



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:08 am GMT

PDB ID : 5ENY  
Title : Ketosynthase from module 6 connected to acyl carrier protein from module 5 (unobservable) of the bacillaene synthase from *Bacillus subtilis* 168  
Authors : Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.  
Deposited on : 2015-11-09  
Resolution : 4.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

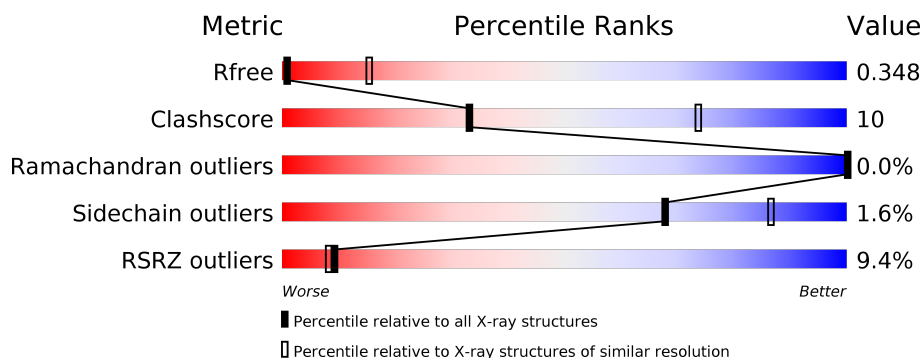
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	764	<div> <div>7%</div> <div> <div></div> <div>62%</div> <div>11%</div> <div>26%</div> </div> </div>
1	B	764	<div> <div>8%</div> <div> <div></div> <div>59%</div> <div>10%</div> <div>30%</div> </div> </div>
1	C	764	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>11%</div> <div>26%</div> </div> </div>
1	D	764	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>9%</div> <div>30%</div> </div> </div>
1	E	764	<div> <div>7%</div> <div> <div></div> <div>62%</div> <div>11%</div> <div>26%</div> </div> </div>
1	F	764	<div> <div>7%</div> <div> <div></div> <div>59%</div> <div>10%</div> <div>30%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	764	<div><div>5%</div><div><div></div><div></div><div></div></div><div>62%11%26%</div></div>
1	H	764	<div><div>10%</div><div><div></div><div></div><div></div></div><div>60%10%30%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34416 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 Polyketide synthase PksL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	B	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			
1	C	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	D	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			
1	E	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	F	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			
1	G	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	H	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-172	MET	-	initiating methionine	UNP Q05470
A	-171	GLY	-	expression tag	UNP Q05470
A	-170	SER	-	expression tag	UNP Q05470
A	-169	SER	-	expression tag	UNP Q05470
A	-168	HIS	-	expression tag	UNP Q05470
A	-167	HIS	-	expression tag	UNP Q05470
A	-166	HIS	-	expression tag	UNP Q05470
A	-165	HIS	-	expression tag	UNP Q05470
A	-164	HIS	-	expression tag	UNP Q05470
A	-163	HIS	-	expression tag	UNP Q05470
A	-162	SER	-	expression tag	UNP Q05470
A	-161	SER	-	expression tag	UNP Q05470
A	-160	GLY	-	expression tag	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-159	LEU	-	expression tag	UNP Q05470
A	-158	VAL	-	expression tag	UNP Q05470
A	-157	PRO	-	expression tag	UNP Q05470
A	-156	ARG	-	expression tag	UNP Q05470
A	-155	GLY	-	expression tag	UNP Q05470
A	-154	SER	-	expression tag	UNP Q05470
A	-153	SER	-	expression tag	UNP Q05470
B	-172	MET	-	initiating methionine	UNP Q05470
B	-171	GLY	-	expression tag	UNP Q05470
B	-170	SER	-	expression tag	UNP Q05470
B	-169	SER	-	expression tag	UNP Q05470
B	-168	HIS	-	expression tag	UNP Q05470
B	-167	HIS	-	expression tag	UNP Q05470
B	-166	HIS	-	expression tag	UNP Q05470
B	-165	HIS	-	expression tag	UNP Q05470
B	-164	HIS	-	expression tag	UNP Q05470
B	-163	HIS	-	expression tag	UNP Q05470
B	-162	SER	-	expression tag	UNP Q05470
B	-161	SER	-	expression tag	UNP Q05470
B	-160	GLY	-	expression tag	UNP Q05470
B	-159	LEU	-	expression tag	UNP Q05470
B	-158	VAL	-	expression tag	UNP Q05470
B	-157	PRO	-	expression tag	UNP Q05470
B	-156	ARG	-	expression tag	UNP Q05470
B	-155	GLY	-	expression tag	UNP Q05470
B	-154	SER	-	expression tag	UNP Q05470
B	-153	SER	-	expression tag	UNP Q05470
C	-172	MET	-	initiating methionine	UNP Q05470
C	-171	GLY	-	expression tag	UNP Q05470
C	-170	SER	-	expression tag	UNP Q05470
C	-169	SER	-	expression tag	UNP Q05470
C	-168	HIS	-	expression tag	UNP Q05470
C	-167	HIS	-	expression tag	UNP Q05470
C	-166	HIS	-	expression tag	UNP Q05470
C	-165	HIS	-	expression tag	UNP Q05470
C	-164	HIS	-	expression tag	UNP Q05470
C	-163	HIS	-	expression tag	UNP Q05470
C	-162	SER	-	expression tag	UNP Q05470
C	-161	SER	-	expression tag	UNP Q05470
C	-160	GLY	-	expression tag	UNP Q05470
C	-159	LEU	-	expression tag	UNP Q05470
C	-158	VAL	-	expression tag	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-157	PRO	-	expression tag	UNP Q05470
C	-156	ARG	-	expression tag	UNP Q05470
C	-155	GLY	-	expression tag	UNP Q05470
C	-154	SER	-	expression tag	UNP Q05470
C	-153	SER	-	expression tag	UNP Q05470
D	-172	MET	-	initiating methionine	UNP Q05470
D	-171	GLY	-	expression tag	UNP Q05470
D	-170	SER	-	expression tag	UNP Q05470
D	-169	SER	-	expression tag	UNP Q05470
D	-168	HIS	-	expression tag	UNP Q05470
D	-167	HIS	-	expression tag	UNP Q05470
D	-166	HIS	-	expression tag	UNP Q05470
D	-165	HIS	-	expression tag	UNP Q05470
D	-164	HIS	-	expression tag	UNP Q05470
D	-163	HIS	-	expression tag	UNP Q05470
D	-162	SER	-	expression tag	UNP Q05470
D	-161	SER	-	expression tag	UNP Q05470
D	-160	GLY	-	expression tag	UNP Q05470
D	-159	LEU	-	expression tag	UNP Q05470
D	-158	VAL	-	expression tag	UNP Q05470
D	-157	PRO	-	expression tag	UNP Q05470
D	-156	ARG	-	expression tag	UNP Q05470
D	-155	GLY	-	expression tag	UNP Q05470
D	-154	SER	-	expression tag	UNP Q05470
D	-153	SER	-	expression tag	UNP Q05470
E	-172	MET	-	initiating methionine	UNP Q05470
E	-171	GLY	-	expression tag	UNP Q05470
E	-170	SER	-	expression tag	UNP Q05470
E	-169	SER	-	expression tag	UNP Q05470
E	-168	HIS	-	expression tag	UNP Q05470
E	-167	HIS	-	expression tag	UNP Q05470
E	-166	HIS	-	expression tag	UNP Q05470
E	-165	HIS	-	expression tag	UNP Q05470
E	-164	HIS	-	expression tag	UNP Q05470
E	-163	HIS	-	expression tag	UNP Q05470
E	-162	SER	-	expression tag	UNP Q05470
E	-161	SER	-	expression tag	UNP Q05470
E	-160	GLY	-	expression tag	UNP Q05470
E	-159	LEU	-	expression tag	UNP Q05470
E	-158	VAL	-	expression tag	UNP Q05470
E	-157	PRO	-	expression tag	UNP Q05470
E	-156	ARG	-	expression tag	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-155	GLY	-	expression tag	UNP Q05470
E	-154	SER	-	expression tag	UNP Q05470
E	-153	SER	-	expression tag	UNP Q05470
F	-172	MET	-	initiating methionine	UNP Q05470
F	-171	GLY	-	expression tag	UNP Q05470
F	-170	SER	-	expression tag	UNP Q05470
F	-169	SER	-	expression tag	UNP Q05470
F	-168	HIS	-	expression tag	UNP Q05470
F	-167	HIS	-	expression tag	UNP Q05470
F	-166	HIS	-	expression tag	UNP Q05470
F	-165	HIS	-	expression tag	UNP Q05470
F	-164	HIS	-	expression tag	UNP Q05470
F	-163	HIS	-	expression tag	UNP Q05470
F	-162	SER	-	expression tag	UNP Q05470
F	-161	SER	-	expression tag	UNP Q05470
F	-160	GLY	-	expression tag	UNP Q05470
F	-159	LEU	-	expression tag	UNP Q05470
F	-158	VAL	-	expression tag	UNP Q05470
F	-157	PRO	-	expression tag	UNP Q05470
F	-156	ARG	-	expression tag	UNP Q05470
F	-155	GLY	-	expression tag	UNP Q05470
F	-154	SER	-	expression tag	UNP Q05470
F	-153	SER	-	expression tag	UNP Q05470
G	-172	MET	-	initiating methionine	UNP Q05470
G	-171	GLY	-	expression tag	UNP Q05470
G	-170	SER	-	expression tag	UNP Q05470
G	-169	SER	-	expression tag	UNP Q05470
G	-168	HIS	-	expression tag	UNP Q05470
G	-167	HIS	-	expression tag	UNP Q05470
G	-166	HIS	-	expression tag	UNP Q05470
G	-165	HIS	-	expression tag	UNP Q05470
G	-164	HIS	-	expression tag	UNP Q05470
G	-163	HIS	-	expression tag	UNP Q05470
G	-162	SER	-	expression tag	UNP Q05470
G	-161	SER	-	expression tag	UNP Q05470
G	-160	GLY	-	expression tag	UNP Q05470
G	-159	LEU	-	expression tag	UNP Q05470
G	-158	VAL	-	expression tag	UNP Q05470
G	-157	PRO	-	expression tag	UNP Q05470
G	-156	ARG	-	expression tag	UNP Q05470
G	-155	GLY	-	expression tag	UNP Q05470
G	-154	SER	-	expression tag	UNP Q05470

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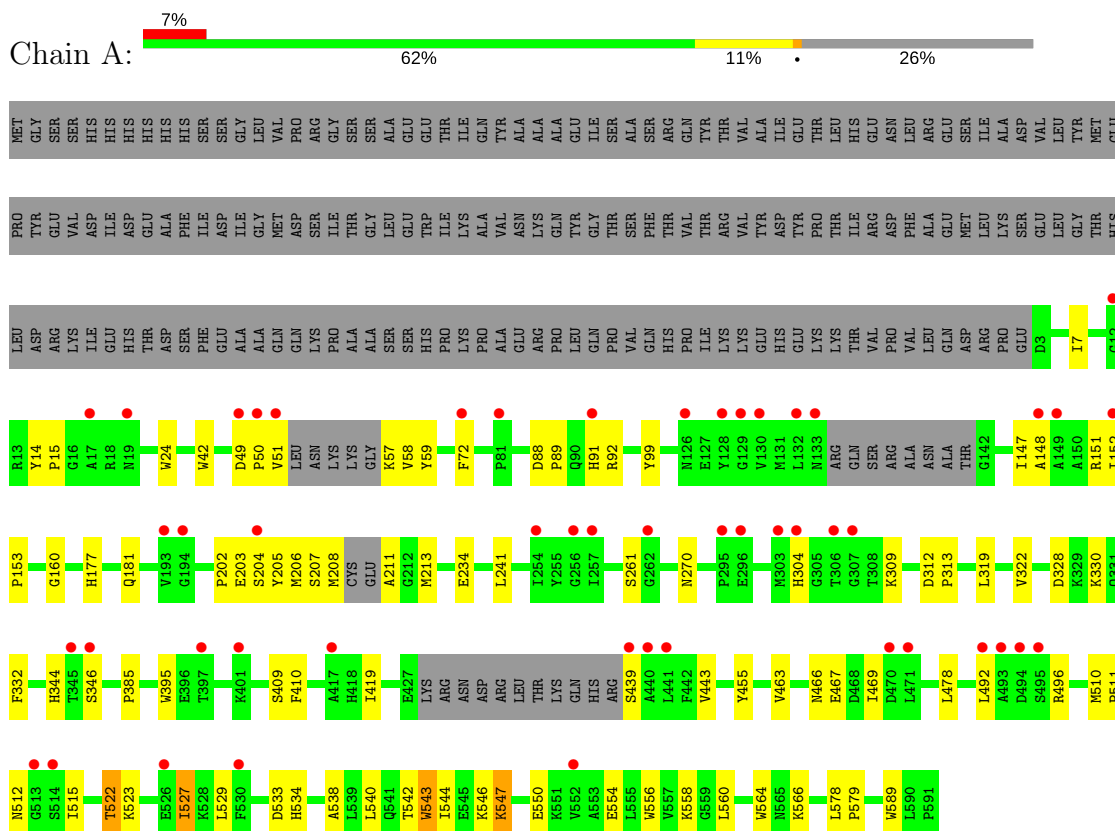
Chain	Residue	Modelled	Actual	Comment	Reference
G	-153	SER	-	expression tag	UNP Q05470
H	-172	MET	-	initiating methionine	UNP Q05470
H	-171	GLY	-	expression tag	UNP Q05470
H	-170	SER	-	expression tag	UNP Q05470
H	-169	SER	-	expression tag	UNP Q05470
H	-168	HIS	-	expression tag	UNP Q05470
H	-167	HIS	-	expression tag	UNP Q05470
H	-166	HIS	-	expression tag	UNP Q05470
H	-165	HIS	-	expression tag	UNP Q05470
H	-164	HIS	-	expression tag	UNP Q05470
H	-163	HIS	-	expression tag	UNP Q05470
H	-162	SER	-	expression tag	UNP Q05470
H	-161	SER	-	expression tag	UNP Q05470
H	-160	GLY	-	expression tag	UNP Q05470
H	-159	LEU	-	expression tag	UNP Q05470
H	-158	VAL	-	expression tag	UNP Q05470
H	-157	PRO	-	expression tag	UNP Q05470
H	-156	ARG	-	expression tag	UNP Q05470
H	-155	GLY	-	expression tag	UNP Q05470
H	-154	SER	-	expression tag	UNP Q05470
H	-153	SER	-	expression tag	UNP Q05470



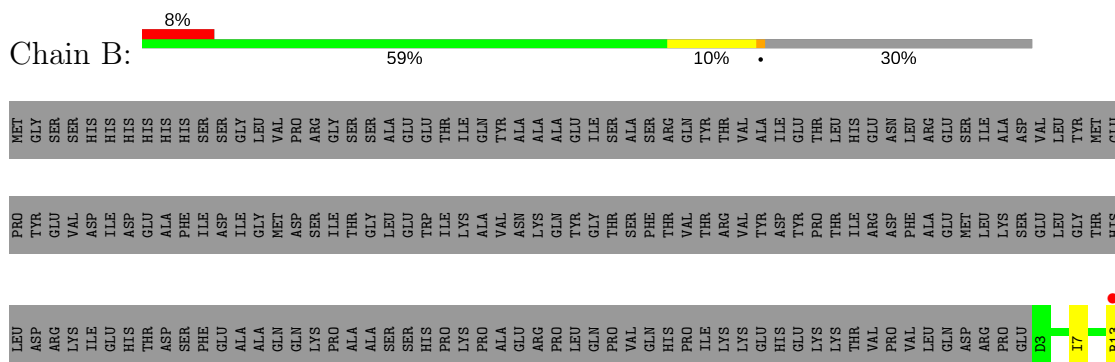
### 3 Residue-property plots

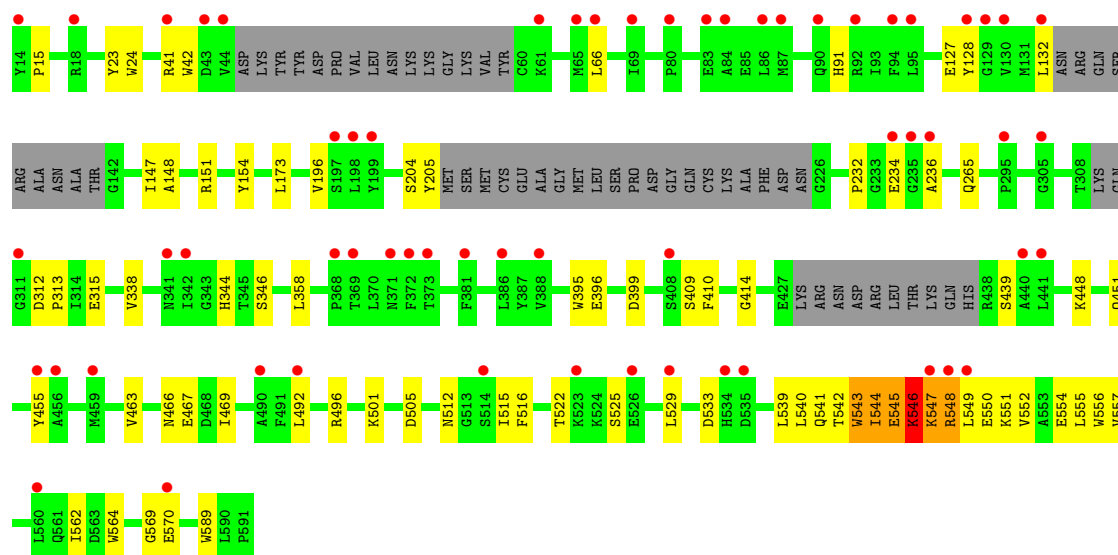
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Polyketide synthase PksL

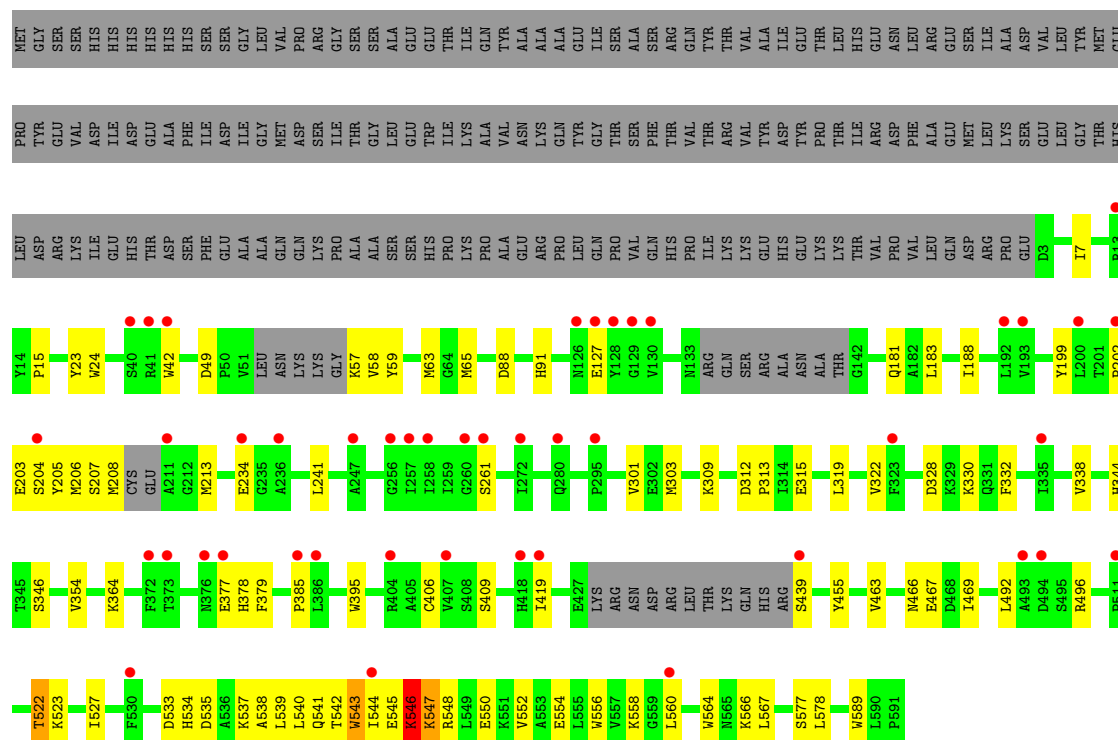


- Molecule 1: Polyketide synthase PksL

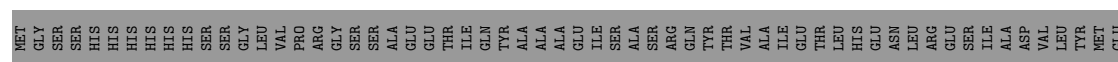


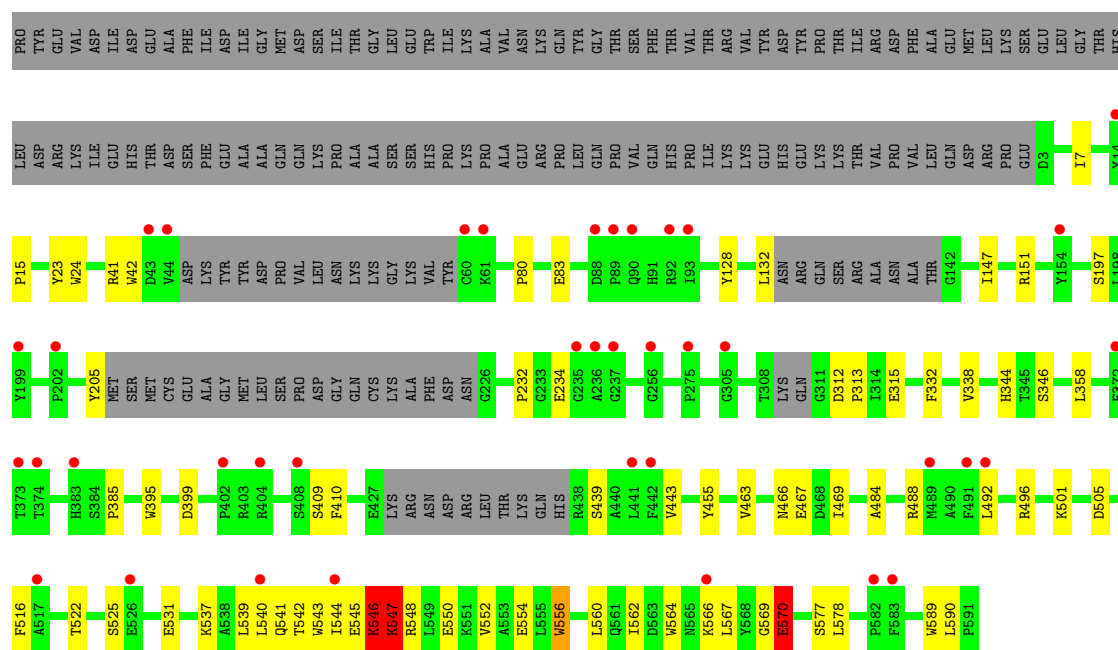


● Molecule 1: Polyketide synthase PksL

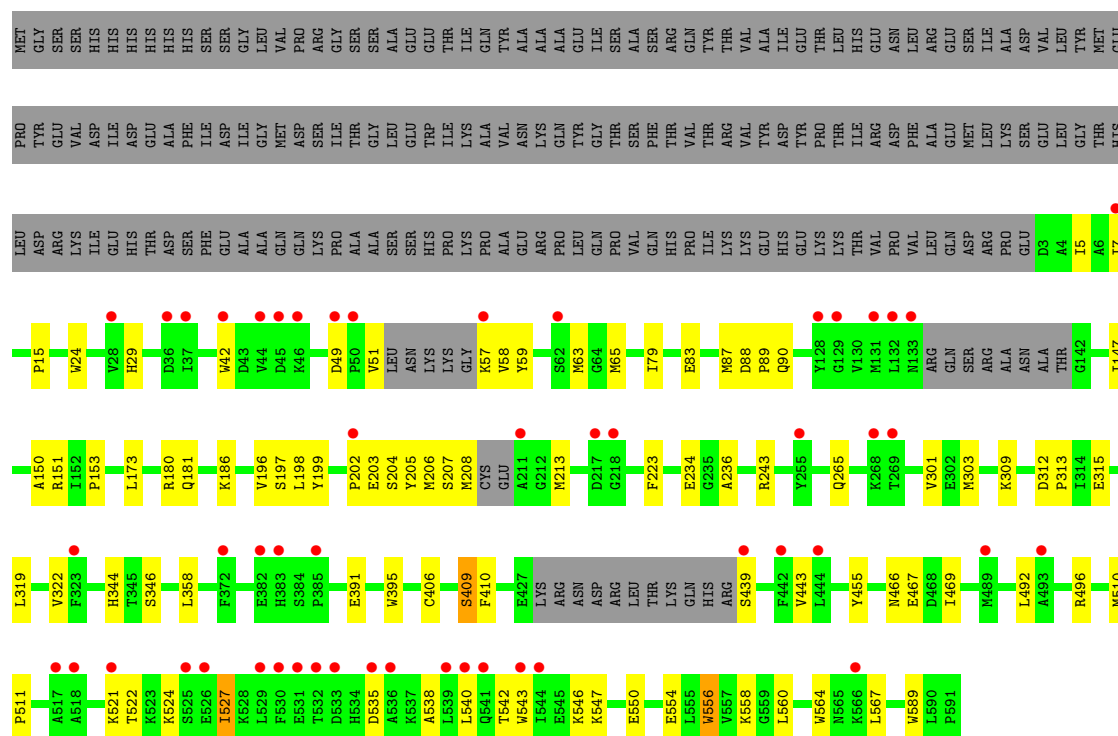


● Molecule 1: Polyketide synthase PksL

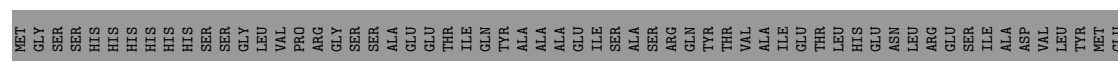




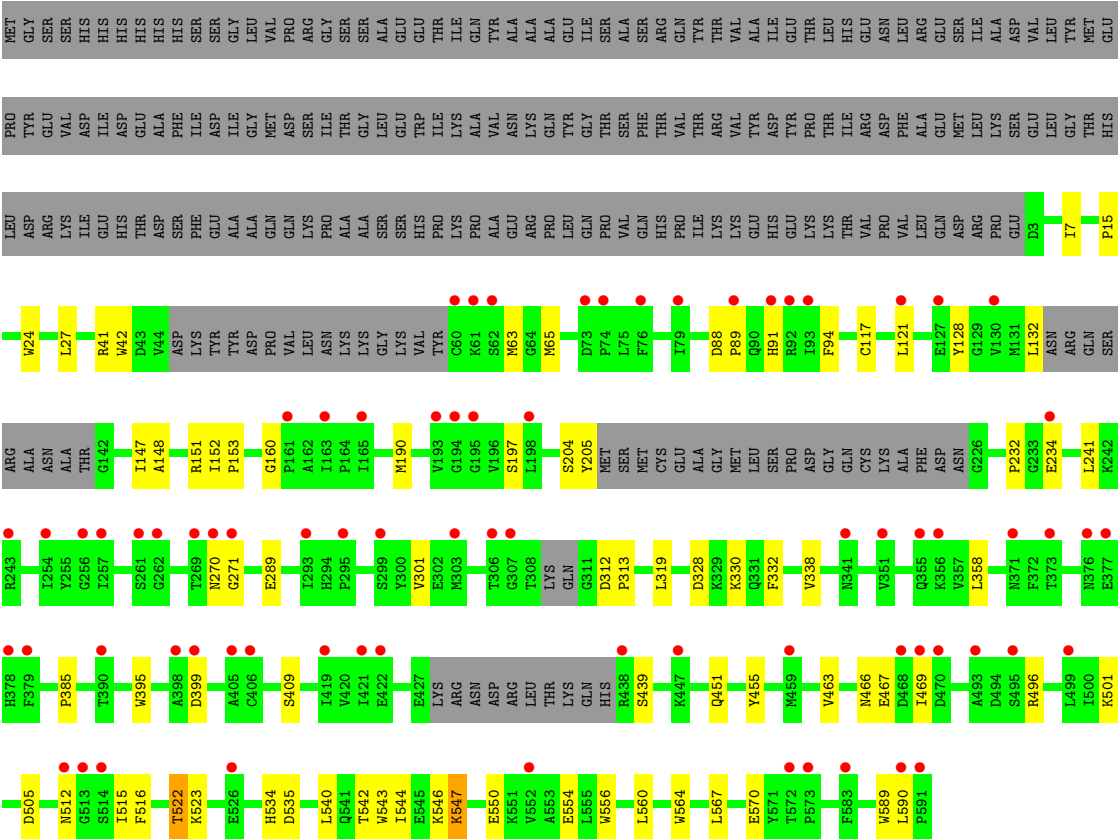
• Molecule 1: Polyketide synthase PksL



• Molecule 1: Polyketide synthase PksL







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.11Å 112.73Å 211.44Å 104.96° 90.07° 106.32°	Depositor
Resolution (Å)	39.77 – 4.00 39.77 – 4.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (39.77-4.00) 84.5 (39.77-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.333 , 0.354 0.327 , 0.348	Depositor DCC
$R_{free}$ test set	2126 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	138.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 102.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.347 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	34416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2714e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.42	7/4518 (0.2%)	0.45	0/6110
1	B	0.43	7/4277 (0.2%)	0.58	7/5784 (0.1%)
1	C	0.42	7/4518 (0.2%)	0.53	2/6110 (0.0%)
1	D	0.41	6/4277 (0.1%)	0.56	7/5784 (0.1%)
1	E	0.42	7/4518 (0.2%)	0.45	0/6110
1	F	0.43	7/4277 (0.2%)	0.54	6/5784 (0.1%)
1	G	0.42	7/4518 (0.2%)	0.45	0/6110
1	H	0.41	6/4277 (0.1%)	0.45	0/5784
All	All	0.42	54/35180 (0.2%)	0.50	22/47576 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	H	0	1
All	All	0	5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	TRP	CD2-CE2	6.34	1.49	1.41
1	F	564	TRP	CD2-CE2	6.24	1.48	1.41
1	G	42	TRP	CD2-CE2	6.24	1.48	1.41
1	E	42	TRP	CD2-CE2	6.23	1.48	1.41
1	E	589	TRP	CD2-CE2	6.21	1.48	1.41
1	H	589	TRP	CD2-CE2	6.19	1.48	1.41
1	A	589	TRP	CD2-CE2	6.17	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	24	TRP	CD2-CE2	6.17	1.48	1.41
1	C	42	TRP	CD2-CE2	6.17	1.48	1.41
1	D	564	TRP	CD2-CE2	6.16	1.48	1.41
1	A	564	TRP	CD2-CE2	6.16	1.48	1.41
1	B	564	TRP	CD2-CE2	6.16	1.48	1.41
1	H	395	TRP	CD2-CE2	6.15	1.48	1.41
1	E	564	TRP	CD2-CE2	6.15	1.48	1.41
1	F	42	TRP	CD2-CE2	6.15	1.48	1.41
1	A	42	TRP	CD2-CE2	6.14	1.48	1.41
1	E	556	TRP	CD2-CE2	6.14	1.48	1.41
1	C	395	TRP	CD2-CE2	6.14	1.48	1.41
1	C	564	TRP	CD2-CE2	6.13	1.48	1.41
1	D	589	TRP	CD2-CE2	6.13	1.48	1.41
1	H	556	TRP	CD2-CE2	6.13	1.48	1.41
1	A	395	TRP	CD2-CE2	6.13	1.48	1.41
1	G	564	TRP	CD2-CE2	6.12	1.48	1.41
1	G	589	TRP	CD2-CE2	6.12	1.48	1.41
1	G	24	TRP	CD2-CE2	6.12	1.48	1.41
1	F	543	TRP	CD2-CE2	6.12	1.48	1.41
1	C	589	TRP	CD2-CE2	6.11	1.48	1.41
1	G	556	TRP	CD2-CE2	6.11	1.48	1.41
1	F	589	TRP	CD2-CE2	6.11	1.48	1.41
1	A	24	TRP	CD2-CE2	6.10	1.48	1.41
1	D	42	TRP	CD2-CE2	6.10	1.48	1.41
1	C	24	TRP	CD2-CE2	6.10	1.48	1.41
1	H	24	TRP	CD2-CE2	6.10	1.48	1.41
1	H	42	TRP	CD2-CE2	6.10	1.48	1.41
1	G	395	TRP	CD2-CE2	6.10	1.48	1.41
1	B	543	TRP	CD2-CE2	6.09	1.48	1.41
1	C	556	TRP	CD2-CE2	6.08	1.48	1.41
1	B	395	TRP	CD2-CE2	6.08	1.48	1.41
1	E	543	TRP	CD2-CE2	6.08	1.48	1.41
1	D	395	TRP	CD2-CE2	6.07	1.48	1.41
1	F	395	TRP	CD2-CE2	6.07	1.48	1.41
1	B	589	TRP	CD2-CE2	6.07	1.48	1.41
1	F	556	TRP	CD2-CE2	6.06	1.48	1.41
1	A	543	TRP	CD2-CE2	6.05	1.48	1.41
1	E	24	TRP	CD2-CE2	6.05	1.48	1.41
1	B	24	TRP	CD2-CE2	6.04	1.48	1.41
1	B	556	TRP	CD2-CE2	6.04	1.48	1.41
1	C	543	TRP	CD2-CE2	6.04	1.48	1.41
1	D	556	TRP	CD2-CE2	6.04	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	556	TRP	CD2-CE2	6.02	1.48	1.41
1	D	24	TRP	CD2-CE2	6.01	1.48	1.41
1	G	543	TRP	CD2-CE2	6.01	1.48	1.41
1	E	395	TRP	CD2-CE2	6.00	1.48	1.41
1	H	564	TRP	CD2-CE2	5.93	1.48	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	546	LYS	CB-CA-C	-19.44	71.52	110.40
1	D	546	LYS	CB-CA-C	-19.21	71.98	110.40
1	B	546	LYS	N-CA-CB	-18.38	77.51	110.60
1	B	545	GLU	CB-CA-C	15.26	140.91	110.40
1	F	546	LYS	N-CA-C	13.36	147.08	111.00
1	F	569	GLY	N-CA-C	-9.54	89.25	113.10
1	B	545	GLU	N-CA-C	-8.93	86.90	111.00
1	F	547	LYS	N-CA-CB	-8.47	95.36	110.60
1	B	548	ARG	N-CA-C	8.01	132.62	111.00
1	B	546	LYS	N-CA-C	7.51	131.28	111.00
1	C	546	LYS	C-N-CA	7.23	139.78	121.70
1	D	569	GLY	N-CA-C	-7.20	95.09	113.10
1	F	548	ARG	CB-CA-C	7.03	124.45	110.40
1	D	570	GLU	N-CA-C	6.91	129.66	111.00
1	D	547	LYS	N-CA-C	6.09	127.43	111.00
1	B	548	ARG	CB-CA-C	-6.07	98.25	110.40
1	D	548	ARG	CB-CA-C	6.06	122.52	110.40
1	D	546	LYS	N-CA-C	6.04	127.30	111.00
1	F	548	ARG	N-CA-C	-5.89	95.09	111.00
1	D	570	GLU	N-CA-CB	-5.77	100.21	110.60
1	B	549	LEU	N-CA-C	5.39	125.55	111.00
1	F	546	LYS	CB-CA-C	-5.29	99.81	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	570	GLU	Peptide
1	C	546	LYS	Peptide
1	D	570	GLU	Peptide
1	F	570	GLU	Peptide
1	H	570	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4419	0	4322	86	2
1	B	4185	0	4102	76	11
1	C	4419	0	4323	84	8
1	D	4185	0	4102	70	2
1	E	4419	0	4323	59	6
1	F	4185	0	4102	193	0
1	G	4419	0	4323	144	0
1	H	4185	0	4102	83	3
All	All	34416	0	33699	670	16

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (670) 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:F:535:ASP:CB	1:G:539:LEU:HB2	1.33	1.56
1:F:535:ASP:HB2	1:G:539:LEU:CB	1.28	1.52
1:F:545:GLU:CA	1:F:546:LYS:HG3	1.36	1.51
1:A:270:ASN:HD21	1:F:378:HIS:CA	1.23	1.51
1:F:539:LEU:CD1	1:G:533:ASP:CG	1.80	1.50
1:F:545:GLU:HA	1:F:546:LYS:CG	1.38	1.49
1:H:542:THR:C	1:H:546:LYS:HG2	1.32	1.46
1:A:270:ASN:CG	1:F:378:HIS:HA	1.35	1.46
1:F:544:ILE:C	1:F:546:LYS:HG2	1.34	1.46
1:H:542:THR:O	1:H:546:LYS:CG	1.68	1.40
1:A:270:ASN:ND2	1:F:378:HIS:HA	1.12	1.40
1:H:542:THR:CG2	1:H:546:LYS:HD3	1.53	1.38
1:C:378:HIS:C	1:H:270:ASN:HD21	1.24	1.38
1:D:540:LEU:HD11	1:D:544:ILE:CD1	1.53	1.38
1:A:270:ASN:OD1	1:F:377:GLU:C	1.65	1.34
1:F:539:LEU:CD2	1:G:536:ALA:HB2	1.57	1.32
1:F:546:LYS:CD	1:F:566:LYS:O	1.77	1.31
1:C:378:HIS:HA	1:H:270:ASN:ND2	1.43	1.31
1:H:546:LYS:O	1:H:547:LYS:HG3	1.19	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:539:LEU:HD22	1:G:536:ALA:CB	1.58	1.30
1:A:270:ASN:HD21	1:F:378:HIS:C	1.34	1.28
1:A:270:ASN:ND2	1:F:378:HIS:CA	1.86	1.27
1:F:544:ILE:O	1:F:546:LYS:CG	1.82	1.26
1:D:541:GLN:O	1:D:545:GLU:HB2	1.35	1.26
1:F:539:LEU:HD11	1:G:533:ASP:CG	0.88	1.25
1:F:546:LYS:HD3	1:F:566:LYS:O	1.14	1.25
1:F:533:ASP:OD2	1:G:539:LEU:CD1	1.85	1.23
1:H:542:THR:CG2	1:H:546:LYS:CD	2.18	1.20
1:C:378:HIS:CA	1:H:270:ASN:HD21	1.55	1.20
1:H:542:THR:HG22	1:H:546:LYS:CG	1.72	1.19
1:C:378:HIS:CA	1:H:270:ASN:ND2	2.06	1.18
1:F:544:ILE:O	1:F:546:LYS:HG2	1.02	1.17
1:C:378:HIS:HA	1:H:270:ASN:CG	1.52	1.17
1:F:539:LEU:HD11	1:G:533:ASP:OD2	1.44	1.17
1:B:540:LEU:O	1:B:544:ILE:HD12	1.44	1.16
1:B:540:LEU:CG	1:B:544:ILE:HD11	1.76	1.16
1:F:539:LEU:HD11	1:G:533:ASP:CB	1.76	1.15
1:H:542:THR:HG23	1:H:546:LYS:CD	1.76	1.13
1:D:540:LEU:CD1	1:D:544:ILE:CD1	2.25	1.12
1:F:539:LEU:CD1	1:G:533:ASP:OD2	1.95	1.12
1:D:541:GLN:NE2	1:D:545:GLU:OE2	1.84	1.11
1:F:545:GLU:CA	1:F:546:LYS:CG	2.08	1.09
1:B:540:LEU:O	1:B:544:ILE:CD1	2.01	1.09
1:B:544:ILE:C	1:B:546:LYS:HB3	1.72	1.09
1:F:539:LEU:CA	1:G:535:ASP:HB2	1.82	1.08
1:B:540:LEU:HG	1:B:544:ILE:CD1	1.82	1.08
1:F:542:THR:CB	1:G:535:ASP:OD2	2.02	1.08
1:H:542:THR:HG22	1:H:546:LYS:HG3	1.33	1.07
1:F:540:LEU:HD11	1:F:544:ILE:HD11	1.36	1.06
1:A:270:ASN:OD1	1:F:378:HIS:N	1.89	1.05
1:A:270:ASN:OD1	1:F:377:GLU:O	1.71	1.05
1:F:539:LEU:HD13	1:G:536:ALA:H	1.20	1.05
1:F:535:ASP:HB2	1:G:539:LEU:CG	1.87	1.04
1:C:541:GLN:O	1:C:545:GLU:HG2	1.55	1.04
1:F:539:LEU:HA	1:G:535:ASP:HB2	1.07	1.03
1:F:543:TRP:CZ2	1:G:533:ASP:HB2	1.92	1.03
1:C:378:HIS:C	1:H:270:ASN:ND2	2.10	1.03
1:B:546:LYS:H	1:B:546:LYS:CD	1.67	1.03
1:F:533:ASP:OD2	1:G:539:LEU:HD11	1.57	1.03
1:B:540:LEU:HG	1:B:544:ILE:HD11	1.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:ASP:CB	1:G:539:LEU:CB	2.10	1.02
1:B:546:LYS:N	1:B:546:LYS:HD3	1.72	1.02
1:D:540:LEU:CD1	1:D:544:ILE:HD11	1.89	1.02
1:B:546:LYS:H	1:B:546:LYS:HD3	0.88	1.01
1:D:540:LEU:CD1	1:D:544:ILE:HD12	1.87	1.01
1:A:270:ASN:OD1	1:F:378:HIS:HA	1.60	1.00
1:D:544:ILE:HG12	1:D:552:VAL:HG13	1.42	1.00
1:F:540:LEU:CD1	1:F:544:ILE:HD11	1.90	1.00
1:H:546:LYS:O	1:H:547:LYS:CG	2.10	1.00
1:F:542:THR:HB	1:G:535:ASP:OD2	1.59	0.99
1:A:270:ASN:CG	1:F:378:HIS:CA	2.26	0.99
1:F:539:LEU:HA	1:G:535:ASP:CB	1.92	0.99
1:H:542:THR:HG22	1:H:546:LYS:CD	1.84	0.99
1:D:540:LEU:HD11	1:D:544:ILE:HD11	1.01	0.98
1:H:542:THR:O	1:H:546:LYS:HG2	0.82	0.98
1:F:536:ALA:N	1:G:539:LEU:HD22	1.79	0.98
1:H:542:THR:C	1:H:546:LYS:CG	2.20	0.98
1:A:270:ASN:OD1	1:F:378:HIS:CA	2.13	0.97
1:F:544:ILE:C	1:F:546:LYS:CG	2.28	0.97
1:F:533:ASP:OD2	1:G:539:LEU:HD13	1.65	0.96
1:F:535:ASP:OD2	1:G:539:LEU:HD12	1.65	0.96
1:F:539:LEU:HD11	1:G:533:ASP:OD1	1.64	0.96
1:E:208:MET:C	1:E:213:MET:H	1.69	0.96
1:G:208:MET:C	1:G:213:MET:H	1.68	0.95
1:C:377:GLU:OE1	1:H:271:GLY:HA2	1.67	0.95
1:F:543:TRP:CE2	1:G:533:ASP:OD2	2.21	0.94
1:F:535:ASP:HB3	1:G:539:LEU:HB2	1.47	0.94
1:C:208:MET:C	1:C:213:MET:H	1.71	0.94
1:F:205:TYR:CE1	1:F:232:PRO:HG2	2.03	0.93
1:H:205:TYR:CE1	1:H:232:PRO:HG2	2.04	0.93
1:A:58:VAL:HB	1:A:208:MET:HE1	1.48	0.93
1:F:545:GLU:N	1:F:546:LYS:HG2	1.83	0.92
1:A:208:MET:C	1:A:213:MET:H	1.73	0.92
1:F:533:ASP:CG	1:G:543:TRP:CZ2	2.43	0.92
1:C:378:HIS:CA	1:H:270:ASN:CG	2.34	0.92
1:D:542:THR:O	1:D:546:LYS:CG	2.18	0.92
1:A:542:THR:O	1:A:546:LYS:N	2.03	0.91
1:F:539:LEU:CG	1:G:533:ASP:OD2	2.18	0.91
1:A:270:ASN:HA	1:F:377:GLU:HG2	1.53	0.91
1:D:542:THR:O	1:D:546:LYS:HG2	1.72	0.90
1:A:59:TYR:CE2	1:A:208:MET:HB3	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LEU:C	1:B:544:ILE:HD12	1.90	0.90
1:A:270:ASN:CG	1:F:377:GLU:O	2.09	0.89
1:D:541:GLN:HE21	1:D:545:GLU:CD	1.74	0.89
1:C:58:VAL:HB	1:C:208:MET:HE1	1.53	0.89
1:F:466:ASN:O	1:F:469:ILE:HG13	1.73	0.89
1:C:542:THR:O	1:C:546:LYS:N	2.05	0.88
1:F:539:LEU:CD1	1:G:533:ASP:OD1	2.20	0.87
1:G:202:PRO:O	1:G:206:MET:HB2	1.75	0.86
1:D:541:GLN:NE2	1:D:545:GLU:CD	2.29	0.86
1:B:540:LEU:CD1	1:B:544:ILE:HD11	2.05	0.86
1:F:546:LYS:CE	1:F:566:LYS:O	2.23	0.85
1:F:533:ASP:CG	1:G:539:LEU:HD11	1.95	0.85
1:F:545:GLU:N	1:F:546:LYS:CG	2.39	0.85
1:A:202:PRO:O	1:A:206:MET:HB2	1.76	0.85
1:H:542:THR:HG23	1:H:546:LYS:HD3	0.87	0.84
1:F:535:ASP:CB	1:G:539:LEU:CA	2.56	0.84
1:A:270:ASN:ND2	1:F:378:HIS:C	2.15	0.83
1:F:535:ASP:HB2	1:G:539:LEU:CD1	2.08	0.83
1:F:546:LYS:HD2	1:F:567:LEU:HA	1.61	0.83
1:F:541:GLN:HB3	1:F:545:GLU:OE2	1.79	0.83
1:F:539:LEU:HD13	1:G:536:ALA:N	1.93	0.83
1:F:533:ASP:OD2	1:G:539:LEU:CD2	2.27	0.82
1:C:59:TYR:CE2	1:C:208:MET:HB3	2.14	0.82
1:E:466:ASN:O	1:E:469:ILE:HG13	1.77	0.82
1:F:535:ASP:HB2	1:G:539:LEU:CA	2.10	0.82
1:H:205:TYR:HE1	1:H:232:PRO:HG2	1.44	0.82
1:C:377:GLU:CD	1:H:271:GLY:HA2	1.99	0.81
1:H:128:TYR:O	1:H:132:LEU:HD13	1.80	0.81
1:B:154:TYR:OH	1:F:377:GLU:CD	2.18	0.81
1:F:539:LEU:HG	1:G:533:ASP:OD2	1.81	0.81
1:E:202:PRO:O	1:E:206:MET:HB2	1.82	0.80
1:F:543:TRP:HZ2	1:G:533:ASP:HB2	1.44	0.80
1:C:202:PRO:O	1:C:206:MET:HB2	1.81	0.80
1:D:542:THR:O	1:D:546:LYS:CB	2.30	0.79
1:G:550:GLU:O	1:G:554:GLU:HG3	1.82	0.79
1:C:466:ASN:O	1:C:469:ILE:HG13	1.83	0.79
1:F:205:TYR:HE1	1:F:232:PRO:HG2	1.47	0.79
1:D:544:ILE:HG12	1:D:552:VAL:CG1	2.11	0.78
1:F:544:ILE:O	1:F:546:LYS:CD	2.30	0.78
1:G:59:TYR:CE2	1:G:208:MET:HB3	2.19	0.78
1:B:544:ILE:CA	1:B:546:LYS:HB3	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:ASP:OD2	1:G:539:LEU:CD1	2.31	0.78
1:B:466:ASN:O	1:B:469:ILE:HG13	1.83	0.78
1:B:544:ILE:O	1:B:545:GLU:C	2.20	0.78
1:A:527:ILE:HD11	1:A:558:LYS:HB2	1.65	0.78
1:D:466:ASN:O	1:D:469:ILE:HG13	1.84	0.78
1:G:58:VAL:HB	1:G:208:MET:HE1	1.66	0.78
1:E:550:GLU:O	1:E:554:GLU:HG3	1.84	0.77
1:H:546:LYS:C	1:H:547:LYS:HG3	2.04	0.77
1:C:364:LYS:HB2	1:F:511:PRO:HD2	1.65	0.77
1:D:540:LEU:CG	1:D:544:ILE:HD12	2.13	0.77
1:G:466:ASN:O	1:G:469:ILE:HG13	1.84	0.77
1:C:550:GLU:O	1:C:554:GLU:HG3	1.83	0.76
1:E:59:TYR:CE2	1:E:208:MET:HB3	2.22	0.75
1:H:91:HIS:CE1	1:H:148:ALA:HB2	2.22	0.75
1:H:543:TRP:HA	1:H:546:LYS:HB2	1.68	0.74
1:C:377:GLU:OE1	1:H:271:GLY:CA	2.35	0.74
1:C:539:LEU:O	1:C:539:LEU:HD12	1.87	0.74
1:B:546:LYS:HG2	1:B:548:ARG:H	1.51	0.74
1:E:466:ASN:HB2	1:E:469:ILE:HD11	1.71	0.73
1:F:546:LYS:HD3	1:F:566:LYS:C	2.06	0.73
1:F:533:ASP:OD1	1:G:543:TRP:NE1	2.21	0.73
1:B:205:TYR:CE1	1:B:232:PRO:HG2	2.23	0.73
1:B:128:TYR:CE2	1:B:132:LEU:HD11	2.25	0.72
1:F:501:LYS:HE2	1:F:505:ASP:OD2	1.88	0.72
1:D:544:ILE:CD1	1:D:562:ILE:HD12	2.20	0.72
1:D:542:THR:O	1:D:546:LYS:HB2	1.89	0.72
1:A:550:GLU:O	1:A:554:GLU:HG3	1.90	0.71
1:A:49:ASP:HB2	1:A:57:LYS:HD3	1.72	0.71
1:A:58:VAL:CB	1:A:208:MET:HE1	2.21	0.71
1:H:550:GLU:O	1:H:554:GLU:HG3	1.90	0.71
1:F:547:LYS:O	1:F:548:ARG:C	2.27	0.71
1:D:466:ASN:HB2	1:D:469:ILE:HD11	1.72	0.71
1:E:527:ILE:HD13	1:E:558:LYS:HB3	1.71	0.71
1:F:545:GLU:HG3	1:F:545:GLU:O	1.89	0.71
1:B:154:TYR:OH	1:F:377:GLU:OE1	2.07	0.70
1:F:535:ASP:CB	1:G:539:LEU:HA	2.20	0.70
1:B:540:LEU:C	1:B:544:ILE:CD1	2.56	0.70
1:D:540:LEU:HG	1:D:544:ILE:HD12	1.74	0.70
1:H:542:THR:O	1:H:546:LYS:CD	2.38	0.70
1:F:535:ASP:CA	1:G:539:LEU:HB2	2.20	0.69
1:H:543:TRP:N	1:H:546:LYS:HG2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ASN:HB3	1:B:515:ILE:HD12	1.73	0.69
1:F:535:ASP:H	1:G:539:LEU:HD13	1.57	0.69
1:E:58:VAL:HB	1:E:208:MET:HE1	1.75	0.69
1:H:128:TYR:CE2	1:H:132:LEU:HD11	2.27	0.69
1:D:205:TYR:CE1	1:D:232:PRO:HG2	2.28	0.68
1:E:527:ILE:HD11	1:E:558:LYS:HB2	1.76	0.68
1:F:543:TRP:CZ2	1:G:533:ASP:CB	2.75	0.68
1:C:377:GLU:CD	1:H:271:GLY:CA	2.61	0.68
1:F:542:THR:HA	1:F:545:GLU:CG	2.24	0.68
1:B:466:ASN:HB2	1:B:469:ILE:HD11	1.75	0.68
1:D:128:TYR:O	1:D:132:LEU:HD13	1.92	0.68
1:D:541:GLN:O	1:D:545:GLU:CB	2.29	0.68
1:F:542:THR:OG1	1:G:535:ASP:OD2	2.12	0.67
1:F:205:TYR:CD1	1:F:232:PRO:HG2	2.29	0.67
1:D:132:LEU:HD12	1:D:590:LEU:CD2	2.24	0.67
1:H:205:TYR:CD1	1:H:232:PRO:HG2	2.29	0.67
1:D:550:GLU:O	1:D:554:GLU:HG3	1.96	0.66
1:B:546:LYS:HG2	1:B:547:LYS:N	2.11	0.66
1:B:128:TYR:O	1:B:132:LEU:HD13	1.95	0.66
1:C:539:LEU:HD11	1:C:543:TRP:CE2	2.31	0.66
1:G:466:ASN:HB2	1:G:469:ILE:HD11	1.78	0.66
1:F:463:VAL:HA	1:F:469:ILE:CD1	2.26	0.66
1:G:49:ASP:OD1	1:G:51:VAL:HG22	1.95	0.66
1:E:206:MET:O	1:E:207:SER:C	2.33	0.66
1:C:206:MET:O	1:C:207:SER:C	2.34	0.65
1:H:542:THR:CG2	1:H:546:LYS:CE	2.74	0.65
1:G:208:MET:C	1:G:213:MET:N	2.46	0.65
1:B:540:LEU:O	1:B:544:ILE:CG1	2.44	0.65
1:B:516:PHE:CE1	1:B:554:GLU:HG2	2.31	0.65
1:F:533:ASP:OD1	1:G:543:TRP:CE2	2.48	0.65
1:D:544:ILE:HD11	1:D:562:ILE:HD12	1.77	0.65
1:G:538:ALA:O	1:G:542:THR:HG23	1.97	0.65
1:F:544:ILE:HG12	1:F:552:VAL:HG22	1.77	0.65
1:F:533:ASP:CG	1:G:543:TRP:HZ2	1.98	0.65
1:F:535:ASP:CB	1:G:539:LEU:CD1	2.75	0.65
1:F:550:GLU:O	1:F:554:GLU:HG3	1.96	0.65
1:A:527:ILE:HD13	1:A:558:LYS:HB3	1.79	0.65
1:A:49:ASP:OD1	1:A:51:VAL:HG22	1.97	0.64
1:C:208:MET:C	1:C:213:MET:N	2.49	0.64
1:C:7:ILE:HG12	1:C:241:LEU:CD2	2.28	0.64
1:B:544:ILE:O	1:B:545:GLU:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:ILE:CD1	1:E:558:LYS:HB3	2.27	0.64
1:B:546:LYS:O	1:B:547:LYS:HB2	1.96	0.64
1:G:527:ILE:HD13	1:G:558:LYS:HB3	1.78	0.64
1:F:543:TRP:CE2	1:G:533:ASP:CG	2.70	0.64
1:F:533:ASP:OD1	1:G:543:TRP:CZ2	2.51	0.64
1:A:527:ILE:CD1	1:A:558:LYS:CB	2.76	0.63
1:C:364:LYS:HE3	1:F:510:MET:SD	2.38	0.63
1:G:527:ILE:HD11	1:G:558:LYS:HB2	1.80	0.63
1:H:466:ASN:HB2	1:H:469:ILE:HD11	1.79	0.63
1:E:208:MET:C	1:E:213:MET:N	2.48	0.63
1:F:535:ASP:CB	1:G:539:LEU:HD13	2.29	0.63
1:H:516:PHE:CE1	1:H:554:GLU:HG2	2.34	0.63
1:F:533:ASP:OD2	1:G:539:LEU:CG	2.47	0.62
1:F:542:THR:HA	1:F:545:GLU:HG3	1.80	0.62
1:C:364:LYS:CB	1:F:511:PRO:HD2	2.30	0.62
1:E:315:GLU:HG3	1:E:410:PHE:HE2	1.64	0.62
1:H:542:THR:CG2	1:H:546:LYS:CG	2.54	0.62
1:H:542:THR:O	1:H:546:LYS:N	2.32	0.62
1:D:544:ILE:O	1:D:567:LEU:HD12	2.00	0.62
1:F:128:TYR:CE2	1:F:132:LEU:HD11	2.34	0.62
1:F:535:ASP:HB2	1:G:539:LEU:HB2	0.80	0.62
1:A:206:MET:O	1:A:207:SER:C	2.37	0.62
1:C:301:VAL:HG22	1:C:406:CYS:HB2	1.82	0.62
1:G:49:ASP:HB2	1:G:57:LYS:HD3	1.81	0.62
1:D:501:LYS:HE2	1:D:505:ASP:OD2	1.99	0.61
1:F:7:ILE:HD13	1:F:358:LEU:HD11	1.82	0.61
1:G:7:ILE:HD13	1:G:358:LEU:HD11	1.81	0.61
1:F:312:ASP:N	1:F:313:PRO:HD2	2.15	0.61
1:A:91:HIS:CE1	1:A:148:ALA:HB2	2.35	0.61
1:G:527:ILE:CD1	1:G:558:LYS:CB	2.79	0.61
1:A:208:MET:C	1:A:213:MET:N	2.52	0.61
1:C:527:ILE:HD13	1:C:558:LYS:HB3	1.82	0.60
1:G:206:MET:O	1:G:207:SER:C	2.38	0.60
1:F:541:GLN:CB	1:F:545:GLU:OE2	2.48	0.60
1:F:533:ASP:CB	1:G:543:TRP:HZ2	2.13	0.60
1:B:545:GLU:N	1:B:546:LYS:HB3	2.15	0.60
1:C:541:GLN:O	1:C:545:GLU:CG	2.41	0.60
1:D:546:LYS:C	1:D:547:LYS:HG3	2.20	0.60
1:D:544:ILE:CG1	1:D:552:VAL:HG22	2.31	0.60
1:C:463:VAL:HA	1:C:469:ILE:CD1	2.32	0.60
1:C:202:PRO:O	1:C:206:MET:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:541:GLN:HB3	1:F:545:GLU:CD	2.21	0.60
1:F:536:ALA:H	1:G:539:LEU:HD22	1.63	0.60
1:G:550:GLU:O	1:G:554:GLU:CG	2.50	0.60
1:A:527:ILE:CD1	1:A:558:LYS:HB3	2.32	0.60
1:B:541:GLN:HA	1:B:544:ILE:HD12	1.84	0.60
1:A:466:ASN:HB2	1:A:469:ILE:HD11	1.84	0.59
1:A:543:TRP:HA	1:A:546:LYS:HB3	1.84	0.59
1:E:527:ILE:CD1	1:E:558:LYS:CB	2.80	0.59
1:H:546:LYS:C	1:H:547:LYS:CG	2.66	0.59
1:A:202:PRO:O	1:A:206:MET:CB	2.51	0.59
1:E:202:PRO:O	1:E:206:MET:CB	2.51	0.59
1:F:533:ASP:HB2	1:G:543:TRP:HZ2	1.67	0.59
1:B:544:ILE:C	1:B:546:LYS:CB	2.62	0.59
1:A:550:GLU:O	1:A:554:GLU:CG	2.51	0.59
1:E:206:MET:O	1:E:208:MET:HE2	2.02	0.59
1:G:527:ILE:CD1	1:G:558:LYS:HB3	2.33	0.59
1:G:202:PRO:O	1:G:206:MET:CB	2.49	0.59
1:F:533:ASP:OD2	1:G:539:LEU:HD21	2.01	0.59
1:E:547:LYS:HE3	1:E:567:LEU:O	2.03	0.59
1:A:319:LEU:O	1:A:322:VAL:HG22	2.04	0.58
1:A:49:ASP:CB	1:A:57:LYS:HD3	2.33	0.58
1:C:542:THR:O	1:C:546:LYS:HG3	2.03	0.58
1:A:546:LYS:O	1:A:547:LYS:HB2	2.03	0.58
1:B:128:TYR:O	1:B:132:LEU:CD1	2.51	0.58
1:A:203:GLU:O	1:A:206:MET:HB3	2.04	0.58
1:C:312:ASP:N	1:C:313:PRO:HD2	2.19	0.58
1:F:128:TYR:O	1:F:132:LEU:HD13	2.04	0.58
1:F:463:VAL:HA	1:F:469:ILE:HD11	1.85	0.58
1:F:492:LEU:N	1:F:492:LEU:HD12	2.20	0.57
1:C:466:ASN:HB2	1:C:469:ILE:HD11	1.85	0.57
1:H:501:LYS:HE2	1:H:505:ASP:OD2	2.04	0.57
1:A:527:ILE:CD1	1:A:558:LYS:HB2	2.33	0.57
1:C:319:LEU:O	1:C:322:VAL:HG22	2.05	0.57
1:F:533:ASP:OD1	1:G:539:LEU:HD11	2.04	0.57
1:C:550:GLU:O	1:C:554:GLU:CG	2.53	0.57
1:G:196:VAL:HG23	1:G:236:ALA:HB2	1.86	0.57
1:H:91:HIS:NE2	1:H:148:ALA:HB2	2.19	0.57
1:F:542:THR:CG2	1:G:535:ASP:OD2	2.52	0.57
1:A:7:ILE:HG12	1:A:241:LEU:CD2	2.34	0.57
1:B:463:VAL:HA	1:B:469:ILE:CD1	2.35	0.57
1:F:535:ASP:CG	1:G:539:LEU:HA	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:492:LEU:HD12	1:G:492:LEU:N	2.19	0.57
1:F:535:ASP:HB3	1:G:539:LEU:CA	2.35	0.57
1:F:540:LEU:HD22	1:F:560:LEU:HD21	1.87	0.56
1:G:344:HIS:HD2	1:G:346:SER:H	1.53	0.56
1:B:550:GLU:O	1:B:554:GLU:HG3	2.06	0.56
1:B:544:ILE:CA	1:B:546:LYS:CB	2.83	0.56
1:D:545:GLU:HG2	1:D:566:LYS:HB3	1.87	0.56
1:D:205:TYR:CD1	1:D:232:PRO:HG2	2.40	0.56
1:G:552:VAL:HG13	1:G:562:ILE:HD12	1.88	0.56
1:G:512:ASN:HB3	1:G:515:ILE:HD12	1.87	0.56
1:F:539:LEU:HB2	1:G:536:ALA:N	2.20	0.56
1:H:128:TYR:O	1:H:132:LEU:CD1	2.53	0.56
1:E:550:GLU:O	1:E:554:GLU:CG	2.53	0.56
1:F:540:LEU:O	1:F:544:ILE:HG13	2.05	0.56
1:G:548:ARG:NH2	1:G:550:GLU:OE1	2.39	0.56
1:A:270:ASN:CA	1:F:377:GLU:HG2	2.32	0.56
1:D:544:ILE:HD13	1:D:562:ILE:HG23	1.87	0.56
1:F:543:TRP:CD2	1:G:533:ASP:OD2	2.59	0.56
1:A:466:ASN:O	1:A:469:ILE:HG13	2.06	0.56
1:C:49:ASP:HB2	1:C:57:LYS:HD3	1.88	0.56
1:D:128:TYR:CE2	1:D:132:LEU:HD11	2.41	0.56
1:F:466:ASN:HB2	1:F:469:ILE:HD11	1.86	0.56
1:F:546:LYS:HD2	1:F:567:LEU:CA	2.35	0.56
1:F:539:LEU:CB	1:G:535:ASP:HB2	2.35	0.55
1:C:181:GLN:HA	1:C:181:GLN:OE1	2.06	0.55
1:C:492:LEU:N	1:C:492:LEU:HD12	2.22	0.55
1:D:544:ILE:HG13	1:D:552:VAL:HG22	1.87	0.55
1:F:199:TYR:HH	1:F:346:SER:HG	1.54	0.55
1:B:205:TYR:CD1	1:B:232:PRO:HG2	2.41	0.55
1:B:205:TYR:HE1	1:B:232:PRO:HG2	1.66	0.55
1:H:205:TYR:HE1	1:H:232:PRO:CG	2.16	0.55
1:F:546:LYS:HE3	1:F:566:LYS:O	2.05	0.55
1:G:344:HIS:CD2	1:G:346:SER:H	2.24	0.55
1:C:377:GLU:OE1	1:H:271:GLY:N	2.40	0.55
1:E:49:ASP:HB2	1:E:57:LYS:HD3	1.88	0.55
1:F:132:LEU:HD12	1:F:590:LEU:CD2	2.36	0.55
1:H:312:ASP:N	1:H:313:PRO:HD2	2.22	0.55
1:E:319:LEU:O	1:E:322:VAL:HG22	2.07	0.55
1:E:7:ILE:HD13	1:E:358:LEU:HD11	1.87	0.55
1:F:539:LEU:HD12	1:G:533:ASP:OD1	2.06	0.55
1:A:15:PRO:HD3	1:A:234:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ASP:HB3	1:C:91:HIS:CD2	2.41	0.54
1:E:63:MET:SD	1:E:65:MET:HG2	2.47	0.54
1:A:204:SER:OG	1:A:205:TYR:N	2.39	0.54
1:H:522:THR:HG22	1:H:523:LYS:HG2	1.89	0.54
1:F:542:THR:OG1	1:G:535:ASP:CG	2.46	0.54
1:D:132:LEU:HD12	1:D:590:LEU:HD21	1.90	0.54
1:H:332:PHE:CE2	1:H:385:PRO:HB3	2.43	0.54
1:F:545:GLU:CG	1:F:545:GLU:O	2.56	0.54
1:G:467:GLU:HA	1:G:496:ARG:NE	2.23	0.54
1:C:542:THR:HA	1:C:545:GLU:HB2	1.90	0.54
1:G:203:GLU:O	1:G:206:MET:HB3	2.08	0.54
1:G:319:LEU:O	1:G:322:VAL:HG22	2.07	0.54
1:G:539:LEU:HD11	1:G:543:TRP:CE2	2.42	0.54
1:G:527:ILE:CD1	1:G:558:LYS:HB2	2.37	0.54
1:D:205:TYR:HE1	1:D:232:PRO:HG2	1.73	0.53
1:E:546:LYS:O	1:E:546:LYS:HG3	2.07	0.53
1:F:543:TRP:NE1	1:G:533:ASP:CG	2.62	0.53
1:H:466:ASN:O	1:H:469:ILE:HG13	2.08	0.53
1:H:543:TRP:HA	1:H:546:LYS:CG	2.38	0.53
1:C:538:ALA:O	1:C:542:THR:HG23	2.09	0.53
1:H:543:TRP:HA	1:H:546:LYS:CB	2.35	0.53
1:C:379:PHE:N	1:H:270:ASN:HD21	1.99	0.53
1:E:204:SER:OG	1:E:205:TYR:N	2.40	0.53
1:H:542:THR:O	1:H:546:LYS:CB	2.52	0.53
1:C:199:TYR:HH	1:C:346:SER:HG	1.56	0.53
1:D:15:PRO:HD3	1:D:234:GLU:O	2.09	0.53
1:F:15:PRO:HD3	1:F:234:GLU:O	2.09	0.53
1:C:204:SER:OG	1:C:205:TYR:N	2.42	0.53
1:C:522:THR:HG22	1:C:523:LYS:HG2	1.90	0.53
1:B:545:GLU:N	1:B:546:LYS:CA	2.72	0.52
1:F:205:TYR:HE1	1:F:232:PRO:CG	2.17	0.52
1:C:58:VAL:CB	1:C:208:MET:HE1	2.31	0.52
1:F:516:PHE:CE1	1:F:554:GLU:HG2	2.44	0.52
1:H:7:ILE:HD13	1:H:358:LEU:HD11	1.92	0.52
1:F:542:THR:CA	1:F:545:GLU:HG2	2.35	0.52
1:F:536:ALA:CA	1:G:539:LEU:HD22	2.38	0.52
1:A:542:THR:O	1:A:546:LYS:HB2	2.10	0.52
1:D:467:GLU:HA	1:D:496:ARG:NE	2.25	0.52
1:C:49:ASP:CB	1:C:57:LYS:HD3	2.39	0.52
1:D:540:LEU:HD22	1:D:560:LEU:HD21	1.91	0.52
1:B:41:ARG:NH1	1:B:234:GLU:OE2	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:328:ASP:O	1:H:330:LYS:HE2	2.09	0.52
1:F:295:PRO:HA	1:F:298:ILE:HD12	1.92	0.52
1:D:315:GLU:HG3	1:D:410:PHE:HE2	1.75	0.51
1:D:516:PHE:CE1	1:D:554:GLU:HG2	2.45	0.51
1:E:467:GLU:HA	1:E:496:ARG:NE	2.24	0.51
1:C:364:LYS:NZ	1:F:510:MET:HB3	2.25	0.51
1:B:552:VAL:HG13	1:B:562:ILE:HD12	1.92	0.51
1:C:467:GLU:HA	1:C:496:ARG:NE	2.25	0.51
1:E:527:ILE:HD11	1:E:558:LYS:CB	2.39	0.51
1:F:88:ASP:HB3	1:F:91:HIS:CD2	2.44	0.51
1:C:548:ARG:O	1:C:552:VAL:HG23	2.11	0.51
1:E:540:LEU:HD22	1:E:560:LEU:HD21	1.90	0.51
1:E:547:LYS:CE	1:E:567:LEU:O	2.59	0.51
1:B:545:GLU:N	1:B:546:LYS:CB	2.73	0.51
1:F:41:ARG:NH1	1:F:234:GLU:OE2	2.33	0.51
1:H:15:PRO:HD3	1:H:234:GLU:O	2.10	0.51
1:E:301:VAL:HG22	1:E:406:CYS:HB2	1.92	0.51
1:F:533:ASP:CB	1:G:543:TRP:CZ2	2.92	0.51
1:B:128:TYR:CD2	1:B:132:LEU:HD11	2.46	0.51
1:B:492:LEU:HD12	1:B:492:LEU:N	2.25	0.51
1:D:132:LEU:CD1	1:D:590:LEU:CD2	2.88	0.51
1:E:206:MET:O	1:E:208:MET:CE	2.59	0.51
1:F:540:LEU:CG	1:F:544:ILE:HD11	2.41	0.51
1:G:91:HIS:CE1	1:G:148:ALA:HB2	2.46	0.51
1:B:23:TYR:OH	1:B:338:VAL:HG21	2.11	0.50
1:E:546:LYS:O	1:E:546:LYS:CG	2.60	0.50
1:D:23:TYR:OH	1:D:338:VAL:HG21	2.12	0.50
1:G:204:SER:OG	1:G:205:TYR:N	2.42	0.50
1:H:132:LEU:HD12	1:H:590:LEU:CD2	2.40	0.50
1:A:59:TYR:CE2	1:A:208:MET:CB	2.89	0.50
1:B:541:GLN:CA	1:B:544:ILE:HD12	2.42	0.50
1:G:49:ASP:CB	1:G:57:LYS:HD3	2.41	0.50
1:B:546:LYS:HE2	1:B:547:LYS:H	1.76	0.50
1:D:312:ASP:N	1:D:313:PRO:HD2	2.27	0.50
1:E:492:LEU:N	1:E:492:LEU:HD12	2.26	0.50
1:E:49:ASP:OD1	1:E:51:VAL:HG22	2.11	0.50
1:G:546:LYS:O	1:G:546:LYS:CG	2.59	0.50
1:A:312:ASP:N	1:A:313:PRO:HD2	2.26	0.50
1:B:344:HIS:CD2	1:B:346:SER:H	2.30	0.50
1:B:467:GLU:HA	1:B:496:ARG:NE	2.26	0.50
1:B:540:LEU:O	1:B:544:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ILE:O	1:D:151:ARG:HG2	2.12	0.50
1:E:196:VAL:HG23	1:E:236:ALA:HB2	1.94	0.50
1:G:463:VAL:HA	1:G:469:ILE:CD1	2.42	0.49
1:C:328:ASP:O	1:C:330:LYS:HE2	2.12	0.49
1:F:542:THR:HA	1:F:545:GLU:HG2	1.93	0.49
1:B:312:ASP:N	1:B:313:PRO:HD2	2.26	0.49
1:C:203:GLU:O	1:C:206:MET:HB3	2.12	0.49
1:D:545:GLU:CG	1:D:566:LYS:HB3	2.42	0.49
1:F:544:ILE:HG12	1:F:552:VAL:CG2	2.42	0.49
1:H:512:ASN:HB3	1:H:515:ILE:HD12	1.94	0.49
1:A:538:ALA:O	1:A:542:THR:HG23	2.12	0.49
1:D:492:LEU:HD12	1:D:492:LEU:N	2.27	0.49
1:D:544:ILE:HA	1:D:552:VAL:HG21	1.95	0.49
1:A:304:HIS:CE1	1:A:410:PHE:O	2.66	0.49
1:B:463:VAL:HA	1:B:469:ILE:HD12	1.94	0.49
1:C:183:LEU:HD23	1:C:188:ILE:HG13	1.93	0.49
1:F:526:GLU:HG3	1:G:526:GLU:HG2	1.95	0.49
1:C:15:PRO:HD3	1:C:234:GLU:O	2.13	0.49
1:G:546:LYS:O	1:G:546:LYS:HG3	2.12	0.49
1:F:467:GLU:HA	1:F:496:ARG:NE	2.27	0.49
1:G:206:MET:O	1:G:208:MET:CE	2.61	0.49
1:G:206:MET:O	1:G:208:MET:HE2	2.13	0.49
1:A:205:TYR:C	1:A:205:TYR:CD1	2.86	0.49
1:C:527:ILE:HD11	1:C:558:LYS:HB2	1.94	0.49
1:E:147:ILE:O	1:E:151:ARG:HG2	2.13	0.49
1:F:541:GLN:C	1:F:545:GLU:OE2	2.50	0.49
1:A:463:VAL:HA	1:A:469:ILE:CD1	2.42	0.49
1:C:545:GLU:OE2	1:C:566:LYS:HB3	2.13	0.49
1:F:540:LEU:HG	1:F:544:ILE:CD1	2.43	0.49
1:G:181:GLN:HA	1:G:181:GLN:OE1	2.12	0.48
1:A:58:VAL:HA	1:A:208:MET:CE	2.43	0.48
1:E:15:PRO:HD3	1:E:234:GLU:O	2.13	0.48
1:C:463:VAL:HA	1:C:469:ILE:HD11	1.94	0.48
1:E:344:HIS:CD2	1:E:346:SER:H	2.31	0.48
1:D:544:ILE:HD13	1:D:562:ILE:HD12	1.92	0.48
1:F:540:LEU:CD1	1:F:544:ILE:CD1	2.79	0.48
1:G:15:PRO:HD3	1:G:234:GLU:O	2.13	0.48
1:F:23:TYR:OH	1:F:338:VAL:HG21	2.14	0.48
1:F:544:ILE:HG23	1:F:567:LEU:HD13	1.96	0.48
1:G:147:ILE:O	1:G:151:ARG:HG2	2.13	0.48
1:F:132:LEU:HD12	1:F:590:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:ASP:C	1:G:539:LEU:HB2	2.34	0.48
1:A:332:PHE:CE2	1:A:385:PRO:HB3	2.49	0.47
1:B:7:ILE:HD13	1:B:358:LEU:HD11	1.94	0.47
1:C:577:SER:O	1:C:578:LEU:HD23	2.14	0.47
1:H:463:VAL:HA	1:H:469:ILE:CD1	2.44	0.47
1:A:542:THR:O	1:A:546:LYS:CB	2.63	0.47
1:A:540:LEU:HD22	1:A:560:LEU:HD21	1.96	0.47
1:F:119:VAL:HG21	1:F:153:PRO:HG3	1.96	0.47
1:G:91:HIS:NE2	1:G:148:ALA:HB2	2.29	0.47
1:G:527:ILE:HD13	1:G:558:LYS:CB	2.43	0.47
1:C:545:GLU:OE2	1:C:566:LYS:HD2	2.14	0.47
1:B:15:PRO:HD3	1:B:234:GLU:O	2.14	0.47
1:F:540:LEU:HG	1:F:544:ILE:HD12	1.97	0.47
1:B:546:LYS:CG	1:B:547:LYS:N	2.76	0.47
1:H:301:VAL:HG21	1:H:319:LEU:HD21	1.95	0.47
1:G:332:PHE:CE2	1:G:385:PRO:HB3	2.50	0.47
1:F:539:LEU:CA	1:G:535:ASP:CB	2.69	0.47
1:F:541:GLN:O	1:F:545:GLU:N	2.48	0.47
1:A:208:MET:O	1:A:211:ALA:HB3	2.15	0.47
1:A:533:ASP:OD1	1:A:534:HIS:N	2.47	0.47
1:A:544:ILE:HG21	1:A:566:LYS:HB2	1.97	0.47
1:A:72:PHE:CD1	1:A:92:ARG:HB3	2.50	0.47
1:F:544:ILE:HG23	1:F:567:LEU:CD1	2.45	0.47
1:G:186:LYS:HD2	1:G:243:ARG:CZ	2.45	0.47
1:C:205:TYR:C	1:C:205:TYR:CD1	2.88	0.46
1:E:223:PHE:CZ	1:E:303:MET:HG3	2.51	0.46
1:A:152:ILE:HB	1:A:153:PRO:HD3	1.97	0.46
1:A:58:VAL:CB	1:A:208:MET:CE	2.93	0.46
1:C:547:LYS:HD3	1:C:547:LYS:HA	1.64	0.46
1:A:328:ASP:O	1:A:330:LYS:HE2	2.15	0.46
1:B:501:LYS:HE2	1:B:505:ASP:OD2	2.15	0.46
1:E:49:ASP:CB	1:E:57:LYS:HD3	2.44	0.46
1:E:88:ASP:OD1	1:E:89:PRO:HD2	2.16	0.46
1:G:205:TYR:CD1	1:G:205:TYR:C	2.88	0.46
1:G:208:MET:HA	1:G:214:LEU:HG	1.98	0.46
1:B:147:ILE:O	1:B:151:ARG:HG2	2.15	0.46
1:E:79:ILE:HG21	1:E:87:MET:HE3	1.98	0.46
1:E:173:LEU:HD22	1:E:409:SER:HB2	1.98	0.46
1:B:315:GLU:HG3	1:B:410:PHE:HE2	1.81	0.46
1:F:535:ASP:HB2	1:G:539:LEU:HD13	1.88	0.46
1:F:542:THR:HG21	1:G:535:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:545:GLU:N	1:F:546:LYS:CA	2.79	0.46
1:B:543:TRP:CE2	1:B:551:LYS:HG3	2.51	0.46
1:D:540:LEU:HD12	1:D:544:ILE:CD1	2.34	0.46
1:E:199:TYR:HH	1:E:346:SER:HG	1.61	0.46
1:A:91:HIS:NE2	1:A:148:ALA:HB2	2.31	0.45
1:A:14:TYR:HB3	1:A:15:PRO:HD2	1.98	0.45
1:C:303:MET:HE1	1:C:315:GLU:HG2	1.99	0.45
1:E:186:LYS:HD2	1:E:243:ARG:CZ	2.46	0.45
1:C:539:LEU:C	1:C:539:LEU:HD12	2.36	0.45
1:F:303:MET:HE1	1:F:315:GLU:HG2	1.99	0.45
1:D:544:ILE:HA	1:D:552:VAL:CG2	2.46	0.45
1:D:488:ARG:HB3	1:D:556:TRP:CZ3	2.52	0.45
1:F:539:LEU:CD1	1:G:533:ASP:CB	2.64	0.45
1:F:539:LEU:HB2	1:G:535:ASP:C	2.37	0.45
1:C:303:MET:CE	1:C:315:GLU:HG2	2.46	0.45
1:C:533:ASP:OD1	1:C:534:HIS:N	2.49	0.45
1:H:7:ILE:HG12	1:H:241:LEU:CD2	2.46	0.45
1:G:312:ASP:N	1:G:313:PRO:HD2	2.30	0.45
1:C:540:LEU:HD22	1:C:560:LEU:HD21	1.99	0.45
1:B:196:VAL:HG23	1:B:236:ALA:HB2	1.98	0.45
1:D:312:ASP:N	1:D:313:PRO:CD	2.80	0.45
1:A:50:PRO:HG3	1:E:83:GLU:OE2	2.17	0.45
1:F:535:ASP:HB3	1:G:539:LEU:CB	2.19	0.45
1:E:203:GLU:O	1:E:206:MET:HB3	2.17	0.45
1:D:7:ILE:HD13	1:D:358:LEU:HD11	1.98	0.44
1:D:344:HIS:CD2	1:D:346:SER:H	2.35	0.44
1:F:312:ASP:N	1:F:313:PRO:CD	2.78	0.44
1:B:543:TRP:HZ3	1:B:555:LEU:HD11	1.80	0.44
1:G:328:ASP:O	1:G:330:LYS:HE2	2.18	0.44
1:D:332:PHE:CE2	1:D:385:PRO:HB3	2.52	0.44
1:D:516:PHE:HZ	1:D:550:GLU:HG3	1.82	0.44
1:E:150:ALA:C	1:E:153:PRO:HD2	2.38	0.44
1:C:364:LYS:O	1:F:511:PRO:HG2	2.17	0.44
1:F:522:THR:HG22	1:F:523:LYS:HG2	1.99	0.44
1:E:344:HIS:HD2	1:E:346:SER:H	1.66	0.44
1:G:13:ARG:HG2	1:G:66:LEU:HD22	2.00	0.44
1:F:188:ILE:HD12	1:F:190:MET:O	2.18	0.44
1:A:177:HIS:CE1	1:A:181:GLN:HE21	2.34	0.44
1:B:344:HIS:HD2	1:B:346:SER:H	1.66	0.44
1:B:539:LEU:HD11	1:B:543:TRP:CE2	2.53	0.44
1:E:538:ALA:O	1:E:542:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:MET:HG2	1:F:347:ALA:HB2	1.99	0.44
1:H:463:VAL:HA	1:H:469:ILE:HD12	2.00	0.44
1:A:88:ASP:OD1	1:A:89:PRO:HD2	2.17	0.44
1:G:265:GLN:HB2	1:H:160:GLY:O	2.18	0.44
1:H:63:MET:SD	1:H:65:MET:HG2	2.58	0.44
1:D:577:SER:O	1:D:578:LEU:HD23	2.18	0.43
1:F:536:ALA:HB2	1:G:539:LEU:CD2	2.48	0.43
1:A:467:GLU:HA	1:A:496:ARG:NE	2.32	0.43
1:B:91:HIS:CE1	1:B:148:ALA:HB2	2.53	0.43
1:C:344:HIS:CD2	1:C:346:SER:H	2.35	0.43
1:F:535:ASP:OD2	1:G:542:THR:OG1	2.36	0.43
1:B:541:GLN:N	1:B:544:ILE:HD12	2.32	0.43
1:C:354:VAL:HG22	1:C:419:ILE:HD11	2.01	0.43
1:E:90:GLN:HG3	1:E:198:LEU:HD12	2.01	0.43
1:F:535:ASP:N	1:G:539:LEU:HD13	2.27	0.43
1:B:541:GLN:O	1:B:545:GLU:HB2	2.18	0.43
1:A:543:TRP:HD1	1:A:546:LYS:HD3	1.84	0.43
1:A:547:LYS:HD3	1:A:547:LYS:HA	1.67	0.43
1:C:539:LEU:HD21	1:C:543:TRP:CZ2	2.53	0.43
1:D:463:VAL:HA	1:D:469:ILE:CD1	2.49	0.43
1:D:80:PRO:HD2	1:D:83:GLU:OE1	2.19	0.43
1:A:160:GLY:O	1:B:265:GLN:HB2	2.18	0.43
1:B:265:GLN:NE2	1:B:414:GLY:C	2.72	0.43
1:F:334:ALA:HB2	1:F:387:TYR:CZ	2.54	0.43
1:H:204:SER:O	1:H:204:SER:OG	2.33	0.43
1:D:544:ILE:HG12	1:D:552:VAL:HG22	2.00	0.43
1:E:443:VAL:HB	1:E:556:TRP:CH2	2.54	0.43
1:F:401:LYS:HE2	1:F:401:LYS:HB3	1.85	0.43
1:A:147:ILE:O	1:A:151:ARG:HG2	2.19	0.43
1:B:128:TYR:CD2	1:B:132:LEU:CD1	3.02	0.43
1:F:544:ILE:O	1:F:546:LYS:HD3	2.15	0.43
1:F:544:ILE:CG2	1:F:567:LEU:HD13	2.49	0.43
1:F:516:PHE:HZ	1:F:550:GLU:HG3	1.84	0.43
1:H:27:LEU:HD21	1:H:338:VAL:HG23	2.01	0.43
1:H:516:PHE:HZ	1:H:550:GLU:HG3	1.83	0.43
1:A:59:TYR:HE2	1:A:208:MET:HB3	1.74	0.42
1:E:206:MET:O	1:E:208:MET:N	2.51	0.42
1:F:547:LYS:C	1:F:548:ARG:O	2.51	0.42
1:G:491:PHE:CE1	1:G:499:LEU:HD12	2.54	0.42
1:F:543:TRP:NE1	1:G:533:ASP:OD2	2.50	0.42
1:F:535:ASP:CG	1:G:539:LEU:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:LEU:HD13	1:G:156:LEU:HD13	2.01	0.42
1:H:152:ILE:HB	1:H:153:PRO:HD3	2.00	0.42
1:H:467:GLU:HA	1:H:496:ARG:NE	2.34	0.42
1:A:181:GLN:OE1	1:A:181:GLN:HA	2.19	0.42
1:A:522:THR:HG22	1:A:523:LYS:HG2	2.01	0.42
1:H:41:ARG:NH1	1:H:234:GLU:OE2	2.33	0.42
1:C:23:TYR:OH	1:C:338:VAL:HG21	2.19	0.42
1:H:544:ILE:O	1:H:567:LEU:HD12	2.19	0.42
1:B:173:LEU:HA	1:B:173:LEU:HD12	1.93	0.42
1:H:94:PHE:CE2	1:H:121:LEU:HD13	2.54	0.42
1:B:91:HIS:NE2	1:B:148:ALA:HB2	2.34	0.42
1:E:5:ILE:HG13	1:E:180:ARG:HG3	2.01	0.42
1:F:541:GLN:NE2	1:F:541:GLN:HA	2.34	0.42
1:H:540:LEU:HD22	1:H:560:LEU:HD21	2.00	0.42
1:D:544:ILE:HD11	1:D:562:ILE:CD1	2.47	0.42
1:G:90:GLN:HG3	1:G:198:LEU:HD12	2.01	0.42
1:A:344:HIS:CD2	1:A:346:SER:H	2.38	0.42
1:D:463:VAL:HA	1:D:469:ILE:HD12	2.01	0.42
1:G:14:TYR:HB3	1:G:15:PRO:HD2	2.00	0.42
1:G:223:PHE:CZ	1:G:303:MET:HG3	2.55	0.42
1:A:510:MET:HA	1:A:511:PRO:HD3	1.90	0.42
1:F:463:VAL:HA	1:F:469:ILE:HD12	1.99	0.42
1:G:463:VAL:HA	1:G:469:ILE:HD12	2.01	0.42
1:G:533:ASP:OD1	1:G:534:HIS:N	2.52	0.42
1:D:443:VAL:HB	1:D:556:TRP:CH2	2.55	0.42
1:E:205:TYR:C	1:E:205:TYR:CD1	2.93	0.42
1:H:543:TRP:CA	1:H:546:LYS:HG2	2.50	0.42
1:E:510:MET:HA	1:E:511:PRO:HD3	1.90	0.41
1:F:512:ASN:HB3	1:F:515:ILE:HD12	2.00	0.41
1:B:542:THR:O	1:B:546:LYS:HA	2.20	0.41
1:C:544:ILE:HG23	1:C:567:LEU:HD13	2.03	0.41
1:C:59:TYR:CE2	1:C:208:MET:CB	2.96	0.41
1:A:512:ASN:HB3	1:A:515:ILE:HD12	2.02	0.41
1:F:577:SER:O	1:F:578:LEU:HD23	2.20	0.41
1:B:540:LEU:HD12	1:B:544:ILE:HD11	1.98	0.41
1:C:63:MET:SD	1:C:65:MET:HG2	2.60	0.41
1:D:484:ALA:HB1	1:D:488:ARG:CZ	2.50	0.41
1:E:312:ASP:N	1:E:313:PRO:HD2	2.36	0.41
1:H:88:ASP:OD1	1:H:89:PRO:HD2	2.21	0.41
1:A:58:VAL:HA	1:A:208:MET:HE3	2.02	0.41
1:B:127:GLU:OE2	1:B:204:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:PHE:CE2	1:C:385:PRO:HB3	2.55	0.41
1:C:527:ILE:CD1	1:C:558:LYS:HB3	2.49	0.41
1:B:13:ARG:HG2	1:B:66:LEU:HD22	2.02	0.41
1:D:41:ARG:NH1	1:D:234:GLU:OE2	2.37	0.41
1:F:173:LEU:HA	1:F:173:LEU:HD12	1.94	0.41
1:F:533:ASP:CG	1:G:543:TRP:CE2	2.92	0.41
1:H:147:ILE:O	1:H:151:ARG:HG2	2.20	0.41
1:A:540:LEU:O	1:A:544:ILE:HG13	2.21	0.41
1:D:544:ILE:CG1	1:D:552:VAL:HG13	2.31	0.41
1:C:364:LYS:HZ2	1:F:510:MET:HB3	1.86	0.41
1:H:312:ASP:N	1:H:313:PRO:CD	2.83	0.41
1:H:542:THR:HG22	1:H:546:LYS:CE	2.45	0.41
1:A:443:VAL:O	1:A:478:LEU:HB3	2.21	0.41
1:C:261:SER:HB2	1:C:419:ILE:HG22	2.02	0.41
1:D:531:GLU:O	1:D:537:LYS:HE3	2.20	0.41
1:G:406:CYS:HB3	1:G:418:HIS:CE1	2.56	0.41
1:H:128:TYR:CD2	1:H:132:LEU:HD11	2.54	0.41
1:E:521:LYS:NZ	1:E:524:LYS:NZ	2.69	0.41
1:H:542:THR:CG2	1:H:546:LYS:HE2	2.50	0.41
1:D:546:LYS:HE3	1:D:546:LYS:HA	2.03	0.41
1:A:578:LEU:HB3	1:A:579:PRO:HD2	2.03	0.41
1:C:364:LYS:HB2	1:F:511:PRO:CD	2.42	0.41
1:E:265:GLN:HB2	1:F:160:GLY:O	2.20	0.41
1:F:543:TRP:CZ2	1:G:533:ASP:OD2	2.72	0.41
1:E:181:GLN:HA	1:E:181:GLN:OE1	2.21	0.40
1:A:261:SER:HB2	1:A:419:ILE:HG22	2.03	0.40
1:A:492:LEU:N	1:A:492:LEU:HD12	2.37	0.40
1:A:99:TYR:CD1	1:A:99:TYR:C	2.94	0.40
1:G:58:VAL:CB	1:G:208:MET:HE1	2.43	0.40
1:H:117:CYS:HA	1:H:190:MET:O	2.21	0.40
1:H:132:LEU:HD12	1:H:590:LEU:HD21	2.02	0.40
1:A:270:ASN:ND2	1:F:378:HIS:O	2.47	0.40
1:C:127:GLU:OE2	1:C:204:SER:OG	2.29	0.40
1:B:448:LYS:HB2	1:B:451:GLN:OE1	2.21	0.40
1:B:554:GLU:O	1:B:557:VAL:HG22	2.22	0.40
1:C:206:MET:O	1:C:208:MET:HE2	2.21	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LYS:O	1:E:29:HIS:NE2[1_665]	1.53	0.67
1:B:547:LYS:O	1:E:29:HIS:CD2[1_665]	1.78	0.42
1:B:539:LEU:CB	1:C:535:ASP:CB[1_655]	1.88	0.32
1:B:539:LEU:CD2	1:C:533:ASP:OD2[1_655]	1.93	0.27
1:E:546:LYS:NZ	1:H:535:ASP:OD2[1_656]	1.96	0.24
1:B:539:LEU:CD1	1:C:533:ASP:OD1[1_655]	2.00	0.20
1:B:543:TRP:CZ2	1:C:533:ASP:CG[1_655]	2.04	0.16
1:B:543:TRP:CH2	1:C:533:ASP:OD2[1_655]	2.05	0.15
1:C:537:LYS:NZ	1:E:391:GLU:OE2[1_565]	2.06	0.14
1:B:547:LYS:C	1:E:29:HIS:NE2[1_665]	2.08	0.12
1:B:543:TRP:CZ2	1:C:533:ASP:OD2[1_655]	2.09	0.11
1:A:529:LEU:CD2	1:D:539:LEU:CD2[1_556]	2.10	0.10
1:B:533:ASP:OD1	1:C:539:LEU:CD1[1_655]	2.11	0.09
1:E:535:ASP:CG	1:H:543:TRP:CZ2[1_656]	2.11	0.09
1:A:529:LEU:CD1	1:D:543:TRP:CZ2[1_556]	2.16	0.04
1:B:396:GLU:OE2	1:H:534:HIS:CD2[1_666]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/764 (72%)	541 (98%)	12 (2%)	0	100	100
1	B	521/764 (68%)	503 (96%)	17 (3%)	1 (0%)	51	84
1	C	553/764 (72%)	539 (98%)	14 (2%)	0	100	100
1	D	521/764 (68%)	508 (98%)	12 (2%)	1 (0%)	51	84
1	E	553/764 (72%)	541 (98%)	12 (2%)	0	100	100
1	F	521/764 (68%)	508 (98%)	13 (2%)	0	100	100
1	G	553/764 (72%)	540 (98%)	13 (2%)	0	100	100
1	H	521/764 (68%)	507 (97%)	14 (3%)	0	100	100
All	All	4296/6112 (70%)	4187 (98%)	107 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	570	GLU
1	B	569	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/644 (73%)	461 (98%)	7 (2%)	70	87
1	B	442/644 (69%)	432 (98%)	10 (2%)	56	80
1	C	468/644 (73%)	462 (99%)	6 (1%)	73	88
1	D	442/644 (69%)	433 (98%)	9 (2%)	60	83
1	E	468/644 (73%)	461 (98%)	7 (2%)	70	87
1	F	442/644 (69%)	436 (99%)	6 (1%)	71	87
1	G	468/644 (73%)	463 (99%)	5 (1%)	78	89
1	H	442/644 (69%)	433 (98%)	9 (2%)	60	83
All	All	3640/5152 (71%)	3581 (98%)	59 (2%)	68	86

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LYS
1	A	409	SER
1	A	439	SER
1	A	455	TYR
1	A	522	THR
1	A	527	ILE
1	A	547	LYS
1	B	399	ASP
1	B	409	SER
1	B	439	SER
1	B	455	TYR
1	B	522	THR

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Mol	Chain	Res	Type
1	B	525	SER
1	B	529	LEU
1	B	544	ILE
1	B	546	LYS
1	B	547	LYS
1	C	309	LYS
1	C	409	SER
1	C	439	SER
1	C	455	TYR
1	C	522	THR
1	C	547	LYS
1	D	197	SER
1	D	399	ASP
1	D	409	SER
1	D	439	SER
1	D	455	TYR
1	D	522	THR
1	D	525	SER
1	D	546	LYS
1	D	547	LYS
1	E	197	SER
1	E	309	LYS
1	E	409	SER
1	E	439	SER
1	E	455	TYR
1	E	522	THR
1	E	527	ILE
1	F	399	ASP
1	F	409	SER
1	F	439	SER
1	F	455	TYR
1	F	522	THR
1	F	525	SER
1	G	309	LYS
1	G	439	SER
1	G	455	TYR
1	G	522	THR
1	G	527	ILE
1	H	197	SER
1	H	289	GLU
1	H	399	ASP
1	H	409	SER

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Mol	Chain	Res	Type
1	H	439	SER
1	H	451	GLN
1	H	455	TYR
1	H	522	THR
1	H	547	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	B	344	HIS
1	B	541	GLN
1	C	91	HIS
1	D	541	GLN
1	E	344	HIS
1	F	541	GLN
1	G	91	HIS
1	G	344	HIS
1	H	324	GLN
1	H	541	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	563/764 (73%)	0.40	50 (8%) 10 9	24, 154, 186, 226	0
1	B	533/764 (69%)	0.46	61 (11%) 6 6	24, 156, 195, 222	0
1	C	563/764 (73%)	0.33	45 (7%) 13 11	24, 153, 185, 226	0
1	D	533/764 (69%)	0.27	38 (7%) 17 12	24, 156, 191, 216	0
1	E	563/764 (73%)	0.32	52 (9%) 10 8	100, 153, 187, 213	0
1	F	533/764 (69%)	0.42	55 (10%) 7 7	24, 156, 189, 216	0
1	G	563/764 (73%)	0.30	39 (6%) 18 13	101, 153, 186, 206	0
1	H	533/764 (69%)	0.53	74 (13%) 3 4	24, 157, 193, 225	0
All	All	4384/6112 (71%)	0.38	414 (9%) 9 8	24, 155, 189, 226	0

All (414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	CYS	9.5
1	A	493	ALA	7.9
1	G	529	LEU	7.6
1	A	513	GLY	7.4
1	F	261	SER	7.3
1	B	526	GLU	7.1
1	B	235	GLY	6.8
1	B	92	ARG	6.6
1	A	50	PRO	6.5
1	E	543	TRP	6.2
1	F	385	PRO	6.2
1	C	126	ASN	6.1
1	B	43	ASP	5.9
1	E	45	ASP	5.8
1	F	384	SER	5.7
1	H	194	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	G	526	GLU	5.5
1	E	533	ASP	5.4
1	A	439	SER	5.4
1	F	470	ASP	5.2
1	C	295	PRO	5.2
1	F	386	LEU	5.2
1	H	257	ILE	5.2
1	B	44	VAL	5.1
1	D	61	LYS	5.1
1	E	544	ILE	5.0
1	E	517	ALA	5.0
1	D	372	PHE	5.0
1	B	197	SER	5.0
1	C	236	ALA	4.8
1	A	306	THR	4.8
1	A	345	THR	4.8
1	H	378	HIS	4.8
1	A	256	GLY	4.8
1	G	61	LYS	4.8
1	A	51	VAL	4.7
1	A	492	LEU	4.7
1	B	535	ASP	4.7
1	E	28	VAL	4.7
1	F	379	PHE	4.7
1	G	42	TRP	4.7
1	H	379	PHE	4.7
1	H	421	ILE	4.7
1	B	66	LEU	4.6
1	A	514	SER	4.6
1	G	41	ARG	4.6
1	B	87	MET	4.6
1	C	258	ILE	4.5
1	D	236	ALA	4.5
1	H	373	THR	4.5
1	D	44	VAL	4.4
1	H	405	ALA	4.4
1	A	148	ALA	4.4
1	E	540	LEU	4.4
1	C	385	PRO	4.4
1	H	459	MET	4.3
1	H	93	ILE	4.3
1	B	234	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	129	GLY	4.3
1	A	19	ASN	4.2
1	F	474	MET	4.2
1	D	373	THR	4.2
1	H	303	MET	4.1
1	H	293	ILE	4.1
1	E	536	ALA	4.1
1	E	218	GLY	4.1
1	C	204	SER	4.1
1	F	447	LYS	4.0
1	G	234	GLU	4.0
1	A	254	ILE	4.0
1	A	346	SER	4.0
1	H	351	VAL	4.0
1	C	439	SER	3.9
1	F	293	ILE	3.9
1	F	236	ALA	3.9
1	B	132	LEU	3.9
1	B	529	LEU	3.9
1	A	12	GLY	3.9
1	B	65	MET	3.9
1	H	513	GLY	3.9
1	E	383	HIS	3.9
1	B	440	ALA	3.9
1	B	492	LEU	3.8
1	H	399	ASP	3.8
1	B	41	ARG	3.8
1	G	527	ILE	3.8
1	H	406	CYS	3.8
1	G	427	GLU	3.8
1	A	152	ILE	3.8
1	F	292	GLY	3.8
1	C	493	ALA	3.8
1	F	235	GLY	3.8
1	F	197	SER	3.8
1	D	544	ILE	3.7
1	B	381	PHE	3.7
1	A	471	LEU	3.7
1	B	373	THR	3.7
1	H	376	ASN	3.7
1	E	44	VAL	3.7
1	B	459	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	307	GLY	3.7
1	G	535	ASP	3.7
1	B	198	LEU	3.6
1	D	442	PHE	3.6
1	C	128	TYR	3.6
1	G	518	ALA	3.6
1	H	161	PRO	3.6
1	B	83	GLU	3.6
1	A	81	PRO	3.6
1	B	84	ALA	3.6
1	D	88	ASP	3.5
1	H	591	PRO	3.5
1	E	532	THR	3.5
1	H	355	GLN	3.5
1	G	36	ASP	3.5
1	F	226	GLY	3.5
1	E	518	ALA	3.5
1	B	371	ASN	3.5
1	F	260	GLY	3.5
1	G	547	LYS	3.4
1	B	199	TYR	3.4
1	A	441	LEU	3.4
1	H	469	ILE	3.4
1	A	440	ALA	3.4
1	H	234	GLU	3.4
1	A	149	ALA	3.3
1	B	341	ASN	3.3
1	F	571	TYR	3.3
1	G	492	LEU	3.3
1	G	65	MET	3.3
1	C	373	THR	3.3
1	D	408	SER	3.3
1	B	368	PRO	3.2
1	D	89	PRO	3.2
1	H	295	PRO	3.2
1	C	418	HIS	3.2
1	H	127	GLU	3.2
1	C	323	PHE	3.2
1	A	470	ASP	3.2
1	D	492	LEU	3.2
1	F	405	ALA	3.2
1	D	199	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	133	ASN	3.1
1	D	237	GLY	3.1
1	H	398	ALA	3.1
1	H	438	ARG	3.1
1	D	540	LEU	3.1
1	G	237	GLY	3.1
1	D	402	PRO	3.1
1	G	560	LEU	3.1
1	F	372	PHE	3.1
1	C	335	ILE	3.1
1	E	539	LEU	3.1
1	H	256	GLY	3.1
1	C	407	VAL	3.1
1	E	521	LYS	3.1
1	G	386	LEU	3.1
1	D	491	PHE	3.0
1	E	531	GLU	3.0
1	A	262	GLY	3.0
1	F	270	ASN	3.0
1	F	323	PHE	3.0
1	H	572	THR	3.0
1	D	202	PRO	3.0
1	C	372	PHE	3.0
1	H	271	GLY	3.0
1	E	493	ALA	3.0
1	E	133	ASN	3.0
1	A	126	ASN	3.0
1	G	202	PRO	3.0
1	D	583	PHE	3.0
1	A	72	PHE	3.0
1	H	552	VAL	3.0
1	B	130	VAL	3.0
1	D	404	ARG	2.9
1	F	258	ILE	2.9
1	H	163	ILE	2.9
1	A	307	GLY	2.9
1	B	86	LEU	2.9
1	H	165	ILE	2.9
1	B	236	ALA	2.9
1	H	130	VAL	2.9
1	F	335	ILE	2.9
1	E	269	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	272	ILE	2.9
1	E	439	SER	2.9
1	B	69	ILE	2.9
1	C	202	PRO	2.9
1	E	36	ASP	2.9
1	F	198	LEU	2.9
1	H	371	ASN	2.9
1	B	311	GLY	2.9
1	C	376	ASN	2.9
1	F	331	GLN	2.9
1	D	60	CYS	2.8
1	D	90	GLN	2.8
1	H	356	LYS	2.8
1	C	377	GLU	2.8
1	G	567	LEU	2.8
1	A	130	VAL	2.8
1	B	295	PRO	2.8
1	C	386	LEU	2.8
1	D	305	GLY	2.8
1	F	506	TYR	2.8
1	H	121	LEU	2.8
1	C	192	LEU	2.8
1	E	382	GLU	2.8
1	B	441	LEU	2.8
1	F	192	LEU	2.8
1	C	280	GLN	2.8
1	B	18	ARG	2.8
1	B	13	ARG	2.8
1	B	514	SER	2.8
1	H	390	THR	2.8
1	H	422	GLU	2.7
1	B	408	SER	2.7
1	E	442	PHE	2.7
1	D	235	GLY	2.7
1	A	303	MET	2.7
1	G	66	LEU	2.7
1	C	511	PRO	2.7
1	E	211	ALA	2.7
1	B	456	ALA	2.7
1	A	204	SER	2.7
1	F	204	SER	2.7
1	A	194	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	374	THR	2.7
1	A	49	ASP	2.7
1	F	412	TYR	2.7
1	F	473	ASP	2.7
1	E	489	MET	2.7
1	G	327	THR	2.7
1	H	61	LYS	2.7
1	F	419	ILE	2.7
1	G	62	SER	2.7
1	A	495	SER	2.6
1	E	128	TYR	2.6
1	D	14	TYR	2.6
1	H	243	ARG	2.6
1	G	295	PRO	2.6
1	H	193	VAL	2.6
1	E	385	PRO	2.6
1	G	517	ALA	2.6
1	E	7	ILE	2.6
1	A	132	LEU	2.6
1	B	90	GLN	2.6
1	F	427	GLU	2.6
1	E	566	LYS	2.6
1	C	200	LEU	2.6
1	E	37	ILE	2.6
1	C	257	ILE	2.6
1	D	582	PRO	2.6
1	E	42	TRP	2.6
1	H	198	LEU	2.6
1	A	17	ALA	2.5
1	H	269	THR	2.5
1	E	525	SER	2.5
1	C	494	ASP	2.5
1	F	97	GLU	2.5
1	B	95	LEU	2.5
1	E	530	PHE	2.5
1	H	514	SER	2.5
1	E	129	GLY	2.5
1	A	296	GLU	2.5
1	E	529	LEU	2.5
1	H	499	LEU	2.5
1	H	73	ASP	2.5
1	D	489	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	306	THR	2.5
1	F	124	MET	2.5
1	H	573	PRO	2.5
1	H	299	SER	2.5
1	B	455	TYR	2.5
1	H	493	ALA	2.5
1	A	526	GLU	2.5
1	D	526	GLU	2.5
1	H	377	GLU	2.5
1	H	470	ASP	2.5
1	D	441	LEU	2.5
1	B	549	LEU	2.4
1	G	571	TYR	2.4
1	C	127	GLU	2.4
1	D	517	ALA	2.4
1	A	128	TYR	2.4
1	D	93	ILE	2.4
1	H	262	GLY	2.4
1	B	570	GLU	2.4
1	A	494	ASP	2.4
1	G	536	ALA	2.4
1	B	14	TYR	2.4
1	F	550	GLU	2.4
1	G	132	LEU	2.4
1	C	261	SER	2.4
1	A	129	GLY	2.4
1	E	132	LEU	2.4
1	B	547	LYS	2.4
1	E	46	LYS	2.4
1	E	50	PRO	2.4
1	G	133	ASN	2.4
1	H	270	ASN	2.4
1	H	341	ASN	2.4
1	F	420	VAL	2.3
1	B	372	PHE	2.3
1	D	256	GLY	2.3
1	E	131	MET	2.3
1	E	202	PRO	2.3
1	B	560	LEU	2.3
1	E	217	ASP	2.3
1	B	369	THR	2.3
1	F	378	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	89	PRO	2.3
1	G	142	GLY	2.3
1	H	92	ARG	2.3
1	E	526	GLU	2.3
1	H	447	LYS	2.3
1	G	131	MET	2.3
1	H	495	SER	2.3
1	G	114	GLU	2.3
1	G	43	ASP	2.3
1	A	530	PHE	2.3
1	A	91	HIS	2.3
1	E	255	TYR	2.3
1	H	261	SER	2.3
1	F	380	GLU	2.3
1	F	572	THR	2.3
1	C	560	LEU	2.3
1	H	419	ILE	2.3
1	F	234	GLU	2.3
1	C	256	GLY	2.3
1	C	404	ARG	2.3
1	H	79	ILE	2.3
1	H	512	ASN	2.3
1	B	490	ALA	2.3
1	E	372	PHE	2.3
1	H	583	PHE	2.3
1	C	419	ILE	2.3
1	C	544	ILE	2.3
1	E	535	ASP	2.3
1	D	92	ARG	2.2
1	H	62	SER	2.2
1	H	590	LEU	2.2
1	A	552	VAL	2.2
1	F	187	GLU	2.2
1	D	275	PRO	2.2
1	B	128	TYR	2.2
1	E	541	GLN	2.2
1	H	76	PHE	2.2
1	A	304	HIS	2.2
1	C	530	PHE	2.2
1	D	383	HIS	2.2
1	G	471	LEU	2.2
1	A	257	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	211	ALA	2.2
1	E	323	PHE	2.2
1	F	19	ASN	2.2
1	H	91	HIS	2.2
1	C	42	TRP	2.2
1	F	387	TYR	2.2
1	F	511	PRO	2.2
1	H	254	ILE	2.2
1	A	193	VAL	2.1
1	C	130	VAL	2.1
1	F	529	LEU	2.1
1	B	61	LYS	2.1
1	D	154	TYR	2.1
1	F	291	TYR	2.1
1	B	129	GLY	2.1
1	B	534	HIS	2.1
1	F	544	ILE	2.1
1	G	543	TRP	2.1
1	B	80	PRO	2.1
1	C	260	GLY	2.1
1	F	320	SER	2.1
1	H	468	ASP	2.1
1	C	193	VAL	2.1
1	E	444	LEU	2.1
1	B	305	GLY	2.1
1	H	195	GLY	2.1
1	E	268	LYS	2.1
1	A	417	ALA	2.1
1	A	397	THR	2.1
1	B	386	LEU	2.1
1	G	459	MET	2.1
1	D	43	ASP	2.1
1	E	62	SER	2.1
1	D	566	LYS	2.1
1	G	407	VAL	2.1
1	B	94	PHE	2.1
1	C	40	SER	2.1
1	E	57	LYS	2.1
1	F	64	GLY	2.1
1	A	295	PRO	2.1
1	C	13	ARG	2.1
1	F	406	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	57	LYS	2.1
1	B	342	ILE	2.1
1	C	247	ALA	2.0
1	G	236	ALA	2.0
1	A	401	LYS	2.0
1	F	41	ARG	2.0
1	H	526	GLU	2.0
1	F	408	SER	2.0
1	G	503	LEU	2.0
1	F	376	ASN	2.0
1	B	388	VAL	2.0
1	B	548	ARG	2.0
1	F	530	PHE	2.0
1	H	74	PRO	2.0
1	F	180	ARG	2.0
1	E	49	ASP	2.0
1	B	523	LYS	2.0
1	C	234	GLU	2.0
1	F	554	GLU	2.0
1	C	41	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.