



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2016 – 05:26 PM EDT

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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	rb-20027939

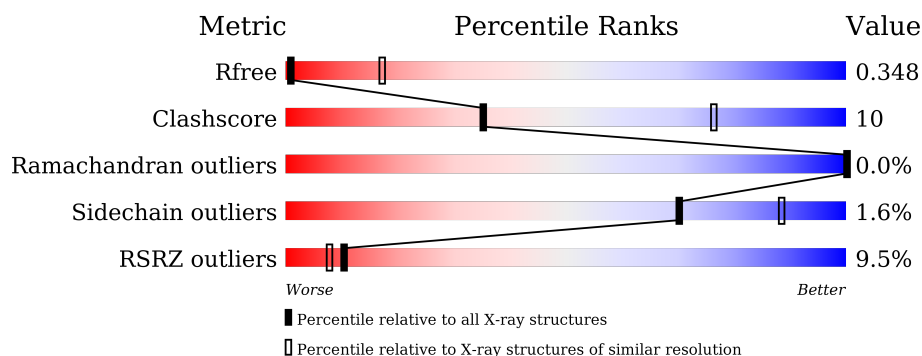
1 Overall quality at a glance

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}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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. 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>62%</div> <div>11%</div> <div>26%</div> </div>
1	B	764	<div> <div>8%</div> <div>59%</div> <div>10%</div> <div>30%</div> </div>
1	C	764	<div> <div>6%</div> <div>62%</div> <div>11%</div> <div>26%</div> </div>
1	D	764	<div> <div>5%</div> <div>60%</div> <div>9%</div> <div>30%</div> </div>
1	E	764	<div> <div>7%</div> <div>62%</div> <div>11%</div> <div>26%</div> </div>
1	F	764	<div> <div>7%</div> <div>59%</div> <div>10%</div> <div>30%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
			5%	62%	11%	26%
1	G	764				
1	H	764				

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

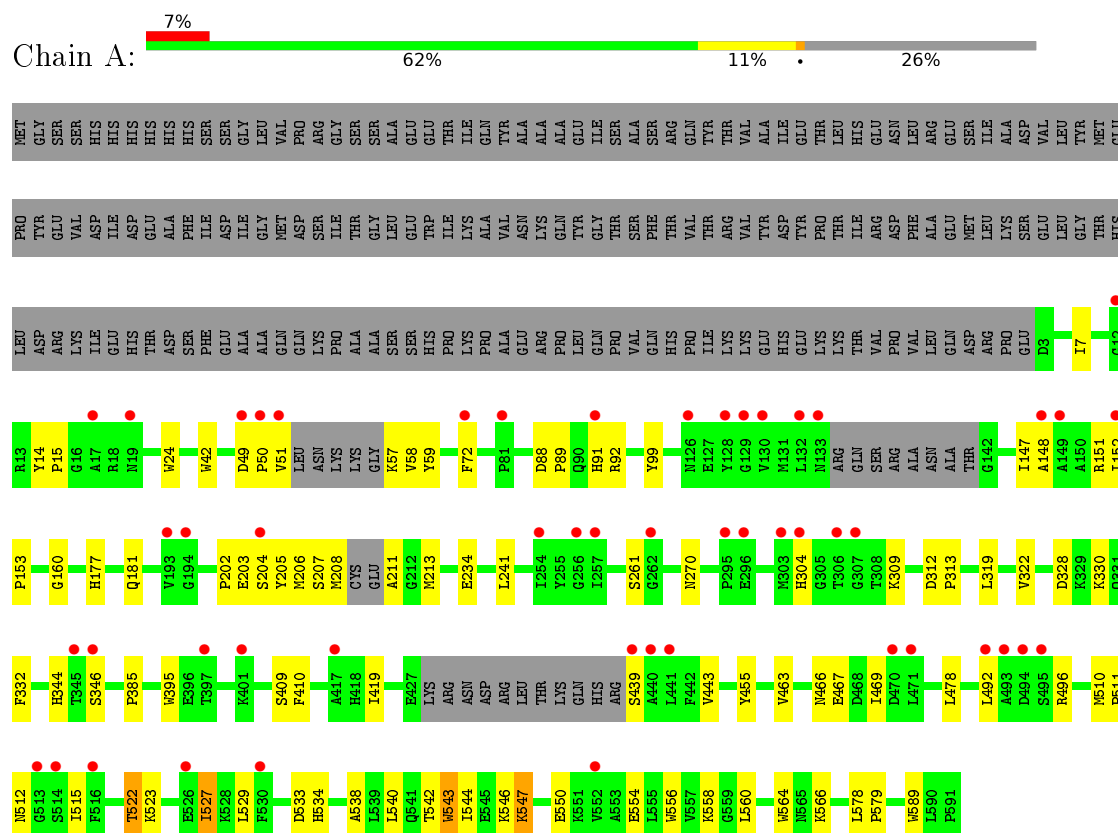
Continued from previous page...

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

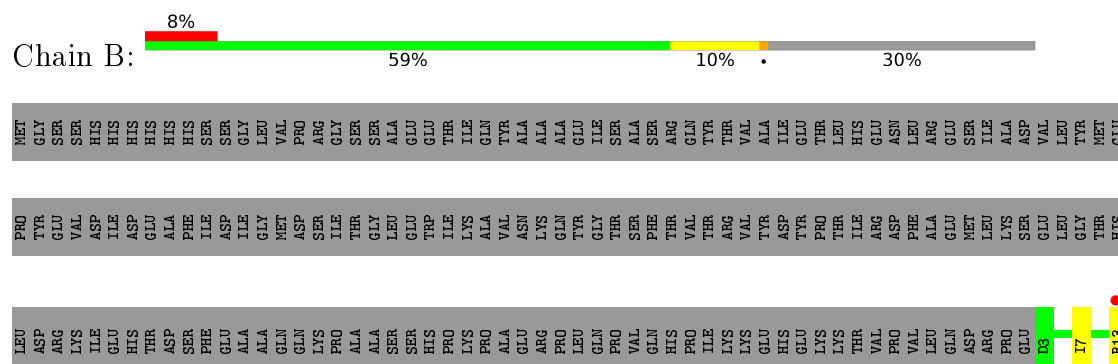
3 Residue-property plots

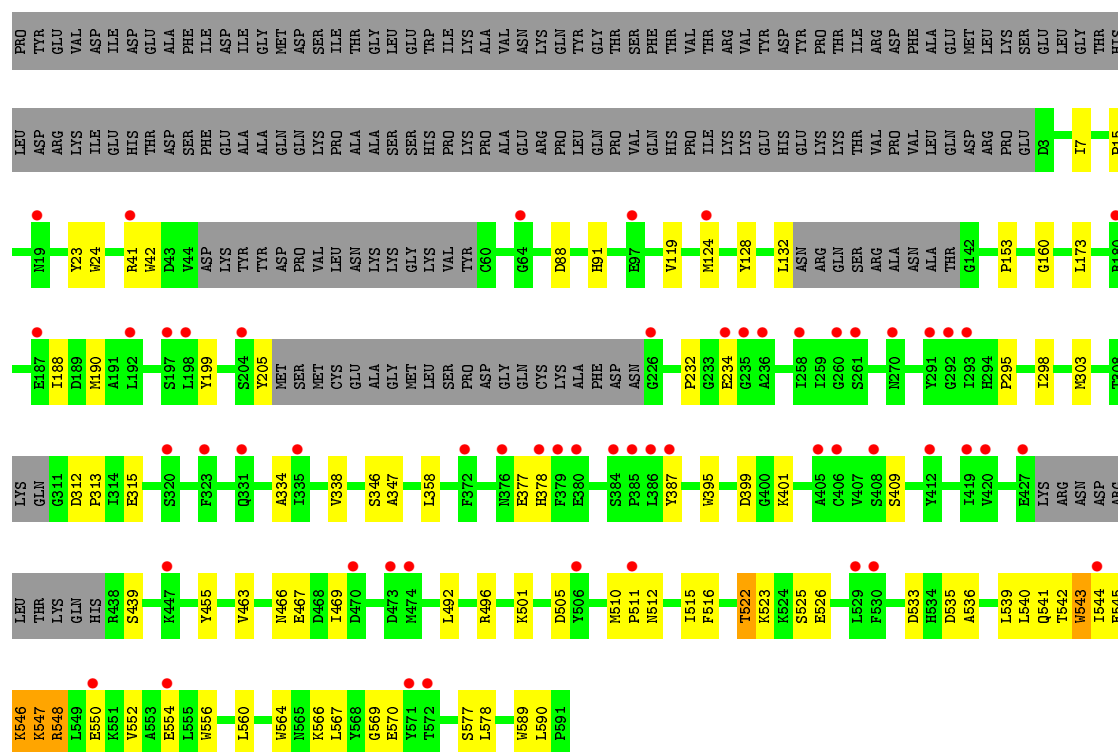
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

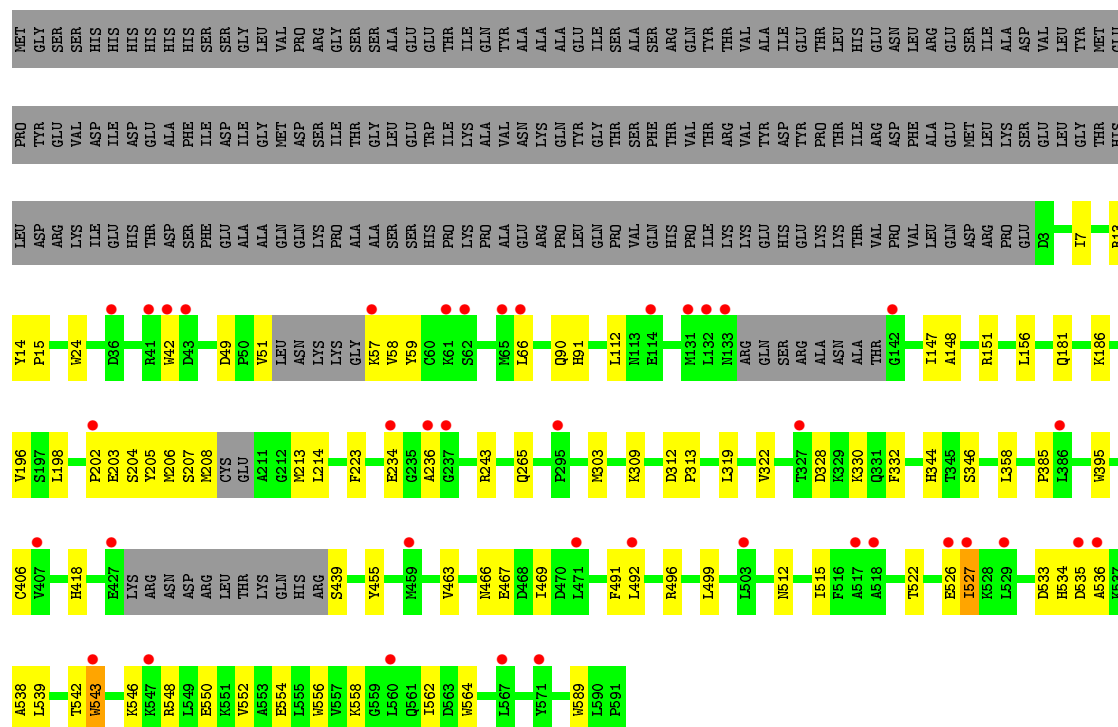


• Molecule 1: Polyketide synthase PksL





● Molecule 1: Polyketide synthase PksL



● Molecule 1: Polyketide synthase PksL





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	138.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 102.3	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.*

¹ Intensities estimated from amplitudes.

² 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:539:LEU:HD11	1:G:533:ASP:OD1	1.64	0.96
1:F:535:ASP:OD2	1:G:539:LEU:HD12	1.65	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

Continued on next page...

Continued from previous page...

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:539:LEU:HD13	1:G:536:ALA:N	1.93	0.83
1:F:541:GLN:HB3	1:F:545:GLU:OE2	1.79	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:H:128:TYR:O	1:H:132:LEU:HD13	1.80	0.81
1:C:377:GLU:CD	1:H:271:GLY:HA2	1.99	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

Continued on next page...

Continued from previous page...

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:D:540:LEU:CG	1:D:544:ILE:HD12	2.13	0.77
1:C:364:LYS:HB2	1:F:511:PRO:HD2	1.65	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

Continued on next page...

Continued from previous page...

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:F:542:THR:HA	1:F:545:GLU:CG	2.24	0.68
1:C:377:GLU:CD	1:H:271:GLY:CA	2.61	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:516:PHE:CE1	1:B:554:GLU:HG2	2.31	0.65
1:B:540:LEU:O	1:B:544:ILE:CG1	2.44	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

Continued on next page...

Continued from previous page...

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:533:ASP:CB	1:G:543:TRP:HZ2	2.13	0.60
1:F:541:GLN:CB	1:F:545:GLU:OE2	2.48	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:544:ILE:CG1	1:D:552:VAL:HG22	2.31	0.60
1:D:546:LYS:C	1:D:547:LYS:HG3	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:536:ALA:H	1:G:539:LEU:HD22	1.63	0.60
1:F:541:GLN:HB3	1:F:545:GLU:CD	2.21	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:HB3	1:G:539:LEU:CA	2.35	0.57

Continued on next page...

Continued from previous page...

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:CG	1:G:539:LEU:HA	2.25	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

Continued on next page...

Continued from previous page...

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:536:ALA:CA	1:G:539:LEU:HD22	2.38	0.52
1:F:542:THR:CA	1:F:545:GLU:HG2	2.35	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

Continued on next page...

Continued from previous page...

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:C:364:LYS:NZ	1:F:510:MET:HB3	2.25	0.51
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: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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:540:LEU:HD22	1:A:560:LEU:HD21	1.96	0.47
1:A:542:THR:O	1:A:546:LYS:CB	2.63	0.47
1:F:119:VAL:HG21	1:F:153:PRO:HG3	1.96	0.47
1:G:527:ILE:HD13	1:G:558:LYS:CB	2.43	0.47
1:G:91:HIS:NE2	1:G:148:ALA:HB2	2.29	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:545:GLU:N	1:F:546:LYS:CA	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:542:THR:HG21	1:G:535:ASP:OD2	2.16	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

Continued on next page...

Continued from previous page...

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:CG2	1:F:567:LEU:HD13	2.49	0.43
1:F:544:ILE:O	1:F:546:LYS:HD3	2.15	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	52	86
1	C	553/764 (72%)	539 (98%)	14 (2%)	0	100	100
1	D	521/764 (68%)	508 (98%)	12 (2%)	1 (0%)	52	86
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%)	72	89
1	B	442/644 (69%)	432 (98%)	10 (2%)	58	83
1	C	468/644 (73%)	462 (99%)	6 (1%)	76	90
1	D	442/644 (69%)	433 (98%)	9 (2%)	63	86
1	E	468/644 (73%)	461 (98%)	7 (2%)	72	89
1	F	442/644 (69%)	436 (99%)	6 (1%)	74	89
1	G	468/644 (73%)	463 (99%)	5 (1%)	80	91
1	H	442/644 (69%)	433 (98%)	9 (2%)	63	86
All	All	3640/5152 (71%)	3581 (98%)	59 (2%)	70	88

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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, 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	51 (9%) 11 8	24, 154, 186, 226	0
1	B	533/764 (69%)	0.46	61 (11%) 7 6	24, 156, 195, 222	0
1	C	563/764 (73%)	0.33	46 (8%) 14 10	24, 153, 185, 226	0
1	D	533/764 (69%)	0.27	39 (7%) 18 13	24, 156, 191, 216	0
1	E	563/764 (73%)	0.32	51 (9%) 11 8	100, 153, 187, 213	0
1	F	533/764 (69%)	0.42	55 (10%) 9 7	24, 156, 189, 216	0
1	G	563/764 (73%)	0.30	39 (6%) 20 13	101, 153, 186, 206	0
1	H	533/764 (69%)	0.53	74 (13%) 4 4	24, 157, 193, 225	0
All	All	4384/6112 (71%)	0.38	416 (9%) 10 8	24, 155, 189, 226	0

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	CYS	9.6
1	A	493	ALA	8.0
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	6.9
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	5.7
1	F	384	SER	5.7
1	H	194	GLY	5.6

Continued on next page...

Continued from previous page...

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	5.3
1	C	295	PRO	5.2
1	F	386	LEU	5.2
1	H	257	ILE	5.2
1	B	44	VAL	5.2
1	D	61	LYS	5.1
1	E	544	ILE	5.0
1	E	517	ALA	5.0
1	B	197	SER	5.0
1	D	372	PHE	5.0
1	C	236	ALA	4.9
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	4.7
1	A	51	VAL	4.7
1	E	28	VAL	4.7
1	A	492	LEU	4.7
1	H	421	ILE	4.7
1	F	379	PHE	4.7
1	G	42	TRP	4.7
1	B	535	ASP	4.7
1	H	379	PHE	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	4.5
1	H	405	ALA	4.5
1	A	148	ALA	4.4
1	C	385	PRO	4.4
1	E	540	LEU	4.4
1	H	459	MET	4.3
1	B	234	GLU	4.3
1	H	93	ILE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	129	GLY	4.3
1	A	19	ASN	4.2
1	F	474	MET	4.2
1	H	303	MET	4.2
1	D	373	THR	4.1
1	H	293	ILE	4.1
1	E	536	ALA	4.1
1	C	204	SER	4.1
1	E	218	GLY	4.1
1	F	447	LYS	4.0
1	G	234	GLU	4.0
1	A	346	SER	4.0
1	A	254	ILE	4.0
1	F	293	ILE	4.0
1	C	439	SER	4.0
1	H	351	VAL	4.0
1	B	65	MET	3.9
1	A	12	GLY	3.9
1	F	236	ALA	3.9
1	B	132	LEU	3.9
1	B	529	LEU	3.9
1	E	383	HIS	3.9
1	H	399	ASP	3.9
1	H	513	GLY	3.9
1	B	440	ALA	3.8
1	B	492	LEU	3.8
1	B	41	ARG	3.8
1	H	406	CYS	3.8
1	G	427	GLU	3.8
1	G	527	ILE	3.8
1	A	152	ILE	3.8
1	F	197	SER	3.8
1	F	292	GLY	3.8
1	F	235	GLY	3.8
1	C	493	ALA	3.8
1	D	544	ILE	3.7
1	B	373	THR	3.7
1	B	381	PHE	3.7
1	A	471	LEU	3.7
1	H	376	ASN	3.7
1	B	198	LEU	3.7
1	B	459	MET	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	44	VAL	3.7
1	G	518	ALA	3.7
1	H	161	PRO	3.7
1	C	128	TYR	3.7
1	G	535	ASP	3.7
1	H	307	GLY	3.7
1	D	442	PHE	3.6
1	B	83	GLU	3.6
1	B	84	ALA	3.6
1	D	88	ASP	3.6
1	H	355	GLN	3.6
1	H	591	PRO	3.6
1	E	532	THR	3.5
1	A	81	PRO	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	B	199	TYR	3.5
1	F	260	GLY	3.4
1	G	547	LYS	3.4
1	A	441	LEU	3.4
1	H	234	GLU	3.4
1	A	440	ALA	3.4
1	H	469	ILE	3.4
1	B	341	ASN	3.4
1	F	571	TYR	3.4
1	A	149	ALA	3.4
1	G	492	LEU	3.3
1	G	65	MET	3.3
1	C	373	THR	3.3
1	D	89	PRO	3.3
1	D	408	SER	3.3
1	B	368	PRO	3.3
1	H	127	GLU	3.3
1	H	295	PRO	3.2
1	C	418	HIS	3.2
1	A	470	ASP	3.2
1	C	323	PHE	3.2
1	D	492	LEU	3.2
1	F	405	ALA	3.2
1	D	199	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	398	ALA	3.2
1	D	237	GLY	3.2
1	A	133	ASN	3.1
1	H	438	ARG	3.1
1	H	256	GLY	3.1
1	D	402	PRO	3.1
1	D	540	LEU	3.1
1	E	539	LEU	3.1
1	G	237	GLY	3.1
1	G	560	LEU	3.1
1	C	335	ILE	3.1
1	C	407	VAL	3.1
1	F	372	PHE	3.1
1	G	386	LEU	3.1
1	E	521	LYS	3.1
1	D	491	PHE	3.0
1	H	572	THR	3.0
1	A	262	GLY	3.0
1	E	531	GLU	3.0
1	F	270	ASN	3.0
1	C	372	PHE	3.0
1	H	271	GLY	3.0
1	D	583	PHE	3.0
1	F	323	PHE	3.0
1	E	133	ASN	3.0
1	D	202	PRO	3.0
1	E	493	ALA	3.0
1	G	202	PRO	3.0
1	A	72	PHE	3.0
1	A	126	ASN	3.0
1	H	552	VAL	3.0
1	B	236	ALA	3.0
1	B	130	VAL	3.0
1	D	404	ARG	3.0
1	H	165	ILE	3.0
1	H	163	ILE	2.9
1	A	307	GLY	2.9
1	E	269	THR	2.9
1	F	258	ILE	2.9
1	H	130	VAL	2.9
1	B	86	LEU	2.9
1	F	335	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	439	SER	2.9
1	F	198	LEU	2.9
1	C	202	PRO	2.9
1	C	272	ILE	2.9
1	H	371	ASN	2.9
1	B	69	ILE	2.9
1	E	36	ASP	2.9
1	D	90	GLN	2.9
1	B	311	GLY	2.9
1	F	331	GLN	2.9
1	H	121	LEU	2.9
1	C	376	ASN	2.8
1	H	356	LYS	2.8
1	C	377	GLU	2.8
1	B	295	PRO	2.8
1	D	60	CYS	2.8
1	G	567	LEU	2.8
1	F	506	TYR	2.8
1	A	130	VAL	2.8
1	C	192	LEU	2.8
1	C	386	LEU	2.8
1	E	382	GLU	2.8
1	D	305	GLY	2.8
1	B	441	LEU	2.8
1	F	192	LEU	2.8
1	H	390	THR	2.8
1	B	13	ARG	2.8
1	C	280	GLN	2.8
1	B	514	SER	2.8
1	H	422	GLU	2.8
1	B	18	ARG	2.8
1	D	235	GLY	2.8
1	B	408	SER	2.7
1	E	442	PHE	2.7
1	G	66	LEU	2.7
1	A	204	SER	2.7
1	B	456	ALA	2.7
1	E	211	ALA	2.7
1	A	49	ASP	2.7
1	A	303	MET	2.7
1	F	473	ASP	2.7
1	H	61	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	327	THR	2.7
1	C	511	PRO	2.7
1	F	204	SER	2.7
1	F	412	TYR	2.7
1	A	495	SER	2.7
1	D	374	THR	2.7
1	A	194	GLY	2.7
1	E	489	MET	2.7
1	F	419	ILE	2.7
1	G	62	SER	2.7
1	E	128	TYR	2.7
1	D	14	TYR	2.6
1	H	243	ARG	2.6
1	B	90	GLN	2.6
1	G	295	PRO	2.6
1	E	7	ILE	2.6
1	H	193	VAL	2.6
1	G	517	ALA	2.6
1	A	132	LEU	2.6
1	F	427	GLU	2.6
1	E	385	PRO	2.6
1	C	200	LEU	2.6
1	D	582	PRO	2.6
1	E	37	ILE	2.6
1	E	566	LYS	2.6
1	H	198	LEU	2.6
1	E	42	TRP	2.6
1	F	97	GLU	2.6
1	C	257	ILE	2.6
1	E	525	SER	2.6
1	C	494	ASP	2.6
1	A	17	ALA	2.5
1	H	269	THR	2.5
1	E	129	GLY	2.5
1	H	573	PRO	2.5
1	B	95	LEU	2.5
1	A	296	GLU	2.5
1	E	530	PHE	2.5
1	H	299	SER	2.5
1	F	124	MET	2.5
1	E	529	LEU	2.5
1	B	455	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	514	SER	2.5
1	H	499	LEU	2.5
1	D	489	MET	2.5
1	H	73	ASP	2.5
1	H	306	THR	2.5
1	A	526	GLU	2.5
1	H	493	ALA	2.5
1	D	526	GLU	2.5
1	H	377	GLU	2.5
1	D	441	LEU	2.5
1	B	549	LEU	2.5
1	G	571	TYR	2.4
1	H	470	ASP	2.4
1	D	93	ILE	2.4
1	A	128	TYR	2.4
1	A	494	ASP	2.4
1	C	127	GLU	2.4
1	B	14	TYR	2.4
1	B	570	GLU	2.4
1	D	517	ALA	2.4
1	E	132	LEU	2.4
1	H	262	GLY	2.4
1	F	550	GLU	2.4
1	G	536	ALA	2.4
1	E	131	MET	2.4
1	G	132	LEU	2.4
1	A	129	GLY	2.4
1	C	261	SER	2.4
1	H	270	ASN	2.4
1	F	378	HIS	2.4
1	H	341	ASN	2.4
1	F	420	VAL	2.4
1	G	133	ASN	2.4
1	B	372	PHE	2.3
1	B	560	LEU	2.3
1	E	50	PRO	2.3
1	B	547	LYS	2.3
1	B	369	THR	2.3
1	D	256	GLY	2.3
1	E	46	LYS	2.3
1	E	217	ASP	2.3
1	E	202	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	89	PRO	2.3
1	H	92	ARG	2.3
1	H	447	LYS	2.3
1	E	255	TYR	2.3
1	F	572	THR	2.3
1	H	495	SER	2.3
1	A	530	PHE	2.3
1	G	131	MET	2.3
1	E	526	GLU	2.3
1	G	43	ASP	2.3
1	A	91	HIS	2.3
1	F	380	GLU	2.3
1	G	114	GLU	2.3
1	H	419	ILE	2.3
1	H	261	SER	2.3
1	G	142	GLY	2.3
1	H	79	ILE	2.3
1	F	234	GLU	2.3
1	C	560	LEU	2.3
1	C	256	GLY	2.3
1	E	372	PHE	2.3
1	C	544	ILE	2.3
1	D	92	ARG	2.3
1	E	535	ASP	2.3
1	H	512	ASN	2.3
1	H	583	PHE	2.3
1	C	404	ARG	2.3
1	C	419	ILE	2.3
1	B	490	ALA	2.3
1	B	128	TYR	2.2
1	A	552	VAL	2.2
1	F	187	GLU	2.2
1	E	541	GLN	2.2
1	H	590	LEU	2.2
1	H	62	SER	2.2
1	H	76	PHE	2.2
1	C	530	PHE	2.2
1	A	304	HIS	2.2
1	F	19	ASN	2.2
1	C	42	TRP	2.2
1	G	471	LEU	2.2
1	D	275	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	387	TYR	2.2
1	C	211	ALA	2.2
1	E	323	PHE	2.2
1	D	383	HIS	2.2
1	H	91	HIS	2.2
1	F	511	PRO	2.2
1	A	257	ILE	2.2
1	B	80	PRO	2.2
1	H	254	ILE	2.2
1	A	193	VAL	2.2
1	C	130	VAL	2.2
1	G	543	TRP	2.2
1	F	291	TYR	2.2
1	D	154	TYR	2.2
1	F	544	ILE	2.2
1	F	529	LEU	2.1
1	B	129	GLY	2.1
1	H	195	GLY	2.1
1	B	61	LYS	2.1
1	B	534	HIS	2.1
1	D	43	ASP	2.1
1	H	468	ASP	2.1
1	F	320	SER	2.1
1	A	397	THR	2.1
1	C	193	VAL	2.1
1	E	268	LYS	2.1
1	C	260	GLY	2.1
1	E	62	SER	2.1
1	B	305	GLY	2.1
1	E	444	LEU	2.1
1	G	459	MET	2.1
1	A	417	ALA	2.1
1	B	386	LEU	2.1
1	G	407	VAL	2.1
1	C	40	SER	2.1
1	D	566	LYS	2.1
1	B	94	PHE	2.1
1	E	57	LYS	2.1
1	F	64	GLY	2.1
1	B	342	ILE	2.1
1	C	247	ALA	2.1
1	A	295	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	406	CYS	2.1
1	C	13	ARG	2.1
1	G	57	LYS	2.0
1	H	526	GLU	2.0
1	H	74	PRO	2.0
1	B	523	LYS	2.0
1	F	41	ARG	2.0
1	F	408	SER	2.0
1	B	388	VAL	2.0
1	A	401	LYS	2.0
1	F	376	ASN	2.0
1	G	236	ALA	2.0
1	G	503	LEU	2.0
1	B	548	ARG	2.0
1	F	180	ARG	2.0
1	D	412	TYR	2.0
1	F	530	PHE	2.0
1	F	554	GLU	2.0
1	C	234	GLU	2.0
1	C	41	ARG	2.0
1	A	516	PHE	2.0
1	C	590	LEU	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.