD2	2.53	0.43
1:D:339:VAL:HG21	1:D:368:GLY:HA2	2.00	0.43
1:I:421:TYR:CE1	1:I:443:ASN:HA	2.54	0.43
1:J:477:ILE:CD1	1:K:464:ARG:HG3	2.48	0.43
1:K:333:LEU:HD11	1:K:392:PRO:HD3	1.99	0.43
1:M:221:GLU:O	1:M:225:ASN:HB2	2.19	0.43
1:S:143:VAL:HB	1:S:480:LEU:HB2	2.01	0.43
1:T:410:ASN:O	1:T:412:THR:N	2.51	0.43
1:V:99:GLU:OE2	1:V:190:SER:OG	2.20	0.43
1:W:479:TYR:CZ	1:W:481:CYS:HB2	2.53	0.43
1:X:150:GLY:O	1:X:178:PRO:HD2	2.18	0.43
1:X:393:LEU:O	1:X:395:PRO:HD3	2.18	0.43
1:Z:184:ALA:C	1:Z:186:SER:N	2.75	0.43
1:5:129:ALA:O	1:5:146:LYS:HE3	2.19	0.43
1:A:393:LEU:O	1:A:395:PRO:HD3	2.18	0.43
1:C:357:MET:HG3	1:L:401:SER:HB3	1.99	0.43
1:E:476:VAL:HG21	1:H:457:VAL:HG12	2.00	0.43
1:F:221:GLU:O	1:F:225:ASN:HB2	2.18	0.43
1:I:427:ARG:O	1:I:431:VAL:HG23	2.18	0.43
1:Q:306:ALA:O	1:Q:310:LYS:HG3	2.19	0.43
1:X:140:LYS:HA	1:X:482:VAL:O	2.19	0.43
1:Z:191:ALA:O	1:Z:210:VAL:HG21	2.17	0.43
1:Z:464:ARG:HE	1:1:477:ILE:HD11	1.82	0.43
1:1:137:ASP:C	1:1:137:ASP:OD1	2.61	0.43
1:C:157:PRO:HD2	1:C:164:MET:HG3	1.99	0.43
1:C:251:VAL:O	1:C:251:VAL:CG1	2.66	0.43
1:F:113:TYR:HE1	1:F:449:ASN:HA	1.82	0.43
1:F:167:ARG:NH2	1:F:465:GLU:OE1	2.32	0.43
1:F:334:ILE:HD13	1:F:334:ILE:O	2.18	0.43
1:H:195:ALA:HB2	1:H:210:VAL:HG21	1.99	0.43
1:H:263:PRO:HD2	1:H:418:ALA:HA	1.99	0.43
1:J:106:GLU:HG3	2:J:515:HOH:O	2.19	0.43
1:L:97:THR:HG23	1:L:102:LYS:O	2.17	0.43
1:M:242:LEU:O	1:M:246:GLN:HG3	2.19	0.43
1:P:251:VAL:HG13	1:P:251:VAL:O	2.19	0.43
1:T:63:TRP:CZ2	1:T:150:GLY:HA2	2.53	0.43
1:U:52:THR:HB	1:U:221:GLU:HG2	1.99	0.43
1:X:47:MET:H	1:X:213:GLY:HA3	1.83	0.43
1:Y:234:THR:HG23	1:Y:257:GLU:HB2	2.00	0.43
1:Y:287:ASN:ND2	1:Y:333:LEU:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:393:LEU:O	1:Y:395:PRO:HD3	2.19	0.43
1:2:139:ASN:O	1:2:484:VAL:HG12	2.18	0.43
1:3:265:ILE:HG23	1:3:405:LEU:HD21	2.00	0.43
1:5:124:GLU:HG2	1:6:127:ARG:HH21	1.84	0.43
1:A:131:ASP:HB2	1:A:144:VAL:HB	2.01	0.43
1:K:135:THR:HG21	1:K:140:LYS:O	2.18	0.43
1:U:29:THR:HG22	1:U:45:PRO:HA	1.99	0.43
1:U:480:LEU:HD22	1:X:442:ILE:HD11	2.00	0.43
1:W:130:GLY:HA3	1:W:144:VAL:O	2.18	0.43
1:Y:404:GLU:HG3	1:Y:407:ARG:HH22	1.84	0.43
1:Y:450:GLU:HG2	1:Y:451:VAL:N	2.32	0.43
1:1:102:LYS:HD3	1:1:106:GLU:HB3	2.00	0.43
1:2:404:GLU:HG2	1:2:408:LEU:CD2	2.48	0.43
1:E:160:PHE:HE2	1:E:290:THR:HG22	1.83	0.43
1:K:250:THR:C	1:K:251:VAL:HG23	2.43	0.43
1:M:188:PRO:HB2	1:M:212:ILE:HD13	2.00	0.43
1:Q:234:THR:HG23	1:Q:257:GLU:HB2	2.01	0.43
1:W:157:PRO:HD2	1:W:164:MET:HG3	2.01	0.43
1:Z:241:ARG:O	1:1:248:ALA:HB1	2.18	0.43
1:E:477:ILE:C	1:E:477:ILE:HD12	2.44	0.43
1:J:228:VAL:O	1:J:252:LYS:NZ	2.46	0.43
1:L:300:HIS:ND1	1:L:302:ARG:HG3	2.34	0.43
1:V:262:ALA:HB3	1:V:294:THR:HA	2.00	0.43
1:2:16:TYR:CZ	1:2:19:GLY:HA2	2.54	0.43
1:A:481:CYS:HB3	1:D:447:ILE:HG22	2.01	0.43
1:E:188:PRO:HB2	1:E:212:ILE:HD13	2.00	0.43
1:H:393:LEU:O	1:H:395:PRO:HD3	2.18	0.43
1:J:477:ILE:HD11	1:K:464:ARG:HG3	2.01	0.43
1:N:265:ILE:HD13	1:N:405:LEU:HD21	2.01	0.43
1:O:265:ILE:HG21	1:O:405:LEU:HD21	2.00	0.43
1:O:272:LEU:H	1:O:272:LEU:HD22	1.82	0.43
1:P:393:LEU:O	1:P:395:PRO:HD3	2.19	0.43
1:Q:124:GLU:HG2	1:R:127:ARG:HH21	1.84	0.43
1:V:246:GLN:O	1:V:249:PRO:HD2	2.19	0.43
1:W:36:ALA:HA	1:W:332:PRO:HG3	2.01	0.43
1:Z:202:GLY:O	1:Z:204:PRO:HD3	2.19	0.43
1:3:194:MET:HE3	1:3:194:MET:HB2	1.76	0.43
1:5:121:PHE:CE2	1:5:171:PRO:HG3	2.54	0.43
1:A:244:MET:HA	1:A:254:LEU:HD21	2.00	0.43
1:H:63:TRP:CZ2	1:H:150:GLY:HA2	2.54	0.43
1:L:160:PHE:HB2	1:L:164:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:29:THR:HB	1:Q:43:THR:HB	2.00	0.43
1:Q:178:PRO:HB3	1:Q:207:VAL:HA	2.00	0.43
1:Z:181:VAL:N	1:Z:209:SER:O	2.51	0.43
1:Z:452:ALA:HA	1:Z:453:PRO:HD3	1.88	0.43
1:2:131:ASP:HB2	1:2:144:VAL:HB	2.00	0.43
1:5:157:PRO:HD3	1:5:234:THR:HB	2.01	0.43
1:A:482:VAL:HA	1:D:442:ILE:HB	2.01	0.42
1:N:183:PRO:HD2	1:N:211:VAL:O	2.19	0.42
1:T:121:PHE:CD2	1:T:171:PRO:HD3	2.54	0.42
1:U:35:PRO:HD2	1:U:98:THR:O	2.17	0.42
1:2:168:LYS:NZ	1:2:465:GLU:OE2	2.45	0.42
1:I:423:ARG:NH1	1:I:443:ASN:ND2	2.67	0.42
1:K:158:TRP:O	1:K:161:PRO:HD3	2.19	0.42
1:M:423:ARG:HD2	1:M:423:ARG:HA	1.64	0.42
1:Y:265:ILE:HG23	1:Y:405:LEU:HD21	1.98	0.42
1:1:282:SER:O	1:1:293:CYS:HA	2.19	0.42
1:2:263:PRO:HA	1:2:296:ARG:O	2.19	0.42
1:3:315:VAL:CG1	1:3:372:PRO:HB2	2.49	0.42
1:A:250:THR:O	1:D:459:GLN:NE2	2.47	0.42
1:D:192:LEU:HD21	1:D:212:ILE:CD1	2.50	0.42
1:F:453:PRO:HG2	1:G:477:ILE:CD1	2.49	0.42
1:G:37:THR:O	1:G:367:HIS:NE2	2.53	0.42
1:G:182:LYS:NZ	1:G:183:PRO:O	2.51	0.42
1:I:424:ASP:O	1:I:428:VAL:HG23	2.19	0.42
1:M:17:ILE:HD12	1:M:211:VAL:HG22	2.01	0.42
1:M:272:LEU:O	1:M:276:VAL:HG23	2.20	0.42
1:P:260:GLY:O	1:P:388:GLU:HG3	2.20	0.42
1:P:350:LEU:HD13	1:P:354:ALA:O	2.19	0.42
1:Q:129:ALA:HB2	1:S:133:LEU:HD23	2.02	0.42
1:Q:248:ALA:N	1:Q:249:PRO:HD2	2.34	0.42
1:T:435:LEU:O	1:T:437:TYR:N	2.51	0.42
1:U:225:ASN:HA	1:U:226:PRO:HD3	1.92	0.42
1:X:192:LEU:HD11	1:X:212:ILE:HD11	2.00	0.42
1:X:371:GLU:HA	1:X:372:PRO:HD2	1.82	0.42
1:Y:84:LEU:HD12	1:Y:201:ALA:HB2	2.01	0.42
1:Z:318:LEU:HB3	1:Z:330:LEU:HD11	2.01	0.42
1:3:480:LEU:HD23	1:6:440:VAL:HB	2.00	0.42
1:4:192:LEU:HD11	1:4:212:ILE:CD1	2.49	0.42
1:6:46:LYS:HA	1:6:213:GLY:HA2	2.01	0.42
1:B:158:TRP:CE3	1:B:334:ILE:HD12	2.55	0.42
1:C:399:PHE:CD1	1:C:405:LEU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:PRO:HD2	1:E:211:VAL:O	2.19	0.42
1:K:375:LEU:O	1:K:396:LEU:HG	2.19	0.42
1:M:440:VAL:HB	1:P:480:LEU:HD23	2.02	0.42
1:Y:59:ALA:HB1	1:Y:178:PRO:HB2	2.02	0.42
1:Y:421:TYR:CE1	1:Y:443:ASN:HA	2.54	0.42
1:5:295:ASN:OD1	1:5:388:GLU:HA	2.19	0.42
1:G:59:ALA:HA	1:G:206:GLY:O	2.19	0.42
1:K:356:LEU:HD21	1:K:360:GLY:HA3	2.01	0.42
1:L:63:TRP:CD1	1:L:178:PRO:HD3	2.55	0.42
1:Q:214:ASP:HB3	1:Q:217:ALA:HB3	2.01	0.42
1:S:131:ASP:H	1:S:144:VAL:HB	1.85	0.42
1:T:297:PHE:HB2	1:T:395:PRO:O	2.19	0.42
1:X:121:PHE:HA	1:X:124:GLU:HB2	2.01	0.42
1:2:214:ASP:HA	1:2:215:PRO:HD3	1.90	0.42
1:5:300:HIS:HB3	1:5:303:VAL:HG22	2.01	0.42
1:B:479:TYR:OH	1:C:447:ILE:O	2.33	0.42
1:D:264:PHE:HA	1:D:419:TYR:HB2	2.00	0.42
1:J:464:ARG:HE	1:K:477:ILE:HG13	1.84	0.42
1:U:239:VAL:HA	1:U:242:LEU:HD12	2.01	0.42
1:1:51:GLU:HG3	1:1:54:ARG:HH12	1.84	0.42
1:3:132:THR:OG1	1:5:130:GLY:HA3	2.20	0.42
1:4:157:PRO:HD2	1:4:164:MET:HG3	2.00	0.42
1:C:192:LEU:HD21	1:C:212:ILE:CD1	2.49	0.42
1:D:315:VAL:HA	1:D:318:LEU:HD12	2.01	0.42
1:E:5:MET:HE2	1:E:8:PRO:HA	2.01	0.42
1:G:157:PRO:HD2	1:G:164:MET:HG3	2.01	0.42
1:I:256:LEU:O	1:I:461:GLY:HA3	2.19	0.42
1:I:309:ASP:HA	1:I:357:MET:HE1	2.02	0.42
1:J:423:ARG:HA	1:J:423:ARG:HD2	1.88	0.42
1:J:439:MET:HE3	1:J:439:MET:HB2	1.97	0.42
1:K:450:GLU:HG2	1:K:451:VAL:HG12	2.02	0.42
1:L:64:ALA:O	1:L:68:MET:HB2	2.18	0.42
1:Z:343:GLU:OE1	1:Z:362:ARG:NH1	2.52	0.42
1:2:128:VAL:HG11	1:2:475:VAL:HG11	2.02	0.42
1:2:378:VAL:HG13	1:2:382:MET:SD	2.59	0.42
1:4:214:ASP:HA	1:4:215:PRO:HD2	1.85	0.42
1:5:195:ALA:HB2	1:5:210:VAL:HG21	2.00	0.42
1:A:267:PHE:CE1	1:A:427:ARG:HD3	2.53	0.42
1:N:114:ALA:HB2	1:N:163:ALA:HA	2.00	0.42
1:P:160:PHE:O	1:P:164:MET:HG2	2.20	0.42
1:U:241:ARG:O	1:X:248:ALA:HB1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:342:VAL:HG22	1:U:389:THR:HG22	2.02	0.42
1:V:30:PHE:HE2	1:V:213:GLY:HA2	1.83	0.42
1:X:230:LYS:O	1:X:230:LYS:HG3	2.19	0.42
1:1:371:GLU:HA	1:1:372:PRO:HD2	1.90	0.42
1:3:345:HIS:HE1	1:3:387:GLU:HB3	1.85	0.42
1:A:451:VAL:HG22	1:D:142:ILE:HD13	2.02	0.42
1:B:185:GLU:CD	1:B:185:GLU:H	2.28	0.42
1:F:155:ILE:HG23	1:F:182:LYS:HE3	2.01	0.42
1:G:214:ASP:HA	1:G:215:PRO:HD3	1.93	0.42
1:G:393:LEU:O	1:G:395:PRO:HD3	2.19	0.42
1:K:450:GLU:OE2	1:L:72:LYS:HE3	2.20	0.42
1:T:84:LEU:HB3	1:T:197:LEU:HD22	2.02	0.42
1:U:352:LYS:HB2	1:U:382:MET:HE2	2.01	0.42
1:1:214:ASP:HA	1:1:215:PRO:HD2	1.90	0.42
1:4:427:ARG:O	1:4:431:VAL:HG23	2.20	0.42
1:B:162:ALA:HB1	1:B:194:MET:HE3	2.02	0.42
1:E:480:LEU:HD23	1:H:440:VAL:HB	2.02	0.42
1:F:393:LEU:O	1:F:395:PRO:HD3	2.20	0.42
1:I:154:ALA:HB2	1:I:179:ILE:HD11	2.02	0.42
1:L:10:LEU:HD21	1:L:197:LEU:HD21	2.02	0.42
1:L:263:PRO:HA	1:L:296:ARG:O	2.20	0.42
1:M:225:ASN:HA	1:M:226:PRO:HD3	1.94	0.42
1:T:117:PHE:CE1	1:T:167:ARG:HG2	2.55	0.42
1:V:284:TYR:HB3	1:V:330:LEU:HD21	2.02	0.42
1:X:69:LYS:O	1:X:74:ARG:NH1	2.52	0.42
1:X:110:GLU:HG3	1:X:163:ALA:HB2	2.00	0.42
1:X:389:THR:O	1:X:390:PHE:HB2	2.19	0.42
1:Y:447:ILE:HG22	1:2:481:CYS:HB2	2.02	0.42
1:5:338:ALA:O	1:5:342:VAL:HG23	2.19	0.42
1:C:225:ASN:HA	1:C:226:PRO:HD3	1.86	0.41
1:N:121:PHE:HA	1:N:124:GLU:HB2	2.02	0.41
1:O:17:ILE:HG13	1:O:47:MET:HE1	2.01	0.41
1:R:417:ALA:HB2	1:R:439:MET:HE3	2.01	0.41
1:S:455:GLY:HA3	1:S:464:ARG:HD3	2.02	0.41
1:U:147:GLU:HB2	1:U:148:PRO:HD2	2.02	0.41
1:U:264:PHE:HB2	1:U:294:THR:HG21	2.01	0.41
1:U:320:VAL:HG22	1:U:330:LEU:HD23	2.02	0.41
1:V:47:MET:HE3	1:V:51:GLU:HB2	1.96	0.41
1:Z:232:SER:HA	1:Z:255:THR:O	2.20	0.41
1:2:264:PHE:HB2	1:2:294:THR:CG2	2.50	0.41
1:3:36:ALA:HB2	1:3:332:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:160:PHE:HE2	1:3:290:THR:HG22	1.85	0.41
1:3:374:VAL:HG22	1:3:394:ALA:HB3	2.01	0.41
1:4:52:THR:O	1:4:56:ILE:HD12	2.20	0.41
1:B:333:LEU:HD23	1:B:339:VAL:HA	2.01	0.41
1:E:279:ALA:O	1:E:283:LYS:HB3	2.21	0.41
1:J:466:GLY:HA3	2:J:509:HOH:O	2.19	0.41
1:M:193:ALA:O	1:M:196:PHE:HB3	2.20	0.41
1:Q:158:TRP:O	1:Q:161:PRO:HD3	2.21	0.41
1:S:256:LEU:O	1:S:461:GLY:HA3	2.20	0.41
1:T:356:LEU:HA	1:T:375:LEU:HD23	2.00	0.41
1:U:248:ALA:N	1:U:249:PRO:CD	2.82	0.41
1:V:154:ALA:HB1	1:V:168:LYS:HD3	2.00	0.41
1:3:160:PHE:CE2	1:3:290:THR:HG22	2.55	0.41
1:4:244:MET:HA	1:4:254:LEU:HD21	2.02	0.41
1:4:297:PHE:HB2	1:4:396:LEU:HD23	2.02	0.41
1:B:251:VAL:O	1:B:251:VAL:CG1	2.67	0.41
1:C:374:VAL:HG22	1:C:394:ALA:HB3	2.02	0.41
1:H:37:THR:O	1:H:367:HIS:CE1	2.73	0.41
1:J:230:LYS:HB2	1:J:253:LYS:HB3	2.02	0.41
1:K:403:GLU:OE2	1:K:407:ARG:NH1	2.53	0.41
1:R:160:PHE:HE2	1:R:290:THR:HG21	1.85	0.41
1:S:300:HIS:HB3	1:S:303:VAL:HG22	2.02	0.41
1:U:66:TRP:CZ2	1:U:74:ARG:HD2	2.55	0.41
1:V:315:VAL:HG13	1:V:372:PRO:HB2	2.02	0.41
1:Y:121:PHE:CD2	1:Y:171:PRO:HD3	2.55	0.41
1:Z:59:ALA:HB1	1:Z:178:PRO:HB2	2.02	0.41
1:Z:81:TRP:HH2	1:Z:169:VAL:HG11	1.85	0.41
1:Z:135:THR:HG23	1:2:70:THR:HG22	2.03	0.41
1:Z:212:ILE:CG2	1:Z:213:GLY:N	2.84	0.41
1:Z:275:ALA:O	1:Z:279:ALA:N	2.54	0.41
1:1:110:GLU:HG3	1:1:160:PHE:HD1	1.86	0.41
1:5:17:ILE:HG13	1:5:47:MET:HE1	2.01	0.41
1:A:165:ILE:O	1:A:169:VAL:HB	2.20	0.41
1:E:283:LYS:O	1:E:288:GLY:HA2	2.21	0.41
1:G:160:PHE:HB3	1:G:163:ALA:HB3	2.02	0.41
1:G:251:VAL:O	1:G:251:VAL:CG1	2.66	0.41
1:L:287:ASN:HD22	1:L:333:LEU:HD13	1.84	0.41
1:1:320:VAL:HG22	1:1:330:LEU:HD12	2.01	0.41
1:5:161:PRO:HB3	1:5:187:THR:OG1	2.20	0.41
1:5:407:ARG:O	1:5:411:ASP:HB2	2.21	0.41
1:A:5:MET:HE3	1:A:8:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:GLU:OE2	1:C:398:ARG:HD3	2.20	0.41
1:D:484:VAL:O	1:D:484:VAL:HG13	2.20	0.41
1:G:230:LYS:HE2	1:G:230:LYS:HB2	1.94	0.41
1:I:140:LYS:O	1:I:141:ARG:HD3	2.20	0.41
1:P:264:PHE:HA	1:P:419:TYR:HB2	2.01	0.41
1:R:132:THR:OG1	1:T:130:GLY:HA3	2.21	0.41
1:3:287:ASN:ND2	1:3:331:GLY:O	2.53	0.41
1:C:267:PHE:CZ	1:C:405:LEU:HD22	2.55	0.41
1:D:164:MET:O	1:D:168:LYS:HG3	2.21	0.41
1:E:363:HIS:HB3	1:E:369:PHE:HB3	2.03	0.41
1:E:407:ARG:HD3	2:E:546:HOH:O	2.20	0.41
1:N:241:ARG:O	1:O:248:ALA:HB1	2.19	0.41
1:P:439:MET:HE3	1:P:439:MET:HB2	1.91	0.41
1:Q:455:GLY:HA3	1:Q:464:ARG:HD3	2.03	0.41
1:R:355:SER:HB2	1:R:376:THR:OG1	2.20	0.41
1:T:300:HIS:HD2	1:T:399:PHE:CE1	2.39	0.41
1:U:298:PHE:HE1	1:U:408:LEU:HD23	1.86	0.41
1:U:378:VAL:HG11	1:U:395:PRO:HB2	2.02	0.41
1:V:180:VAL:HG22	1:V:209:SER:HB2	2.02	0.41
1:Z:121:PHE:HA	1:Z:124:GLU:HB2	2.03	0.41
1:6:59:ALA:O	1:6:178:PRO:HG3	2.19	0.41
1:C:141:ARG:HG3	1:D:429:TRP:CZ3	2.55	0.41
1:D:5:MET:HE3	1:D:5:MET:HB2	1.93	0.41
1:F:457:VAL:HG11	1:G:476:VAL:HG11	2.03	0.41
1:G:315:VAL:CG1	1:G:372:PRO:HB2	2.51	0.41
1:H:17:ILE:CD1	1:H:211:VAL:HG22	2.51	0.41
1:J:168:LYS:HE2	1:J:232:SER:OG	2.21	0.41
1:J:188:PRO:HB3	1:J:212:ILE:HD13	2.02	0.41
1:L:182:LYS:HE2	1:L:215:PRO:HA	2.02	0.41
1:M:152:CYS:SG	1:M:230:LYS:HG2	2.60	0.41
1:W:75:ALA:O	1:W:79:ARG:HB2	2.20	0.41
1:X:147:GLU:HB2	1:X:148:PRO:HD2	2.02	0.41
1:Z:136:PRO:HD3	1:1:451:VAL:HG11	2.03	0.41
1:1:24:ALA:HA	1:1:47:MET:HG2	2.02	0.41
1:3:96:LEU:HG	1:3:161:PRO:HG2	2.03	0.41
1:3:285:ARG:HH21	1:3:446:LEU:HD21	1.85	0.41
1:6:156:THR:HG21	1:6:165:ILE:HD13	2.02	0.41
1:A:137:ASP:OD1	1:A:137:ASP:C	2.62	0.41
1:A:188:PRO:HB2	1:A:212:ILE:HD13	2.01	0.41
1:J:47:MET:HE3	1:J:51:GLU:CB	2.48	0.41
1:N:230:LYS:HB2	1:N:253:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:479:TYR:CD1	1:U:480:LEU:N	2.89	0.41
1:V:81:TRP:O	1:V:85:VAL:HG23	2.20	0.41
1:V:398:ARG:HG3	2:V:524:HOH:O	2.20	0.41
1:W:141:ARG:HG2	1:X:429:TRP:CZ3	2.54	0.41
1:Y:237:THR:HA	1:Y:258:LEU:HD13	2.02	0.41
1:Z:12:ARG:HD3	2:Z:520:HOH:O	2.20	0.41
1:Z:372:PRO:HA	1:Z:392:PRO:HB2	2.03	0.41
1:4:241:ARG:O	1:5:248:ALA:HB1	2.21	0.41
1:A:5:MET:HE3	1:A:5:MET:HB2	2.00	0.41
1:A:251:VAL:HG12	1:A:251:VAL:O	2.21	0.41
1:C:287:ASN:ND2	1:C:333:LEU:HD13	2.36	0.41
1:C:413:GLU:CB	2:C:508:HOH:O	2.69	0.41
1:D:255:THR:HG21	2:D:511:HOH:O	2.21	0.41
1:E:149:ILE:HD13	1:E:230:LYS:HB3	2.03	0.41
1:G:287:ASN:ND2	1:G:333:LEU:HD13	2.36	0.41
1:I:92:LEU:HD21	1:I:197:LEU:HD11	2.02	0.41
1:J:59:ALA:HB1	1:J:178:PRO:HB2	2.02	0.41
1:L:13:HIS:CE1	1:L:42:GLY:HA3	2.56	0.41
1:N:15:ALA:H	1:N:45:PRO:HG2	1.84	0.41
1:O:45:PRO:O	1:O:212:ILE:HG22	2.21	0.41
1:Q:162:ALA:O	1:Q:194:MET:HE1	2.21	0.41
1:R:225:ASN:HA	1:R:226:PRO:HD2	1.97	0.41
1:S:264:PHE:HB2	1:S:294:THR:CG2	2.50	0.41
1:T:283:LYS:HA	1:T:283:LYS:HD2	1.90	0.41
1:U:13:HIS:HE1	1:U:42:GLY:HA3	1.86	0.41
1:U:279:ALA:O	1:U:283:LYS:HB3	2.21	0.41
1:V:233:PHE:CZ	1:V:235:GLY:HA3	2.56	0.41
1:W:29:THR:HB	1:W:43:THR:HB	2.03	0.41
1:Y:371:GLU:HA	1:Y:372:PRO:HD2	1.80	0.41
1:1:17:ILE:HD11	1:1:47:MET:HE1	2.03	0.41
1:1:232:SER:HA	1:1:255:THR:O	2.21	0.41
1:1:239:VAL:HG12	1:1:243:LEU:CD1	2.51	0.41
1:1:381:ASP:O	1:1:382:MET:HG3	2.21	0.41
1:2:121:PHE:O	1:2:122:ALA:C	2.63	0.41
1:2:160:PHE:HB2	1:2:164:MET:HE2	2.03	0.41
1:3:265:ILE:HG21	1:3:405:LEU:HD21	2.01	0.41
1:3:407:ARG:O	1:3:411:ASP:HB2	2.21	0.41
1:5:300:HIS:CE1	1:5:302:ARG:HG3	2.55	0.41
1:B:465:GLU:HG2	2:B:502:HOH:O	2.21	0.41
1:C:372:PRO:HA	1:C:392:PRO:HB2	2.03	0.41
1:E:142:ILE:CD1	1:H:451:VAL:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:384:VAL:HG21	1:F:395:PRO:HG3	2.03	0.41
1:F:423:ARG:HA	1:F:423:ARG:HD2	1.87	0.41
1:F:464:ARG:NE	2:F:560:HOH:O	2.48	0.41
1:H:286:ASN:O	1:H:289:GLN:HB2	2.21	0.41
1:Q:476:VAL:CG2	1:T:457:VAL:HG12	2.50	0.41
1:X:349:ALA:O	1:X:354:ALA:HB3	2.21	0.41
1:Z:111:ILE:HD13	1:Z:111:ILE:HA	1.77	0.41
1:1:29:THR:HG22	1:1:45:PRO:HA	2.03	0.41
1:1:247:SER:HB3	1:1:252:LYS:HG3	2.03	0.41
1:3:418:ALA:O	1:3:440:VAL:HA	2.20	0.41
1:4:423:ARG:HG3	1:6:424:ASP:OD1	2.21	0.41
1:E:25:ASP:OD2	1:E:54:ARG:NH1	2.53	0.40
1:R:246:GLN:O	1:R:249:PRO:HD2	2.20	0.40
1:W:79:ARG:NH2	1:W:119:GLU:HG3	2.36	0.40
1:X:51:GLU:HA	1:X:54:ARG:NH1	2.36	0.40
1:Z:10:LEU:HB3	1:Z:95:ILE:CD1	2.50	0.40
1:Z:67:ARG:HG3	1:Z:68:MET:N	2.36	0.40
1:2:357:MET:O	1:3:309:ASP:HB3	2.21	0.40
1:3:63:TRP:CZ2	1:3:150:GLY:HA2	2.56	0.40
1:F:271:ASP:OD1	1:F:271:ASP:C	2.64	0.40
1:R:283:LYS:CE	1:R:393:LEU:O	2.69	0.40
1:B:47:MET:CE	1:B:51:GLU:CB	2.84	0.40
1:B:410:ASN:O	1:B:412:THR:N	2.51	0.40
1:C:15:ALA:O	1:C:21:TRP:HA	2.21	0.40
1:D:17:ILE:HG23	1:D:55:ALA:HB2	2.03	0.40
1:D:161:PRO:HB2	1:D:190:SER:HB2	2.03	0.40
1:F:157:PRO:HD3	1:F:234:THR:HB	2.03	0.40
1:I:183:PRO:HD2	1:I:211:VAL:O	2.21	0.40
1:O:214:ASP:HA	1:O:215:PRO:HD2	1.92	0.40
1:P:140:LYS:O	1:P:141:ARG:HD3	2.22	0.40
1:U:5:MET:HE3	1:U:5:MET:H	1.86	0.40
1:U:226:PRO:HA	1:U:250:THR:CG2	2.51	0.40
1:X:436:GLU:HB3	1:X:458:LYS:HD2	2.04	0.40
1:Z:172:ALA:O	1:Z:177:CYS:HB2	2.21	0.40
1:Z:230:LYS:HG3	1:Z:231:LEU:N	2.37	0.40
1:6:121:PHE:O	1:6:122:ALA:C	2.64	0.40
1:E:121:PHE:HA	1:E:124:GLU:HB2	2.02	0.40
1:E:157:PRO:HD2	1:E:164:MET:HG3	2.03	0.40
1:E:447:ILE:HG22	1:H:481:CYS:HB3	2.04	0.40
1:G:131:ASP:OD1	1:G:131:ASP:N	2.53	0.40
1:M:484:VAL:O	1:M:484:VAL:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:423:ARG:HA	1:N:423:ARG:HD2	1.80	0.40
1:S:300:HIS:CE1	1:S:302:ARG:HG3	2.56	0.40
1:U:256:LEU:O	1:U:461:GLY:HA3	2.21	0.40
1:V:264:PHE:CD1	1:V:419:TYR:HB2	2.56	0.40
1:C:141:ARG:CG	1:D:429:TRP:CZ3	3.05	0.40
1:D:286:ASN:O	1:D:289:GLN:HG3	2.22	0.40
1:E:221:GLU:O	1:E:225:ASN:HB2	2.21	0.40
1:E:230:LYS:HB2	1:E:253:LYS:HB3	2.03	0.40
1:F:214:ASP:HA	1:F:215:PRO:HD2	1.97	0.40
1:I:244:MET:HA	1:I:254:LEU:HD21	2.04	0.40
1:J:287:ASN:O	1:J:392:PRO:HD3	2.21	0.40
1:M:338:ALA:O	1:M:342:VAL:HG23	2.21	0.40
1:N:113:TYR:CZ	1:N:117:PHE:HE2	2.39	0.40
1:N:415:GLY:HA2	1:N:437:TYR:CD1	2.56	0.40
1:Q:346:ILE:O	1:Q:350:LEU:HD22	2.21	0.40
1:Q:415:GLY:HA2	1:Q:437:TYR:CE1	2.56	0.40
1:V:477:ILE:HD11	1:W:453:PRO:CB	2.49	0.40
1:W:113:TYR:O	1:W:116:SER:OG	2.38	0.40
1:W:182:LYS:HG3	1:W:218:ILE:HG21	2.03	0.40
1:Y:47:MET:HE2	1:Y:51:GLU:HG2	2.04	0.40
1:Z:29:THR:HB	1:Z:43:THR:HB	2.03	0.40
1:Z:237:THR:O	1:Z:241:ARG:HG3	2.22	0.40
1:1:263:PRO:HD2	1:1:418:ALA:HA	2.03	0.40
1:2:421:TYR:HA	1:2:443:ASN:OD1	2.22	0.40
1:3:234:THR:HA	1:3:257:GLU:O	2.22	0.40
1:4:84:LEU:HD12	1:4:201:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	480/484 (99%)	441 (92%)	33 (7%)	6 (1%)	9	25
1	2	480/484 (99%)	443 (92%)	31 (6%)	6 (1%)	9	25
1	3	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	30	54
1	4	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	21	44
1	5	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	21	44
1	6	480/484 (99%)	463 (96%)	13 (3%)	4 (1%)	16	37
1	A	480/484 (99%)	457 (95%)	21 (4%)	2 (0%)	30	54
1	B	480/484 (99%)	464 (97%)	13 (3%)	3 (1%)	21	44
1	C	480/484 (99%)	465 (97%)	14 (3%)	1 (0%)	43	68
1	D	480/484 (99%)	450 (94%)	27 (6%)	3 (1%)	21	44
1	E	480/484 (99%)	456 (95%)	24 (5%)	0	100	100
1	F	480/484 (99%)	463 (96%)	15 (3%)	2 (0%)	30	54
1	G	480/484 (99%)	462 (96%)	16 (3%)	2 (0%)	30	54
1	H	480/484 (99%)	454 (95%)	24 (5%)	2 (0%)	30	54
1	I	480/484 (99%)	445 (93%)	32 (7%)	3 (1%)	21	44
1	J	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	30	54
1	K	480/484 (99%)	459 (96%)	19 (4%)	2 (0%)	30	54
1	L	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	43	68
1	M	480/484 (99%)	458 (95%)	19 (4%)	3 (1%)	21	44
1	N	480/484 (99%)	463 (96%)	16 (3%)	1 (0%)	43	68
1	O	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	43	68
1	P	480/484 (99%)	458 (95%)	22 (5%)	0	100	100
1	Q	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	21	44
1	R	480/484 (99%)	458 (95%)	17 (4%)	5 (1%)	12	32
1	S	480/484 (99%)	462 (96%)	17 (4%)	1 (0%)	43	68
1	T	480/484 (99%)	447 (93%)	29 (6%)	4 (1%)	16	37
1	U	480/484 (99%)	438 (91%)	41 (8%)	1 (0%)	43	68
1	V	480/484 (99%)	443 (92%)	33 (7%)	4 (1%)	16	37
1	W	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	21	44
1	X	480/484 (99%)	429 (89%)	48 (10%)	3 (1%)	21	44
1	Y	480/484 (99%)	427 (89%)	45 (9%)	8 (2%)	7	19
1	Z	480/484 (99%)	430 (90%)	45 (9%)	5 (1%)	12	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	15360/15488 (99%)	14487 (94%)	784 (5%)	89 (1%)	21	44

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	ASP
1	D	261	ASN
1	D	268	ASP
1	G	268	ASP
1	H	268	ASP
1	I	268	ASP
1	J	268	ASP
1	J	367	HIS
1	N	268	ASP
1	Y	27	ASP
1	Y	287	ASN
1	3	27	ASP
1	5	268	ASP
1	6	268	ASP
1	I	185	GLU
1	T	367	HIS
1	T	411	ASP
1	Y	330	LEU
1	Y	425	ILE
1	Z	128	VAL
1	Z	334	ILE
1	Z	367	HIS
1	2	139	ASN
1	2	261	ASN
1	F	268	ASP
1	M	261	ASN
1	R	261	ASN
1	T	261	ASN
1	V	25	ASP
1	Y	261	ASN
1	Y	367	HIS
1	1	261	ASN
1	1	264	PHE
1	1	423	ARG
1	6	261	ASN
1	A	27	ASP
1	C	261	ASN

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Mol	Chain	Res	Type
1	D	367	HIS
1	K	261	ASN
1	L	467	SER
1	M	139	ASN
1	M	467	SER
1	Q	27	ASP
1	R	268	ASP
1	V	467	SER
1	W	301	GLU
1	X	377	GLY
1	Z	4	SER
1	2	25	ASP
1	2	367	HIS
1	2	392	PRO
1	4	268	ASP
1	4	411	ASP
1	5	367	HIS
1	B	261	ASN
1	B	411	ASP
1	V	261	ASN
1	W	467	SER
1	1	467	SER
1	4	367	HIS
1	5	4	SER
1	H	326	SER
1	K	467	SER
1	Q	261	ASN
1	Q	415	GLY
1	R	4	SER
1	T	436	GLU
1	X	157	PRO
1	Z	188	PRO
1	U	415	GLY
1	V	392	PRO
1	Y	157	PRO
1	Y	415	GLY
1	1	263	PRO
1	A	425	ILE
1	F	415	GLY
1	I	415	GLY
1	O	128	VAL
1	W	415	GLY

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Mol	Chain	Res	Type
1	X	457	VAL
1	6	415	GLY
1	R	251	VAL
1	1	251	VAL
1	3	415	GLY
1	G	395	PRO
1	R	157	PRO
1	S	415	GLY
1	2	395	PRO
1	6	380	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	1	341/363 (94%)	314 (92%)	27 (8%)	11	28
1	2	349/363 (96%)	327 (94%)	22 (6%)	16	39
1	3	349/363 (96%)	325 (93%)	24 (7%)	14	34
1	4	349/363 (96%)	329 (94%)	20 (6%)	18	43
1	5	349/363 (96%)	327 (94%)	22 (6%)	16	39
1	6	349/363 (96%)	330 (95%)	19 (5%)	20	45
1	A	350/363 (96%)	334 (95%)	16 (5%)	24	51
1	B	351/363 (97%)	334 (95%)	17 (5%)	23	50
1	C	350/363 (96%)	324 (93%)	26 (7%)	13	32
1	D	350/363 (96%)	331 (95%)	19 (5%)	20	45
1	E	350/363 (96%)	330 (94%)	20 (6%)	18	43
1	F	350/363 (96%)	335 (96%)	15 (4%)	26	54
1	G	350/363 (96%)	329 (94%)	21 (6%)	17	41
1	H	350/363 (96%)	330 (94%)	20 (6%)	18	43
1	I	344/363 (95%)	315 (92%)	29 (8%)	10	26
1	J	350/363 (96%)	330 (94%)	20 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	349/363 (96%)	332 (95%)	17 (5%)	22	49
1	L	348/363 (96%)	326 (94%)	22 (6%)	16	39
1	M	349/363 (96%)	325 (93%)	24 (7%)	14	34
1	N	349/363 (96%)	329 (94%)	20 (6%)	18	43
1	O	349/363 (96%)	331 (95%)	18 (5%)	21	47
1	P	349/363 (96%)	333 (95%)	16 (5%)	24	51
1	Q	349/363 (96%)	325 (93%)	24 (7%)	14	34
1	R	349/363 (96%)	322 (92%)	27 (8%)	12	30
1	S	349/363 (96%)	332 (95%)	17 (5%)	22	49
1	T	346/363 (95%)	331 (96%)	15 (4%)	26	54
1	U	344/363 (95%)	321 (93%)	23 (7%)	15	36
1	V	346/363 (95%)	322 (93%)	24 (7%)	14	34
1	W	349/363 (96%)	334 (96%)	15 (4%)	26	54
1	X	340/363 (94%)	317 (93%)	23 (7%)	14	35
1	Y	349/363 (96%)	327 (94%)	22 (6%)	16	39
1	Z	346/363 (95%)	324 (94%)	22 (6%)	16	38
All	All	11141/11616 (96%)	10475 (94%)	666 (6%)	17	41

All (666) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	141	ARG
1	A	185	GLU
1	A	186	SER
1	A	230	LYS
1	A	272	LEU
1	A	285	ARG
1	A	291	CYS
1	A	302	ARG
1	A	333	LEU
1	A	334	ILE
1	A	408	LEU
1	A	425	ILE
1	A	451	VAL
1	A	462	LEU

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Mol	Chain	Res	Type
1	A	477	ILE
1	B	57	GLU
1	B	141	ARG
1	B	230	LYS
1	B	254	LEU
1	B	257	GLU
1	B	272	LEU
1	B	285	ARG
1	B	333	LEU
1	B	334	ILE
1	B	336	GLU
1	B	350	LEU
1	B	408	LEU
1	B	425	ILE
1	B	451	VAL
1	B	476	VAL
1	B	477	ILE
1	B	484	VAL
1	C	20	GLU
1	C	44	VAL
1	C	94	LEU
1	C	141	ARG
1	C	159	ASN
1	C	185	GLU
1	C	230	LYS
1	C	254	LEU
1	C	255	THR
1	C	272	LEU
1	C	290	THR
1	C	291	CYS
1	C	301	GLU
1	C	324	THR
1	C	333	LEU
1	C	336	GLU
1	C	355	SER
1	C	376	THR
1	C	405	LEU
1	C	408	LEU
1	C	423	ARG
1	C	425	ILE
1	C	451	VAL
1	C	476	VAL

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Mol	Chain	Res	Type
1	C	477	ILE
1	C	484	VAL
1	D	6	LYS
1	D	20	GLU
1	D	37	THR
1	D	57	GLU
1	D	94	LEU
1	D	104	LEU
1	D	131	ASP
1	D	159	ASN
1	D	230	LYS
1	D	253	LYS
1	D	254	LEU
1	D	276	VAL
1	D	283	LYS
1	D	293	CYS
1	D	324	THR
1	D	350	LEU
1	D	408	LEU
1	D	425	ILE
1	D	476	VAL
1	E	5	MET
1	E	20	GLU
1	E	27	ASP
1	E	96	LEU
1	E	104	LEU
1	E	159	ASN
1	E	185	GLU
1	E	230	LYS
1	E	242	LEU
1	E	254	LEU
1	E	272	LEU
1	E	283	LYS
1	E	333	LEU
1	E	408	LEU
1	E	425	ILE
1	E	448	SER
1	E	451	VAL
1	E	462	LEU
1	E	476	VAL
1	E	477	ILE
1	F	20	GLU

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Mol	Chain	Res	Type
1	F	96	LEU
1	F	141	ARG
1	F	185	GLU
1	F	254	LEU
1	F	285	ARG
1	F	333	LEU
1	F	334	ILE
1	F	350	LEU
1	F	405	LEU
1	F	408	LEU
1	F	423	ARG
1	F	451	VAL
1	F	476	VAL
1	F	477	ILE
1	G	20	GLU
1	G	57	GLU
1	G	89	SER
1	G	94	LEU
1	G	104	LEU
1	G	131	ASP
1	G	182	LYS
1	G	185	GLU
1	G	230	LYS
1	G	254	LEU
1	G	291	CYS
1	G	326	SER
1	G	333	LEU
1	G	336	GLU
1	G	376	THR
1	G	405	LEU
1	G	407	ARG
1	G	408	LEU
1	G	451	VAL
1	G	476	VAL
1	G	477	ILE
1	H	20	GLU
1	H	94	LEU
1	H	104	LEU
1	H	182	LYS
1	H	230	LYS
1	H	253	LYS
1	H	254	LEU

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Mol	Chain	Res	Type
1	H	283	LYS
1	H	291	CYS
1	H	293	CYS
1	H	324	THR
1	H	326	SER
1	H	334	ILE
1	H	396	LEU
1	H	403	GLU
1	H	408	LEU
1	H	425	ILE
1	H	451	VAL
1	H	476	VAL
1	H	477	ILE
1	I	43	THR
1	I	44	VAL
1	I	57	GLU
1	I	72	LYS
1	I	141	ARG
1	I	159	ASN
1	I	186	SER
1	I	230	LYS
1	I	231	LEU
1	I	253	LYS
1	I	291	CYS
1	I	324	THR
1	I	330	LEU
1	I	333	LEU
1	I	334	ILE
1	I	336	GLU
1	I	350	LEU
1	I	356	LEU
1	I	371	GLU
1	I	396	LEU
1	I	403	GLU
1	I	408	LEU
1	I	423	ARG
1	I	425	ILE
1	I	427	ARG
1	I	451	VAL
1	I	462	LEU
1	I	476	VAL
1	I	477	ILE

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Mol	Chain	Res	Type
1	J	20	GLU
1	J	27	ASP
1	J	39	GLU
1	J	44	VAL
1	J	57	GLU
1	J	104	LEU
1	J	141	ARG
1	J	159	ASN
1	J	186	SER
1	J	230	LYS
1	J	253	LYS
1	J	272	LEU
1	J	285	ARG
1	J	326	SER
1	J	333	LEU
1	J	350	LEU
1	J	408	LEU
1	J	423	ARG
1	J	451	VAL
1	J	477	ILE
1	K	40	SER
1	K	131	ASP
1	K	230	LYS
1	K	251	VAL
1	K	253	LYS
1	K	254	LEU
1	K	272	LEU
1	K	299	VAL
1	K	336	GLU
1	K	350	LEU
1	K	356	LEU
1	K	376	THR
1	K	425	ILE
1	K	451	VAL
1	K	475	VAL
1	K	476	VAL
1	K	477	ILE
1	L	57	GLU
1	L	104	LEU
1	L	142	ILE
1	L	159	ASN
1	L	186	SER

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Mol	Chain	Res	Type
1	L	211	VAL
1	L	230	LYS
1	L	253	LYS
1	L	254	LEU
1	L	272	LEU
1	L	283	LYS
1	L	333	LEU
1	L	334	ILE
1	L	336	GLU
1	L	348	ASP
1	L	356	LEU
1	L	403	GLU
1	L	408	LEU
1	L	425	ILE
1	L	451	VAL
1	L	476	VAL
1	L	477	ILE
1	M	20	GLU
1	M	57	GLU
1	M	78	LEU
1	M	131	ASP
1	M	159	ASN
1	M	200	ARG
1	M	230	LYS
1	M	251	VAL
1	M	272	LEU
1	M	285	ARG
1	M	291	CYS
1	M	333	LEU
1	M	334	ILE
1	M	396	LEU
1	M	408	LEU
1	M	412	THR
1	M	423	ARG
1	M	425	ILE
1	M	427	ARG
1	M	448	SER
1	M	451	VAL
1	M	462	LEU
1	M	476	VAL
1	M	477	ILE
1	N	6	LYS

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Mol	Chain	Res	Type
1	N	20	GLU
1	N	57	GLU
1	N	194	MET
1	N	230	LYS
1	N	251	VAL
1	N	253	LYS
1	N	254	LEU
1	N	272	LEU
1	N	333	LEU
1	N	350	LEU
1	N	376	THR
1	N	408	LEU
1	N	423	ARG
1	N	425	ILE
1	N	427	ARG
1	N	451	VAL
1	N	476	VAL
1	N	477	ILE
1	N	484	VAL
1	O	96	LEU
1	O	143	VAL
1	O	159	ASN
1	O	253	LYS
1	O	254	LEU
1	O	268	ASP
1	O	272	LEU
1	O	292	VAL
1	O	333	LEU
1	O	336	GLU
1	O	341	LYS
1	O	350	LEU
1	O	425	ILE
1	O	451	VAL
1	O	476	VAL
1	O	477	ILE
1	O	482	VAL
1	O	484	VAL
1	P	57	GLU
1	P	104	LEU
1	P	141	ARG
1	P	159	ASN
1	P	230	LYS

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Mol	Chain	Res	Type
1	P	250	THR
1	P	253	LYS
1	P	285	ARG
1	P	333	LEU
1	P	334	ILE
1	P	362	ARG
1	P	408	LEU
1	P	425	ILE
1	P	451	VAL
1	P	476	VAL
1	P	477	ILE
1	Q	31	GLU
1	Q	37	THR
1	Q	40	SER
1	Q	44	VAL
1	Q	73	GLU
1	Q	104	LEU
1	Q	131	ASP
1	Q	141	ARG
1	Q	159	ASN
1	Q	165	ILE
1	Q	182	LYS
1	Q	230	LYS
1	Q	253	LYS
1	Q	257	GLU
1	Q	272	LEU
1	Q	333	LEU
1	Q	341	LYS
1	Q	350	LEU
1	Q	371	GLU
1	Q	403	GLU
1	Q	405	LEU
1	Q	408	LEU
1	Q	425	ILE
1	Q	451	VAL
1	R	68	MET
1	R	77	ILE
1	R	104	LEU
1	R	131	ASP
1	R	141	ARG
1	R	147	GLU
1	R	237	THR

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Mol	Chain	Res	Type
1	R	253	LYS
1	R	254	LEU
1	R	267	PHE
1	R	272	LEU
1	R	289	GLN
1	R	291	CYS
1	R	305	ASP
1	R	336	GLU
1	R	350	LEU
1	R	355	SER
1	R	405	LEU
1	R	408	LEU
1	R	423	ARG
1	R	425	ILE
1	R	444	THR
1	R	451	VAL
1	R	462	LEU
1	R	476	VAL
1	R	477	ILE
1	R	484	VAL
1	S	4	SER
1	S	182	LYS
1	S	236	SER
1	S	253	LYS
1	S	268	ASP
1	S	272	LEU
1	S	285	ARG
1	S	326	SER
1	S	333	LEU
1	S	371	GLU
1	S	405	LEU
1	S	408	LEU
1	S	425	ILE
1	S	451	VAL
1	S	462	LEU
1	S	476	VAL
1	S	477	ILE
1	T	57	GLU
1	T	212	ILE
1	T	230	LYS
1	T	242	LEU
1	T	254	LEU

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Mol	Chain	Res	Type
1	T	301	GLU
1	T	320	VAL
1	T	350	LEU
1	T	397	PHE
1	T	408	LEU
1	T	423	ARG
1	T	451	VAL
1	T	471	ILE
1	T	476	VAL
1	T	477	ILE
1	U	5	MET
1	U	9	SER
1	U	57	GLU
1	U	60	GLN
1	U	91	ASP
1	U	94	LEU
1	U	95	ILE
1	U	104	LEU
1	U	131	ASP
1	U	141	ARG
1	U	165	ILE
1	U	194	MET
1	U	212	ILE
1	U	250	THR
1	U	272	LEU
1	U	320	VAL
1	U	324	THR
1	U	333	LEU
1	U	408	LEU
1	U	423	ARG
1	U	440	VAL
1	U	451	VAL
1	U	477	ILE
1	V	34	ASP
1	V	37	THR
1	V	57	GLU
1	V	68	MET
1	V	90	ASP
1	V	126	LYS
1	V	131	ASP
1	V	141	ARG
1	V	159	ASN

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Mol	Chain	Res	Type
1	V	186	SER
1	V	251	VAL
1	V	253	LYS
1	V	299	VAL
1	V	333	LEU
1	V	358	THR
1	V	398	ARG
1	V	403	GLU
1	V	405	LEU
1	V	408	LEU
1	V	425	ILE
1	V	446	LEU
1	V	451	VAL
1	V	476	VAL
1	V	477	ILE
1	W	57	GLU
1	W	79	ARG
1	W	96	LEU
1	W	104	LEU
1	W	159	ASN
1	W	253	LYS
1	W	287	ASN
1	W	333	LEU
1	W	334	ILE
1	W	336	GLU
1	W	389	THR
1	W	405	LEU
1	W	408	LEU
1	W	425	ILE
1	W	476	VAL
1	X	20	GLU
1	X	37	THR
1	X	141	ARG
1	X	212	ILE
1	X	230	LYS
1	X	254	LEU
1	X	272	LEU
1	X	285	ARG
1	X	320	VAL
1	X	325	GLU
1	X	334	ILE
1	X	339	VAL

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Mol	Chain	Res	Type
1	X	350	LEU
1	X	373	THR
1	X	376	THR
1	X	403	GLU
1	X	404	GLU
1	X	405	LEU
1	X	425	ILE
1	X	451	VAL
1	X	476	VAL
1	X	477	ILE
1	X	482	VAL
1	Y	6	LYS
1	Y	29	THR
1	Y	78	LEU
1	Y	104	LEU
1	Y	131	ASP
1	Y	141	ARG
1	Y	194	MET
1	Y	230	LYS
1	Y	257	GLU
1	Y	290	THR
1	Y	291	CYS
1	Y	303	VAL
1	Y	305	ASP
1	Y	325	GLU
1	Y	330	LEU
1	Y	350	LEU
1	Y	358	THR
1	Y	396	LEU
1	Y	403	GLU
1	Y	425	ILE
1	Y	476	VAL
1	Y	477	ILE
1	Z	33	PHE
1	Z	44	VAL
1	Z	92	LEU
1	Z	95	ILE
1	Z	111	ILE
1	Z	209	SER
1	Z	230	LYS
1	Z	242	LEU
1	Z	250	THR

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Mol	Chain	Res	Type
1	Z	251	VAL
1	Z	254	LEU
1	Z	272	LEU
1	Z	283	LYS
1	Z	291	CYS
1	Z	293	CYS
1	Z	299	VAL
1	Z	320	VAL
1	Z	396	LEU
1	Z	425	ILE
1	Z	448	SER
1	Z	451	VAL
1	Z	477	ILE
1	1	20	GLU
1	1	27	ASP
1	1	39	GLU
1	1	57	GLU
1	1	97	THR
1	1	99	GLU
1	1	104	LEU
1	1	141	ARG
1	1	165	ILE
1	1	194	MET
1	1	273	ASP
1	1	325	GLU
1	1	333	LEU
1	1	334	ILE
1	1	339	VAL
1	1	350	LEU
1	1	357	MET
1	1	376	THR
1	1	387	GLU
1	1	396	LEU
1	1	408	LEU
1	1	412	THR
1	1	425	ILE
1	1	446	LEU
1	1	451	VAL
1	1	477	ILE
1	1	484	VAL
1	2	6	LYS
1	2	44	VAL

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Mol	Chain	Res	Type
1	2	104	LEU
1	2	135	THR
1	2	141	ARG
1	2	182	LYS
1	2	250	THR
1	2	254	LEU
1	2	272	LEU
1	2	293	CYS
1	2	325	GLU
1	2	348	ASP
1	2	350	LEU
1	2	403	GLU
1	2	408	LEU
1	2	420	LEU
1	2	425	ILE
1	2	451	VAL
1	2	476	VAL
1	2	477	ILE
1	2	481	CYS
1	2	482	VAL
1	3	20	GLU
1	3	22	GLN
1	3	37	THR
1	3	44	VAL
1	3	104	LEU
1	3	194	MET
1	3	212	ILE
1	3	230	LYS
1	3	253	LYS
1	3	254	LEU
1	3	255	THR
1	3	257	GLU
1	3	272	LEU
1	3	291	CYS
1	3	336	GLU
1	3	350	LEU
1	3	382	MET
1	3	390	PHE
1	3	396	LEU
1	3	408	LEU
1	3	420	LEU
1	3	425	ILE

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Mol	Chain	Res	Type
1	3	476	VAL
1	3	477	ILE
1	4	44	VAL
1	4	56	ILE
1	4	57	GLU
1	4	131	ASP
1	4	141	ARG
1	4	149	ILE
1	4	230	LYS
1	4	251	VAL
1	4	254	LEU
1	4	272	LEU
1	4	285	ARG
1	4	334	ILE
1	4	350	LEU
1	4	357	MET
1	4	408	LEU
1	4	423	ARG
1	4	425	ILE
1	4	448	SER
1	4	451	VAL
1	4	477	ILE
1	5	20	GLU
1	5	57	GLU
1	5	104	LEU
1	5	141	ARG
1	5	230	LYS
1	5	251	VAL
1	5	254	LEU
1	5	272	LEU
1	5	285	ARG
1	5	291	CYS
1	5	302	ARG
1	5	333	LEU
1	5	350	LEU
1	5	355	SER
1	5	356	LEU
1	5	396	LEU
1	5	403	GLU
1	5	408	LEU
1	5	425	ILE
1	5	451	VAL

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Mol	Chain	Res	Type
1	5	476	VAL
1	5	477	ILE
1	6	9	SER
1	6	96	LEU
1	6	159	ASN
1	6	211	VAL
1	6	230	LYS
1	6	242	LEU
1	6	251	VAL
1	6	253	LYS
1	6	254	LEU
1	6	272	LEU
1	6	283	LYS
1	6	350	LEU
1	6	358	THR
1	6	396	LEU
1	6	408	LEU
1	6	451	VAL
1	6	476	VAL
1	6	477	ILE
1	6	484	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	367	HIS
1	B	159	ASN
1	B	367	HIS
1	D	261	ASN
1	D	287	ASN
1	E	88	ASN
1	E	246	GLN
1	E	287	ASN
1	F	14	GLN
1	F	60	GLN
1	F	159	ASN
1	H	363	HIS
1	I	246	GLN
1	J	13	HIS
1	J	159	ASN
1	J	287	ASN

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Mol	Chain	Res	Type
1	K	14	GLN
1	L	246	GLN
1	L	367	HIS
1	M	345	HIS
1	M	367	HIS
1	N	246	GLN
1	O	60	GLN
1	P	88	ASN
1	P	246	GLN
1	Q	468	HIS
1	R	289	GLN
1	R	367	HIS
1	R	468	HIS
1	S	246	GLN
1	T	14	GLN
1	U	88	ASN
1	V	100	GLN
1	W	246	GLN
1	X	286	ASN
1	X	289	GLN
1	Y	13	HIS
1	Y	287	ASN
1	Z	13	HIS
1	Z	22	GLN
1	1	14	GLN
1	1	60	GLN
1	1	289	GLN
1	1	443	ASN
1	1	449	ASN
1	3	88	ASN
1	3	261	ASN
1	3	345	HIS
1	4	289	GLN
1	4	295	ASN
1	6	459	GLN
1	6	468	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	482/484 (99%)	1.05	53 (10%) 10 9	36, 52, 63, 68	1 (0%)
1	2	482/484 (99%)	0.40	11 (2%) 61 58	28, 42, 57, 62	1 (0%)
1	3	482/484 (99%)	0.41	8 (1%) 69 67	27, 43, 56, 64	1 (0%)
1	4	482/484 (99%)	0.25	5 (1%) 79 78	33, 44, 57, 64	1 (0%)
1	5	482/484 (99%)	0.26	3 (0%) 85 85	31, 44, 58, 63	1 (0%)
1	6	482/484 (99%)	0.06	1 (0%) 91 90	26, 37, 51, 55	1 (0%)
1	A	482/484 (99%)	0.11	2 (0%) 88 87	29, 41, 52, 64	1 (0%)
1	B	482/484 (99%)	0.05	2 (0%) 88 87	26, 38, 49, 59	1 (0%)
1	C	482/484 (99%)	0.08	1 (0%) 91 90	25, 38, 51, 62	1 (0%)
1	D	482/484 (99%)	0.26	12 (2%) 58 55	25, 40, 54, 63	1 (0%)
1	E	482/484 (99%)	0.05	1 (0%) 91 90	24, 37, 47, 59	1 (0%)
1	F	482/484 (99%)	0.03	3 (0%) 85 85	25, 36, 47, 58	1 (0%)
1	G	482/484 (99%)	0.08	2 (0%) 88 87	26, 38, 51, 61	1 (0%)
1	H	482/484 (99%)	0.13	6 (1%) 76 75	25, 39, 53, 62	1 (0%)
1	I	482/484 (99%)	0.74	34 (7%) 22 19	33, 49, 62, 67	1 (0%)
1	J	482/484 (99%)	0.21	2 (0%) 88 87	29, 43, 54, 63	1 (0%)
1	K	482/484 (99%)	0.12	4 (0%) 82 81	28, 41, 57, 60	1 (0%)
1	L	482/484 (99%)	0.05	6 (1%) 76 75	28, 39, 47, 54	1 (0%)
1	M	482/484 (99%)	0.26	9 (1%) 66 63	32, 43, 55, 63	1 (0%)
1	N	482/484 (99%)	0.11	5 (1%) 79 78	29, 41, 51, 62	1 (0%)
1	O	482/484 (99%)	0.16	4 (0%) 82 81	28, 42, 56, 61	1 (0%)
1	P	482/484 (99%)	-0.02	4 (0%) 82 81	28, 36, 46, 54	1 (0%)
1	Q	482/484 (99%)	0.45	6 (1%) 76 75	38, 50, 61, 67	1 (0%)
1	R	482/484 (99%)	0.24	8 (1%) 69 67	31, 43, 57, 60	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	S	482/484 (99%)	0.04	2 (0%) 88 87	32, 40, 49, 58	1 (0%)
1	T	482/484 (99%)	0.56	12 (2%) 58 55	39, 51, 62, 68	1 (0%)
1	U	482/484 (99%)	0.88	24 (4%) 34 30	43, 53, 64, 69	1 (0%)
1	V	482/484 (99%)	0.56	13 (2%) 56 53	38, 47, 60, 64	1 (0%)
1	W	482/484 (99%)	0.27	4 (0%) 82 81	35, 44, 52, 59	1 (0%)
1	X	482/484 (99%)	0.97	29 (6%) 27 24	43, 54, 63, 69	1 (0%)
1	Y	482/484 (99%)	0.74	27 (5%) 30 26	30, 48, 59, 67	1 (0%)
1	Z	482/484 (99%)	1.06	43 (8%) 15 13	40, 52, 62, 71	1 (0%)
All	All	15424/15488 (99%)	0.33	346 (2%) 62 59	24, 43, 59, 71	32 (0%)

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	3	GLY	5.5
1	L	3	GLY	4.8
1	2	3	GLY	4.5
1	V	3	GLY	4.4
1	U	32	VAL	4.2
1	W	3	GLY	4.2
1	1	298	PHE	4.1
1	T	291	CYS	4.1
1	2	484	VAL	4.0
1	1	266	VAL	3.8
1	1	434	ALA	3.8
1	U	3	GLY	3.7
1	1	384	VAL	3.7
1	K	291	CYS	3.6
1	N	291	CYS	3.6
1	Z	291	CYS	3.6
1	Q	3	GLY	3.6
1	R	429	TRP	3.5
1	1	417	ALA	3.5
1	T	365	LEU	3.4
1	I	36	ALA	3.4
1	Z	32	VAL	3.4
1	I	3	GLY	3.3
1	2	143	VAL	3.3
1	W	470	GLY	3.3
1	Y	291	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	3	291	CYS	3.2
1	U	390	PHE	3.2
1	Z	65	GLY	3.2
1	1	41	LEU	3.2
1	Y	281	ALA	3.2
1	I	350	LEU	3.1
1	U	185	GLU	3.1
1	1	291	CYS	3.1
1	2	360	GLY	3.1
1	X	41	LEU	3.1
1	Y	8	PRO	3.1
1	T	3	GLY	3.1
1	Z	211	VAL	3.1
1	5	291	CYS	3.1
1	I	291	CYS	3.1
1	D	317	LYS	3.0
1	X	3	GLY	3.0
1	U	5	MET	3.0
1	Y	327	GLY	3.0
1	V	429	TRP	2.9
1	X	43	THR	2.9
1	I	374	VAL	2.9
1	1	378	VAL	2.9
1	P	3	GLY	2.9
1	Y	280	ILE	2.9
1	X	373	THR	2.9
1	R	396	LEU	2.9
1	X	32	VAL	2.9
1	1	405	LEU	2.9
1	B	3	GLY	2.9
1	I	284	TYR	2.9
1	S	3	GLY	2.9
1	X	42	GLY	2.9
1	I	37	THR	2.9
1	I	328	ALA	2.9
1	Z	41	LEU	2.9
1	Z	245	ALA	2.9
1	X	30	PHE	2.9
1	Z	233	PHE	2.9
1	I	104	LEU	2.8
1	N	470	GLY	2.8
1	1	101	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	Y	275	ALA	2.8
1	Q	291	CYS	2.8
1	D	3	GLY	2.8
1	Y	368	GLY	2.8
1	Z	196	PHE	2.8
1	Z	54	ARG	2.8
1	D	316	SER	2.7
1	I	373	THR	2.7
1	U	245	ALA	2.7
1	Y	320	VAL	2.7
1	1	62	ALA	2.7
1	G	3	GLY	2.7
1	I	327	GLY	2.7
1	W	429	TRP	2.7
1	3	357	MET	2.7
1	M	320	VAL	2.7
1	X	337	ALA	2.7
1	I	365	LEU	2.7
1	6	3	GLY	2.7
1	I	105	ALA	2.7
1	I	394	ALA	2.7
1	1	276	VAL	2.7
1	1	279	ALA	2.7
1	1	454	PHE	2.7
1	A	5	MET	2.7
1	1	3	GLY	2.7
1	X	376	THR	2.7
1	Z	24	ALA	2.7
1	1	297	PHE	2.7
1	1	390	PHE	2.7
1	Z	161	PRO	2.7
1	I	393	LEU	2.6
1	1	277	GLU	2.6
1	D	370	PHE	2.6
1	I	347	ALA	2.6
1	D	5	MET	2.6
1	I	318	LEU	2.6
1	4	3	GLY	2.6
1	Z	33	PHE	2.6
1	Y	273	ASP	2.6
1	X	272	LEU	2.6
1	D	293	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	39	GLU	2.6
1	Z	191	ALA	2.6
1	1	299	VAL	2.6
1	I	370	PHE	2.6
1	H	293	CYS	2.6
1	Z	55	ALA	2.6
1	5	429	TRP	2.5
1	X	322	ARG	2.5
1	3	317	LYS	2.5
1	K	3	GLY	2.5
1	3	3	GLY	2.5
1	I	372	PRO	2.5
1	1	457	VAL	2.5
1	2	320	VAL	2.5
1	U	291	CYS	2.5
1	1	429	TRP	2.5
1	1	419	TYR	2.5
1	Q	24	ALA	2.5
1	1	418	ALA	2.5
1	U	334	ILE	2.5
1	H	365	LEU	2.5
1	O	365	LEU	2.5
1	1	469	TYR	2.5
1	O	3	GLY	2.5
1	1	292	VAL	2.5
1	V	390	PHE	2.5
1	Z	193	ALA	2.5
1	Z	238	ALA	2.5
1	Y	330	LEU	2.5
1	Z	192	LEU	2.5
1	3	5	MET	2.5
1	D	313	ALA	2.5
1	U	24	ALA	2.5
1	Z	58	ALA	2.5
1	U	324	THR	2.4
1	U	285	ARG	2.4
1	V	288	GLY	2.4
1	R	307	PHE	2.4
1	Z	172	ALA	2.4
1	1	400	ALA	2.4
1	4	364	ALA	2.4
1	O	291	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	185	GLU	2.4
1	M	359	GLY	2.4
1	H	5	MET	2.4
1	1	319	LYS	2.4
1	V	210	VAL	2.4
1	X	315	VAL	2.4
1	Y	303	VAL	2.4
1	1	339	VAL	2.4
1	U	284	TYR	2.4
1	V	356	LEU	2.4
1	X	29	THR	2.4
1	Z	227	ILE	2.4
1	A	355	SER	2.4
1	F	268	ASP	2.4
1	F	291	CYS	2.4
1	V	392	PRO	2.4
1	Y	288	GLY	2.4
1	1	320	VAL	2.4
1	1	407	ARG	2.4
1	M	364	ALA	2.4
1	X	189	PHE	2.4
1	I	317	LYS	2.3
1	1	386	LYS	2.3
1	J	291	CYS	2.3
1	Z	3	GLY	2.3
1	1	406	VAL	2.3
1	I	369	PHE	2.3
1	Z	11	LEU	2.3
1	1	337	ALA	2.3
1	2	41	LEU	2.3
1	B	268	ASP	2.3
1	M	429	TRP	2.3
1	Y	19	GLY	2.3
1	Y	323	GLY	2.3
1	4	291	CYS	2.3
1	Q	292	VAL	2.3
1	Z	207	VAL	2.3
1	1	428	VAL	2.3
1	I	94	LEU	2.3
1	O	397	PHE	2.3
1	U	11	LEU	2.3
1	X	347	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	Y	11	LEU	2.3
1	1	160	PHE	2.3
1	1	399	PHE	2.3
1	Z	364	ALA	2.3
1	Z	452	ALA	2.3
1	Y	5	MET	2.3
1	Z	68	MET	2.3
1	N	465	GLU	2.3
1	T	26	SER	2.3
1	C	3	GLY	2.3
1	I	323	GLY	2.3
1	Z	18	GLY	2.3
1	Z	331	GLY	2.3
1	D	318	LEU	2.3
1	F	208	LEU	2.3
1	1	231	LEU	2.3
1	M	5	MET	2.3
1	W	465	GLU	2.3
1	T	322	ARG	2.3
1	I	276	VAL	2.3
1	X	44	VAL	2.3
1	X	184	ALA	2.2
1	1	346	ILE	2.2
1	V	6	LYS	2.2
1	U	215	PRO	2.2
1	Z	226	PRO	2.2
1	U	4	SER	2.2
1	Z	190	SER	2.2
1	G	18	GLY	2.2
1	H	3	GLY	2.2
1	P	38	GLY	2.2
1	Y	3	GLY	2.2
1	1	445	GLY	2.2
1	T	272	LEU	2.2
1	T	484	VAL	2.2
1	X	104	LEU	2.2
1	Y	420	LEU	2.2
1	I	334	ILE	2.2
1	I	390	PHE	2.2
1	Z	165	ILE	2.2
1	Z	5	MET	2.2
1	1	274	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	481	CYS	2.2
1	V	395	PRO	2.2
1	3	309	ASP	2.2
1	U	292	VAL	2.2
1	I	5	MET	2.2
1	Z	390	PHE	2.2
1	1	414	PHE	2.2
1	4	68	MET	2.2
1	Y	105	ALA	2.2
1	3	354	ALA	2.2
1	R	350	LEU	2.2
1	Z	235	GLY	2.2
1	U	44	VAL	2.2
1	X	374	VAL	2.2
1	I	367	HIS	2.2
1	X	390	PHE	2.2
1	K	347	ALA	2.2
1	R	394	ALA	2.2
1	2	138	ALA	2.2
1	R	398	ARG	2.2
1	Q	14	GLN	2.2
1	3	396	LEU	2.2
1	J	5	MET	2.2
1	L	268	ASP	2.2
1	P	5	MET	2.2
1	Q	40	SER	2.2
1	U	9	SER	2.2
1	V	4	SER	2.2
1	D	334	ILE	2.2
1	X	442	ILE	2.2
1	Z	457	VAL	2.2
1	Y	196	PHE	2.2
1	1	307	PHE	2.2
1	X	122	ALA	2.1
1	Y	36	ALA	2.1
1	P	291	CYS	2.1
1	E	41	LEU	2.1
1	M	365	LEU	2.1
1	Y	10	LEU	2.1
1	1	408	LEU	2.1
1	M	360	GLY	2.1
1	V	391	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	262	ALA	2.1
1	R	36	ALA	2.1
1	U	28	ALA	2.1
1	Z	166	ALA	2.1
1	1	58	ALA	2.1
1	S	429	TRP	2.1
1	T	257	GLU	2.1
1	D	322	ARG	2.1
1	1	398	ARG	2.1
1	T	317	LYS	2.1
1	U	8	PRO	2.1
1	2	361	LYS	2.1
1	L	291	CYS	2.1
1	V	357	MET	2.1
1	2	365	LEU	2.1
1	Z	461	GLY	2.1
1	Z	212	ILE	2.1
1	5	378	VAL	2.1
1	M	390	PHE	2.1
1	T	50	ALA	2.1
1	X	153	ALA	2.1
1	K	429	TRP	2.1
1	L	5	MET	2.1
1	I	396	LEU	2.1
1	X	393	LEU	2.1
1	2	356	LEU	2.1
1	Y	206	GLY	2.1
1	1	368	GLY	2.1
1	U	212	ILE	2.1
1	1	381	ASP	2.1
1	H	312	ALA	2.1
1	H	316	SER	2.1
1	I	409	ALA	2.1
1	Z	4	SER	2.1
1	N	429	TRP	2.1
1	N	5	MET	2.1
1	D	375	LEU	2.1
1	U	446	LEU	2.1
1	Z	10	LEU	2.1
1	X	291	CYS	2.1
1	X	463	GLY	2.1
1	T	346	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	484	VAL	2.1
1	1	342	VAL	2.1
1	1	264	PHE	2.1
1	X	429	TRP	2.0
1	D	358	THR	2.0
1	Y	329	THR	2.0
1	2	358	THR	2.0
1	1	395	PRO	2.0
1	1	365	LEU	2.0
1	Y	331	GLY	2.0
1	Z	374	VAL	2.0
1	I	397	PHE	2.0
1	T	33	PHE	2.0
1	1	370	PHE	2.0
1	U	163	ALA	2.0
1	Y	310	LYS	2.0
1	Z	28	ALA	2.0
1	Y	332	PRO	2.0
1	Z	183	PRO	2.0
1	U	350	LEU	2.0
1	X	333	LEU	2.0
1	I	335	ASN	2.0
1	1	288	GLY	2.0
1	V	322	ARG	2.0
1	X	484	VAL	2.0
1	4	322	ARG	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.