



Full wwPDB X-ray Structure Validation Report i

May 27, 2020 – 03:34 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

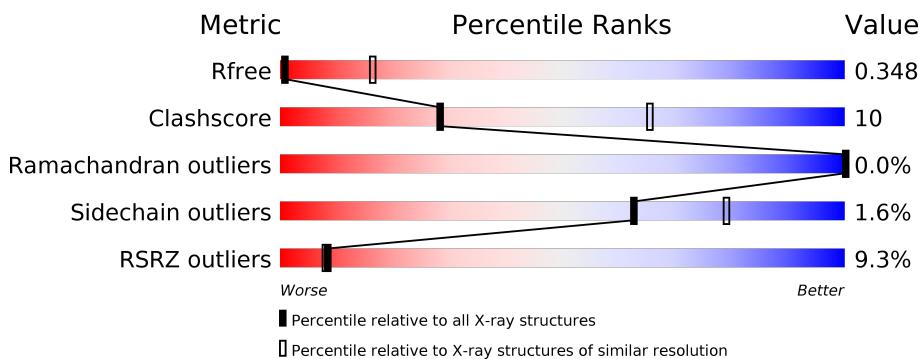
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

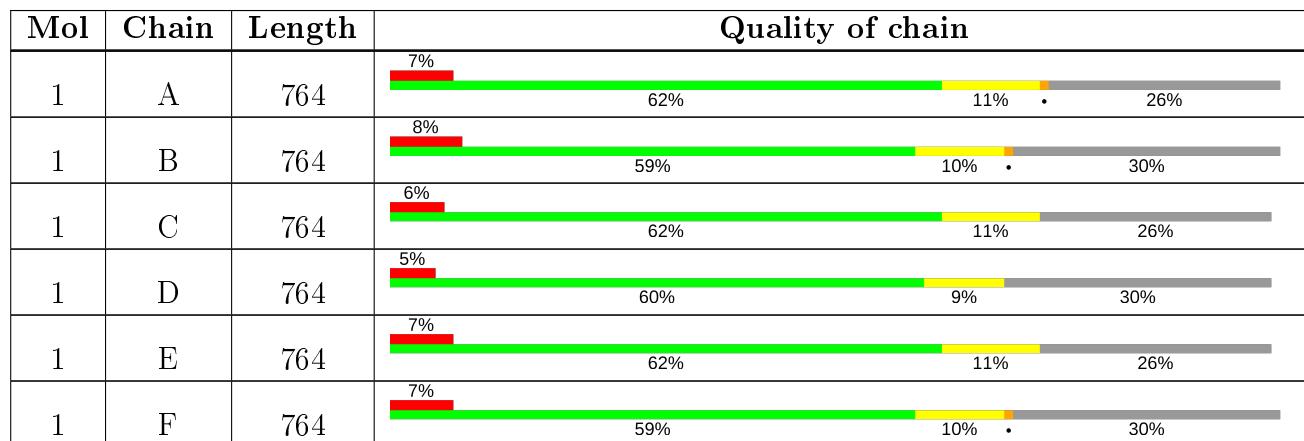
The reported resolution of this entry is 4.00 Å.

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.



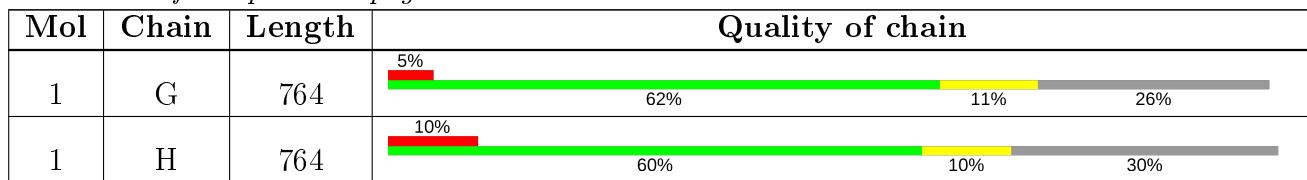
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 >=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.



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2 Entry composition (i)

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 4419	N 2811	O 738	S 844	26	0	0
1	B	533	Total	C 4185	N 2663	O 703	S 797	22	0	0
1	C	563	Total	C 4419	N 2811	O 738	S 844	26	0	0
1	D	533	Total	C 4185	N 2663	O 703	S 797	22	0	0
1	E	563	Total	C 4419	N 2811	O 738	S 844	26	0	0
1	F	533	Total	C 4185	N 2663	O 703	S 797	22	0	0
1	G	563	Total	C 4419	N 2811	O 738	S 844	26	0	0
1	H	533	Total	C 4185	N 2663	O 703	S 797	22	0	0

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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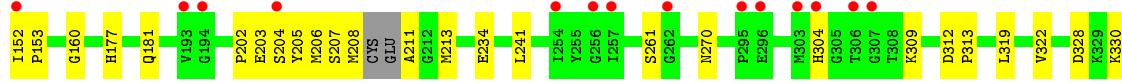
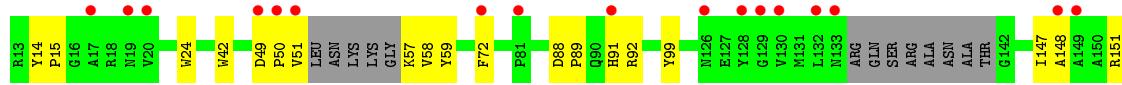
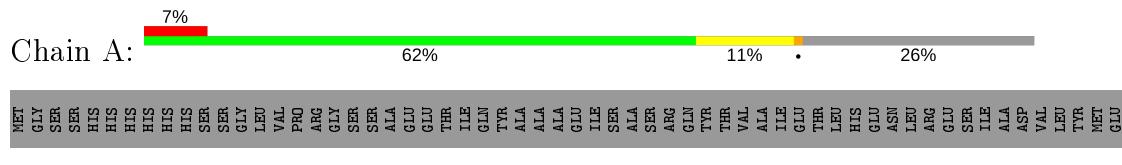
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-153	SER	-	expression tag	UNP Q05470
H	-172	MET	-	initiating methionine	UNP Q05470
H	-171	GLY	-	expression tag	UNP Q05470
H	-170	SER	-	expression tag	UNP Q05470
H	-169	SER	-	expression tag	UNP Q05470
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

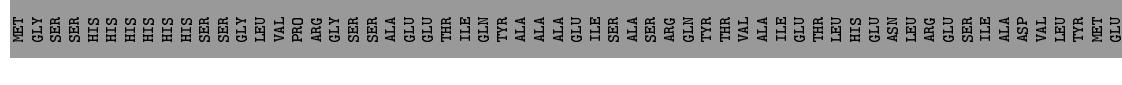
3 Residue-property plots

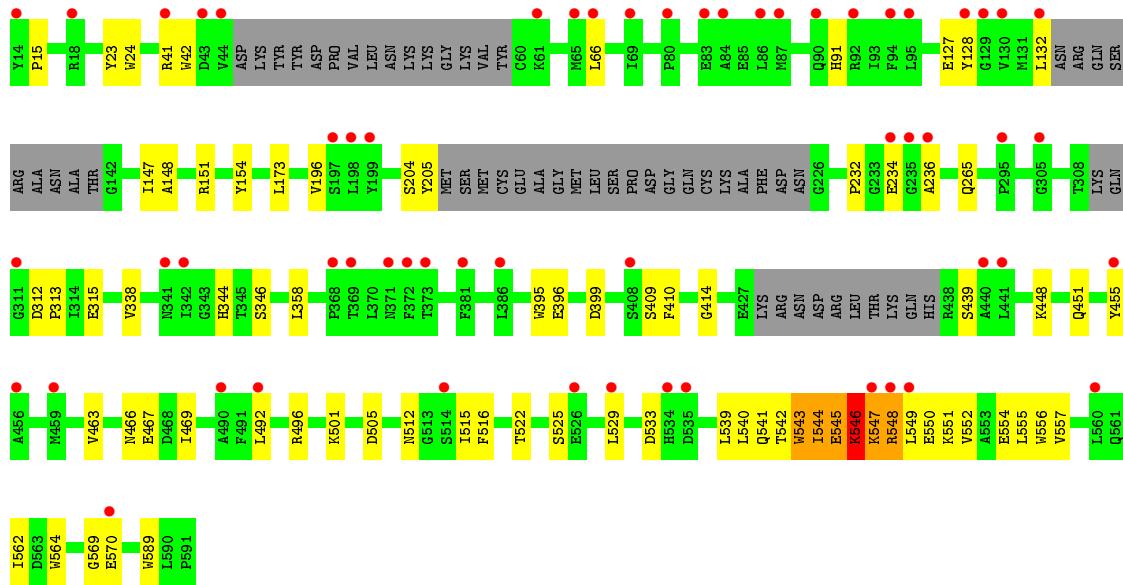
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

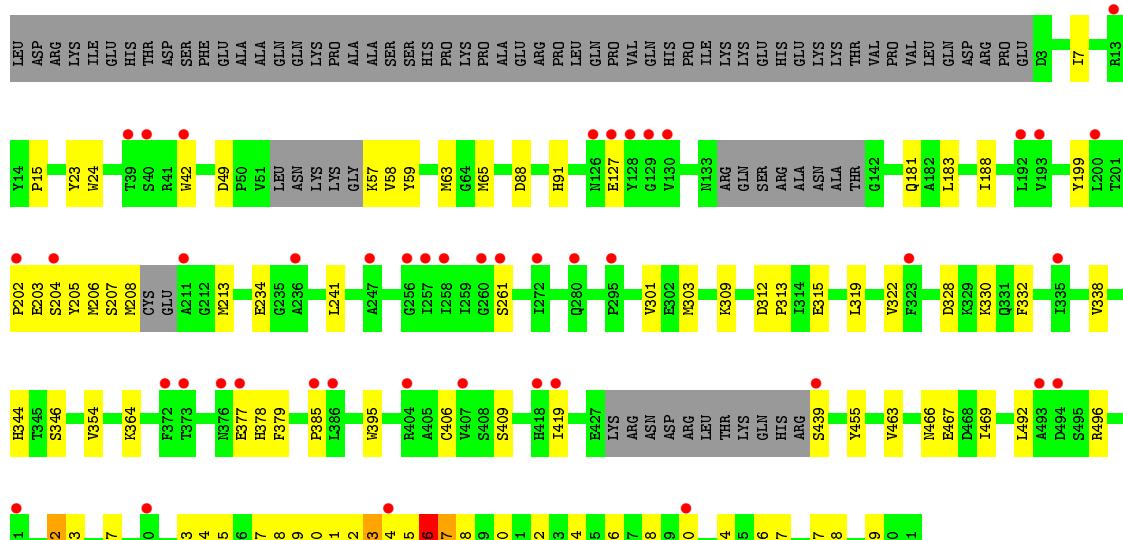
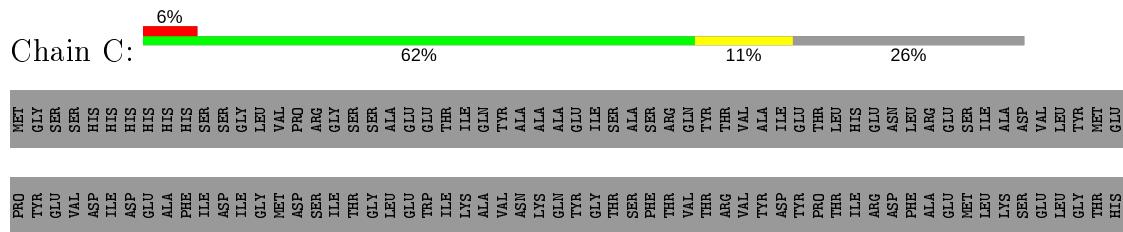


- Molecule 1: Polyketide synthase PksL



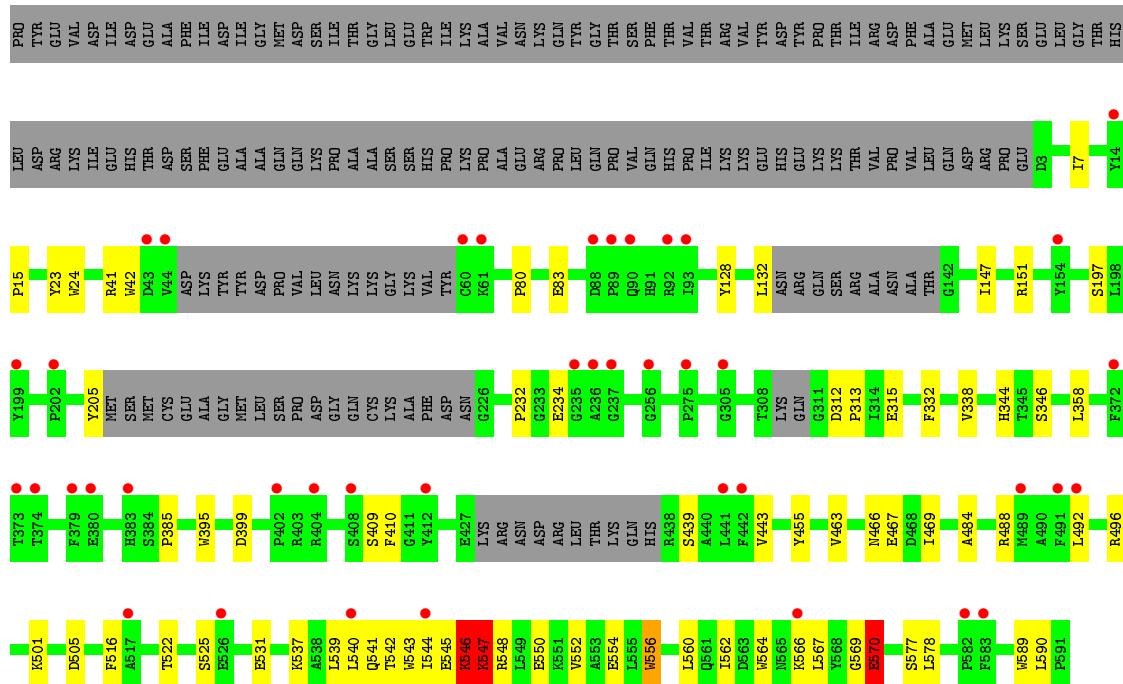


- Molecule 1: Polyketide synthase PksL

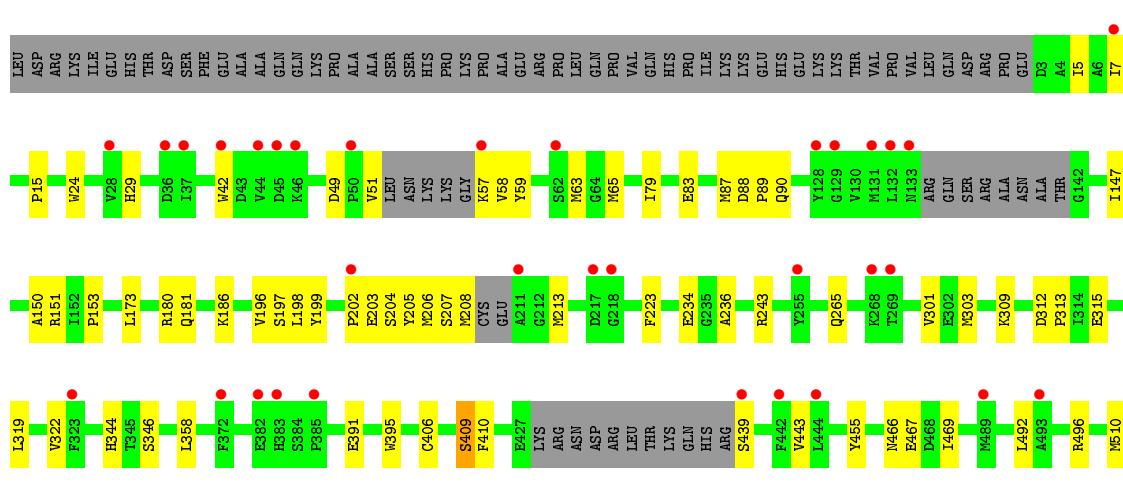
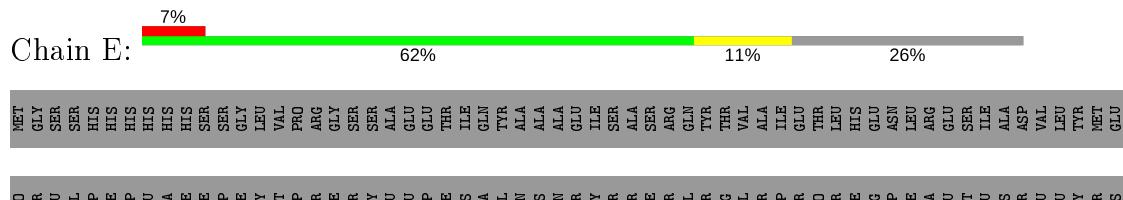


- Molecule 1: Polyketide synthase PksL



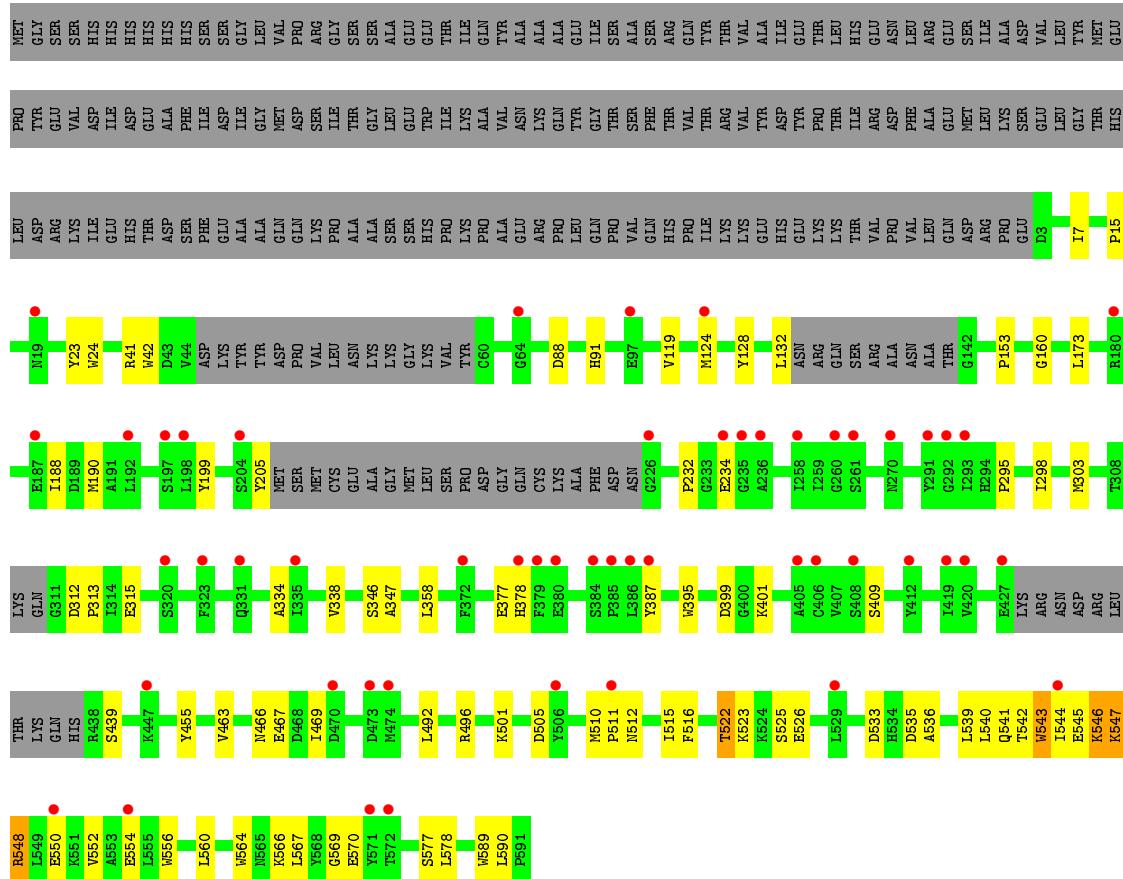


- Molecule 1: Polyketide synthase PksL

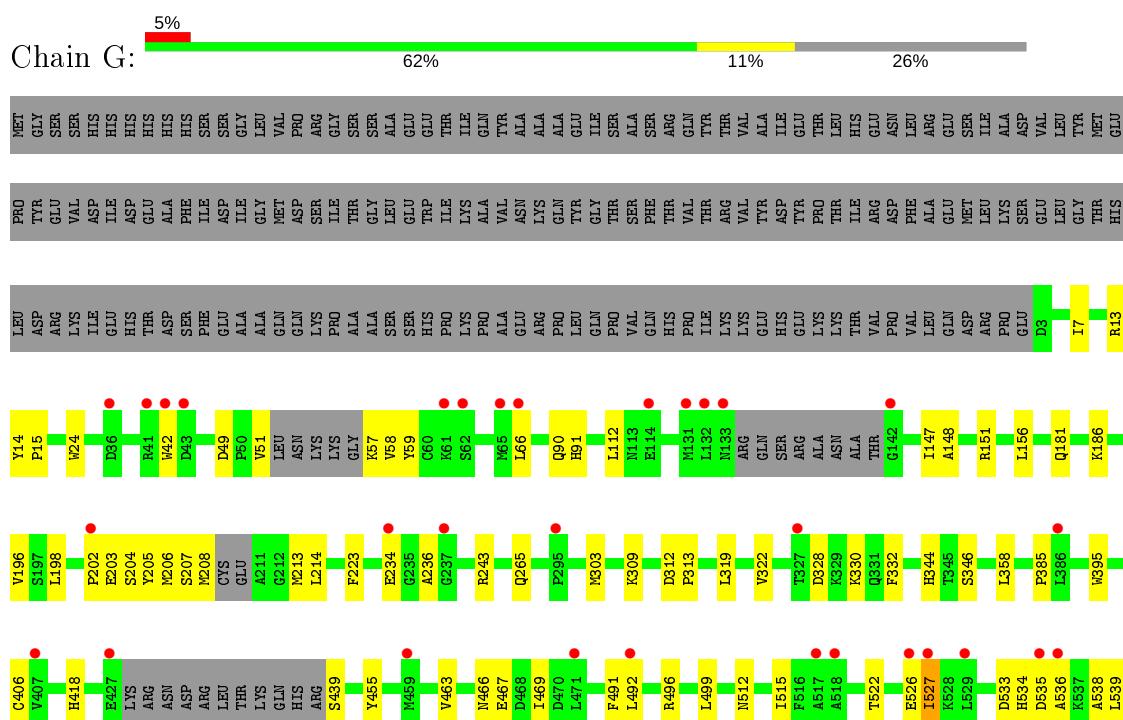


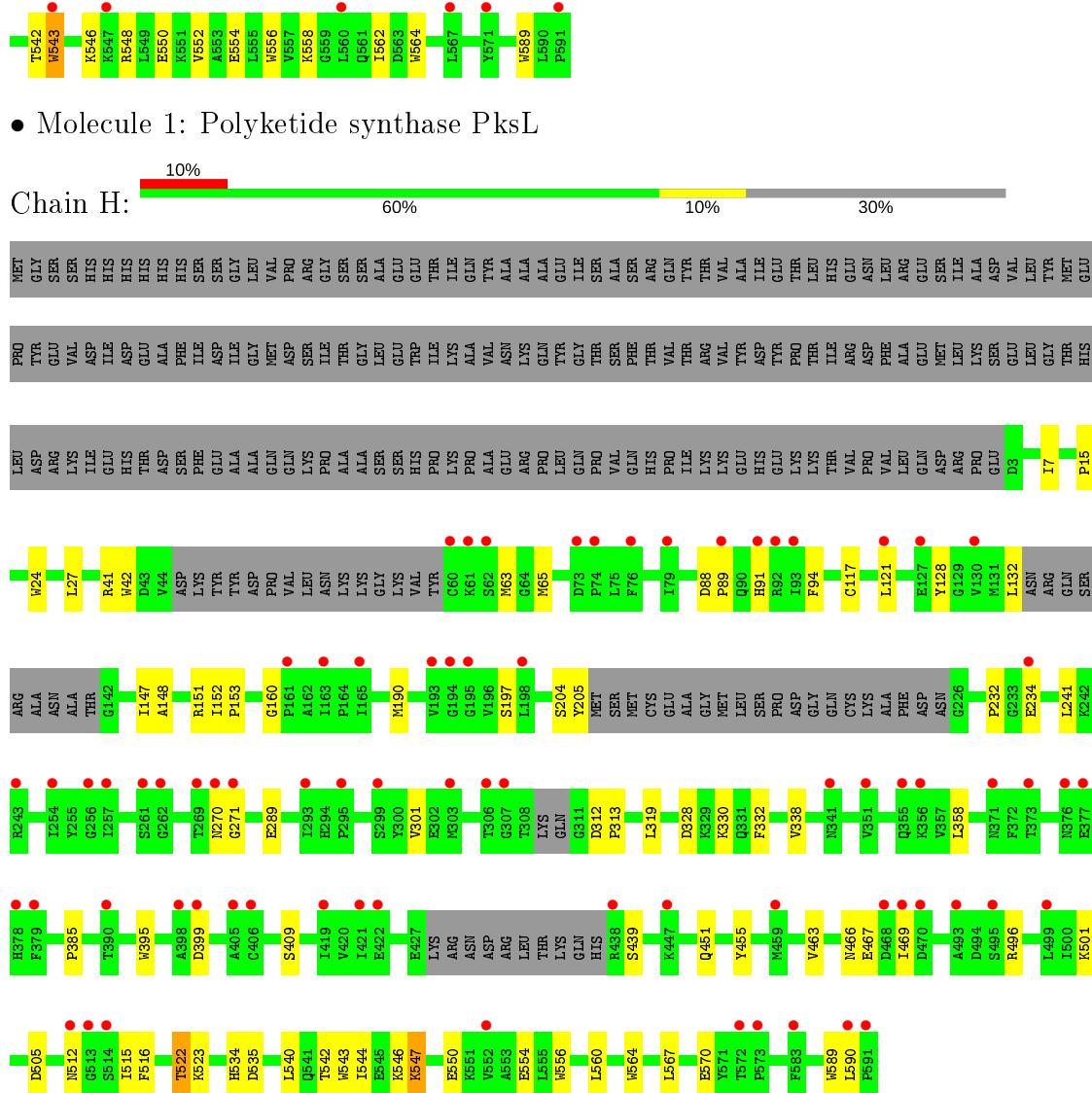
- Molecule 1: Polyketide synthase PksL





- Molecule 1: Polyketide synthase PksL





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.11 Å 112.73 Å 211.44 Å 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) 92.5 (39.77-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.12 (at 4.00 Å)	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 (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	138.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 100.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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 [\(i\)](#)

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	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	553/764 (72%)	541 (98%)	12 (2%)	0	100 100
1	B	521/764 (68%)	503 (96%)	17 (3%)	1 (0%)	47 79
1	C	553/764 (72%)	539 (98%)	14 (2%)	0	100 100
1	D	521/764 (68%)	508 (98%)	12 (2%)	1 (0%)	47 79
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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	468/644 (73%)	461 (98%)	7 (2%)	65 80
1	B	442/644 (69%)	432 (98%)	10 (2%)	50 70
1	C	468/644 (73%)	462 (99%)	6 (1%)	69 82
1	D	442/644 (69%)	433 (98%)	9 (2%)	55 73
1	E	468/644 (73%)	461 (98%)	7 (2%)	65 80
1	F	442/644 (69%)	436 (99%)	6 (1%)	67 81
1	G	468/644 (73%)	463 (99%)	5 (1%)	73 85
1	H	442/644 (69%)	433 (98%)	9 (2%)	55 73
All	All	3640/5152 (71%)	3581 (98%)	59 (2%)	62 79

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 (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	A	563/764 (73%)	0.40	52 (9%) 9 8	24, 154, 186, 226	0
1	B	533/764 (69%)	0.46	59 (11%) 5 5	24, 156, 195, 222	0
1	C	563/764 (73%)	0.33	44 (7%) 13 11	24, 153, 185, 226	0
1	D	533/764 (69%)	0.27	41 (7%) 13 11	24, 156, 191, 216	0
1	E	563/764 (73%)	0.32	51 (9%) 9 8	100, 153, 187, 213	0
1	F	533/764 (69%)	0.42	52 (9%) 7 7	24, 156, 189, 216	0
1	G	563/764 (73%)	0.30	37 (6%) 18 14	101, 153, 186, 206	0
1	H	533/764 (69%)	0.53	73 (13%) 3 3	24, 157, 193, 225	0
All	All	4384/6112 (71%)	0.38	409 (9%) 8 8	24, 155, 189, 226	0

All (409) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	CYS	9.8
1	A	493	ALA	7.9
1	G	529	LEU	7.7
1	A	513	GLY	7.6
1	F	261	SER	7.2
1	B	526	GLU	7.0
1	B	235	GLY	6.8
1	B	92	ARG	6.6
1	A	50	PRO	6.4
1	E	543	TRP	6.2
1	F	385	PRO	6.1
1	C	126	ASN	6.1
1	B	43	ASP	5.9
1	E	45	ASP	5.7
1	F	384	SER	5.7
1	H	194	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	533	ASP	5.4
1	G	526	GLU	5.3
1	A	439	SER	5.3
1	B	44	VAL	5.2
1	F	470	ASP	5.2
1	C	295	PRO	5.2
1	F	386	LEU	5.2
1	D	61	LYS	5.1
1	H	257	ILE	5.1
1	B	197	SER	5.0
1	E	517	ALA	5.0
1	E	544	ILE	5.0
1	D	372	PHE	4.9
1	A	345	THR	4.8
1	C	236	ALA	4.8
1	A	306	THR	4.8
1	H	378	HIS	4.8
1	G	42	TRP	4.7
1	H	379	PHE	4.7
1	B	66	LEU	4.7
1	F	379	PHE	4.7
1	G	41	ARG	4.7
1	D	44	VAL	4.6
1	A	51	VAL	4.6
1	B	535	ASP	4.6
1	H	421	ILE	4.6
1	G	61	LYS	4.6
1	E	28	VAL	4.6
1	B	87	MET	4.6
1	A	514	SER	4.6
1	A	256	GLY	4.6
1	A	492	LEU	4.6
1	C	385	PRO	4.5
1	C	258	ILE	4.5
1	E	540	LEU	4.4
1	A	148	ALA	4.4
1	D	236	ALA	4.4
1	H	405	ALA	4.4
1	H	373	THR	4.4
1	H	93	ILE	4.4
1	H	459	MET	4.3
1	B	234	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	129	GLY	4.3
1	E	536	ALA	4.2
1	A	19	ASN	4.2
1	F	474	MET	4.2
1	H	293	ILE	4.1
1	D	373	THR	4.1
1	H	303	MET	4.1
1	C	204	SER	4.1
1	A	346	SER	4.0
1	F	293	ILE	4.0
1	F	447	LYS	4.0
1	A	12	GLY	4.0
1	H	406	CYS	4.0
1	B	65	MET	3.9
1	E	218	GLY	3.9
1	A	254	ILE	3.9
1	G	234	GLU	3.9
1	B	529	LEU	3.9
1	H	399	ASP	3.9
1	H	351	VAL	3.9
1	C	439	SER	3.9
1	E	383	HIS	3.9
1	G	527	ILE	3.9
1	B	132	LEU	3.9
1	F	292	GLY	3.8
1	B	373	THR	3.8
1	F	235	GLY	3.8
1	B	440	ALA	3.8
1	C	493	ALA	3.8
1	F	197	SER	3.8
1	F	236	ALA	3.8
1	B	41	ARG	3.8
1	A	152	ILE	3.8
1	H	513	GLY	3.8
1	G	427	GLU	3.8
1	B	492	LEU	3.8
1	G	36	ASP	3.7
1	B	83	GLU	3.7
1	G	535	ASP	3.7
1	B	381	PHE	3.7
1	D	88	ASP	3.7
1	G	518	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	198	LEU	3.7
1	D	544	ILE	3.7
1	H	591	PRO	3.7
1	A	471	LEU	3.7
1	H	376	ASN	3.7
1	H	161	PRO	3.7
1	C	128	TYR	3.7
1	H	307	GLY	3.6
1	B	459	MET	3.6
1	E	44	VAL	3.6
1	B	84	ALA	3.6
1	E	532	THR	3.6
1	H	355	GLN	3.6
1	B	371	ASN	3.5
1	D	442	PHE	3.5
1	B	199	TYR	3.5
1	E	518	ALA	3.5
1	C	373	THR	3.4
1	G	547	LYS	3.4
1	A	81	PRO	3.4
1	F	260	GLY	3.4
1	F	226	GLY	3.4
1	F	571	TYR	3.4
1	H	469	ILE	3.4
1	A	441	LEU	3.4
1	A	149	ALA	3.4
1	B	341	ASN	3.3
1	H	234	GLU	3.3
1	B	368	PRO	3.3
1	A	440	ALA	3.3
1	H	127	GLU	3.3
1	G	492	LEU	3.3
1	G	65	MET	3.3
1	A	470	ASP	3.3
1	D	89	PRO	3.3
1	D	199	TYR	3.3
1	H	398	ALA	3.2
1	H	295	PRO	3.2
1	E	521	LYS	3.2
1	H	438	ARG	3.2
1	F	405	ALA	3.2
1	D	408	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	418	HIS	3.2
1	C	323	PHE	3.2
1	D	402	PRO	3.1
1	E	531	GLU	3.1
1	D	540	LEU	3.1
1	G	560	LEU	3.1
1	A	133	ASN	3.1
1	F	270	ASN	3.1
1	E	539	LEU	3.1
1	D	237	GLY	3.1
1	C	335	ILE	3.1
1	G	237	GLY	3.1
1	H	271	GLY	3.0
1	F	198	LEU	3.0
1	G	386	LEU	3.0
1	D	202	PRO	3.0
1	F	372	PHE	3.0
1	C	372	PHE	3.0
1	D	491	PHE	3.0
1	C	407	VAL	3.0
1	E	269	THR	3.0
1	A	262	GLY	3.0
1	D	404	ARG	3.0
1	G	202	PRO	3.0
1	E	36	ASP	3.0
1	D	492	LEU	3.0
1	H	572	THR	3.0
1	D	583	PHE	3.0
1	A	72	PHE	3.0
1	B	130	VAL	3.0
1	A	126	ASN	3.0
1	H	256	GLY	3.0
1	B	311	GLY	3.0
1	E	133	ASN	3.0
1	H	163	ILE	3.0
1	B	236	ALA	3.0
1	H	165	ILE	2.9
1	A	307	GLY	2.9
1	H	371	ASN	2.9
1	D	90	GLN	2.9
1	F	323	PHE	2.9
1	H	552	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	272	ILE	2.9
1	F	335	ILE	2.9
1	H	356	LYS	2.9
1	B	86	LEU	2.9
1	F	258	ILE	2.9
1	E	493	ALA	2.9
1	C	202	PRO	2.9
1	E	439	SER	2.9
1	H	130	VAL	2.9
1	H	121	LEU	2.9
1	F	331	GLN	2.9
1	D	60	CYS	2.9
1	C	192	LEU	2.8
1	B	69	ILE	2.8
1	B	514	SER	2.8
1	E	382	GLU	2.8
1	C	376	ASN	2.8
1	C	386	LEU	2.8
1	G	567	LEU	2.8
1	C	377	GLU	2.8
1	B	18	ARG	2.8
1	A	49	ASP	2.8
1	A	130	VAL	2.8
1	F	506	TYR	2.8
1	H	422	GLU	2.8
1	E	442	PHE	2.8
1	D	305	GLY	2.8
1	B	441	LEU	2.8
1	B	295	PRO	2.8
1	H	390	THR	2.8
1	C	280	GLN	2.7
1	B	13	ARG	2.7
1	E	211	ALA	2.7
1	F	192	LEU	2.7
1	A	495	SER	2.7
1	B	456	ALA	2.7
1	G	66	LEU	2.7
1	F	412	TYR	2.7
1	A	204	SER	2.7
1	H	61	LYS	2.7
1	E	128	TYR	2.7
1	D	235	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	408	SER	2.7
1	G	517	ALA	2.7
1	G	327	THR	2.7
1	G	62	SER	2.7
1	F	204	SER	2.7
1	F	419	ILE	2.7
1	D	14	TYR	2.6
1	F	473	ASP	2.6
1	C	511	PRO	2.6
1	H	243	ARG	2.6
1	C	200	LEU	2.6
1	E	385	PRO	2.6
1	E	489	MET	2.6
1	F	97	GLU	2.6
1	D	374	THR	2.6
1	D	582	PRO	2.6
1	E	7	ILE	2.6
1	E	566	LYS	2.6
1	H	193	VAL	2.6
1	H	198	LEU	2.6
1	H	306	THR	2.6
1	A	132	LEU	2.6
1	B	90	GLN	2.6
1	A	303	MET	2.6
1	G	295	PRO	2.6
1	A	194	GLY	2.5
1	C	494	ASP	2.5
1	C	257	ILE	2.5
1	A	296	GLU	2.5
1	E	129	GLY	2.5
1	E	525	SER	2.5
1	E	529	LEU	2.5
1	H	73	ASP	2.5
1	E	37	ILE	2.5
1	F	427	GLU	2.5
1	H	269	THR	2.5
1	B	570	GLU	2.5
1	H	299	SER	2.5
1	H	573	PRO	2.5
1	E	42	TRP	2.5
1	D	517	ALA	2.5
1	G	536	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	571	TYR	2.5
1	D	526	GLU	2.5
1	E	530	PHE	2.5
1	H	377	GLU	2.5
1	H	493	ALA	2.5
1	A	526	GLU	2.5
1	A	494	ASP	2.5
1	B	549	LEU	2.5
1	F	124	MET	2.5
1	H	499	LEU	2.4
1	B	455	TYR	2.4
1	D	489	MET	2.4
1	C	127	GLU	2.4
1	H	470	ASP	2.4
1	B	95	LEU	2.4
1	D	441	LEU	2.4
1	H	514	SER	2.4
1	B	14	TYR	2.4
1	E	132	LEU	2.4
1	D	93	ILE	2.4
1	F	550	GLU	2.4
1	A	128	TYR	2.4
1	G	132	LEU	2.4
1	F	380	GLU	2.4
1	F	420	VAL	2.4
1	H	89	PRO	2.4
1	E	131	MET	2.4
1	B	372	PHE	2.4
1	G	131	MET	2.4
1	B	560	LEU	2.4
1	H	495	SER	2.4
1	H	270	ASN	2.4
1	H	419	ILE	2.4
1	E	46	LYS	2.3
1	B	547	LYS	2.3
1	C	261	SER	2.3
1	A	17	ALA	2.3
1	A	129	GLY	2.3
1	F	378	HIS	2.3
1	H	262	GLY	2.3
1	B	128	TYR	2.3
1	B	369	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	261	SER	2.3
1	H	341	ASN	2.3
1	G	142	GLY	2.3
1	E	202	PRO	2.3
1	H	79	ILE	2.3
1	G	43	ASP	2.3
1	H	62	SER	2.3
1	E	541	GLN	2.3
1	H	447	LYS	2.3
1	E	535	ASP	2.3
1	H	92	ARG	2.3
1	A	530	PHE	2.3
1	E	372	PHE	2.3
1	D	256	GLY	2.3
1	E	50	PRO	2.3
1	C	560	LEU	2.3
1	E	217	ASP	2.3
1	F	572	THR	2.3
1	D	92	ARG	2.3
1	G	133	ASN	2.3
1	A	91	HIS	2.3
1	E	255	TYR	2.2
1	F	19	ASN	2.2
1	H	91	HIS	2.2
1	C	544	ILE	2.2
1	H	512	ASN	2.2
1	H	76	PHE	2.2
1	E	526	GLU	2.2
1	F	234	GLU	2.2
1	C	530	PHE	2.2
1	H	583	PHE	2.2
1	F	529	LEU	2.2
1	D	43	ASP	2.2
1	F	320	SER	2.2
1	C	256	GLY	2.2
1	G	543	TRP	2.2
1	B	490	ALA	2.2
1	G	114	GLU	2.2
1	G	471	LEU	2.2
1	D	275	PRO	2.2
1	C	42	TRP	2.2
1	H	590	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	HIS	2.2
1	E	323	PHE	2.2
1	C	404	ARG	2.2
1	A	552	VAL	2.2
1	C	211	ALA	2.2
1	D	383	HIS	2.2
1	F	387	TYR	2.2
1	H	195	GLY	2.2
1	D	154	TYR	2.2
1	E	57	LYS	2.2
1	F	511	PRO	2.2
1	H	254	ILE	2.2
1	F	544	ILE	2.2
1	B	80	PRO	2.1
1	F	187	GLU	2.1
1	H	468	ASP	2.1
1	B	129	GLY	2.1
1	C	419	ILE	2.1
1	F	291	TYR	2.1
1	F	64	GLY	2.1
1	C	40	SER	2.1
1	A	257	ILE	2.1
1	B	534	HIS	2.1
1	A	193	VAL	2.1
1	B	61	LYS	2.1
1	E	444	LEU	2.1
1	C	130	VAL	2.1
1	C	39	THR	2.1
1	C	193	VAL	2.1
1	D	380	GLU	2.1
1	A	397	THR	2.1
1	E	62	SER	2.1
1	B	548	ARG	2.1
1	G	459	MET	2.1
1	F	554	GLU	2.1
1	B	94	PHE	2.1
1	D	412	TYR	2.1
1	C	247	ALA	2.1
1	B	305	GLY	2.1
1	G	407	VAL	2.1
1	D	566	LYS	2.1
1	H	74	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	417	ALA	2.0
1	B	342	ILE	2.0
1	B	386	LEU	2.0
1	C	13	ARG	2.0
1	E	268	LYS	2.0
1	F	406	CYS	2.0
1	C	260	GLY	2.0
1	A	491	PHE	2.0
1	A	295	PRO	2.0
1	G	591	PRO	2.0
1	A	20	VAL	2.0
1	A	516	PHE	2.0
1	D	379	PHE	2.0
1	F	408	SER	2.0
1	F	180	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.