



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:45 AM UTC

PDB ID : 6VY9 / pdb_00006vy9
Title : Crystal structure of NotF prenyltransferase
Authors : Dan, Q.; Smith, J.L.
Deposited on : 2020-02-25
Resolution : 3.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

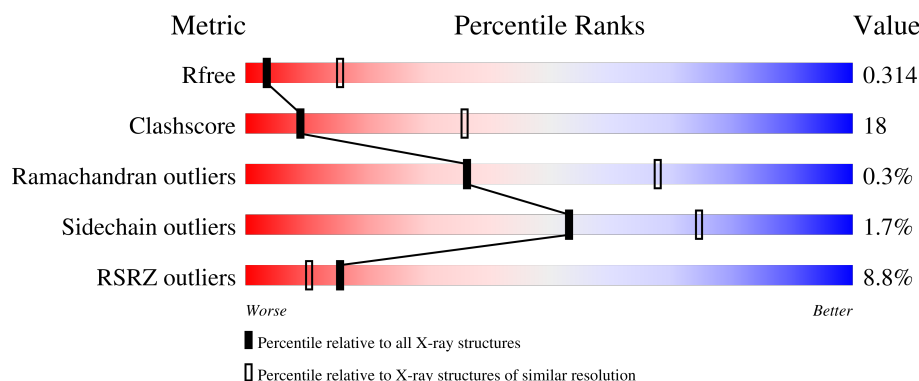
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	472	6% 53% 30% • 16%
1	B	472	6% 53% 30% • 16%
1	C	472	6% 54% 29% • 16%
1	D	472	7% 54% 29% 16%
1	E	472	8% 54% 29% • 16%

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Mol	Chain	Length	Quality of chain
1	F	472	 8% 54% 29% • 16%
1	G	472	 8% 53% 30% • 16%
1	H	472	 10% 53% 30% • 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25720 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 Deoxybrevianamide E synthase notF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			
1	B	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			
1	G	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			
1	H	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			
1	F	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			
1	D	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			
1	E	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			
1	C	396	Total	C	N	O	S	0	0	0
			3215	2083	541	584	7			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E0Y3X1
A	-18	GLY	-	expression tag	UNP E0Y3X1
A	-17	SER	-	expression tag	UNP E0Y3X1
A	-16	SER	-	expression tag	UNP E0Y3X1
A	-15	HIS	-	expression tag	UNP E0Y3X1
A	-14	HIS	-	expression tag	UNP E0Y3X1
A	-13	HIS	-	expression tag	UNP E0Y3X1
A	-12	HIS	-	expression tag	UNP E0Y3X1
A	-11	HIS	-	expression tag	UNP E0Y3X1
A	-10	HIS	-	expression tag	UNP E0Y3X1
A	-9	SER	-	expression tag	UNP E0Y3X1
A	-8	SER	-	expression tag	UNP E0Y3X1
A	-7	GLY	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP E0Y3X1
A	-5	VAL	-	expression tag	UNP E0Y3X1
A	-4	PRO	-	expression tag	UNP E0Y3X1
A	-3	ARG	-	expression tag	UNP E0Y3X1
A	-2	GLY	-	expression tag	UNP E0Y3X1
A	-1	SER	-	expression tag	UNP E0Y3X1
A	0	HIS	-	expression tag	UNP E0Y3X1
B	-19	MET	-	initiating methionine	UNP E0Y3X1
B	-18	GLY	-	expression tag	UNP E0Y3X1
B	-17	SER	-	expression tag	UNP E0Y3X1
B	-16	SER	-	expression tag	UNP E0Y3X1
B	-15	HIS	-	expression tag	UNP E0Y3X1
B	-14	HIS	-	expression tag	UNP E0Y3X1
B	-13	HIS	-	expression tag	UNP E0Y3X1
B	-12	HIS	-	expression tag	UNP E0Y3X1
B	-11	HIS	-	expression tag	UNP E0Y3X1
B	-10	HIS	-	expression tag	UNP E0Y3X1
B	-9	SER	-	expression tag	UNP E0Y3X1
B	-8	SER	-	expression tag	UNP E0Y3X1
B	-7	GLY	-	expression tag	UNP E0Y3X1
B	-6	LEU	-	expression tag	UNP E0Y3X1
B	-5	VAL	-	expression tag	UNP E0Y3X1
B	-4	PRO	-	expression tag	UNP E0Y3X1
B	-3	ARG	-	expression tag	UNP E0Y3X1
B	-2	GLY	-	expression tag	UNP E0Y3X1
B	-1	SER	-	expression tag	UNP E0Y3X1
B	0	HIS	-	expression tag	UNP E0Y3X1
G	-19	MET	-	initiating methionine	UNP E0Y3X1
G	-18	GLY	-	expression tag	UNP E0Y3X1
G	-17	SER	-	expression tag	UNP E0Y3X1
G	-16	SER	-	expression tag	UNP E0Y3X1
G	-15	HIS	-	expression tag	UNP E0Y3X1
G	-14	HIS	-	expression tag	UNP E0Y3X1
G	-13	HIS	-	expression tag	UNP E0Y3X1
G	-12	HIS	-	expression tag	UNP E0Y3X1
G	-11	HIS	-	expression tag	UNP E0Y3X1
G	-10	HIS	-	expression tag	UNP E0Y3X1
G	-9	SER	-	expression tag	UNP E0Y3X1
G	-8	SER	-	expression tag	UNP E0Y3X1
G	-7	GLY	-	expression tag	UNP E0Y3X1
G	-6	LEU	-	expression tag	UNP E0Y3X1
G	-5	VAL	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	PRO	-	expression tag	UNP E0Y3X1
G	-3	ARG	-	expression tag	UNP E0Y3X1
G	-2	GLY	-	expression tag	UNP E0Y3X1
G	-1	SER	-	expression tag	UNP E0Y3X1
G	0	HIS	-	expression tag	UNP E0Y3X1
H	-19	MET	-	initiating methionine	UNP E0Y3X1
H	-18	GLY	-	expression tag	UNP E0Y3X1
H	-17	SER	-	expression tag	UNP E0Y3X1
H	-16	SER	-	expression tag	UNP E0Y3X1
H	-15	HIS	-	expression tag	UNP E0Y3X1
H	-14	HIS	-	expression tag	UNP E0Y3X1
H	-13	HIS	-	expression tag	UNP E0Y3X1
H	-12	HIS	-	expression tag	UNP E0Y3X1
H	-11	HIS	-	expression tag	UNP E0Y3X1
H	-10	HIS	-	expression tag	UNP E0Y3X1
H	-9	SER	-	expression tag	UNP E0Y3X1
H	-8	SER	-	expression tag	UNP E0Y3X1
H	-7	GLY	-	expression tag	UNP E0Y3X1
H	-6	LEU	-	expression tag	UNP E0Y3X1
H	-5	VAL	-	expression tag	UNP E0Y3X1
H	-4	PRO	-	expression tag	UNP E0Y3X1
H	-3	ARG	-	expression tag	UNP E0Y3X1
H	-2	GLY	-	expression tag	UNP E0Y3X1
H	-1	SER	-	expression tag	UNP E0Y3X1
H	0	HIS	-	expression tag	UNP E0Y3X1
F	-19	MET	-	initiating methionine	UNP E0Y3X1
F	-18	GLY	-	expression tag	UNP E0Y3X1
F	-17	SER	-	expression tag	UNP E0Y3X1
F	-16	SER	-	expression tag	UNP E0Y3X1
F	-15	HIS	-	expression tag	UNP E0Y3X1
F	-14	HIS	-	expression tag	UNP E0Y3X1
F	-13	HIS	-	expression tag	UNP E0Y3X1
F	-12	HIS	-	expression tag	UNP E0Y3X1
F	-11	HIS	-	expression tag	UNP E0Y3X1
F	-10	HIS	-	expression tag	UNP E0Y3X1
F	-9	SER	-	expression tag	UNP E0Y3X1
F	-8	SER	-	expression tag	UNP E0Y3X1
F	-7	GLY	-	expression tag	UNP E0Y3X1
F	-6	LEU	-	expression tag	UNP E0Y3X1
F	-5	VAL	-	expression tag	UNP E0Y3X1
F	-4	PRO	-	expression tag	UNP E0Y3X1
F	-3	ARG	-	expression tag	UNP E0Y3X1

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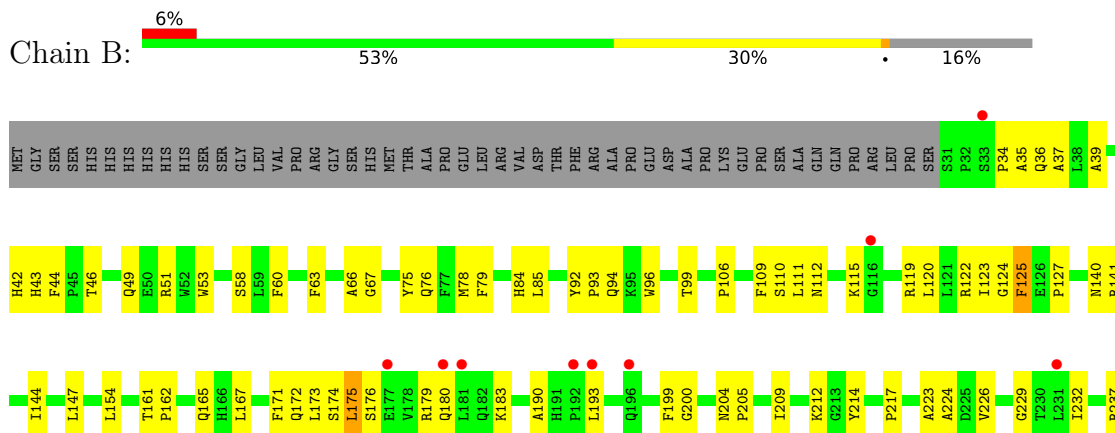
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F	-1	SER	-	expression tag	UNP E0Y3X1
F	0	HIS	-	expression tag	UNP E0Y3X1
D	-19	MET	-	initiating methionine	UNP E0Y3X1
D	-18	GLY	-	expression tag	UNP E0Y3X1
D	-17	SER	-	expression tag	UNP E0Y3X1
D	-16	SER	-	expression tag	UNP E0Y3X1
D	-15	HIS	-	expression tag	UNP E0Y3X1
D	-14	HIS	-	expression tag	UNP E0Y3X1
D	-13	HIS	-	expression tag	UNP E0Y3X1
D	-12	HIS	-	expression tag	UNP E0Y3X1
D	-11	HIS	-	expression tag	UNP E0Y3X1
D	-10	HIS	-	expression tag	UNP E0Y3X1
D	-9	SER	-	expression tag	UNP E0Y3X1
D	-8	SER	-	expression tag	UNP E0Y3X1
D	-7	GLY	-	expression tag	UNP E0Y3X1
D	-6	LEU	-	expression tag	UNP E0Y3X1
D	-5	VAL	-	expression tag	UNP E0Y3X1
D	-4	PRO	-	expression tag	UNP E0Y3X1
D	-3	ARG	-	expression tag	UNP E0Y3X1
D	-2	GLY	-	expression tag	UNP E0Y3X1
D	-1	SER	-	expression tag	UNP E0Y3X1
D	0	HIS	-	expression tag	UNP E0Y3X1
E	-19	MET	-	initiating methionine	UNP E0Y3X1
E	-18	GLY	-	expression tag	UNP E0Y3X1
E	-17	SER	-	expression tag	UNP E0Y3X1
E	-16	SER	-	expression tag	UNP E0Y3X1
E	-15	HIS	-	expression tag	UNP E0Y3X1
E	-14	HIS	-	expression tag	UNP E0Y3X1
E	-13	HIS	-	expression tag	UNP E0Y3X1
E	-12	HIS	-	expression tag	UNP E0Y3X1
E	-11	HIS	-	expression tag	UNP E0Y3X1
E	-10	HIS	-	expression tag	UNP E0Y3X1
E	-9	SER	-	expression tag	UNP E0Y3X1
E	-8	SER	-	expression tag	UNP E0Y3X1
E	-7	GLY	-	expression tag	UNP E0Y3X1
E	-6	LEU	-	expression tag	UNP E0Y3X1
E	-5	VAL	-	expression tag	UNP E0Y3X1
E	-4	PRO	-	expression tag	UNP E0Y3X1
E	-3	ARG	-	expression tag	UNP E0Y3X1
E	-2	GLY	-	expression tag	UNP E0Y3X1
E	-1	SER	-	expression tag	UNP E0Y3X1

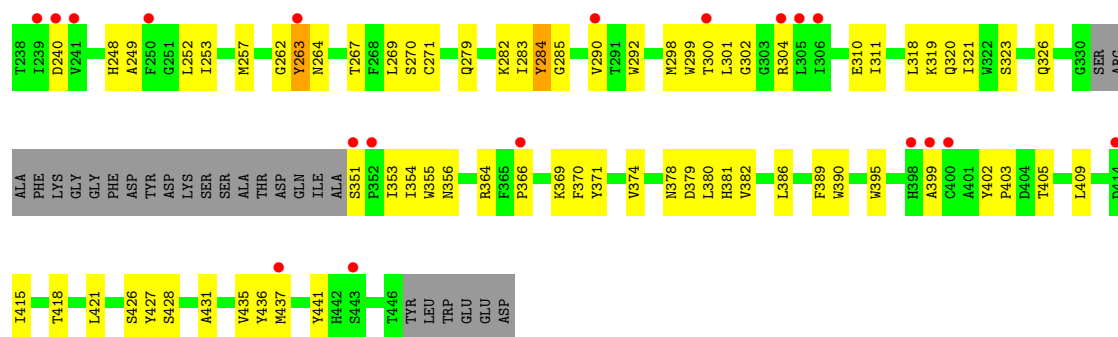
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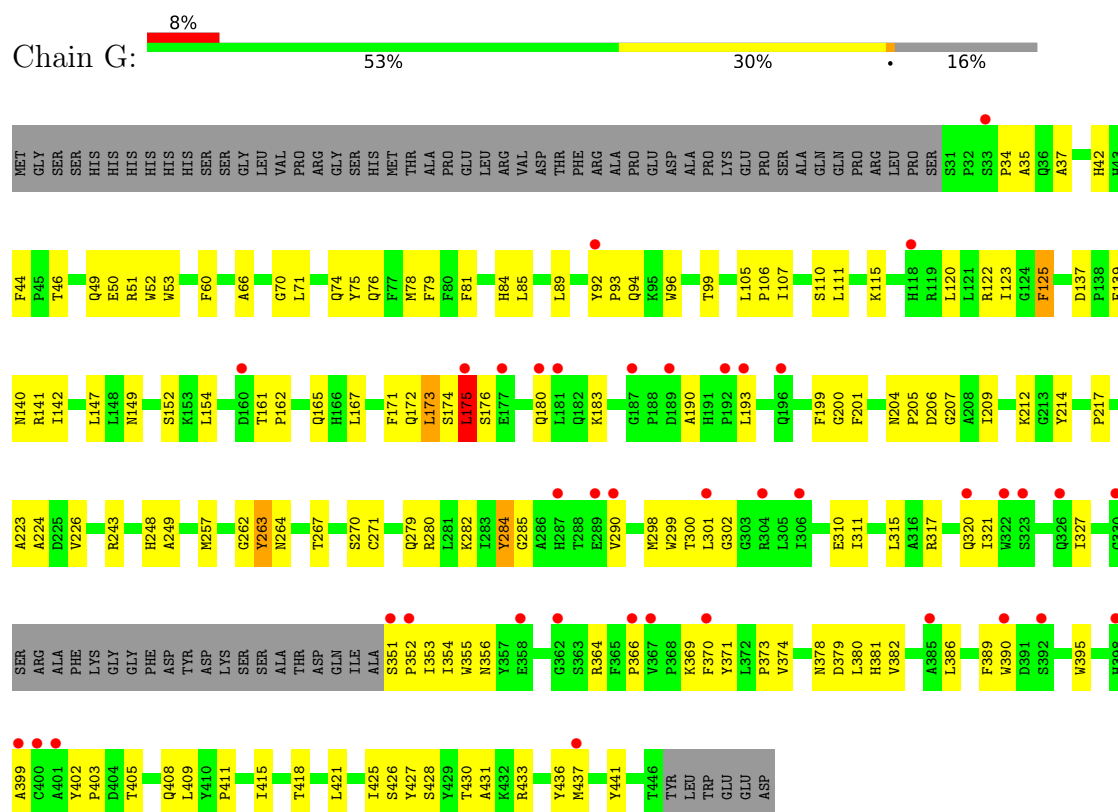
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP E0Y3X1
C	-19	MET	-	initiating methionine	UNP E0Y3X1
C	-18	GLY	-	expression tag	UNP E0Y3X1
C	-17	SER	-	expression tag	UNP E0Y3X1
C	-16	SER	-	expression tag	UNP E0Y3X1
C	-15	HIS	-	expression tag	UNP E0Y3X1
C	-14	HIS	-	expression tag	UNP E0Y3X1
C	-13	HIS	-	expression tag	UNP E0Y3X1
C	-12	HIS	-	expression tag	UNP E0Y3X1
C	-11	HIS	-	expression tag	UNP E0Y3X1
C	-10	HIS	-	expression tag	UNP E0Y3X1
C	-9	SER	-	expression tag	UNP E0Y3X1
C	-8	SER	-	expression tag	UNP E0Y3X1
C	-7	GLY	-	expression tag	UNP E0Y3X1
C	-6	LEU	-	expression tag	UNP E0Y3X1
C	-5	VAL	-	expression tag	UNP E0Y3X1
C	-4	PRO	-	expression tag	UNP E0Y3X1
C	-3	ARG	-	expression tag	UNP E0Y3X1
C	-2	GLY	-	expression tag	UNP E0Y3X1
C	-1	SER	-	expression tag	UNP E0Y3X1
C	0	HIS	-	expression tag	UNP E0Y3X1

- Molecule 1: Deoxybrevianamide E synthase notF

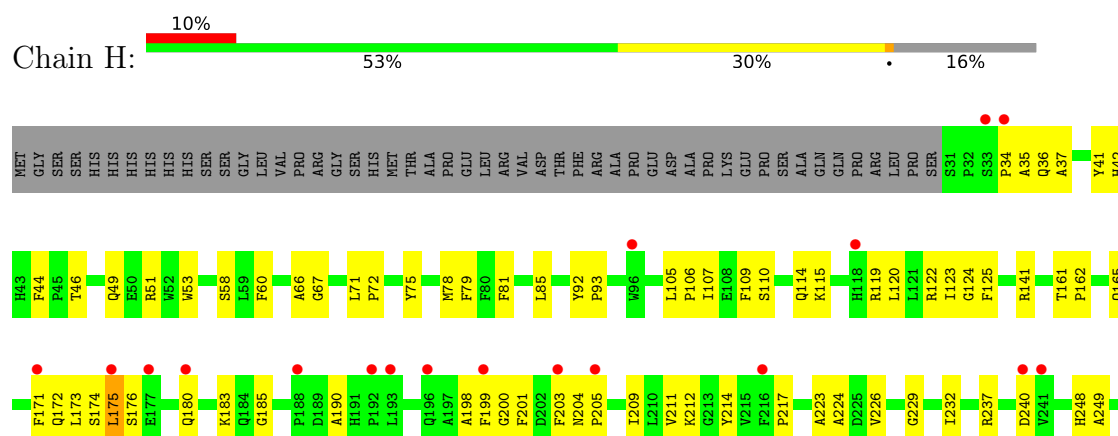


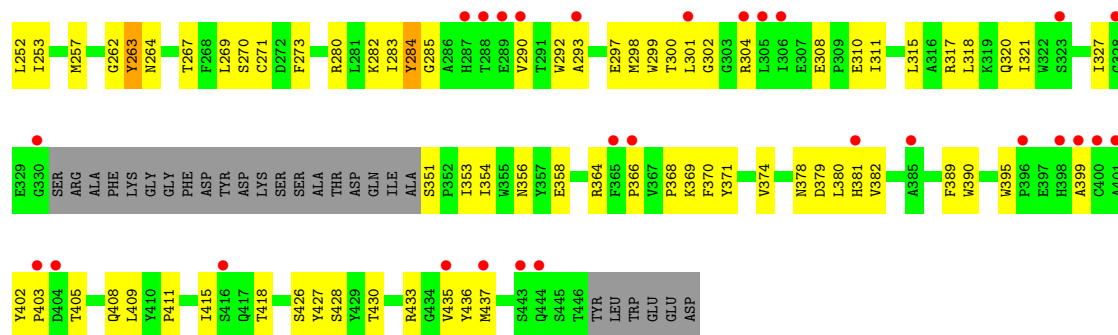


• Molecule 1: Deoxybrevianamide E synthase notF

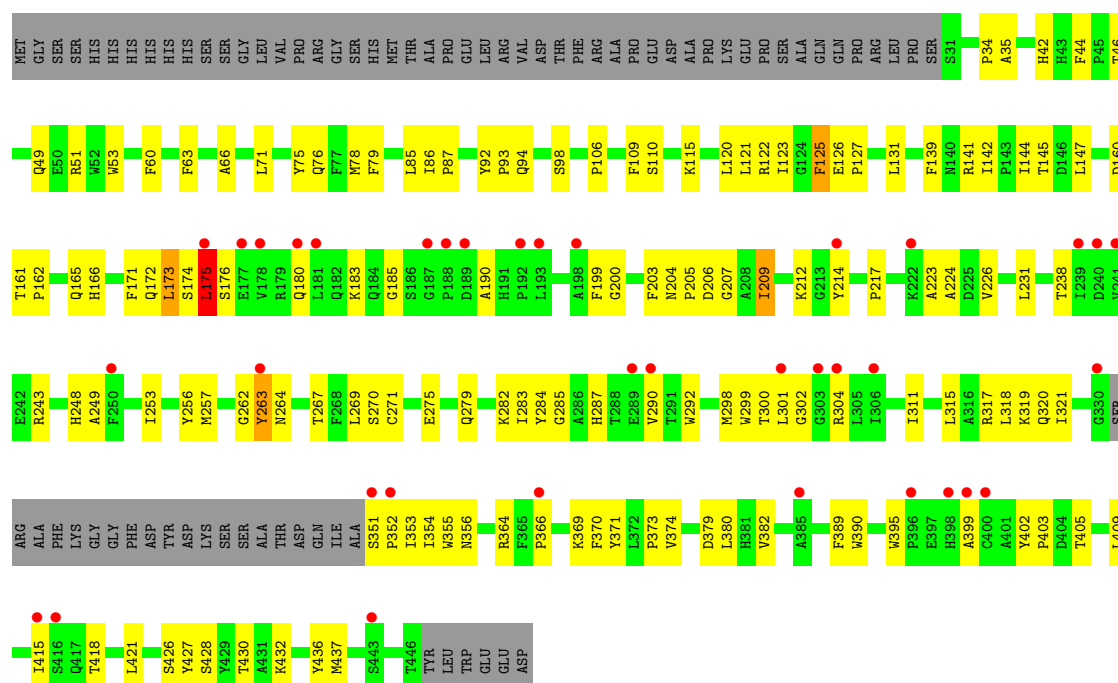


• Molecule 1: Deoxybrevianamide E synthase notF

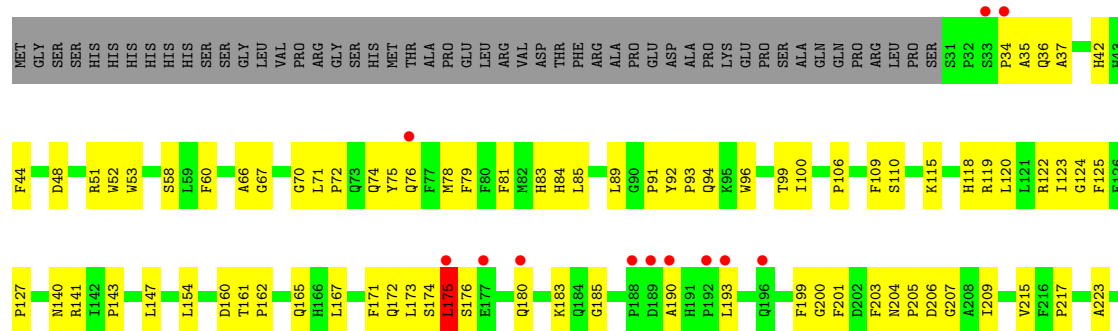


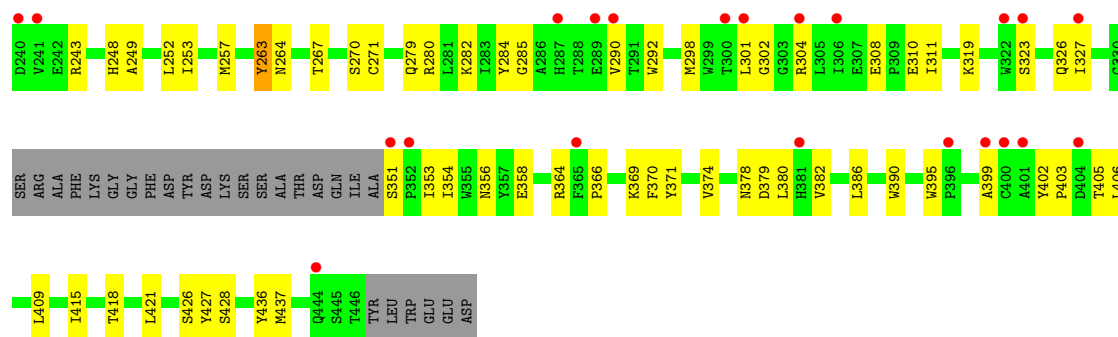


• Molecule 1: Deoxybrevianamide E synthase notF

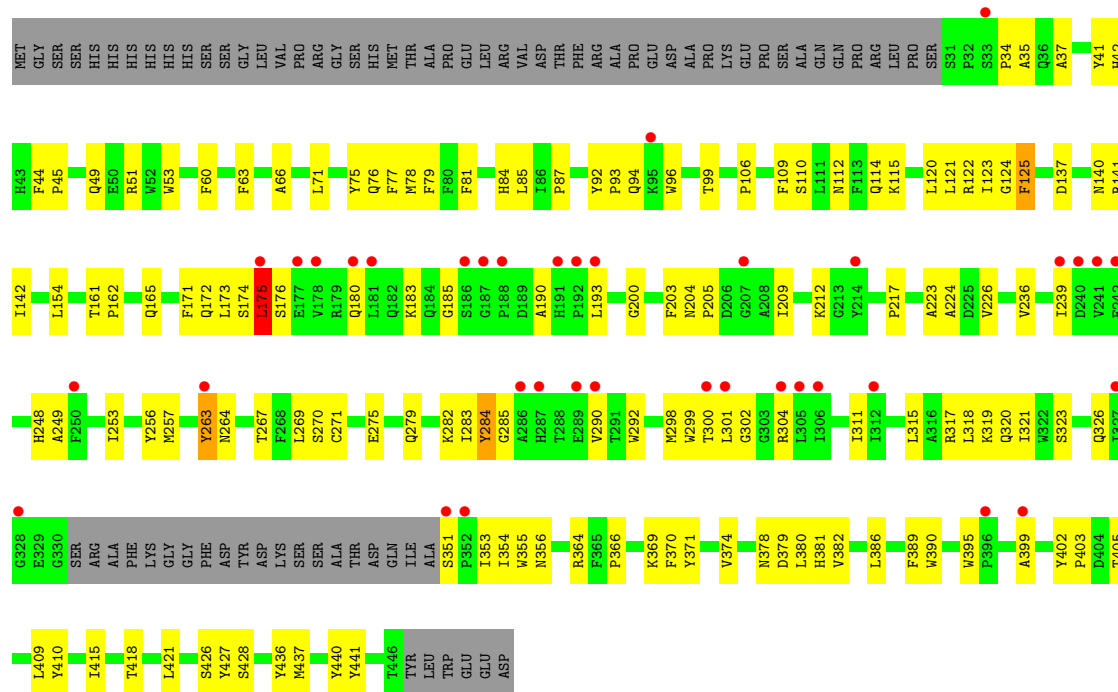


• Molecule 1: Deoxybrevianamide E synthase notF

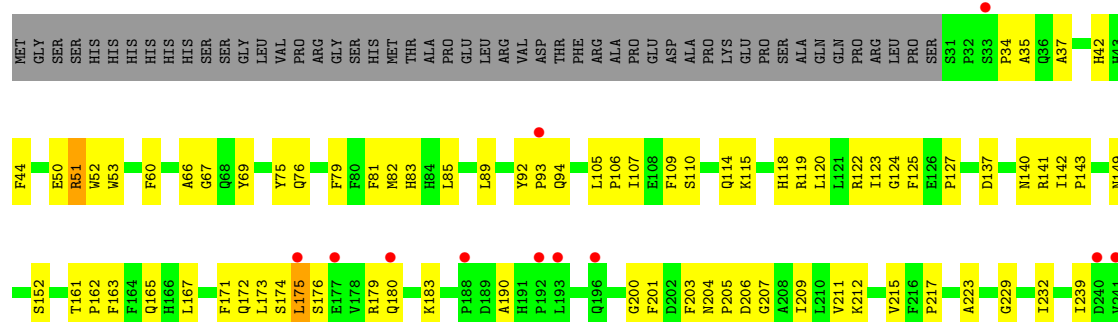


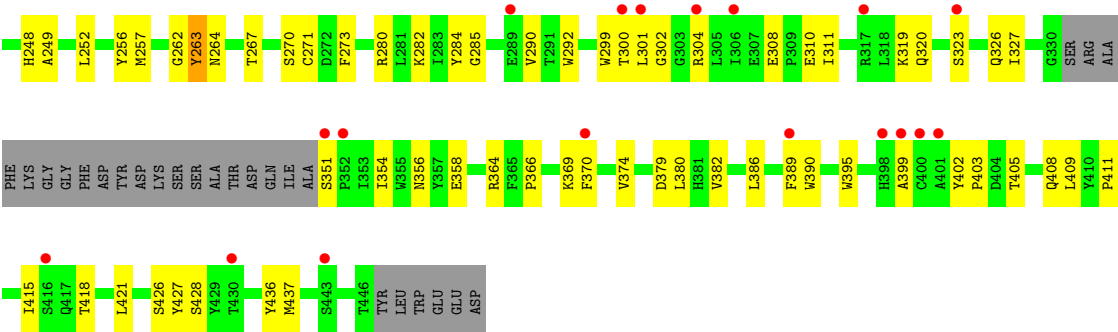


• Molecule 1: Deoxybrevianamide E synthase notF



• Molecule 1: Deoxybrevianamide E synthase notF





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.59Å 208.29Å 217.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.19 49.32 – 3.19	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.32-3.19) 92.7 (49.32-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.307 , 0.316 0.306 , 0.314	Depositor DCC
R_{free} test set	1902 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25720	wwPDB-VP
Average B, all atoms (Å ²)	102.0	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 35.84 % 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 5.4788e-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	0.38	0/3319	0.64	0/4514
1	B	0.38	0/3319	0.66	0/4514
1	C	0.43	1/3319 (0.0%)	0.69	2/4514 (0.0%)
1	D	0.37	0/3319	0.64	0/4514
1	E	0.37	0/3319	0.64	0/4514
1	F	0.39	0/3319	0.66	0/4514
1	G	0.39	0/3319	0.67	0/4514
1	H	0.38	0/3319	0.65	0/4514
All	All	0.39	1/26552 (0.0%)	0.66	2/36112 (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	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	ARG	CA-CB	-7.87	1.40	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	ARG	CB-CG-CD	11.25	137.18	111.30
1	C	51	ARG	NE-CZ-NH1	6.11	127.61	121.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	175	LEU	Peptide
1	E	175	LEU	Peptide
1	F	175	LEU	Peptide
1	G	175	LEU	Peptide
1	H	175	LEU	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	3215	0	3093	131	0
1	B	3215	0	3093	134	0
1	C	3215	0	3093	124	0
1	D	3215	0	3093	126	0
1	E	3215	0	3093	128	0
1	F	3215	0	3093	120	0
1	G	3215	0	3093	128	0
1	H	3215	0	3093	120	0
All	All	25720	0	24744	930	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (930) 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:A:162:PRO:HG2	1:G:174:SER:HB3	1.35	1.08
1:G:290:VAL:HG21	1:G:351:SER:HB2	1.45	0.98
1:H:290:VAL:HG21	1:H:351:SER:HB2	1.48	0.95
1:F:165:GLN:HG3	1:C:172:GLN:HE22	1.31	0.94
1:B:174:SER:HB3	1:H:162:PRO:HG2	1.48	0.94
1:B:290:VAL:HG21	1:B:351:SER:HB2	1.47	0.94
1:D:290:VAL:HG21	1:D:351:SER:HB2	1.51	0.93
1:A:172:GLN:HE22	1:G:165:GLN:HG3	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:SER:HB3	1:E:162:PRO:HG2	1.52	0.92
1:F:162:PRO:HG2	1:C:174:SER:HB3	1.51	0.91
1:E:290:VAL:HG21	1:E:351:SER:HB2	1.52	0.88
1:C:290:VAL:HG21	1:C:351:SER:HB2	1.56	0.88
1:E:110:SER:HB2	1:E:122:ARG:HB2	1.55	0.87
1:F:174:SER:HB3	1:C:162:PRO:HG2	1.57	0.87
1:C:301:LEU:HD12	1:C:302:GLY:H	1.41	0.85
1:B:110:SER:HB2	1:B:122:ARG:HB2	1.58	0.85
1:H:75:TYR:HD2	1:F:75:TYR:HD2	1.21	0.85
1:B:180:GLN:HE21	1:B:223:ALA:HB2	1.42	0.85
1:F:172:GLN:HE22	1:C:165:GLN:HG3	1.41	0.85
1:F:290:VAL:HG21	1:F:351:SER:HB2	1.57	0.84
1:B:270:SER:HB3	1:B:282:LYS:HB2	1.59	0.84
1:A:174:SER:HB3	1:G:162:PRO:HG2	1.58	0.84
1:B:162:PRO:HG2	1:H:174:SER:HB3	1.58	0.84
1:H:35:ALA:HA	1:H:75:TYR:HE1	1.43	0.84
1:E:44:PHE:HE2	1:E:53:TRP:HB2	1.42	0.84
1:B:165:GLN:HG3	1:H:172:GLN:HE22	1.42	0.84
1:G:44:PHE:HE2	1:G:53:TRP:HB2	1.43	0.83
1:B:75:TYR:HD2	1:C:75:TYR:HD2	1.24	0.83
1:D:374:VAL:HG13	1:D:382:VAL:HG21	1.58	0.83
1:A:290:VAL:HG21	1:A:351:SER:HB2	1.58	0.83
1:D:301:LEU:HD12	1:D:302:GLY:H	1.43	0.83
1:H:374:VAL:HG13	1:H:382:VAL:HG21	1.60	0.82
1:B:257:MET:HE2	1:B:263:TYR:HB3	1.62	0.82
1:H:110:SER:HB2	1:H:122:ARG:HB2	1.62	0.82
1:A:75:TYR:HD2	1:E:75:TYR:HD2	1.26	0.81
1:D:172:GLN:HE22	1:E:165:GLN:HG3	1.42	0.81
1:F:282:LYS:HD3	1:F:356:ASN:HD21	1.45	0.81
1:E:257:MET:HE2	1:E:263:TYR:HB3	1.61	0.81
1:A:110:SER:HB2	1:A:122:ARG:HB2	1.63	0.81
1:F:428:SER:HB3	1:F:436:TYR:HB2	1.63	0.80
1:D:257:MET:HE2	1:D:263:TYR:HB3	1.63	0.80
1:F:257:MET:HE2	1:F:263:TYR:HB3	1.63	0.80
1:G:428:SER:HB3	1:G:436:TYR:HB2	1.64	0.80
1:B:374:VAL:HG13	1:B:382:VAL:HG21	1.62	0.80
1:F:110:SER:HB2	1:F:122:ARG:HB2	1.63	0.80
1:F:263:TYR:HD1	1:F:263:TYR:H	1.29	0.80
1:F:249:ALA:HB1	1:F:366:PRO:HG3	1.62	0.79
1:A:301:LEU:HD12	1:A:302:GLY:H	1.48	0.79
1:D:162:PRO:HG2	1:E:174:SER:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:TYR:HD1	1:D:263:TYR:H	1.27	0.79
1:G:257:MET:HE2	1:G:263:TYR:HB3	1.63	0.79
1:D:249:ALA:HB1	1:D:366:PRO:HG3	1.65	0.79
1:D:165:GLN:HG3	1:E:172:GLN:HE22	1.47	0.78
1:E:249:ALA:HB1	1:E:366:PRO:HG3	1.65	0.78
1:H:301:LEU:HD12	1:H:302:GLY:H	1.48	0.78
1:F:44:PHE:HE2	1:F:53:TRP:HB2	1.49	0.78
1:A:44:PHE:HE2	1:A:53:TRP:HB2	1.48	0.77
1:G:110:SER:HB2	1:G:122:ARG:HB2	1.66	0.77
1:C:374:VAL:HG13	1:C:382:VAL:HG21	1.66	0.77
1:F:301:LEU:HD12	1:F:302:GLY:H	1.50	0.77
1:B:263:TYR:HD1	1:B:263:TYR:H	1.32	0.77
1:C:263:TYR:HD1	1:C:263:TYR:H	1.29	0.77
1:A:374:VAL:HG13	1:A:382:VAL:HG21	1.67	0.77
1:H:263:TYR:HD1	1:H:263:TYR:H	1.31	0.76
1:E:428:SER:HB3	1:E:436:TYR:HB2	1.68	0.76
1:E:263:TYR:H	1:E:263:TYR:HD1	1.33	0.76
1:G:374:VAL:HG13	1:G:382:VAL:HG21	1.66	0.76
1:G:249:ALA:HB1	1:G:366:PRO:HG3	1.67	0.76
1:A:75:TYR:CD2	1:E:75:TYR:HD2	2.04	0.75
1:E:301:LEU:HD12	1:E:302:GLY:H	1.52	0.75
1:C:270:SER:HB3	1:C:282:LYS:HB2	1.69	0.75
1:B:428:SER:HB3	1:B:436:TYR:HB2	1.68	0.75
1:G:180:GLN:HE21	1:G:223:ALA:HB2	1.52	0.75
1:E:271:CYS:SG	1:E:279:GLN:NE2	2.60	0.75
1:A:180:GLN:HE21	1:A:223:ALA:HB2	1.52	0.74
1:H:180:GLN:HE21	1:H:223:ALA:HB2	1.52	0.74
1:D:180:GLN:HE21	1:D:223:ALA:HB2	1.52	0.74
1:C:44:PHE:HE2	1:C:53:TRP:HB2	1.50	0.74
1:E:44:PHE:CE2	1:E:53:TRP:HB2	2.21	0.74
1:E:180:GLN:HE21	1:E:223:ALA:HB2	1.51	0.74
1:F:35:ALA:HA	1:F:75:TYR:HE1	1.52	0.74
1:C:249:ALA:HB1	1:C:366:PRO:HG3	1.69	0.74
1:B:44:PHE:HE2	1:B:53:TRP:HB2	1.52	0.73
1:B:301:LEU:HD12	1:B:302:GLY:H	1.51	0.73
1:E:35:ALA:HA	1:E:75:TYR:HE1	1.52	0.73
1:B:298:MET:HE1	1:B:353:ILE:HD11	1.71	0.73
1:D:35:ALA:HA	1:D:75:TYR:HE1	1.52	0.73
1:A:263:TYR:HD1	1:A:263:TYR:H	1.34	0.73
1:E:282:LYS:HD3	1:E:356:ASN:HD21	1.53	0.73
1:B:75:TYR:CD2	1:C:75:TYR:HD2	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:SER:HB3	1:A:436:TYR:HB2	1.72	0.72
1:C:35:ALA:HA	1:C:75:TYR:HE1	1.53	0.72
1:D:110:SER:HB2	1:D:122:ARG:HB2	1.72	0.72
1:G:75:TYR:HD2	1:D:75:TYR:HD2	1.37	0.72
1:G:263:TYR:HD1	1:G:263:TYR:H	1.36	0.72
1:B:249:ALA:HB1	1:B:366:PRO:HG3	1.71	0.72
1:G:75:TYR:CD2	1:D:75:TYR:HD2	2.08	0.71
1:D:60:PHE:HE1	1:D:123:ILE:HD11	1.53	0.71
1:H:229:GLY:HA2	1:H:232:ILE:HD12	1.73	0.71
1:D:428:SER:HB3	1:D:436:TYR:HB2	1.71	0.71
1:G:85:LEU:HD22	1:G:125:PHE:CE1	2.26	0.71
1:H:81:PHE:HD1	1:H:85:LEU:HD12	1.55	0.70
1:G:79:PHE:HE2	1:D:42:HIS:HB2	1.56	0.70
1:H:44:PHE:CE2	1:H:53:TRP:HB2	2.26	0.70
1:C:257:MET:HE2	1:C:263:TYR:HB3	1.73	0.70
1:F:374:VAL:HG13	1:F:382:VAL:HG21	1.72	0.70
1:G:301:LEU:HD12	1:G:302:GLY:H	1.55	0.70
1:D:60:PHE:CE1	1:D:123:ILE:HD11	2.27	0.70
1:F:141:ARG:CZ	1:F:172:GLN:HE21	2.05	0.69
1:H:75:TYR:HD2	1:F:75:TYR:CD2	2.07	0.69
1:G:35:ALA:HA	1:G:75:TYR:HE1	1.57	0.69
1:A:249:ALA:HB1	1:A:366:PRO:HG3	1.74	0.69
1:B:172:GLN:HE22	1:H:165:GLN:HG3	1.58	0.69
1:H:257:MET:HE2	1:H:263:TYR:HB3	1.74	0.69
1:D:380:LEU:HB2	1:D:415:ILE:HG22	1.75	0.69
1:E:374:VAL:HG13	1:E:382:VAL:HG21	1.75	0.69
1:G:75:TYR:HD2	1:D:75:TYR:CD2	2.10	0.68
1:H:249:ALA:HB1	1:H:366:PRO:HG3	1.74	0.68
1:G:183:LYS:NZ	1:G:190:ALA:O	2.25	0.68
1:C:248:HIS:CE1	1:C:364:ARG:HD2	2.29	0.68
1:A:44:PHE:CE2	1:A:53:TRP:HB2	2.28	0.68
1:C:282:LYS:HD3	1:C:356:ASN:HD21	1.59	0.68
1:C:110:SER:HB2	1:C:122:ARG:HB2	1.74	0.67
1:C:60:PHE:CE1	1:C:123:ILE:HD11	2.29	0.67
1:A:257:MET:HE2	1:A:263:TYR:HB3	1.75	0.67
1:F:44:PHE:CE2	1:F:53:TRP:HB2	2.28	0.67
1:F:183:LYS:NZ	1:F:190:ALA:O	2.27	0.67
1:D:183:LYS:NZ	1:D:190:ALA:O	2.27	0.67
1:H:379:ASP:HB2	1:H:418:THR:HG23	1.76	0.67
1:G:37:ALA:HB1	1:D:76:GLN:HE21	1.60	0.67
1:G:44:PHE:CE2	1:G:53:TRP:HB2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:MET:HE1	1:F:353:ILE:HD11	1.75	0.66
1:G:271:CYS:SG	1:G:279:GLN:NE2	2.67	0.66
1:C:206:ASP:OD1	1:C:207:GLY:N	2.27	0.66
1:E:85:LEU:HD22	1:E:125:PHE:CE1	2.30	0.66
1:B:35:ALA:HA	1:B:75:TYR:HE1	1.59	0.66
1:B:264:ASN:O	1:B:267:THR:HG22	1.95	0.66
1:H:141:ARG:CZ	1:H:172:GLN:HE21	2.08	0.66
1:F:270:SER:HB3	1:F:282:LYS:HB2	1.78	0.66
1:G:76:GLN:HE21	1:D:37:ALA:HB1	1.60	0.66
1:E:379:ASP:HB2	1:E:418:THR:HG23	1.76	0.66
1:A:85:LEU:HD22	1:A:125:PHE:CE1	2.30	0.66
1:H:85:LEU:HD22	1:H:125:PHE:CE1	2.31	0.65
1:A:66:ALA:HB2	1:A:409:LEU:HD11	1.78	0.65
1:A:248:HIS:CE1	1:A:364:ARG:HD2	2.32	0.65
1:C:85:LEU:HD22	1:C:125:PHE:CE1	2.32	0.65
1:H:75:TYR:CD2	1:F:75:TYR:HD2	2.08	0.65
1:A:35:ALA:HA	1:A:75:TYR:CE1	2.32	0.64
1:E:120:LEU:HD21	1:E:205:PRO:HD3	1.78	0.64
1:C:141:ARG:CZ	1:C:172:GLN:HE21	2.10	0.64
1:A:35:ALA:HA	1:A:75:TYR:HE1	1.62	0.64
1:B:66:ALA:HB2	1:B:409:LEU:HD11	1.79	0.64
1:B:183:LYS:NZ	1:B:190:ALA:O	2.29	0.64
1:G:264:ASN:O	1:G:267:THR:HG22	1.98	0.64
1:C:69:TYR:OH	1:C:203:PHE:O	2.13	0.64
1:D:35:ALA:HA	1:D:75:TYR:CE1	2.32	0.64
1:A:75:TYR:HD2	1:E:75:TYR:CD2	2.13	0.64
1:B:75:TYR:HD2	1:C:75:TYR:CD2	2.11	0.64
1:F:98:SER:OG	1:F:126:GLU:OE1	2.14	0.64
1:D:123:ILE:O	1:D:201:PHE:N	2.23	0.64
1:E:141:ARG:CZ	1:E:172:GLN:HE21	2.11	0.64
1:A:53:TRP:CH2	1:A:78:MET:HE2	2.34	0.63
1:B:79:PHE:HE2	1:C:42:HIS:HB2	1.62	0.63
1:E:115:LYS:HG2	1:E:395:TRP:HE1	1.62	0.63
1:F:35:ALA:HA	1:F:75:TYR:CE1	2.32	0.63
1:H:35:ALA:HA	1:H:75:TYR:CE1	2.30	0.63
1:H:44:PHE:HE2	1:H:53:TRP:HB2	1.62	0.63
1:F:180:GLN:HE21	1:F:223:ALA:HB2	1.63	0.63
1:H:115:LYS:HG2	1:H:395:TRP:HE1	1.64	0.63
1:C:44:PHE:CE2	1:C:53:TRP:HB2	2.33	0.63
1:C:183:LYS:NZ	1:C:190:ALA:O	2.32	0.63
1:A:60:PHE:CE1	1:A:123:ILE:HD11	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:354:ILE:HB	1:H:371:TYR:HB2	1.80	0.63
1:D:390:TRP:HB2	1:D:399:ALA:HB2	1.81	0.63
1:E:390:TRP:HB2	1:E:399:ALA:HB2	1.80	0.63
1:C:180:GLN:HE21	1:C:223:ALA:HB2	1.64	0.63
1:H:428:SER:HB3	1:H:436:TYR:HB2	1.80	0.62
1:G:79:PHE:CE2	1:D:42:HIS:HB2	2.33	0.62
1:F:418:THR:HG21	1:F:421:LEU:HD12	1.82	0.62
1:D:124:GLY:HA2	1:D:200:GLY:HA2	1.80	0.62
1:H:66:ALA:HB2	1:H:409:LEU:HD11	1.80	0.62
1:D:354:ILE:HB	1:D:371:TYR:HB2	1.82	0.62
1:H:380:LEU:HB2	1:H:415:ILE:HG22	1.81	0.62
1:E:35:ALA:HA	1:E:75:TYR:CE1	2.34	0.62
1:G:270:SER:HB3	1:G:282:LYS:HB2	1.82	0.61
1:D:282:LYS:HD3	1:D:356:ASN:HD21	1.64	0.61
1:E:183:LYS:NZ	1:E:190:ALA:O	2.33	0.61
1:G:171:PHE:HE1	1:G:217:PRO:HB3	1.65	0.61
1:F:390:TRP:HB2	1:F:399:ALA:HB2	1.81	0.61
1:G:35:ALA:HA	1:G:75:TYR:CE1	2.35	0.61
1:B:76:GLN:HE21	1:C:37:ALA:HB1	1.65	0.61
1:D:44:PHE:HE2	1:D:53:TRP:HB2	1.65	0.61
1:D:405:THR:O	1:D:409:LEU:HD13	2.00	0.61
1:A:123:ILE:O	1:A:201:PHE:N	2.29	0.61
1:B:380:LEU:HB2	1:B:415:ILE:HG22	1.83	0.60
1:A:60:PHE:HE1	1:A:123:ILE:HD11	1.67	0.60
1:B:115:LYS:HG2	1:B:395:TRP:HE1	1.65	0.60
1:E:53:TRP:CH2	1:E:78:MET:HE2	2.36	0.60
1:B:415:ILE:HA	1:B:418:THR:HG22	1.84	0.60
1:E:390:TRP:HB3	1:E:395:TRP:HB2	1.84	0.60
1:C:81:PHE:HD1	1:C:85:LEU:HD12	1.67	0.60
1:H:298:MET:HE1	1:H:353:ILE:HD11	1.83	0.60
1:D:85:LEU:HD22	1:D:125:PHE:CE1	2.37	0.60
1:F:66:ALA:HB2	1:F:409:LEU:HD11	1.84	0.60
1:E:270:SER:HB3	1:E:282:LYS:HB2	1.83	0.60
1:G:298:MET:HE1	1:G:353:ILE:HD11	1.84	0.59
1:A:37:ALA:HB1	1:E:76:GLN:HE21	1.66	0.59
1:F:85:LEU:HD22	1:F:125:PHE:CE1	2.38	0.59
1:B:35:ALA:HA	1:B:75:TYR:CE1	2.36	0.59
1:B:248:HIS:CE1	1:B:364:ARG:HD2	2.38	0.59
1:B:79:PHE:CE2	1:C:42:HIS:HB2	2.37	0.59
1:H:267:THR:HA	1:H:285:GLY:HA2	1.85	0.59
1:C:35:ALA:HA	1:C:75:TYR:CE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:GLN:HE22	1:H:436:TYR:HE1	1.50	0.59
1:A:174:SER:C	1:A:176:SER:H	2.11	0.59
1:F:318:LEU:HD12	1:F:427:TYR:CD2	2.38	0.59
1:D:248:HIS:CE1	1:D:364:ARG:HD2	2.38	0.59
1:C:428:SER:HB3	1:C:436:TYR:HB2	1.83	0.59
1:A:141:ARG:CZ	1:A:172:GLN:HE21	2.16	0.59
1:H:60:PHE:CE1	1:H:123:ILE:HD11	2.38	0.59
1:D:415:ILE:HA	1:D:418:THR:HG22	1.84	0.58
1:E:66:ALA:HB2	1:E:409:LEU:HD11	1.84	0.58
1:C:418:THR:HG21	1:C:421:LEU:HD12	1.85	0.58
1:B:379:ASP:HB2	1:B:418:THR:HG23	1.85	0.58
1:F:115:LYS:HG2	1:F:395:TRP:HE1	1.68	0.58
1:B:85:LEU:HD22	1:B:125:PHE:CE1	2.38	0.58
1:B:354:ILE:HB	1:B:371:TYR:HB2	1.83	0.58
1:G:290:VAL:HG11	1:G:351:SER:N	2.18	0.58
1:G:418:THR:HG21	1:G:421:LEU:HD12	1.86	0.58
1:H:415:ILE:HA	1:H:418:THR:HG22	1.86	0.58
1:C:51:ARG:HG3	1:C:51:ARG:O	2.02	0.58
1:C:174:SER:C	1:C:176:SER:H	2.11	0.58
1:E:42:HIS:HD1	1:E:44:PHE:HD1	1.51	0.58
1:A:165:GLN:HG3	1:G:172:GLN:HE22	1.69	0.58
1:B:42:HIS:HD1	1:B:44:PHE:HD1	1.51	0.58
1:H:42:HIS:HD1	1:H:44:PHE:HD1	1.52	0.58
1:F:415:ILE:HA	1:F:418:THR:HG22	1.85	0.58
1:D:67:GLY:HA2	1:D:119:ARG:HG3	1.86	0.58
1:E:248:HIS:CE1	1:E:364:ARG:HD2	2.38	0.58
1:D:418:THR:HG21	1:D:421:LEU:HD12	1.84	0.57
1:B:229:GLY:HA2	1:B:232:ILE:HD12	1.85	0.57
1:H:42:HIS:HB2	1:F:79:PHE:HE2	1.69	0.57
1:H:390:TRP:HB2	1:H:399:ALA:HB2	1.87	0.57
1:B:92:TYR:O	1:B:94:GLN:N	2.38	0.57
1:G:370:PHE:O	1:G:426:SER:HA	2.04	0.57
1:H:270:SER:HB3	1:H:282:LYS:HB2	1.85	0.57
1:C:390:TRP:HB2	1:C:399:ALA:HB2	1.86	0.57
1:A:81:PHE:HD1	1:A:85:LEU:HD12	1.69	0.57
1:F:200:GLY:N	1:F:212:LYS:O	2.37	0.57
1:E:298:MET:HE1	1:E:353:ILE:HD11	1.85	0.57
1:C:92:TYR:HB3	1:C:93:PRO:HD3	1.86	0.57
1:C:415:ILE:HA	1:C:418:THR:HG22	1.87	0.57
1:C:379:ASP:HB2	1:C:418:THR:HG23	1.86	0.57
1:B:147:LEU:HD23	1:B:199:PHE:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:430:THR:HB	1:H:433:ARG:HB2	1.87	0.56
1:B:174:SER:C	1:B:176:SER:H	2.13	0.56
1:H:183:LYS:NZ	1:H:190:ALA:O	2.33	0.56
1:D:66:ALA:HB2	1:D:409:LEU:HD11	1.85	0.56
1:B:147:LEU:HD23	1:B:199:PHE:HD2	1.69	0.56
1:B:290:VAL:HG11	1:B:351:SER:N	2.19	0.56
1:G:66:ALA:HB2	1:G:409:LEU:HD11	1.87	0.56
1:H:369:LYS:HA	1:H:427:TYR:O	2.05	0.56
1:F:380:LEU:HB2	1:F:415:ILE:HG22	1.86	0.56
1:E:354:ILE:HB	1:E:371:TYR:HB2	1.87	0.56
1:F:299:TRP:CD1	1:F:315:LEU:HD12	2.40	0.56
1:A:92:TYR:HB3	1:A:93:PRO:HD3	1.87	0.56
1:A:106:PRO:O	1:A:125:PHE:HB2	2.04	0.56
1:B:141:ARG:CZ	1:B:172:GLN:HE21	2.19	0.56
1:G:299:TRP:CD1	1:G:311:ILE:HG23	2.41	0.56
1:F:120:LEU:HD21	1:F:205:PRO:HD3	1.88	0.56
1:B:171:PHE:HE1	1:B:217:PRO:HB3	1.71	0.56
1:G:354:ILE:HB	1:G:371:TYR:HB2	1.87	0.56
1:G:42:HIS:HD1	1:G:44:PHE:HD1	1.53	0.56
1:F:390:TRP:HB3	1:F:395:TRP:HB2	1.88	0.56
1:E:415:ILE:HA	1:E:418:THR:HG22	1.87	0.56
1:B:390:TRP:HB2	1:B:399:ALA:HB2	1.88	0.55
1:G:380:LEU:HB2	1:G:415:ILE:HG22	1.88	0.55
1:F:121:LEU:HD23	1:F:203:PHE:HD2	1.71	0.55
1:A:183:LYS:NZ	1:A:190:ALA:O	2.36	0.55
1:A:379:ASP:HB2	1:A:418:THR:HG23	1.87	0.55
1:G:120:LEU:HD21	1:G:205:PRO:HD3	1.88	0.55
1:G:300:THR:O	1:G:301:LEU:HG	2.06	0.55
1:E:121:LEU:HD23	1:E:203:PHE:HD2	1.71	0.55
1:D:44:PHE:CE2	1:D:53:TRP:HB2	2.40	0.55
1:D:115:LYS:HG2	1:D:395:TRP:HE1	1.72	0.55
1:G:282:LYS:HD3	1:G:356:ASN:HD21	1.72	0.55
1:G:311:ILE:HD12	1:G:311:ILE:H	1.71	0.55
1:A:267:THR:HA	1:A:285:GLY:HA2	1.87	0.55
1:B:323:SER:O	1:B:326:GLN:NE2	2.39	0.55
1:D:402:TYR:HB3	1:D:403:PRO:HD3	1.88	0.55
1:H:248:HIS:CE1	1:H:364:ARG:HD2	2.42	0.55
1:C:51:ARG:HG2	1:C:92:TYR:CD2	2.41	0.55
1:A:173:LEU:HB2	1:A:176:SER:HB2	1.89	0.55
1:D:174:SER:C	1:D:176:SER:H	2.14	0.54
1:C:167:LEU:HB3	1:C:215:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:264:ASN:O	1:H:267:THR:HG22	2.08	0.54
1:D:81:PHE:HD1	1:D:85:LEU:HD12	1.72	0.54
1:C:171:PHE:HE1	1:C:217:PRO:HB3	1.71	0.54
1:E:249:ALA:HB1	1:E:366:PRO:CG	2.35	0.54
1:A:79:PHE:HE2	1:E:42:HIS:HB2	1.72	0.54
1:G:75:TYR:CD2	1:D:75:TYR:CD2	2.90	0.54
1:H:115:LYS:HG2	1:H:395:TRP:NE1	2.22	0.54
1:F:206:ASP:OD1	1:F:207:GLY:N	2.40	0.54
1:D:147:LEU:HD23	1:D:199:PHE:HD2	1.71	0.54
1:C:257:MET:HB3	1:C:263:TYR:CD1	2.42	0.54
1:A:51:ARG:HG3	1:A:92:TYR:CD2	2.42	0.54
1:A:124:GLY:HA2	1:A:200:GLY:HA2	1.88	0.54
1:H:92:TYR:HB3	1:H:93:PRO:HD3	1.89	0.54
1:A:270:SER:HB3	1:A:282:LYS:HB2	1.89	0.54
1:D:42:HIS:HD1	1:D:44:PHE:HE1	1.55	0.54
1:C:171:PHE:CE1	1:C:217:PRO:HB3	2.43	0.54
1:G:200:GLY:N	1:G:212:LYS:O	2.41	0.54
1:H:42:HIS:HB2	1:F:79:PHE:CE2	2.42	0.54
1:F:171:PHE:HE1	1:F:217:PRO:HB3	1.73	0.54
1:F:212:LYS:HG3	1:F:271:CYS:O	2.08	0.54
1:E:174:SER:C	1:E:176:SER:H	2.16	0.54
1:B:171:PHE:CE1	1:B:217:PRO:HB3	2.42	0.54
1:A:402:TYR:HB3	1:A:403:PRO:HD3	1.89	0.53
1:A:426:SER:O	1:A:437:MET:HG3	2.08	0.53
1:H:282:LYS:HD3	1:H:356:ASN:HD21	1.73	0.53
1:D:252:LEU:HD22	1:D:304:ARG:HH21	1.72	0.53
1:E:418:THR:HG21	1:E:421:LEU:HD12	1.89	0.53
1:C:120:LEU:HD21	1:C:205:PRO:HD3	1.90	0.53
1:A:253:ILE:HD11	1:A:304:ARG:HH22	1.73	0.53
1:A:282:LYS:HD3	1:A:356:ASN:HD21	1.73	0.53
1:B:405:THR:O	1:B:409:LEU:HD13	2.08	0.53
1:G:415:ILE:HA	1:G:418:THR:HG22	1.89	0.53
1:F:311:ILE:HD12	1:F:311:ILE:H	1.73	0.53
1:D:171:PHE:HE1	1:D:217:PRO:HB3	1.71	0.53
1:H:426:SER:O	1:H:437:MET:HG3	2.09	0.53
1:E:311:ILE:H	1:E:311:ILE:HD12	1.73	0.53
1:C:426:SER:O	1:C:437:MET:HG3	2.09	0.53
1:A:264:ASN:O	1:A:267:THR:HG22	2.09	0.53
1:F:42:HIS:HD1	1:F:44:PHE:HD1	1.51	0.53
1:C:66:ALA:HB2	1:C:409:LEU:HD11	1.90	0.53
1:A:370:PHE:O	1:A:426:SER:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TRP:HB2	1:A:399:ALA:HB2	1.90	0.53
1:C:109:PHE:CD1	1:C:123:ILE:HG12	2.44	0.53
1:B:299:TRP:CD1	1:B:311:ILE:HG23	2.44	0.53
1:G:141:ARG:CZ	1:G:172:GLN:HE21	2.22	0.53
1:H:106:PRO:O	1:H:125:PHE:HB2	2.08	0.53
1:H:290:VAL:HG11	1:H:351:SER:N	2.24	0.53
1:C:267:THR:HA	1:C:285:GLY:HA2	1.89	0.53
1:A:299:TRP:CD1	1:A:311:ILE:HG23	2.43	0.53
1:F:173:LEU:HB2	1:F:176:SER:HB2	1.89	0.53
1:F:354:ILE:HB	1:F:371:TYR:HB2	1.90	0.53
1:E:370:PHE:O	1:E:426:SER:HA	2.09	0.53
1:A:418:THR:HG21	1:A:421:LEU:HD12	1.91	0.53
1:A:79:PHE:CE2	1:E:42:HIS:HB2	2.44	0.53
1:H:180:GLN:O	1:H:183:LYS:HG2	2.09	0.53
1:G:115:LYS:HG2	1:G:395:TRP:HE1	1.74	0.53
1:G:430:THR:HB	1:G:433:ARG:HB2	1.91	0.53
1:H:224:ALA:O	1:H:226:VAL:HG23	2.08	0.53
1:F:275:GLU:OE1	1:C:175:LEU:HD23	2.09	0.53
1:D:171:PHE:CE1	1:D:217:PRO:HB3	2.44	0.53
1:B:37:ALA:HB1	1:C:76:GLN:HE21	1.75	0.52
1:G:92:TYR:HB3	1:G:93:PRO:HD3	1.91	0.52
1:E:253:ILE:HD11	1:E:304:ARG:HH22	1.73	0.52
1:C:256:TYR:CD1	1:C:301:LEU:HB2	2.44	0.52
1:B:92:TYR:HB3	1:B:93:PRO:HD3	1.91	0.52
1:H:37:ALA:HB1	1:F:76:GLN:HE21	1.73	0.52
1:C:248:HIS:HE1	1:C:364:ARG:HD2	1.75	0.52
1:B:300:THR:O	1:B:301:LEU:HG	2.08	0.52
1:G:42:HIS:CD2	1:D:79:PHE:HZ	2.27	0.52
1:D:379:ASP:HB2	1:D:418:THR:HG23	1.91	0.52
1:E:60:PHE:CE1	1:E:123:ILE:HD11	2.44	0.52
1:C:252:LEU:HD22	1:C:304:ARG:HH21	1.74	0.52
1:G:402:TYR:HB3	1:G:403:PRO:HD3	1.91	0.52
1:F:248:HIS:CE1	1:F:364:ARG:HD2	2.44	0.52
1:F:379:ASP:OD2	1:F:421:LEU:HB2	2.09	0.52
1:D:120:LEU:HD21	1:D:205:PRO:HD3	1.92	0.52
1:C:67:GLY:HA2	1:C:119:ARG:HG3	1.91	0.52
1:A:123:ILE:HD12	1:A:203:PHE:CZ	2.44	0.52
1:G:42:HIS:CD2	1:D:79:PHE:CZ	2.98	0.52
1:G:257:MET:O	1:G:262:GLY:HA2	2.09	0.52
1:F:162:PRO:HA	1:C:172:GLN:OE1	2.09	0.52
1:B:321:ILE:HG23	1:B:389:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:TYR:O	1:G:94:GLN:N	2.43	0.52
1:D:426:SER:O	1:D:437:MET:HG3	2.10	0.52
1:E:84:HIS:CE1	1:E:154:LEU:HD11	2.44	0.52
1:E:292:TRP:CE2	1:E:319:LYS:HD3	2.44	0.52
1:A:405:THR:O	1:A:409:LEU:HD13	2.09	0.52
1:D:180:GLN:O	1:D:183:LYS:HG2	2.09	0.52
1:E:200:GLY:N	1:E:212:LYS:O	2.42	0.52
1:A:53:TRP:HH2	1:A:78:MET:HE2	1.74	0.51
1:F:317:ARG:HH11	1:F:320:GLN:HE22	1.58	0.51
1:D:92:TYR:HB3	1:D:93:PRO:HD3	1.91	0.51
1:C:311:ILE:H	1:C:311:ILE:HD12	1.74	0.51
1:B:46:THR:OG1	1:B:49:GLN:HG3	2.11	0.51
1:F:405:THR:O	1:F:409:LEU:HD13	2.10	0.51
1:H:171:PHE:CE1	1:H:217:PRO:HB3	2.45	0.51
1:H:249:ALA:HB1	1:H:366:PRO:CG	2.40	0.51
1:F:165:GLN:HG3	1:C:172:GLN:NE2	2.14	0.51
1:F:176:SER:O	1:F:180:GLN:HG2	2.11	0.51
1:D:280:ARG:HD3	1:D:358:GLU:CD	2.36	0.51
1:D:386:LEU:HD13	1:D:390:TRP:NE1	2.26	0.51
1:B:94:GLN:OE1	1:B:106:PRO:HD3	2.11	0.51
1:G:96:TRP:NE1	1:G:140:ASN:HD22	2.09	0.51
1:H:402:TYR:HB3	1:H:403:PRO:HD3	1.92	0.51
1:F:171:PHE:CE1	1:F:217:PRO:HB3	2.45	0.51
1:F:370:PHE:O	1:F:426:SER:HA	2.10	0.51
1:D:96:TRP:NE1	1:D:140:ASN:HD22	2.09	0.51
1:D:206:ASP:OD1	1:D:207:GLY:N	2.42	0.51
1:H:171:PHE:HE1	1:H:217:PRO:HB3	1.75	0.51
1:F:92:TYR:O	1:F:94:GLN:N	2.44	0.51
1:D:204:ASN:HB2	1:D:205:PRO:HD2	1.91	0.51
1:B:311:ILE:HD12	1:B:311:ILE:H	1.76	0.51
1:G:390:TRP:HB2	1:G:399:ALA:HB2	1.92	0.51
1:H:71:LEU:HD23	1:F:71:LEU:HD23	1.93	0.51
1:H:405:THR:O	1:H:409:LEU:HD13	2.10	0.51
1:C:42:HIS:HD1	1:C:44:PHE:HE1	1.56	0.51
1:B:44:PHE:CE2	1:B:53:TRP:HB2	2.40	0.51
1:H:81:PHE:CD1	1:H:85:LEU:HD12	2.43	0.51
1:A:430:THR:HB	1:A:433:ARG:HB2	1.93	0.51
1:G:428:SER:HB3	1:G:436:TYR:CB	2.39	0.51
1:B:282:LYS:HD3	1:B:356:ASN:HD21	1.76	0.50
1:F:174:SER:C	1:F:176:SER:H	2.19	0.50
1:E:299:TRP:CD1	1:E:315:LEU:HD12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLN:O	1:B:183:LYS:HG2	2.10	0.50
1:H:317:ARG:HH11	1:H:320:GLN:HE22	1.59	0.50
1:F:53:TRP:CH2	1:F:78:MET:HE2	2.46	0.50
1:D:271:CYS:SG	1:D:279:GLN:NE2	2.84	0.50
1:C:212:LYS:HG3	1:C:271:CYS:O	2.11	0.50
1:A:180:GLN:O	1:A:183:LYS:HG2	2.11	0.50
1:G:42:HIS:HB2	1:D:79:PHE:CE2	2.46	0.50
1:H:253:ILE:HD11	1:H:304:ARG:HH22	1.76	0.50
1:E:410:TYR:OH	1:E:441:TYR:HB3	2.12	0.50
1:A:369:LYS:HA	1:A:427:TYR:O	2.12	0.50
1:A:380:LEU:HB2	1:A:415:ILE:HG22	1.91	0.50
1:B:115:LYS:HA	1:B:395:TRP:CE2	2.47	0.50
1:C:292:TRP:CE2	1:C:319:LYS:HD3	2.46	0.50
1:A:248:HIS:HE1	1:A:364:ARG:HD2	1.74	0.50
1:A:298:MET:HE1	1:A:353:ILE:HD11	1.92	0.50
1:F:379:ASP:HB2	1:F:418:THR:HG23	1.93	0.50
1:G:94:GLN:OE1	1:G:106:PRO:HD3	2.12	0.50
1:F:92:TYR:HB3	1:F:93:PRO:HD3	1.93	0.50
1:D:290:VAL:HG11	1:D:351:SER:N	2.26	0.50
1:B:257:MET:O	1:B:262:GLY:HA2	2.12	0.50
1:G:356:ASN:HB3	1:G:369:LYS:HB3	1.93	0.50
1:D:257:MET:HB3	1:D:263:TYR:CD1	2.46	0.50
1:E:402:TYR:HB3	1:E:403:PRO:HD3	1.94	0.50
1:C:60:PHE:HE1	1:C:123:ILE:HD11	1.76	0.50
1:B:180:GLN:NE2	1:B:223:ALA:HB2	2.21	0.50
1:G:369:LYS:HA	1:G:427:TYR:O	2.12	0.50
1:F:60:PHE:CE1	1:F:123:ILE:HD11	2.47	0.50
1:C:369:LYS:HA	1:C:427:TYR:O	2.12	0.50
1:B:290:VAL:CG2	1:B:351:SER:HB2	2.32	0.50
1:F:257:MET:HB3	1:F:263:TYR:CD1	2.45	0.50
1:C:402:TYR:HB3	1:C:403:PRO:HD3	1.93	0.50
1:G:320:GLN:HE21	1:G:389:PHE:HE1	1.59	0.49
1:B:426:SER:O	1:B:437:MET:HG3	2.12	0.49
1:H:174:SER:C	1:H:176:SER:H	2.20	0.49
1:H:311:ILE:H	1:H:311:ILE:HD12	1.77	0.49
1:B:378:ASN:HB3	1:B:381:HIS:HB3	1.94	0.49
1:G:204:ASN:HB2	1:G:205:PRO:HD2	1.93	0.49
1:G:174:SER:C	1:G:176:SER:H	2.20	0.49
1:D:270:SER:HB3	1:D:282:LYS:HB2	1.93	0.49
1:B:252:LEU:HD22	1:B:304:ARG:HH21	1.77	0.49
1:C:123:ILE:O	1:C:201:PHE:N	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ASN:HB3	1:E:120:LEU:HB2	1.94	0.49
1:B:162:PRO:HA	1:H:172:GLN:OE1	2.13	0.49
1:H:318:LEU:HD12	1:H:427:TYR:CD2	2.48	0.49
1:F:253:ILE:HD11	1:F:304:ARG:HH22	1.77	0.49
1:B:42:HIS:CD2	1:C:79:PHE:HZ	2.31	0.49
1:B:79:PHE:HE1	1:C:83:HIS:HE1	1.61	0.49
1:G:99:THR:HG23	1:G:193:LEU:HD22	1.94	0.49
1:F:51:ARG:HG3	1:F:92:TYR:CD2	2.47	0.49
1:F:63:PHE:HE2	1:F:109:PHE:HB2	1.78	0.49
1:E:290:VAL:CG2	1:E:351:SER:HB2	2.34	0.49
1:B:43:HIS:NE2	1:F:131:LEU:HD11	2.28	0.49
1:G:248:HIS:CE1	1:G:364:ARG:HD2	2.47	0.49
1:E:405:THR:O	1:E:409:LEU:HD13	2.13	0.49
1:B:51:ARG:HG3	1:B:92:TYR:CG	2.48	0.48
1:G:180:GLN:O	1:G:183:LYS:HG2	2.12	0.48
1:H:37:ALA:HB1	1:F:76:GLN:NE2	2.28	0.48
1:E:180:GLN:O	1:E:183:LYS:HG2	2.12	0.48
1:A:206:ASP:OD1	1:A:207:GLY:N	2.43	0.48
1:B:402:TYR:HB3	1:B:403:PRO:HD3	1.95	0.48
1:E:380:LEU:HB2	1:E:415:ILE:HG22	1.95	0.48
1:B:267:THR:HA	1:B:285:GLY:HA2	1.94	0.48
1:A:167:LEU:O	1:A:171:PHE:HD2	1.97	0.48
1:A:311:ILE:HD12	1:A:311:ILE:H	1.78	0.48
1:B:42:HIS:CD2	1:C:79:PHE:CZ	3.01	0.48
1:C:204:ASN:HB2	1:C:205:PRO:HD2	1.94	0.48
1:A:42:HIS:HD1	1:A:44:PHE:HD1	1.59	0.48
1:A:42:HIS:ND1	1:A:44:PHE:CE1	2.81	0.48
1:A:204:ASN:HB2	1:A:205:PRO:HD2	1.95	0.48
1:F:290:VAL:HG11	1:F:351:SER:N	2.28	0.48
1:D:249:ALA:HB1	1:D:366:PRO:CG	2.41	0.48
1:C:115:LYS:HG2	1:C:395:TRP:HE1	1.79	0.48
1:A:42:HIS:HB2	1:E:79:PHE:CE2	2.49	0.48
1:B:418:THR:HG21	1:B:421:LEU:HD12	1.96	0.48
1:H:46:THR:OG1	1:H:49:GLN:HG3	2.14	0.48
1:F:212:LYS:HE3	1:F:214:TYR:OH	2.14	0.48
1:D:161:THR:N	1:D:162:PRO:CD	2.77	0.48
1:A:105:LEU:CD1	1:A:107:ILE:HG22	2.44	0.48
1:B:53:TRP:CH2	1:B:78:MET:HE2	2.48	0.48
1:B:84:HIS:NE2	1:B:154:LEU:HD11	2.29	0.48
1:E:299:TRP:HB3	1:E:315:LEU:HD12	1.96	0.48
1:A:100:ILE:CD1	1:A:125:PHE:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:378:ASN:HB3	1:G:381:HIS:HB3	1.96	0.48
1:F:292:TRP:CE2	1:F:319:LYS:HD3	2.48	0.48
1:A:37:ALA:HB1	1:E:76:GLN:NE2	2.28	0.48
1:A:415:ILE:HA	1:A:418:THR:HG22	1.96	0.48
1:C:124:GLY:HA2	1:C:200:GLY:HA2	1.95	0.48
1:C:327:ILE:HG21	1:C:351:SER:OG	2.13	0.48
1:A:120:LEU:HD21	1:A:205:PRO:HD3	1.96	0.48
1:A:200:GLY:N	1:A:212:LYS:O	2.44	0.48
1:H:79:PHE:CE2	1:F:42:HIS:HB2	2.48	0.48
1:D:253:ILE:HD11	1:D:304:ARG:HH22	1.79	0.48
1:C:380:LEU:HB2	1:C:415:ILE:HG22	1.96	0.48
1:C:405:THR:O	1:C:409:LEU:HD13	2.14	0.48
1:G:379:ASP:HB2	1:G:418:THR:HG23	1.96	0.47
1:E:115:LYS:HG2	1:E:395:TRP:NE1	2.27	0.47
1:E:269:LEU:CD1	1:E:283:ILE:HG13	2.44	0.47
1:E:300:THR:O	1:E:301:LEU:HG	2.14	0.47
1:E:317:ARG:HB2	1:E:427:TYR:OH	2.14	0.47
1:A:75:TYR:CD2	1:E:75:TYR:CD2	2.94	0.47
1:A:229:GLY:HA2	1:A:232:ILE:HD12	1.96	0.47
1:C:161:THR:N	1:C:162:PRO:CD	2.77	0.47
1:A:408:GLN:O	1:A:411:PRO:HD3	2.14	0.47
1:G:426:SER:O	1:G:437:MET:HG3	2.14	0.47
1:H:36:GLN:OE1	1:H:58:SER:HA	2.14	0.47
1:H:53:TRP:CH2	1:H:78:MET:HE2	2.50	0.47
1:D:162:PRO:HA	1:E:172:GLN:OE1	2.14	0.47
1:H:204:ASN:HB2	1:H:205:PRO:HD2	1.95	0.47
1:H:269:LEU:CD1	1:H:283:ILE:HG13	2.45	0.47
1:H:282:LYS:CB	1:H:284:TYR:HE1	2.27	0.47
1:F:94:GLN:OE1	1:F:106:PRO:HD3	2.14	0.47
1:F:271:CYS:SG	1:F:279:GLN:NE2	2.87	0.47
1:E:94:GLN:OE1	1:E:106:PRO:HD3	2.13	0.47
1:B:67:GLY:HA2	1:B:119:ARG:HG3	1.97	0.47
1:B:271:CYS:SG	1:B:279:GLN:NE2	2.88	0.47
1:G:115:LYS:HG2	1:G:395:TRP:NE1	2.30	0.47
1:E:63:PHE:HE2	1:E:109:PHE:HB2	1.80	0.47
1:E:171:PHE:CE1	1:E:217:PRO:HB3	2.49	0.47
1:H:60:PHE:HE1	1:H:123:ILE:HD11	1.78	0.47
1:H:105:LEU:CD1	1:H:107:ILE:HG22	2.45	0.47
1:H:124:GLY:HA2	1:H:200:GLY:HA2	1.97	0.47
1:F:402:TYR:HB3	1:F:403:PRO:HD3	1.96	0.47
1:D:92:TYR:O	1:D:94:GLN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:TRP:CE2	1:D:319:LYS:HD3	2.50	0.47
1:E:321:ILE:HG23	1:E:389:PHE:CD1	2.49	0.47
1:C:180:GLN:O	1:C:183:LYS:HG2	2.15	0.47
1:C:229:GLY:HA2	1:C:232:ILE:HD12	1.96	0.47
1:A:42:HIS:ND1	1:A:44:PHE:CD1	2.81	0.47
1:B:39:ALA:HB2	1:B:53:TRP:CZ2	2.49	0.47
1:B:96:TRP:NE1	1:B:140:ASN:HD22	2.12	0.47
1:B:112:ASN:HB3	1:B:120:LEU:HB2	1.97	0.47
1:A:115:LYS:HG2	1:A:395:TRP:HE1	1.80	0.47
1:B:204:ASN:HB2	1:B:205:PRO:HD2	1.96	0.47
1:F:180:GLN:O	1:F:183:LYS:HG2	2.15	0.47
1:B:369:LYS:HA	1:B:427:TYR:O	2.15	0.47
1:G:290:VAL:CG2	1:G:351:SER:HB2	2.31	0.47
1:C:137:ASP:CG	1:C:142:ILE:HG12	2.40	0.47
1:F:127:PRO:HD2	1:F:144:ILE:HD13	1.97	0.46
1:C:52:TRP:CE2	1:C:89:LEU:HB3	2.50	0.46
1:A:42:HIS:CD2	1:E:79:PHE:HZ	2.33	0.46
1:B:60:PHE:HD1	1:B:109:PHE:CE1	2.33	0.46
1:E:318:LEU:HD12	1:E:427:TYR:CD2	2.50	0.46
1:G:70:GLY:O	1:G:74:GLN:HG3	2.14	0.46
1:C:211:VAL:HG12	1:C:273:PHE:CD2	2.50	0.46
1:A:212:LYS:HG3	1:A:271:CYS:O	2.15	0.46
1:G:171:PHE:CE1	1:G:217:PRO:HB3	2.47	0.46
1:G:257:MET:HB3	1:G:263:TYR:CD1	2.50	0.46
1:H:284:TYR:CD1	1:H:284:TYR:N	2.84	0.46
1:C:300:THR:O	1:C:301:LEU:HG	2.15	0.46
1:A:176:SER:O	1:A:180:GLN:HG2	2.16	0.46
1:A:280:ARG:HH11	1:A:358:GLU:CD	2.23	0.46
1:G:249:ALA:HB1	1:G:366:PRO:CG	2.40	0.46
1:F:264:ASN:O	1:F:267:THR:HG22	2.15	0.46
1:F:290:VAL:CG2	1:F:351:SER:HB2	2.36	0.46
1:D:147:LEU:HD23	1:D:199:PHE:CD2	2.50	0.46
1:E:264:ASN:O	1:E:267:THR:HG22	2.15	0.46
1:H:293:ALA:O	1:H:297:GLU:HG3	2.16	0.46
1:F:249:ALA:HB1	1:F:366:PRO:CG	2.38	0.46
1:D:428:SER:HB3	1:D:436:TYR:CB	2.42	0.46
1:E:356:ASN:HB3	1:E:369:LYS:HB3	1.96	0.46
1:H:300:THR:O	1:H:301:LEU:HG	2.15	0.46
1:E:290:VAL:HG11	1:E:351:SER:N	2.30	0.46
1:H:120:LEU:HD21	1:H:205:PRO:HD3	1.98	0.46
1:F:115:LYS:HA	1:F:395:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:ASN:HB2	1:F:205:PRO:HD2	1.97	0.46
1:D:99:THR:HG23	1:D:193:LEU:HD22	1.96	0.46
1:D:323:SER:O	1:D:326:GLN:NE2	2.49	0.46
1:E:51:ARG:HB3	1:E:92:TYR:CD2	2.51	0.46
1:E:99:THR:HG23	1:E:193:LEU:HD22	1.97	0.46
1:G:285:GLY:HA3	1:G:355:TRP:CZ2	2.51	0.46
1:H:51:ARG:HG3	1:H:92:TYR:CG	2.50	0.46
1:H:321:ILE:HG23	1:H:389:PHE:CD1	2.50	0.46
1:D:308:GLU:HB3	1:D:310:GLU:OE1	2.16	0.46
1:A:63:PHE:HE2	1:A:109:PHE:HB2	1.81	0.46
1:A:51:ARG:HG3	1:A:92:TYR:CG	2.50	0.45
1:A:321:ILE:HG23	1:A:389:PHE:CD1	2.51	0.45
1:A:356:ASN:HB3	1:A:369:LYS:HB3	1.99	0.45
1:B:292:TRP:CE2	1:B:319:LYS:HD3	2.50	0.45
1:B:370:PHE:O	1:B:426:SER:HA	2.15	0.45
1:G:224:ALA:O	1:G:226:VAL:HG23	2.15	0.45
1:D:81:PHE:CD1	1:D:85:LEU:HD12	2.52	0.45
1:C:264:ASN:O	1:C:267:THR:HG22	2.15	0.45
1:A:410:TYR:OH	1:A:441:TYR:HB3	2.16	0.45
1:D:51:ARG:HG3	1:D:92:TYR:CD2	2.51	0.45
1:E:53:TRP:HH2	1:E:78:MET:HE2	1.76	0.45
1:E:92:TYR:HB3	1:E:93:PRO:HD3	1.99	0.45
1:E:224:ALA:O	1:E:226:VAL:HG23	2.16	0.45
1:C:60:PHE:CZ	1:C:203:PHE:HE2	2.35	0.45
1:C:280:ARG:HD3	1:C:358:GLU:CD	2.41	0.45
1:B:115:LYS:HG2	1:B:395:TRP:NE1	2.30	0.45
1:F:145:THR:OG1	1:C:149:ASN:OD1	2.24	0.45
1:D:311:ILE:HD12	1:D:311:ILE:H	1.80	0.45
1:E:171:PHE:HE1	1:E:217:PRO:HB3	1.81	0.45
1:A:161:THR:N	1:A:162:PRO:CD	2.79	0.45
1:H:67:GLY:HA2	1:H:119:ARG:HG3	1.97	0.45
1:H:263:TYR:CD1	1:H:263:TYR:N	2.80	0.45
1:F:106:PRO:O	1:F:125:PHE:HB2	2.16	0.45
1:D:53:TRP:CH2	1:D:78:MET:HE2	2.51	0.45
1:C:106:PRO:O	1:C:125:PHE:HB2	2.16	0.45
1:C:301:LEU:CD1	1:C:302:GLY:H	2.22	0.45
1:H:51:ARG:HG3	1:H:92:TYR:CD2	2.51	0.45
1:C:320:GLN:HE21	1:C:389:PHE:HE1	1.64	0.45
1:A:161:THR:N	1:A:162:PRO:HD3	2.31	0.45
1:F:257:MET:O	1:F:262:GLY:HA2	2.16	0.45
1:D:115:LYS:HG2	1:D:395:TRP:NE1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ASP:OD2	1:E:175:LEU:HD21	2.16	0.45
1:E:390:TRP:HD1	1:E:399:ALA:HA	1.82	0.45
1:A:280:ARG:NH1	1:A:358:GLU:OE2	2.46	0.45
1:B:66:ALA:O	1:B:119:ARG:HD2	2.17	0.45
1:B:257:MET:HB3	1:B:263:TYR:CD1	2.51	0.45
1:G:147:LEU:HD23	1:G:199:PHE:CD2	2.51	0.45
1:G:386:LEU:HD13	1:G:390:TRP:NE1	2.31	0.45
1:H:123:ILE:O	1:H:201:PHE:N	2.35	0.45
1:E:284:TYR:N	1:E:284:TYR:CD1	2.84	0.45
1:C:163:PHE:CE1	1:C:239:ILE:HG12	2.51	0.45
1:A:86:ILE:HB	1:A:87:PRO:HD3	1.99	0.45
1:G:84:HIS:NE2	1:G:154:LEU:HD11	2.32	0.45
1:G:94:GLN:HE22	1:G:105:LEU:HA	1.81	0.45
1:G:167:LEU:O	1:G:171:PHE:HD2	1.99	0.45
1:G:310:GLU:OE2	1:G:431:ALA:HB2	2.17	0.45
1:H:161:THR:N	1:H:162:PRO:HD3	2.32	0.45
1:D:36:GLN:OE1	1:D:58:SER:HA	2.17	0.45
1:C:299:TRP:CD1	1:C:311:ILE:HG23	2.52	0.45
1:A:60:PHE:HZ	1:A:203:PHE:HE2	1.64	0.45
1:G:111:LEU:HD12	1:G:441:TYR:CE2	2.52	0.45
1:D:71:LEU:HB3	1:D:72:PRO:HD3	1.98	0.45
1:E:317:ARG:HH11	1:E:320:GLN:HE22	1.65	0.45
1:A:171:PHE:CE1	1:A:217:PRO:HB3	2.52	0.45
1:G:96:TRP:CE2	1:G:140:ASN:ND2	2.84	0.45
1:G:173:LEU:HB2	1:G:176:SER:HB2	1.99	0.45
1:D:280:ARG:NH1	1:D:358:GLU:OE2	2.38	0.45
1:E:204:ASN:HB2	1:E:205:PRO:HD2	1.99	0.45
1:C:386:LEU:HD13	1:C:390:TRP:NE1	2.32	0.45
1:A:356:ASN:HD22	1:A:369:LYS:HD2	1.82	0.44
1:B:51:ARG:HG3	1:B:92:TYR:CD2	2.52	0.44
1:B:119:ARG:NH2	1:B:405:THR:HG21	2.33	0.44
1:F:320:GLN:HE21	1:F:389:PHE:HE1	1.65	0.44
1:D:386:LEU:HD13	1:D:390:TRP:HE1	1.82	0.44
1:B:60:PHE:CE1	1:B:123:ILE:HD11	2.53	0.44
1:B:285:GLY:HA3	1:B:355:TRP:CZ2	2.52	0.44
1:C:390:TRP:HB3	1:C:395:TRP:HB2	1.99	0.44
1:A:257:MET:HB3	1:A:263:TYR:CD1	2.52	0.44
1:A:285:GLY:HA3	1:A:355:TRP:CZ2	2.52	0.44
1:F:161:THR:N	1:F:162:PRO:CD	2.81	0.44
1:D:175:LEU:HD23	1:E:275:GLU:OE1	2.17	0.44
1:A:66:ALA:O	1:A:119:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLN:NE2	1:A:436:TYR:HE1	2.15	0.44
1:B:36:GLN:OE1	1:B:58:SER:HA	2.18	0.44
1:G:42:HIS:ND1	1:G:44:PHE:CD1	2.83	0.44
1:G:279:GLN:HG3	1:G:280:ARG:N	2.32	0.44
1:G:390:TRP:HB3	1:G:395:TRP:HB2	1.99	0.44
1:E:256:TYR:CD1	1:E:301:LEU:HB2	2.52	0.44
1:A:171:PHE:HE1	1:A:217:PRO:HB3	1.82	0.44
1:A:378:ASN:HB3	1:A:381:HIS:HB3	1.98	0.44
1:B:37:ALA:HB1	1:C:76:GLN:NE2	2.32	0.44
1:B:174:SER:C	1:B:176:SER:N	2.75	0.44
1:G:52:TRP:CD2	1:G:89:LEU:HD13	2.52	0.44
1:G:139:PHE:CZ	1:G:180:GLN:HB3	2.53	0.44
1:G:147:LEU:HD23	1:G:199:PHE:HD2	1.83	0.44
1:H:211:VAL:HG12	1:H:273:PHE:CD2	2.51	0.44
1:H:308:GLU:HB3	1:H:310:GLU:OE1	2.18	0.44
1:D:100:ILE:HD11	1:D:125:PHE:HA	1.99	0.44
1:C:249:ALA:HB1	1:C:366:PRO:CG	2.42	0.44
1:B:269:LEU:CD1	1:B:283:ILE:HG13	2.47	0.44
1:G:81:PHE:HD1	1:G:85:LEU:HD12	1.83	0.44
1:H:370:PHE:O	1:H:426:SER:HA	2.18	0.44
1:E:137:ASP:OD2	1:E:142:ILE:HG12	2.17	0.44
1:E:174:SER:C	1:E:175:LEU:HD22	2.43	0.44
1:B:161:THR:N	1:B:162:PRO:CD	2.81	0.44
1:G:212:LYS:HE3	1:G:214:TYR:OH	2.18	0.44
1:G:321:ILE:HG23	1:G:389:PHE:CD1	2.52	0.44
1:D:290:VAL:CG2	1:D:351:SER:HB2	2.33	0.44
1:E:115:LYS:HA	1:E:395:TRP:CE2	2.53	0.44
1:E:323:SER:O	1:E:326:GLN:NE2	2.49	0.44
1:A:327:ILE:HG21	1:A:351:SER:OG	2.16	0.44
1:B:99:THR:HG23	1:B:193:LEU:HD22	2.00	0.44
1:H:428:SER:HB3	1:H:436:TYR:CB	2.47	0.44
1:D:141:ARG:CZ	1:D:172:GLN:HE21	2.31	0.44
1:E:257:MET:HB3	1:E:263:TYR:CD1	2.52	0.44
1:E:378:ASN:HB3	1:E:381:HIS:HB3	1.99	0.44
1:C:105:LEU:CD1	1:C:107:ILE:HG22	2.48	0.44
1:A:172:GLN:OE1	1:G:162:PRO:HA	2.18	0.44
1:B:389:PHE:CE2	1:B:437:MET:HE1	2.52	0.44
1:H:115:LYS:HE3	1:H:435:VAL:H	1.83	0.44
1:C:323:SER:O	1:C:326:GLN:NE2	2.50	0.44
1:B:386:LEU:HD13	1:B:390:TRP:NE1	2.33	0.43
1:G:42:HIS:ND1	1:G:44:PHE:CE1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LEU:HD23	1:F:199:PHE:HD2	1.82	0.43
1:E:45:PRO:HD2	1:E:49:GLN:OE1	2.18	0.43
1:C:257:MET:O	1:C:262:GLY:HA2	2.18	0.43
1:A:71:LEU:HD23	1:E:71:LEU:HD23	2.00	0.43
1:B:253:ILE:HD11	1:B:304:ARG:HH22	1.83	0.43
1:B:427:TYR:HD1	1:B:437:MET:CE	2.30	0.43
1:G:149:ASN:O	1:G:152:SER:OG	2.27	0.43
1:H:212:LYS:HE3	1:H:214:TYR:OH	2.18	0.43
1:F:269:LEU:CD1	1:F:283:ILE:HG13	2.48	0.43
1:F:390:TRP:HD1	1:F:399:ALA:HA	1.83	0.43
1:D:48:ASP:CG	1:D:91:PRO:HA	2.43	0.43
1:C:252:LEU:HD22	1:C:304:ARG:NH2	2.33	0.43
1:A:390:TRP:HB3	1:A:395:TRP:HB2	1.99	0.43
1:B:310:GLU:OE2	1:B:431:ALA:HB2	2.18	0.43
1:G:37:ALA:HB1	1:D:76:GLN:NE2	2.30	0.43
1:H:282:LYS:HB3	1:H:284:TYR:HE1	1.82	0.43
1:H:284:TYR:N	1:H:284:TYR:HD1	2.16	0.43
1:D:285:GLY:O	1:D:354:ILE:HG23	2.18	0.43
1:C:123:ILE:HD12	1:C:203:PHE:CZ	2.53	0.43
1:A:354:ILE:HB	1:A:371:TYR:HB2	1.99	0.43
1:B:124:GLY:HA2	1:B:200:GLY:HA2	2.00	0.43
1:G:79:PHE:HE1	1:D:83:HIS:HE1	1.66	0.43
1:H:114:GLN:NE2	1:H:436:TYR:HE1	2.13	0.43
1:F:300:THR:O	1:F:301:LEU:HG	2.19	0.43
1:F:356:ASN:HB3	1:F:369:LYS:HB3	1.99	0.43
1:F:426:SER:O	1:F:437:MET:HG3	2.18	0.43
1:D:252:LEU:HD22	1:D:304:ARG:NH2	2.34	0.43
1:D:370:PHE:O	1:D:426:SER:HA	2.18	0.43
1:A:42:HIS:CD2	1:E:79:PHE:CZ	3.07	0.43
1:A:94:GLN:OE1	1:A:106:PRO:HD3	2.18	0.43
1:B:176:SER:O	1:B:180:GLN:HG2	2.19	0.43
1:H:212:LYS:HG3	1:H:271:CYS:O	2.19	0.43
1:F:46:THR:OG1	1:F:49:GLN:HG3	2.18	0.43
1:E:285:GLY:HA3	1:E:355:TRP:CZ2	2.53	0.43
1:C:290:VAL:HG11	1:C:351:SER:N	2.33	0.43
1:A:114:GLN:HE22	1:A:436:TYR:HE1	1.67	0.43
1:H:252:LEU:HD22	1:H:304:ARG:HH21	1.84	0.43
1:H:299:TRP:CZ2	1:H:368:PRO:HG2	2.54	0.43
1:F:160:ASP:OD2	1:C:175:LEU:HD21	2.19	0.43
1:D:174:SER:C	1:D:176:SER:N	2.76	0.43
1:E:106:PRO:O	1:E:125:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:SER:C	1:C:176:SER:N	2.75	0.43
1:B:127:PRO:HD2	1:B:144:ILE:HD13	2.00	0.43
1:B:252:LEU:HD22	1:B:304:ARG:NH2	2.33	0.43
1:B:304:ARG:HG2	1:B:311:ILE:CD1	2.49	0.43
1:G:53:TRP:CH2	1:G:78:MET:HE2	2.53	0.43
1:G:212:LYS:HG3	1:G:271:CYS:O	2.18	0.43
1:F:427:TYR:HD1	1:F:437:MET:CE	2.32	0.43
1:D:123:ILE:HD12	1:D:203:PHE:CZ	2.53	0.43
1:D:263:TYR:CD1	1:D:263:TYR:N	2.77	0.43
1:A:234:GLU:O	1:A:238:THR:HG23	2.18	0.43
1:B:42:HIS:ND1	1:B:44:PHE:CE1	2.87	0.43
1:B:200:GLY:N	1:B:212:LYS:O	2.46	0.43
1:G:161:THR:N	1:G:162:PRO:CD	2.81	0.43
1:H:327:ILE:HG21	1:H:351:SER:OG	2.18	0.43
1:C:285:GLY:O	1:C:354:ILE:HG23	2.18	0.43
1:B:75:TYR:CD2	1:C:75:TYR:CD2	2.96	0.43
1:B:165:GLN:HG3	1:H:172:GLN:NE2	2.22	0.43
1:F:430:THR:HG22	1:F:432:LYS:H	1.84	0.43
1:D:70:GLY:O	1:D:74:GLN:HG3	2.19	0.43
1:C:42:HIS:ND1	1:C:44:PHE:CE1	2.80	0.43
1:C:140:ASN:OD1	1:C:143:PRO:HG2	2.19	0.43
1:A:60:PHE:CZ	1:A:203:PHE:HE2	2.37	0.43
1:F:243:ARG:HA	1:F:243:ARG:NE	2.33	0.43
1:E:121:LEU:HD23	1:E:203:PHE:CD2	2.53	0.43
1:B:63:PHE:HE2	1:B:109:PHE:HB2	1.84	0.42
1:B:263:TYR:CD1	1:B:263:TYR:N	2.80	0.42
1:G:123:ILE:O	1:G:201:PHE:N	2.37	0.42
1:F:287:HIS:CE1	1:F:355:TRP:HE1	2.37	0.42
1:D:298:MET:HE1	1:D:353:ILE:HD11	2.00	0.42
1:E:81:PHE:CD1	1:E:85:LEU:HD12	2.54	0.42
1:E:284:TYR:N	1:E:284:TYR:HD1	2.16	0.42
1:B:167:LEU:O	1:B:171:PHE:HD2	2.02	0.42
1:D:264:ASN:O	1:D:267:THR:HG22	2.18	0.42
1:G:137:ASP:OD2	1:G:142:ILE:HG12	2.19	0.42
1:D:94:GLN:OE1	1:D:106:PRO:HD3	2.19	0.42
1:A:236:VAL:O	1:A:239:ILE:HG22	2.20	0.42
1:B:179:ARG:NH2	1:B:223:ALA:O	2.53	0.42
1:G:125:PHE:CE1	1:G:201:PHE:HE2	2.37	0.42
1:H:161:THR:N	1:H:162:PRO:CD	2.83	0.42
1:H:257:MET:O	1:H:262:GLY:HA2	2.20	0.42
1:H:280:ARG:HD3	1:H:358:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:408:GLN:O	1:H:411:PRO:HD3	2.19	0.42
1:F:267:THR:HA	1:F:285:GLY:HA2	2.01	0.42
1:D:243:ARG:HA	1:D:243:ARG:NE	2.34	0.42
1:E:282:LYS:HB2	1:E:284:TYR:HE1	1.85	0.42
1:E:371:TYR:CE1	1:E:426:SER:HB3	2.55	0.42
1:E:390:TRP:CH2	1:E:437:MET:SD	3.12	0.42
1:B:282:LYS:HB3	1:B:284:TYR:HE1	1.85	0.42
1:H:257:MET:HB3	1:H:263:TYR:CD1	2.55	0.42
1:H:292:TRP:HZ2	1:H:315:LEU:HD21	1.84	0.42
1:C:60:PHE:HZ	1:C:203:PHE:HE2	1.67	0.42
1:B:320:GLN:HE21	1:B:389:PHE:HE1	1.68	0.42
1:G:51:ARG:HG3	1:G:92:TYR:CD2	2.54	0.42
1:G:408:GLN:O	1:G:411:PRO:HD3	2.20	0.42
1:H:66:ALA:O	1:H:119:ARG:HD2	2.20	0.42
1:F:183:LYS:O	1:F:185:GLY:N	2.53	0.42
1:E:96:TRP:NE1	1:E:140:ASN:HD22	2.18	0.42
1:A:209:ILE:HD12	1:E:41:TYR:HE2	1.84	0.42
1:A:243:ARG:HA	1:A:243:ARG:NE	2.34	0.42
1:G:60:PHE:CE1	1:G:123:ILE:HD11	2.54	0.42
1:G:243:ARG:HA	1:G:243:ARG:NE	2.35	0.42
1:F:426:SER:O	1:F:437:MET:HA	2.19	0.42
1:H:237:ARG:HA	1:H:240:ASP:OD2	2.19	0.42
1:F:115:LYS:HG2	1:F:395:TRP:NE1	2.33	0.42
1:C:44:PHE:CD2	1:C:50:GLU:HA	2.54	0.42
1:A:237:ARG:HA	1:A:240:ASP:OD2	2.20	0.42
1:F:224:ALA:O	1:F:226:VAL:HG23	2.20	0.42
1:D:106:PRO:O	1:D:125:PHE:HB2	2.20	0.42
1:D:167:LEU:HB3	1:D:215:VAL:HG21	2.01	0.42
1:E:114:GLN:HE22	1:E:436:TYR:HE1	1.68	0.42
1:B:249:ALA:HB1	1:B:366:PRO:CG	2.45	0.41
1:H:183:LYS:O	1:H:185:GLY:N	2.53	0.41
1:H:198:ALA:O	1:H:199:PHE:HD1	2.03	0.41
1:H:304:ARG:HG2	1:H:311:ILE:CD1	2.50	0.41
1:H:378:ASN:HB3	1:H:381:HIS:HB3	2.02	0.41
1:F:256:TYR:CD1	1:F:301:LEU:HB2	2.56	0.41
1:F:263:TYR:CD1	1:F:263:TYR:N	2.78	0.41
1:A:256:TYR:CD1	1:A:301:LEU:HB2	2.55	0.41
1:A:386:LEU:HD13	1:A:390:TRP:NE1	2.35	0.41
1:B:318:LEU:HD12	1:B:427:TYR:CD2	2.55	0.41
1:B:427:TYR:HD1	1:B:437:MET:HE2	1.85	0.41
1:H:60:PHE:HD1	1:H:109:PHE:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ILE:HG21	1:D:351:SER:OG	2.19	0.41
1:E:292:TRP:CZ2	1:E:319:LYS:HD3	2.55	0.41
1:C:82:MET:HE3	1:C:82:MET:HB2	1.95	0.41
1:A:183:LYS:O	1:A:185:GLY:N	2.54	0.41
1:A:224:ALA:O	1:A:226:VAL:HG23	2.20	0.41
1:B:44:PHE:HE2	1:B:53:TRP:CB	2.28	0.41
1:B:120:LEU:HD21	1:B:205:PRO:HD3	2.03	0.41
1:H:123:ILE:HD12	1:H:203:PHE:CZ	2.55	0.41
1:E:161:THR:N	1:E:162:PRO:CD	2.84	0.41
1:C:127:PRO:HB2	1:C:143:PRO:HB2	2.02	0.41
1:A:53:TRP:CZ3	1:A:82:MET:HG2	2.56	0.41
1:F:139:PHE:CZ	1:F:180:GLN:HB3	2.55	0.41
1:D:127:PRO:HB2	1:D:143:PRO:HB2	2.02	0.41
1:E:85:LEU:HD22	1:E:125:PHE:CZ	2.55	0.41
1:E:183:LYS:O	1:E:185:GLY:N	2.53	0.41
1:E:386:LEU:HD13	1:E:390:TRP:NE1	2.34	0.41
1:A:76:GLN:NE2	1:E:37:ALA:HB1	2.36	0.41
1:A:209:ILE:HD12	1:E:41:TYR:CE2	2.56	0.41
1:G:327:ILE:HD12	1:G:327:ILE:HG23	1.85	0.41
1:D:52:TRP:CE3	1:D:89:LEU:HD13	2.55	0.41
1:D:280:ARG:HH11	1:D:358:GLU:CD	2.24	0.41
1:E:174:SER:C	1:E:176:SER:N	2.77	0.41
1:B:42:HIS:ND1	1:B:44:PHE:CD1	2.84	0.41
1:G:174:SER:C	1:G:175:LEU:HD22	2.44	0.41
1:F:142:ILE:HD12	1:C:152:SER:OG	2.21	0.41
1:E:49:GLN:NE2	1:E:87:PRO:HG3	2.35	0.41
1:F:147:LEU:HD23	1:F:199:PHE:CD2	2.55	0.41
1:D:140:ASN:OD1	1:D:143:PRO:HG2	2.21	0.41
1:C:179:ARG:NH2	1:C:223:ALA:O	2.53	0.41
1:C:292:TRP:CZ2	1:C:319:LYS:HD3	2.55	0.41
1:A:299:TRP:CZ2	1:A:368:PRO:HG2	2.56	0.41
1:B:111:LEU:HD12	1:B:441:TYR:CE2	2.56	0.41
1:G:285:GLY:HA3	1:G:355:TRP:CE2	2.56	0.41
1:F:166:HIS:NE2	1:F:238:THR:OG1	2.50	0.41
1:F:352:PRO:O	1:F:373:PRO:HG3	2.21	0.41
1:A:109:PHE:CD1	1:A:123:ILE:HG12	2.56	0.41
1:A:166:HIS:NE2	1:A:238:THR:OG1	2.50	0.41
1:A:290:VAL:HG11	1:A:351:SER:N	2.35	0.41
1:A:308:GLU:HB3	1:A:310:GLU:OE1	2.21	0.41
1:B:290:VAL:HG13	1:B:290:VAL:O	2.21	0.41
1:G:105:LEU:CD1	1:G:107:ILE:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:VAL:HG21	1:G:425:ILE:HG13	2.02	0.41
1:H:41:TYR:HE2	1:F:209:ILE:HD12	1.85	0.41
1:H:42:HIS:ND1	1:H:44:PHE:CE1	2.88	0.41
1:H:301:LEU:HD12	1:H:302:GLY:N	2.26	0.41
1:F:174:SER:C	1:F:175:LEU:HD22	2.46	0.41
1:F:321:ILE:HG23	1:F:389:PHE:CD1	2.55	0.41
1:D:378:ASN:O	1:D:382:VAL:HG23	2.21	0.41
1:E:124:GLY:HA2	1:E:200:GLY:HA2	2.02	0.41
1:E:236:VAL:O	1:E:239:ILE:HG22	2.21	0.41
1:E:267:THR:HA	1:E:285:GLY:HA2	2.02	0.41
1:C:370:PHE:O	1:C:426:SER:HA	2.20	0.41
1:A:174:SER:C	1:A:176:SER:N	2.74	0.41
1:B:115:LYS:HE3	1:B:435:VAL:H	1.86	0.41
1:B:212:LYS:HE3	1:B:214:TYR:OH	2.21	0.41
1:B:237:ARG:HA	1:B:240:ASP:OD2	2.21	0.41
1:B:390:TRP:HB3	1:B:395:TRP:HB2	2.02	0.41
1:G:42:HIS:HD2	1:D:79:PHE:CZ	2.38	0.41
1:F:86:ILE:HB	1:F:87:PRO:HD3	2.02	0.41
1:D:109:PHE:CD1	1:D:123:ILE:HG12	2.56	0.41
1:D:304:ARG:HG2	1:D:311:ILE:CD1	2.51	0.41
1:E:77:PHE:CD1	1:E:203:PHE:CD1	3.09	0.41
1:C:408:GLN:O	1:C:411:PRO:HD3	2.20	0.41
1:A:211:VAL:HG12	1:A:273:PHE:CD2	2.55	0.40
1:A:280:ARG:HD2	1:A:280:ARG:O	2.21	0.40
1:A:300:THR:O	1:A:301:LEU:HG	2.21	0.40
1:B:161:THR:N	1:B:162:PRO:HD3	2.35	0.40
1:G:46:THR:OG1	1:G:49:GLN:HG3	2.19	0.40
1:G:176:SER:O	1:G:180:GLN:HG2	2.21	0.40
1:C:118:HIS:NE2	1:C:205:PRO:HG3	2.36	0.40
1:B:224:ALA:O	1:B:226:VAL:HG23	2.21	0.40
1:G:44:PHE:HD2	1:G:50:GLU:HA	1.86	0.40
1:G:405:THR:O	1:G:409:LEU:HD13	2.22	0.40
1:E:42:HIS:ND1	1:E:44:PHE:CE1	2.89	0.40
1:C:94:GLN:OE1	1:C:106:PRO:HD3	2.20	0.40
1:D:118:HIS:NE2	1:D:205:PRO:HG3	2.37	0.40
1:D:183:LYS:O	1:D:185:GLY:N	2.55	0.40
1:D:267:THR:HA	1:D:285:GLY:HA2	2.02	0.40
1:E:440:TYR:N	1:E:440:TYR:CD1	2.89	0.40
1:C:109:PHE:HD1	1:C:123:ILE:HG12	1.84	0.40
1:C:114:GLN:NE2	1:C:436:TYR:HE1	2.19	0.40
1:B:356:ASN:HB3	1:B:369:LYS:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:ASP:OD1	1:G:207:GLY:N	2.51	0.40
1:G:282:LYS:CB	1:G:284:TYR:HE1	2.33	0.40
1:G:317:ARG:HB2	1:G:427:TYR:OH	2.22	0.40
1:H:71:LEU:HB3	1:H:72:PRO:HD3	2.04	0.40
1:F:318:LEU:HD23	1:F:318:LEU:O	2.21	0.40
1:D:84:HIS:CE1	1:D:154:LEU:HD21	2.56	0.40
1:D:327:ILE:HD12	1:D:327:ILE:HG23	1.88	0.40
1:D:379:ASP:OD2	1:D:421:LEU:HB2	2.22	0.40
1:C:115:LYS:HG2	1:C:395:TRP:NE1	2.36	0.40
1:C:308:GLU:HB3	1:C:310:GLU:OE1	2.22	0.40
1:A:280:ARG:HD3	1:A:358:GLU:CD	2.47	0.40
1:G:71:LEU:HD23	1:D:71:LEU:HD23	2.04	0.40
1:G:299:TRP:CD1	1:G:315:LEU:HD12	2.56	0.40
1:G:352:PRO:O	1:G:373:PRO:HG3	2.21	0.40
1:D:167:LEU:O	1:D:171:PHE:HD2	2.04	0.40
1:D:369:LYS:HA	1:D:427:TYR:O	2.22	0.40
1:E:176:SER:O	1:E:180:GLN:HG2	2.22	0.40
1:E:282:LYS:CB	1:E:284:TYR:HE1	2.34	0.40
1:C:52:TRP:CE3	1:C:89:LEU:HD13	2.56	0.40
1:C:53:TRP:CZ3	1:C:82:MET:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	392/472 (83%)	368 (94%)	23 (6%)	1 (0%)	36 68
1	B	392/472 (83%)	368 (94%)	22 (6%)	2 (0%)	24 59
1	C	392/472 (83%)	367 (94%)	24 (6%)	1 (0%)	36 68
1	D	392/472 (83%)	370 (94%)	21 (5%)	1 (0%)	36 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	392/472 (83%)	366 (93%)	25 (6%)	1 (0%)	36	68
1	F	392/472 (83%)	365 (93%)	26 (7%)	1 (0%)	36	68
1	G	392/472 (83%)	366 (93%)	25 (6%)	1 (0%)	36	68
1	H	392/472 (83%)	366 (93%)	25 (6%)	1 (0%)	36	68
All	All	3136/3776 (83%)	2936 (94%)	191 (6%)	9 (0%)	36	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	34	PRO
1	E	34	PRO
1	C	34	PRO
1	A	34	PRO
1	G	34	PRO
1	D	34	PRO
1	B	34	PRO
1	B	175	LEU
1	H	34	PRO

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	344/408 (84%)	339 (98%)	5 (2%)	57	76
1	B	344/408 (84%)	338 (98%)	6 (2%)	53	75
1	C	344/408 (84%)	339 (98%)	5 (2%)	57	76
1	D	344/408 (84%)	338 (98%)	6 (2%)	53	75
1	E	344/408 (84%)	338 (98%)	6 (2%)	53	75
1	F	344/408 (84%)	337 (98%)	7 (2%)	48	72
1	G	344/408 (84%)	338 (98%)	6 (2%)	53	75
1	H	344/408 (84%)	339 (98%)	5 (2%)	57	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2752/3264 (84%)	2706 (98%)	46 (2%)	53 75

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LEU
1	A	175	LEU
1	A	209	ILE
1	A	263	TYR
1	A	284	TYR
1	B	125	PHE
1	B	173	LEU
1	B	175	LEU
1	B	209	ILE
1	B	263	TYR
1	B	284	TYR
1	G	125	PHE
1	G	173	LEU
1	G	175	LEU
1	G	209	ILE
1	G	263	TYR
1	G	284	TYR
1	H	173	LEU
1	H	175	LEU
1	H	209	ILE
1	H	263	TYR
1	H	284	TYR
1	F	125	PHE
1	F	173	LEU
1	F	175	LEU
1	F	209	ILE
1	F	231	LEU
1	F	263	TYR
1	F	284	TYR
1	D	173	LEU
1	D	175	LEU
1	D	209	ILE
1	D	263	TYR
1	D	284	TYR
1	D	406	LEU
1	E	125	PHE
1	E	173	LEU

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Mol	Chain	Res	Type
1	E	175	LEU
1	E	209	ILE
1	E	263	TYR
1	E	284	TYR
1	C	173	LEU
1	C	175	LEU
1	C	209	ILE
1	C	263	TYR
1	C	284	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	172	GLN
1	A	180	GLN
1	A	245	GLN
1	A	422	GLN
1	A	442	HIS
1	B	76	GLN
1	B	165	GLN
1	B	172	GLN
1	B	180	GLN
1	B	196	GLN
1	B	245	GLN
1	B	320	GLN
1	B	388	GLN
1	B	422	GLN
1	B	442	HIS
1	G	76	GLN
1	G	149	ASN
1	G	165	GLN
1	G	172	GLN
1	G	182	GLN
1	G	184	GLN
1	G	245	GLN
1	G	279	GLN
1	G	388	GLN
1	G	422	GLN
1	G	442	HIS
1	H	165	GLN
1	H	172	GLN

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Mol	Chain	Res	Type
1	H	180	GLN
1	H	245	GLN
1	H	320	GLN
1	H	388	GLN
1	H	422	GLN
1	H	442	HIS
1	F	172	GLN
1	F	180	GLN
1	F	245	GLN
1	F	279	GLN
1	F	320	GLN
1	F	388	GLN
1	F	422	GLN
1	D	76	GLN
1	D	165	GLN
1	D	172	GLN
1	D	180	GLN
1	D	320	GLN
1	D	422	GLN
1	D	442	HIS
1	E	76	GLN
1	E	84	HIS
1	E	165	GLN
1	E	172	GLN
1	E	180	GLN
1	E	184	GLN
1	E	245	GLN
1	E	279	GLN
1	E	320	GLN
1	E	422	GLN
1	C	76	GLN
1	C	136	GLN
1	C	172	GLN
1	C	180	GLN
1	C	245	GLN
1	C	320	GLN
1	C	422	GLN
1	C	442	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/472 (83%)	0.54	30 (7%) 20 13	61, 98, 168, 261	0
1	B	396/472 (83%)	0.64	28 (7%) 22 14	58, 94, 169, 261	0
1	C	396/472 (83%)	0.61	29 (7%) 21 13	64, 101, 169, 261	0
1	D	396/472 (83%)	0.64	34 (8%) 16 11	63, 100, 169, 261	0
1	E	396/472 (83%)	0.63	37 (9%) 14 9	59, 97, 169, 261	0
1	F	396/472 (83%)	0.61	36 (9%) 15 9	60, 96, 169, 261	0
1	G	396/472 (83%)	0.67	39 (9%) 13 9	58, 94, 169, 261	0
1	H	396/472 (83%)	0.77	46 (11%) 9 7	62, 101, 170, 261	0
All	All	3168/3776 (83%)	0.64	279 (8%) 15 10	58, 97, 169, 261	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	LEU	6.1
1	A	304	ARG	5.7
1	E	306	ILE	5.4
1	C	180	GLN	5.3
1	B	304	ARG	5.1
1	G	304	ARG	5.1
1	B	193	LEU	4.9
1	G	193	LEU	4.9
1	H	304	ARG	4.8
1	D	306	ILE	4.6
1	D	180	GLN	4.6
1	F	180	GLN	4.6
1	B	351	SER	4.5
1	G	392	SER	4.4
1	C	306	ILE	4.2
1	D	240	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	398	HIS	4.2
1	E	193	LEU	4.1
1	E	396	PRO	4.1
1	C	177	GLU	4.0
1	G	180	GLN	4.0
1	H	306	ILE	4.0
1	D	304	ARG	4.0
1	C	193	LEU	3.9
1	G	351	SER	3.9
1	H	404	ASP	3.9
1	A	177	GLU	3.8
1	A	306	ILE	3.8
1	H	180	GLN	3.7
1	C	323	SER	3.7
1	E	304	ARG	3.7
1	C	399	ALA	3.7
1	E	241	VAL	3.7
1	F	304	ARG	3.7
1	F	239	ILE	3.7
1	B	177	GLU	3.7
1	H	192	PRO	3.6
1	D	196	GLN	3.6
1	C	301	LEU	3.6
1	G	362	GLY	3.6
1	G	177	GLU	3.6
1	G	399	ALA	3.5
1	B	399	ALA	3.5
1	F	396	PRO	3.5
1	E	180	GLN	3.5
1	D	177	GLU	3.4
1	H	330	GLY	3.4
1	D	192	PRO	3.4
1	E	192	PRO	3.4
1	E	177	GLU	3.4
1	F	399	ALA	3.4
1	B	306	ILE	3.4
1	C	304	ARG	3.4
1	H	396	PRO	3.4
1	F	290	VAL	3.3
1	C	241	VAL	3.3
1	H	33	SER	3.3
1	H	290	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	306	ILE	3.3
1	A	34	PRO	3.3
1	A	370	PHE	3.2
1	D	300	THR	3.2
1	H	289	GLU	3.2
1	E	300	THR	3.1
1	F	189	ASP	3.1
1	B	180	GLN	3.1
1	E	286	ALA	3.1
1	G	367	VAL	3.1
1	D	399	ALA	3.1
1	B	192	PRO	3.1
1	D	189	ASP	3.1
1	D	400	CYS	3.1
1	A	399	ALA	3.0
1	B	33	SER	3.0
1	F	241	VAL	3.0
1	E	301	LEU	3.0
1	H	293	ALA	3.0
1	B	241	VAL	3.0
1	H	400	CYS	3.0
1	G	301	LEU	3.0
1	E	399	ALA	3.0
1	G	160	ASP	3.0
1	D	327	ILE	3.0
1	H	205	PRO	2.9
1	G	187	GLY	2.9
1	E	240	ASP	2.9
1	F	250	PHE	2.9
1	D	444	GLN	2.9
1	H	175	LEU	2.9
1	C	443	SER	2.9
1	D	287	HIS	2.9
1	C	196	GLN	2.9
1	F	301	LEU	2.9
1	E	175	LEU	2.9
1	B	290	VAL	2.9
1	B	400	CYS	2.9
1	B	196	GLN	2.8
1	G	196	GLN	2.8
1	C	351	SER	2.8
1	G	192	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	186	SER	2.8
1	D	290	VAL	2.8
1	F	306	ILE	2.8
1	G	352	PRO	2.8
1	A	193	LEU	2.8
1	H	328	GLY	2.8
1	D	241	VAL	2.8
1	A	322	TRP	2.8
1	G	437	MET	2.8
1	A	263	TYR	2.8
1	A	398	HIS	2.7
1	E	178	VAL	2.7
1	A	188	PRO	2.7
1	A	181	LEU	2.7
1	H	399	ALA	2.7
1	C	401	ALA	2.7
1	A	400	CYS	2.7
1	F	192	PRO	2.7
1	C	240	ASP	2.7
1	H	437	MET	2.7
1	F	351	SER	2.7
1	F	366	PRO	2.7
1	G	330	GLY	2.7
1	B	352	PRO	2.6
1	C	389	PHE	2.6
1	B	300	THR	2.6
1	F	443	SER	2.6
1	C	175	LEU	2.6
1	B	366	PRO	2.6
1	F	177	GLU	2.6
1	A	240	ASP	2.6
1	D	301	LEU	2.6
1	G	401	ALA	2.6
1	A	239	ILE	2.6
1	F	181	LEU	2.6
1	F	178	VAL	2.6
1	A	33	SER	2.6
1	E	351	SER	2.6
1	G	175	LEU	2.5
1	A	118	HIS	2.5
1	E	181	LEU	2.5
1	E	187	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	289	GLU	2.5
1	A	180	GLN	2.5
1	G	290	VAL	2.5
1	F	385	ALA	2.5
1	B	414	ASP	2.5
1	H	199	PHE	2.5
1	D	381	HIS	2.5
1	G	358	GLU	2.5
1	B	240	ASP	2.5
1	G	322	TRP	2.5
1	A	243	ARG	2.5
1	A	192	PRO	2.5
1	E	263	TYR	2.5
1	H	241	VAL	2.5
1	D	289	GLU	2.4
1	A	175	LEU	2.4
1	G	366	PRO	2.4
1	C	33	SER	2.4
1	A	199	PHE	2.4
1	C	352	PRO	2.4
1	E	289	GLU	2.4
1	F	416	SER	2.4
1	D	323	SER	2.4
1	F	175	LEU	2.4
1	H	118	HIS	2.4
1	F	415	ILE	2.4
1	G	370	PHE	2.4
1	H	301	LEU	2.4
1	C	400	CYS	2.4
1	D	404	ASP	2.4
1	H	305	LEU	2.4
1	H	398	HIS	2.3
1	G	92	TYR	2.3
1	H	240	ASP	2.3
1	A	305	LEU	2.3
1	D	188	PRO	2.3
1	E	33	SER	2.3
1	C	430	THR	2.3
1	A	191	HIS	2.3
1	H	381	HIS	2.3
1	B	231	LEU	2.3
1	H	435	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	222	LYS	2.3
1	D	351	SER	2.3
1	H	287	HIS	2.3
1	B	263	TYR	2.3
1	B	305	LEU	2.3
1	E	305	LEU	2.3
1	B	239	ILE	2.3
1	G	390	TRP	2.3
1	H	171	PHE	2.3
1	D	352	PRO	2.3
1	C	93	PRO	2.3
1	B	437	MET	2.3
1	G	118	HIS	2.3
1	F	398	HIS	2.3
1	G	33	SER	2.3
1	G	323	SER	2.3
1	E	290	VAL	2.3
1	G	287	HIS	2.2
1	H	365	PHE	2.2
1	E	250	PHE	2.2
1	E	287	HIS	2.2
1	A	245	GLN	2.2
1	F	352	PRO	2.2
1	E	352	PRO	2.2
1	C	192	PRO	2.2
1	F	193	LEU	2.2
1	C	300	THR	2.2
1	A	290	VAL	2.2
1	B	116	GLY	2.2
1	G	181	LEU	2.2
1	F	240	ASP	2.2
1	H	188	PRO	2.2
1	D	34	PRO	2.2
1	D	396	PRO	2.2
1	E	191	HIS	2.2
1	A	352	PRO	2.2
1	H	34	PRO	2.2
1	H	385	ALA	2.2
1	D	322	TRP	2.2
1	A	288	THR	2.2
1	G	398	HIS	2.2
1	G	289	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	317	ARG	2.2
1	B	250	PHE	2.2
1	H	288	THR	2.1
1	F	214	TYR	2.1
1	B	181	LEU	2.1
1	H	444	GLN	2.1
1	H	443	SER	2.1
1	H	177	GLU	2.1
1	E	207	GLY	2.1
1	C	188	PRO	2.1
1	G	189	ASP	2.1
1	H	193	LEU	2.1
1	D	175	LEU	2.1
1	F	303	GLY	2.1
1	E	242	GLU	2.1
1	E	328	GLY	2.1
1	H	96	TRP	2.1
1	F	400	CYS	2.1
1	E	214	TYR	2.1
1	F	330	GLY	2.1
1	H	416	SER	2.1
1	D	401	ALA	2.1
1	G	326	GLN	2.1
1	H	196	GLN	2.1
1	F	187	GLY	2.1
1	H	203	PHE	2.1
1	H	366	PRO	2.1
1	H	403	PRO	2.1
1	C	370	PHE	2.1
1	H	323	SER	2.1
1	D	33	SER	2.1
1	A	401	ALA	2.1
1	F	198	ALA	2.1
1	C	416	SER	2.0
1	E	239	ILE	2.0
1	G	385	ALA	2.0
1	G	400	CYS	2.0
1	H	401	ALA	2.0
1	D	76	GLN	2.0
1	F	188	PRO	2.0
1	B	443	SER	2.0
1	E	312	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	327	ILE	2.0
1	A	287	HIS	2.0
1	B	398	HIS	2.0
1	D	190	ALA	2.0
1	F	263	TYR	2.0
1	H	216	PHE	2.0
1	D	365	PHE	2.0
1	G	320	GLN	2.0
1	E	95	LYS	2.0
1	E	188	PRO	2.0
1	C	289	GLU	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 oligosaccharides 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.