Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 01:00 AM EDT

PDB ID	:	3NQ4
Title	:	30mer structure of Lumazine synthase from Salmonella typhimurium LT2
Authors	:	Kumar, P.; Singh, M.; Karthikeyan, S.
Deposited on	:	2010-06-29
Resolution	:	3.50 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 (i) 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 (i)) were used in the production of this report:

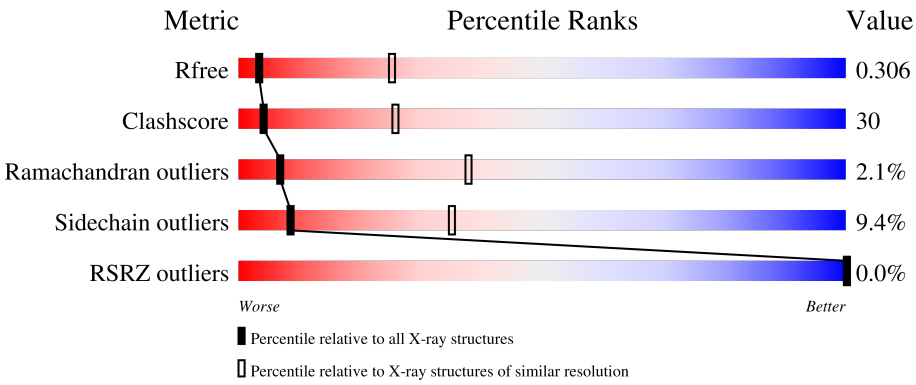
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	156	57% 37% • •
1	2	156	51% 43% 5% •
1	3	156	52% 40% 6% ••
1	4	156	52% 42% • ••
1	A	156	54% 40% • ••

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Mol	Chain	Length	Quality of chain
1	B	156	51% 43%
1	C	156	% 49% 44% 5%
1	D	156	% 52% 40% 6%
1	E	156	53% 41%
1	F	156	47% 48%
1	G	156	49% 44% 6%
1	H	156	52% 42%
1	I	156	52% 42%
1	J	156	52% 41% 6%
1	K	156	54% 39% 5%
1	L	156	55% 38% 5%
1	M	156	54% 38% 6%
1	N	156	53% 39% 6%
1	O	156	54% 40% 5%
1	P	156	46% 47% 6%
1	Q	156	51% 42% 5%
1	R	156	48% 46% 5%
1	S	156	47% 46% 6%
1	T	156	55% 38%
1	U	156	49% 44% 6%
1	V	156	46% 47% 5%
1	W	156	56% 38%
1	X	156	48% 45% 5%
1	Y	156	54% 38% 5%
1	Z	156	55% 38% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	1	157	-	-	X	-
2	SO4	F	158	-	-	X	-
2	SO4	H	157	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 33262 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 6,7-dimethyl-8-ribityllumazine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	154	1102	696	187	217	2	0	0	0
1	B	154	1102	696	187	217	2	0	0	0
1	C	154	1102	696	187	217	2	0	0	0
1	D	154	1106	699	188	217	2	0	0	0
1	E	154	1102	696	187	217	2	0	0	0
1	F	154	1102	696	187	217	2	0	0	0
1	G	154	1102	696	187	217	2	0	0	0
1	H	154	1102	696	187	217	2	0	0	0
1	I	154	1102	696	187	217	2	0	0	0
1	J	154	1102	696	187	217	2	0	0	0
1	K	154	1102	696	187	217	2	0	0	0
1	L	154	1102	696	187	217	2	0	0	0
1	M	154	1102	696	187	217	2	0	0	0
1	N	154	1102	696	187	217	2	0	0	0
1	O	154	1102	696	187	217	2	0	0	0
1	P	154	1099	695	187	215	2	0	0	0

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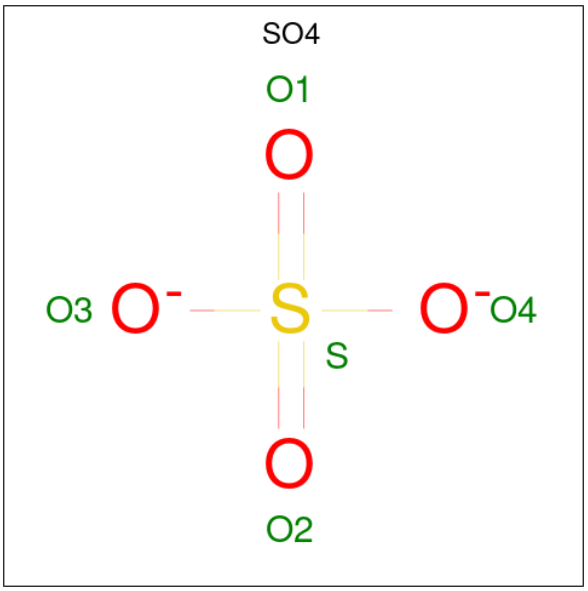
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	R	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	S	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	T	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	U	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	V	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	W	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	X	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	Y	154	1099	695	187	215	2	0	0	0
			Total	C	N	O	S			
1	Z	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	1	154	1106	699	188	217	2	0	0	0
			Total	C	N	O	S			
1	2	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	3	154	1102	696	187	217	2	0	0	0
			Total	C	N	O	S			
1	4	154	1102	696	187	217	2	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	J	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	K	1	5	4	1	0	0
			Total	O	S		
2	L	1	5	4	1	0	0
			Total	O	S		
2	L	1	5	4	1	0	0
			Total	O	S		
2	M	1	5	4	1	0	0
			Total	O	S		
2	M	1	5	4	1	0	0
			Total	O	S		
2	M	1	5	4	1	0	0
			Total	O	S		
2	N	1	5	4	1	0	0
			Total	O	S		
2	P	1	5	4	1	0	0
			Total	O	S		
2	Q	1	5	4	1	0	0
			Total	O	S		
2	Q	1	5	4	1	0	0
			Total	O	S		
2	Q	1	5	4	1	0	0
			Total	O	S		
2	R	1	5	4	1	0	0
			Total	O	S		
2	S	1	5	4	1	0	0
			Total	O	S		
2	U	1	5	4	1	0	0
			Total	O	S		
2	V	1	5	4	1	0	0
			Total	O	S		
2	V	1	5	4	1	0	0
			Total	O	S		
2	X	1	5	4	1	0	0
			Total	O	S		
2	X	1	5	4	1	0	0
			Total	O	S		
2	Z	1	5	4	1	0	0
			Total	O	S		
2	Z	1	5	4	1	0	0
			Total	O	S		
2	1	1	5	4	1	0	0

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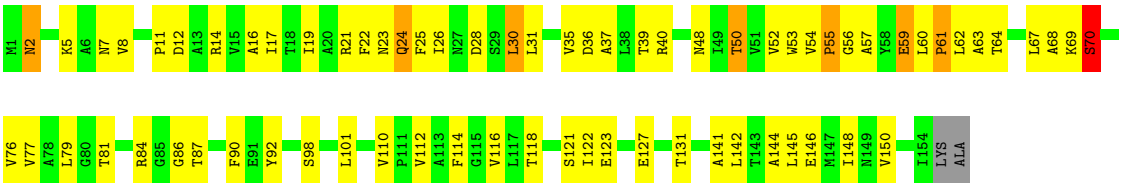
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	1	1	5	4	1	0	0
			Total	O	S		
2	2	1	5	4	1	0	0
			Total	O	S		
2	2	1	5	4	1	0	0
			Total	O	S		
2	2	1	5	4	1	0	0
			Total	O	S		
2	3	1	5	4	1	0	0

3 Residue-property plots (i)

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

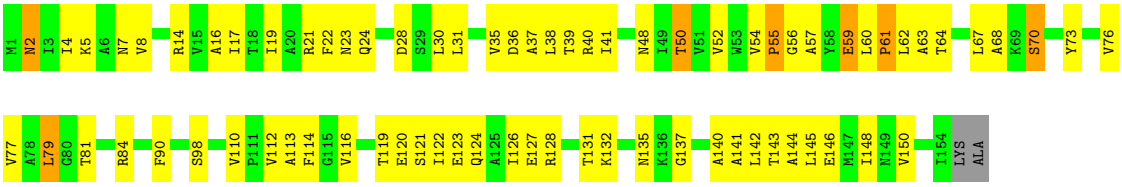
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain A:



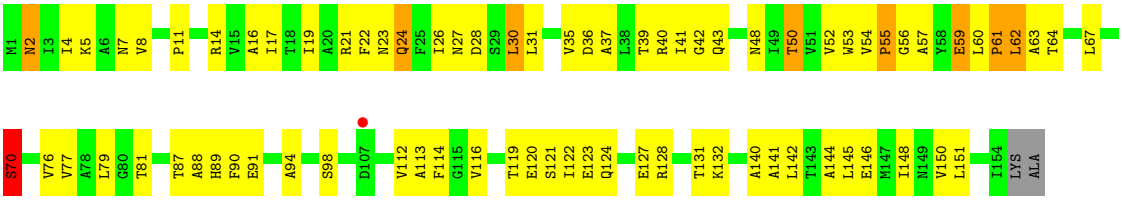
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B:



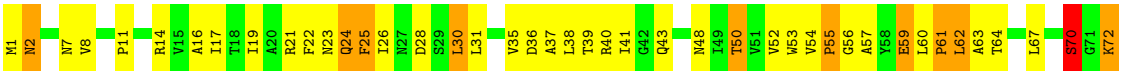
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C:



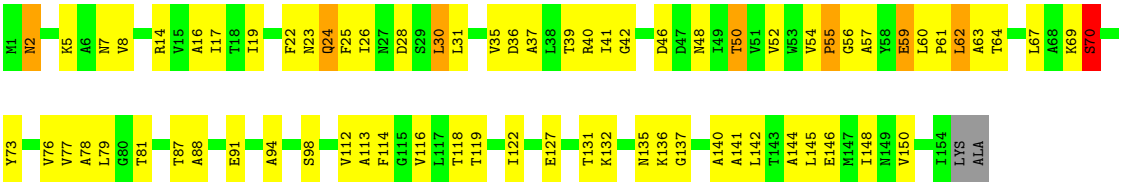
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain D:



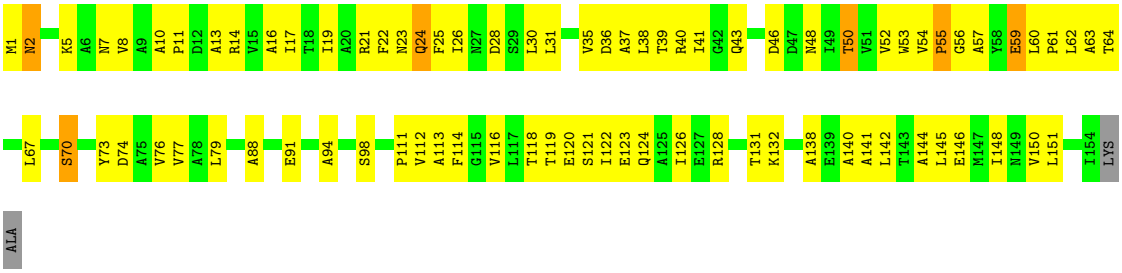
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain E:



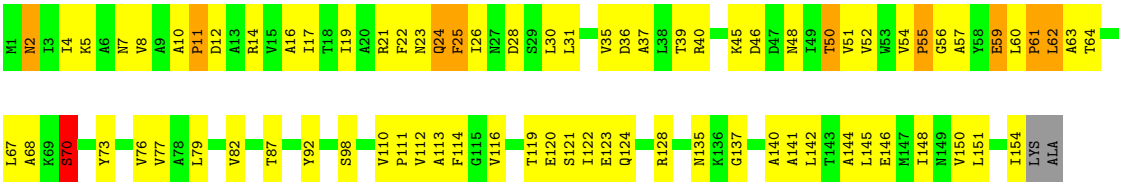
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F:



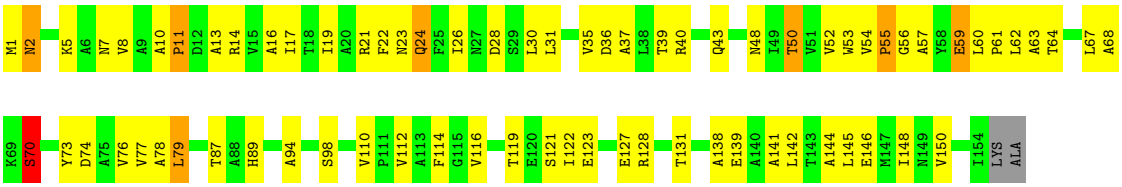
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain G:



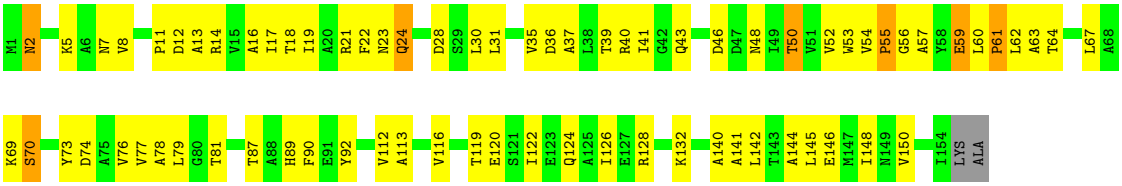
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain H:



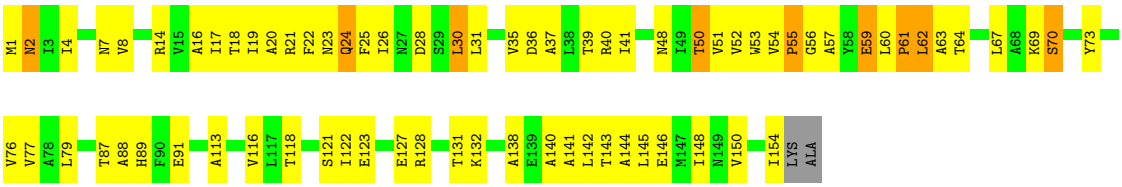
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain I:



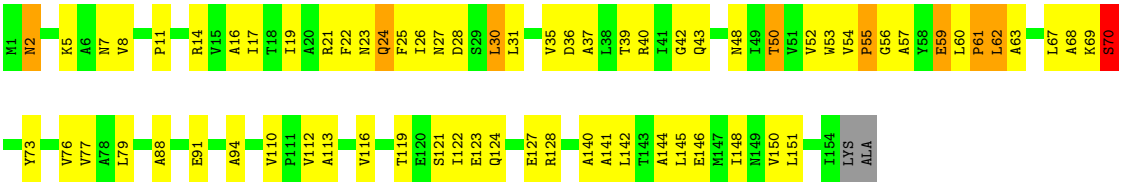
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J: 52% 41% 6% •



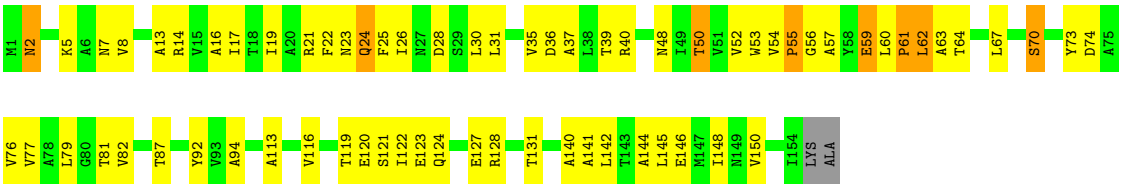
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain K: 54% 39% 5% ••



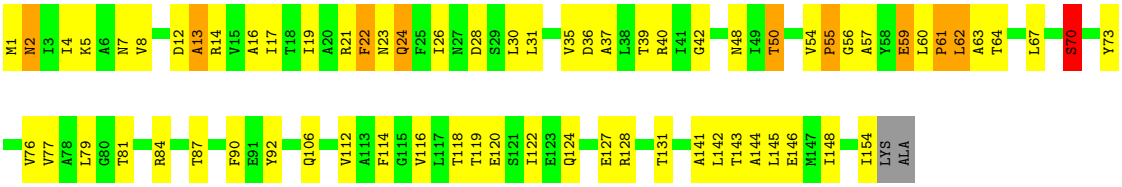
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain L: 55% 38% 5% •



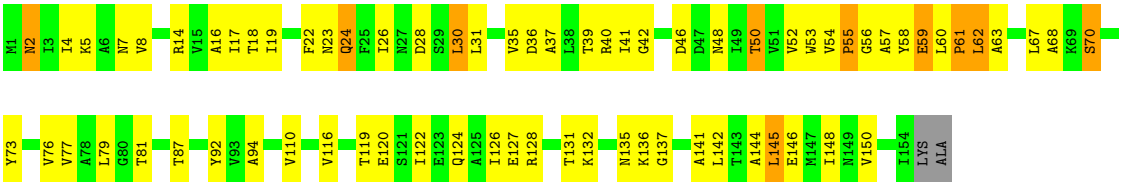
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain M: 54% 38% 6% ••



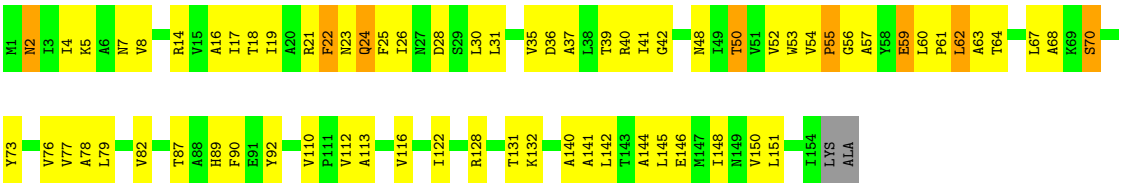
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain N: 53% 39% 6% •



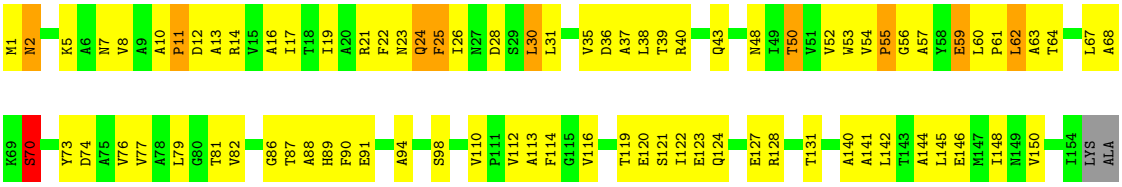
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain O: 54% 40% 5%



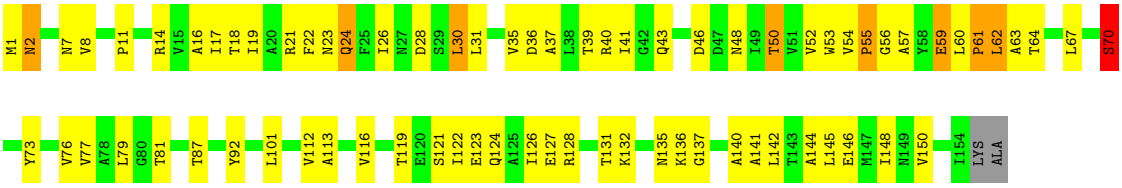
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain P: 46% 47% 6%



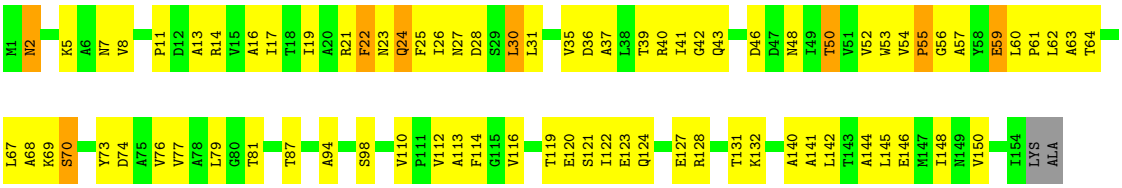
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Q: 51% 42% 5%



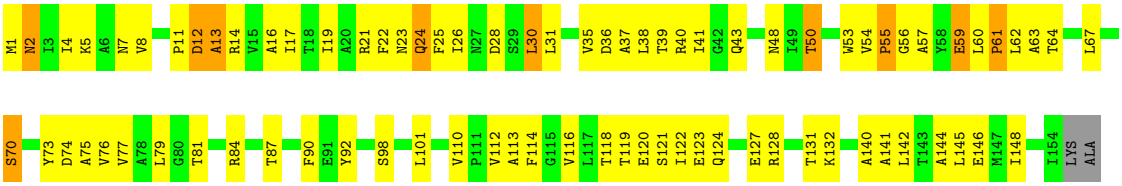
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain R: 48% 46% 5%



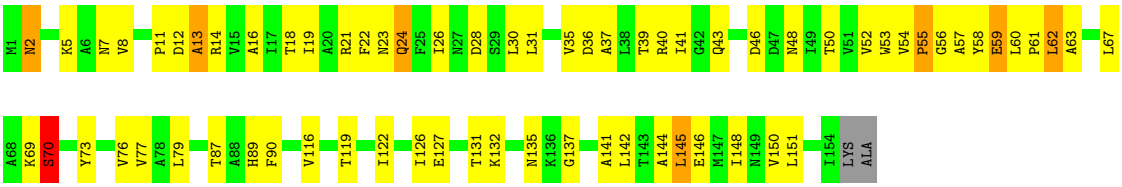
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain S: 47% 46% 6%



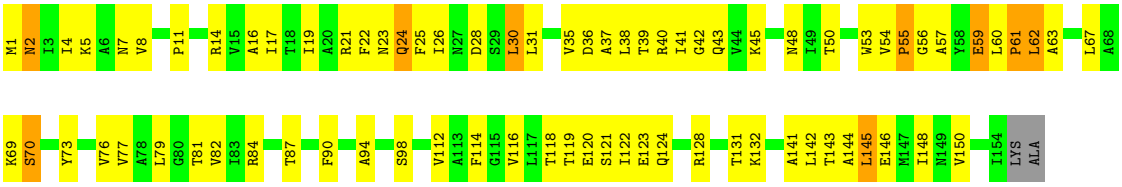
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain T:



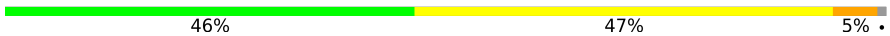
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain U:



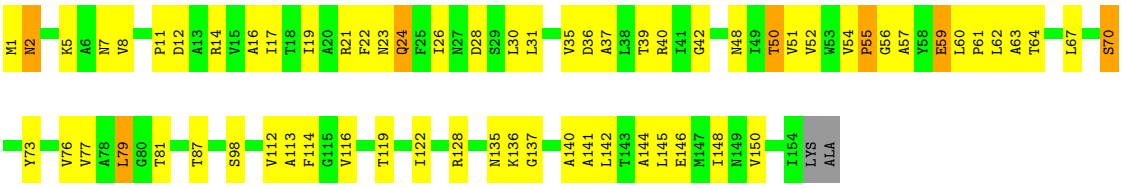
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain V:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain W:



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain X: 48% 45% 5% ••

M1 N2 K5 A6 N7 V8 P11 R14 V15 A16 I17 T18 I19 A20 R21 F22 N23 Q24 F25 I26 N27 D28 S29 L30 L31 V35 D36 A37 L38 T39 R40 I41 G42 Q43 V44 K45 D46 D47 N48 I49 T50 W53 V54 P55 G56 A57 Y58 E59 L60 P61 L62 A63 T64 L67

A68 K69 S70 Y73 V76 V77 A78 L79 V82 I83 R84 T87 A88 H89 F90 E91 A94 S98 V110 P111 V112 A113 F114 G115 V116 T119 E120 S121 I122 E123 E127 R128 T131 K132 A140 A141 L142 T143 A144 L145 E146 M147 I148 N149 V150 L151 I154 LYS

ALA

- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Y: 54% 38% 5% ••

M1 N2 K5 A6 N7 V8 R14 V15 A16 I17 T18 I19 A20 R21 F22 N23 Q24 F25 I26 N27 D28 S29 L30 L31 V35 D36 A37 L38 T39 R40 I41 K45 N48 I49 T50 V54 P55 G56 A57 Y58 E59 L60 P61 L62 A63 T64 L67 A68 K69 S70 Y73

V76 V77 A78 L79 G80 T81 V82 I83 R84 T87 A88 H89 F90 E91 Y92 V112 A113 V116 T119 I122 E127 R128 T131 K132 A138 E139 A140 A141 L142 T143 A144 L145 E146 M147 I148 N149 V150 I154 LYS ALA

- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Z: 55% 38% 5% ••

M1 N2 I3 I4 K5 A6 N7 V8 R14 V15 A16 I17 T18 I19 A20 R21 F22 N23 Q24 F25 I26 N27 D28 S29 L30 L31 A37 L38 T39 R40 N48 I49 T50 W53 V54 P55 G56 A57 Y58 E59 L60 P61 L62 A63 T64 L67 A68 K69 S70 Y73 V76 V77 A78

L79 G80 T81 T87 A88 E91 Y92 S98 V110 P111 V112 A113 F114 G115 V116 I122 E127 R128 T131 N135 K136 G137 A140 A141 L142 T143 A144 L145 E146 M147 I148 N149 V150 I154 LYS ALA

- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 1: 57% 37% • •

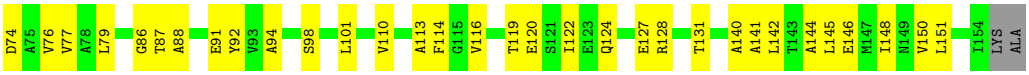
M1 N2 I3 I4 K5 A6 N7 V8 P11 R14 V15 A16 I17 T18 I19 A20 R21 F22 N23 Q24 F25 I26 N27 D28 S29 L30 L31 V35 D36 A37 L38 T39 R40 K45 D46 D47 N48 I49 T50 V51 V52 W53 V54 P55 G56 A57 Y58 E59 L60 P61 L62 A63 T64 L67

S70 V76 V77 A78 L79 G85 G86 T87 A94 S98 V112 A113 F114 G115 V116 T119 I122 E127 R128 T131 A141 L142 T143 A144 L145 E146 M147 I148 N149 V150 I154 LYS ALA

- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

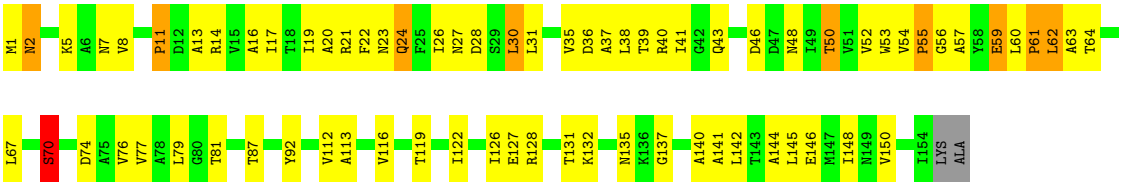
Chain 2: 51% 43% 5% •

M1 N2 K5 A6 N7 V8 P11 D12 A13 R14 V15 A16 I17 T18 I19 A20 R21 F22 N23 Q24 D28 S29 L30 L31 V35 D36 A37 L38 T39 R40 Q43 N48 I49 T50 V51 V52 W53 V54 P55 G56 A57 Y58 E59 L60 P61 L62 A63 L67 A68 K69 S70 Y73



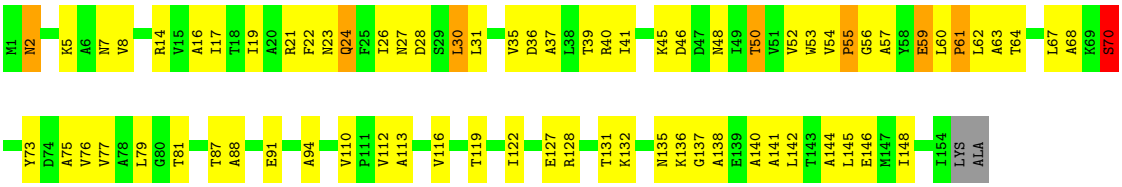
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 3:



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.43Å 157.49Å 202.79Å 90.00° 91.58° 90.00°	Depositor
Resolution (Å)	78.75 – 3.50 78.75 – 3.50	Depositor EDS
% Data completeness (in resolution range)	66.0 (78.75-3.50) 62.2 (78.75-3.50)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.255 , 0.299 0.265 , 0.306	Depositor DCC
R_{free} test set	1139 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	33262	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.40	0/1119	0.53	0/1524
1	2	0.41	0/1115	0.53	0/1520
1	3	0.42	0/1115	0.53	0/1520
1	4	0.43	0/1115	0.54	0/1520
1	A	0.40	0/1115	0.53	0/1520
1	B	0.41	0/1115	0.53	0/1520
1	C	0.43	0/1115	0.54	0/1520
1	D	0.40	0/1119	0.54	0/1524
1	E	0.45	0/1115	0.54	0/1520
1	F	0.42	0/1115	0.54	0/1520
1	G	0.42	0/1115	0.55	0/1520
1	H	0.41	0/1115	0.54	0/1520
1	I	0.43	0/1115	0.52	0/1520
1	J	0.41	0/1115	0.55	0/1520
1	K	0.43	0/1115	0.54	0/1520
1	L	0.41	0/1115	0.53	0/1520
1	M	0.42	0/1115	0.54	0/1520
1	N	0.44	0/1115	0.55	0/1520
1	O	0.41	0/1115	0.54	0/1520
1	P	0.41	0/1112	0.54	0/1516
1	Q	0.40	0/1115	0.54	0/1520
1	R	0.43	0/1115	0.54	0/1520
1	S	0.41	0/1115	0.53	0/1520
1	T	0.41	0/1115	0.53	0/1520
1	U	0.42	0/1115	0.54	0/1520
1	V	0.40	0/1115	0.53	0/1520
1	W	0.40	0/1115	0.52	0/1520
1	X	0.43	0/1115	0.53	0/1520
1	Y	0.40	0/1112	0.54	0/1516
1	Z	0.42	0/1115	0.53	0/1520
All	All	0.42	0/33452	0.54	0/45600

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1106	0	1126	63	0
1	2	1102	0	1115	74	0
1	3	1102	0	1115	73	0
1	4	1102	0	1115	80	0
1	A	1102	0	1115	64	0
1	B	1102	0	1115	70	0
1	C	1102	0	1115	83	0
1	D	1106	0	1126	85	0
1	E	1102	0	1115	75	0
1	F	1102	0	1115	92	0
1	G	1102	0	1115	73	0
1	H	1102	0	1115	75	0
1	I	1102	0	1115	73	0
1	J	1102	0	1115	84	0
1	K	1102	0	1115	71	0
1	L	1102	0	1115	68	0
1	M	1102	0	1115	72	0
1	N	1102	0	1115	83	0
1	O	1102	0	1115	74	0
1	P	1099	0	1113	78	0
1	Q	1102	0	1115	77	0
1	R	1102	0	1115	83	0
1	S	1102	0	1115	87	0
1	T	1102	0	1115	70	0
1	U	1102	0	1115	86	0
1	V	1102	0	1115	80	0
1	W	1102	0	1115	56	0
1	X	1102	0	1115	76	0
1	Y	1099	0	1113	78	0
1	Z	1102	0	1115	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	10	0	0	3	0
2	2	15	0	0	1	0
2	3	5	0	0	0	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
2	E	5	0	0	0	0
2	F	10	0	0	3	0
2	G	5	0	0	0	0
2	H	15	0	0	4	0
2	J	5	0	0	1	0
2	K	5	0	0	0	0
2	L	10	0	0	0	0
2	M	15	0	0	0	0
2	N	5	0	0	0	0
2	P	5	0	0	1	0
2	Q	15	0	0	1	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	U	5	0	0	0	0
2	V	10	0	0	0	0
2	X	10	0	0	0	0
2	Z	10	0	0	0	0
All	All	33262	0	33468	1980	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 30.

All (1980) 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:P:11:PRO:HB3	1:P:43:GLN:HB3	1.41	1.03
1:F:11:PRO:HB3	1:F:43:GLN:HB3	1.40	1.01
1:S:7:ASN:ND2	1:Y:41:ILE:HA	1.77	0.99
1:P:122:ILE:HD12	1:P:122:ILE:H	1.28	0.98
1:S:41:ILE:HA	1:Y:7:ASN:ND2	1.82	0.95
1:Q:122:ILE:H	1:Q:122:ILE:HD12	1.33	0.93
1:Y:122:ILE:H	1:Y:122:ILE:HD12	1.34	0.92
1:J:122:ILE:H	1:J:122:ILE:HD12	1.33	0.92
1:X:122:ILE:HD12	1:X:122:ILE:H	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:122:ILE:H	1:N:122:ILE:HD12	1.35	0.91
1:U:122:ILE:H	1:U:122:ILE:HD12	1.36	0.91
1:H:122:ILE:HD12	1:H:122:ILE:H	1.33	0.91
1:V:122:ILE:H	1:V:122:ILE:HD12	1.36	0.91
1:M:122:ILE:H	1:M:122:ILE:HD12	1.36	0.91
1:1:122:ILE:H	1:1:122:ILE:HD12	1.34	0.91
1:L:122:ILE:H	1:L:122:ILE:HD12	1.35	0.90
1:C:122:ILE:H	1:C:122:ILE:HD12	1.35	0.90
1:I:55:PRO:HG2	1:I:59:GLU:HG3	1.53	0.90
1:E:122:ILE:H	1:E:122:ILE:HD12	1.38	0.89
1:4:122:ILE:H	1:4:122:ILE:HD12	1.37	0.89
1:S:122:ILE:HD12	1:S:122:ILE:H	1.37	0.89
1:G:122:ILE:H	1:G:122:ILE:HD12	1.36	0.89
1:K:122:ILE:HD12	1:K:122:ILE:H	1.35	0.89
1:D:41:ILE:HA	1:J:7:ASN:ND2	1.89	0.88
1:I:122:ILE:H	1:I:122:ILE:HD12	1.38	0.88
1:R:122:ILE:H	1:R:122:ILE:HD12	1.40	0.87
1:B:122:ILE:H	1:B:122:ILE:HD12	1.41	0.86
1:T:122:ILE:H	1:T:122:ILE:HD12	1.38	0.86
1:F:122:ILE:H	1:F:122:ILE:HD12	1.38	0.86
1:A:122:ILE:H	1:A:122:ILE:HD12	1.39	0.86
1:O:55:PRO:HG2	1:O:59:GLU:HG3	1.57	0.85
1:W:122:ILE:H	1:W:122:ILE:HD12	1.40	0.85
1:Z:122:ILE:H	1:Z:122:ILE:HD12	1.40	0.85
1:A:55:PRO:HG2	1:A:59:GLU:HG3	1.58	0.84
1:L:55:PRO:HG2	1:L:59:GLU:HG3	1.59	0.84
1:W:55:PRO:HG2	1:W:59:GLU:HG3	1.59	0.84
1:B:55:PRO:HG2	1:B:59:GLU:HG3	1.58	0.84
1:3:55:PRO:HG2	1:3:59:GLU:HG3	1.58	0.83
1:Y:55:PRO:HG2	1:Y:59:GLU:HG3	1.60	0.83
1:X:55:PRO:HG2	1:X:59:GLU:HG3	1.61	0.83
1:H:13:ALA:HB1	1:H:74:ASP:OD2	1.79	0.83
1:M:55:PRO:HG2	1:M:59:GLU:HG3	1.61	0.83
1:O:122:ILE:H	1:O:122:ILE:HD12	1.43	0.83
1:3:11:PRO:HB3	1:3:43:GLN:HB3	1.61	0.83
1:2:122:ILE:H	1:2:122:ILE:HD12	1.41	0.82
1:3:122:ILE:H	1:3:122:ILE:HD12	1.43	0.82
1:D:55:PRO:HG2	1:D:59:GLU:HG3	1.61	0.82
1:P:55:PRO:HG2	1:P:59:GLU:HG3	1.62	0.82
1:H:13:ALA:HB1	1:H:74:ASP:CG	2.01	0.81
1:S:55:PRO:HG2	1:S:59:GLU:HG3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:55:PRO:HG2	1:1:59:GLU:HG3	1.63	0.81
1:T:55:PRO:HG2	1:T:59:GLU:HG3	1.60	0.81
1:4:55:PRO:HG2	1:4:59:GLU:HG3	1.61	0.81
1:R:55:PRO:HG2	1:R:59:GLU:HG3	1.62	0.81
1:J:55:PRO:HG2	1:J:59:GLU:HG3	1.63	0.80
1:H:55:PRO:HG2	1:H:59:GLU:HG3	1.64	0.80
1:F:55:PRO:HG2	1:F:59:GLU:HG3	1.64	0.80
1:K:55:PRO:HG2	1:K:59:GLU:HG3	1.62	0.79
1:Q:55:PRO:HG2	1:Q:59:GLU:HG3	1.65	0.79
1:Y:122:ILE:HD11	1:4:132:LYS:HD2	1.65	0.79
1:D:7:ASN:ND2	1:J:41:ILE:HA	1.97	0.79
1:D:122:ILE:H	1:D:122:ILE:HD12	1.45	0.79
1:2:55:PRO:HG2	1:2:59:GLU:HG3	1.64	0.79
1:K:11:PRO:HB3	1:K:43:GLN:HB3	1.65	0.78
1:S:7:ASN:HD22	1:Y:41:ILE:HD13	1.48	0.78
1:U:55:PRO:HG2	1:U:59:GLU:HG3	1.65	0.78
1:V:55:PRO:HG2	1:V:59:GLU:HG3	1.66	0.78
1:K:50:THR:HG22	1:O:2:ASN:HD21	1.49	0.77
1:E:55:PRO:HG2	1:E:59:GLU:HG3	1.63	0.77
1:P:11:PRO:CB	1:P:43:GLN:HB3	2.14	0.77
1:D:41:ILE:HD13	1:J:7:ASN:HD22	1.50	0.77
1:Z:55:PRO:HG2	1:Z:59:GLU:HG3	1.64	0.77
1:N:55:PRO:HG2	1:N:59:GLU:HG3	1.67	0.77
1:C:55:PRO:HG2	1:C:59:GLU:HG3	1.67	0.76
1:F:7:ASN:ND2	1:Q:41:ILE:HA	2.02	0.74
1:F:7:ASN:HD22	1:Q:41:ILE:HD13	1.52	0.74
1:C:132:LYS:HD2	1:S:122:ILE:HD11	1.70	0.74
1:P:50:THR:HG22	1:T:2:ASN:HD21	1.52	0.74
1:H:56:GLY:O	1:H:59:GLU:HG2	1.88	0.73
1:S:11:PRO:HG3	1:S:43:GLN:HB3	1.68	0.73
1:D:2:ASN:H	1:D:2:ASN:HD22	1.37	0.73
1:C:11:PRO:HB3	1:C:43:GLN:HB3	1.71	0.73
1:E:56:GLY:O	1:E:59:GLU:HG2	1.87	0.73
1:M:56:GLY:O	1:M:59:GLU:HG2	1.89	0.73
1:I:7:ASN:ND2	1:O:41:ILE:HA	2.03	0.72
1:U:2:ASN:H	1:U:2:ASN:HD22	1.37	0.72
1:I:56:GLY:O	1:I:59:GLU:HG2	1.90	0.72
1:E:16:ALA:HB1	1:E:67:LEU:HD13	1.69	0.72
1:D:122:ILE:HD11	1:R:132:LYS:HD2	1.72	0.72
1:R:2:ASN:H	1:R:2:ASN:HD22	1.36	0.72
1:G:55:PRO:HG2	1:G:59:GLU:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:ASN:H	1:M:2:ASN:HD22	1.37	0.72
1:A:16:ALA:HB1	1:A:67:LEU:HD13	1.72	0.72
1:1:77:VAL:HG12	1:1:79:LEU:HD13	1.72	0.71
1:X:7:ASN:HD22	1:4:41:ILE:HD13	1.55	0.71
1:2:56:GLY:O	1:2:59:GLU:HG2	1.90	0.71
1:I:7:ASN:HD22	1:O:41:ILE:HD13	1.53	0.71
1:K:2:ASN:HD22	1:K:2:ASN:H	1.39	0.71
1:A:122:ILE:HD11	1:N:132:LYS:HD2	1.73	0.71
1:S:7:ASN:HD22	1:Y:41:ILE:HA	1.54	0.71
1:T:7:ASN:HD22	1:3:41:ILE:HD13	1.54	0.71
1:K:16:ALA:HB1	1:K:67:LEU:HD13	1.72	0.71
1:O:77:VAL:HG12	1:O:79:LEU:HD13	1.73	0.71
1:S:16:ALA:HB1	1:S:67:LEU:HD13	1.73	0.70
1:B:41:ILE:HA	1:U:7:ASN:ND2	2.06	0.70
1:D:16:ALA:HB1	1:D:67:LEU:HD13	1.71	0.70
1:K:141:ALA:O	1:K:144:ALA:HB3	1.91	0.70
1:T:7:ASN:ND2	1:3:41:ILE:HA	2.06	0.70
1:S:2:ASN:HD22	1:S:2:ASN:H	1.40	0.70
1:A:77:VAL:HG12	1:A:79:LEU:HD13	1.74	0.70
1:3:2:ASN:HD22	1:3:2:ASN:H	1.40	0.70
1:B:2:ASN:H	1:B:2:ASN:HD22	1.39	0.69
1:E:7:ASN:ND2	1:N:41:ILE:HA	2.07	0.69
1:N:16:ALA:HB1	1:N:67:LEU:HD13	1.74	0.69
1:L:2:ASN:H	1:L:2:ASN:HD22	1.38	0.69
1:C:122:ILE:HD11	1:U:132:LYS:HD2	1.75	0.69
1:I:2:ASN:HD22	1:I:2:ASN:H	1.41	0.69
1:M:2:ASN:HD21	1:N:50:THR:HG22	1.57	0.69
1:T:41:ILE:HA	1:3:7:ASN:ND2	2.08	0.69
1:E:41:ILE:HA	1:N:7:ASN:ND2	2.08	0.69
1:P:2:ASN:HD22	1:P:2:ASN:H	1.40	0.69
1:V:2:ASN:HD22	1:V:2:ASN:H	1.41	0.69
1:4:16:ALA:HB1	1:4:67:LEU:HD13	1.73	0.69
1:F:2:ASN:HD22	1:F:2:ASN:H	1.41	0.69
1:G:2:ASN:H	1:G:2:ASN:HD22	1.40	0.69
1:G:2:ASN:HD21	1:H:50:THR:HG22	1.58	0.69
1:G:56:GLY:O	1:G:59:GLU:HG2	1.92	0.69
1:T:77:VAL:HG12	1:T:79:LEU:HD13	1.75	0.68
1:Z:2:ASN:H	1:Z:2:ASN:HD22	1.41	0.68
1:C:2:ASN:HD22	1:C:2:ASN:H	1.39	0.68
1:L:16:ALA:HB1	1:L:67:LEU:HD13	1.74	0.68
1:S:41:ILE:HA	1:Y:7:ASN:HD22	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:7:ASN:ND2	1:4:41:ILE:HA	2.08	0.68
1:2:77:VAL:HG12	1:2:79:LEU:HD13	1.75	0.68
1:Q:2:ASN:HD22	1:Q:2:ASN:H	1.41	0.68
1:G:77:VAL:HG12	1:G:79:LEU:HD13	1.76	0.68
1:B:7:ASN:HD22	1:U:41:ILE:HD13	1.59	0.68
1:I:41:ILE:HA	1:O:7:ASN:ND2	2.09	0.68
1:Y:7:ASN:ND2	1:Y:8:VAL:H	1.91	0.68
1:Y:77:VAL:HG12	1:Y:79:LEU:HD13	1.75	0.68
1:N:56:GLY:O	1:N:59:GLU:HG2	1.93	0.68
1:1:2:ASN:H	1:1:2:ASN:HD22	1.41	0.68
1:T:2:ASN:H	1:T:2:ASN:HD22	1.41	0.68
1:W:16:ALA:HB1	1:W:67:LEU:HD13	1.76	0.68
2:1:158:SO4:O2	1:2:86:GLY:HA3	1.93	0.68
1:E:2:ASN:H	1:E:2:ASN:HD22	1.42	0.68
1:S:132:LYS:HD2	1:U:122:ILE:HD11	1.75	0.68
1:V:77:VAL:HG12	1:V:79:LEU:HD13	1.76	0.68
1:W:56:GLY:O	1:W:59:GLU:HG2	1.94	0.68
1:H:2:ASN:HD22	1:H:2:ASN:H	1.39	0.67
1:J:2:ASN:H	1:J:2:ASN:HD22	1.41	0.67
1:U:2:ASN:HD21	1:V:50:THR:HG22	1.59	0.67
1:C:41:ILE:HD13	1:R:7:ASN:HD22	1.59	0.67
1:E:132:LYS:HD2	1:O:122:ILE:HD11	1.77	0.67
1:N:2:ASN:HD22	1:N:2:ASN:H	1.43	0.67
1:P:16:ALA:HB1	1:P:67:LEU:HD13	1.77	0.67
1:Y:2:ASN:HD22	1:Y:2:ASN:H	1.42	0.67
1:B:67:LEU:O	1:B:70:SER:HB3	1.95	0.67
1:J:67:LEU:O	1:J:70:SER:HB3	1.94	0.67
1:J:77:VAL:HG12	1:J:79:LEU:HD13	1.76	0.67
1:Z:67:LEU:O	1:Z:70:SER:HB3	1.94	0.67
1:3:16:ALA:HB1	1:3:67:LEU:HD13	1.74	0.67
1:C:7:ASN:ND2	1:R:41:ILE:HA	2.10	0.67
1:3:7:ASN:ND2	1:3:8:VAL:H	1.92	0.67
1:B:7:ASN:ND2	1:U:41:ILE:HA	2.10	0.67
1:O:2:ASN:H	1:O:2:ASN:HD22	1.42	0.67
1:P:122:ILE:HD11	1:3:132:LYS:HD2	1.76	0.67
1:M:7:ASN:ND2	1:M:8:VAL:H	1.91	0.67
1:A:2:ASN:H	1:A:2:ASN:HD22	1.42	0.66
1:D:131:THR:HA	1:F:23:ASN:HA	1.76	0.66
1:N:141:ALA:O	1:N:144:ALA:HB3	1.95	0.66
1:P:7:ASN:ND2	1:P:8:VAL:H	1.94	0.66
1:R:16:ALA:HB1	1:R:67:LEU:HD13	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2:ASN:HD22	1:X:2:ASN:H	1.42	0.66
1:1:85:GLY:HA3	2:1:157:SO4:O4	1.96	0.66
1:4:56:GLY:O	1:4:59:GLU:HG2	1.96	0.66
1:U:21:ARG:HH22	1:Y:5:LYS:HD3	1.60	0.66
1:F:13:ALA:HB1	1:F:74:ASP:CG	2.16	0.66
1:M:16:ALA:HB1	1:M:67:LEU:HD13	1.77	0.66
1:B:56:GLY:O	1:B:59:GLU:HG2	1.95	0.66
1:F:56:GLY:O	1:F:59:GLU:HG2	1.96	0.66
1:N:77:VAL:HG12	1:N:79:LEU:HD13	1.75	0.66
1:4:77:VAL:HG12	1:4:79:LEU:HD13	1.77	0.66
1:K:77:VAL:HG12	1:K:79:LEU:HD13	1.77	0.66
1:1:56:GLY:O	1:1:59:GLU:HG2	1.94	0.66
1:3:77:VAL:HG12	1:3:79:LEU:HD13	1.78	0.66
1:B:141:ALA:O	1:B:144:ALA:HB3	1.96	0.66
1:M:141:ALA:O	1:M:144:ALA:HB3	1.96	0.66
1:Q:56:GLY:O	1:Q:59:GLU:HG2	1.96	0.66
1:A:87:THR:HB	1:E:119:THR:HA	1.78	0.65
1:D:56:GLY:O	1:D:59:GLU:HG2	1.96	0.65
1:I:13:ALA:HB1	1:I:74:ASP:HB2	1.79	0.65
1:I:132:LYS:HD2	1:K:122:ILE:HD11	1.77	0.65
1:E:67:LEU:O	1:E:70:SER:HB3	1.95	0.65
1:Q:77:VAL:HG12	1:Q:79:LEU:HD13	1.77	0.65
1:T:7:ASN:ND2	1:T:8:VAL:H	1.93	0.65
1:B:41:ILE:HD13	1:U:7:ASN:HD22	1.61	0.65
1:B:145:LEU:HA	1:B:148:ILE:HD12	1.79	0.65
1:C:16:ALA:HB1	1:C:67:LEU:HD13	1.78	0.65
1:G:16:ALA:HB1	1:G:67:LEU:HD13	1.77	0.65
1:Z:2:ASN:HD21	1:1:50:THR:HG22	1.60	0.65
1:Q:16:ALA:HB1	1:Q:67:LEU:HD13	1.79	0.65
1:Z:16:ALA:HB1	1:Z:67:LEU:HD13	1.78	0.65
1:F:7:ASN:ND2	1:F:8:VAL:H	1.94	0.65
1:L:56:GLY:O	1:L:59:GLU:HG2	1.97	0.65
1:Z:56:GLY:O	1:Z:59:GLU:HG2	1.96	0.65
1:1:16:ALA:HB1	1:1:67:LEU:HD13	1.78	0.65
1:O:16:ALA:HB1	1:O:67:LEU:HD13	1.77	0.65
1:Y:145:LEU:HA	1:Y:148:ILE:HD12	1.78	0.65
1:O:67:LEU:O	1:O:70:SER:HB3	1.97	0.65
1:T:16:ALA:HB1	1:T:67:LEU:HD13	1.79	0.65
1:X:16:ALA:HB1	1:X:67:LEU:HD13	1.79	0.65
1:3:56:GLY:O	1:3:59:GLU:HG2	1.96	0.65
1:F:132:LYS:HD2	1:R:122:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:16:ALA:HB1	1:2:67:LEU:HD13	1.77	0.65
1:4:2:ASN:H	1:4:2:ASN:HD22	1.43	0.65
1:D:11:PRO:HA	1:D:43:GLN:O	1.96	0.64
1:I:5:LYS:HD3	1:J:21:ARG:HH22	1.62	0.64
1:K:7:ASN:ND2	1:K:8:VAL:H	1.95	0.64
1:A:7:ASN:ND2	1:A:8:VAL:H	1.95	0.64
1:C:77:VAL:HG12	1:C:79:LEU:HD13	1.78	0.64
1:R:5:LYS:HD3	1:S:21:ARG:HH22	1.62	0.64
1:Y:56:GLY:O	1:Y:59:GLU:HG2	1.96	0.64
1:A:11:PRO:HG2	1:A:12:ASP:OD2	1.96	0.64
1:C:41:ILE:HA	1:R:7:ASN:ND2	2.13	0.64
1:3:67:LEU:O	1:3:70:SER:HB3	1.98	0.64
1:R:7:ASN:ND2	1:R:8:VAL:H	1.95	0.64
1:2:2:ASN:H	1:2:2:ASN:HD22	1.44	0.64
1:B:16:ALA:HB1	1:B:67:LEU:HD13	1.79	0.64
1:F:50:THR:HG22	1:J:2:ASN:HD21	1.61	0.64
1:V:56:GLY:O	1:V:59:GLU:HG2	1.98	0.64
1:M:77:VAL:HG12	1:M:79:LEU:HD13	1.79	0.64
1:V:13:ALA:HB1	1:V:74:ASP:CG	2.19	0.64
1:2:22:PHE:O	1:2:23:ASN:HB2	1.97	0.64
1:I:16:ALA:HB1	1:I:67:LEU:HD13	1.78	0.64
1:I:77:VAL:HG12	1:I:79:LEU:HD13	1.80	0.64
1:M:67:LEU:O	1:M:70:SER:HB3	1.98	0.64
1:R:56:GLY:O	1:R:59:GLU:HG2	1.98	0.64
1:F:41:ILE:HA	1:Q:7:ASN:ND2	2.13	0.64
1:S:7:ASN:ND2	1:S:8:VAL:H	1.95	0.64
1:C:7:ASN:ND2	1:C:8:VAL:H	1.96	0.63
1:C:56:GLY:O	1:C:59:GLU:HG2	1.97	0.63
1:F:13:ALA:HB1	1:F:74:ASP:OD2	1.98	0.63
1:P:56:GLY:O	1:P:59:GLU:HG2	1.98	0.63
1:W:2:ASN:H	1:W:2:ASN:HD22	1.46	0.63
1:W:67:LEU:O	1:W:70:SER:HB3	1.97	0.63
1:H:77:VAL:HG12	1:H:79:LEU:HD13	1.80	0.63
1:O:56:GLY:O	1:O:59:GLU:HG2	1.98	0.63
1:O:141:ALA:O	1:O:144:ALA:HB3	1.99	0.63
1:F:77:VAL:HG12	1:F:79:LEU:HD13	1.79	0.63
1:L:7:ASN:ND2	1:L:8:VAL:H	1.95	0.63
1:X:56:GLY:O	1:X:59:GLU:HG2	1.98	0.63
1:H:67:LEU:O	1:H:70:SER:HB3	1.99	0.63
1:Z:145:LEU:HA	1:Z:148:ILE:HD12	1.81	0.63
1:F:7:ASN:CG	1:F:8:VAL:H	2.01	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:ASN:CG	1:F:8:VAL:N	2.52	0.62
1:P:77:VAL:HG12	1:P:79:LEU:HD13	1.79	0.62
1:R:77:VAL:HG12	1:R:79:LEU:HD13	1.79	0.62
1:X:145:LEU:HA	1:X:148:ILE:HD12	1.81	0.62
1:U:56:GLY:O	1:U:59:GLU:HG2	1.99	0.62
1:G:10:ALA:N	1:G:11:PRO:CD	2.61	0.62
1:X:141:ALA:O	1:X:144:ALA:HB3	1.99	0.62
1:4:141:ALA:O	1:4:144:ALA:HB3	1.99	0.62
1:L:77:VAL:HG12	1:L:79:LEU:HD13	1.81	0.62
1:O:7:ASN:ND2	1:O:8:VAL:H	1.96	0.62
1:E:41:ILE:HD13	1:N:7:ASN:HD22	1.65	0.62
1:O:145:LEU:HA	1:O:148:ILE:HD12	1.81	0.62
1:X:119:THR:HA	1:Y:87:THR:HB	1.79	0.62
1:Y:16:ALA:HB1	1:Y:67:LEU:HD13	1.80	0.62
1:4:37:ALA:HB1	1:4:142:LEU:HD21	1.81	0.62
1:K:122:ILE:HD12	1:K:122:ILE:N	2.13	0.62
1:C:145:LEU:HA	1:C:148:ILE:HD12	1.82	0.62
1:L:7:ASN:CG	1:L:8:VAL:H	2.03	0.62
1:U:54:VAL:HG11	1:U:63:ALA:HB2	1.81	0.62
1:F:16:ALA:HB1	1:F:67:LEU:HD13	1.81	0.61
1:M:7:ASN:CG	1:M:8:VAL:N	2.52	0.61
1:P:145:LEU:HA	1:P:148:ILE:HD12	1.82	0.61
1:Q:67:LEU:O	1:Q:70:SER:HB3	1.99	0.61
1:S:77:VAL:HG12	1:S:79:LEU:HD13	1.81	0.61
1:M:7:ASN:CG	1:M:8:VAL:H	2.04	0.61
1:1:67:LEU:O	1:1:70:SER:HB3	2.00	0.61
1:3:2:ASN:HD21	1:4:50:THR:HG22	1.66	0.61
1:W:77:VAL:HG12	1:W:79:LEU:HD13	1.82	0.61
1:2:2:ASN:HD21	1:3:50:THR:HG22	1.65	0.61
1:C:54:VAL:HG11	1:C:63:ALA:HB2	1.83	0.61
1:F:67:LEU:O	1:F:70:SER:HB3	1.99	0.61
1:U:16:ALA:HB1	1:U:67:LEU:HD13	1.82	0.61
1:X:41:ILE:HD13	1:4:7:ASN:HD22	1.63	0.61
1:2:7:ASN:ND2	1:2:8:VAL:H	1.98	0.61
1:D:22:PHE:O	1:D:23:ASN:HB2	2.01	0.61
1:I:22:PHE:O	1:I:23:ASN:HB2	2.01	0.61
1:L:122:ILE:H	1:L:122:ILE:CD1	2.11	0.61
1:R:67:LEU:O	1:R:70:SER:HB3	1.99	0.61
1:T:37:ALA:HB1	1:T:142:LEU:HD21	1.83	0.61
1:Z:4:ILE:HD12	1:1:52:VAL:HG22	1.83	0.61
1:B:14:ARG:HA	1:B:48:ASN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:LEU:HA	1:F:148:ILE:HD12	1.83	0.61
1:I:128:ARG:HH11	1:I:128:ARG:HG3	1.64	0.60
1:J:7:ASN:ND2	1:J:8:VAL:H	1.98	0.60
1:R:145:LEU:HA	1:R:148:ILE:HD12	1.83	0.60
1:T:67:LEU:O	1:T:70:SER:HB3	2.01	0.60
1:E:7:ASN:ND2	1:E:8:VAL:H	1.98	0.60
1:A:37:ALA:HB1	1:A:142:LEU:HD21	1.84	0.60
1:B:7:ASN:ND2	1:B:8:VAL:H	1.98	0.60
1:J:16:ALA:HB1	1:J:67:LEU:HD13	1.84	0.60
1:X:5:LYS:HD3	1:Y:21:ARG:HH22	1.66	0.60
1:X:41:ILE:HA	1:4:7:ASN:ND2	2.16	0.60
1:D:77:VAL:HG12	1:D:79:LEU:HD13	1.82	0.60
1:E:7:ASN:CG	1:E:8:VAL:H	2.05	0.60
1:R:7:ASN:CG	1:R:8:VAL:H	2.05	0.60
1:V:16:ALA:HB1	1:V:67:LEU:HD13	1.84	0.60
1:D:7:ASN:HD22	1:J:41:ILE:HD13	1.65	0.60
1:G:122:ILE:HD11	1:Q:132:LYS:HD2	1.82	0.60
1:L:7:ASN:CG	1:L:8:VAL:N	2.55	0.60
1:T:41:ILE:HD13	1:3:7:ASN:HD22	1.66	0.60
1:J:56:GLY:O	1:J:59:GLU:HG2	2.01	0.60
1:P:13:ALA:HB1	1:P:74:ASP:HB2	1.82	0.60
1:T:56:GLY:O	1:T:59:GLU:HG2	2.01	0.60
1:U:37:ALA:HB1	1:U:142:LEU:HD21	1.83	0.60
1:2:141:ALA:O	1:2:144:ALA:HB3	2.02	0.60
1:E:7:ASN:HD22	1:N:41:ILE:HD13	1.65	0.60
1:M:54:VAL:HG11	1:M:63:ALA:HB2	1.82	0.60
1:1:54:VAL:HG11	1:1:63:ALA:HB2	1.84	0.60
1:F:54:VAL:HG11	1:F:63:ALA:HB2	1.83	0.60
1:X:77:VAL:HG12	1:X:79:LEU:HD13	1.82	0.60
1:C:37:ALA:HB1	1:C:142:LEU:HD21	1.84	0.59
1:F:124:GLN:HG2	2:F:158:SO4:O4	2.01	0.59
1:K:119:THR:HA	1:L:87:THR:HB	1.82	0.59
1:A:122:ILE:HD11	1:N:132:LYS:CD	2.32	0.59
1:D:145:LEU:HA	1:D:148:ILE:HD12	1.84	0.59
1:H:16:ALA:HB1	1:H:67:LEU:HD13	1.83	0.59
1:N:22:PHE:O	1:N:23:ASN:HB2	2.03	0.59
1:U:119:THR:HA	1:V:87:THR:HB	1.84	0.59
1:Z:77:VAL:HG12	1:Z:79:LEU:HD13	1.84	0.59
1:G:67:LEU:O	1:G:70:SER:HB3	2.01	0.59
1:H:10:ALA:N	1:H:11:PRO:CD	2.64	0.59
1:S:41:ILE:HD13	1:Y:7:ASN:HD22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:41:ILE:HD13	1:O:7:ASN:HD22	1.68	0.59
1:J:122:ILE:HD11	1:O:132:LYS:HD2	1.85	0.59
1:K:56:GLY:O	1:K:59:GLU:HG2	2.02	0.59
1:S:54:VAL:HG11	1:S:63:ALA:HB2	1.83	0.59
1:A:56:GLY:O	1:A:59:GLU:HG2	2.02	0.59
1:V:37:ALA:HB1	1:V:142:LEU:HD21	1.83	0.59
1:1:37:ALA:HB1	1:1:142:LEU:HD21	1.84	0.59
1:D:7:ASN:ND2	1:D:8:VAL:H	2.00	0.59
1:Y:67:LEU:O	1:Y:70:SER:HB3	2.03	0.59
1:Y:122:ILE:HD12	1:Y:122:ILE:N	2.13	0.59
1:Z:7:ASN:ND2	1:Z:8:VAL:H	2.00	0.59
1:A:14:ARG:HA	1:A:48:ASN:HB3	1.85	0.59
1:3:22:PHE:O	1:3:23:ASN:HB2	2.02	0.59
1:D:146:GLU:O	1:D:150:VAL:HG23	2.03	0.59
1:I:54:VAL:HG11	1:I:63:ALA:HB2	1.85	0.59
1:J:37:ALA:HB1	1:J:142:LEU:HD21	1.83	0.59
1:K:145:LEU:HA	1:K:148:ILE:HD12	1.85	0.59
1:V:145:LEU:HA	1:V:148:ILE:HD12	1.85	0.59
1:H:2:ASN:HD21	1:I:50:THR:HG22	1.67	0.59
1:I:7:ASN:ND2	1:I:8:VAL:H	2.00	0.59
1:K:21:ARG:HH22	1:O:5:LYS:HD3	1.68	0.59
1:L:54:VAL:HG11	1:L:63:ALA:HB2	1.84	0.59
1:P:119:THR:HA	1:Q:87:THR:HB	1.84	0.59
1:V:141:ALA:O	1:V:144:ALA:HB3	2.03	0.59
1:E:7:ASN:CG	1:E:8:VAL:N	2.56	0.58
1:U:122:ILE:H	1:U:122:ILE:CD1	2.12	0.58
1:C:22:PHE:O	1:C:23:ASN:HB2	2.03	0.58
1:D:54:VAL:HG11	1:D:63:ALA:HB2	1.85	0.58
1:L:67:LEU:O	1:L:70:SER:HB3	2.02	0.58
1:S:56:GLY:O	1:S:59:GLU:HG2	2.03	0.58
1:1:141:ALA:O	1:1:144:ALA:HB3	2.03	0.58
1:3:141:ALA:O	1:3:144:ALA:HB3	2.02	0.58
1:4:54:VAL:HG11	1:4:63:ALA:HB2	1.84	0.58
1:A:22:PHE:O	1:A:23:ASN:HB2	2.03	0.58
1:G:7:ASN:ND2	1:G:8:VAL:H	2.01	0.58
1:M:14:ARG:HA	1:M:48:ASN:HB3	1.85	0.58
1:V:7:ASN:ND2	1:V:8:VAL:H	2.01	0.58
1:W:141:ALA:O	1:W:144:ALA:HB3	2.03	0.58
1:C:5:LYS:HD3	1:D:21:ARG:HH22	1.68	0.58
1:P:7:ASN:CG	1:P:8:VAL:N	2.56	0.58
1:P:67:LEU:O	1:P:70:SER:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:7:ASN:CG	1:S:8:VAL:H	2.07	0.58
1:A:67:LEU:O	1:A:70:SER:HB3	2.04	0.58
1:I:2:ASN:HD21	1:J:50:THR:HG22	1.68	0.58
1:L:119:THR:HA	1:M:87:THR:HB	1.86	0.58
1:M:122:ILE:H	1:M:122:ILE:CD1	2.14	0.58
1:Q:122:ILE:HD12	1:Q:122:ILE:N	2.12	0.58
1:X:67:LEU:O	1:X:70:SER:HB3	2.03	0.58
1:J:141:ALA:O	1:J:144:ALA:HB3	2.04	0.58
1:Y:141:ALA:O	1:Y:144:ALA:HB3	2.04	0.58
1:3:7:ASN:CG	1:3:8:VAL:N	2.57	0.58
1:L:5:LYS:HD3	1:M:21:ARG:HH22	1.69	0.58
1:L:67:LEU:HD22	1:L:73:TYR:CE2	2.39	0.58
1:M:128:ARG:HG3	1:M:128:ARG:HH11	1.69	0.58
1:U:77:VAL:HG12	1:U:79:LEU:HD13	1.86	0.58
1:B:132:LYS:HD2	1:V:122:ILE:HD11	1.86	0.58
1:E:77:VAL:HG12	1:E:79:LEU:HD13	1.84	0.58
1:G:145:LEU:HA	1:G:148:ILE:HD12	1.86	0.58
1:J:122:ILE:H	1:J:122:ILE:CD1	2.10	0.58
1:Z:21:ARG:HH22	1:4:5:LYS:HD3	1.68	0.58
1:4:67:LEU:O	1:4:70:SER:HB3	2.04	0.58
1:H:7:ASN:ND2	1:H:8:VAL:H	2.02	0.58
1:P:11:PRO:HB3	1:P:43:GLN:O	2.04	0.58
1:S:40:ARG:O	1:Y:7:ASN:HB2	2.03	0.58
1:V:11:PRO:HA	1:V:43:GLN:O	2.03	0.58
1:Z:14:ARG:HA	1:Z:48:ASN:HB3	1.85	0.58
1:1:7:ASN:ND2	1:1:8:VAL:H	2.01	0.58
1:C:7:ASN:CG	1:C:8:VAL:H	2.06	0.58
1:Y:7:ASN:CG	1:Y:8:VAL:N	2.58	0.58
1:E:37:ALA:HB1	1:E:142:LEU:HD21	1.86	0.57
1:H:11:PRO:HA	1:H:43:GLN:O	2.04	0.57
1:P:11:PRO:HA	1:P:43:GLN:O	2.04	0.57
1:R:19:ILE:HD11	1:R:31:LEU:HB2	1.86	0.57
1:X:2:ASN:HD21	1:Y:50:THR:HG22	1.69	0.57
1:E:122:ILE:HD11	1:J:132:LYS:HD2	1.85	0.57
1:O:7:ASN:CG	1:O:8:VAL:N	2.58	0.57
1:S:7:ASN:CG	1:S:8:VAL:N	2.57	0.57
1:W:145:LEU:HA	1:W:148:ILE:HD12	1.85	0.57
1:1:5:LYS:HD3	1:2:21:ARG:HH22	1.70	0.57
1:3:7:ASN:CG	1:3:8:VAL:H	2.06	0.57
1:D:14:ARG:HA	1:D:48:ASN:HB3	1.86	0.57
1:F:52:VAL:HG22	1:J:4:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:LEU:O	1:K:70:SER:HB3	2.05	0.57
1:P:141:ALA:O	1:P:144:ALA:HB3	2.04	0.57
1:C:7:ASN:CG	1:C:8:VAL:N	2.58	0.57
1:T:141:ALA:O	1:T:144:ALA:HB3	2.04	0.57
1:Z:5:LYS:HD3	1:1:21:ARG:HH22	1.69	0.57
1:4:122:ILE:H	1:4:122:ILE:CD1	2.14	0.57
1:E:16:ALA:O	1:E:76:VAL:HA	2.04	0.57
1:L:145:LEU:HA	1:L:148:ILE:HD12	1.87	0.57
1:J:54:VAL:HG11	1:J:63:ALA:HB2	1.86	0.57
1:P:14:ARG:HA	1:P:48:ASN:HB3	1.86	0.57
1:T:12:ASP:O	1:T:13:ALA:O	2.20	0.57
1:Z:54:VAL:HG11	1:Z:63:ALA:HB2	1.86	0.57
1:2:128:ARG:NE	2:2:159:SO4:O3	2.36	0.57
1:A:5:LYS:HD3	1:B:21:ARG:HH22	1.69	0.57
1:A:7:ASN:CG	1:A:8:VAL:H	2.07	0.57
1:C:7:ASN:HD22	1:R:41:ILE:HD13	1.69	0.57
1:K:7:ASN:CG	1:K:8:VAL:N	2.58	0.57
1:O:54:VAL:HG11	1:O:63:ALA:HB2	1.86	0.57
1:T:14:ARG:HA	1:T:48:ASN:HB3	1.86	0.57
1:U:7:ASN:ND2	1:U:8:VAL:H	2.03	0.57
1:4:7:ASN:ND2	1:4:8:VAL:H	2.03	0.57
1:4:14:ARG:HA	1:4:48:ASN:HB3	1.87	0.57
1:P:37:ALA:HB1	1:P:142:LEU:HD21	1.87	0.57
1:F:119:THR:HA	1:G:87:THR:HB	1.87	0.57
1:F:146:GLU:O	1:F:150:VAL:HG23	2.05	0.57
1:H:141:ALA:O	1:H:144:ALA:HB3	2.04	0.57
1:P:7:ASN:CG	1:P:8:VAL:H	2.08	0.57
1:P:86:GLY:N	2:P:157:SO4:O1	2.37	0.57
1:R:22:PHE:O	1:R:23:ASN:HB2	2.04	0.57
1:W:37:ALA:HB1	1:W:142:LEU:HD21	1.85	0.57
1:W:54:VAL:HG11	1:W:63:ALA:HB2	1.87	0.57
1:X:54:VAL:HG11	1:X:63:ALA:HB2	1.86	0.57
1:A:23:ASN:HA	1:N:131:THR:HA	1.85	0.56
1:D:67:LEU:O	1:D:70:SER:HB3	2.05	0.56
1:I:35:VAL:HG23	1:I:36:ASP:N	2.20	0.56
1:K:54:VAL:HG11	1:K:63:ALA:HB2	1.87	0.56
1:K:146:GLU:O	1:K:150:VAL:HG23	2.05	0.56
1:O:37:ALA:HB1	1:O:142:LEU:HD21	1.86	0.56
1:T:122:ILE:HD11	1:Y:132:LYS:HD2	1.86	0.56
1:1:14:ARG:HA	1:1:48:ASN:HB3	1.87	0.56
1:A:7:ASN:CG	1:A:8:VAL:N	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:54:VAL:HG11	1:2:63:ALA:HB2	1.87	0.56
1:L:22:PHE:O	1:L:23:ASN:HB2	2.06	0.56
1:N:5:LYS:HD3	1:O:21:ARG:HH22	1.70	0.56
1:Y:122:ILE:H	1:Y:122:ILE:CD1	2.10	0.56
1:1:122:ILE:H	1:1:122:ILE:CD1	2.11	0.56
1:A:145:LEU:HA	1:A:148:ILE:HD12	1.87	0.56
1:E:141:ALA:O	1:E:144:ALA:HB3	2.05	0.56
1:J:7:ASN:CG	1:J:8:VAL:H	2.07	0.56
1:N:2:ASN:HD21	1:O:50:THR:HG22	1.70	0.56
1:Y:54:VAL:HG11	1:Y:63:ALA:HB2	1.88	0.56
1:Q:14:ARG:HA	1:Q:48:ASN:HB3	1.87	0.56
1:2:67:LEU:O	1:2:70:SER:HB3	2.05	0.56
1:G:14:ARG:HA	1:G:48:ASN:HB3	1.86	0.56
1:S:141:ALA:O	1:S:144:ALA:HB3	2.06	0.56
1:T:7:ASN:CG	1:T:8:VAL:N	2.58	0.56
1:V:2:ASN:HD21	1:W:50:THR:HG22	1.70	0.56
1:J:89:HIS:ND1	2:J:158:SO4:O2	2.39	0.56
1:R:7:ASN:CG	1:R:8:VAL:N	2.58	0.56
1:S:7:ASN:HB2	1:Y:40:ARG:O	2.06	0.56
1:T:145:LEU:HA	1:T:148:ILE:HD12	1.87	0.56
1:U:67:LEU:O	1:U:70:SER:HB3	2.05	0.56
1:V:67:LEU:O	1:V:70:SER:HB3	2.06	0.56
1:Y:14:ARG:HA	1:Y:48:ASN:HB3	1.88	0.56
1:K:7:ASN:CG	1:K:8:VAL:H	2.08	0.56
1:Q:146:GLU:O	1:Q:150:VAL:HG23	2.06	0.56
1:R:19:ILE:CD1	1:R:31:LEU:HB2	2.36	0.56
1:U:22:PHE:O	1:U:23:ASN:HB2	2.06	0.56
1:Y:122:ILE:HD11	1:4:132:LYS:CD	2.34	0.56
1:Z:22:PHE:O	1:Z:23:ASN:HB2	2.04	0.56
1:F:128:ARG:NH2	2:F:158:SO4:O4	2.38	0.56
1:R:54:VAL:HG11	1:R:63:ALA:HB2	1.86	0.56
1:Y:7:ASN:CG	1:Y:8:VAL:H	2.09	0.56
1:Z:37:ALA:HB1	1:Z:142:LEU:HD21	1.88	0.56
1:B:2:ASN:HD21	1:C:50:THR:HG22	1.70	0.56
1:F:11:PRO:CB	1:F:43:GLN:HB3	2.27	0.56
1:M:145:LEU:HA	1:M:148:ILE:HD12	1.88	0.56
1:R:11:PRO:HB3	1:R:43:GLN:HB3	1.87	0.56
1:R:37:ALA:HB1	1:R:142:LEU:HD21	1.87	0.56
1:G:122:ILE:HD12	1:G:122:ILE:N	2.16	0.55
1:J:7:ASN:CG	1:J:8:VAL:N	2.58	0.55
1:M:143:THR:HG22	1:N:55:PRO:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:5:LYS:HD3	1:T:21:ARG:HH22	1.70	0.55
1:S:35:VAL:HG23	1:S:36:ASP:N	2.20	0.55
1:1:145:LEU:HA	1:1:148:ILE:HD12	1.89	0.55
1:3:37:ALA:HB1	1:3:142:LEU:HD21	1.87	0.55
1:B:54:VAL:HG11	1:B:63:ALA:HB2	1.88	0.55
1:I:7:ASN:CG	1:I:8:VAL:H	2.10	0.55
1:J:14:ARG:HA	1:J:48:ASN:HB3	1.88	0.55
1:O:14:ARG:HA	1:O:48:ASN:HB3	1.88	0.55
1:V:54:VAL:HG11	1:V:63:ALA:HB2	1.88	0.55
1:B:77:VAL:HG12	1:B:79:LEU:HD13	1.87	0.55
1:C:14:ARG:HA	1:C:48:ASN:HB3	1.88	0.55
1:E:60:LEU:O	1:E:64:THR:HG23	2.07	0.55
1:L:141:ALA:O	1:L:144:ALA:HB3	2.06	0.55
1:N:37:ALA:HB1	1:N:142:LEU:HD21	1.88	0.55
1:O:7:ASN:CG	1:O:8:VAL:H	2.10	0.55
1:Q:37:ALA:HB1	1:Q:142:LEU:HD21	1.89	0.55
1:Y:22:PHE:O	1:Y:23:ASN:HB2	2.07	0.55
1:D:7:ASN:CG	1:D:8:VAL:H	2.10	0.55
1:F:22:PHE:O	1:F:23:ASN:HB2	2.06	0.55
1:G:23:ASN:HA	1:Q:131:THR:HA	1.89	0.55
1:I:67:LEU:O	1:I:70:SER:HB3	2.07	0.55
1:N:7:ASN:ND2	1:N:8:VAL:H	2.05	0.55
1:S:67:LEU:O	1:S:70:SER:HB3	2.05	0.55
1:W:7:ASN:ND2	1:W:8:VAL:H	2.03	0.55
1:J:60:LEU:O	1:J:64:THR:HG23	2.05	0.55
1:U:11:PRO:HB3	1:U:43:GLN:O	2.06	0.55
1:X:7:ASN:ND2	1:X:8:VAL:H	2.04	0.55
1:Y:37:ALA:HB1	1:Y:142:LEU:HD21	1.88	0.55
1:D:41:ILE:HD13	1:J:7:ASN:ND2	2.20	0.55
1:J:146:GLU:O	1:J:150:VAL:HG23	2.06	0.55
1:L:14:ARG:HA	1:L:48:ASN:HB3	1.89	0.55
1:E:22:PHE:O	1:E:23:ASN:HB2	2.07	0.55
1:B:22:PHE:O	1:B:23:ASN:HB2	2.07	0.55
1:E:54:VAL:HG11	1:E:63:ALA:HB2	1.89	0.55
1:A:2:ASN:HD21	1:B:50:THR:HG22	1.71	0.55
1:F:2:ASN:HD21	1:G:50:THR:HG22	1.72	0.54
1:H:145:LEU:HA	1:H:148:ILE:HD12	1.87	0.54
1:K:122:ILE:H	1:K:122:ILE:CD1	2.12	0.54
1:2:7:ASN:CG	1:2:8:VAL:N	2.60	0.54
1:E:122:ILE:H	1:E:122:ILE:CD1	2.14	0.54
1:H:11:PRO:HB3	1:H:43:GLN:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:ARG:HA	1:I:48:ASN:HB3	1.88	0.54
1:N:54:VAL:HG11	1:N:63:ALA:HB2	1.90	0.54
1:T:7:ASN:CG	1:T:8:VAL:H	2.10	0.54
1:V:7:ASN:CG	1:V:8:VAL:N	2.61	0.54
1:X:132:LYS:HD2	1:Z:122:ILE:HD11	1.88	0.54
1:D:41:ILE:HA	1:J:7:ASN:HD22	1.69	0.54
1:K:5:LYS:HD3	1:L:21:ARG:HH22	1.71	0.54
1:X:14:ARG:HA	1:X:48:ASN:HB3	1.89	0.54
1:Z:50:THR:HG22	1:4:2:ASN:HD21	1.72	0.54
1:Z:128:ARG:HH11	1:Z:128:ARG:HG3	1.73	0.54
1:B:122:ILE:H	1:B:122:ILE:CD1	2.17	0.54
1:C:67:LEU:O	1:C:70:SER:HB3	2.07	0.54
1:D:7:ASN:CG	1:D:8:VAL:N	2.61	0.54
1:F:14:ARG:HA	1:F:48:ASN:HB3	1.88	0.54
1:Q:54:VAL:HG11	1:Q:63:ALA:HB2	1.88	0.54
1:S:7:ASN:ND2	1:Y:41:ILE:HD13	2.20	0.54
1:Z:19:ILE:CD1	1:Z:31:LEU:HB2	2.37	0.54
1:I:141:ALA:O	1:I:144:ALA:HB3	2.06	0.54
1:T:131:THR:HA	1:4:23:ASN:HA	1.89	0.54
1:3:5:LYS:HD3	1:4:21:ARG:HH22	1.73	0.54
1:A:54:VAL:HG11	1:A:63:ALA:HB2	1.88	0.54
1:F:25:PHE:O	1:F:25:PHE:CD1	2.61	0.54
1:F:131:THR:HA	1:R:23:ASN:HA	1.89	0.54
1:K:35:VAL:HG23	1:K:36:ASP:N	2.23	0.54
1:V:5:LYS:HD3	1:W:21:ARG:HH22	1.72	0.54
1:W:22:PHE:O	1:W:23:ASN:HB2	2.07	0.54
1:2:119:THR:HA	1:3:87:THR:HB	1.89	0.54
1:D:37:ALA:HB1	1:D:142:LEU:HD21	1.89	0.54
1:G:54:VAL:HG11	1:G:63:ALA:HB2	1.90	0.54
1:G:146:GLU:O	1:G:150:VAL:HG23	2.08	0.54
1:I:146:GLU:O	1:I:150:VAL:HG23	2.08	0.54
1:K:22:PHE:O	1:K:23:ASN:HB2	2.07	0.54
1:U:5:LYS:HD3	1:V:21:ARG:HH22	1.72	0.54
1:U:7:ASN:CG	1:U:8:VAL:H	2.11	0.54
1:V:13:ALA:HB1	1:V:74:ASP:CB	2.38	0.54
1:X:37:ALA:HB1	1:X:142:LEU:HD21	1.90	0.54
1:B:68:ALA:HB1	1:B:110:VAL:HG21	1.90	0.54
1:C:76:VAL:HB	1:C:112:VAL:HG22	1.90	0.54
1:C:141:ALA:O	1:C:144:ALA:HB3	2.06	0.54
1:E:23:ASN:HA	1:J:131:THR:HA	1.88	0.54
1:E:35:VAL:HG23	1:E:36:ASP:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:ILE:HG12	1:G:77:VAL:HB	1.89	0.54
1:H:35:VAL:HG23	1:H:36:ASP:N	2.22	0.54
1:P:122:ILE:HD12	1:P:122:ILE:N	2.12	0.54
1:W:35:VAL:HG23	1:W:36:ASP:N	2.22	0.54
1:H:54:VAL:HG11	1:H:63:ALA:HB2	1.90	0.54
1:N:145:LEU:HA	1:N:148:ILE:HD12	1.90	0.54
1:U:39:THR:OG1	1:U:40:ARG:N	2.41	0.54
1:3:54:VAL:HG11	1:3:63:ALA:HB2	1.90	0.54
1:4:7:ASN:CG	1:4:8:VAL:N	2.61	0.54
1:I:7:ASN:CG	1:I:8:VAL:N	2.61	0.54
1:J:145:LEU:HA	1:J:148:ILE:HD12	1.90	0.54
1:S:14:ARG:HA	1:S:48:ASN:HB3	1.90	0.54
1:W:7:ASN:CG	1:W:8:VAL:N	2.61	0.54
1:H:37:ALA:HB1	1:H:142:LEU:HD21	1.89	0.53
1:P:39:THR:OG1	1:P:40:ARG:N	2.41	0.53
1:X:11:PRO:HA	1:X:43:GLN:O	2.08	0.53
1:4:145:LEU:HA	1:4:148:ILE:HD12	1.90	0.53
1:H:14:ARG:HA	1:H:48:ASN:HB3	1.90	0.53
1:K:57:ALA:HA	1:K:60:LEU:HG	1.90	0.53
1:T:11:PRO:HA	1:T:43:GLN:O	2.08	0.53
1:X:7:ASN:CG	1:X:8:VAL:N	2.61	0.53
1:Y:145:LEU:O	1:Y:146:GLU:C	2.46	0.53
1:4:7:ASN:CG	1:4:8:VAL:H	2.11	0.53
1:G:37:ALA:HB1	1:G:142:LEU:HD21	1.90	0.53
1:J:22:PHE:O	1:J:23:ASN:HB2	2.09	0.53
1:P:94:ALA:HB3	1:Q:92:TYR:OH	2.08	0.53
1:1:76:VAL:HB	1:1:112:VAL:HG22	1.91	0.53
1:P:10:ALA:C	1:P:12:ASP:H	2.11	0.53
1:U:141:ALA:O	1:U:144:ALA:HB3	2.09	0.53
1:X:7:ASN:CG	1:X:8:VAL:H	2.11	0.53
1:2:7:ASN:CG	1:2:8:VAL:H	2.11	0.53
1:F:39:THR:OG1	1:F:40:ARG:N	2.40	0.53
1:H:7:ASN:CG	1:H:8:VAL:H	2.12	0.53
1:H:7:ASN:CG	1:H:8:VAL:N	2.62	0.53
1:Q:22:PHE:O	1:Q:23:ASN:HB2	2.08	0.53
1:R:146:GLU:O	1:R:150:VAL:HG23	2.08	0.53
1:C:132:LYS:CD	1:S:122:ILE:HD11	2.38	0.53
1:M:37:ALA:HB1	1:M:142:LEU:HD21	1.89	0.53
1:2:145:LEU:HA	1:2:148:ILE:HD12	1.89	0.53
1:F:7:ASN:HD22	1:Q:41:ILE:HA	1.74	0.53
1:F:141:ALA:O	1:F:144:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:LEU:O	1:H:148:ILE:N	2.41	0.53
1:N:145:LEU:O	1:N:146:GLU:C	2.46	0.53
1:Q:121:SER:OG	1:Q:123:GLU:HB3	2.09	0.53
1:W:7:ASN:CG	1:W:8:VAL:H	2.11	0.53
1:B:35:VAL:HG23	1:B:36:ASP:N	2.24	0.53
1:N:14:ARG:HA	1:N:48:ASN:HB3	1.91	0.53
1:S:145:LEU:HA	1:S:148:ILE:HD12	1.89	0.53
1:T:22:PHE:O	1:T:23:ASN:HB2	2.08	0.53
1:C:122:ILE:HD12	1:C:122:ILE:N	2.15	0.53
1:V:14:ARG:HA	1:V:48:ASN:HB3	1.91	0.53
1:D:7:ASN:HD22	1:J:41:ILE:HA	1.73	0.53
1:F:94:ALA:HB3	1:G:92:TYR:OH	2.08	0.53
1:H:22:PHE:O	1:H:23:ASN:HB2	2.09	0.53
1:I:145:LEU:HA	1:I:148:ILE:HD12	1.91	0.53
1:T:54:VAL:HG11	1:T:63:ALA:HB2	1.90	0.53
1:U:7:ASN:CG	1:U:8:VAL:N	2.63	0.53
1:Z:141:ALA:O	1:Z:144:ALA:HB3	2.09	0.53
1:D:60:LEU:O	1:D:64:THR:HG23	2.09	0.52
1:G:141:ALA:O	1:G:144:ALA:HB3	2.09	0.52
1:Q:145:LEU:HA	1:Q:148:ILE:HD12	1.91	0.52
1:W:146:GLU:O	1:W:150:VAL:HG23	2.10	0.52
1:X:131:THR:HA	1:Z:23:ASN:HA	1.90	0.52
1:4:22:PHE:O	1:4:23:ASN:HB2	2.09	0.52
1:E:14:ARG:HA	1:E:48:ASN:HB3	1.90	0.52
1:F:122:ILE:H	1:F:122:ILE:CD1	2.13	0.52
1:M:122:ILE:HD12	1:M:122:ILE:N	2.16	0.52
1:Q:7:ASN:ND2	1:Q:8:VAL:H	2.06	0.52
1:Q:35:VAL:HG23	1:Q:36:ASP:N	2.23	0.52
1:S:37:ALA:HB1	1:S:142:LEU:HD21	1.92	0.52
1:V:128:ARG:HH11	1:V:128:ARG:HG3	1.75	0.52
1:Z:7:ASN:CG	1:Z:8:VAL:N	2.62	0.52
1:1:154:ILE:HD13	1:2:67:LEU:CD2	2.39	0.52
1:4:145:LEU:O	1:4:146:GLU:C	2.46	0.52
1:D:141:ALA:O	1:D:144:ALA:HB3	2.09	0.52
1:R:35:VAL:HG23	1:R:36:ASP:N	2.25	0.52
1:T:23:ASN:HA	1:Y:131:THR:HA	1.91	0.52
1:Y:35:VAL:HG23	1:Y:36:ASP:N	2.25	0.52
1:G:22:PHE:O	1:G:23:ASN:HB2	2.09	0.52
1:J:145:LEU:O	1:J:146:GLU:C	2.46	0.52
1:M:22:PHE:O	1:M:23:ASN:HB2	2.08	0.52
1:O:22:PHE:O	1:O:23:ASN:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:119:THR:HA	1:2:87:THR:HB	1.91	0.52
1:4:76:VAL:HB	1:4:112:VAL:HG22	1.91	0.52
1:F:17:ILE:HG12	1:F:77:VAL:HB	1.92	0.52
1:K:37:ALA:HB1	1:K:142:LEU:HD21	1.89	0.52
1:N:67:LEU:O	1:N:70:SER:HB3	2.09	0.52
1:X:24:GLN:O	1:X:26:ILE:N	2.43	0.52
1:I:128:ARG:HG3	1:I:128:ARG:NH1	2.25	0.52
1:2:11:PRO:HB3	1:2:43:GLN:HB3	1.90	0.52
1:H:119:THR:HA	1:I:87:THR:HB	1.90	0.52
1:K:94:ALA:HB3	1:L:92:TYR:OH	2.10	0.52
1:C:2:ASN:HD21	1:D:50:THR:HG22	1.75	0.52
1:G:7:ASN:CG	1:G:8:VAL:H	2.13	0.52
1:G:121:SER:OG	1:G:123:GLU:HB3	2.10	0.52
1:Q:39:THR:OG1	1:Q:40:ARG:N	2.40	0.52
1:U:14:ARG:HA	1:U:48:ASN:HB3	1.92	0.52
1:U:145:LEU:HA	1:U:148:ILE:HD12	1.90	0.52
1:2:127:GLU:HA	1:2:131:THR:OG1	2.10	0.52
1:2:128:ARG:HG3	1:2:128:ARG:HH11	1.74	0.52
1:C:17:ILE:HG12	1:C:77:VAL:HB	1.91	0.52
1:U:87:THR:HB	1:Y:119:THR:HA	1.92	0.52
1:1:24:GLN:O	1:1:26:ILE:N	2.43	0.52
1:L:39:THR:OG1	1:L:40:ARG:N	2.43	0.52
1:2:35:VAL:HG23	1:2:36:ASP:N	2.25	0.52
1:O:146:GLU:O	1:O:150:VAL:HG23	2.10	0.51
1:V:22:PHE:O	1:V:23:ASN:HB2	2.09	0.51
1:D:128:ARG:HH11	1:D:128:ARG:HG3	1.75	0.51
1:F:5:LYS:HD3	1:G:21:ARG:HH22	1.74	0.51
1:T:145:LEU:O	1:T:146:GLU:C	2.49	0.51
1:Z:87:THR:HB	1:4:119:THR:HA	1.91	0.51
1:A:92:TYR:OH	1:E:94:ALA:HB3	2.10	0.51
1:F:37:ALA:HB1	1:F:142:LEU:HD21	1.92	0.51
1:G:7:ASN:CG	1:G:8:VAL:N	2.63	0.51
1:H:19:ILE:CD1	1:H:31:LEU:HB2	2.40	0.51
1:J:23:ASN:HA	1:O:131:THR:HA	1.92	0.51
1:P:23:ASN:HA	1:3:131:THR:HA	1.93	0.51
1:P:54:VAL:HG11	1:P:63:ALA:HB2	1.92	0.51
1:1:35:VAL:HG23	1:1:36:ASP:N	2.24	0.51
1:H:122:ILE:HD12	1:H:122:ILE:N	2.14	0.51
1:M:119:THR:HA	1:N:87:THR:HB	1.91	0.51
1:X:94:ALA:HB3	1:Y:92:TYR:OH	2.10	0.51
1:A:21:ARG:HH22	1:E:5:LYS:HD3	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ALA:HB1	1:C:142:LEU:CD2	2.41	0.51
1:H:94:ALA:HB3	1:I:92:TYR:OH	2.11	0.51
1:I:13:ALA:HB1	1:I:74:ASP:CB	2.40	0.51
1:K:2:ASN:HD21	1:L:50:THR:HG22	1.75	0.51
1:W:122:ILE:H	1:W:122:ILE:CD1	2.15	0.51
1:X:19:ILE:CD1	1:X:31:LEU:HB2	2.40	0.51
1:1:7:ASN:CG	1:1:8:VAL:N	2.64	0.51
1:2:13:ALA:HB1	1:2:74:ASP:HB2	1.93	0.51
1:D:1:MET:HE2	1:E:46:ASP:HB2	1.92	0.51
1:K:16:ALA:CB	1:K:67:LEU:HD13	2.40	0.51
1:O:35:VAL:HG23	1:O:36:ASP:N	2.26	0.51
1:R:60:LEU:O	1:R:64:THR:HG23	2.11	0.51
1:U:37:ALA:HB1	1:U:142:LEU:CD2	2.41	0.51
1:2:13:ALA:HB1	1:2:74:ASP:CB	2.40	0.51
1:B:131:THR:HA	1:V:23:ASN:HA	1.91	0.51
1:D:19:ILE:CD1	1:D:31:LEU:HB2	2.41	0.51
1:G:25:PHE:CE1	1:Q:126:ILE:HD13	2.46	0.51
1:2:17:ILE:HG12	1:2:77:VAL:HB	1.93	0.51
1:H:128:ARG:HG3	1:H:128:ARG:HH11	1.76	0.51
1:H:146:GLU:O	1:H:150:VAL:HG23	2.11	0.51
1:I:39:THR:OG1	1:I:40:ARG:N	2.44	0.51
1:O:22:PHE:HD1	1:O:23:ASN:H	1.59	0.51
1:O:67:LEU:HD22	1:O:73:TYR:CE2	2.46	0.51
1:W:14:ARG:HA	1:W:48:ASN:HB3	1.93	0.51
1:3:19:ILE:CG2	1:3:53:TRP:CZ3	2.94	0.51
1:R:37:ALA:HB1	1:R:142:LEU:CD2	2.41	0.51
1:S:17:ILE:HG12	1:S:77:VAL:HB	1.93	0.51
1:X:22:PHE:O	1:X:23:ASN:HB2	2.11	0.51
1:Y:122:ILE:CD1	1:4:132:LYS:HD2	2.40	0.51
1:B:19:ILE:CD1	1:B:31:LEU:HB2	2.42	0.50
1:K:19:ILE:CD1	1:K:31:LEU:HB2	2.42	0.50
1:Q:7:ASN:CG	1:Q:8:VAL:N	2.64	0.50
1:1:22:PHE:O	1:1:23:ASN:HB2	2.10	0.50
1:4:21:ARG:O	1:4:24:GLN:HB2	2.11	0.50
1:B:7:ASN:CG	1:B:8:VAL:N	2.65	0.50
1:I:37:ALA:HB1	1:I:142:LEU:HD21	1.92	0.50
1:N:16:ALA:O	1:N:76:VAL:HA	2.11	0.50
1:P:122:ILE:H	1:P:122:ILE:CD1	2.06	0.50
1:U:25:PHE:CD1	1:U:25:PHE:O	2.63	0.50
1:D:67:LEU:HD22	1:D:73:TYR:CE2	2.46	0.50
1:F:132:LYS:CD	1:R:122:ILE:HD11	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:GLU:HB2	1:G:124:GLN:OE1	2.11	0.50
1:I:76:VAL:HB	1:I:112:VAL:HG22	1.92	0.50
1:L:37:ALA:HB1	1:L:142:LEU:HD21	1.92	0.50
1:1:145:LEU:O	1:1:148:ILE:N	2.44	0.50
1:C:146:GLU:O	1:C:150:VAL:HG23	2.11	0.50
1:N:7:ASN:CG	1:N:8:VAL:N	2.65	0.50
1:S:22:PHE:O	1:S:23:ASN:HB2	2.12	0.50
1:3:11:PRO:CB	1:3:43:GLN:HB3	2.38	0.50
1:X:146:GLU:O	1:X:150:VAL:HG23	2.11	0.50
1:2:19:ILE:CG2	1:2:53:TRP:CZ3	2.95	0.50
1:4:19:ILE:CD1	1:4:31:LEU:HB2	2.41	0.50
1:I:126:ILE:HG21	1:K:122:ILE:HG21	1.94	0.50
1:K:25:PHE:O	1:K:25:PHE:CD1	2.65	0.50
1:Q:24:GLN:O	1:Q:26:ILE:N	2.45	0.50
1:1:4:ILE:HD12	1:2:52:VAL:HG22	1.94	0.50
1:2:19:ILE:CD1	1:2:31:LEU:HB2	2.41	0.50
1:3:57:ALA:HA	1:3:60:LEU:HG	1.92	0.50
1:K:22:PHE:HD1	1:K:23:ASN:H	1.60	0.50
1:Q:11:PRO:HA	1:Q:43:GLN:O	2.12	0.50
1:R:67:LEU:HD22	1:R:73:TYR:CE2	2.46	0.50
1:T:57:ALA:HA	1:T:60:LEU:HG	1.93	0.50
1:U:57:ALA:HA	1:U:60:LEU:HG	1.94	0.50
1:X:35:VAL:HG23	1:X:36:ASP:N	2.27	0.50
1:B:145:LEU:O	1:B:146:GLU:C	2.50	0.50
1:D:132:LYS:HD2	1:F:122:ILE:HD11	1.94	0.50
1:N:7:ASN:CG	1:N:8:VAL:H	2.15	0.50
1:N:94:ALA:HB3	1:O:92:TYR:OH	2.12	0.50
1:Q:7:ASN:CG	1:Q:8:VAL:H	2.15	0.50
1:Q:16:ALA:O	1:Q:76:VAL:HA	2.12	0.50
1:Q:19:ILE:HG12	1:Q:79:LEU:HB2	1.93	0.50
1:T:37:ALA:HB1	1:T:142:LEU:CD2	2.40	0.50
1:T:132:LYS:HD2	1:4:122:ILE:HD11	1.92	0.50
1:U:4:ILE:HD12	1:V:52:VAL:HG22	1.93	0.50
1:U:35:VAL:HG23	1:U:36:ASP:N	2.26	0.50
1:E:16:ALA:CB	1:E:67:LEU:HD13	2.41	0.50
1:H:89:HIS:CB	2:H:157:SO4:O4	2.60	0.50
1:I:67:LEU:HD22	1:I:73:TYR:CE2	2.47	0.50
1:M:12:ASP:O	1:M:13:ALA:C	2.48	0.50
1:N:39:THR:OG1	1:N:40:ARG:N	2.45	0.50
1:S:145:LEU:O	1:S:146:GLU:C	2.50	0.50
1:T:39:THR:OG1	1:T:40:ARG:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:7:ASN:CG	1:V:8:VAL:H	2.14	0.50
1:Z:7:ASN:CG	1:Z:8:VAL:H	2.15	0.50
1:Z:57:ALA:HA	1:Z:60:LEU:HG	1.94	0.50
1:4:39:THR:OG1	1:4:40:ARG:N	2.44	0.50
1:A:37:ALA:HB1	1:A:142:LEU:CD2	2.42	0.49
1:C:131:THR:HA	1:S:23:ASN:HA	1.94	0.49
1:J:121:SER:OG	1:J:123:GLU:HB3	2.11	0.49
1:J:122:ILE:HD12	1:J:122:ILE:N	2.16	0.49
1:M:17:ILE:HG12	1:M:77:VAL:HB	1.93	0.49
1:N:37:ALA:HB1	1:N:142:LEU:CD2	2.42	0.49
1:Q:1:MET:HE2	1:R:46:ASP:HB2	1.93	0.49
1:Q:113:ALA:HB1	1:Q:140:ALA:HB1	1.94	0.49
1:Q:119:THR:HA	1:R:87:THR:HB	1.93	0.49
1:B:57:ALA:HA	1:B:60:LEU:HG	1.94	0.49
1:B:128:ARG:HH11	1:B:128:ARG:HG3	1.77	0.49
1:D:23:ASN:HA	1:R:131:THR:HA	1.94	0.49
1:G:76:VAL:HB	1:G:112:VAL:HG22	1.94	0.49
1:L:19:ILE:CD1	1:L:31:LEU:HB2	2.42	0.49
1:N:19:ILE:CD1	1:N:31:LEU:HB2	2.41	0.49
1:X:7:ASN:ND2	1:4:41:ILE:HD13	2.25	0.49
1:3:119:THR:HA	1:4:87:THR:HB	1.94	0.49
1:B:67:LEU:HD22	1:B:73:TYR:CE2	2.47	0.49
1:C:24:GLN:O	1:C:26:ILE:N	2.45	0.49
1:J:22:PHE:HD1	1:J:23:ASN:H	1.61	0.49
1:M:35:VAL:HG23	1:M:36:ASP:N	2.28	0.49
1:R:76:VAL:HB	1:R:112:VAL:HG22	1.93	0.49
1:R:122:ILE:H	1:R:122:ILE:CD1	2.15	0.49
1:V:24:GLN:O	1:V:26:ILE:N	2.45	0.49
1:2:122:ILE:H	1:2:122:ILE:CD1	2.17	0.49
1:D:2:ASN:HD21	1:E:50:THR:HG22	1.77	0.49
1:E:19:ILE:CD1	1:E:31:LEU:HB2	2.42	0.49
1:E:145:LEU:O	1:E:146:GLU:C	2.51	0.49
1:F:41:ILE:HA	1:Q:7:ASN:HD22	1.77	0.49
1:G:19:ILE:CD1	1:G:31:LEU:HB2	2.42	0.49
1:K:19:ILE:HD11	1:K:31:LEU:HB2	1.94	0.49
1:K:128:ARG:HH11	1:K:128:ARG:HG3	1.77	0.49
1:L:2:ASN:HD21	1:M:50:THR:HG22	1.76	0.49
1:V:19:ILE:CD1	1:V:31:LEU:HB2	2.42	0.49
1:W:39:THR:OG1	1:W:40:ARG:N	2.45	0.49
1:Z:76:VAL:HB	1:Z:112:VAL:HG22	1.93	0.49
1:D:122:ILE:H	1:D:122:ILE:CD1	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:ALA:HA	1:H:60:LEU:HG	1.94	0.49
1:N:35:VAL:HG23	1:N:36:ASP:N	2.27	0.49
1:P:24:GLN:O	1:P:26:ILE:N	2.45	0.49
1:R:119:THR:HA	1:S:87:THR:HB	1.94	0.49
1:V:119:THR:HA	1:W:87:THR:HB	1.93	0.49
1:V:145:LEU:O	1:V:146:GLU:C	2.49	0.49
1:1:57:ALA:HA	1:1:60:LEU:HG	1.95	0.49
1:A:16:ALA:CB	1:A:67:LEU:HD13	2.41	0.49
1:A:24:GLN:O	1:A:26:ILE:N	2.46	0.49
1:D:16:ALA:CB	1:D:67:LEU:HD13	2.42	0.49
1:E:146:GLU:O	1:E:150:VAL:HG23	2.12	0.49
1:F:16:ALA:O	1:F:76:VAL:HA	2.13	0.49
1:M:22:PHE:HD1	1:M:23:ASN:H	1.59	0.49
1:S:121:SER:OG	1:S:123:GLU:HB3	2.13	0.49
1:Y:17:ILE:HG12	1:Y:77:VAL:HB	1.95	0.49
1:H:145:LEU:O	1:H:148:ILE:HB	2.13	0.49
1:M:19:ILE:CD1	1:M:31:LEU:HB2	2.43	0.49
1:O:22:PHE:HD1	1:O:23:ASN:N	2.11	0.49
1:T:135:ASN:O	1:T:137:GLY:N	2.44	0.49
1:U:128:ARG:HG3	1:U:128:ARG:HH11	1.77	0.49
1:J:37:ALA:HB1	1:J:142:LEU:CD2	2.43	0.49
1:P:35:VAL:HG23	1:P:36:ASP:N	2.27	0.49
1:P:87:THR:HB	1:T:119:THR:HA	1.95	0.49
1:1:7:ASN:CG	1:1:8:VAL:H	2.15	0.49
1:2:145:LEU:O	1:2:146:GLU:C	2.51	0.49
1:3:19:ILE:HG21	1:3:53:TRP:CZ3	2.48	0.49
1:E:57:ALA:HA	1:E:60:LEU:HG	1.94	0.49
1:K:67:LEU:HD22	1:K:73:TYR:CE2	2.48	0.49
1:N:22:PHE:HD1	1:N:23:ASN:H	1.60	0.49
1:S:76:VAL:HB	1:S:112:VAL:HG22	1.95	0.49
1:W:57:ALA:HA	1:W:60:LEU:HG	1.94	0.49
1:W:128:ARG:HH11	1:W:128:ARG:HG3	1.78	0.49
1:B:145:LEU:O	1:B:148:ILE:N	2.45	0.49
1:O:57:ALA:HA	1:O:60:LEU:HG	1.94	0.49
1:U:145:LEU:O	1:U:146:GLU:C	2.50	0.49
1:W:11:PRO:HG2	1:W:12:ASP:OD2	2.12	0.49
1:W:24:GLN:O	1:W:26:ILE:N	2.46	0.49
1:2:5:LYS:HD3	1:3:21:ARG:HH22	1.78	0.49
1:O:113:ALA:HB1	1:O:140:ALA:HB1	1.95	0.48
1:Q:145:LEU:O	1:Q:146:GLU:C	2.51	0.48
1:V:39:THR:OG1	1:V:40:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:37:ALA:HB1	1:W:142:LEU:CD2	2.43	0.48
1:X:19:ILE:HD11	1:X:31:LEU:HB2	1.95	0.48
1:2:146:GLU:O	1:2:150:VAL:HG23	2.12	0.48
1:3:14:ARG:HA	1:3:48:ASN:HB3	1.95	0.48
1:M:2:ASN:O	1:N:50:THR:HA	2.13	0.48
1:M:118:THR:HG21	1:N:92:TYR:CE2	2.48	0.48
1:P:120:GLU:HB2	1:P:124:GLN:OE1	2.13	0.48
1:S:22:PHE:HD1	1:S:23:ASN:H	1.60	0.48
1:U:24:GLN:O	1:U:26:ILE:N	2.46	0.48
1:2:57:ALA:HA	1:2:60:LEU:HG	1.94	0.48
1:C:16:ALA:O	1:C:76:VAL:HA	2.14	0.48
1:I:7:ASN:ND2	1:O:41:ILE:HD13	2.24	0.48
1:J:57:ALA:HA	1:J:60:LEU:HG	1.95	0.48
1:L:128:ARG:HH11	1:L:128:ARG:HG3	1.77	0.48
1:O:19:ILE:CD1	1:O:31:LEU:HB2	2.43	0.48
1:X:113:ALA:HB1	1:X:140:ALA:HB1	1.95	0.48
1:2:142:LEU:HD22	1:2:142:LEU:H	1.76	0.48
1:3:16:ALA:O	1:3:76:VAL:HA	2.13	0.48
1:C:127:GLU:HA	1:C:131:THR:OG1	2.13	0.48
1:D:35:VAL:HG23	1:D:36:ASP:N	2.29	0.48
1:G:145:LEU:O	1:G:146:GLU:C	2.51	0.48
1:S:120:GLU:HB2	1:S:124:GLN:OE1	2.14	0.48
1:T:35:VAL:HG23	1:T:36:ASP:N	2.28	0.48
1:V:120:GLU:HB2	1:V:124:GLN:OE1	2.13	0.48
1:Y:60:LEU:O	1:Y:64:THR:HG23	2.13	0.48
1:Z:145:LEU:O	1:Z:146:GLU:C	2.52	0.48
1:2:37:ALA:HB1	1:2:142:LEU:HD21	1.95	0.48
1:A:25:PHE:CE1	1:N:126:ILE:HD13	2.48	0.48
1:D:24:GLN:O	1:D:26:ILE:N	2.46	0.48
1:L:57:ALA:HA	1:L:60:LEU:HG	1.96	0.48
1:P:22:PHE:O	1:P:23:ASN:HB2	2.14	0.48
1:Q:19:ILE:CD1	1:Q:31:LEU:HB2	2.43	0.48
1:Q:145:LEU:O	1:Q:148:ILE:N	2.45	0.48
1:T:7:ASN:ND2	1:3:41:ILE:HD13	2.27	0.48
1:Y:22:PHE:HD1	1:Y:23:ASN:H	1.61	0.48
1:2:1:MET:HE2	1:3:46:ASP:HB2	1.95	0.48
1:4:135:ASN:O	1:4:137:GLY:N	2.47	0.48
1:A:122:ILE:CD1	1:N:132:LYS:HD2	2.42	0.48
1:B:126:ILE:CG2	1:V:122:ILE:HG21	2.44	0.48
1:D:145:LEU:O	1:D:148:ILE:N	2.47	0.48
1:G:35:VAL:HG23	1:G:36:ASP:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:GLN:O	1:L:26:ILE:N	2.47	0.48
1:M:5:LYS:HE2	1:N:53:TRP:CD2	2.49	0.48
1:R:14:ARG:HA	1:R:48:ASN:HB3	1.96	0.48
1:Y:16:ALA:CB	1:Y:67:LEU:HD13	2.44	0.48
1:G:4:ILE:HD12	1:H:52:VAL:HG22	1.95	0.48
1:H:17:ILE:HG12	1:H:77:VAL:HB	1.94	0.48
1:N:22:PHE:HD1	1:N:23:ASN:N	2.12	0.48
1:P:21:ARG:HH22	1:T:5:LYS:HD3	1.77	0.48
1:R:13:ALA:HB1	1:R:74:ASP:HB2	1.95	0.48
1:Z:38:LEU:CD2	1:Z:141:ALA:HB1	2.44	0.48
1:4:24:GLN:O	1:4:26:ILE:N	2.46	0.48
1:A:146:GLU:O	1:A:150:VAL:HG23	2.14	0.48
1:B:37:ALA:HB1	1:B:142:LEU:HD21	1.95	0.48
1:E:37:ALA:HB1	1:E:142:LEU:CD2	2.43	0.48
1:F:22:PHE:HD1	1:F:23:ASN:H	1.61	0.48
1:F:76:VAL:HB	1:F:112:VAL:HG22	1.95	0.48
1:G:24:GLN:O	1:G:26:ILE:N	2.46	0.48
1:G:122:ILE:H	1:G:122:ILE:CD1	2.13	0.48
1:M:114:PHE:HB2	1:N:58:TYR:CE2	2.48	0.48
1:N:128:ARG:HH11	1:N:128:ARG:HG3	1.79	0.48
1:P:10:ALA:N	1:P:11:PRO:CD	2.76	0.48
1:R:128:ARG:HH11	1:R:128:ARG:HG3	1.79	0.48
1:V:37:ALA:HB1	1:V:142:LEU:CD2	2.42	0.48
1:Z:37:ALA:HB1	1:Z:142:LEU:CD2	2.44	0.48
1:A:35:VAL:HG23	1:A:36:ASP:N	2.28	0.48
1:B:52:VAL:HG21	1:B:67:LEU:HD11	1.95	0.48
1:R:121:SER:OG	1:R:123:GLU:HB3	2.13	0.48
1:V:35:VAL:HG23	1:V:36:ASP:N	2.29	0.48
1:W:19:ILE:CD1	1:W:31:LEU:HB2	2.44	0.48
1:W:76:VAL:HB	1:W:112:VAL:HG22	1.96	0.48
1:Y:37:ALA:HB1	1:Y:142:LEU:CD2	2.43	0.48
1:1:145:LEU:O	1:1:146:GLU:C	2.52	0.48
1:2:16:ALA:O	1:2:76:VAL:HA	2.14	0.48
1:3:145:LEU:O	1:3:146:GLU:C	2.53	0.48
1:A:16:ALA:O	1:A:76:VAL:HA	2.13	0.48
1:C:145:LEU:O	1:C:148:ILE:HB	2.14	0.48
1:E:145:LEU:HA	1:E:148:ILE:HD12	1.95	0.48
1:I:126:ILE:CG2	1:K:122:ILE:HG21	2.43	0.48
1:O:19:ILE:HD11	1:O:31:LEU:HB2	1.96	0.48
1:O:145:LEU:O	1:O:146:GLU:C	2.52	0.48
1:Z:39:THR:OG1	1:Z:40:ARG:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ILE:HD12	1:D:122:ILE:N	2.24	0.47
1:H:39:THR:OG1	1:H:40:ARG:N	2.47	0.47
1:L:35:VAL:HG23	1:L:36:ASP:N	2.29	0.47
1:O:19:ILE:CG2	1:O:53:TRP:CZ3	2.97	0.47
1:T:145:LEU:O	1:T:148:ILE:N	2.47	0.47
1:V:19:ILE:HD11	1:V:31:LEU:HB2	1.96	0.47
1:W:67:LEU:HD22	1:W:73:TYR:CE2	2.49	0.47
1:Z:92:TYR:OH	1:4:94:ALA:HB3	2.14	0.47
1:1:17:ILE:HG12	1:1:77:VAL:HB	1.96	0.47
1:4:17:ILE:HG12	1:4:77:VAL:HB	1.95	0.47
1:4:35:VAL:HG23	1:4:36:ASP:N	2.30	0.47
1:4:52:VAL:HG21	1:4:67:LEU:HD11	1.95	0.47
1:E:22:PHE:HD1	1:E:23:ASN:H	1.62	0.47
1:F:19:ILE:HG12	1:F:79:LEU:HB2	1.95	0.47
1:G:39:THR:OG1	1:G:40:ARG:N	2.47	0.47
1:G:142:LEU:HD22	1:G:142:LEU:H	1.79	0.47
1:N:57:ALA:HA	1:N:60:LEU:HG	1.95	0.47
1:N:122:ILE:H	1:N:122:ILE:CD1	2.11	0.47
1:R:120:GLU:HB2	1:R:124:GLN:OE1	2.14	0.47
1:1:22:PHE:HD1	1:1:23:ASN:H	1.62	0.47
1:M:4:ILE:HD12	1:N:52:VAL:HG22	1.97	0.47
1:P:37:ALA:HB1	1:P:142:LEU:CD2	2.45	0.47
1:T:19:ILE:CD1	1:T:31:LEU:HB2	2.45	0.47
1:A:57:ALA:HA	1:A:60:LEU:HG	1.96	0.47
1:C:11:PRO:HA	1:C:43:GLN:O	2.15	0.47
1:F:57:ALA:HA	1:F:60:LEU:HG	1.97	0.47
1:J:39:THR:OG1	1:J:40:ARG:N	2.46	0.47
1:L:22:PHE:HD1	1:L:23:ASN:H	1.60	0.47
1:Q:135:ASN:O	1:Q:137:GLY:N	2.48	0.47
1:R:17:ILE:HG12	1:R:77:VAL:HB	1.96	0.47
1:R:27:ASN:O	1:R:30:LEU:HB2	2.15	0.47
1:W:113:ALA:HB1	1:W:140:ALA:HB1	1.96	0.47
1:B:135:ASN:O	1:B:137:GLY:N	2.47	0.47
1:I:122:ILE:H	1:I:122:ILE:CD1	2.15	0.47
1:K:88:ALA:HB1	1:K:91:GLU:HB2	1.96	0.47
1:Q:141:ALA:O	1:Q:144:ALA:HB3	2.14	0.47
1:R:68:ALA:HB1	1:R:110:VAL:HG21	1.96	0.47
1:S:19:ILE:CD1	1:S:31:LEU:HB2	2.45	0.47
1:A:68:ALA:HB1	1:A:110:VAL:HG21	1.97	0.47
1:3:19:ILE:CD1	1:3:31:LEU:HB2	2.44	0.47
1:B:39:THR:OG1	1:B:40:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ASN:HD22	1:R:41:ILE:HA	1.79	0.47
1:K:145:LEU:O	1:K:148:ILE:N	2.46	0.47
1:M:128:ARG:HG3	1:M:128:ARG:NH1	2.28	0.47
1:U:19:ILE:CD1	1:U:31:LEU:HB2	2.44	0.47
1:W:135:ASN:O	1:W:137:GLY:N	2.48	0.47
1:X:60:LEU:O	1:X:64:THR:HG23	2.14	0.47
1:X:145:LEU:O	1:X:148:ILE:HB	2.14	0.47
1:1:16:ALA:O	1:1:76:VAL:HA	2.14	0.47
1:1:94:ALA:HB3	1:2:92:TYR:OH	2.15	0.47
1:2:19:ILE:HG21	1:2:53:TRP:CZ3	2.49	0.47
1:3:19:ILE:HD11	1:3:31:LEU:HB2	1.96	0.47
1:3:145:LEU:HA	1:3:148:ILE:HD12	1.95	0.47
1:A:19:ILE:CD1	1:A:31:LEU:HB2	2.44	0.47
1:D:122:ILE:HD11	1:R:132:LYS:CD	2.41	0.47
1:L:22:PHE:HD1	1:L:23:ASN:N	2.13	0.47
1:L:120:GLU:HB2	1:L:124:GLN:OE1	2.14	0.47
1:O:37:ALA:HB1	1:O:142:LEU:CD2	2.44	0.47
1:P:76:VAL:HB	1:P:112:VAL:HG22	1.96	0.47
1:S:1:MET:HE2	1:T:46:ASP:HB2	1.96	0.47
1:T:146:GLU:O	1:T:150:VAL:HG23	2.15	0.47
1:U:11:PRO:HB3	1:U:43:GLN:HB3	1.96	0.47
1:I:132:LYS:CD	1:K:122:ILE:HD11	2.44	0.47
1:T:126:ILE:HG21	1:4:122:ILE:HG21	1.96	0.47
1:Y:128:ARG:HH11	1:Y:128:ARG:HG3	1.80	0.47
1:Z:19:ILE:HD11	1:Z:31:LEU:HB2	1.96	0.47
1:1:19:ILE:HD11	1:1:31:LEU:HB2	1.97	0.47
1:A:50:THR:HG22	1:E:2:ASN:HD21	1.80	0.47
1:B:41:ILE:HD13	1:U:7:ASN:ND2	2.29	0.47
1:F:11:PRO:HA	1:F:43:GLN:O	2.16	0.47
1:F:25:PHE:O	1:F:25:PHE:CG	2.68	0.47
1:F:145:LEU:O	1:F:148:ILE:HB	2.15	0.47
1:H:22:PHE:HD1	1:H:23:ASN:H	1.63	0.47
1:L:19:ILE:HD11	1:L:31:LEU:HB2	1.97	0.47
1:M:62:LEU:HA	1:M:62:LEU:HD23	1.76	0.47
1:P:2:ASN:HD21	1:Q:50:THR:HG22	1.80	0.47
1:Y:19:ILE:CD1	1:Y:31:LEU:HB2	2.45	0.47
1:Y:39:THR:OG1	1:Y:40:ARG:N	2.47	0.47
1:3:135:ASN:O	1:3:137:GLY:N	2.48	0.47
1:A:17:ILE:HG12	1:A:77:VAL:HB	1.97	0.46
1:A:69:LYS:O	1:A:70:SER:C	2.52	0.46
1:F:19:ILE:CG2	1:F:53:TRP:CZ3	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ALA:O	1:F:145:LEU:HG	2.14	0.46
1:L:146:GLU:O	1:L:150:VAL:HG23	2.15	0.46
1:Q:17:ILE:HG12	1:Q:77:VAL:HB	1.97	0.46
1:R:57:ALA:HA	1:R:60:LEU:HG	1.97	0.46
1:Z:19:ILE:HG12	1:Z:79:LEU:CB	2.45	0.46
1:1:19:ILE:CD1	1:1:31:LEU:HB2	2.45	0.46
1:C:4:ILE:HD12	1:D:52:VAL:HG22	1.98	0.46
1:C:19:ILE:CD1	1:C:31:LEU:HB2	2.45	0.46
1:E:67:LEU:HD22	1:E:73:TYR:CE2	2.51	0.46
1:F:118:THR:HG21	1:G:92:TYR:CE2	2.50	0.46
1:F:120:GLU:HB2	1:F:124:GLN:OE1	2.15	0.46
1:I:122:ILE:HD12	1:I:122:ILE:N	2.19	0.46
1:L:145:LEU:O	1:L:148:ILE:HB	2.16	0.46
1:M:1:MET:HE2	1:N:46:ASP:HB2	1.96	0.46
1:O:128:ARG:HH11	1:O:128:ARG:HG3	1.79	0.46
1:P:17:ILE:HG12	1:P:77:VAL:HB	1.98	0.46
1:U:25:PHE:O	1:U:25:PHE:CG	2.67	0.46
1:1:37:ALA:HB1	1:1:142:LEU:CD2	2.45	0.46
1:1:154:ILE:HG21	1:2:67:LEU:HD23	1.97	0.46
1:A:92:TYR:CE2	1:E:118:THR:HG21	2.51	0.46
1:B:119:THR:HA	1:C:87:THR:HB	1.98	0.46
1:D:145:LEU:O	1:D:146:GLU:C	2.54	0.46
1:F:35:VAL:HG23	1:F:36:ASP:N	2.30	0.46
1:G:10:ALA:N	1:G:11:PRO:HD2	2.24	0.46
1:G:113:ALA:HB1	1:G:140:ALA:HB1	1.98	0.46
1:M:39:THR:OG1	1:M:40:ARG:N	2.48	0.46
1:N:4:ILE:HD12	1:O:52:VAL:HG22	1.95	0.46
1:S:41:ILE:HD12	1:Y:8:VAL:HG22	1.97	0.46
1:T:24:GLN:O	1:T:26:ILE:N	2.48	0.46
1:V:13:ALA:HB1	1:V:74:ASP:HB2	1.97	0.46
1:Y:22:PHE:HD1	1:Y:23:ASN:N	2.13	0.46
1:1:2:ASN:HD21	1:2:50:THR:HG22	1.80	0.46
1:2:16:ALA:CB	1:2:67:LEU:HD13	2.45	0.46
1:2:19:ILE:HG12	1:2:79:LEU:HB2	1.97	0.46
1:B:4:ILE:HD12	1:C:52:VAL:HG22	1.98	0.46
1:F:138:ALA:O	1:F:142:LEU:HD22	2.15	0.46
1:I:22:PHE:HD1	1:I:23:ASN:H	1.63	0.46
1:K:22:PHE:HD1	1:K:23:ASN:N	2.13	0.46
1:M:154:ILE:HD13	1:N:67:LEU:CD2	2.45	0.46
1:O:17:ILE:HG12	1:O:77:VAL:HB	1.97	0.46
1:P:121:SER:OG	1:P:123:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:145:LEU:O	1:P:148:ILE:HB	2.15	0.46
1:Q:76:VAL:HB	1:Q:112:VAL:HG22	1.97	0.46
1:Q:122:ILE:H	1:Q:122:ILE:CD1	2.10	0.46
1:U:22:PHE:HD1	1:U:23:ASN:H	1.63	0.46
1:H:89:HIS:HB3	2:H:157:SO4:O4	2.16	0.46
1:I:145:LEU:O	1:I:146:GLU:C	2.54	0.46
1:P:146:GLU:O	1:P:150:VAL:HG23	2.16	0.46
1:R:13:ALA:HB1	1:R:74:ASP:CB	2.45	0.46
1:X:22:PHE:HD1	1:X:23:ASN:H	1.63	0.46
1:C:19:ILE:CG2	1:C:53:TRP:CZ3	2.98	0.46
1:D:126:ILE:HD13	1:F:25:PHE:CE1	2.50	0.46
1:M:22:PHE:HD1	1:M:23:ASN:N	2.14	0.46
1:M:143:THR:HG22	1:N:55:PRO:HB2	1.97	0.46
1:P:22:PHE:HD1	1:P:23:ASN:H	1.62	0.46
1:W:119:THR:HA	1:X:87:THR:HB	1.98	0.46
1:3:37:ALA:HB1	1:3:142:LEU:CD2	2.45	0.46
1:A:39:THR:OG1	1:A:40:ARG:N	2.48	0.46
1:B:132:LYS:CD	1:V:122:ILE:HD11	2.46	0.46
1:C:62:LEU:HD23	1:C:62:LEU:HA	1.76	0.46
1:E:41:ILE:HA	1:N:7:ASN:HD22	1.81	0.46
1:I:35:VAL:HG23	1:I:36:ASP:H	1.81	0.46
1:N:24:GLN:O	1:N:26:ILE:N	2.49	0.46
1:S:16:ALA:CB	1:S:67:LEU:HD13	2.43	0.46
1:T:19:ILE:HG12	1:T:79:LEU:HB2	1.98	0.46
1:U:145:LEU:O	1:U:148:ILE:N	2.49	0.46
1:W:17:ILE:HG12	1:W:77:VAL:HB	1.98	0.46
1:Y:24:GLN:O	1:Y:26:ILE:N	2.49	0.46
1:3:146:GLU:O	1:3:150:VAL:HG23	2.15	0.46
1:A:141:ALA:O	1:A:144:ALA:HB3	2.14	0.46
1:D:39:THR:OG1	1:D:40:ARG:N	2.47	0.46
1:E:7:ASN:HD22	1:N:41:ILE:HA	1.76	0.46
1:F:128:ARG:NH2	2:F:158:SO4:O3	2.48	0.46
1:I:17:ILE:HG12	1:I:77:VAL:HB	1.98	0.46
1:O:16:ALA:CB	1:O:67:LEU:HD13	2.44	0.46
1:T:22:PHE:HD1	1:T:23:ASN:H	1.63	0.46
1:U:16:ALA:O	1:U:76:VAL:HA	2.16	0.46
1:U:118:THR:HG21	1:V:92:TYR:CE2	2.50	0.46
1:3:17:ILE:HG12	1:3:77:VAL:HB	1.97	0.46
1:4:19:ILE:HD11	1:4:31:LEU:HB2	1.97	0.46
1:A:52:VAL:HG21	1:A:67:LEU:HD11	1.97	0.46
1:J:22:PHE:HD1	1:J:23:ASN:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:145:LEU:O	1:N:148:ILE:N	2.49	0.46
1:P:62:LEU:HD13	1:T:151:LEU:HD11	1.97	0.46
1:Q:19:ILE:HG21	1:Q:53:TRP:CZ3	2.51	0.46
1:Q:22:PHE:HD1	1:Q:23:ASN:H	1.64	0.46
1:W:60:LEU:O	1:W:64:THR:HG23	2.15	0.46
1:A:19:ILE:HD11	1:A:31:LEU:HB2	1.98	0.46
1:D:22:PHE:HD1	1:D:23:ASN:H	1.62	0.46
1:J:60:LEU:HB2	1:J:61:PRO:HD3	1.96	0.46
1:Z:141:ALA:O	1:Z:145:LEU:HG	2.16	0.46
1:B:7:ASN:CG	1:B:8:VAL:H	2.19	0.45
1:K:17:ILE:HG12	1:K:77:VAL:HB	1.99	0.45
1:L:17:ILE:HG12	1:L:77:VAL:HB	1.98	0.45
1:P:113:ALA:HB1	1:P:140:ALA:HB1	1.97	0.45
1:S:145:LEU:O	1:S:148:ILE:HB	2.17	0.45
1:Z:67:LEU:HD22	1:Z:73:TYR:CE2	2.51	0.45
1:1:128:ARG:HH11	1:1:128:ARG:HG3	1.81	0.45
1:3:39:THR:OG1	1:3:40:ARG:N	2.48	0.45
1:4:57:ALA:HA	1:4:60:LEU:HG	1.98	0.45
1:B:17:ILE:HG12	1:B:77:VAL:HB	1.97	0.45
1:C:141:ALA:O	1:C:145:LEU:HG	2.16	0.45
1:D:57:ALA:HA	1:D:60:LEU:HG	1.98	0.45
1:E:19:ILE:HD11	1:E:31:LEU:HB2	1.98	0.45
1:G:5:LYS:HD3	1:H:21:ARG:HH22	1.80	0.45
1:H:1:MET:HE2	1:I:46:ASP:HB2	1.98	0.45
1:N:16:ALA:CB	1:N:67:LEU:HD13	2.45	0.45
1:P:67:LEU:HD22	1:P:73:TYR:CE2	2.50	0.45
1:R:113:ALA:HB1	1:R:140:ALA:HB1	1.97	0.45
1:T:67:LEU:HD22	1:T:73:TYR:CE2	2.51	0.45
1:Z:128:ARG:HG3	1:Z:128:ARG:NH1	2.31	0.45
1:4:127:GLU:HA	1:4:131:THR:OG1	2.16	0.45
1:B:22:PHE:HD1	1:B:23:ASN:N	2.14	0.45
1:C:19:ILE:HG12	1:C:79:LEU:HB2	1.97	0.45
1:C:119:THR:HA	1:D:87:THR:HB	1.98	0.45
1:E:39:THR:OG1	1:E:40:ARG:N	2.49	0.45
1:F:37:ALA:HB1	1:F:142:LEU:CD2	2.47	0.45
1:H:19:ILE:HD11	1:H:31:LEU:HB2	1.97	0.45
1:N:127:GLU:HA	1:N:131:THR:OG1	2.17	0.45
1:O:19:ILE:HG12	1:O:79:LEU:HB2	1.98	0.45
1:O:19:ILE:HG21	1:O:53:TRP:CZ3	2.52	0.45
1:P:16:ALA:O	1:P:76:VAL:HA	2.16	0.45
1:U:22:PHE:HD1	1:U:23:ASN:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:11:PRO:HA	1:2:43:GLN:O	2.16	0.45
1:D:22:PHE:HD1	1:D:23:ASN:N	2.14	0.45
1:F:22:PHE:HD1	1:F:23:ASN:N	2.15	0.45
1:K:16:ALA:O	1:K:76:VAL:HA	2.16	0.45
1:M:145:LEU:O	1:M:146:GLU:C	2.54	0.45
1:P:11:PRO:CB	1:P:43:GLN:O	2.64	0.45
1:R:145:LEU:O	1:R:146:GLU:C	2.55	0.45
1:T:126:ILE:CG2	1:4:122:ILE:HG21	2.46	0.45
1:W:16:ALA:O	1:W:76:VAL:HA	2.15	0.45
1:Y:16:ALA:O	1:Y:76:VAL:HA	2.17	0.45
1:1:145:LEU:O	1:1:148:ILE:HB	2.15	0.45
1:2:14:ARG:HA	1:2:48:ASN:HB3	1.97	0.45
1:F:41:ILE:HD13	1:Q:7:ASN:HD22	1.81	0.45
1:I:19:ILE:CD1	1:I:31:LEU:HB2	2.47	0.45
1:I:37:ALA:HB1	1:I:142:LEU:CD2	2.47	0.45
1:K:14:ARG:HA	1:K:48:ASN:HB3	1.97	0.45
1:N:19:ILE:HA	1:N:79:LEU:O	2.17	0.45
1:N:60:LEU:N	1:N:61:PRO:CD	2.80	0.45
1:Q:19:ILE:CG2	1:Q:53:TRP:CZ3	3.00	0.45
1:S:19:ILE:CG2	1:S:53:TRP:CZ3	3.00	0.45
1:U:5:LYS:HE2	1:V:53:TRP:CD2	2.52	0.45
1:Y:145:LEU:O	1:Y:148:ILE:N	2.49	0.45
1:Z:16:ALA:O	1:Z:76:VAL:HA	2.16	0.45
1:Z:98:SER:HA	1:Z:114:PHE:HE1	1.81	0.45
1:2:94:ALA:HB3	1:3:92:TYR:OH	2.17	0.45
1:3:35:VAL:HG23	1:3:36:ASP:N	2.31	0.45
1:B:145:LEU:O	1:B:148:ILE:HB	2.16	0.45
1:D:76:VAL:HB	1:D:112:VAL:HG22	1.98	0.45
1:E:19:ILE:HG12	1:E:79:LEU:HB2	1.98	0.45
1:E:78:ALA:O	1:E:79:LEU:HD12	2.17	0.45
1:F:122:ILE:HD12	1:F:122:ILE:N	2.19	0.45
1:G:62:LEU:HD23	1:G:62:LEU:HA	1.79	0.45
1:I:22:PHE:HD1	1:I:23:ASN:N	2.14	0.45
1:M:19:ILE:HD11	1:M:31:LEU:HB2	1.99	0.45
1:T:22:PHE:HD1	1:T:23:ASN:N	2.15	0.45
1:V:122:ILE:H	1:V:122:ILE:CD1	2.12	0.45
1:Y:57:ALA:HA	1:Y:60:LEU:HG	1.99	0.45
1:C:128:ARG:HH11	1:C:128:ARG:HG3	1.81	0.45
1:D:37:ALA:HB1	1:D:142:LEU:CD2	2.46	0.45
1:E:76:VAL:HB	1:E:112:VAL:HG22	1.99	0.45
1:F:7:ASN:ND2	1:Q:41:ILE:HD13	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:ALA:HB1	1:G:110:VAL:HG21	1.99	0.45
1:H:10:ALA:N	1:H:11:PRO:HD2	2.32	0.45
1:P:11:PRO:CA	1:P:43:GLN:O	2.65	0.45
1:U:19:ILE:HD11	1:U:31:LEU:HB2	1.98	0.45
1:1:122:ILE:HD12	1:1:122:ILE:N	2.15	0.45
1:A:76:VAL:HB	1:A:112:VAL:HG22	1.99	0.45
1:A:145:LEU:O	1:A:146:GLU:C	2.53	0.45
1:C:131:THR:HG23	1:S:25:PHE:HB3	1.98	0.45
1:D:141:ALA:O	1:D:145:LEU:HG	2.17	0.45
1:F:88:ALA:HB1	1:F:91:GLU:HB2	1.98	0.45
1:K:121:SER:OG	1:K:123:GLU:HB3	2.16	0.45
1:M:154:ILE:HD13	1:N:67:LEU:HD23	1.97	0.45
1:N:30:LEU:HD12	1:N:30:LEU:HA	1.81	0.45
1:P:62:LEU:HD23	1:P:62:LEU:HA	1.78	0.45
1:S:57:ALA:HA	1:S:60:LEU:HG	1.99	0.45
1:S:122:ILE:H	1:S:122:ILE:CD1	2.13	0.45
1:T:19:ILE:CG2	1:T:53:TRP:CZ3	3.00	0.45
1:U:19:ILE:HG21	1:U:53:TRP:CZ3	2.51	0.45
1:U:38:LEU:CD2	1:U:141:ALA:HB1	2.47	0.45
1:Z:1:MET:HA	1:1:46:ASP:O	2.16	0.45
1:Z:19:ILE:CG2	1:Z:53:TRP:CZ3	2.99	0.45
1:2:98:SER:HA	1:2:114:PHE:HE1	1.81	0.45
1:E:17:ILE:HG12	1:E:77:VAL:HB	1.99	0.45
1:F:67:LEU:CD2	1:J:154:ILE:HD13	2.47	0.45
1:F:126:ILE:CG2	1:R:122:ILE:HG21	2.47	0.45
1:R:141:ALA:O	1:R:145:LEU:HG	2.16	0.45
1:3:60:LEU:HB2	1:3:61:PRO:HD3	1.99	0.45
1:B:5:LYS:HD3	1:C:21:ARG:HH22	1.82	0.45
1:C:30:LEU:HD12	1:C:30:LEU:HA	1.83	0.45
1:C:94:ALA:HB3	1:D:92:TYR:OH	2.17	0.45
1:E:135:ASN:O	1:E:137:GLY:N	2.50	0.45
1:H:19:ILE:CG2	1:H:53:TRP:CZ3	3.00	0.45
1:H:122:ILE:H	1:H:122:ILE:CD1	2.12	0.45
1:L:60:LEU:O	1:L:64:THR:HG23	2.17	0.45
1:L:145:LEU:O	1:L:146:GLU:C	2.56	0.45
1:Q:61:PRO:O	1:Q:64:THR:N	2.50	0.45
1:W:145:LEU:O	1:W:148:ILE:HB	2.17	0.45
1:X:88:ALA:HB1	1:X:91:GLU:HB2	1.99	0.45
1:2:67:LEU:HD22	1:2:73:TYR:CE2	2.52	0.45
1:E:22:PHE:HD1	1:E:23:ASN:N	2.15	0.44
1:G:60:LEU:HB2	1:G:61:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:ALA:HB1	1:K:142:LEU:CD2	2.46	0.44
1:M:1:MET:CB	1:N:46:ASP:O	2.65	0.44
1:U:60:LEU:N	1:U:61:PRO:CD	2.79	0.44
1:U:94:ALA:HB3	1:V:92:TYR:OH	2.18	0.44
1:W:5:LYS:HD3	1:X:21:ARG:HH22	1.82	0.44
1:W:42:GLY:HA3	1:W:145:LEU:CD1	2.47	0.44
1:2:69:LYS:O	1:2:70:SER:C	2.56	0.44
1:4:128:ARG:HH11	1:4:128:ARG:HG3	1.82	0.44
1:F:21:ARG:O	1:F:24:GLN:HB2	2.17	0.44
1:I:16:ALA:O	1:I:76:VAL:HA	2.17	0.44
1:L:52:VAL:HG21	1:L:67:LEU:HD11	1.98	0.44
1:O:145:LEU:O	1:O:148:ILE:N	2.51	0.44
1:P:16:ALA:CB	1:P:67:LEU:HD13	2.47	0.44
1:P:50:THR:HA	1:T:2:ASN:O	2.16	0.44
1:Q:52:VAL:HG21	1:Q:67:LEU:HD11	1.99	0.44
1:Q:61:PRO:HA	1:Q:101:LEU:HD23	1.99	0.44
1:R:16:ALA:O	1:R:76:VAL:HA	2.17	0.44
1:R:16:ALA:CB	1:R:67:LEU:HD13	2.45	0.44
1:U:145:LEU:O	1:U:148:ILE:HB	2.17	0.44
1:V:16:ALA:O	1:V:76:VAL:HA	2.17	0.44
1:D:19:ILE:CG2	1:D:53:TRP:CZ3	3.01	0.44
1:E:88:ALA:HB1	1:E:91:GLU:HB2	1.99	0.44
1:G:19:ILE:HD11	1:G:31:LEU:HB2	1.98	0.44
1:H:19:ILE:HG12	1:H:79:LEU:HB2	1.99	0.44
1:L:121:SER:OG	1:L:123:GLU:HB3	2.18	0.44
1:M:1:MET:HA	1:N:46:ASP:O	2.18	0.44
1:M:54:VAL:CG1	1:M:63:ALA:HB2	2.47	0.44
1:R:22:PHE:HD1	1:R:23:ASN:N	2.15	0.44
1:X:37:ALA:HB1	1:X:142:LEU:CD2	2.47	0.44
1:1:60:LEU:HB2	1:1:61:PRO:HD3	2.00	0.44
1:3:13:ALA:HB1	1:3:74:ASP:CG	2.38	0.44
1:3:145:LEU:O	1:3:148:ILE:N	2.51	0.44
1:4:22:PHE:HD1	1:4:23:ASN:H	1.63	0.44
1:H:52:VAL:HG21	1:H:67:LEU:HD11	2.00	0.44
1:H:121:SER:OG	1:H:123:GLU:HB3	2.17	0.44
1:K:50:THR:HA	1:O:2:ASN:O	2.17	0.44
1:L:94:ALA:HB3	1:M:92:TYR:OH	2.17	0.44
1:M:76:VAL:HB	1:M:112:VAL:HG22	1.99	0.44
1:P:88:ALA:HB1	1:P:91:GLU:HB2	2.00	0.44
1:S:54:VAL:HB	1:S:55:PRO:HD2	1.98	0.44
1:U:54:VAL:CG1	1:U:63:ALA:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:HG23	1:C:36:ASP:N	2.32	0.44
1:C:60:LEU:O	1:C:64:THR:HG23	2.18	0.44
1:D:19:ILE:HG12	1:D:79:LEU:HB2	1.99	0.44
1:E:131:THR:HA	1:O:23:ASN:HA	1.99	0.44
1:G:154:ILE:HD13	1:H:67:LEU:CD2	2.48	0.44
1:H:16:ALA:O	1:H:76:VAL:HA	2.17	0.44
1:K:76:VAL:HB	1:K:112:VAL:HG22	1.99	0.44
1:M:24:GLN:O	1:M:26:ILE:N	2.50	0.44
1:U:62:LEU:HD23	1:U:62:LEU:HA	1.78	0.44
1:V:22:PHE:HD1	1:V:23:ASN:N	2.16	0.44
1:V:128:ARG:HG3	1:V:128:ARG:NH1	2.32	0.44
1:X:142:LEU:HD22	1:X:142:LEU:H	1.83	0.44
1:Y:113:ALA:HB1	1:Y:140:ALA:HB1	2.00	0.44
1:2:120:GLU:HB2	1:2:124:GLN:OE1	2.18	0.44
1:A:30:LEU:HD12	1:A:30:LEU:HA	1.89	0.44
1:A:86:GLY:N	2:A:157:SO4:O1	2.50	0.44
1:D:25:PHE:CE1	1:F:25:PHE:HZ	2.36	0.44
1:D:41:ILE:HD12	1:J:8:VAL:HG22	2.00	0.44
1:J:19:ILE:CG2	1:J:53:TRP:CZ3	3.01	0.44
1:J:69:LYS:O	1:J:70:SER:C	2.56	0.44
1:L:22:PHE:CD1	1:L:23:ASN:N	2.86	0.44
1:M:1:MET:HB2	1:N:46:ASP:O	2.18	0.44
1:M:16:ALA:CB	1:M:67:LEU:HD13	2.47	0.44
1:N:22:PHE:CD1	1:N:23:ASN:N	2.86	0.44
1:O:22:PHE:CD1	1:O:23:ASN:N	2.85	0.44
1:Q:37:ALA:HB1	1:Q:142:LEU:CD2	2.47	0.44
1:Q:57:ALA:HA	1:Q:60:LEU:HG	1.98	0.44
1:W:16:ALA:CB	1:W:67:LEU:HD13	2.46	0.44
1:W:145:LEU:O	1:W:146:GLU:C	2.56	0.44
1:X:98:SER:HA	1:X:114:PHE:HE1	1.83	0.44
1:Y:62:LEU:HD23	1:Y:62:LEU:HA	1.81	0.44
1:2:62:LEU:HD23	1:2:62:LEU:HA	1.79	0.44
1:2:88:ALA:HB1	1:2:91:GLU:HB2	1.99	0.44
1:3:128:ARG:HH11	1:3:128:ARG:HG3	1.83	0.44
1:3:141:ALA:O	1:3:145:LEU:HG	2.17	0.44
1:A:54:VAL:HB	1:A:55:PRO:HD2	2.00	0.44
1:C:19:ILE:HG21	1:C:53:TRP:CZ3	2.52	0.44
1:D:16:ALA:O	1:D:76:VAL:HA	2.18	0.44
1:D:19:ILE:HG21	1:D:53:TRP:CZ3	2.52	0.44
1:F:128:ARG:HH11	1:F:128:ARG:HG3	1.82	0.44
1:G:37:ALA:HB1	1:G:142:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:18:THR:HG22	1:J:52:VAL:HB	2.00	0.44
1:M:16:ALA:O	1:M:76:VAL:HA	2.17	0.44
1:M:145:LEU:O	1:M:148:ILE:HB	2.18	0.44
1:O:19:ILE:HG12	1:O:79:LEU:CB	2.48	0.44
1:P:1:MET:HE2	1:Q:46:ASP:HB2	2.00	0.44
1:P:22:PHE:HD1	1:P:23:ASN:N	2.15	0.44
1:P:128:ARG:HG3	1:P:128:ARG:HH11	1.83	0.44
1:S:119:THR:HA	1:T:87:THR:HB	1.99	0.44
1:V:4:ILE:HD12	1:W:52:VAL:HG22	1.99	0.44
1:V:22:PHE:HD1	1:V:23:ASN:H	1.66	0.44
1:Z:19:ILE:HG12	1:Z:79:LEU:HB2	2.00	0.44
1:2:128:ARG:HG3	1:2:128:ARG:NH1	2.32	0.44
1:B:128:ARG:HG3	1:B:128:ARG:NH1	2.33	0.44
1:C:57:ALA:HA	1:C:60:LEU:HG	1.98	0.44
1:C:132:LYS:HD2	1:S:122:ILE:CD1	2.43	0.44
1:G:135:ASN:O	1:G:137:GLY:N	2.51	0.44
1:K:22:PHE:CD1	1:K:23:ASN:N	2.86	0.44
1:K:25:PHE:O	1:K:25:PHE:CG	2.71	0.44
1:L:145:LEU:O	1:L:148:ILE:N	2.50	0.44
1:R:145:LEU:O	1:R:148:ILE:HB	2.18	0.44
1:S:37:ALA:HB1	1:S:142:LEU:CD2	2.47	0.44
1:U:19:ILE:CG2	1:U:53:TRP:CZ3	3.00	0.44
1:V:19:ILE:CG2	1:V:53:TRP:CZ3	3.01	0.44
1:V:76:VAL:HB	1:V:112:VAL:HG22	2.00	0.44
1:V:135:ASN:O	1:V:137:GLY:N	2.51	0.44
1:Z:19:ILE:HG21	1:Z:53:TRP:CZ3	2.53	0.44
1:Z:27:ASN:O	1:Z:30:LEU:HB2	2.18	0.44
1:1:19:ILE:HG12	1:1:79:LEU:HB2	1.99	0.44
1:1:22:PHE:HD1	1:1:23:ASN:N	2.16	0.44
1:2:52:VAL:HG21	1:2:67:LEU:HD11	2.00	0.44
1:B:2:ASN:H	1:B:2:ASN:ND2	2.13	0.44
1:C:122:ILE:H	1:C:122:ILE:CD1	2.12	0.44
1:E:30:LEU:HD12	1:E:30:LEU:HA	1.81	0.44
1:E:145:LEU:O	1:E:148:ILE:HB	2.18	0.44
1:F:19:ILE:CD1	1:F:31:LEU:HB2	2.48	0.44
1:F:24:GLN:O	1:F:26:ILE:N	2.51	0.44
1:I:19:ILE:HG12	1:I:79:LEU:CB	2.48	0.44
1:P:57:ALA:HA	1:P:60:LEU:HG	2.00	0.44
1:Q:24:GLN:C	1:Q:26:ILE:N	2.70	0.44
1:V:12:ASP:O	1:V:48:ASN:ND2	2.51	0.44
1:V:68:ALA:HB1	1:V:110:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:21:ARG:O	1:Y:24:GLN:HB2	2.18	0.44
1:Z:30:LEU:HD12	1:Z:30:LEU:HA	1.82	0.44
1:F:55:PRO:CB	1:J:143:THR:HG22	2.48	0.43
1:G:22:PHE:HD1	1:G:23:ASN:H	1.65	0.43
1:G:141:ALA:O	1:G:145:LEU:HG	2.18	0.43
1:H:19:ILE:HG21	1:H:53:TRP:CZ3	2.53	0.43
1:H:76:VAL:HB	1:H:112:VAL:HG22	2.00	0.43
1:L:16:ALA:O	1:L:76:VAL:HA	2.18	0.43
1:N:19:ILE:HD11	1:N:31:LEU:HB2	1.99	0.43
1:N:19:ILE:HG12	1:N:79:LEU:CB	2.48	0.43
1:R:2:ASN:HD21	1:S:50:THR:HG22	1.83	0.43
1:R:69:LYS:O	1:R:70:SER:C	2.57	0.43
1:S:127:GLU:HA	1:S:131:THR:OG1	2.16	0.43
1:V:19:ILE:HG21	1:V:53:TRP:CZ3	2.53	0.43
1:X:145:LEU:O	1:X:146:GLU:C	2.57	0.43
1:2:19:ILE:HD11	1:2:31:LEU:HB2	1.99	0.43
1:4:22:PHE:HD1	1:4:23:ASN:N	2.16	0.43
1:D:135:ASN:O	1:D:137:GLY:N	2.51	0.43
1:G:54:VAL:HB	1:G:55:PRO:HD2	2.00	0.43
1:G:67:LEU:HD22	1:G:73:TYR:CE2	2.53	0.43
1:H:60:LEU:O	1:H:64:THR:HG23	2.18	0.43
1:K:145:LEU:O	1:K:148:ILE:HB	2.18	0.43
1:R:124:GLN:O	1:R:127:GLU:HB2	2.19	0.43
1:T:19:ILE:HG21	1:T:53:TRP:CZ3	2.53	0.43
1:U:17:ILE:HG12	1:U:77:VAL:HB	1.99	0.43
1:U:120:GLU:HB2	1:U:124:GLN:OE1	2.18	0.43
1:V:98:SER:HA	1:V:114:PHE:HE1	1.84	0.43
1:V:145:LEU:O	1:V:148:ILE:N	2.51	0.43
1:Y:67:LEU:HD22	1:Y:73:TYR:CE2	2.53	0.43
1:B:60:LEU:O	1:B:64:THR:HG23	2.19	0.43
1:C:98:SER:HA	1:C:114:PHE:HE1	1.82	0.43
1:D:19:ILE:HD11	1:D:31:LEU:HB2	1.99	0.43
1:E:122:ILE:HD11	1:J:132:LYS:CD	2.46	0.43
1:F:19:ILE:HG21	1:F:53:TRP:CZ3	2.53	0.43
1:K:21:ARG:O	1:K:24:GLN:HB2	2.19	0.43
1:K:60:LEU:HB2	1:K:61:PRO:HD3	2.01	0.43
1:L:19:ILE:HG12	1:L:79:LEU:HB2	2.00	0.43
1:P:98:SER:HA	1:P:114:PHE:HE1	1.83	0.43
1:P:145:LEU:O	1:P:148:ILE:N	2.51	0.43
1:R:42:GLY:HA3	1:R:145:LEU:CD1	2.48	0.43
1:X:128:ARG:HG3	1:X:128:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:22:PHE:HD1	1:Z:23:ASN:H	1.66	0.43
1:1:60:LEU:O	1:1:64:THR:HG23	2.18	0.43
1:1:154:ILE:HD13	1:2:67:LEU:HD21	2.00	0.43
1:C:27:ASN:O	1:C:30:LEU:HB2	2.18	0.43
1:F:10:ALA:N	1:F:11:PRO:CD	2.81	0.43
1:F:60:LEU:O	1:F:64:THR:HG23	2.18	0.43
1:G:128:ARG:HH11	1:G:128:ARG:HG3	1.84	0.43
1:H:127:GLU:HA	1:H:131:THR:OG1	2.17	0.43
1:H:128:ARG:HG3	1:H:128:ARG:NH1	2.33	0.43
1:I:19:ILE:CG2	1:I:53:TRP:CZ3	3.01	0.43
1:I:19:ILE:HD11	1:I:31:LEU:HB2	1.99	0.43
1:K:68:ALA:HB1	1:K:110:VAL:HG21	2.01	0.43
1:L:19:ILE:CG2	1:L:53:TRP:CZ3	3.01	0.43
1:L:113:ALA:HB1	1:L:140:ALA:HB1	2.00	0.43
1:N:17:ILE:HG12	1:N:77:VAL:HB	2.00	0.43
1:N:146:GLU:O	1:N:150:VAL:HG23	2.18	0.43
1:O:62:LEU:HA	1:O:62:LEU:HD23	1.74	0.43
1:T:41:ILE:HA	1:3:7:ASN:HD22	1.83	0.43
1:X:16:ALA:O	1:X:76:VAL:HA	2.17	0.43
1:Z:60:LEU:O	1:Z:64:THR:HG23	2.18	0.43
1:4:75:ALA:HA	1:4:110:VAL:HG12	2.00	0.43
1:B:22:PHE:HD1	1:B:23:ASN:H	1.65	0.43
1:B:120:GLU:HB2	1:B:124:GLN:OE1	2.17	0.43
1:F:19:ILE:HG12	1:F:79:LEU:CB	2.48	0.43
1:I:120:GLU:HB2	1:I:124:GLN:OE1	2.19	0.43
1:K:62:LEU:HD13	1:O:151:LEU:HD11	1.99	0.43
1:K:113:ALA:HB1	1:K:140:ALA:HB1	2.00	0.43
1:L:37:ALA:HB1	1:L:142:LEU:CD2	2.48	0.43
1:P:30:LEU:HD12	1:P:30:LEU:HA	1.90	0.43
1:P:52:VAL:HG21	1:P:67:LEU:HD11	2.00	0.43
1:Q:2:ASN:HD21	1:R:50:THR:HG22	1.84	0.43
1:Q:128:ARG:NE	2:Q:159:SO4:O3	2.49	0.43
1:S:141:ALA:O	1:S:145:LEU:HG	2.18	0.43
1:T:52:VAL:HG21	1:T:67:LEU:HD11	2.00	0.43
1:V:17:ILE:HG12	1:V:77:VAL:HB	2.01	0.43
1:X:24:GLN:C	1:X:26:ILE:N	2.71	0.43
1:1:146:GLU:O	1:1:150:VAL:HG23	2.18	0.43
1:3:16:ALA:CB	1:3:67:LEU:HD13	2.43	0.43
1:4:60:LEU:N	1:4:61:PRO:CD	2.82	0.43
1:4:142:LEU:HD22	1:4:142:LEU:H	1.84	0.43
1:D:72:LYS:HE2	1:D:72:LYS:HB2	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:PRO:HG3	1:F:151:LEU:HD12	2.00	0.43
1:F:113:ALA:HB1	1:F:140:ALA:HB1	2.00	0.43
1:G:122:ILE:HD11	1:Q:132:LYS:CD	2.48	0.43
1:Q:60:LEU:O	1:Q:64:THR:HG23	2.18	0.43
1:Q:124:GLN:O	1:Q:127:GLU:HB2	2.19	0.43
1:R:19:ILE:HG21	1:R:53:TRP:CZ3	2.54	0.43
1:S:22:PHE:HD1	1:S:23:ASN:N	2.16	0.43
1:U:142:LEU:HD22	1:U:142:LEU:H	1.82	0.43
1:E:54:VAL:HB	1:E:55:PRO:HD2	2.01	0.43
1:E:98:SER:HA	1:E:114:PHE:HE1	1.84	0.43
1:H:2:ASN:H	1:H:2:ASN:ND2	2.13	0.43
1:K:27:ASN:O	1:K:30:LEU:HB2	2.18	0.43
1:M:1:MET:CE	1:N:46:ASP:HB2	2.49	0.43
1:M:5:LYS:HE2	1:N:53:TRP:CG	2.54	0.43
1:M:57:ALA:HA	1:M:60:LEU:HG	2.00	0.43
1:S:19:ILE:HD11	1:S:31:LEU:HB2	2.01	0.43
1:S:19:ILE:HG12	1:S:79:LEU:HB2	1.99	0.43
1:2:19:ILE:HG22	1:2:53:TRP:CZ3	2.54	0.43
1:C:24:GLN:C	1:C:26:ILE:N	2.72	0.43
1:D:120:GLU:HB2	1:D:124:GLN:OE1	2.18	0.43
1:M:120:GLU:HB2	1:M:124:GLN:OE1	2.19	0.43
1:O:76:VAL:HB	1:O:112:VAL:HG22	2.01	0.43
1:P:5:LYS:HD3	1:Q:21:ARG:HH22	1.82	0.43
1:P:68:ALA:HB1	1:P:110:VAL:HG21	2.01	0.43
1:R:25:PHE:CD1	1:R:25:PHE:O	2.71	0.43
1:X:122:ILE:HD12	1:X:122:ILE:N	2.17	0.43
1:X:145:LEU:O	1:X:148:ILE:N	2.51	0.43
1:Y:23:ASN:HA	1:4:131:THR:HA	2.00	0.43
1:4:16:ALA:O	1:4:76:VAL:HA	2.19	0.43
1:A:141:ALA:O	1:A:145:LEU:HG	2.18	0.43
1:B:126:ILE:HG21	1:V:122:ILE:HG21	2.00	0.43
1:F:126:ILE:HG21	1:R:122:ILE:HG21	2.01	0.43
1:H:67:LEU:HD22	1:H:73:TYR:CE2	2.54	0.43
1:J:113:ALA:HB1	1:J:140:ALA:HB1	2.00	0.43
1:M:141:ALA:O	1:M:145:LEU:HG	2.19	0.43
1:P:38:LEU:HD23	1:P:38:LEU:HA	1.87	0.43
1:Q:145:LEU:O	1:Q:148:ILE:HB	2.18	0.43
1:S:16:ALA:O	1:S:76:VAL:HA	2.19	0.43
1:S:19:ILE:HG21	1:S:53:TRP:CZ3	2.54	0.43
1:V:42:GLY:HA3	1:V:145:LEU:CD1	2.49	0.43
1:Z:22:PHE:HD1	1:Z:23:ASN:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:52:VAL:HG21	1:3:67:LEU:HD11	2.00	0.43
1:B:127:GLU:HA	1:B:131:THR:OG1	2.19	0.43
1:D:128:ARG:HG3	1:D:128:ARG:NH1	2.34	0.43
1:J:67:LEU:HD22	1:J:73:TYR:CE2	2.54	0.43
1:P:127:GLU:HA	1:P:131:THR:OG1	2.19	0.43
1:R:19:ILE:CG2	1:R:53:TRP:CZ3	3.02	0.43
1:U:2:ASN:O	1:V:50:THR:HA	2.19	0.43
1:U:42:GLY:HA3	1:U:145:LEU:CD1	2.49	0.43
1:W:1:MET:HE2	1:X:46:ASP:HB2	2.00	0.43
1:W:19:ILE:HG12	1:W:79:LEU:HB2	2.00	0.43
1:Y:84:ARG:HA	1:Y:90:PHE:HB2	2.01	0.43
1:Z:127:GLU:HA	1:Z:131:THR:OG1	2.19	0.43
1:B:122:ILE:HD12	1:B:122:ILE:N	2.21	0.42
1:C:60:LEU:HB2	1:C:61:PRO:HD3	2.01	0.42
1:C:145:LEU:O	1:C:146:GLU:C	2.58	0.42
1:D:22:PHE:CD1	1:D:23:ASN:N	2.87	0.42
1:F:98:SER:HA	1:F:114:PHE:HE1	1.84	0.42
1:F:145:LEU:O	1:F:146:GLU:C	2.57	0.42
1:H:37:ALA:HB1	1:H:142:LEU:CD2	2.48	0.42
1:H:127:GLU:OE2	2:H:158:SO4:O4	2.37	0.42
1:I:18:THR:HG21	1:I:64:THR:HG22	2.01	0.42
1:K:19:ILE:HA	1:K:79:LEU:O	2.19	0.42
1:K:39:THR:OG1	1:K:40:ARG:N	2.53	0.42
1:N:119:THR:HA	1:O:87:THR:HB	2.01	0.42
1:P:22:PHE:CD1	1:P:23:ASN:N	2.87	0.42
1:P:24:GLN:C	1:P:26:ILE:N	2.72	0.42
1:Q:54:VAL:CG1	1:Q:63:ALA:HB2	2.50	0.42
1:S:22:PHE:CD1	1:S:23:ASN:N	2.87	0.42
1:S:128:ARG:HH11	1:S:128:ARG:HG3	1.84	0.42
1:U:69:LYS:O	1:U:70:SER:C	2.57	0.42
1:X:21:ARG:O	1:X:24:GLN:HB2	2.19	0.42
1:C:16:ALA:CB	1:C:67:LEU:HD13	2.47	0.42
1:I:57:ALA:HA	1:I:60:LEU:HG	2.01	0.42
1:K:42:GLY:HA3	1:K:145:LEU:CD1	2.49	0.42
1:L:16:ALA:CB	1:L:67:LEU:HD13	2.43	0.42
1:R:24:GLN:O	1:R:26:ILE:N	2.52	0.42
1:R:94:ALA:HB3	1:S:92:TYR:OH	2.19	0.42
1:S:113:ALA:HB1	1:S:140:ALA:HB1	2.00	0.42
1:T:145:LEU:O	1:T:148:ILE:HB	2.19	0.42
1:V:24:GLN:C	1:V:26:ILE:N	2.72	0.42
1:X:30:LEU:HD12	1:X:30:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:60:LEU:N	1:Y:61:PRO:CD	2.83	0.42
1:3:127:GLU:HA	1:3:131:THR:OG1	2.19	0.42
1:B:7:ASN:ND2	1:U:41:ILE:HD13	2.29	0.42
1:B:143:THR:HG22	1:C:55:PRO:CB	2.49	0.42
1:C:113:ALA:HB1	1:C:140:ALA:HB1	2.01	0.42
1:G:60:LEU:N	1:G:61:PRO:CD	2.82	0.42
1:I:54:VAL:CG1	1:I:63:ALA:HB2	2.49	0.42
1:J:138:ALA:O	1:J:142:LEU:HD22	2.20	0.42
1:L:21:ARG:O	1:L:24:GLN:HB2	2.19	0.42
1:L:52:VAL:CG2	1:L:67:LEU:HD11	2.50	0.42
1:L:128:ARG:HG3	1:L:128:ARG:NH1	2.34	0.42
1:P:145:LEU:O	1:P:146:GLU:C	2.57	0.42
1:Q:24:GLN:C	1:Q:26:ILE:H	2.23	0.42
1:R:22:PHE:HD1	1:R:23:ASN:H	1.65	0.42
1:T:16:ALA:O	1:T:76:VAL:HA	2.19	0.42
1:U:21:ARG:O	1:U:24:GLN:HB2	2.18	0.42
1:U:141:ALA:O	1:U:145:LEU:HG	2.18	0.42
1:V:30:LEU:HD12	1:V:30:LEU:HA	1.82	0.42
1:X:42:GLY:HA3	1:X:145:LEU:CD1	2.49	0.42
1:X:54:VAL:CG1	1:X:63:ALA:HB2	2.48	0.42
1:Y:69:LYS:O	1:Y:70:SER:C	2.58	0.42
1:Y:127:GLU:HA	1:Y:131:THR:OG1	2.20	0.42
1:4:19:ILE:HG12	1:4:79:LEU:HB2	2.00	0.42
1:4:88:ALA:HB1	1:4:91:GLU:HB2	2.01	0.42
1:A:145:LEU:O	1:A:148:ILE:N	2.52	0.42
1:B:19:ILE:HD11	1:B:31:LEU:HB2	2.00	0.42
1:B:146:GLU:O	1:B:150:VAL:HG23	2.20	0.42
1:C:120:GLU:HB2	1:C:124:GLN:OE1	2.19	0.42
1:F:50:THR:HA	1:J:2:ASN:O	2.19	0.42
1:F:132:LYS:HD2	1:R:122:ILE:CD1	2.49	0.42
1:G:119:THR:HA	1:H:87:THR:HB	2.02	0.42
1:I:19:ILE:HG12	1:I:79:LEU:HB2	2.02	0.42
1:I:69:LYS:O	1:I:70:SER:C	2.57	0.42
1:J:19:ILE:HG21	1:J:53:TRP:CZ3	2.54	0.42
1:J:30:LEU:HD12	1:J:30:LEU:HA	1.92	0.42
1:J:60:LEU:N	1:J:61:PRO:CD	2.83	0.42
1:J:88:ALA:HB1	1:J:91:GLU:HB2	2.00	0.42
1:K:52:VAL:HG22	1:O:4:ILE:HD12	2.01	0.42
1:K:62:LEU:HA	1:K:62:LEU:HD23	1.80	0.42
1:K:145:LEU:O	1:K:146:GLU:C	2.57	0.42
1:L:2:ASN:H	1:L:2:ASN:ND2	2.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:ALA:HB1	1:M:142:LEU:CD2	2.48	0.42
1:O:78:ALA:O	1:O:79:LEU:HD12	2.20	0.42
1:R:2:ASN:H	1:R:2:ASN:ND2	2.10	0.42
1:U:122:ILE:HD12	1:U:122:ILE:N	2.17	0.42
1:V:57:ALA:HA	1:V:60:LEU:HG	2.00	0.42
1:1:24:GLN:C	1:1:26:ILE:N	2.71	0.42
1:2:39:THR:OG1	1:2:40:ARG:N	2.52	0.42
1:2:68:ALA:HB1	1:2:110:VAL:HG21	2.00	0.42
1:4:67:LEU:HD22	1:4:73:TYR:CE2	2.54	0.42
1:4:68:ALA:HB1	1:4:110:VAL:HG21	2.02	0.42
1:A:121:SER:OG	1:A:123:GLU:HB3	2.20	0.42
1:D:17:ILE:HG12	1:D:77:VAL:HB	2.01	0.42
1:E:132:LYS:CD	1:O:122:ILE:HD11	2.46	0.42
1:H:22:PHE:HD1	1:H:23:ASN:N	2.18	0.42
1:I:60:LEU:N	1:I:61:PRO:CD	2.83	0.42
1:M:21:ARG:O	1:M:24:GLN:HB2	2.19	0.42
1:M:60:LEU:O	1:M:64:THR:HG23	2.20	0.42
1:Q:142:LEU:HD22	1:Q:142:LEU:N	2.34	0.42
1:S:98:SER:HA	1:S:114:PHE:HE1	1.85	0.42
1:U:98:SER:HA	1:U:114:PHE:HE1	1.85	0.42
1:U:121:SER:OG	1:U:123:GLU:HB3	2.19	0.42
1:Y:22:PHE:CD1	1:Y:23:ASN:N	2.88	0.42
1:Z:62:LEU:HA	1:Z:62:LEU:HD23	1.82	0.42
1:Z:88:ALA:HB1	1:Z:91:GLU:HB2	2.02	0.42
1:2:21:ARG:O	1:2:24:GLN:HB2	2.20	0.42
1:3:19:ILE:HG22	1:3:53:TRP:CZ3	2.54	0.42
1:A:19:ILE:HA	1:A:79:LEU:O	2.20	0.42
1:A:145:LEU:O	1:A:148:ILE:HB	2.20	0.42
1:B:76:VAL:HB	1:B:112:VAL:HG22	2.01	0.42
1:E:62:LEU:HA	1:E:62:LEU:HD23	1.76	0.42
1:E:113:ALA:HB1	1:E:140:ALA:HB1	2.02	0.42
1:G:16:ALA:O	1:G:76:VAL:HA	2.19	0.42
1:J:22:PHE:CD1	1:J:23:ASN:N	2.88	0.42
1:J:24:GLN:O	1:J:26:ILE:N	2.52	0.42
1:J:142:LEU:HD22	1:J:142:LEU:H	1.83	0.42
1:J:145:LEU:O	1:J:148:ILE:N	2.52	0.42
1:K:19:ILE:HG12	1:K:79:LEU:HB2	2.01	0.42
1:O:54:VAL:HB	1:O:55:PRO:HD2	2.02	0.42
1:Q:128:ARG:HH11	1:Q:128:ARG:HG3	1.85	0.42
1:X:45:LYS:HD3	1:X:45:LYS:HA	1.82	0.42
1:X:57:ALA:HA	1:X:60:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:78:ALA:O	1:X:79:LEU:HD12	2.20	0.42
1:X:84:ARG:HA	1:X:90:PHE:HB2	2.02	0.42
1:2:145:LEU:O	1:2:148:ILE:HB	2.20	0.42
1:2:145:LEU:O	1:2:148:ILE:N	2.53	0.42
1:3:11:PRO:HA	1:3:43:GLN:O	2.19	0.42
1:3:24:GLN:O	1:3:26:ILE:N	2.53	0.42
1:D:7:ASN:ND2	1:J:41:ILE:HD13	2.34	0.42
1:E:22:PHE:CD1	1:E:23:ASN:N	2.88	0.42
1:F:67:LEU:HD22	1:F:73:TYR:CE2	2.54	0.42
1:G:16:ALA:CB	1:G:67:LEU:HD13	2.46	0.42
1:G:17:ILE:O	1:G:51:VAL:HA	2.20	0.42
1:H:78:ALA:O	1:H:79:LEU:HD12	2.20	0.42
1:I:52:VAL:HG21	1:I:67:LEU:HD11	2.01	0.42
1:J:19:ILE:CD1	1:J:31:LEU:HB2	2.50	0.42
1:J:20:ALA:HA	1:J:54:VAL:O	2.19	0.42
1:K:128:ARG:HG3	1:K:128:ARG:NH1	2.34	0.42
1:L:13:ALA:HB1	1:L:74:ASP:HB2	2.02	0.42
1:M:22:PHE:CD1	1:M:23:ASN:N	2.87	0.42
1:O:89:HIS:O	1:O:90:PHE:C	2.58	0.42
1:R:13:ALA:HB1	1:R:74:ASP:CG	2.40	0.42
1:S:41:ILE:HA	1:Y:7:ASN:HD21	1.77	0.42
1:T:19:ILE:HD11	1:T:31:LEU:HB2	2.02	0.42
1:V:19:ILE:HG12	1:V:79:LEU:HB2	2.01	0.42
1:V:146:GLU:O	1:V:150:VAL:HG23	2.20	0.42
1:W:2:ASN:HD21	1:X:50:THR:HG22	1.85	0.42
1:W:21:ARG:O	1:W:24:GLN:HB2	2.19	0.42
1:X:17:ILE:HG12	1:X:77:VAL:HB	2.00	0.42
1:1:39:THR:OG1	1:1:40:ARG:N	2.50	0.42
1:C:151:LEU:HD11	1:D:62:LEU:HD13	2.01	0.42
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.82	0.42
1:F:138:ALA:O	1:F:142:LEU:CD2	2.68	0.42
1:J:138:ALA:O	1:J:142:LEU:CD2	2.68	0.42
1:O:39:THR:OG1	1:O:40:ARG:N	2.52	0.42
1:O:42:GLY:HA3	1:O:145:LEU:CD1	2.50	0.42
1:Q:19:ILE:HG12	1:Q:79:LEU:CB	2.50	0.42
1:Q:19:ILE:HD11	1:Q:31:LEU:HB2	2.02	0.42
1:S:38:LEU:HD23	1:S:38:LEU:HA	1.90	0.42
1:T:69:LYS:O	1:T:70:SER:C	2.58	0.42
1:T:141:ALA:O	1:T:145:LEU:HG	2.19	0.42
1:W:128:ARG:HG3	1:W:128:ARG:NH1	2.35	0.42
1:X:127:GLU:HA	1:X:131:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:128:ARG:HG3	1:Y:128:ARG:NH1	2.35	0.42
1:2:113:ALA:HB1	1:2:140:ALA:HB1	2.01	0.42
1:4:22:PHE:CD1	1:4:23:ASN:N	2.88	0.42
1:I:119:THR:HA	1:J:87:THR:HB	2.00	0.42
1:J:16:ALA:O	1:J:76:VAL:HA	2.20	0.42
1:J:35:VAL:HG23	1:J:36:ASP:N	2.34	0.42
1:L:142:LEU:H	1:L:142:LEU:HD22	1.85	0.42
1:M:60:LEU:N	1:M:61:PRO:CD	2.82	0.42
1:P:10:ALA:O	1:P:12:ASP:N	2.49	0.42
1:U:24:GLN:C	1:U:26:ILE:H	2.23	0.42
1:U:76:VAL:HB	1:U:112:VAL:HG22	2.01	0.42
1:U:128:ARG:HG3	1:U:128:ARG:NH1	2.34	0.42
1:V:67:LEU:HD22	1:V:73:TYR:CE2	2.53	0.42
1:X:122:ILE:H	1:X:122:ILE:CD1	2.12	0.42
1:3:22:PHE:HD1	1:3:23:ASN:H	1.65	0.42
1:4:145:LEU:O	1:4:148:ILE:N	2.53	0.42
1:A:127:GLU:HA	1:A:131:THR:OG1	2.19	0.42
1:B:37:ALA:HB1	1:B:142:LEU:CD2	2.49	0.42
1:D:38:LEU:HD23	1:D:38:LEU:HA	1.89	0.42
1:D:122:ILE:CD1	1:R:132:LYS:HD2	2.47	0.42
1:F:54:VAL:HB	1:F:55:PRO:HD2	2.01	0.42
1:H:24:GLN:O	1:H:26:ILE:N	2.53	0.42
1:I:60:LEU:O	1:I:64:THR:HG23	2.20	0.42
1:J:141:ALA:O	1:J:145:LEU:HG	2.20	0.42
1:M:145:LEU:O	1:M:148:ILE:N	2.52	0.42
1:R:98:SER:HA	1:R:114:PHE:HE1	1.85	0.42
1:S:12:ASP:O	1:S:13:ALA:O	2.38	0.42
1:S:114:PHE:HB2	1:T:58:TYR:CE2	2.55	0.42
1:T:12:ASP:O	1:T:13:ALA:C	2.58	0.42
1:V:60:LEU:N	1:V:61:PRO:CD	2.83	0.42
1:X:41:ILE:HD13	1:4:7:ASN:ND2	2.33	0.42
1:X:121:SER:OG	1:X:123:GLU:HB3	2.20	0.42
1:Z:122:ILE:H	1:Z:122:ILE:CD1	2.17	0.42
1:3:60:LEU:N	1:3:61:PRO:CD	2.82	0.42
1:A:61:PRO:HA	1:A:101:LEU:HD23	2.02	0.41
1:B:54:VAL:CG1	1:B:63:ALA:HB2	2.50	0.41
1:D:113:ALA:HB1	1:D:140:ALA:HB1	2.02	0.41
1:G:24:GLN:C	1:G:26:ILE:N	2.74	0.41
1:G:52:VAL:HG21	1:G:67:LEU:HD11	2.01	0.41
1:G:154:ILE:HD13	1:H:67:LEU:HD23	2.02	0.41
1:J:128:ARG:HH11	1:J:128:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:67:LEU:HD22	1:M:73:TYR:CE2	2.54	0.41
1:O:24:GLN:O	1:O:26:ILE:N	2.53	0.41
1:O:54:VAL:CG1	1:O:63:ALA:HB2	2.50	0.41
1:P:19:ILE:CG2	1:P:53:TRP:CZ3	3.03	0.41
1:P:89:HIS:O	1:P:90:PHE:C	2.58	0.41
1:S:54:VAL:CG1	1:S:63:ALA:HB2	2.48	0.41
1:T:21:ARG:O	1:T:24:GLN:HB2	2.20	0.41
1:U:45:LYS:HD3	1:U:45:LYS:HA	1.83	0.41
1:U:142:LEU:HD22	1:U:142:LEU:N	2.35	0.41
1:Y:141:ALA:O	1:Y:145:LEU:HG	2.20	0.41
1:Z:60:LEU:N	1:Z:61:PRO:CD	2.83	0.41
1:2:38:LEU:HD23	1:2:38:LEU:HA	1.87	0.41
1:4:19:ILE:CG2	1:4:53:TRP:CZ3	3.03	0.41
1:4:138:ALA:O	1:4:142:LEU:HD22	2.20	0.41
1:4:142:LEU:HD22	1:4:142:LEU:N	2.35	0.41
1:A:24:GLN:C	1:A:26:ILE:N	2.72	0.41
1:A:60:LEU:O	1:A:64:THR:HG23	2.20	0.41
1:C:60:LEU:N	1:C:61:PRO:CD	2.82	0.41
1:D:62:LEU:HA	1:D:62:LEU:HD23	1.79	0.41
1:F:46:ASP:O	1:J:1:MET:HA	2.19	0.41
1:L:5:LYS:NZ	1:M:21:ARG:NH2	2.68	0.41
1:L:127:GLU:HA	1:L:131:THR:OG1	2.19	0.41
1:N:68:ALA:HB1	1:N:110:VAL:HG21	2.02	0.41
1:R:128:ARG:HG3	1:R:128:ARG:NH1	2.35	0.41
1:U:30:LEU:HD12	1:U:30:LEU:HA	1.86	0.41
1:U:84:ARG:HA	1:U:90:PHE:HB2	2.02	0.41
1:V:13:ALA:HB1	1:V:74:ASP:OD2	2.19	0.41
1:X:39:THR:OG1	1:X:40:ARG:N	2.52	0.41
1:X:54:VAL:HB	1:X:55:PRO:HD2	2.02	0.41
1:X:111:PRO:HG3	1:X:151:LEU:HD12	2.01	0.41
1:1:60:LEU:N	1:1:61:PRO:CD	2.84	0.41
1:1:127:GLU:HA	1:1:131:THR:OG1	2.20	0.41
1:2:151:LEU:HD11	1:3:62:LEU:HD13	2.02	0.41
1:3:62:LEU:HA	1:3:62:LEU:HD23	1.74	0.41
1:B:113:ALA:HB1	1:B:140:ALA:HB1	2.02	0.41
1:D:1:MET:CE	1:E:46:ASP:HB2	2.50	0.41
1:D:119:THR:HA	1:E:87:THR:HB	2.01	0.41
1:E:2:ASN:H	1:E:2:ASN:ND2	2.15	0.41
1:E:42:GLY:HA3	1:E:145:LEU:CD1	2.49	0.41
1:G:57:ALA:HA	1:G:60:LEU:HG	2.01	0.41
1:H:145:LEU:O	1:H:146:GLU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:PHE:CD1	1:I:23:ASN:N	2.88	0.41
1:M:84:ARG:HA	1:M:90:PHE:HB2	2.02	0.41
1:O:25:PHE:O	1:O:25:PHE:CD1	2.73	0.41
1:Q:67:LEU:HD22	1:Q:73:TYR:CE2	2.55	0.41
1:V:60:LEU:O	1:V:64:THR:HG23	2.20	0.41
1:V:84:ARG:HA	1:V:90:PHE:HB2	2.02	0.41
1:V:141:ALA:O	1:V:145:LEU:HG	2.21	0.41
1:X:68:ALA:HB1	1:X:110:VAL:HG21	2.01	0.41
1:Y:19:ILE:HA	1:Y:79:LEU:O	2.20	0.41
1:Z:17:ILE:HG12	1:Z:77:VAL:HB	2.03	0.41
1:Z:135:ASN:O	1:Z:137:GLY:N	2.53	0.41
1:1:19:ILE:HG12	1:1:79:LEU:CB	2.50	0.41
1:3:76:VAL:HB	1:3:112:VAL:HG22	2.01	0.41
1:A:22:PHE:HD1	1:A:23:ASN:H	1.69	0.41
1:A:98:SER:HA	1:A:114:PHE:HE1	1.85	0.41
1:C:88:ALA:HB1	1:C:91:GLU:HB2	2.01	0.41
1:D:88:ALA:HB1	1:D:91:GLU:HB2	2.02	0.41
1:E:52:VAL:HG21	1:E:67:LEU:HD11	2.02	0.41
1:E:145:LEU:O	1:E:148:ILE:N	2.53	0.41
1:F:22:PHE:CD1	1:F:23:ASN:N	2.88	0.41
1:H:22:PHE:CD1	1:H:23:ASN:N	2.88	0.41
1:J:17:ILE:HG12	1:J:77:VAL:HB	2.02	0.41
1:K:124:GLN:O	1:K:127:GLU:HB2	2.20	0.41
1:N:62:LEU:HD23	1:N:62:LEU:HA	1.78	0.41
1:O:145:LEU:O	1:O:148:ILE:HB	2.21	0.41
1:R:39:THR:OG1	1:R:40:ARG:N	2.51	0.41
1:R:141:ALA:O	1:R:144:ALA:HB3	2.21	0.41
1:V:78:ALA:O	1:V:79:LEU:HD12	2.21	0.41
1:W:24:GLN:C	1:W:26:ILE:N	2.72	0.41
1:W:54:VAL:HB	1:W:55:PRO:HD2	2.02	0.41
1:W:98:SER:HA	1:W:114:PHE:HE1	1.86	0.41
1:X:67:LEU:HD22	1:X:73:TYR:CE2	2.55	0.41
1:2:22:PHE:HD1	1:2:23:ASN:H	1.68	0.41
1:4:45:LYS:HA	1:4:45:LYS:HD3	1.82	0.41
1:D:24:GLN:C	1:D:26:ILE:N	2.74	0.41
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.88	0.41
1:E:69:LYS:O	1:E:70:SER:C	2.59	0.41
1:E:127:GLU:HA	1:E:131:THR:OG1	2.19	0.41
1:H:68:ALA:HB1	1:H:110:VAL:HG21	2.03	0.41
1:I:113:ALA:HB1	1:I:140:ALA:HB1	2.01	0.41
1:N:128:ARG:HG3	1:N:128:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:22:PHE:HD1	1:Q:23:ASN:N	2.18	0.41
1:R:127:GLU:HA	1:R:131:THR:OG1	2.20	0.41
1:S:21:ARG:O	1:S:24:GLN:HB2	2.20	0.41
1:S:39:THR:OG1	1:S:40:ARG:N	2.53	0.41
1:X:142:LEU:HD22	1:X:142:LEU:N	2.36	0.41
1:Y:19:ILE:HD11	1:Y:31:LEU:HB2	2.02	0.41
1:Y:45:LYS:HD3	1:Y:45:LYS:HA	1.81	0.41
1:Y:146:GLU:O	1:Y:150:VAL:HG23	2.21	0.41
1:1:45:LYS:HA	1:1:45:LYS:HD3	1.86	0.41
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.89	0.41
1:C:41:ILE:HA	1:R:7:ASN:HD22	1.84	0.41
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.89	0.41
1:C:89:HIS:O	1:C:90:PHE:C	2.57	0.41
1:H:19:ILE:HG12	1:H:79:LEU:CB	2.51	0.41
1:J:17:ILE:O	1:J:51:VAL:HA	2.20	0.41
1:J:127:GLU:HA	1:J:131:THR:OG1	2.20	0.41
1:K:19:ILE:HG21	1:K:53:TRP:CZ3	2.56	0.41
1:K:151:LEU:HD11	1:L:62:LEU:HD13	2.02	0.41
1:L:19:ILE:HG21	1:L:53:TRP:CZ3	2.55	0.41
1:L:60:LEU:N	1:L:61:PRO:CD	2.83	0.41
1:W:19:ILE:HD11	1:W:31:LEU:HB2	2.01	0.41
1:X:19:ILE:HG12	1:X:79:LEU:HB2	2.01	0.41
1:3:113:ALA:HB1	1:3:140:ALA:HB1	2.01	0.41
1:4:24:GLN:C	1:4:26:ILE:N	2.73	0.41
1:4:145:LEU:O	1:4:148:ILE:HB	2.20	0.41
1:B:16:ALA:CB	1:B:67:LEU:HD13	2.48	0.41
1:C:128:ARG:NE	2:D:157:SO4:O2	2.45	0.41
1:G:45:LYS:HA	1:G:45:LYS:HD3	1.81	0.41
1:H:11:PRO:CB	1:H:43:GLN:HB3	2.50	0.41
1:H:89:HIS:HB2	2:H:157:SO4:O4	2.21	0.41
1:I:11:PRO:O	1:I:12:ASP:OD1	2.38	0.41
1:M:106:GLN:HG2	1:M:106:GLN:O	2.21	0.41
1:N:52:VAL:HG21	1:N:67:LEU:HD11	2.02	0.41
1:N:67:LEU:HD22	1:N:73:TYR:CE2	2.55	0.41
1:P:19:ILE:CD1	1:P:31:LEU:HB2	2.51	0.41
1:P:25:PHE:CE1	1:3:126:ILE:HD13	2.55	0.41
1:Q:18:THR:HG22	1:Q:52:VAL:HB	2.03	0.41
1:Q:135:ASN:O	1:Q:136:LYS:C	2.59	0.41
1:S:13:ALA:HB1	1:S:74:ASP:HB2	2.02	0.41
1:S:84:ARG:HA	1:S:90:PHE:HB2	2.02	0.41
1:V:121:SER:OG	1:V:123:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:127:GLU:HA	1:V:131:THR:OG1	2.20	0.41
1:Y:76:VAL:HB	1:Y:112:VAL:HG22	2.02	0.41
1:Z:21:ARG:O	1:Z:24:GLN:HB2	2.20	0.41
1:2:22:PHE:HD1	1:2:23:ASN:N	2.18	0.41
1:3:27:ASN:O	1:3:30:LEU:HB2	2.19	0.41
1:3:38:LEU:CD2	1:3:141:ALA:HB1	2.50	0.41
1:4:37:ALA:HB1	1:4:142:LEU:CD2	2.46	0.41
1:4:52:VAL:CG2	1:4:67:LEU:HD11	2.51	0.41
1:4:113:ALA:HB1	1:4:140:ALA:HB1	2.02	0.41
1:A:19:ILE:CG2	1:A:53:TRP:CZ3	3.03	0.41
1:A:60:LEU:N	1:A:61:PRO:CD	2.83	0.41
1:B:54:VAL:HB	1:B:55:PRO:HD2	2.03	0.41
1:C:124:GLN:O	1:C:127:GLU:HB2	2.21	0.41
1:G:12:ASP:O	1:G:48:ASN:ND2	2.49	0.41
1:H:54:VAL:HB	1:H:55:PRO:HD2	2.02	0.41
1:J:19:ILE:HD11	1:J:31:LEU:HB2	2.03	0.41
1:P:54:VAL:HB	1:P:55:PRO:HD2	2.02	0.41
1:S:8:VAL:HG22	1:Y:41:ILE:HD12	2.01	0.41
1:S:36:ASP:OD1	1:U:21:ARG:NH2	2.54	0.41
1:T:67:LEU:HD23	1:T:67:LEU:HA	1.87	0.41
1:T:89:HIS:O	1:T:90:PHE:C	2.59	0.41
1:U:22:PHE:CD1	1:U:23:ASN:N	2.88	0.41
1:1:54:VAL:CG1	1:1:63:ALA:HB2	2.50	0.41
1:3:145:LEU:O	1:3:148:ILE:HB	2.20	0.41
1:4:54:VAL:CG1	1:4:63:ALA:HB2	2.50	0.41
1:A:142:LEU:HD22	1:A:142:LEU:N	2.36	0.41
1:B:60:LEU:N	1:B:61:PRO:CD	2.84	0.41
1:C:39:THR:OG1	1:C:40:ARG:N	2.52	0.41
1:C:42:GLY:HA3	1:C:145:LEU:CD1	2.50	0.41
1:C:145:LEU:O	1:C:148:ILE:N	2.53	0.41
1:E:122:ILE:HD12	1:E:122:ILE:N	2.20	0.41
1:F:121:SER:OG	1:F:123:GLU:HB3	2.21	0.41
1:H:5:LYS:HD3	1:I:21:ARG:HH22	1.84	0.41
1:H:138:ALA:O	1:H:139:GLU:C	2.57	0.41
1:I:89:HIS:O	1:I:90:PHE:C	2.60	0.41
1:J:21:ARG:O	1:J:24:GLN:HB2	2.21	0.41
1:K:24:GLN:O	1:K:26:ILE:N	2.54	0.41
1:L:62:LEU:HA	1:L:62:LEU:HD23	1.84	0.41
1:N:120:GLU:HB2	1:N:124:GLN:OE1	2.21	0.41
1:O:16:ALA:O	1:O:76:VAL:HA	2.21	0.41
1:P:19:ILE:HG21	1:P:53:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:75:ALA:HA	1:S:110:VAL:HG12	2.03	0.41
1:U:1:MET:HE2	1:V:46:ASP:HB2	2.02	0.41
1:U:19:ILE:HG12	1:U:79:LEU:HB2	2.01	0.41
1:U:67:LEU:HD22	1:U:73:TYR:CE2	2.55	0.41
1:W:67:LEU:HD23	1:W:67:LEU:HA	1.86	0.41
1:X:60:LEU:N	1:X:61:PRO:CD	2.84	0.41
1:Y:61:PRO:O	1:Y:64:THR:N	2.54	0.41
1:Y:89:HIS:O	1:Y:90:PHE:C	2.59	0.41
1:Z:54:VAL:HB	1:Z:55:PRO:HD2	2.02	0.41
1:Z:68:ALA:HB1	1:Z:110:VAL:HG21	2.03	0.41
1:Z:113:ALA:HB1	1:Z:140:ALA:HB1	2.03	0.41
1:1:19:ILE:HA	1:1:79:LEU:O	2.21	0.41
1:1:87:THR:HG23	2:1:157:SO4:O1	2.21	0.41
1:2:61:PRO:HA	1:2:101:LEU:HD23	2.03	0.41
1:3:60:LEU:O	1:3:64:THR:HG23	2.21	0.41
1:4:19:ILE:HG21	1:4:53:TRP:CZ3	2.56	0.41
1:C:23:ASN:HA	1:U:131:THR:HA	2.03	0.41
1:D:60:LEU:HB2	1:D:61:PRO:HD3	2.02	0.41
1:E:19:ILE:HG12	1:E:79:LEU:CB	2.51	0.41
1:G:98:SER:HA	1:G:114:PHE:HE1	1.86	0.41
1:I:11:PRO:HB3	1:I:43:GLN:HB3	2.03	0.41
1:K:60:LEU:N	1:K:61:PRO:CD	2.84	0.41
1:L:24:GLN:C	1:L:26:ILE:N	2.74	0.41
1:N:18:THR:HG22	1:N:52:VAL:HB	2.03	0.41
1:O:19:ILE:HG22	1:O:53:TRP:CZ3	2.56	0.41
1:P:60:LEU:O	1:P:64:THR:HG23	2.21	0.41
1:Q:61:PRO:O	1:Q:62:LEU:C	2.59	0.41
1:R:21:ARG:O	1:R:24:GLN:HB2	2.20	0.41
1:S:4:ILE:HD12	1:T:52:VAL:HG22	2.02	0.41
1:S:67:LEU:HD22	1:S:73:TYR:CE2	2.56	0.41
1:Z:16:ALA:CB	1:Z:67:LEU:HD13	2.48	0.41
1:Z:146:GLU:O	1:Z:150:VAL:HG23	2.20	0.41
1:1:38:LEU:HD23	1:1:38:LEU:HA	1.89	0.41
1:2:60:LEU:N	1:2:61:PRO:CD	2.84	0.41
1:4:27:ASN:O	1:4:30:LEU:HB2	2.21	0.41
1:A:84:ARG:HA	1:A:90:PHE:HB2	2.02	0.40
1:B:121:SER:OG	1:B:123:GLU:HB3	2.20	0.40
1:C:22:PHE:HD1	1:C:23:ASN:N	2.19	0.40
1:D:21:ARG:O	1:D:24:GLN:HB2	2.21	0.40
1:F:38:LEU:HD23	1:F:38:LEU:HA	1.94	0.40
1:I:19:ILE:HG21	1:I:53:TRP:CZ3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2:ASN:H	1:J:2:ASN:ND2	2.15	0.40
1:J:16:ALA:CB	1:J:67:LEU:HD13	2.51	0.40
1:J:62:LEU:HD23	1:J:62:LEU:HA	1.81	0.40
1:N:24:GLN:C	1:N:26:ILE:N	2.74	0.40
1:N:42:GLY:HA3	1:N:145:LEU:CD1	2.52	0.40
1:O:19:ILE:HA	1:O:79:LEU:O	2.21	0.40
1:O:68:ALA:HB1	1:O:110:VAL:HG21	2.02	0.40
1:R:52:VAL:HG21	1:R:67:LEU:HD11	2.03	0.40
1:S:60:LEU:N	1:S:61:PRO:CD	2.84	0.40
1:S:60:LEU:O	1:S:64:THR:HG23	2.21	0.40
1:U:143:THR:HG22	1:V:55:PRO:CB	2.51	0.40
1:W:17:ILE:O	1:W:51:VAL:HA	2.22	0.40
1:Y:88:ALA:HB1	1:Y:91:GLU:HB2	2.02	0.40
1:1:128:ARG:HG3	1:1:128:ARG:NH1	2.36	0.40
1:3:20:ALA:HA	1:3:54:VAL:O	2.21	0.40
1:4:16:ALA:CB	1:4:67:LEU:HD13	2.45	0.40
1:A:122:ILE:H	1:A:122:ILE:CD1	2.15	0.40
1:B:98:SER:HA	1:B:114:PHE:HE1	1.86	0.40
1:C:22:PHE:HD1	1:C:23:ASN:H	1.69	0.40
1:D:25:PHE:O	1:D:25:PHE:CD1	2.75	0.40
1:G:111:PRO:HG3	1:G:151:LEU:HD12	2.03	0.40
1:I:78:ALA:O	1:I:79:LEU:HD12	2.20	0.40
1:L:61:PRO:O	1:L:64:THR:N	2.54	0.40
1:N:135:ASN:O	1:N:136:LYS:C	2.59	0.40
1:S:61:PRO:HA	1:S:101:LEU:HD23	2.03	0.40
1:S:132:LYS:CD	1:U:122:ILE:HD11	2.47	0.40
1:T:18:THR:HG22	1:T:52:VAL:HB	2.04	0.40
1:T:22:PHE:CD1	1:T:23:ASN:N	2.89	0.40
1:V:21:ARG:O	1:V:24:GLN:HB2	2.20	0.40
1:V:22:PHE:CD1	1:V:23:ASN:N	2.90	0.40
1:V:113:ALA:HB1	1:V:140:ALA:HB1	2.03	0.40
1:W:122:ILE:HD12	1:W:122:ILE:N	2.22	0.40
1:X:19:ILE:CG2	1:X:53:TRP:CZ3	3.04	0.40
1:X:24:GLN:C	1:X:26:ILE:H	2.25	0.40
1:Z:22:PHE:CD1	1:Z:23:ASN:N	2.89	0.40
1:4:60:LEU:O	1:4:64:THR:HG23	2.21	0.40
1:B:22:PHE:CD1	1:B:23:ASN:N	2.89	0.40
1:B:84:ARG:HA	1:B:90:PHE:HB2	2.04	0.40
1:F:1:MET:HE2	1:G:46:ASP:HB2	2.02	0.40
1:G:19:ILE:HG12	1:G:79:LEU:HB2	2.04	0.40
1:G:145:LEU:O	1:G:148:ILE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:ARG:O	1:I:24:GLN:HB2	2.22	0.40
1:L:25:PHE:CD1	1:L:25:PHE:O	2.74	0.40
1:L:142:LEU:HD22	1:L:142:LEU:N	2.37	0.40
1:O:18:THR:HG21	1:O:64:THR:HG22	2.04	0.40
1:O:128:ARG:HG3	1:O:128:ARG:NH1	2.37	0.40
1:W:135:ASN:O	1:W:136:LYS:C	2.60	0.40
1:Y:138:ALA:O	1:Y:142:LEU:HD22	2.21	0.40
1:1:142:LEU:N	1:1:142:LEU:HD22	2.36	0.40
1:2:37:ALA:HB1	1:2:142:LEU:CD2	2.50	0.40
1:C:121:SER:OG	1:C:123:GLU:HB3	2.21	0.40
1:D:41:ILE:HA	1:J:7:ASN:HD21	1.79	0.40
1:E:24:GLN:O	1:E:26:ILE:N	2.54	0.40
1:G:60:LEU:O	1:G:64:THR:HG23	2.21	0.40
1:H:142:LEU:H	1:H:142:LEU:HD22	1.87	0.40
1:K:69:LYS:O	1:K:70:SER:C	2.59	0.40
1:M:127:GLU:HA	1:M:131:THR:OG1	2.21	0.40
1:N:135:ASN:O	1:N:137:GLY:N	2.54	0.40
1:O:122:ILE:HD12	1:O:122:ILE:N	2.23	0.40
1:Q:30:LEU:HD12	1:Q:30:LEU:HA	1.90	0.40
1:R:123:GLU:O	1:R:127:GLU:HG3	2.21	0.40
1:R:142:LEU:HD13	1:R:142:LEU:HA	1.91	0.40
1:S:30:LEU:HD12	1:S:30:LEU:HA	1.85	0.40
1:S:35:VAL:HG23	1:S:36:ASP:H	1.87	0.40
1:T:62:LEU:HD23	1:T:62:LEU:HA	1.79	0.40
1:U:24:GLN:C	1:U:26:ILE:N	2.73	0.40
1:U:146:GLU:O	1:U:150:VAL:HG23	2.22	0.40
1:X:16:ALA:CB	1:X:67:LEU:HD13	2.50	0.40
1:Y:24:GLN:C	1:Y:26:ILE:N	2.73	0.40
1:3:54:VAL:HB	1:3:55:PRO:HD2	2.03	0.40
1:E:25:PHE:HZ	1:J:25:PHE:CE1	2.40	0.40
1:H:98:SER:HA	1:H:114:PHE:HE1	1.86	0.40
1:I:145:LEU:O	1:I:148:ILE:HB	2.21	0.40
1:J:52:VAL:HG21	1:J:67:LEU:HD11	2.04	0.40
1:L:122:ILE:HD12	1:L:122:ILE:N	2.17	0.40
1:M:42:GLY:HA3	1:M:145:LEU:CD1	2.52	0.40
1:S:24:GLN:O	1:S:26:ILE:N	2.54	0.40
1:T:127:GLU:HA	1:T:131:THR:OG1	2.21	0.40
1:X:27:ASN:HA	1:X:30:LEU:HD22	2.04	0.40
1:Z:25:PHE:O	1:Z:25:PHE:CG	2.75	0.40
1:1:98:SER:HA	1:1:114:PHE:HE1	1.87	0.40
1:2:54:VAL:HB	1:2:55:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1:MET:HE2	1:4:46:ASP:HB2	2.04	0.40
1:3:22:PHE:HD1	1:3:23:ASN:N	2.19	0.40
1:4:62:LEU:HA	1:4:62:LEU:HD23	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	152/156 (97%)	127 (84%)	21 (14%)	4 (3%)	5	33
1	2	152/156 (97%)	122 (80%)	28 (18%)	2 (1%)	12	48
1	3	152/156 (97%)	124 (82%)	24 (16%)	4 (3%)	5	33
1	4	152/156 (97%)	126 (83%)	22 (14%)	4 (3%)	5	33
1	A	152/156 (97%)	124 (82%)	25 (16%)	3 (2%)	7	39
1	B	152/156 (97%)	124 (82%)	26 (17%)	2 (1%)	12	48
1	C	152/156 (97%)	127 (84%)	22 (14%)	3 (2%)	7	39
1	D	152/156 (97%)	124 (82%)	24 (16%)	4 (3%)	5	33
1	E	152/156 (97%)	121 (80%)	27 (18%)	4 (3%)	5	33
1	F	152/156 (97%)	122 (80%)	28 (18%)	2 (1%)	12	48
1	G	152/156 (97%)	122 (80%)	25 (16%)	5 (3%)	4	28
1	H	152/156 (97%)	123 (81%)	25 (16%)	4 (3%)	5	33
1	I	152/156 (97%)	121 (80%)	29 (19%)	2 (1%)	12	48
1	J	152/156 (97%)	125 (82%)	25 (16%)	2 (1%)	12	48
1	K	152/156 (97%)	122 (80%)	27 (18%)	3 (2%)	7	39
1	L	152/156 (97%)	126 (83%)	24 (16%)	2 (1%)	12	48
1	M	152/156 (97%)	123 (81%)	25 (16%)	4 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	152/156 (97%)	126 (83%)	23 (15%)	3 (2%)	7	39
1	O	152/156 (97%)	126 (83%)	24 (16%)	2 (1%)	12	48
1	P	152/156 (97%)	124 (82%)	23 (15%)	5 (3%)	4	28
1	Q	152/156 (97%)	126 (83%)	23 (15%)	3 (2%)	7	39
1	R	152/156 (97%)	125 (82%)	25 (16%)	2 (1%)	12	48
1	S	152/156 (97%)	124 (82%)	24 (16%)	4 (3%)	5	33
1	T	152/156 (97%)	125 (82%)	22 (14%)	5 (3%)	4	28
1	U	152/156 (97%)	125 (82%)	24 (16%)	3 (2%)	7	39
1	V	152/156 (97%)	123 (81%)	27 (18%)	2 (1%)	12	48
1	W	152/156 (97%)	123 (81%)	27 (18%)	2 (1%)	12	48
1	X	152/156 (97%)	125 (82%)	24 (16%)	3 (2%)	7	39
1	Y	152/156 (97%)	125 (82%)	24 (16%)	3 (2%)	7	39
1	Z	152/156 (97%)	125 (82%)	24 (16%)	3 (2%)	7	39
All	All	4560/4680 (97%)	3725 (82%)	741 (16%)	94 (2%)	7	38

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	11	PRO
1	S	12	ASP
1	S	13	ALA
1	T	13	ALA
1	H	11	PRO
1	A	55	PRO
1	B	55	PRO
1	C	55	PRO
1	D	55	PRO
1	D	70	SER
1	E	55	PRO
1	E	70	SER
1	F	55	PRO
1	G	55	PRO
1	H	55	PRO
1	I	55	PRO
1	J	55	PRO
1	K	55	PRO
1	K	70	SER

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Mol	Chain	Res	Type
1	L	55	PRO
1	M	13	ALA
1	M	55	PRO
1	N	55	PRO
1	O	55	PRO
1	P	55	PRO
1	Q	55	PRO
1	R	55	PRO
1	S	55	PRO
1	T	55	PRO
1	U	55	PRO
1	V	55	PRO
1	W	55	PRO
1	X	55	PRO
1	Y	55	PRO
1	Z	55	PRO
1	1	55	PRO
1	2	55	PRO
1	3	55	PRO
1	4	55	PRO
1	A	61	PRO
1	E	136	LYS
1	M	70	SER
1	P	11	PRO
1	Q	61	PRO
1	U	61	PRO
1	X	61	PRO
1	Z	61	PRO
1	Z	70	SER
1	1	25	PHE
1	A	70	SER
1	B	61	PRO
1	D	25	PHE
1	D	61	PRO
1	E	61	PRO
1	F	61	PRO
1	L	61	PRO
1	N	61	PRO
1	N	145	LEU
1	P	25	PHE
1	P	61	PRO
1	P	70	SER

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Mol	Chain	Res	Type
1	Q	70	SER
1	T	70	SER
1	T	145	LEU
1	U	145	LEU
1	V	61	PRO
1	Y	61	PRO
1	Y	70	SER
1	3	61	PRO
1	4	70	SER
1	4	136	LYS
1	C	61	PRO
1	C	70	SER
1	G	25	PHE
1	G	70	SER
1	H	61	PRO
1	H	70	SER
1	K	61	PRO
1	R	61	PRO
1	T	61	PRO
1	W	61	PRO
1	X	70	SER
1	1	61	PRO
1	2	61	PRO
1	3	70	SER
1	4	61	PRO
1	G	61	PRO
1	J	61	PRO
1	S	61	PRO
1	3	11	PRO
1	M	61	PRO
1	I	61	PRO
1	O	61	PRO
1	1	11	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	110/112 (98%)	101 (92%)	9 (8%)	11	40
1	2	109/112 (97%)	100 (92%)	9 (8%)	11	40
1	3	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	4	109/112 (97%)	100 (92%)	9 (8%)	11	40
1	A	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	B	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	C	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	D	110/112 (98%)	99 (90%)	11 (10%)	7	32
1	E	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	F	109/112 (97%)	100 (92%)	9 (8%)	11	40
1	G	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	H	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	I	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	J	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	K	109/112 (97%)	100 (92%)	9 (8%)	11	40
1	L	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	M	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	N	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	O	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	P	108/112 (96%)	97 (90%)	11 (10%)	7	32
1	Q	109/112 (97%)	99 (91%)	10 (9%)	9	36
1	R	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	S	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	T	109/112 (97%)	100 (92%)	9 (8%)	11	40
1	U	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	V	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	W	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	X	109/112 (97%)	98 (90%)	11 (10%)	7	32
1	Y	108/112 (96%)	96 (89%)	12 (11%)	6	28
1	Z	109/112 (97%)	99 (91%)	10 (9%)	9	36
All	All	3270/3360 (97%)	2961 (91%)	309 (9%)	8	35

All (309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	24	GLN
1	A	28	ASP
1	A	30	LEU
1	A	50	THR
1	A	59	GLU
1	A	62	LEU
1	A	70	SER
1	A	81	THR
1	A	116	VAL
1	A	118	THR
1	B	2	ASN
1	B	24	GLN
1	B	28	ASP
1	B	30	LEU
1	B	50	THR
1	B	59	GLU
1	B	62	LEU
1	B	70	SER
1	B	79	LEU
1	B	81	THR
1	B	116	VAL
1	C	2	ASN
1	C	24	GLN
1	C	28	ASP
1	C	30	LEU
1	C	50	THR
1	C	59	GLU
1	C	62	LEU
1	C	70	SER
1	C	81	THR
1	C	116	VAL
1	D	2	ASN
1	D	24	GLN
1	D	28	ASP
1	D	30	LEU
1	D	50	THR
1	D	59	GLU
1	D	62	LEU
1	D	70	SER
1	D	72	LYS
1	D	81	THR
1	D	116	VAL

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Mol	Chain	Res	Type
1	E	2	ASN
1	E	24	GLN
1	E	28	ASP
1	E	30	LEU
1	E	50	THR
1	E	59	GLU
1	E	62	LEU
1	E	70	SER
1	E	81	THR
1	E	116	VAL
1	F	2	ASN
1	F	24	GLN
1	F	28	ASP
1	F	30	LEU
1	F	50	THR
1	F	59	GLU
1	F	62	LEU
1	F	70	SER
1	F	116	VAL
1	G	2	ASN
1	G	24	GLN
1	G	28	ASP
1	G	30	LEU
1	G	50	THR
1	G	59	GLU
1	G	62	LEU
1	G	70	SER
1	G	82	VAL
1	G	116	VAL
1	H	2	ASN
1	H	24	GLN
1	H	28	ASP
1	H	30	LEU
1	H	50	THR
1	H	59	GLU
1	H	62	LEU
1	H	70	SER
1	H	79	LEU
1	H	116	VAL
1	I	2	ASN
1	I	24	GLN
1	I	28	ASP

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Mol	Chain	Res	Type
1	I	30	LEU
1	I	50	THR
1	I	59	GLU
1	I	62	LEU
1	I	70	SER
1	I	81	THR
1	I	116	VAL
1	J	2	ASN
1	J	24	GLN
1	J	28	ASP
1	J	30	LEU
1	J	50	THR
1	J	59	GLU
1	J	62	LEU
1	J	70	SER
1	J	116	VAL
1	J	118	THR
1	K	2	ASN
1	K	24	GLN
1	K	28	ASP
1	K	30	LEU
1	K	50	THR
1	K	59	GLU
1	K	62	LEU
1	K	70	SER
1	K	116	VAL
1	L	2	ASN
1	L	24	GLN
1	L	28	ASP
1	L	30	LEU
1	L	50	THR
1	L	59	GLU
1	L	62	LEU
1	L	70	SER
1	L	81	THR
1	L	82	VAL
1	L	116	VAL
1	M	2	ASN
1	M	22	PHE
1	M	24	GLN
1	M	28	ASP
1	M	30	LEU

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Mol	Chain	Res	Type
1	M	50	THR
1	M	59	GLU
1	M	62	LEU
1	M	70	SER
1	M	81	THR
1	M	116	VAL
1	N	2	ASN
1	N	24	GLN
1	N	28	ASP
1	N	30	LEU
1	N	50	THR
1	N	59	GLU
1	N	62	LEU
1	N	70	SER
1	N	81	THR
1	N	116	VAL
1	O	2	ASN
1	O	22	PHE
1	O	24	GLN
1	O	28	ASP
1	O	30	LEU
1	O	50	THR
1	O	59	GLU
1	O	62	LEU
1	O	70	SER
1	O	82	VAL
1	O	116	VAL
1	P	2	ASN
1	P	24	GLN
1	P	28	ASP
1	P	30	LEU
1	P	50	THR
1	P	59	GLU
1	P	62	LEU
1	P	70	SER
1	P	81	THR
1	P	82	VAL
1	P	116	VAL
1	Q	2	ASN
1	Q	24	GLN
1	Q	28	ASP
1	Q	30	LEU

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Mol	Chain	Res	Type
1	Q	50	THR
1	Q	59	GLU
1	Q	62	LEU
1	Q	70	SER
1	Q	81	THR
1	Q	116	VAL
1	R	2	ASN
1	R	22	PHE
1	R	24	GLN
1	R	28	ASP
1	R	30	LEU
1	R	50	THR
1	R	59	GLU
1	R	62	LEU
1	R	70	SER
1	R	81	THR
1	R	116	VAL
1	S	2	ASN
1	S	24	GLN
1	S	28	ASP
1	S	30	LEU
1	S	50	THR
1	S	59	GLU
1	S	62	LEU
1	S	70	SER
1	S	81	THR
1	S	116	VAL
1	S	118	THR
1	T	2	ASN
1	T	24	GLN
1	T	28	ASP
1	T	30	LEU
1	T	50	THR
1	T	59	GLU
1	T	62	LEU
1	T	70	SER
1	T	116	VAL
1	U	2	ASN
1	U	24	GLN
1	U	28	ASP
1	U	30	LEU
1	U	50	THR

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Mol	Chain	Res	Type
1	U	59	GLU
1	U	62	LEU
1	U	70	SER
1	U	81	THR
1	U	82	VAL
1	U	116	VAL
1	V	2	ASN
1	V	24	GLN
1	V	28	ASP
1	V	30	LEU
1	V	50	THR
1	V	59	GLU
1	V	62	LEU
1	V	70	SER
1	V	81	THR
1	V	116	VAL
1	V	118	THR
1	W	2	ASN
1	W	24	GLN
1	W	28	ASP
1	W	30	LEU
1	W	50	THR
1	W	59	GLU
1	W	62	LEU
1	W	70	SER
1	W	79	LEU
1	W	81	THR
1	W	116	VAL
1	X	2	ASN
1	X	24	GLN
1	X	28	ASP
1	X	30	LEU
1	X	50	THR
1	X	59	GLU
1	X	62	LEU
1	X	70	SER
1	X	82	VAL
1	X	87	THR
1	X	116	VAL
1	Y	2	ASN
1	Y	22	PHE
1	Y	24	GLN

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Mol	Chain	Res	Type
1	Y	28	ASP
1	Y	30	LEU
1	Y	50	THR
1	Y	59	GLU
1	Y	62	LEU
1	Y	70	SER
1	Y	81	THR
1	Y	82	VAL
1	Y	116	VAL
1	Z	2	ASN
1	Z	24	GLN
1	Z	28	ASP
1	Z	30	LEU
1	Z	50	THR
1	Z	59	GLU
1	Z	62	LEU
1	Z	70	SER
1	Z	81	THR
1	Z	116	VAL
1	1	2	ASN
1	1	24	GLN
1	1	28	ASP
1	1	30	LEU
1	1	50	THR
1	1	59	GLU
1	1	62	LEU
1	1	70	SER
1	1	116	VAL
1	2	2	ASN
1	2	24	GLN
1	2	28	ASP
1	2	30	LEU
1	2	50	THR
1	2	59	GLU
1	2	62	LEU
1	2	70	SER
1	2	116	VAL
1	3	2	ASN
1	3	24	GLN
1	3	28	ASP
1	3	30	LEU
1	3	50	THR

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Mol	Chain	Res	Type
1	3	59	GLU
1	3	62	LEU
1	3	70	SER
1	3	81	THR
1	3	116	VAL
1	4	2	ASN
1	4	24	GLN
1	4	28	ASP
1	4	30	LEU
1	4	50	THR
1	4	59	GLU
1	4	70	SER
1	4	81	THR
1	4	116	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	B	2	ASN
1	B	7	ASN
1	C	2	ASN
1	C	7	ASN
1	D	2	ASN
1	D	7	ASN
1	E	2	ASN
1	E	7	ASN
1	F	2	ASN
1	F	7	ASN
1	G	2	ASN
1	H	2	ASN
1	I	2	ASN
1	I	7	ASN
1	J	2	ASN
1	J	7	ASN
1	K	2	ASN
1	K	24	GLN
1	L	2	ASN
1	M	2	ASN
1	N	2	ASN
1	N	7	ASN
1	O	2	ASN

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Mol	Chain	Res	Type
1	O	7	ASN
1	P	2	ASN
1	Q	2	ASN
1	Q	7	ASN
1	R	2	ASN
1	R	7	ASN
1	S	2	ASN
1	S	7	ASN
1	T	2	ASN
1	T	7	ASN
1	U	2	ASN
1	U	7	ASN
1	V	2	ASN
1	W	2	ASN
1	X	2	ASN
1	X	7	ASN
1	Y	2	ASN
1	Y	7	ASN
1	Z	2	ASN
1	1	2	ASN
1	2	2	ASN
1	3	2	ASN
1	3	7	ASN
1	4	2	ASN
1	4	7	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

40 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	F	157	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	J	158	-	4,4,4	0.15	0	6,6,6	0.55	0
2	SO4	Z	158	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	2	158	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	D	158	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	A	157	-	4,4,4	0.15	0	6,6,6	0.41	0
2	SO4	U	157	-	4,4,4	0.26	0	6,6,6	0.49	0
2	SO4	V	158	-	4,4,4	0.18	0	6,6,6	0.26	0
2	SO4	L	158	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	X	157	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	2	159	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	C	158	-	4,4,4	0.12	0	6,6,6	0.24	0
2	SO4	1	157	-	4,4,4	0.24	0	6,6,6	0.35	0
2	SO4	K	157	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	S	157	-	4,4,4	0.17	0	6,6,6	0.34	0
2	SO4	N	157	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	G	157	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	M	158	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	M	159	-	4,4,4	0.11	0	6,6,6	0.55	0
2	SO4	E	157	-	4,4,4	0.15	0	6,6,6	0.38	0
2	SO4	D	157	-	4,4,4	0.16	0	6,6,6	0.33	0
2	SO4	Q	157	-	4,4,4	0.23	0	6,6,6	0.27	0
2	SO4	F	158	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	H	157	-	4,4,4	0.29	0	6,6,6	0.66	0
2	SO4	H	158	-	4,4,4	0.27	0	6,6,6	0.35	0
2	SO4	L	157	-	4,4,4	0.26	0	6,6,6	0.57	0
2	SO4	Q	158	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	V	157	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	C	157	-	4,4,4	0.17	0	6,6,6	0.51	0
2	SO4	P	157	-	4,4,4	0.29	0	6,6,6	0.46	0
2	SO4	B	157	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	2	157	-	4,4,4	0.22	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	X	158	-	4,4,4	0.20	0	6,6,6	0.39	0
2	SO4	Z	157	-	4,4,4	0.11	0	6,6,6	0.24	0
2	SO4	Q	159	-	4,4,4	0.13	0	6,6,6	0.23	0
2	SO4	M	157	-	4,4,4	0.12	0	6,6,6	0.51	0
2	SO4	R	158	-	4,4,4	0.14	0	6,6,6	0.28	0
2	SO4	H	159	-	4,4,4	0.06	0	6,6,6	0.48	0
2	SO4	3	157	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	1	158	-	4,4,4	0.24	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	158	SO4	1	0
2	A	157	SO4	1	0
2	2	159	SO4	1	0
2	1	157	SO4	2	0
2	D	157	SO4	1	0
2	F	158	SO4	3	0
2	H	157	SO4	3	0
2	H	158	SO4	1	0
2	P	157	SO4	1	0
2	Q	159	SO4	1	0
2	1	158	SO4	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	154/156 (98%)	-0.22	0	100	100	15, 27, 51, 63	0
1	2	154/156 (98%)	-0.22	0	100	100	12, 27, 48, 61	0
1	3	154/156 (98%)	-0.33	0	100	100	16, 27, 47, 61	0
1	4	154/156 (98%)	-0.27	0	100	100	12, 27, 47, 58	0
1	A	154/156 (98%)	-0.27	0	100	100	8, 27, 48, 59	0
1	B	154/156 (98%)	-0.24	0	100	100	15, 27, 49, 63	0
1	C	154/156 (98%)	-0.31	1 (0%)	89	86	16, 28, 45, 66	0
1	D	154/156 (98%)	-0.20	1 (0%)	89	86	15, 28, 48, 63	0
1	E	154/156 (98%)	-0.25	0	100	100	16, 28, 50, 65	0
1	F	154/156 (98%)	-0.24	0	100	100	15, 28, 51, 63	0
1	G	154/156 (98%)	-0.30	0	100	100	16, 28, 50, 65	0
1	H	154/156 (98%)	-0.26	0	100	100	15, 28, 46, 62	0
1	I	154/156 (98%)	-0.29	0	100	100	16, 28, 50, 63	0
1	J	154/156 (98%)	-0.24	0	100	100	14, 28, 50, 61	0
1	K	154/156 (98%)	-0.26	0	100	100	16, 27, 46, 65	0
1	L	154/156 (98%)	-0.27	0	100	100	9, 27, 47, 64	0
1	M	154/156 (98%)	-0.28	0	100	100	13, 27, 49, 62	0
1	N	154/156 (98%)	-0.30	0	100	100	15, 26, 47, 63	0
1	O	154/156 (98%)	-0.27	0	100	100	16, 27, 48, 62	0
1	P	154/156 (98%)	-0.31	0	100	100	15, 27, 46, 60	0
1	Q	154/156 (98%)	-0.28	0	100	100	16, 27, 49, 63	0
1	R	154/156 (98%)	-0.29	0	100	100	6, 27, 45, 66	0
1	S	154/156 (98%)	-0.24	0	100	100	14, 28, 48, 64	0
1	T	154/156 (98%)	-0.29	0	100	100	15, 27, 48, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	U	154/156 (98%)	-0.27	0	100	100	13, 27, 49, 69	0
1	V	154/156 (98%)	-0.30	0	100	100	15, 28, 47, 64	0
1	W	154/156 (98%)	-0.25	0	100	100	17, 28, 51, 71	0
1	X	154/156 (98%)	-0.25	0	100	100	15, 28, 47, 65	0
1	Y	154/156 (98%)	-0.21	0	100	100	16, 27, 48, 61	0
1	Z	154/156 (98%)	-0.31	0	100	100	16, 28, 50, 63	0
All	All	4620/4680 (98%)	-0.27	2 (0%)	100	100	6, 27, 50, 71	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	107	ASP	2.5
1	D	106	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	L	158	5/5	0.80	0.37	26,45,126,127	0
2	SO4	C	158	5/5	0.83	0.30	4,65,108,137	0
2	SO4	Z	158	5/5	0.84	0.40	54,54,136,173	0
2	SO4	2	158	5/5	0.87	0.47	7,125,158,173	0
2	SO4	D	158	5/5	0.89	0.22	18,61,108,122	0
2	SO4	1	158	5/5	0.91	0.22	11,20,56,96	0
2	SO4	H	158	5/5	0.92	0.24	14,15,75,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	F	157	5/5	0.92	0.19	15,42,63,77	0
2	SO4	M	158	5/5	0.92	0.22	24,29,94,96	0
2	SO4	F	158	5/5	0.93	0.32	35,65,98,122	0
2	SO4	1	157	5/5	0.93	0.19	21,23,40,43	0
2	SO4	N	157	5/5	0.93	0.18	0,0,65,84	0
2	SO4	Q	158	5/5	0.93	0.17	19,27,92,107	0
2	SO4	P	157	5/5	0.94	0.18	3,10,40,41	0
2	SO4	L	157	5/5	0.94	0.21	0,24,71,90	0
2	SO4	Q	157	5/5	0.95	0.20	6,18,40,85	0
2	SO4	C	157	5/5	0.95	0.17	7,25,31,40	0
2	SO4	S	157	5/5	0.95	0.15	11,18,71,72	0
2	SO4	U	157	5/5	0.95	0.16	24,26,45,80	0
2	SO4	Z	157	5/5	0.95	0.17	4,23,45,51	0
2	SO4	A	157	5/5	0.95	0.16	0,9,46,48	0
2	SO4	G	157	5/5	0.95	0.17	0,46,65,90	0
2	SO4	E	157	5/5	0.95	0.17	4,23,38,53	0
2	SO4	J	158	5/5	0.95	0.15	10,11,62,73	0
2	SO4	K	157	5/5	0.96	0.16	16,22,50,65	0
2	SO4	V	157	5/5	0.96	0.21	17,23,44,50	0
2	SO4	X	157	5/5	0.96	0.20	12,22,75,95	0
2	SO4	X	158	5/5	0.96	0.20	10,29,35,40	0
2	SO4	B	157	5/5	0.96	0.14	3,28,29,50	0
2	SO4	H	159	5/5	0.96	0.16	17,32,71,89	0
2	SO4	M	157	5/5	0.96	0.15	10,13,15,17	0
2	SO4	Q	159	5/5	0.96	0.18	23,35,38,63	0
2	SO4	2	157	5/5	0.96	0.14	3,17,46,60	0
2	SO4	H	157	5/5	0.96	0.12	7,9,42,76	0
2	SO4	3	157	5/5	0.96	0.17	33,41,74,81	0
2	SO4	D	157	5/5	0.97	0.17	1,22,30,51	0
2	SO4	M	159	5/5	0.97	0.16	3,6,18,57	0
2	SO4	2	159	5/5	0.97	0.13	1,22,38,44	0
2	SO4	V	158	5/5	0.97	0.14	15,38,53,59	0
2	SO4	R	158	5/5	0.98	0.12	8,20,44,67	0

6.5 Other polymers (i)

There are no such residues in this entry.