



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DAO  
Title : COVALENT ADDUCT OF D-AMINO ACID OXIDASE FROM PIG KIDNEY WITH 3-METHYL-2-OXO-VALERIC ACID  
Authors : Todone, F.; Mattevi, A.  
Deposited on : 1997-01-16  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

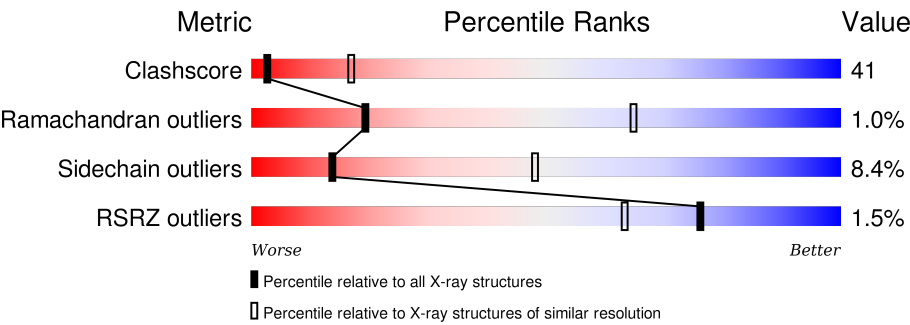
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	347	<div><div></div><div>42%42%12%..</div></div>
1	B	347	<div><div>2%</div><div>41%43%12%..</div></div>
1	C	347	<div><div>2%</div><div>40%44%11%..</div></div>
1	D	347	<div><div>2%</div><div>41%45%11%..</div></div>
1	E	347	<div><div>%</div><div>41%44%11%..</div></div>
1	F	347	<div><div>%</div><div>44%41%12%..</div></div>
1	G	347	<div><div>2%</div><div>40%45%11%..</div></div>

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Mol	Chain	Length	Quality of chain
1	H	347	<div><div></div><div>2%</div><div>42%</div><div>43%</div><div>12%</div><div>••</div></div>

## 2 Entry composition

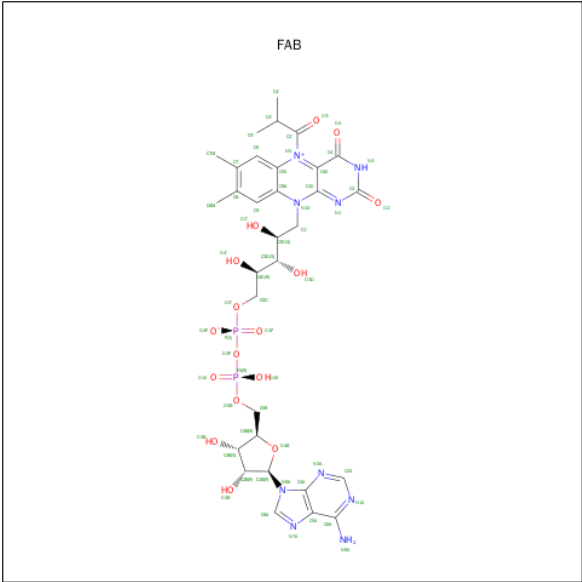
There are 3 unique types of molecules in this entry. The entry contains 22232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-AMINO ACID OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	103	0	0
			2720	1749	473	489	9			
1	B	339	Total	C	N	O	S	104	0	0
			2720	1749	473	489	9			
1	C	339	Total	C	N	O	S	109	0	0
			2720	1749	473	489	9			
1	D	339	Total	C	N	O	S	99	0	0
			2720	1749	473	489	9			
1	E	339	Total	C	N	O	S	113	0	0
			2720	1749	473	489	9			
1	F	339	Total	C	N	O	S	111	0	0
			2720	1749	473	489	9			
1	G	339	Total	C	N	O	S	116	0	0
			2720	1749	473	489	9			
1	H	339	Total	C	N	O	S	112	0	0
			2720	1749	473	489	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE-N5-ISOBUTYL KETONE (three-letter code: FAB) (formula: C<sub>31</sub>H<sub>39</sub>N<sub>9</sub>O<sub>16</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	C	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	D	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	E	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	F	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	G	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	H	1	Total	C	N	O	P	0	0
			58	31	9	16	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

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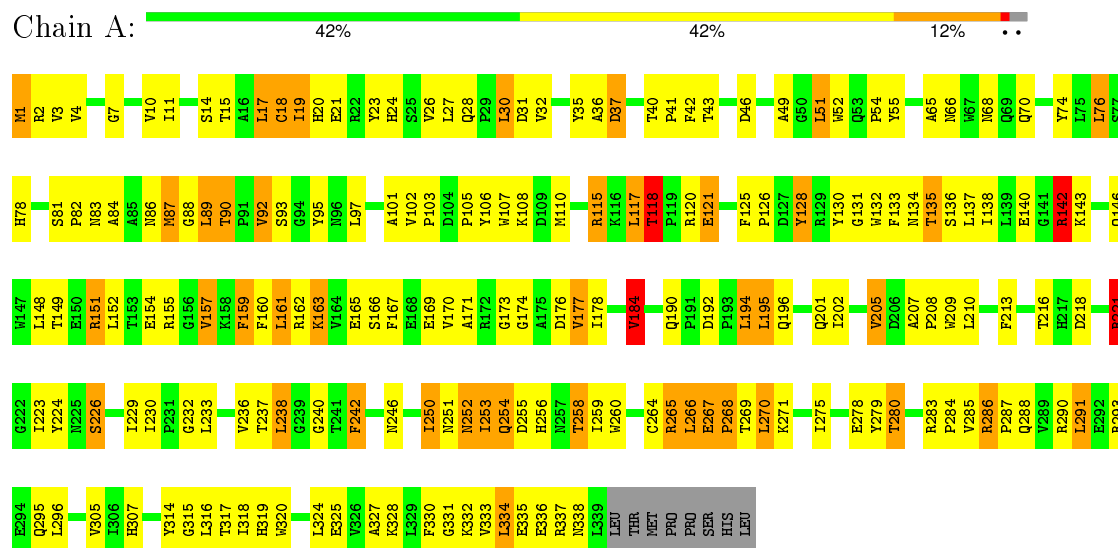
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0

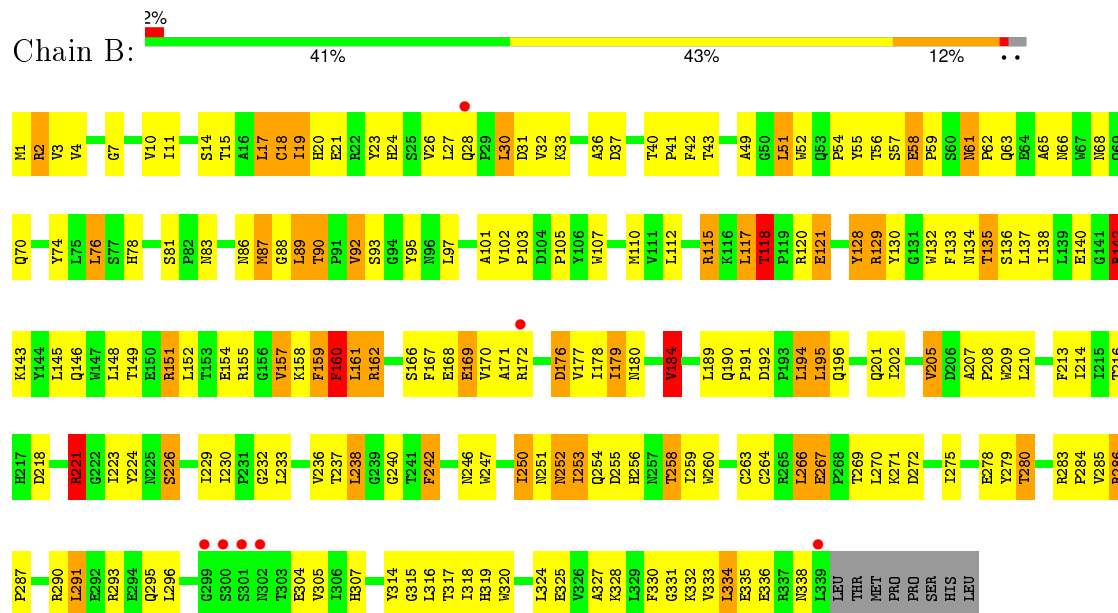
### 3 Residue-property plots

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.

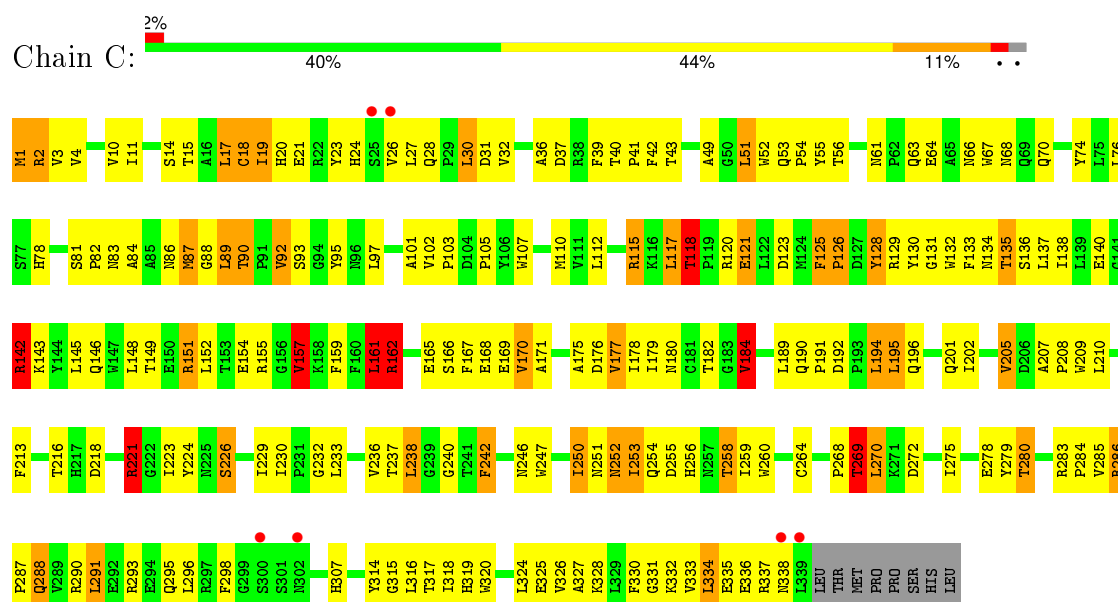
#### • Molecule 1: D-AMINO ACID OXIDASE



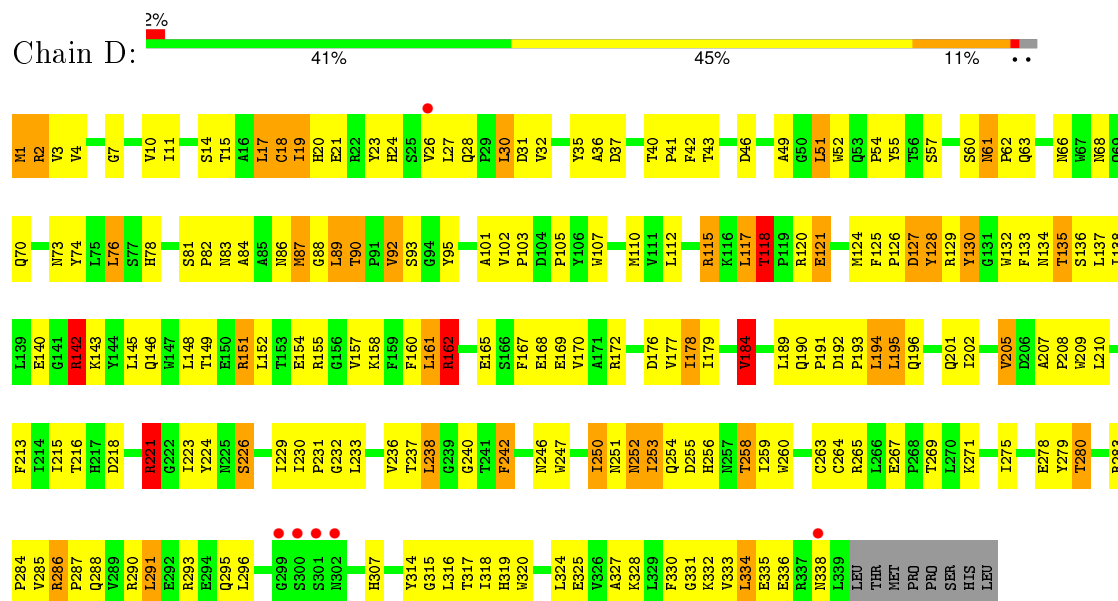
#### • Molecule 1: D-AMINO ACID OXIDASE



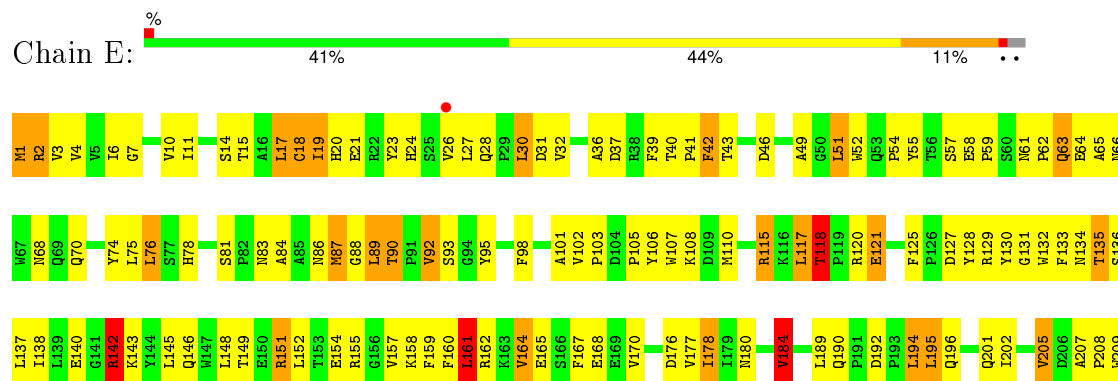
#### • Molecule 1: D-AMINO ACID OXIDASE



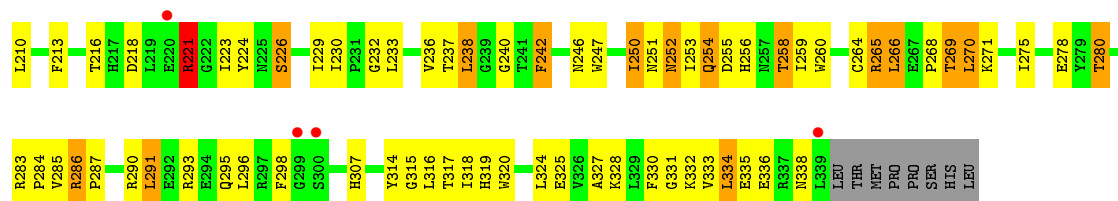
• Molecule 1: D-AMINO ACID OXIDASE



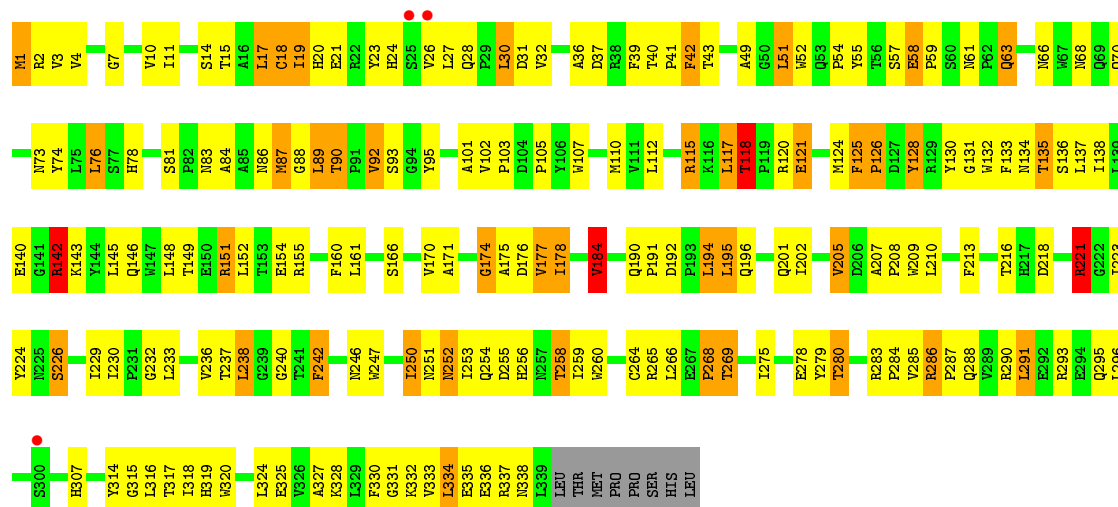
• Molecule 1: D-AMINO ACID OXIDASE



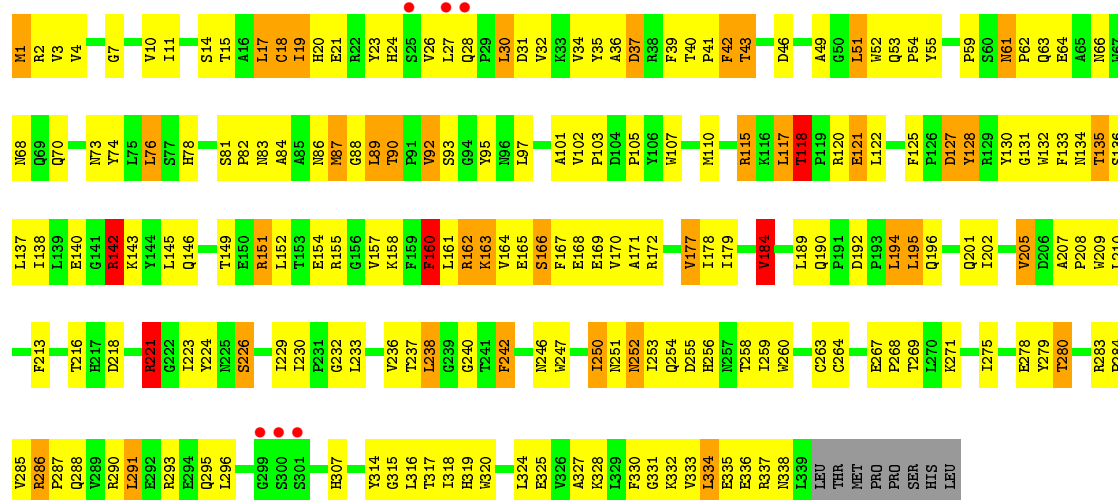




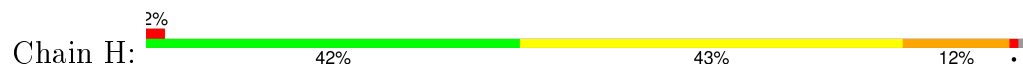
• Molecule 1: D-AMINO ACID OXIDASE

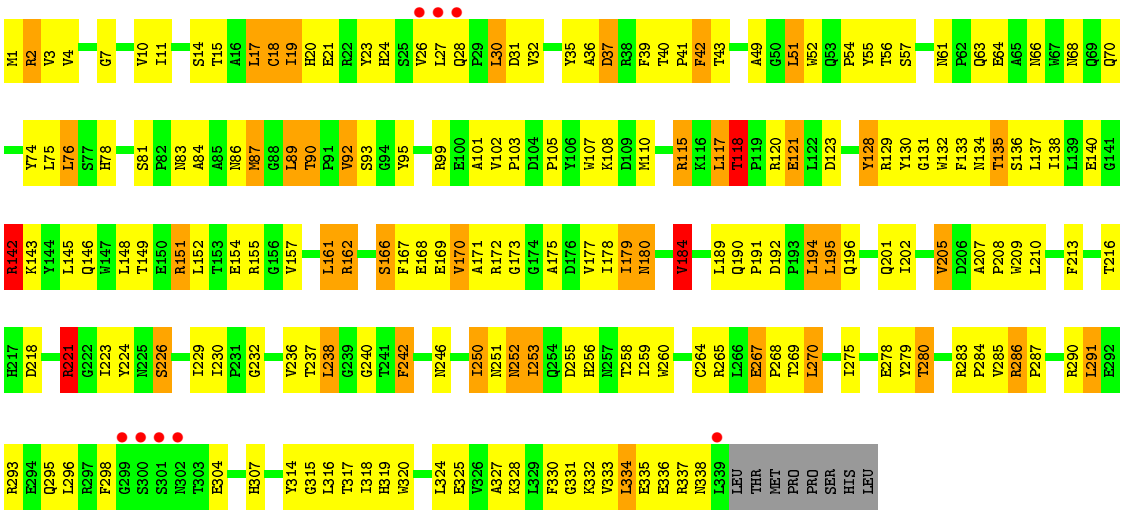


• Molecule 1: D-AMINO ACID OXIDASE



• Molecule 1: D-AMINO ACID OXIDASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	326.40 Å   136.90 Å   196.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-3.20) 99.7 (19.96-3.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.32 (at 3.22 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.232   ,   0.260 0.249   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 113.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.28$ , $\langle L^2 \rangle = 0.12$	Xtriage
Outliers	0 of 72258 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	22232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.83	1/2796 (0.0%)	1.60	48/3808 (1.3%)
1	B	0.80	1/2796 (0.0%)	1.57	49/3808 (1.3%)
1	C	0.81	1/2796 (0.0%)	1.60	46/3808 (1.2%)
1	D	0.83	1/2796 (0.0%)	1.70	50/3808 (1.3%)
1	E	0.80	1/2796 (0.0%)	1.58	48/3808 (1.3%)
1	F	0.82	1/2796 (0.0%)	1.57	42/3808 (1.1%)
1	G	0.86	3/2796 (0.1%)	1.57	45/3808 (1.2%)
1	H	0.81	1/2796 (0.0%)	1.58	45/3808 (1.2%)
All	All	0.82	10/22368 (0.0%)	1.60	373/30464 (1.2%)

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	A	0	1
1	C	0	1
1	G	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	163	LYS	CE-NZ	-15.43	1.10	1.49
1	G	166	SER	CB-OG	-6.10	1.34	1.42
1	C	143	LYS	CE-NZ	5.09	1.61	1.49
1	F	143	LYS	CE-NZ	5.08	1.61	1.49
1	E	143	LYS	CE-NZ	5.07	1.61	1.49
1	B	143	LYS	CE-NZ	5.06	1.61	1.49
1	D	143	LYS	CE-NZ	5.06	1.61	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	LYS	CE-NZ	5.06	1.61	1.49
1	H	143	LYS	CE-NZ	5.06	1.61	1.49
1	G	143	LYS	CE-NZ	5.05	1.61	1.49

All (373) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ARG	NE-CZ-NH1	-29.91	105.34	120.30
1	D	129	ARG	NE-CZ-NH2	21.15	130.87	120.30
1	D	127	ASP	CB-CG-OD1	-12.02	107.48	118.30
1	E	120	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	A	120	ARG	NE-CZ-NH1	-11.23	114.68	120.30
1	C	120	ARG	NE-CZ-NH1	-11.23	114.69	120.30
1	D	120	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	B	266	LEU	CB-CG-CD1	-11.21	91.93	111.00
1	B	120	ARG	NE-CZ-NH1	-11.20	114.70	120.30
1	H	120	ARG	NE-CZ-NH1	-11.19	114.71	120.30
1	G	120	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	F	120	ARG	NE-CZ-NH1	-11.17	114.72	120.30
1	B	266	LEU	CB-CG-CD2	10.31	128.53	111.00
1	C	161	LEU	CB-CG-CD1	10.31	128.53	111.00
1	D	126	PRO	C-N-CA	-9.98	96.76	121.70
1	F	125	PHE	C-N-CD	-9.52	99.66	120.60
1	A	270	LEU	CB-CG-CD1	-9.45	94.94	111.00
1	C	162	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	C	92	VAL	CB-CA-C	-9.30	93.72	111.40
1	F	92	VAL	CB-CA-C	-9.29	93.74	111.40
1	A	92	VAL	CB-CA-C	-9.28	93.76	111.40
1	B	92	VAL	CB-CA-C	-9.28	93.77	111.40
1	E	92	VAL	CB-CA-C	-9.28	93.77	111.40
1	D	92	VAL	CB-CA-C	-9.28	93.77	111.40
1	G	92	VAL	CB-CA-C	-9.27	93.78	111.40
1	H	92	VAL	CB-CA-C	-9.26	93.81	111.40
1	H	270	LEU	CB-CG-CD2	-8.84	95.97	111.00
1	E	270	LEU	CB-CG-CD2	-8.65	96.30	111.00
1	F	142	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	B	142	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	G	142	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	C	142	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	H	142	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	142	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	D	142	ARG	NE-CZ-NH2	-8.45	116.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	90	THR	N-CA-CB	8.06	125.61	110.30
1	E	90	THR	N-CA-CB	8.04	125.57	110.30
1	D	90	THR	N-CA-CB	8.04	125.57	110.30
1	A	90	THR	N-CA-CB	8.03	125.56	110.30
1	C	90	THR	N-CA-CB	8.03	125.56	110.30
1	H	90	THR	N-CA-CB	8.02	125.53	110.30
1	F	90	THR	N-CA-CB	8.01	125.52	110.30
1	G	90	THR	N-CA-CB	8.00	125.51	110.30
1	C	194	LEU	CA-CB-CG	-7.87	97.19	115.30
1	H	194	LEU	CA-CB-CG	-7.87	97.19	115.30
1	E	194	LEU	CA-CB-CG	-7.87	97.20	115.30
1	D	194	LEU	CA-CB-CG	-7.87	97.21	115.30
1	A	194	LEU	CA-CB-CG	-7.86	97.22	115.30
1	B	194	LEU	CA-CB-CG	-7.86	97.23	115.30
1	G	194	LEU	CA-CB-CG	-7.86	97.23	115.30
1	F	194	LEU	CA-CB-CG	-7.84	97.26	115.30
1	B	162	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	A	177	VAL	CA-CB-CG2	-7.74	99.29	110.90
1	B	283	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	283	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	E	283	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	H	283	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	G	283	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	283	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	283	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	F	283	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	161	LEU	CA-CB-CG	-7.49	98.07	115.30
1	B	221	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	E	221	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	G	221	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	G	177	VAL	CB-CA-C	-7.31	97.50	111.40
1	F	221	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	221	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	D	221	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	H	221	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	C	221	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	C	270	LEU	CB-CG-CD2	-7.22	98.73	111.00
1	E	266	LEU	CB-CG-CD2	-7.11	98.91	111.00
1	F	286	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	D	286	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	A	286	ARG	NE-CZ-NH1	-7.06	116.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	E	286	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	C	286	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	H	286	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	H	170	VAL	CB-CA-C	-6.93	98.23	111.40
1	G	286	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	B	61	ASN	N-CA-C	-6.85	92.50	111.00
1	G	160	PHE	CB-CG-CD1	-6.79	116.05	120.80
1	G	162	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	C	159	PHE	CB-CA-C	-6.69	97.02	110.40
1	A	163	LYS	N-CA-C	-6.68	92.95	111.00
1	A	128	TYR	CA-CB-CG	-6.62	100.83	113.40
1	B	202	ILE	CB-CA-C	-6.55	98.50	111.60
1	H	202	ILE	CB-CA-C	-6.55	98.51	111.60
1	C	202	ILE	CB-CA-C	-6.54	98.52	111.60
1	E	202	ILE	CB-CA-C	-6.53	98.53	111.60
1	F	202	ILE	CB-CA-C	-6.53	98.54	111.60
1	D	202	ILE	CB-CA-C	-6.53	98.54	111.60
1	G	202	ILE	CB-CA-C	-6.53	98.54	111.60
1	A	202	ILE	CB-CA-C	-6.52	98.57	111.60
1	D	179	ILE	CB-CA-C	6.49	124.57	111.60
1	D	149	THR	CA-CB-CG2	-6.46	103.36	112.40
1	B	149	THR	CA-CB-CG2	-6.45	103.37	112.40
1	A	149	THR	CA-CB-CG2	-6.45	103.38	112.40
1	G	149	THR	CA-CB-CG2	-6.45	103.38	112.40
1	F	149	THR	CA-CB-CG2	-6.44	103.39	112.40
1	C	149	THR	CA-CB-CG2	-6.43	103.39	112.40
1	E	149	THR	CA-CB-CG2	-6.43	103.39	112.40
1	H	149	THR	CA-CB-CG2	-6.43	103.40	112.40
1	F	178	ILE	CB-CA-C	-6.42	98.75	111.60
1	B	89	LEU	CB-CG-CD1	-6.40	100.12	111.00
1	D	89	LEU	CB-CG-CD1	-6.40	100.12	111.00
1	C	89	LEU	CB-CG-CD1	-6.40	100.13	111.00
1	H	89	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	A	89	LEU	CB-CG-CD1	-6.39	100.14	111.00
1	C	157	VAL	CG1-CB-CG2	6.37	121.09	110.90
1	E	89	LEU	CB-CG-CD1	-6.37	100.17	111.00
1	F	89	LEU	CB-CG-CD1	-6.37	100.18	111.00
1	G	89	LEU	CB-CG-CD1	-6.36	100.19	111.00
1	H	140	GLU	OE1-CD-OE2	6.34	130.90	123.30
1	H	162	ARG	CG-CD-NE	-6.33	98.51	111.80
1	D	140	GLU	OE1-CD-OE2	6.29	130.85	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	140	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	B	140	GLU	OE1-CD-OE2	6.27	130.83	123.30
1	E	140	GLU	OE1-CD-OE2	6.27	130.82	123.30
1	G	128	TYR	N-CA-CB	6.27	121.88	110.60
1	A	140	GLU	OE1-CD-OE2	6.26	130.82	123.30
1	G	140	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	C	140	GLU	OE1-CD-OE2	6.25	130.81	123.30
1	D	128	TYR	CB-CA-C	6.24	122.87	110.40
1	G	163	LYS	CG-CD-CE	6.23	130.59	111.90
1	H	162	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	H	184	VAL	CB-CA-C	-6.20	99.62	111.40
1	A	266	LEU	CB-CG-CD2	-6.20	100.46	111.00
1	D	184	VAL	CB-CA-C	-6.19	99.64	111.40
1	G	184	VAL	CB-CA-C	-6.19	99.64	111.40
1	F	184	VAL	CB-CA-C	-6.18	99.66	111.40
1	A	184	VAL	CB-CA-C	-6.18	99.66	111.40
1	E	184	VAL	CB-CA-C	-6.17	99.68	111.40
1	D	162	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	C	184	VAL	CB-CA-C	-6.16	99.70	111.40
1	B	172	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	B	184	VAL	CB-CA-C	-6.15	99.71	111.40
1	B	334	LEU	CB-CG-CD1	-6.14	100.56	111.00
1	G	37	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	37	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	2	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	A	334	LEU	CB-CG-CD1	-6.12	100.60	111.00
1	C	334	LEU	CB-CG-CD1	-6.12	100.60	111.00
1	A	37	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	37	ASP	CB-CG-OD2	6.11	123.80	118.30
1	H	334	LEU	CB-CG-CD1	-6.11	100.61	111.00
1	E	334	LEU	CB-CG-CD1	-6.11	100.62	111.00
1	C	89	LEU	CB-CA-C	-6.11	98.60	110.20
1	E	89	LEU	CB-CA-C	-6.11	98.60	110.20
1	A	89	LEU	CB-CA-C	-6.10	98.61	110.20
1	F	334	LEU	CB-CG-CD1	-6.10	100.63	111.00
1	G	334	LEU	CB-CG-CD1	-6.10	100.63	111.00
1	D	37	ASP	CB-CG-OD2	6.10	123.79	118.30
1	F	37	ASP	CB-CG-OD2	6.09	123.78	118.30
1	H	89	LEU	CB-CA-C	-6.09	98.62	110.20
1	H	37	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	334	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	B	89	LEU	CB-CA-C	-6.08	98.65	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	ASP	CB-CG-OD2	6.08	123.77	118.30
1	G	89	LEU	CB-CA-C	-6.08	98.65	110.20
1	F	117	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	H	117	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	D	89	LEU	CB-CA-C	-6.07	98.66	110.20
1	F	89	LEU	CB-CA-C	-6.07	98.67	110.20
1	A	117	LEU	CB-CG-CD1	-6.07	100.69	111.00
1	F	2	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	H	2	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	C	117	LEU	CB-CG-CD1	-6.07	100.69	111.00
1	E	117	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	G	2	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	D	117	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	G	117	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	A	2	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	E	265	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	117	LEU	CB-CG-CD1	-6.04	100.74	111.00
1	E	2	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	B	2	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	G	1	MET	CA-CB-CG	-6.02	103.07	113.30
1	B	1	MET	CA-CB-CG	-6.01	103.08	113.30
1	E	1	MET	CA-CB-CG	-6.01	103.08	113.30
1	D	1	MET	CA-CB-CG	-6.01	103.08	113.30
1	F	1	MET	CA-CB-CG	-6.01	103.08	113.30
1	A	1	MET	CA-CB-CG	-6.01	103.09	113.30
1	H	1	MET	CA-CB-CG	-6.01	103.09	113.30
1	C	2	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	C	1	MET	CA-CB-CG	-6.00	103.10	113.30
1	B	65	ALA	CB-CA-C	-5.98	101.13	110.10
1	H	56	THR	CA-CB-CG2	-5.97	104.04	112.40
1	F	266	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	A	268	PRO	N-CD-CG	-5.88	94.39	103.20
1	E	254	GLN	CA-CB-CG	5.87	126.32	113.40
1	C	269	THR	OG1-CB-CG2	-5.86	96.53	110.00
1	G	166	SER	N-CA-CB	-5.86	101.72	110.50
1	B	129	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	C	177	VAL	CB-CA-C	-5.82	100.34	111.40
1	B	157	VAL	CA-CB-CG1	-5.80	102.20	110.90
1	B	121	GLU	CG-CD-OE1	-5.79	106.72	118.30
1	C	18	CYS	N-CA-CB	-5.79	100.18	110.60
1	F	43	THR	CA-CB-CG2	-5.79	104.30	112.40
1	C	121	GLU	CG-CD-OE1	-5.78	106.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	E	121	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	F	18	CYS	N-CA-CB	-5.78	100.19	110.60
1	A	121	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	D	18	CYS	N-CA-CB	-5.78	100.21	110.60
1	A	18	CYS	N-CA-CB	-5.77	100.21	110.60
1	A	43	THR	CA-CB-CG2	-5.77	104.32	112.40
1	B	43	THR	CA-CB-CG2	-5.77	104.32	112.40
1	F	121	GLU	CG-CD-OE1	-5.77	106.76	118.30
1	H	43	THR	CA-CB-CG2	-5.77	104.32	112.40
1	B	18	CYS	N-CA-CB	-5.77	100.22	110.60
1	C	43	THR	CA-CB-CG2	-5.77	104.33	112.40
1	E	43	THR	CA-CB-CG2	-5.77	104.33	112.40
1	H	121	GLU	CG-CD-OE1	-5.77	106.76	118.30
1	G	43	THR	CA-CB-CG2	-5.77	104.33	112.40
1	G	121	GLU	CG-CD-OE1	-5.76	106.78	118.30
1	D	43	THR	CA-CB-CG2	-5.76	104.34	112.40
1	G	18	CYS	N-CA-CB	-5.75	100.24	110.60
1	E	18	CYS	N-CA-CB	-5.75	100.25	110.60
1	H	18	CYS	N-CA-CB	-5.75	100.26	110.60
1	E	161	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	F	266	LEU	CA-CB-CG	5.71	128.44	115.30
1	F	128	TYR	CA-CB-CG	-5.71	102.55	113.40
1	H	128	TYR	CA-CB-CG	-5.71	102.56	113.40
1	D	128	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
1	H	250	ILE	CB-CA-C	-5.69	100.22	111.60
1	D	250	ILE	CB-CA-C	-5.69	100.23	111.60
1	B	250	ILE	CB-CA-C	-5.68	100.24	111.60
1	G	250	ILE	CB-CA-C	-5.68	100.24	111.60
1	A	250	ILE	CB-CA-C	-5.68	100.25	111.60
1	E	250	ILE	CB-CA-C	-5.68	100.25	111.60
1	F	250	ILE	CB-CA-C	-5.68	100.25	111.60
1	C	250	ILE	CB-CA-C	-5.67	100.27	111.60
1	B	128	TYR	N-CA-CB	-5.66	100.41	110.60
1	D	265	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	G	160	PHE	CD1-CE1-CZ	-5.65	113.33	120.10
1	A	176	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	D	129	ARG	CB-CA-C	-5.62	99.15	110.40
1	C	128	TYR	CA-CB-CG	-5.59	102.77	113.40
1	B	159	PHE	CB-CA-C	-5.59	99.22	110.40
1	D	178	ILE	CG1-CB-CG2	5.57	123.65	111.40
1	F	63	GLN	CB-CA-C	-5.52	99.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	177	VAL	CA-CB-CG2	-5.52	102.62	110.90
1	H	118	THR	CA-CB-CG2	-5.52	104.68	112.40
1	D	127	ASP	CB-CG-OD2	5.51	123.25	118.30
1	G	118	THR	CA-CB-CG2	-5.50	104.69	112.40
1	A	118	THR	CA-CB-CG2	-5.49	104.71	112.40
1	B	160	PHE	CB-CA-C	-5.49	99.41	110.40
1	H	267	GLU	CB-CA-C	-5.49	99.41	110.40
1	E	118	THR	CA-CB-CG2	-5.49	104.72	112.40
1	B	118	THR	CA-CB-CG2	-5.48	104.72	112.40
1	A	265	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	F	118	THR	CA-CB-CG2	-5.47	104.74	112.40
1	E	164	VAL	CB-CA-C	-5.47	101.02	111.40
1	D	118	THR	CA-CB-CG2	-5.46	104.75	112.40
1	G	164	VAL	N-CA-C	-5.46	96.27	111.00
1	C	118	THR	CA-CB-CG2	-5.45	104.77	112.40
1	C	120	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	57	SER	N-CA-CB	-5.43	102.35	110.50
1	C	170	VAL	CG1-CB-CG2	5.43	119.59	110.90
1	E	266	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	E	178	ILE	CB-CA-C	-5.43	100.74	111.60
1	H	2	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	E	129	ARG	C-N-CA	-5.41	108.18	121.70
1	F	120	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	E	120	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	F	17	LEU	CA-CB-CG	-5.39	102.89	115.30
1	G	120	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	B	120	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	D	17	LEU	CA-CB-CG	-5.39	102.91	115.30
1	F	2	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	B	17	LEU	CA-CB-CG	-5.38	102.93	115.30
1	A	17	LEU	CA-CB-CG	-5.38	102.93	115.30
1	A	120	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	G	17	LEU	CA-CB-CG	-5.38	102.94	115.30
1	C	17	LEU	CA-CB-CG	-5.36	102.97	115.30
1	H	166	SER	C-N-CA	-5.36	108.30	121.70
1	B	2	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	E	17	LEU	CA-CB-CG	-5.36	102.97	115.30
1	H	17	LEU	CA-CB-CG	-5.36	102.98	115.30
1	D	2	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	H	120	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	2	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	C	2	ARG	NE-CZ-NH1	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	D	120	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	E	127	ASP	C-N-CA	-5.30	108.44	121.70
1	B	19	ILE	CB-CA-C	-5.30	101.00	111.60
1	H	19	ILE	CB-CA-C	-5.30	101.00	111.60
1	D	19	ILE	CB-CA-C	-5.29	101.01	111.60
1	F	37	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	F	142	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	19	ILE	CB-CA-C	-5.29	101.02	111.60
1	E	19	ILE	CB-CA-C	-5.29	101.02	111.60
1	F	19	ILE	CB-CA-C	-5.29	101.02	111.60
1	C	19	ILE	CB-CA-C	-5.29	101.03	111.60
1	B	37	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	G	142	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	37	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	G	19	ILE	CB-CA-C	-5.28	101.05	111.60
1	G	195	LEU	CB-CG-CD1	-5.27	102.03	111.00
1	H	195	LEU	CB-CG-CD1	-5.27	102.05	111.00
1	D	179	ILE	CA-CB-CG1	-5.26	101.00	111.00
1	D	195	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	A	37	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	161	LEU	N-CA-C	-5.26	96.81	111.00
1	A	195	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	G	37	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	C	87	MET	CG-SD-CE	-5.25	91.80	100.20
1	E	195	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	F	195	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	D	1	MET	CB-CG-SD	-5.25	96.66	112.40
1	F	1	MET	CB-CG-SD	-5.25	96.66	112.40
1	G	128	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	B	87	MET	CG-SD-CE	-5.24	91.81	100.20
1	G	1	MET	CB-CG-SD	-5.24	96.68	112.40
1	E	1	MET	CB-CG-SD	-5.24	96.69	112.40
1	F	87	MET	CG-SD-CE	-5.24	91.82	100.20
1	B	1	MET	CB-CG-SD	-5.24	96.69	112.40
1	D	42	PHE	N-CA-C	5.23	125.13	111.00
1	H	37	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	C	1	MET	CB-CG-SD	-5.23	96.70	112.40
1	A	1	MET	CB-CG-SD	-5.23	96.71	112.40
1	C	37	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	195	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	C	42	PHE	N-CA-C	5.23	125.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	H	1	MET	CB-CG-SD	-5.23	96.72	112.40
1	C	195	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	E	42	PHE	N-CA-C	5.22	125.11	111.00
1	A	87	MET	CG-SD-CE	-5.22	91.85	100.20
1	A	42	PHE	N-CA-C	5.22	125.09	111.00
1	E	37	ASP	CB-CG-OD1	-5.22	113.61	118.30
1	G	87	MET	CG-SD-CE	-5.22	91.85	100.20
1	F	42	PHE	N-CA-C	5.21	125.08	111.00
1	G	42	PHE	N-CA-C	5.21	125.08	111.00
1	H	42	PHE	N-CA-C	5.21	125.07	111.00
1	D	87	MET	CG-SD-CE	-5.20	91.87	100.20
1	B	42	PHE	N-CA-C	5.20	125.04	111.00
1	C	142	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	87	MET	CG-SD-CE	-5.20	91.88	100.20
1	A	142	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	270	LEU	CA-CB-CG	-5.20	103.35	115.30
1	A	126	PRO	C-N-CA	-5.19	108.72	121.70
1	H	142	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	269	THR	CA-CB-CG2	-5.18	105.15	112.40
1	H	87	MET	CG-SD-CE	-5.18	91.92	100.20
1	B	51	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	B	142	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	51	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	E	51	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	D	51	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	51	LEU	CB-CG-CD1	-5.16	102.24	111.00
1	E	142	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	F	51	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	D	142	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	H	51	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	G	51	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	H	179	ILE	CG1-CB-CG2	5.12	122.67	111.40
1	H	166	SER	CB-CA-C	-5.12	100.38	110.10
1	A	265	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	G	288	GLN	N-CA-CB	5.12	119.81	110.60
1	A	268	PRO	CA-CB-CG	-5.11	94.30	104.00
1	E	162	ARG	N-CA-CB	-5.09	101.43	110.60
1	C	161	LEU	CB-CA-C	5.06	119.82	110.20
1	D	127	ASP	N-CA-C	5.06	124.67	111.00
1	D	288	GLN	N-CA-C	-5.06	97.35	111.00
1	B	179	ILE	CG1-CB-CG2	-5.04	100.31	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	THR	N-CA-CB	5.02	119.84	110.30
1	B	17	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	PHE	Sidechain
1	C	125	PHE	Sidechain
1	G	160	PHE	Sidechain

## 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	2720	0	2675	221	0
1	B	2720	0	2675	218	0
1	C	2720	0	2675	214	3
1	D	2720	0	2675	211	1
1	E	2720	0	2675	234	1
1	F	2720	0	2675	207	1
1	G	2720	0	2675	222	1
1	H	2720	0	2675	208	3
2	A	58	0	38	6	0
2	B	58	0	38	7	0
2	C	58	0	38	5	0
2	D	58	0	38	6	0
2	E	58	0	38	7	0
2	F	58	0	38	7	0
2	G	58	0	38	7	0
2	H	58	0	38	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	1	0
3	H	1	0	0	0	0
All	All	22232	0	21704	1695	5

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 41.

All (1695) 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:E:61:ASN:ND2	1:E:63:GLN:HG3	1.11	1.38
1:E:61:ASN:ND2	1:E:63:GLN:CG	1.89	1.35
1:E:61:ASN:HD21	1:E:63:GLN:NE2	1.40	1.19
1:A:253:ILE:HG13	1:F:42:PHE:CD1	1.88	1.08
1:B:250:ILE:HD11	1:E:250:ILE:CD1	1.88	1.04
1:F:1:MET:CE	1:F:177:VAL:HG23	1.90	1.02
1:E:61:ASN:ND2	1:E:63:GLN:HE21	1.56	1.02
1:B:23:TYR:HD1	1:B:26:VAL:HG11	1.26	1.01
1:A:23:TYR:HD1	1:A:26:VAL:HG11	1.25	1.00
1:C:23:TYR:HD1	1:C:26:VAL:HG11	1.25	1.00
1:H:23:TYR:HD1	1:H:26:VAL:HG11	1.25	1.00
1:B:253:ILE:HG13	1:E:42:PHE:CD1	1.96	0.99
1:G:23:TYR:HD1	1:G:26:VAL:HG11	1.25	0.98
1:D:23:TYR:HD1	1:D:26:VAL:HG11	1.25	0.97
1:E:23:TYR:HD1	1:E:26:VAL:HG11	1.26	0.97
1:F:23:TYR:HD1	1:F:26:VAL:HG11	1.26	0.97
1:G:53:GLN:HG2	3:G:349:HOH:O	1.65	0.96
1:C:101:ALA:HA	1:C:130:TYR:CD2	1.99	0.96
1:F:209:TRP:HE1	1:F:269:THR:HG1	1.12	0.95
1:B:250:ILE:HD11	1:E:250:ILE:HD11	1.48	0.94
1:F:61:ASN:OD1	1:F:63:GLN:HG3	1.68	0.94
1:F:256:HIS:ND1	1:F:278:GLU:OE2	2.01	0.93
1:G:167:PHE:CE1	1:G:189:LEU:HB3	2.02	0.93
1:E:256:HIS:ND1	1:E:278:GLU:OE2	2.01	0.93
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.34	0.93
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.34	0.93
1:C:256:HIS:ND1	1:C:278:GLU:OE2	2.02	0.93
1:B:256:HIS:ND1	1:B:278:GLU:OE2	2.02	0.93
1:D:142:ARG:HG3	1:D:142:ARG:HH11	1.34	0.93
1:G:142:ARG:HG3	1:G:142:ARG:HH11	1.34	0.93
1:A:256:HIS:ND1	1:A:278:GLU:OE2	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:HIS:ND1	1:G:278:GLU:OE2	2.01	0.92
1:E:61:ASN:HD21	1:E:63:GLN:CD	1.71	0.92
1:H:256:HIS:ND1	1:H:278:GLU:OE2	2.01	0.92
1:F:142:ARG:HG3	1:F:142:ARG:HH11	1.34	0.92
1:D:256:HIS:ND1	1:D:278:GLU:OE2	2.02	0.91
1:H:142:ARG:HH11	1:H:142:ARG:HG3	1.34	0.91
1:E:61:ASN:HD22	1:E:63:GLN:HG3	1.32	0.91
1:C:142:ARG:HH11	1:C:142:ARG:HG3	1.34	0.90
1:E:61:ASN:HD21	1:E:63:GLN:HE21	1.04	0.90
1:E:61:ASN:ND2	1:E:63:GLN:NE2	2.14	0.90
1:E:142:ARG:HH11	1:E:142:ARG:HG3	1.34	0.90
1:E:93:SER:OG	1:E:135:THR:HB	1.73	0.89
1:D:93:SER:OG	1:D:135:THR:HB	1.73	0.89
1:G:93:SER:OG	1:G:135:THR:HB	1.72	0.89
1:A:93:SER:OG	1:A:135:THR:HB	1.73	0.89
1:C:93:SER:OG	1:C:135:THR:HB	1.73	0.89
1:B:250:ILE:CD1	1:E:250:ILE:CD1	2.51	0.88
1:F:93:SER:OG	1:F:135:THR:HB	1.72	0.88
1:B:93:SER:OG	1:B:135:THR:HB	1.73	0.88
1:H:167:PHE:CE2	1:H:189:LEU:HB3	2.08	0.88
1:E:92:VAL:CG2	1:E:138:ILE:HG13	2.04	0.88
1:D:92:VAL:CG2	1:D:138:ILE:HG13	2.04	0.87
1:E:61:ASN:CG	1:E:63:GLN:CG	2.42	0.87
1:H:93:SER:OG	1:H:135:THR:HB	1.72	0.87
1:G:92:VAL:CG2	1:G:138:ILE:HG13	2.04	0.87
1:B:92:VAL:CG2	1:B:138:ILE:HG13	2.04	0.86
1:A:92:VAL:CG2	1:A:138:ILE:HG13	2.04	0.86
1:A:23:TYR:CD1	1:A:26:VAL:HG11	2.10	0.86
1:C:23:TYR:CD1	1:C:26:VAL:HG11	2.10	0.86
1:E:23:TYR:CD1	1:E:26:VAL:HG11	2.10	0.86
1:C:92:VAL:CG2	1:C:138:ILE:HG13	2.04	0.86
1:H:92:VAL:CG2	1:H:138:ILE:HG13	2.04	0.86
1:F:92:VAL:CG2	1:F:138:ILE:HG13	2.04	0.86
1:D:23:TYR:CD1	1:D:26:VAL:HG11	2.10	0.86
1:B:33:LYS:HB3	1:B:160:PHE:HE1	1.41	0.86
1:F:1:MET:HE2	1:F:177:VAL:HG23	1.56	0.86
1:B:23:TYR:CD1	1:B:26:VAL:HG11	2.10	0.86
1:H:23:TYR:CD1	1:H:26:VAL:HG11	2.10	0.85
1:E:61:ASN:CG	1:E:63:GLN:HG3	1.96	0.85
1:F:125:PHE:N	1:F:126:PRO:HD3	1.92	0.85
1:G:23:TYR:CD1	1:G:26:VAL:HG11	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:TYR:CD1	1:F:26:VAL:HG11	2.10	0.84
1:C:20:HIS:CE1	1:C:155:ARG:HH11	1.95	0.84
1:A:20:HIS:CE1	1:A:155:ARG:HH11	1.95	0.84
1:B:20:HIS:CE1	1:B:155:ARG:HH11	1.95	0.84
1:H:20:HIS:CE1	1:H:155:ARG:HH11	1.95	0.84
1:B:21:GLU:HG3	1:B:155:ARG:NH2	1.93	0.84
1:D:20:HIS:CE1	1:D:155:ARG:HH11	1.95	0.84
1:F:21:GLU:HG3	1:F:155:ARG:NH2	1.93	0.84
1:C:21:GLU:HG3	1:C:155:ARG:NH2	1.93	0.84
1:F:20:HIS:CE1	1:F:155:ARG:HH11	1.95	0.83
1:G:21:GLU:HG3	1:G:155:ARG:NH2	1.93	0.83
1:E:20:HIS:CE1	1:E:155:ARG:HH11	1.95	0.83
1:A:24:HIS:HA	1:A:30:LEU:HD23	1.61	0.83
1:E:21:GLU:HG3	1:E:155:ARG:NH2	1.93	0.83
1:F:24:HIS:HA	1:F:30:LEU:HD23	1.61	0.83
1:G:20:HIS:CE1	1:G:155:ARG:HH11	1.95	0.83
1:D:21:GLU:HG3	1:D:155:ARG:NH2	1.92	0.83
1:E:252:ASN:HD21	1:E:255:ASP:CG	1.83	0.83
1:H:21:GLU:HG3	1:H:155:ARG:NH2	1.93	0.83
1:G:24:HIS:HA	1:G:30:LEU:HD23	1.61	0.83
1:B:24:HIS:HA	1:B:30:LEU:HD23	1.61	0.82
1:A:21:GLU:HG3	1:A:155:ARG:NH2	1.92	0.82
1:D:252:ASN:HD21	1:D:255:ASP:CG	1.83	0.82
1:A:250:ILE:HD11	1:F:250:ILE:CD1	2.08	0.82
1:G:252:ASN:HD21	1:G:255:ASP:CG	1.83	0.82
1:B:252:ASN:HD21	1:B:255:ASP:CG	1.83	0.82
1:F:252:ASN:HD21	1:F:255:ASP:CG	1.83	0.82
1:A:253:ILE:CG1	1:F:42:PHE:CD1	2.63	0.82
1:D:82:PRO:HA	1:H:268:PRO:HB2	1.60	0.82
1:H:24:HIS:HA	1:H:30:LEU:HD23	1.61	0.82
1:E:24:HIS:HA	1:E:30:LEU:HD23	1.61	0.81
1:B:128:TYR:N	1:B:128:TYR:CD1	2.45	0.81
1:H:118:THR:HG23	1:H:121:GLU:OE1	1.81	0.81
1:C:24:HIS:HA	1:C:30:LEU:HD23	1.61	0.81
1:F:118:THR:HG23	1:F:121:GLU:OE1	1.81	0.81
1:H:168:GLU:O	1:H:171:ALA:HB3	1.81	0.81
1:A:118:THR:HG23	1:A:121:GLU:OE1	1.81	0.81
1:H:252:ASN:HD21	1:H:255:ASP:CG	1.83	0.81
1:C:118:THR:HG23	1:C:121:GLU:OE1	1.81	0.81
1:E:118:THR:HG23	1:E:121:GLU:OE1	1.81	0.81
1:G:118:THR:HG23	1:G:121:GLU:OE1	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:HD21	1:A:255:ASP:CG	1.83	0.81
1:B:250:ILE:HD11	1:E:250:ILE:HD13	1.63	0.81
1:C:252:ASN:HD21	1:C:255:ASP:CG	1.83	0.81
1:D:24:HIS:HA	1:D:30:LEU:HD23	1.61	0.80
1:B:118:THR:HG23	1:B:121:GLU:OE1	1.81	0.80
1:D:2:ARG:O	1:D:176:ASP:N	2.13	0.80
1:C:61:ASN:HB3	1:C:64:GLU:HG3	1.64	0.80
1:D:167:PHE:HE1	1:D:189:LEU:HD13	1.46	0.80
1:D:118:THR:HG23	1:D:121:GLU:OE1	1.81	0.80
1:B:253:ILE:CG1	1:E:42:PHE:CD1	2.65	0.79
1:C:54:PRO:HG2	1:C:107:TRP:CD1	2.18	0.79
1:E:54:PRO:HG2	1:E:107:TRP:CD1	2.18	0.79
1:F:1:MET:CE	1:F:177:VAL:CG2	2.60	0.79
1:D:60:SER:C	1:D:61:ASN:HD22	1.86	0.79
1:B:54:PRO:HG2	1:B:107:TRP:CD1	2.18	0.79
1:H:54:PRO:HG2	1:H:107:TRP:CD1	2.18	0.79
1:A:101:ALA:HA	1:A:130:TYR:CD2	2.18	0.78
1:D:54:PRO:HG2	1:D:107:TRP:CD1	2.18	0.78
1:D:286:ARG:HG2	1:D:287:PRO:HD2	1.65	0.78
1:A:54:PRO:HG2	1:A:107:TRP:CD1	2.18	0.78
1:B:250:ILE:CD1	1:E:250:ILE:HD13	2.13	0.78
1:F:115:ARG:NH2	1:F:121:GLU:OE1	2.17	0.78
1:G:54:PRO:HG2	1:G:107:TRP:CD1	2.18	0.78
1:F:286:ARG:HG2	1:F:287:PRO:HD2	1.66	0.78
1:A:286:ARG:HG2	1:A:287:PRO:HD2	1.66	0.78
1:G:286:ARG:HG2	1:G:287:PRO:HD2	1.66	0.78
1:F:54:PRO:HG2	1:F:107:TRP:CD1	2.18	0.77
1:F:1:MET:HE1	1:F:177:VAL:CG2	2.14	0.77
1:F:36:ALA:O	1:F:161:LEU:HD12	1.84	0.77
1:A:115:ARG:NH2	1:A:121:GLU:OE1	2.17	0.77
1:E:286:ARG:HG2	1:E:287:PRO:HD2	1.65	0.77
1:H:286:ARG:HG2	1:H:287:PRO:HD2	1.65	0.77
1:H:115:ARG:NH2	1:H:121:GLU:OE1	2.17	0.77
1:C:115:ARG:NH2	1:C:121:GLU:OE1	2.17	0.77
1:G:115:ARG:NH2	1:G:121:GLU:OE1	2.17	0.77
1:B:115:ARG:NH2	1:B:121:GLU:OE1	2.17	0.77
1:G:177:VAL:HG12	1:G:178:ILE:N	1.99	0.77
1:D:115:ARG:NH2	1:D:121:GLU:OE1	2.17	0.77
1:E:115:ARG:NH2	1:E:121:GLU:OE1	2.17	0.77
1:E:266:LEU:O	1:E:266:LEU:HD12	1.84	0.76
1:A:286:ARG:CG	1:A:287:PRO:HD2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:286:ARG:CG	1:H:287:PRO:HD2	2.16	0.76
1:B:286:ARG:HG2	1:B:287:PRO:HD2	1.66	0.76
1:E:286:ARG:CG	1:E:287:PRO:HD2	2.16	0.76
1:C:286:ARG:CG	1:C:287:PRO:HD2	2.16	0.76
1:E:61:ASN:OD1	1:E:62:PRO:HD2	1.84	0.76
1:C:286:ARG:HG2	1:C:287:PRO:HD2	1.66	0.76
1:B:214:ILE:HG21	1:B:266:LEU:HD21	1.66	0.76
1:D:286:ARG:CG	1:D:287:PRO:HD2	2.16	0.75
1:G:286:ARG:CG	1:G:287:PRO:HD2	2.16	0.75
1:B:286:ARG:CG	1:B:287:PRO:HD2	2.16	0.75
1:F:286:ARG:CG	1:F:287:PRO:HD2	2.16	0.75
1:C:209:TRP:HE1	1:C:269:THR:HG1	1.33	0.75
1:D:252:ASN:OD1	1:D:254:GLN:HB2	1.87	0.74
1:B:252:ASN:OD1	1:B:254:GLN:HG2	1.86	0.74
1:D:253:ILE:HG13	1:G:42:PHE:CD1	2.22	0.74
1:D:167:PHE:HE1	1:D:189:LEU:CD1	1.99	0.74
1:A:51:LEU:HD12	1:A:52:TRP:H	1.53	0.73
1:F:51:LEU:HD12	1:F:52:TRP:H	1.53	0.73
1:G:51:LEU:HD12	1:G:52:TRP:H	1.53	0.73
1:G:179:ILE:N	1:G:179:ILE:HD12	2.02	0.73
1:G:61:ASN:HD22	1:G:62:PRO:N	1.87	0.73
1:B:20:HIS:ND1	1:B:155:ARG:NH1	2.37	0.73
1:G:66:ASN:O	1:G:70:GLN:HG3	1.89	0.73
1:A:20:HIS:ND1	1:A:155:ARG:NH1	2.37	0.73
1:G:177:VAL:CG1	1:G:178:ILE:N	2.51	0.73
1:E:61:ASN:ND2	1:E:63:GLN:CD	2.37	0.73
1:H:92:VAL:HG21	1:H:138:ILE:HG13	1.71	0.72
1:H:20:HIS:ND1	1:H:155:ARG:NH1	2.37	0.72
1:D:167:PHE:CE1	1:D:189:LEU:HD13	2.23	0.72
1:D:66:ASN:O	1:D:70:GLN:HG3	1.89	0.72
1:B:51:LEU:HD12	1:B:52:TRP:H	1.53	0.72
1:E:115:ARG:HH22	1:E:121:GLU:CD	1.93	0.72
1:A:255:ASP:O	1:A:259:ILE:HG13	1.89	0.72
1:F:20:HIS:ND1	1:F:155:ARG:NH1	2.37	0.72
1:H:115:ARG:HH22	1:H:121:GLU:CD	1.93	0.72
1:A:115:ARG:HH22	1:A:121:GLU:CD	1.93	0.72
1:D:51:LEU:HD12	1:D:52:TRP:H	1.53	0.72
1:B:255:ASP:O	1:B:259:ILE:HG13	1.89	0.72
1:C:115:ARG:HH22	1:C:121:GLU:CD	1.93	0.72
1:C:254:GLN:O	1:C:258:THR:HG23	1.90	0.72
1:D:255:ASP:O	1:D:259:ILE:HG13	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ASN:O	1:E:70:GLN:HG3	1.89	0.72
1:A:92:VAL:HG22	1:A:138:ILE:HG13	1.72	0.72
1:C:92:VAL:HG22	1:C:138:ILE:HG13	1.71	0.72
1:D:20:HIS:ND1	1:D:155:ARG:NH1	2.37	0.72
1:G:255:ASP:O	1:G:259:ILE:HG13	1.89	0.72
1:C:66:ASN:O	1:C:70:GLN:HG3	1.89	0.72
1:C:130:TYR:CD1	1:C:131:GLY:N	2.58	0.72
1:E:92:VAL:HG21	1:E:138:ILE:HG13	1.71	0.72
1:D:92:VAL:HG21	1:D:138:ILE:HG13	1.71	0.72
1:C:20:HIS:ND1	1:C:155:ARG:NH1	2.37	0.72
1:D:167:PHE:CE1	1:D:189:LEU:HB3	2.24	0.72
1:G:20:HIS:ND1	1:G:155:ARG:NH1	2.37	0.72
1:G:92:VAL:HG22	1:G:138:ILE:HG13	1.72	0.72
1:C:92:VAL:HG21	1:C:138:ILE:HG13	1.71	0.72
1:B:115:ARG:HH22	1:B:121:GLU:CD	1.93	0.72
1:H:51:LEU:HD12	1:H:52:TRP:H	1.53	0.72
1:E:51:LEU:HD12	1:E:52:TRP:H	1.53	0.72
1:C:166:SER:OG	1:C:169:GLU:HB2	1.89	0.72
1:D:115:ARG:HH22	1:D:121:GLU:CD	1.93	0.71
1:C:51:LEU:HD12	1:C:52:TRP:H	1.53	0.71
1:F:66:ASN:O	1:F:70:GLN:HG3	1.89	0.71
1:B:66:ASN:O	1:B:70:GLN:HG3	1.89	0.71
1:E:255:ASP:O	1:E:259:ILE:HG13	1.89	0.71
1:G:252:ASN:OD1	1:G:254:GLN:HG2	1.90	0.71
1:F:115:ARG:HH22	1:F:121:GLU:CD	1.93	0.71
1:C:255:ASP:O	1:C:259:ILE:HG13	1.89	0.71
1:F:255:ASP:O	1:F:259:ILE:HG13	1.89	0.71
1:G:92:VAL:HG21	1:G:138:ILE:HG13	1.71	0.71
1:A:66:ASN:O	1:A:70:GLN:HG3	1.89	0.71
1:E:92:VAL:HG22	1:E:138:ILE:HG13	1.71	0.71
1:F:20:HIS:CE1	1:F:155:ARG:HD2	2.26	0.71
1:E:20:HIS:CE1	1:E:155:ARG:HD2	2.26	0.71
1:H:255:ASP:O	1:H:259:ILE:HG13	1.89	0.71
1:H:66:ASN:O	1:H:70:GLN:HG3	1.89	0.71
1:E:20:HIS:ND1	1:E:155:ARG:NH1	2.37	0.71
1:G:61:ASN:HD22	1:G:62:PRO:CD	2.04	0.71
1:G:36:ALA:O	1:G:161:LEU:HD12	1.91	0.71
1:F:92:VAL:HG22	1:F:138:ILE:HG13	1.72	0.71
1:G:20:HIS:CE1	1:G:155:ARG:HD2	2.26	0.71
1:F:92:VAL:HG21	1:F:138:ILE:HG13	1.71	0.71
1:A:20:HIS:CE1	1:A:155:ARG:HD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:HIS:CE1	1:D:155:ARG:HD2	2.26	0.71
1:A:166:SER:OG	1:A:169:GLU:HB2	1.91	0.71
1:A:165:GLU:N	1:A:169:GLU:OE1	2.19	0.71
1:E:164:VAL:HG12	1:E:165:GLU:N	2.06	0.71
1:E:49:ALA:HB3	2:E:348:FAB:H3'	1.73	0.71
1:B:92:VAL:HG21	1:B:138:ILE:HG13	1.71	0.70
1:F:49:ALA:HB3	2:F:348:FAB:H3'	1.73	0.70
1:B:49:ALA:HB3	2:B:348:FAB:H3'	1.73	0.70
1:H:166:SER:OG	1:H:169:GLU:N	2.22	0.70
1:A:92:VAL:HG21	1:A:138:ILE:HG13	1.71	0.70
1:B:105:PRO:HD3	1:B:132:TRP:CZ2	2.27	0.70
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.26	0.70
1:F:105:PRO:HD3	1:F:132:TRP:CZ2	2.26	0.70
1:D:92:VAL:HG22	1:D:138:ILE:HG13	1.72	0.70
1:G:115:ARG:HH22	1:G:121:GLU:CD	1.93	0.70
1:E:78:HIS:CD2	1:E:87:MET:HE1	2.25	0.70
1:H:101:ALA:HA	1:H:130:TYR:CD2	2.24	0.70
1:C:162:ARG:HH11	1:C:162:ARG:HG3	1.55	0.70
1:D:61:ASN:N	1:D:61:ASN:HD22	1.89	0.70
1:E:105:PRO:HD3	1:E:132:TRP:CZ2	2.27	0.70
1:C:20:HIS:CE1	1:C:155:ARG:HD2	2.26	0.70
1:F:254:GLN:O	1:F:258:THR:HG23	1.91	0.70
1:G:267:GLU:OE1	1:G:269:THR:HG23	1.92	0.70
1:D:161:LEU:HD12	1:D:162:ARG:N	2.06	0.70
1:H:105:PRO:HD3	1:H:132:TRP:CZ2	2.26	0.70
1:F:142:ARG:HH11	1:F:142:ARG:CG	2.05	0.70
1:H:20:HIS:CE1	1:H:155:ARG:HD2	2.26	0.70
1:G:105:PRO:HD3	1:G:132:TRP:CZ2	2.26	0.70
1:B:20:HIS:CE1	1:B:155:ARG:HD2	2.26	0.70
1:A:250:ILE:HD11	1:F:250:ILE:HD13	1.74	0.70
1:C:105:PRO:HD3	1:C:132:TRP:CZ2	2.26	0.70
1:E:254:GLN:O	1:E:258:THR:HG23	1.92	0.70
1:H:92:VAL:HG22	1:H:138:ILE:HG13	1.72	0.70
1:A:49:ALA:HB3	2:A:348:FAB:H3'	1.73	0.69
1:D:49:ALA:HB3	2:D:348:FAB:H3'	1.73	0.69
1:B:92:VAL:HG22	1:B:138:ILE:HG13	1.72	0.69
1:C:23:TYR:HD1	1:C:26:VAL:CG1	2.05	0.69
1:B:253:ILE:HG12	1:E:42:PHE:CE1	2.27	0.69
1:D:23:TYR:HD1	1:D:26:VAL:CG1	2.04	0.69
1:G:142:ARG:CG	1:G:142:ARG:HH11	2.05	0.69
1:G:61:ASN:ND2	1:G:63:GLN:H	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:HB3	2:C:348:FAB:H3'	1.73	0.69
1:D:105:PRO:HD3	1:D:132:TRP:CZ2	2.26	0.69
1:B:23:TYR:HD1	1:B:26:VAL:CG1	2.05	0.69
1:G:166:SER:O	1:G:170:VAL:HG23	1.93	0.69
1:B:214:ILE:CG2	1:B:266:LEU:HD21	2.23	0.69
1:H:40:THR:OG1	1:H:41:PRO:HA	1.93	0.69
1:H:49:ALA:HB3	2:H:348:FAB:H3'	1.73	0.69
1:G:35:TYR:HE1	1:G:160:PHE:CD2	2.11	0.69
1:C:40:THR:OG1	1:C:41:PRO:HA	1.93	0.69
1:D:40:THR:OG1	1:D:41:PRO:HA	1.93	0.69
1:A:250:ILE:HD11	1:F:250:ILE:HD11	1.74	0.69
1:C:39:PHE:CD2	1:C:161:LEU:HD23	2.27	0.69
1:G:40:THR:OG1	1:G:41:PRO:HA	1.93	0.68
1:A:152:LEU:O	1:A:157:VAL:HG23	1.93	0.68
1:G:39:PHE:CD2	1:G:161:LEU:HD13	2.28	0.68
1:C:253:ILE:HG13	1:H:42:PHE:CD1	2.29	0.68
1:B:142:ARG:HH11	1:B:142:ARG:CG	2.05	0.68
1:E:40:THR:OG1	1:E:41:PRO:HA	1.93	0.68
1:H:295:GLN:O	1:H:296:LEU:HD23	1.93	0.68
1:F:40:THR:OG1	1:F:41:PRO:HA	1.93	0.68
1:C:295:GLN:O	1:C:296:LEU:HD23	1.93	0.68
1:C:142:ARG:CG	1:C:142:ARG:HH11	2.05	0.68
1:G:49:ALA:HB3	2:G:348:FAB:H3'	1.73	0.68
1:F:251:ASN:HA	1:F:280:THR:HG21	1.76	0.68
1:D:142:ARG:CG	1:D:142:ARG:HH11	2.05	0.68
1:D:161:LEU:HD12	1:D:161:LEU:C	2.13	0.68
1:F:295:GLN:O	1:F:296:LEU:HD23	1.93	0.68
1:B:251:ASN:HA	1:B:280:THR:HG21	1.76	0.68
1:H:23:TYR:HD1	1:H:26:VAL:CG1	2.04	0.68
1:H:251:ASN:HA	1:H:280:THR:HG21	1.76	0.68
1:G:251:ASN:HA	1:G:280:THR:HG21	1.76	0.68
1:A:101:ALA:HA	1:A:130:TYR:CG	2.29	0.68
1:E:51:LEU:HD12	1:E:52:TRP:N	2.09	0.68
1:A:40:THR:OG1	1:A:41:PRO:HA	1.93	0.68
1:C:251:ASN:HA	1:C:280:THR:HG21	1.76	0.68
1:G:295:GLN:O	1:G:296:LEU:HD23	1.93	0.68
1:E:142:ARG:HH11	1:E:142:ARG:CG	2.05	0.67
1:E:295:GLN:O	1:E:296:LEU:HD23	1.93	0.67
1:B:295:GLN:O	1:B:296:LEU:HD23	1.93	0.67
1:H:166:SER:OG	1:H:169:GLU:HB2	1.93	0.67
1:F:39:PHE:CD2	1:F:161:LEU:HD13	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD12	1:A:52:TRP:N	2.09	0.67
1:G:51:LEU:HD12	1:G:52:TRP:N	2.09	0.67
1:H:51:LEU:HD12	1:H:52:TRP:N	2.09	0.67
1:G:105:PRO:HD3	1:G:132:TRP:CH2	2.30	0.67
1:B:40:THR:OG1	1:B:41:PRO:HA	1.93	0.67
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.05	0.67
1:C:51:LEU:HD12	1:C:52:TRP:N	2.09	0.67
1:A:295:GLN:O	1:A:296:LEU:HD23	1.93	0.67
1:D:1:MET:HG3	1:D:176:ASP:HB2	1.77	0.67
1:C:162:ARG:HH11	1:C:162:ARG:CG	2.07	0.67
1:E:23:TYR:HD1	1:E:26:VAL:CG1	2.05	0.67
1:E:105:PRO:HD3	1:E:132:TRP:CH2	2.30	0.67
1:E:251:ASN:HA	1:E:280:THR:HG21	1.76	0.67
1:E:61:ASN:HB3	1:E:64:GLU:HG3	1.74	0.67
1:D:170:VAL:CG1	1:D:178:ILE:HD13	2.24	0.67
1:C:105:PRO:HD3	1:C:132:TRP:CH2	2.30	0.67
1:D:105:PRO:HD3	1:D:132:TRP:CH2	2.30	0.67
1:D:251:ASN:HA	1:D:280:THR:HG21	1.76	0.67
1:D:51:LEU:HD12	1:D:52:TRP:N	2.09	0.67
1:A:253:ILE:HG12	1:F:42:PHE:CE1	2.30	0.67
1:H:142:ARG:HH11	1:H:142:ARG:CG	2.05	0.67
1:E:2:ARG:O	1:E:176:ASP:HB2	1.95	0.67
1:A:105:PRO:HD3	1:A:132:TRP:CH2	2.30	0.66
1:D:295:GLN:O	1:D:296:LEU:HD23	1.93	0.66
1:F:51:LEU:HD12	1:F:52:TRP:N	2.09	0.66
1:E:39:PHE:HD2	1:E:161:LEU:HD12	1.60	0.66
1:B:51:LEU:HD12	1:B:52:TRP:N	2.09	0.66
1:B:105:PRO:HD3	1:B:132:TRP:CH2	2.30	0.66
1:F:105:PRO:HD3	1:F:132:TRP:CH2	2.30	0.66
1:D:193:PRO:HG2	1:F:73:ASN:HB2	1.76	0.66
1:H:105:PRO:HD3	1:H:132:TRP:CH2	2.30	0.66
1:E:266:LEU:C	1:E:266:LEU:HD12	2.16	0.66
1:B:170:VAL:HG12	1:B:178:ILE:HD11	1.77	0.65
1:A:253:ILE:CG1	1:F:42:PHE:CE1	2.79	0.65
1:G:127:ASP:OD1	1:G:127:ASP:N	2.28	0.65
1:E:39:PHE:HE2	1:E:161:LEU:HA	1.60	0.65
1:A:251:ASN:HA	1:A:280:THR:HG21	1.76	0.65
1:G:23:TYR:HD1	1:G:26:VAL:CG1	2.04	0.65
1:F:209:TRP:NE1	1:F:269:THR:OG1	2.19	0.65
1:G:78:HIS:CD2	1:G:87:MET:HE1	2.32	0.65
1:G:196:GLN:O	1:G:285:VAL:HB	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLN:O	1:B:285:VAL:HB	1.97	0.65
1:D:254:GLN:O	1:D:258:THR:HG23	1.97	0.65
1:A:78:HIS:CD2	1:A:87:MET:HE1	2.32	0.65
1:D:208:PRO:HD2	1:D:209:TRP:CE3	2.32	0.65
1:G:208:PRO:HD2	1:G:209:TRP:CE3	2.32	0.65
1:G:1:MET:CE	1:G:177:VAL:HG23	2.27	0.65
1:G:59:PRO:HB3	1:G:64:GLU:OE2	1.96	0.64
1:A:23:TYR:HD1	1:A:26:VAL:CG1	2.05	0.64
1:E:208:PRO:HD2	1:E:209:TRP:CE3	2.32	0.64
1:A:287:PRO:HB2	1:A:288:GLN:NE2	2.12	0.64
1:C:196:GLN:O	1:C:285:VAL:HB	1.97	0.64
1:C:93:SER:HG	1:C:135:THR:HB	1.62	0.64
1:C:165:GLU:HB2	1:C:169:GLU:OE1	1.96	0.64
1:D:196:GLN:O	1:D:285:VAL:HB	1.97	0.64
1:F:208:PRO:HD2	1:F:209:TRP:CE3	2.32	0.64
1:E:196:GLN:O	1:E:285:VAL:HB	1.97	0.64
1:F:23:TYR:HD1	1:F:26:VAL:CG1	2.04	0.64
1:H:208:PRO:HD2	1:H:209:TRP:CE3	2.32	0.64
1:A:208:PRO:HD2	1:A:209:TRP:CE3	2.32	0.64
1:D:168:GLU:O	1:D:172:ARG:HG3	1.98	0.64
1:F:196:GLN:O	1:F:285:VAL:HB	1.97	0.64
1:B:208:PRO:HD2	1:B:209:TRP:CE3	2.32	0.64
1:A:159:PHE:HD1	1:A:159:PHE:N	1.96	0.64
1:A:196:GLN:O	1:A:285:VAL:HB	1.97	0.64
1:F:39:PHE:CE2	1:F:161:LEU:HD13	2.33	0.63
1:C:78:HIS:CD2	1:C:87:MET:HE1	2.33	0.63
1:H:196:GLN:O	1:H:285:VAL:HB	1.97	0.63
1:D:177:VAL:HG12	1:D:178:ILE:N	2.11	0.63
1:D:128:TYR:N	1:D:128:TYR:CD1	2.64	0.63
1:A:177:VAL:HG12	1:A:178:ILE:N	2.14	0.63
1:D:78:HIS:CD2	1:D:87:MET:HE1	2.33	0.63
1:H:267:GLU:O	1:H:270:LEU:HB2	1.98	0.63
1:C:208:PRO:HD2	1:C:209:TRP:CE3	2.32	0.63
1:A:250:ILE:CD1	1:F:250:ILE:CD1	2.76	0.62
1:H:168:GLU:OE2	1:H:172:ARG:NH1	2.32	0.62
1:F:224:TYR:HB2	1:F:242:PHE:HD2	1.64	0.62
1:H:78:HIS:CD2	1:H:87:MET:HE1	2.34	0.62
1:F:1:MET:HE1	1:F:177:VAL:HG21	1.81	0.62
1:B:78:HIS:CD2	1:B:87:MET:HE1	2.34	0.62
1:C:325:GLU:O	1:C:328:LYS:HB3	2.00	0.62
1:D:325:GLU:O	1:D:328:LYS:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:HIS:ND1	1:D:155:ARG:HD2	2.15	0.62
1:D:177:VAL:CG1	1:D:178:ILE:N	2.63	0.62
1:E:224:TYR:HB2	1:E:242:PHE:HD2	1.64	0.62
1:A:254:GLN:O	1:A:258:THR:HG23	2.00	0.62
1:B:253:ILE:HG13	1:E:42:PHE:CG	2.34	0.62
1:H:20:HIS:ND1	1:H:155:ARG:HD2	2.15	0.62
1:A:35:TYR:CD1	1:A:160:PHE:HB2	2.35	0.62
1:H:325:GLU:O	1:H:328:LYS:HB3	2.00	0.62
1:C:39:PHE:CE2	1:C:161:LEU:HD23	2.33	0.62
1:A:325:GLU:O	1:A:328:LYS:HB3	2.00	0.62
1:A:224:TYR:HB2	1:A:242:PHE:HD2	1.64	0.62
1:G:20:HIS:ND1	1:G:155:ARG:HD2	2.15	0.61
1:F:325:GLU:O	1:F:328:LYS:HB3	2.00	0.61
1:E:325:GLU:O	1:E:328:LYS:HB3	2.00	0.61
1:F:20:HIS:ND1	1:F:155:ARG:HD2	2.15	0.61
1:C:252:ASN:OD1	1:C:254:GLN:HB3	1.99	0.61
1:A:20:HIS:ND1	1:A:155:ARG:HD2	2.15	0.61
1:H:224:TYR:HB2	1:H:242:PHE:HD2	1.64	0.61
1:H:332:LYS:O	1:H:336:GLU:HG3	2.01	0.61
1:E:61:ASN:CG	1:E:63:GLN:HE21	2.03	0.61
1:C:20:HIS:ND1	1:C:155:ARG:HD2	2.15	0.61
1:B:128:TYR:N	1:B:128:TYR:HD1	1.99	0.61
1:B:224:TYR:HB2	1:B:242:PHE:HD2	1.64	0.61
1:G:325:GLU:O	1:G:328:LYS:HB3	2.00	0.61
1:G:35:TYR:CE1	1:G:160:PHE:CD2	2.89	0.61
1:C:224:TYR:HB2	1:C:242:PHE:HD2	1.64	0.61
1:C:293:ARG:HH22	1:C:336:GLU:CD	2.04	0.61
1:E:293:ARG:HH22	1:E:336:GLU:CD	2.04	0.61
1:A:159:PHE:N	1:A:159:PHE:CD1	2.67	0.61
1:B:325:GLU:O	1:B:328:LYS:HB3	2.00	0.61
1:D:293:ARG:HH22	1:D:336:GLU:CD	2.04	0.61
1:G:224:TYR:HB2	1:G:242:PHE:HD2	1.64	0.61
1:E:332:LYS:O	1:E:336:GLU:HG3	2.01	0.61
1:A:332:LYS:O	1:A:336:GLU:HG3	2.01	0.61
1:B:293:ARG:HH22	1:B:336:GLU:CD	2.04	0.61
1:B:20:HIS:ND1	1:B:155:ARG:HD2	2.15	0.60
1:E:20:HIS:ND1	1:E:155:ARG:HD2	2.15	0.60
1:G:61:ASN:ND2	1:G:63:GLN:HB2	2.16	0.60
1:A:293:ARG:HH22	1:A:336:GLU:CD	2.04	0.60
1:F:293:ARG:HH22	1:F:336:GLU:CD	2.04	0.60
1:G:293:ARG:HH22	1:G:336:GLU:CD	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:ARG:HH22	1:H:336:GLU:CD	2.04	0.60
1:B:332:LYS:O	1:B:336:GLU:HG3	2.01	0.60
1:H:99:ARG:O	1:H:129:ARG:HB3	2.00	0.60
1:G:170:VAL:HB	1:G:178:ILE:CD1	2.31	0.60
1:D:193:PRO:HG2	1:F:73:ASN:CB	2.30	0.60
1:D:224:TYR:HB2	1:D:242:PHE:HD2	1.65	0.60
1:A:291:LEU:HA	1:A:307:HIS:O	2.02	0.60
1:G:291:LEU:HA	1:G:307:HIS:O	2.02	0.60
1:A:36:ALA:O	1:A:161:LEU:HD12	2.01	0.60
1:C:332:LYS:O	1:C:336:GLU:HG3	2.01	0.60
1:B:253:ILE:CG1	1:E:42:PHE:CE1	2.84	0.60
1:C:291:LEU:HA	1:C:307:HIS:O	2.02	0.60
1:F:332:LYS:O	1:F:336:GLU:HG3	2.01	0.60
1:F:166:SER:O	1:F:170:VAL:HG23	2.02	0.60
1:B:291:LEU:HA	1:B:307:HIS:O	2.02	0.60
1:F:78:HIS:CD2	1:F:87:MET:HE1	2.37	0.60
1:C:101:ALA:CA	1:C:130:TYR:CD2	2.80	0.60
1:B:201:GLN:HG3	1:B:280:THR:HG22	1.84	0.60
1:E:201:GLN:HG3	1:E:280:THR:HG22	1.84	0.60
1:D:201:GLN:HG3	1:D:280:THR:HG22	1.84	0.60
1:G:332:LYS:O	1:G:336:GLU:HG3	2.01	0.60
1:C:130:TYR:HD1	1:C:131:GLY:N	2.00	0.59
1:H:291:LEU:HA	1:H:307:HIS:O	2.02	0.59
1:C:165:GLU:HB2	1:C:169:GLU:CD	2.22	0.59
1:F:291:LEU:HA	1:F:307:HIS:O	2.02	0.59
1:C:101:ALA:HA	1:C:130:TYR:CG	2.38	0.59
1:H:267:GLU:OE1	1:H:269:THR:HG23	2.02	0.59
1:A:78:HIS:CD2	1:A:87:MET:CE	2.86	0.59
1:C:125:PHE:N	1:C:126:PRO:HD3	2.17	0.59
1:G:102:VAL:HG13	1:G:103:PRO:HD2	1.84	0.59
1:C:165:GLU:HB2	1:C:169:GLU:OE2	2.03	0.59
1:A:159:PHE:C	1:A:160:PHE:CD1	2.76	0.59
1:D:332:LYS:O	1:D:336:GLU:HG3	2.01	0.59
1:H:260:TRP:O	1:H:264:CYS:HB2	2.03	0.59
1:B:260:TRP:O	1:B:264:CYS:HB2	2.03	0.59
1:E:61:ASN:CG	1:E:63:GLN:HG2	2.23	0.59
1:A:161:LEU:O	1:A:162:ARG:HG2	2.02	0.59
1:D:35:TYR:HE1	1:D:160:PHE:CD2	2.20	0.59
1:F:201:GLN:HG3	1:F:280:THR:HG22	1.84	0.59
1:G:201:GLN:HG3	1:G:280:THR:HG22	1.84	0.59
1:C:260:TRP:O	1:C:264:CYS:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:HIS:CD2	1:C:87:MET:CE	2.86	0.59
1:H:78:HIS:CD2	1:H:87:MET:CE	2.86	0.59
1:B:78:HIS:CD2	1:B:87:MET:CE	2.86	0.59
1:F:260:TRP:O	1:F:264:CYS:HB2	2.03	0.59
1:G:122:LEU:O	1:G:125:PHE:O	2.21	0.59
1:D:291:LEU:HA	1:D:307:HIS:O	2.02	0.59
1:E:78:HIS:CD2	1:E:87:MET:CE	2.86	0.59
1:H:201:GLN:HG3	1:H:280:THR:HG22	1.84	0.59
1:C:102:VAL:HG13	1:C:103:PRO:HD2	1.84	0.59
1:B:263:CYS:O	1:B:267:GLU:N	2.36	0.59
1:C:1:MET:CE	1:C:177:VAL:HG23	2.32	0.59
1:E:10:VAL:HG13	1:E:11:ILE:N	2.18	0.59
1:B:250:ILE:CD1	1:E:250:ILE:HD11	2.24	0.58
1:H:102:VAL:HG13	1:H:103:PRO:HD2	1.84	0.58
1:A:201:GLN:HG3	1:A:280:THR:HG22	1.84	0.58
1:C:61:ASN:OD1	1:C:63:GLN:N	2.35	0.58
1:E:291:LEU:HA	1:E:307:HIS:O	2.02	0.58
1:G:10:VAL:HG13	1:G:11:ILE:N	2.18	0.58
1:A:102:VAL:HG13	1:A:103:PRO:HD2	1.84	0.58
1:D:195:LEU:HD12	1:D:285:VAL:O	2.04	0.58
1:G:167:PHE:HE1	1:G:189:LEU:O	1.85	0.58
1:B:195:LEU:HD12	1:B:285:VAL:O	2.04	0.58
1:B:269:THR:C	1:B:271:LYS:N	2.57	0.58
1:G:260:TRP:O	1:G:264:CYS:HB2	2.03	0.58
1:E:260:TRP:O	1:E:264:CYS:HB2	2.03	0.58
1:D:260:TRP:O	1:D:264:CYS:HB2	2.03	0.58
1:A:253:ILE:HA	1:F:42:PHE:CZ	2.39	0.58
1:D:102:VAL:HG13	1:D:103:PRO:HD2	1.84	0.58
1:A:260:TRP:O	1:A:264:CYS:HB2	2.03	0.58
1:F:128:TYR:CD1	1:F:128:TYR:N	2.72	0.58
1:G:195:LEU:HD12	1:G:285:VAL:O	2.04	0.58
1:D:78:HIS:CD2	1:D:87:MET:CE	2.86	0.58
1:F:78:HIS:CD2	1:F:87:MET:CE	2.86	0.58
1:G:78:HIS:CD2	1:G:87:MET:CE	2.86	0.58
1:H:195:LEU:HD12	1:H:285:VAL:O	2.04	0.58
1:F:10:VAL:HG13	1:F:11:ILE:N	2.18	0.58
1:E:102:VAL:HG13	1:E:103:PRO:HD2	1.84	0.58
1:C:205:VAL:HG23	1:C:275:ILE:HA	1.86	0.58
1:B:33:LYS:HB3	1:B:160:PHE:CE1	2.31	0.58
1:G:166:SER:OG	1:G:169:GLU:HB2	2.02	0.58
1:B:10:VAL:HG13	1:B:11:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:VAL:HG23	1:D:275:ILE:HA	1.86	0.58
1:C:201:GLN:HG3	1:C:280:THR:HG22	1.84	0.58
1:E:195:LEU:HD12	1:E:285:VAL:O	2.04	0.58
1:E:205:VAL:HG23	1:E:275:ILE:HA	1.86	0.58
1:D:125:PHE:N	1:D:125:PHE:CD1	2.71	0.58
1:H:205:VAL:HG23	1:H:275:ILE:HA	1.86	0.58
1:C:152:LEU:O	1:C:157:VAL:HG13	2.04	0.57
1:B:102:VAL:HG13	1:B:103:PRO:HD2	1.85	0.57
1:H:10:VAL:HG13	1:H:11:ILE:N	2.18	0.57
1:H:35:TYR:CZ	1:H:162:ARG:NH1	2.72	0.57
1:E:168:GLU:HG3	1:E:298:PHE:CE1	2.39	0.57
1:C:195:LEU:HD12	1:C:285:VAL:O	2.04	0.57
1:A:250:ILE:CD1	1:F:250:ILE:HD13	2.33	0.57
1:F:195:LEU:HD12	1:F:285:VAL:O	2.04	0.57
1:A:10:VAL:HG13	1:A:11:ILE:N	2.18	0.57
1:C:128:TYR:CD1	1:C:128:TYR:N	2.71	0.57
1:F:102:VAL:HG13	1:F:103:PRO:HD2	1.84	0.57
1:C:10:VAL:HG13	1:C:11:ILE:N	2.18	0.57
1:H:130:TYR:CD1	1:H:131:GLY:N	2.73	0.57
1:D:10:VAL:HG13	1:D:11:ILE:N	2.18	0.57
1:H:293:ARG:NH2	1:H:336:GLU:OE1	2.38	0.57
1:A:195:LEU:HD12	1:A:285:VAL:O	2.04	0.57
1:D:293:ARG:NH2	1:D:336:GLU:OE1	2.38	0.57
1:D:170:VAL:HG11	1:D:178:ILE:HD13	1.87	0.57
1:F:293:ARG:NH2	1:F:336:GLU:OE1	2.38	0.57
1:G:130:TYR:CD1	1:G:131:GLY:N	2.73	0.57
1:D:165:GLU:HA	1:D:165:GLU:OE1	2.03	0.57
1:A:293:ARG:NH2	1:A:336:GLU:OE1	2.38	0.56
1:E:293:ARG:NH2	1:E:336:GLU:OE1	2.38	0.56
1:D:170:VAL:HG12	1:D:178:ILE:HD13	1.87	0.56
1:C:293:ARG:NH2	1:C:336:GLU:OE1	2.38	0.56
1:G:293:ARG:NH2	1:G:336:GLU:OE1	2.38	0.56
1:A:205:VAL:HG23	1:A:275:ILE:HA	1.86	0.56
1:A:93:SER:HA	1:A:135:THR:HA	1.88	0.56
1:F:93:SER:HA	1:F:135:THR:HA	1.88	0.56
1:H:152:LEU:HD22	1:H:157:VAL:HG21	1.87	0.56
1:A:177:VAL:CG1	1:A:178:ILE:N	2.69	0.56
1:B:293:ARG:NH2	1:B:336:GLU:OE1	2.38	0.56
1:H:128:TYR:CD1	1:H:128:TYR:N	2.73	0.56
1:F:205:VAL:HG23	1:F:275:ILE:HA	1.86	0.56
1:E:93:SER:HG	1:E:135:THR:HB	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:VAL:HG23	1:G:275:ILE:HA	1.86	0.56
1:D:93:SER:HA	1:D:135:THR:HA	1.88	0.56
1:G:93:SER:HA	1:G:135:THR:HA	1.88	0.56
1:H:168:GLU:CG	1:H:172:ARG:HD2	2.35	0.56
1:E:2:ARG:N	1:E:176:ASP:OD2	2.23	0.56
1:B:205:VAL:HG23	1:B:275:ILE:HA	1.86	0.56
1:D:236:VAL:HG12	1:D:237:THR:N	2.21	0.56
1:B:160:PHE:N	1:B:160:PHE:CD1	2.74	0.56
1:E:24:HIS:O	1:E:27:LEU:O	2.24	0.56
1:A:24:HIS:O	1:A:27:LEU:O	2.24	0.55
1:G:24:HIS:O	1:G:27:LEU:O	2.24	0.55
1:G:190:GLN:NE2	1:G:290:ARG:HH12	2.05	0.55
1:C:36:ALA:O	1:C:161:LEU:HD22	2.06	0.55
1:A:190:GLN:NE2	1:A:290:ARG:HH12	2.05	0.55
1:C:190:GLN:NE2	1:C:290:ARG:HH12	2.05	0.55
1:C:1:MET:HE1	1:C:177:VAL:CG2	2.35	0.55
1:B:93:SER:HA	1:B:135:THR:HA	1.88	0.55
1:D:24:HIS:O	1:D:27:LEU:O	2.24	0.55
1:H:190:GLN:NE2	1:H:290:ARG:HH12	2.05	0.55
1:C:1:MET:HE2	1:C:177:VAL:HG23	1.87	0.55
1:B:236:VAL:HG12	1:B:237:THR:N	2.21	0.55
1:B:24:HIS:O	1:B:27:LEU:O	2.24	0.55
1:F:190:GLN:NE2	1:F:290:ARG:HH12	2.05	0.55
1:D:124:MET:HB2	1:D:125:PHE:CE1	2.42	0.55
1:B:190:GLN:NE2	1:B:290:ARG:HH12	2.05	0.55
1:G:35:TYR:CG	1:G:162:ARG:HD2	2.42	0.55
1:E:93:SER:HA	1:E:135:THR:HA	1.88	0.55
1:H:24:HIS:O	1:H:27:LEU:O	2.24	0.55
1:F:101:ALA:HA	1:F:130:TYR:CD2	2.42	0.55
1:C:24:HIS:O	1:C:27:LEU:O	2.24	0.55
1:F:142:ARG:HG3	1:F:142:ARG:NH1	2.14	0.55
1:A:290:ARG:NH2	1:A:307:HIS:CE1	2.75	0.55
1:G:290:ARG:NH2	1:G:307:HIS:CE1	2.75	0.55
1:E:190:GLN:NE2	1:E:290:ARG:HH12	2.05	0.55
1:C:236:VAL:HG12	1:C:237:THR:N	2.21	0.55
1:B:290:ARG:NH2	1:B:307:HIS:CE1	2.75	0.55
1:D:128:TYR:H	1:D:128:TYR:HD1	1.54	0.55
1:F:236:VAL:HG12	1:F:237:THR:N	2.21	0.55
1:E:138:ILE:HD13	1:E:232:GLY:HA2	1.89	0.55
1:D:138:ILE:HD13	1:D:232:GLY:HA2	1.89	0.55
1:F:316:LEU:HB2	2:F:348:FAB:O2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ARG:NH2	1:C:307:HIS:CE1	2.75	0.55
1:E:164:VAL:CG1	1:E:165:GLU:N	2.69	0.55
1:B:166:SER:OG	1:B:169:GLU:HB3	2.06	0.55
1:E:128:TYR:CD1	1:E:128:TYR:N	2.74	0.55
1:H:316:LEU:HB2	2:H:348:FAB:O2	2.07	0.55
1:A:236:VAL:HG12	1:A:237:THR:N	2.21	0.55
1:H:290:ARG:NH2	1:H:307:HIS:CE1	2.75	0.54
1:B:269:THR:C	1:B:271:LYS:H	2.10	0.54
1:E:236:VAL:HG12	1:E:237:THR:N	2.21	0.54
1:C:93:SER:HA	1:C:135:THR:HA	1.88	0.54
1:G:138:ILE:HD13	1:G:232:GLY:HA2	1.89	0.54
1:F:89:LEU:O	1:F:90:THR:HG23	2.08	0.54
1:E:290:ARG:NH2	1:E:307:HIS:CE1	2.75	0.54
1:D:316:LEU:HB2	2:D:348:FAB:O2	2.07	0.54
1:G:15:THR:O	1:G:19:ILE:HG12	2.08	0.54
1:H:177:VAL:CG1	1:H:178:ILE:N	2.70	0.54
1:D:15:THR:O	1:D:19:ILE:HG12	2.08	0.54
1:H:93:SER:HA	1:H:135:THR:HA	1.88	0.54
1:A:138:ILE:HD13	1:A:232:GLY:HA2	1.89	0.54
1:D:290:ARG:NH2	1:D:307:HIS:CE1	2.75	0.54
1:F:290:ARG:NH2	1:F:307:HIS:CE1	2.75	0.54
1:H:37:ASP:O	1:H:161:LEU:HD11	2.07	0.54
1:H:136:SER:O	1:H:137:LEU:HD23	2.08	0.54
1:B:136:SER:O	1:B:137:LEU:HD23	2.08	0.54
1:D:136:SER:O	1:D:137:LEU:HD23	2.08	0.54
1:E:15:THR:O	1:E:19:ILE:HG12	2.08	0.54
1:E:180:ASN:HD22	1:E:307:HIS:CD2	2.26	0.54
1:G:316:LEU:HB2	2:G:348:FAB:O2	2.07	0.54
1:C:136:SER:O	1:C:137:LEU:HD23	2.08	0.54
1:E:61:ASN:HD21	1:E:63:GLN:CG	1.75	0.54
1:A:93:SER:HG	1:A:135:THR:HB	1.72	0.54
1:F:138:ILE:HD13	1:F:232:GLY:HA2	1.89	0.54
1:F:24:HIS:O	1:F:27:LEU:O	2.24	0.54
1:E:316:LEU:HB2	2:E:348:FAB:O2	2.07	0.54
1:F:136:SER:O	1:F:137:LEU:HD23	2.08	0.54
1:A:291:LEU:HD12	1:A:291:LEU:C	2.28	0.54
1:C:291:LEU:HD12	1:C:291:LEU:C	2.28	0.54
1:A:165:GLU:HB3	1:A:169:GLU:OE1	2.07	0.54
1:C:316:LEU:HB2	2:C:348:FAB:O2	2.07	0.54
1:E:136:SER:O	1:E:137:LEU:HD23	2.08	0.54
1:G:136:SER:O	1:G:137:LEU:HD23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:VAL:HG12	1:G:237:THR:N	2.21	0.54
1:E:89:LEU:O	1:E:90:THR:HG23	2.08	0.54
1:D:89:LEU:O	1:D:90:THR:HG23	2.08	0.54
1:D:24:HIS:CD2	1:D:24:HIS:O	2.61	0.54
1:D:190:GLN:NE2	1:D:290:ARG:HH12	2.05	0.54
1:H:236:VAL:HG12	1:H:237:THR:N	2.21	0.54
1:H:24:HIS:CD2	1:H:24:HIS:O	2.61	0.54
1:E:291:LEU:C	1:E:291:LEU:HD12	2.28	0.54
1:B:291:LEU:HD12	1:B:291:LEU:C	2.28	0.54
1:G:89:LEU:O	1:G:90:THR:HG23	2.08	0.54
1:A:89:LEU:O	1:A:90:THR:HG23	2.08	0.54
1:H:101:ALA:HA	1:H:130:TYR:CG	2.43	0.54
1:F:15:THR:O	1:F:19:ILE:HG12	2.08	0.54
1:B:15:THR:O	1:B:19:ILE:HG12	2.08	0.54
1:C:15:THR:O	1:C:19:ILE:HG12	2.08	0.54
1:C:24:HIS:O	1:C:24:HIS:CD2	2.61	0.54
1:B:138:ILE:HD13	1:B:232:GLY:HA2	1.89	0.54
1:D:291:LEU:C	1:D:291:LEU:HD12	2.28	0.54
1:F:291:LEU:C	1:F:291:LEU:HD12	2.28	0.54
1:E:39:PHE:HE2	1:E:161:LEU:CA	2.20	0.54
1:A:316:LEU:HB2	2:A:348:FAB:O2	2.07	0.54
1:A:15:THR:O	1:A:19:ILE:HG12	2.08	0.53
1:G:24:HIS:CD2	1:G:24:HIS:O	2.61	0.53
1:C:21:GLU:HG3	1:C:155:ARG:HH21	1.73	0.53
1:E:24:HIS:CD2	1:E:24:HIS:O	2.61	0.53
1:G:39:PHE:CE2	1:G:161:LEU:HD13	2.43	0.53
1:B:316:LEU:HB2	2:B:348:FAB:O2	2.07	0.53
1:H:15:THR:O	1:H:19:ILE:HG12	2.08	0.53
1:F:209:TRP:NE1	1:F:210:LEU:HD21	2.24	0.53
1:H:89:LEU:O	1:H:90:THR:HG23	2.08	0.53
1:A:21:GLU:HG3	1:A:155:ARG:HH21	1.72	0.53
1:H:291:LEU:C	1:H:291:LEU:HD12	2.28	0.53
1:B:210:LEU:HD11	1:B:270:LEU:HD21	1.91	0.53
1:H:177:VAL:HG22	1:H:304:GLU:HB2	1.89	0.53
1:B:24:HIS:CD2	1:B:24:HIS:O	2.61	0.53
1:B:253:ILE:HA	1:E:42:PHE:CZ	2.44	0.53
1:F:24:HIS:O	1:F:24:HIS:CD2	2.61	0.53
1:B:89:LEU:O	1:B:90:THR:HG23	2.08	0.53
1:F:293:ARG:NE	1:F:333:VAL:HG23	2.24	0.53
1:F:93:SER:HG	1:F:135:THR:HB	1.70	0.53
1:C:89:LEU:O	1:C:90:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:VAL:HG12	1:E:158:LYS:N	2.22	0.53
1:C:168:GLU:O	1:C:171:ALA:N	2.41	0.53
1:F:124:MET:C	1:F:126:PRO:HD3	2.28	0.53
1:B:90:THR:HG21	1:F:209:TRP:HD1	1.74	0.53
1:A:24:HIS:O	1:A:24:HIS:CD2	2.61	0.53
1:B:254:GLN:O	1:B:258:THR:HG23	2.08	0.53
1:F:252:ASN:ND2	1:F:255:ASP:HB2	2.24	0.53
1:B:209:TRP:NE1	1:B:210:LEU:HD21	2.24	0.53
1:E:293:ARG:NE	1:E:333:VAL:HG23	2.24	0.53
1:D:293:ARG:NE	1:D:333:VAL:HG23	2.24	0.53
1:B:293:ARG:NE	1:B:333:VAL:HG23	2.24	0.53
1:A:208:PRO:HB2	1:E:233:LEU:O	2.09	0.53
1:D:252:ASN:ND2	1:D:255:ASP:HB2	2.24	0.53
1:G:291:LEU:C	1:G:291:LEU:HD12	2.28	0.53
1:F:24:HIS:C	1:F:24:HIS:CD2	2.81	0.52
1:C:293:ARG:NE	1:C:333:VAL:HG23	2.24	0.52
1:A:293:ARG:NE	1:A:333:VAL:HG23	2.24	0.52
1:D:102:VAL:O	1:D:130:TYR:OH	2.18	0.52
1:B:101:ALA:HA	1:B:130:TYR:CD2	2.44	0.52
1:A:136:SER:O	1:A:137:LEU:HD23	2.08	0.52
1:A:252:ASN:ND2	1:A:255:ASP:HB2	2.24	0.52
1:E:142:ARG:CG	1:E:142:ARG:NH1	2.69	0.52
1:C:138:ILE:HD13	1:C:232:GLY:HA2	1.89	0.52
1:H:138:ILE:HD13	1:H:232:GLY:HA2	1.89	0.52
1:D:117:LEU:CD2	1:D:133:PHE:HB2	2.40	0.52
1:G:117:LEU:CD2	1:G:133:PHE:HB2	2.40	0.52
1:H:168:GLU:HG2	1:H:172:ARG:HD2	1.92	0.52
1:A:209:TRP:NE1	1:A:210:LEU:HD21	2.24	0.52
1:E:209:TRP:NE1	1:E:210:LEU:HD21	2.24	0.52
1:C:209:TRP:NE1	1:C:210:LEU:HD21	2.24	0.52
1:D:209:TRP:NE1	1:D:210:LEU:HD21	2.24	0.52
1:A:35:TYR:HD1	1:A:160:PHE:HB2	1.73	0.52
1:H:293:ARG:NE	1:H:333:VAL:HG23	2.24	0.52
1:G:293:ARG:NE	1:G:333:VAL:HG23	2.24	0.52
1:E:61:ASN:OD1	1:E:63:GLN:NE2	2.43	0.52
1:A:233:LEU:O	1:E:208:PRO:HB2	2.10	0.52
1:E:252:ASN:ND2	1:E:255:ASP:HB2	2.24	0.52
1:H:209:TRP:NE1	1:H:210:LEU:HD21	2.24	0.52
1:F:184:VAL:HG13	1:F:284:PRO:HA	1.92	0.52
1:F:117:LEU:CD2	1:F:133:PHE:HB2	2.40	0.52
1:F:136:SER:OG	1:F:137:LEU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:SER:O	1:F:18:CYS:HB2	2.10	0.52
1:E:184:VAL:HG13	1:E:284:PRO:HA	1.92	0.52
1:D:14:SER:O	1:D:18:CYS:HB2	2.10	0.52
1:D:267:GLU:OE1	1:D:269:THR:HG23	2.10	0.52
1:G:136:SER:OG	1:G:137:LEU:N	2.43	0.52
1:A:142:ARG:NH1	1:A:142:ARG:HG3	2.14	0.52
1:G:209:TRP:NE1	1:G:210:LEU:HD21	2.24	0.52
1:B:252:ASN:ND2	1:B:255:ASP:HB2	2.24	0.52
1:C:252:ASN:ND2	1:C:255:ASP:HB2	2.24	0.52
1:D:61:ASN:HB2	1:D:63:GLN:HB2	1.92	0.52
1:C:161:LEU:HD11	1:H:253:ILE:HG21	1.92	0.52
1:A:136:SER:OG	1:A:137:LEU:N	2.43	0.52
1:B:184:VAL:HG13	1:B:284:PRO:HA	1.92	0.52
1:C:117:LEU:CD2	1:C:133:PHE:HB2	2.40	0.52
1:B:14:SER:O	1:B:18:CYS:HB2	2.10	0.51
1:A:271:LYS:NZ	1:E:83:ASN:OD1	2.42	0.51
1:G:40:THR:OG1	1:G:46:ASP:OD1	2.18	0.51
1:B:55:TYR:CE2	1:B:314:TYR:HE2	2.29	0.51
1:D:55:TYR:CE2	1:D:314:TYR:HE2	2.29	0.51
1:F:55:TYR:CE2	1:F:314:TYR:HE2	2.29	0.51
1:B:24:HIS:CD2	1:B:24:HIS:C	2.81	0.51
1:A:208:PRO:HD2	1:A:209:TRP:HE3	1.76	0.51
1:E:24:HIS:CD2	1:E:24:HIS:C	2.81	0.51
1:H:252:ASN:ND2	1:H:255:ASP:HB2	2.24	0.51
1:C:55:TYR:CE2	1:C:314:TYR:HE2	2.29	0.51
1:C:14:SER:O	1:C:18:CYS:HB2	2.10	0.51
1:F:142:ARG:CG	1:F:142:ARG:NH1	2.69	0.51
1:G:168:GLU:O	1:G:172:ARG:N	2.27	0.51
1:E:117:LEU:CD2	1:E:133:PHE:HB2	2.40	0.51
1:A:125:PHE:CD1	1:A:125:PHE:N	2.76	0.51
1:D:184:VAL:HG13	1:D:284:PRO:HA	1.92	0.51
1:B:208:PRO:HD2	1:B:209:TRP:HE3	1.76	0.51
1:H:117:LEU:CD2	1:H:133:PHE:HB2	2.40	0.51
1:B:117:LEU:CD2	1:B:133:PHE:HB2	2.40	0.51
1:F:160:PHE:N	1:F:160:PHE:CD2	2.78	0.51
1:E:39:PHE:CE2	1:E:161:LEU:HA	2.44	0.51
1:D:101:ALA:HA	1:D:130:TYR:CG	2.46	0.51
1:C:19:ILE:HD11	1:C:179:ILE:CD1	2.40	0.51
1:C:184:VAL:HG13	1:C:284:PRO:HA	1.92	0.51
1:A:55:TYR:CE2	1:A:314:TYR:HE2	2.29	0.51
1:E:14:SER:O	1:E:18:CYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:PRO:HD2	1:F:209:TRP:HE3	1.76	0.51
1:E:21:GLU:HA	1:E:155:ARG:NH1	2.26	0.51
1:G:252:ASN:ND2	1:G:255:ASP:HB2	2.24	0.51
1:C:3:VAL:HB	1:C:32:VAL:HG22	1.93	0.51
1:A:1:MET:CE	1:A:177:VAL:HG23	2.41	0.51
1:G:14:SER:O	1:G:18:CYS:HB2	2.10	0.51
1:E:55:TYR:CE2	1:E:314:TYR:HE2	2.29	0.51
1:A:21:GLU:HA	1:A:155:ARG:NH1	2.26	0.51
1:D:21:GLU:HA	1:D:155:ARG:NH1	2.26	0.51
1:G:3:VAL:HB	1:G:32:VAL:HG22	1.93	0.51
1:A:14:SER:O	1:A:18:CYS:HB2	2.10	0.51
1:H:14:SER:O	1:H:18:CYS:HB2	2.10	0.51
1:F:3:VAL:HB	1:F:32:VAL:HG22	1.93	0.51
1:A:117:LEU:CD2	1:A:133:PHE:HB2	2.40	0.51
1:F:21:GLU:HA	1:F:155:ARG:NH1	2.26	0.51
1:B:93:SER:HG	1:B:135:THR:HB	1.72	0.50
1:A:184:VAL:HG13	1:A:284:PRO:HA	1.92	0.50
1:A:3:VAL:HB	1:A:32:VAL:HG22	1.93	0.50
1:C:21:GLU:HA	1:C:155:ARG:NH1	2.26	0.50
1:A:21:GLU:CG	1:A:155:ARG:NH2	2.71	0.50
1:B:21:GLU:HA	1:B:155:ARG:NH1	2.26	0.50
1:H:21:GLU:HA	1:H:155:ARG:NH1	2.26	0.50
1:D:83:ASN:O	1:D:86:ASN:N	2.45	0.50
1:G:55:TYR:CE2	1:G:314:TYR:HE2	2.29	0.50
1:H:171:ALA:HB1	1:H:298:PHE:CD2	2.46	0.50
1:H:83:ASN:O	1:H:86:ASN:N	2.45	0.50
1:E:3:VAL:HB	1:E:32:VAL:HG22	1.93	0.50
1:D:3:VAL:HB	1:D:32:VAL:HG22	1.93	0.50
1:G:21:GLU:HA	1:G:155:ARG:NH1	2.26	0.50
1:D:61:ASN:HB3	1:D:62:PRO:HD2	1.92	0.50
1:B:36:ALA:O	1:B:161:LEU:HD12	2.12	0.50
1:E:83:ASN:O	1:E:86:ASN:N	2.45	0.50
1:E:61:ASN:CG	1:E:63:GLN:NE2	2.64	0.50
1:A:253:ILE:HG13	1:F:42:PHE:CG	2.43	0.50
1:C:83:ASN:O	1:C:86:ASN:N	2.45	0.50
1:F:83:ASN:O	1:F:86:ASN:N	2.45	0.50
1:H:3:VAL:HB	1:H:32:VAL:HG22	1.93	0.50
1:A:89:LEU:HD23	1:A:138:ILE:O	2.12	0.50
1:E:136:SER:OG	1:E:137:LEU:N	2.43	0.50
1:F:265:ARG:O	1:F:268:PRO:HD3	2.11	0.50
1:H:184:VAL:HG13	1:H:284:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:TYR:CE2	1:H:314:TYR:HE2	2.29	0.50
1:A:83:ASN:O	1:A:86:ASN:N	2.45	0.50
1:C:24:HIS:C	1:C:24:HIS:CD2	2.81	0.50
1:H:142:ARG:NH1	1:H:142:ARG:CG	2.69	0.50
1:C:89:LEU:HD23	1:C:138:ILE:O	2.12	0.50
1:E:21:GLU:CG	1:E:155:ARG:NH2	2.72	0.50
1:C:162:ARG:HG3	1:C:162:ARG:NH1	2.26	0.50
1:B:178:ILE:HB	1:B:305:VAL:HG22	1.93	0.50
1:B:89:LEU:HD23	1:B:138:ILE:O	2.12	0.50
1:E:40:THR:OG1	1:E:142:ARG:HD3	2.12	0.50
1:B:21:GLU:HG3	1:B:155:ARG:HH21	1.73	0.50
1:G:34:VAL:N	1:G:158:LYS:O	2.42	0.50
1:B:40:THR:OG1	1:B:142:ARG:HD3	2.12	0.50
1:G:165:GLU:HB2	1:G:169:GLU:OE1	2.12	0.50
1:H:128:TYR:CZ	1:H:216:THR:HB	2.47	0.50
1:D:95:TYR:N	1:D:95:TYR:CD1	2.80	0.50
1:G:208:PRO:HD2	1:G:209:TRP:HE3	1.76	0.49
1:H:89:LEU:HD23	1:H:138:ILE:O	2.12	0.49
1:B:17:LEU:O	1:B:21:GLU:HB2	2.12	0.49
1:D:17:LEU:O	1:D:21:GLU:HB2	2.12	0.49
1:G:184:VAL:HG13	1:G:284:PRO:HA	1.92	0.49
1:A:40:THR:OG1	1:A:142:ARG:HD3	2.12	0.49
1:D:318:ILE:HG12	1:D:318:ILE:O	2.12	0.49
1:C:318:ILE:HG12	1:C:318:ILE:O	2.12	0.49
1:B:3:VAL:HB	1:B:32:VAL:HG22	1.93	0.49
1:C:95:TYR:N	1:C:95:TYR:CD1	2.80	0.49
1:H:40:THR:OG1	1:H:142:ARG:HD3	2.12	0.49
1:C:40:THR:OG1	1:C:142:ARG:HD3	2.12	0.49
1:G:89:LEU:HD23	1:G:138:ILE:O	2.12	0.49
1:A:17:LEU:O	1:A:21:GLU:HB2	2.12	0.49
1:D:167:PHE:N	1:D:167:PHE:CD1	2.80	0.49
1:G:251:ASN:OD1	1:G:280:THR:HG22	2.13	0.49
1:A:128:TYR:CD2	1:A:128:TYR:N	2.79	0.49
1:F:95:TYR:N	1:F:95:TYR:CD1	2.80	0.49
1:C:101:ALA:CB	1:C:130:TYR:CD2	2.96	0.49
1:G:40:THR:OG1	1:G:142:ARG:HD3	2.12	0.49
1:F:89:LEU:HD23	1:F:138:ILE:O	2.12	0.49
1:E:318:ILE:O	1:E:318:ILE:HG12	2.12	0.49
1:G:17:LEU:O	1:G:21:GLU:HB2	2.12	0.49
1:E:20:HIS:CE1	1:E:155:ARG:CD	2.96	0.49
1:G:24:HIS:CD2	1:G:24:HIS:C	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:PRO:HD2	1:C:209:TRP:HE3	1.76	0.49
1:E:251:ASN:OD1	1:E:280:THR:HG22	2.13	0.49
1:H:177:VAL:HG12	1:H:178:ILE:N	2.28	0.49
1:B:83:ASN:O	1:B:86:ASN:N	2.45	0.49
1:G:83:ASN:O	1:G:86:ASN:N	2.45	0.49
1:H:21:GLU:HG3	1:H:155:ARG:HH21	1.73	0.49
1:D:20:HIS:CE1	1:D:155:ARG:CD	2.96	0.49
1:B:251:ASN:OD1	1:B:280:THR:HG22	2.13	0.49
1:C:251:ASN:OD1	1:C:280:THR:HG22	2.13	0.49
1:F:318:ILE:HG12	1:F:318:ILE:O	2.12	0.49
1:A:95:TYR:CD1	1:A:95:TYR:N	2.80	0.49
1:C:17:LEU:O	1:C:21:GLU:HB2	2.12	0.49
1:D:24:HIS:CD2	1:D:24:HIS:C	2.81	0.49
1:H:208:PRO:HD2	1:H:209:TRP:HE3	1.76	0.49
1:D:35:TYR:CE1	1:D:160:PHE:CD2	3.00	0.49
1:E:59:PRO:HB2	1:E:61:ASN:O	2.12	0.49
1:E:17:LEU:O	1:E:21:GLU:HB2	2.12	0.49
1:G:61:ASN:ND2	1:G:63:GLN:N	2.59	0.49
1:G:35:TYR:CD1	1:G:160:PHE:HB2	2.47	0.49
1:H:251:ASN:OD1	1:H:280:THR:HG22	2.13	0.49
1:D:208:PRO:HD2	1:D:209:TRP:HE3	1.76	0.49
1:F:133:PHE:CD1	1:F:133:PHE:C	2.86	0.49
1:A:267:GLU:O	1:A:270:LEU:HB2	2.13	0.49
1:B:318:ILE:HG12	1:B:318:ILE:O	2.12	0.49
1:B:95:TYR:N	1:B:95:TYR:CD1	2.80	0.49
1:F:335:GLU:O	1:F:338:ASN:N	2.43	0.49
1:D:89:LEU:HD23	1:D:138:ILE:O	2.12	0.49
1:H:93:SER:HG	1:H:135:THR:HB	1.73	0.49
1:C:20:HIS:CE1	1:C:155:ARG:CD	2.96	0.49
1:D:251:ASN:OD1	1:D:280:THR:HG22	2.13	0.49
1:H:318:ILE:HG12	1:H:318:ILE:O	2.12	0.49
1:C:268:PRO:HB2	1:G:82:PRO:HA	1.95	0.49
1:A:318:ILE:HG12	1:A:318:ILE:O	2.12	0.49
1:H:95:TYR:CD1	1:H:95:TYR:N	2.80	0.49
1:F:178:ILE:HG22	1:F:178:ILE:O	2.10	0.49
1:G:23:TYR:CE2	1:G:330:PHE:HD2	2.31	0.49
1:E:23:TYR:CE2	1:E:330:PHE:HD2	2.31	0.49
1:B:128:TYR:CE2	1:B:216:THR:HB	2.47	0.49
1:C:74:TYR:CE1	1:C:78:HIS:HE1	2.31	0.49
1:H:136:SER:OG	1:H:137:LEU:N	2.43	0.49
1:D:133:PHE:CD1	1:D:133:PHE:C	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:HB3	1:A:163:LYS:HG3	1.95	0.49
1:G:21:GLU:CG	1:G:155:ARG:NH2	2.72	0.48
1:H:190:GLN:HG2	1:H:190:GLN:O	2.13	0.48
1:F:251:ASN:OD1	1:F:280:THR:HG22	2.13	0.48
1:A:251:ASN:OD1	1:A:280:THR:HG22	2.13	0.48
1:B:74:TYR:CE1	1:B:78:HIS:HE1	2.31	0.48
1:C:133:PHE:C	1:C:133:PHE:CD1	2.86	0.48
1:B:23:TYR:CE2	1:B:330:PHE:HD2	2.31	0.48
1:B:142:ARG:NH1	1:B:142:ARG:CG	2.69	0.48
1:A:142:ARG:NH1	1:A:142:ARG:CG	2.69	0.48
1:D:21:GLU:CG	1:D:155:ARG:NH2	2.71	0.48
1:E:180:ASN:HD22	1:E:307:HIS:HD2	1.60	0.48
1:E:74:TYR:CE1	1:E:78:HIS:HE1	2.31	0.48
1:C:253:ILE:HG21	1:H:161:LEU:HD21	1.94	0.48
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.61	0.48
1:A:23:TYR:CE2	1:A:330:PHE:HD2	2.31	0.48
1:H:23:TYR:CE2	1:H:330:PHE:HD2	2.31	0.48
1:D:40:THR:OG1	1:D:142:ARG:HD3	2.12	0.48
1:F:40:THR:OG1	1:F:142:ARG:HD3	2.12	0.48
1:F:17:LEU:O	1:F:21:GLU:HB2	2.13	0.48
1:A:166:SER:OG	1:A:169:GLU:N	2.41	0.48
1:F:74:TYR:CE1	1:F:78:HIS:HE1	2.31	0.48
1:B:133:PHE:CD1	1:B:133:PHE:C	2.86	0.48
1:A:133:PHE:C	1:A:133:PHE:CD1	2.86	0.48
1:C:23:TYR:CE2	1:C:330:PHE:HD2	2.31	0.48
1:E:190:GLN:HG2	1:E:190:GLN:O	2.13	0.48
1:E:133:PHE:CD1	1:E:133:PHE:C	2.86	0.48
1:H:151:ARG:O	1:H:154:GLU:HG2	2.14	0.48
1:A:252:ASN:OD1	1:A:254:GLN:HB2	2.14	0.48
1:G:142:ARG:CG	1:G:142:ARG:NH1	2.69	0.48
1:C:151:ARG:O	1:C:154:GLU:HG2	2.14	0.48
1:G:318:ILE:O	1:G:318:ILE:HG12	2.12	0.48
1:B:238:LEU:CD1	1:B:238:LEU:N	2.74	0.48
1:E:95:TYR:N	1:E:95:TYR:CD1	2.80	0.48
1:A:252:ASN:ND2	1:A:255:ASP:OD2	2.44	0.48
1:D:23:TYR:CE2	1:D:330:PHE:HD2	2.31	0.48
1:E:89:LEU:HD23	1:E:138:ILE:O	2.12	0.48
1:C:1:MET:CE	1:C:177:VAL:CG2	2.91	0.48
1:A:171:ALA:O	1:A:174:GLY:N	2.43	0.48
1:A:24:HIS:C	1:A:24:HIS:CD2	2.81	0.48
1:H:190:GLN:HE22	1:H:290:ARG:HH22	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:GLN:HE22	1:C:290:ARG:HH22	1.62	0.48
1:E:6:ILE:HD13	1:E:164:VAL:HG21	1.95	0.48
1:A:269:THR:C	1:A:271:LYS:H	2.15	0.48
1:E:151:ARG:O	1:E:154:GLU:HG2	2.14	0.48
1:G:95:TYR:CD1	1:G:95:TYR:N	2.80	0.48
1:F:151:ARG:O	1:F:154:GLU:HG2	2.14	0.48
1:B:20:HIS:CE1	1:B:155:ARG:CD	2.96	0.48
1:G:252:ASN:ND2	1:G:255:ASP:OD2	2.44	0.48
1:C:107:TRP:HA	1:C:110:MET:HG3	1.96	0.48
1:B:190:GLN:HG2	1:B:190:GLN:O	2.13	0.48
1:A:37:ASP:CB	1:A:163:LYS:HG3	2.43	0.48
1:F:125:PHE:CD1	1:F:125:PHE:N	2.81	0.48
1:H:107:TRP:HA	1:H:110:MET:HG3	1.96	0.48
1:H:74:TYR:CE1	1:H:78:HIS:HE1	2.32	0.48
1:E:117:LEU:HD21	1:E:133:PHE:HB2	1.96	0.48
1:G:107:TRP:HA	1:G:110:MET:HG3	1.96	0.48
1:H:20:HIS:CE1	1:H:155:ARG:CD	2.96	0.48
1:D:107:TRP:HA	1:D:110:MET:HG3	1.96	0.48
1:A:74:TYR:CE1	1:A:78:HIS:HE1	2.32	0.48
1:A:267:GLU:N	1:A:268:PRO:HD3	2.26	0.48
1:E:335:GLU:O	1:E:338:ASN:N	2.43	0.48
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.26	0.48
1:H:17:LEU:O	1:H:21:GLU:HB2	2.12	0.47
1:E:21:GLU:HG3	1:E:155:ARG:HH21	1.73	0.47
1:B:107:TRP:HA	1:B:110:MET:HG3	1.96	0.47
1:B:190:GLN:HE22	1:B:290:ARG:HH22	1.62	0.47
1:C:209:TRP:CD1	1:C:210:LEU:CD2	2.97	0.47
1:G:267:GLU:O	1:G:269:THR:N	2.47	0.47
1:H:39:PHE:HE2	1:H:161:LEU:HA	1.79	0.47
1:G:133:PHE:C	1:G:133:PHE:CD1	2.86	0.47
1:D:238:LEU:CD1	1:D:238:LEU:N	2.74	0.47
1:G:327:ALA:O	1:G:330:PHE:HB3	2.14	0.47
1:H:167:PHE:CE2	1:H:189:LEU:CB	2.88	0.47
1:F:107:TRP:HA	1:F:110:MET:HG3	1.96	0.47
1:G:3:VAL:HG13	1:G:179:ILE:HD11	1.96	0.47
1:D:101:ALA:HA	1:D:130:TYR:CD1	2.49	0.47
1:D:136:SER:OG	1:D:137:LEU:N	2.43	0.47
1:A:151:ARG:O	1:A:154:GLU:HG2	2.14	0.47
1:D:151:ARG:O	1:D:154:GLU:HG2	2.14	0.47
1:C:238:LEU:N	1:C:238:LEU:CD1	2.74	0.47
1:A:327:ALA:O	1:A:330:PHE:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ALA:O	1:C:330:PHE:HB3	2.14	0.47
1:A:209:TRP:CD1	1:A:210:LEU:CD2	2.97	0.47
1:A:209:TRP:CD1	1:A:210:LEU:HD23	2.49	0.47
1:B:252:ASN:ND2	1:B:255:ASP:OD2	2.44	0.47
1:D:190:GLN:O	1:D:190:GLN:HG2	2.13	0.47
1:A:190:GLN:O	1:A:190:GLN:HG2	2.13	0.47
1:G:269:THR:C	1:G:271:LYS:H	2.16	0.47
1:B:209:TRP:CD1	1:B:210:LEU:CD2	2.98	0.47
1:G:117:LEU:HD21	1:G:133:PHE:HB2	1.96	0.47
1:H:133:PHE:C	1:H:133:PHE:CD1	2.86	0.47
1:D:335:GLU:O	1:D:338:ASN:N	2.43	0.47
1:E:327:ALA:O	1:E:330:PHE:HB3	2.14	0.47
1:F:209:TRP:CD1	1:F:210:LEU:HD23	2.49	0.47
1:F:207:ALA:HA	1:F:209:TRP:CZ3	2.50	0.47
1:H:170:VAL:HG12	1:H:175:ALA:CB	2.44	0.47
1:A:17:LEU:HD12	1:A:17:LEU:HA	1.47	0.47
1:H:17:LEU:HD12	1:H:17:LEU:HA	1.47	0.47
1:D:21:GLU:HG3	1:D:155:ARG:HH21	1.73	0.47
1:F:190:GLN:HG2	1:F:190:GLN:O	2.13	0.47
1:D:209:TRP:CD1	1:D:210:LEU:CD2	2.98	0.47
1:D:209:TRP:CD1	1:D:210:LEU:HD23	2.49	0.47
1:F:238:LEU:CD1	1:F:238:LEU:N	2.74	0.47
1:D:327:ALA:O	1:D:330:PHE:HB3	2.14	0.47
1:F:23:TYR:CE2	1:F:330:PHE:HD2	2.31	0.47
1:A:207:ALA:HA	1:A:209:TRP:CZ3	2.49	0.47
1:B:128:TYR:HD1	1:B:128:TYR:H	1.59	0.47
1:E:190:GLN:HE22	1:E:290:ARG:HH22	1.62	0.47
1:G:1:MET:HE1	1:G:177:VAL:HG23	1.94	0.47
1:G:74:TYR:CE1	1:G:78:HIS:HE1	2.31	0.47
1:C:270:LEU:C	1:C:272:ASP:N	2.64	0.47
1:G:151:ARG:O	1:G:154:GLU:HG2	2.14	0.47
1:B:157:VAL:CG1	1:B:158:LYS:N	2.72	0.47
1:G:250:ILE:HD12	1:G:250:ILE:HG23	1.42	0.47
1:H:265:ARG:O	1:H:265:ARG:HG2	2.15	0.47
1:F:209:TRP:CD1	1:F:210:LEU:CD2	2.98	0.47
1:D:170:VAL:HG12	1:D:178:ILE:CD1	2.44	0.47
1:E:107:TRP:HA	1:E:110:MET:HG3	1.96	0.47
1:G:170:VAL:HB	1:G:178:ILE:HD11	1.96	0.47
1:G:3:VAL:CG1	1:G:179:ILE:CD1	2.92	0.47
1:B:133:PHE:CD1	1:B:134:ASN:N	2.83	0.47
1:B:157:VAL:HG12	1:B:158:LYS:N	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:O	1:B:154:GLU:HG2	2.14	0.47
1:E:65:ALA:HB2	1:E:106:TYR:CE2	2.50	0.47
1:H:238:LEU:CD1	1:H:238:LEU:N	2.74	0.47
1:B:327:ALA:O	1:B:330:PHE:HB3	2.14	0.47
1:H:327:ALA:O	1:H:330:PHE:HB3	2.14	0.47
1:F:327:ALA:O	1:F:330:PHE:HB3	2.14	0.47
1:H:167:PHE:HE2	1:H:189:LEU:O	1.96	0.47
1:A:209:TRP:HD1	1:E:90:THR:HG21	1.80	0.47
1:G:207:ALA:HA	1:G:209:TRP:CZ3	2.50	0.47
1:D:190:GLN:HE22	1:D:290:ARG:HH22	1.62	0.47
1:A:107:TRP:HA	1:A:110:MET:HG3	1.96	0.47
1:F:36:ALA:O	1:F:161:LEU:HA	2.15	0.47
1:C:207:ALA:HA	1:C:209:TRP:CZ3	2.50	0.47
1:C:83:ASN:OD1	1:G:271:LYS:NZ	2.45	0.47
1:H:209:TRP:CD1	1:H:210:LEU:CD2	2.98	0.47
1:B:136:SER:OG	1:B:137:LEU:N	2.43	0.47
1:D:117:LEU:HD21	1:D:133:PHE:HB2	1.96	0.47
1:C:133:PHE:CD1	1:C:134:ASN:N	2.83	0.47
1:A:133:PHE:CD1	1:A:134:ASN:N	2.83	0.47
1:E:209:TRP:CD1	1:E:210:LEU:HD23	2.49	0.47
1:A:90:THR:HG21	1:E:209:TRP:HD1	1.80	0.47
1:G:21:GLU:HG3	1:G:155:ARG:HH21	1.73	0.47
1:G:286:ARG:CG	1:G:287:PRO:CD	2.92	0.47
1:H:207:ALA:HA	1:H:209:TRP:CZ3	2.50	0.47
1:B:207:ALA:HA	1:B:209:TRP:CZ3	2.50	0.47
1:E:270:LEU:O	1:E:271:LYS:C	2.51	0.47
1:G:209:TRP:CD1	1:G:210:LEU:CD2	2.98	0.47
1:C:209:TRP:CD1	1:C:210:LEU:HD23	2.49	0.47
1:A:166:SER:O	1:A:169:GLU:HB3	2.15	0.47
1:C:171:ALA:CB	1:C:298:PHE:CD2	2.98	0.47
1:H:166:SER:HG	1:H:169:GLU:HB2	1.77	0.47
1:E:207:ALA:HA	1:E:209:TRP:CZ3	2.50	0.47
1:C:90:THR:HG21	1:G:209:TRP:HD1	1.80	0.47
1:F:190:GLN:HE22	1:F:290:ARG:HH22	1.62	0.47
1:G:39:PHE:HD2	1:G:161:LEU:HD13	1.74	0.47
1:D:207:ALA:HA	1:D:209:TRP:CZ3	2.50	0.47
1:D:74:TYR:CE1	1:D:78:HIS:HE1	2.32	0.47
1:H:117:LEU:HD21	1:H:133:PHE:HB2	1.96	0.47
1:H:133:PHE:CD1	1:H:134:ASN:N	2.83	0.47
1:B:177:VAL:HG22	1:B:304:GLU:HB2	1.97	0.47
1:B:256:HIS:HD1	1:B:278:GLU:CD	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:TRP:CD1	1:G:210:LEU:HD23	2.49	0.46
1:B:159:PHE:C	1:B:160:PHE:CD1	2.89	0.46
1:E:252:ASN:ND2	1:E:255:ASP:OD2	2.44	0.46
1:G:133:PHE:CD1	1:G:134:ASN:N	2.83	0.46
1:F:1:MET:HG3	1:F:176:ASP:HB2	1.98	0.46
1:C:233:LEU:O	1:G:208:PRO:HB2	2.14	0.46
1:H:21:GLU:HA	1:H:155:ARG:CZ	2.46	0.46
1:H:21:GLU:CG	1:H:155:ARG:NH2	2.72	0.46
1:G:20:HIS:CE1	1:G:155:ARG:CD	2.96	0.46
1:G:267:GLU:N	1:G:268:PRO:HD3	2.29	0.46
1:B:209:TRP:CD1	1:B:210:LEU:HD23	2.49	0.46
1:F:78:HIS:CD2	1:F:87:MET:HE3	2.49	0.46
1:F:101:ALA:HA	1:F:130:TYR:CG	2.50	0.46
1:F:59:PRO:HB2	1:F:61:ASN:O	2.15	0.46
1:E:209:TRP:CD1	1:E:210:LEU:CD2	2.98	0.46
1:G:21:GLU:HA	1:G:155:ARG:CZ	2.46	0.46
1:H:267:GLU:HB3	1:H:270:LEU:HG	1.98	0.46
1:F:118:THR:O	1:F:121:GLU:HB2	2.16	0.46
1:A:190:GLN:HE22	1:A:290:ARG:HH22	1.62	0.46
1:E:36:ALA:O	1:E:161:LEU:HA	2.15	0.46
1:E:133:PHE:CD1	1:E:134:ASN:N	2.83	0.46
1:F:194:LEU:HD23	1:F:194:LEU:HA	1.26	0.46
1:A:21:GLU:HA	1:A:155:ARG:CZ	2.46	0.46
1:A:250:ILE:HG23	1:A:250:ILE:HD12	1.43	0.46
1:D:133:PHE:CD1	1:D:134:ASN:N	2.83	0.46
1:D:238:LEU:HD12	1:D:238:LEU:HA	1.50	0.46
1:H:209:TRP:CD1	1:H:210:LEU:HD23	2.49	0.46
1:D:263:CYS:O	1:D:267:GLU:N	2.48	0.46
1:C:117:LEU:HD21	1:C:133:PHE:HB2	1.96	0.46
1:A:335:GLU:O	1:A:338:ASN:N	2.43	0.46
1:G:37:ASP:HB3	1:G:163:LYS:HA	1.96	0.46
1:F:145:LEU:HA	1:F:145:LEU:HD23	1.77	0.46
1:C:250:ILE:HD12	1:C:250:ILE:HG23	1.42	0.46
1:A:40:THR:OG1	1:A:46:ASP:OD1	2.18	0.46
1:B:21:GLU:HA	1:B:155:ARG:CZ	2.46	0.46
1:D:118:THR:O	1:D:121:GLU:HB2	2.16	0.46
1:G:269:THR:C	1:G:271:LYS:N	2.68	0.46
1:B:117:LEU:HD21	1:B:133:PHE:HB2	1.96	0.46
1:H:335:GLU:O	1:H:338:ASN:N	2.43	0.46
1:F:58:GLU:CG	1:F:59:PRO:HD2	2.46	0.46
1:A:20:HIS:CE1	1:A:155:ARG:CD	2.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLU:CG	1:B:155:ARG:NH2	2.72	0.46
1:F:20:HIS:CE1	1:F:155:ARG:CD	2.96	0.46
1:E:21:GLU:HA	1:E:155:ARG:CZ	2.46	0.46
1:A:118:THR:H	1:A:118:THR:HG23	1.36	0.46
1:G:118:THR:O	1:G:121:GLU:HB2	2.16	0.46
1:A:117:LEU:HD21	1:A:133:PHE:HB2	1.96	0.46
1:A:171:ALA:O	1:A:173:GLY:N	2.49	0.46
1:E:208:PRO:HD2	1:E:209:TRP:HE3	1.76	0.46
1:D:17:LEU:CA	1:D:152:LEU:HD21	2.46	0.46
1:A:118:THR:O	1:A:121:GLU:HB2	2.16	0.46
1:C:190:GLN:O	1:C:190:GLN:HG2	2.13	0.46
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.76	0.46
1:C:21:GLU:HA	1:C:155:ARG:NH2	2.31	0.46
1:D:21:GLU:HA	1:D:155:ARG:CZ	2.46	0.46
1:H:24:HIS:C	1:H:24:HIS:CD2	2.81	0.46
1:H:118:THR:O	1:H:121:GLU:HB2	2.16	0.46
1:F:133:PHE:CD1	1:F:134:ASN:N	2.83	0.46
1:B:250:ILE:HD13	1:E:250:ILE:CD1	2.39	0.46
1:B:17:LEU:CA	1:B:152:LEU:HD21	2.46	0.46
1:E:21:GLU:HA	1:E:155:ARG:NH2	2.31	0.46
1:C:118:THR:O	1:C:121:GLU:HB2	2.16	0.46
1:E:118:THR:HG23	1:E:118:THR:H	1.36	0.46
1:E:118:THR:O	1:E:121:GLU:HB2	2.16	0.46
1:G:190:GLN:HE22	1:G:290:ARG:HH22	1.62	0.46
1:B:61:ASN:HB3	1:B:63:GLN:HG3	1.98	0.46
1:E:130:TYR:CD1	1:E:131:GLY:N	2.84	0.46
1:C:180:ASN:ND2	1:C:182:THR:HG23	2.31	0.46
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.60	0.46
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.77	0.46
1:G:256:HIS:HD1	1:G:278:GLU:CD	2.12	0.45
1:F:21:GLU:HA	1:F:155:ARG:NH2	2.31	0.45
1:F:21:GLU:HA	1:F:155:ARG:CZ	2.46	0.45
1:G:21:GLU:HA	1:G:155:ARG:NH2	2.31	0.45
1:E:17:LEU:CA	1:E:152:LEU:HD21	2.46	0.45
1:H:286:ARG:CG	1:H:287:PRO:CD	2.92	0.45
1:G:157:VAL:HG12	1:G:158:LYS:N	2.31	0.45
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.50	0.45
1:A:171:ALA:C	1:A:173:GLY:N	2.68	0.45
1:H:319:HIS:CG	1:H:320:TRP:N	2.85	0.45
1:B:229:ILE:C	1:B:230:ILE:HG13	2.37	0.45
1:D:23:TYR:OH	1:D:331:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:CA	1:C:152:LEU:HD21	2.46	0.45
1:C:107:TRP:HB3	1:C:110:MET:HE3	1.98	0.45
1:F:229:ILE:C	1:F:230:ILE:HG13	2.37	0.45
1:E:286:ARG:HG3	1:E:287:PRO:HD2	1.98	0.45
1:C:82:PRO:HA	1:G:268:PRO:HB2	1.97	0.45
1:B:319:HIS:CG	1:B:320:TRP:N	2.84	0.45
1:E:319:HIS:CG	1:E:320:TRP:N	2.84	0.45
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.61	0.45
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.76	0.45
1:G:319:HIS:CG	1:G:320:TRP:N	2.85	0.45
1:H:166:SER:O	1:H:170:VAL:HG23	2.16	0.45
1:A:21:GLU:HA	1:A:155:ARG:NH2	2.31	0.45
1:C:286:ARG:HG3	1:C:287:PRO:HD2	1.98	0.45
1:G:61:ASN:ND2	1:G:62:PRO:CD	2.78	0.45
1:C:253:ILE:HG13	1:H:42:PHE:CE1	2.51	0.45
1:F:117:LEU:HD21	1:F:133:PHE:HB2	1.96	0.45
1:A:266:LEU:C	1:A:268:PRO:HD3	2.36	0.45
1:D:23:TYR:O	1:D:26:VAL:HG12	2.17	0.45
1:C:142:ARG:CG	1:C:142:ARG:NH1	2.69	0.45
1:C:21:GLU:HA	1:C:155:ARG:CZ	2.46	0.45
1:A:17:LEU:CA	1:A:152:LEU:HD21	2.46	0.45
1:B:21:GLU:HA	1:B:155:ARG:NH2	2.31	0.45
1:H:21:GLU:HA	1:H:155:ARG:NH2	2.31	0.45
1:F:17:LEU:CA	1:F:152:LEU:HD21	2.46	0.45
1:G:286:ARG:CZ	1:G:290:ARG:HB2	2.47	0.45
1:F:130:TYR:CD1	1:F:131:GLY:N	2.84	0.45
1:C:229:ILE:C	1:C:230:ILE:HG13	2.36	0.45
1:F:148:LEU:HD23	1:F:148:LEU:HA	1.76	0.45
1:A:82:PRO:HA	1:E:268:PRO:HB2	1.99	0.45
1:E:23:TYR:O	1:E:26:VAL:HG12	2.17	0.45
1:F:23:TYR:OH	1:F:331:GLY:HA3	2.17	0.45
1:E:40:THR:OG1	1:E:46:ASP:OD1	2.18	0.45
1:D:286:ARG:CZ	1:D:290:ARG:HB2	2.47	0.45
1:F:286:ARG:CZ	1:F:290:ARG:HB2	2.47	0.45
1:A:286:ARG:CG	1:A:287:PRO:CD	2.92	0.45
1:G:61:ASN:ND2	1:G:62:PRO:HD2	2.32	0.45
1:A:319:HIS:CG	1:A:320:TRP:N	2.84	0.45
1:C:167:PHE:CE2	1:C:189:LEU:HB3	2.52	0.45
1:E:170:VAL:CG1	1:E:178:ILE:HD13	2.46	0.45
1:C:23:TYR:O	1:C:26:VAL:HG12	2.16	0.45
1:C:23:TYR:OH	1:C:331:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:LEU:CA	1:H:152:LEU:HD21	2.46	0.45
1:B:118:THR:O	1:B:121:GLU:HB2	2.16	0.45
1:H:286:ARG:CZ	1:H:290:ARG:HB2	2.47	0.45
1:C:286:ARG:CZ	1:C:290:ARG:HB2	2.47	0.45
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.68	0.45
1:E:151:ARG:NH2	1:E:154:GLU:OE1	2.40	0.45
1:C:319:HIS:CG	1:C:320:TRP:N	2.84	0.45
1:D:319:HIS:CG	1:D:320:TRP:N	2.84	0.45
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.61	0.45
1:E:238:LEU:N	1:E:238:LEU:CD1	2.74	0.45
1:G:17:LEU:CA	1:G:152:LEU:HD21	2.46	0.45
1:B:286:ARG:CZ	1:B:290:ARG:HB2	2.47	0.45
1:H:229:ILE:C	1:H:230:ILE:HG13	2.37	0.45
1:B:168:GLU:O	1:B:170:VAL:N	2.49	0.45
1:A:229:ILE:C	1:A:230:ILE:HG13	2.37	0.45
1:G:335:GLU:O	1:G:338:ASN:N	2.43	0.45
1:F:252:ASN:ND2	1:F:255:ASP:OD2	2.44	0.45
1:H:252:ASN:ND2	1:H:255:ASP:OD2	2.44	0.45
1:C:286:ARG:CG	1:C:287:PRO:CD	2.92	0.45
1:D:229:ILE:C	1:D:230:ILE:HG13	2.37	0.45
1:F:195:LEU:HD12	1:F:195:LEU:HA	1.63	0.45
1:H:78:HIS:CD2	1:H:87:MET:HE3	2.52	0.45
1:G:293:ARG:HD3	1:G:293:ARG:HH11	1.61	0.45
1:A:23:TYR:OH	1:A:331:GLY:HA3	2.17	0.45
1:F:23:TYR:O	1:F:26:VAL:HG12	2.16	0.45
1:G:54:PRO:HG2	1:G:107:TRP:CG	2.52	0.45
1:E:256:HIS:HD1	1:E:278:GLU:CD	2.12	0.45
1:F:89:LEU:HA	1:F:138:ILE:O	2.17	0.45
1:C:17:LEU:HD12	1:C:17:LEU:HA	1.47	0.45
1:F:21:GLU:CG	1:F:155:ARG:NH2	2.72	0.45
1:F:21:GLU:HG3	1:F:155:ARG:HH21	1.73	0.45
1:G:17:LEU:HA	1:G:17:LEU:HD12	1.47	0.45
1:E:286:ARG:CZ	1:E:290:ARG:HB2	2.47	0.45
1:G:61:ASN:HD22	1:G:62:PRO:HD2	1.79	0.45
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.50	0.45
1:C:246:ASN:OD1	1:C:246:ASN:C	2.56	0.45
1:A:246:ASN:OD1	1:A:246:ASN:C	2.56	0.45
1:G:229:ILE:C	1:G:230:ILE:HG13	2.37	0.45
1:H:89:LEU:HA	1:H:138:ILE:O	2.17	0.45
1:F:124:MET:HB2	1:F:125:PHE:CE1	2.52	0.45
1:F:286:ARG:CG	1:F:287:PRO:CD	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:CZ	1:A:290:ARG:HB2	2.47	0.45
1:B:166:SER:HG	1:B:169:GLU:H	1.60	0.45
1:A:128:TYR:CZ	1:A:216:THR:HB	2.52	0.45
1:H:61:ASN:HB3	1:H:64:GLU:HG3	1.99	0.45
1:G:238:LEU:CD1	1:G:238:LEU:N	2.74	0.45
1:A:238:LEU:N	1:A:238:LEU:CD1	2.74	0.45
1:H:23:TYR:O	1:H:26:VAL:HG12	2.17	0.44
1:E:23:TYR:OH	1:E:331:GLY:HA3	2.17	0.44
1:D:169:GLU:HG2	1:D:170:VAL:N	2.32	0.44
1:G:190:GLN:HG2	1:G:190:GLN:O	2.13	0.44
1:F:319:HIS:CG	1:F:320:TRP:N	2.84	0.44
1:B:246:ASN:C	1:B:246:ASN:OD1	2.56	0.44
1:B:23:TYR:O	1:B:26:VAL:HG12	2.17	0.44
1:B:23:TYR:OH	1:B:331:GLY:HA3	2.17	0.44
1:G:107:TRP:CA	1:G:110:MET:HG3	2.48	0.44
1:D:21:GLU:HA	1:D:155:ARG:NH2	2.31	0.44
1:A:107:TRP:CA	1:A:110:MET:HG3	2.48	0.44
1:G:286:ARG:HG3	1:G:287:PRO:HD2	1.98	0.44
1:G:145:LEU:HD23	1:G:145:LEU:HA	1.77	0.44
1:C:21:GLU:CG	1:C:155:ARG:NH2	2.72	0.44
1:C:252:ASN:ND2	1:C:255:ASP:OD2	2.44	0.44
1:E:107:TRP:CA	1:E:110:MET:HG3	2.48	0.44
1:D:190:GLN:HA	1:D:191:PRO:HD3	1.74	0.44
1:D:286:ARG:CG	1:D:287:PRO:CD	2.92	0.44
1:B:286:ARG:HG3	1:B:287:PRO:HD2	1.98	0.44
1:E:39:PHE:CD2	1:E:161:LEU:HD12	2.44	0.44
1:E:168:GLU:HG3	1:E:298:PHE:CD1	2.51	0.44
1:D:269:THR:C	1:D:271:LYS:H	2.21	0.44
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.26	0.44
1:H:23:TYR:OH	1:H:331:GLY:HA3	2.17	0.44
1:G:23:TYR:OH	1:G:331:GLY:HA3	2.17	0.44
1:B:89:LEU:HA	1:B:138:ILE:O	2.17	0.44
1:D:89:LEU:HA	1:D:138:ILE:O	2.17	0.44
1:D:252:ASN:HD21	1:D:255:ASP:CB	2.31	0.44
1:C:252:ASN:HD21	1:C:255:ASP:CB	2.31	0.44
1:H:107:TRP:HB3	1:H:110:MET:HE3	2.00	0.44
1:B:266:LEU:HD12	1:B:266:LEU:HA	1.44	0.44
1:G:23:TYR:O	1:G:26:VAL:HG12	2.17	0.44
1:H:167:PHE:CE2	1:H:189:LEU:O	2.71	0.44
1:C:89:LEU:HA	1:C:138:ILE:O	2.17	0.44
1:E:17:LEU:HD12	1:E:17:LEU:HA	1.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:TRP:CA	1:D:110:MET:HG3	2.48	0.44
1:F:107:TRP:CA	1:F:110:MET:HG3	2.48	0.44
1:H:190:GLN:HA	1:H:191:PRO:HD3	1.74	0.44
2:G:348:FAB:H9	2:G:348:FAB:O2'	2.18	0.44
2:C:348:FAB:H9	2:C:348:FAB:O2'	2.18	0.44
1:E:157:VAL:CG1	1:E:158:LYS:N	2.80	0.44
1:C:168:GLU:O	1:C:171:ALA:HB3	2.17	0.44
1:C:335:GLU:O	1:C:338:ASN:N	2.43	0.44
1:A:65:ALA:HB2	1:A:106:TYR:CE2	2.53	0.44
1:F:246:ASN:C	1:F:246:ASN:OD1	2.56	0.44
1:A:331:GLY:O	1:A:334:LEU:HB2	2.17	0.44
1:E:89:LEU:HA	1:E:138:ILE:O	2.17	0.44
1:E:36:ALA:HA	2:E:348:FAB:N3A	2.33	0.44
2:D:348:FAB:H9	2:D:348:FAB:O2'	2.18	0.44
1:C:179:ILE:HD13	1:C:326:VAL:HG11	1.99	0.44
1:G:315:GLY:O	1:G:319:HIS:HB3	2.18	0.44
1:A:315:GLY:O	1:A:319:HIS:HB3	2.18	0.44
1:G:246:ASN:OD1	1:G:246:ASN:C	2.56	0.44
1:E:192:ASP:OD1	1:E:194:LEU:HB2	2.18	0.44
1:C:194:LEU:HA	1:C:194:LEU:HD23	1.26	0.44
1:D:246:ASN:C	1:D:246:ASN:OD1	2.56	0.44
1:E:167:PHE:CE1	1:E:189:LEU:HD13	2.53	0.44
1:F:213:PHE:CD1	1:F:213:PHE:C	2.91	0.44
1:B:331:GLY:O	1:B:334:LEU:HB2	2.18	0.44
1:H:166:SER:HG	1:H:169:GLU:CB	2.31	0.44
1:F:250:ILE:HD12	1:F:250:ILE:HG23	1.42	0.44
1:D:54:PRO:HG2	1:D:107:TRP:CG	2.52	0.44
2:F:348:FAB:O2'	2:F:348:FAB:H9	2.18	0.44
1:G:263:CYS:O	1:G:267:GLU:N	2.50	0.44
1:A:36:ALA:HA	2:A:348:FAB:N3A	2.33	0.44
1:C:36:ALA:HA	2:C:348:FAB:N3A	2.33	0.44
2:H:348:FAB:O2'	2:H:348:FAB:H9	2.18	0.44
1:H:36:ALA:HA	2:H:348:FAB:N3A	2.33	0.44
1:B:269:THR:O	1:B:271:LYS:N	2.51	0.44
1:A:236:VAL:CG1	1:A:237:THR:N	2.81	0.44
1:G:236:VAL:CG1	1:G:237:THR:N	2.81	0.44
1:B:315:GLY:O	1:B:319:HIS:HB3	2.18	0.44
1:D:213:PHE:CD1	1:D:213:PHE:C	2.91	0.44
1:A:23:TYR:O	1:A:26:VAL:HG12	2.17	0.44
1:E:331:GLY:O	1:E:334:LEU:HB2	2.18	0.44
1:F:252:ASN:HD21	1:F:255:ASP:CB	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:TRP:CA	1:H:110:MET:HG3	2.48	0.44
1:A:287:PRO:HB2	1:A:288:GLN:CD	2.38	0.44
1:B:190:GLN:HA	1:B:191:PRO:HD3	1.74	0.44
2:E:348:FAB:H9	2:E:348:FAB:O2'	2.18	0.44
1:A:271:LYS:HE2	1:E:86:ASN:HD21	1.83	0.44
1:C:238:LEU:HD12	1:C:238:LEU:HA	1.50	0.44
1:E:269:THR:C	1:E:271:LYS:N	2.68	0.44
1:E:315:GLY:O	1:E:319:HIS:HB3	2.18	0.44
1:C:315:GLY:O	1:C:319:HIS:HB3	2.18	0.44
1:D:315:GLY:O	1:D:319:HIS:HB3	2.18	0.44
1:G:238:LEU:HD12	1:G:238:LEU:HA	1.50	0.44
1:H:192:ASP:OD1	1:H:194:LEU:HB2	2.18	0.44
1:H:250:ILE:HD12	1:H:250:ILE:HG23	1.43	0.44
1:H:179:ILE:O	1:H:179:ILE:HG22	2.17	0.44
1:A:89:LEU:HA	1:A:138:ILE:O	2.17	0.44
1:H:252:ASN:HD21	1:H:255:ASP:CB	2.31	0.44
1:C:54:PRO:HG2	1:C:107:TRP:CG	2.52	0.44
1:B:54:PRO:HG2	1:B:107:TRP:CG	2.52	0.44
1:G:36:ALA:HA	2:G:348:FAB:N3A	2.33	0.44
1:E:229:ILE:C	1:E:230:ILE:HG13	2.37	0.44
1:B:78:HIS:CD2	1:B:87:MET:HE3	2.52	0.44
1:C:293:ARG:HH11	1:C:293:ARG:HD3	1.61	0.44
1:A:97:LEU:HB3	1:A:128:TYR:CG	2.53	0.44
1:B:63:GLN:H	1:B:63:GLN:HG2	1.48	0.44
1:E:246:ASN:C	1:E:246:ASN:OD1	2.56	0.44
1:C:213:PHE:C	1:C:213:PHE:CD1	2.91	0.44
1:E:213:PHE:C	1:E:213:PHE:CD1	2.91	0.44
1:B:270:LEU:C	1:B:272:ASP:N	2.71	0.43
1:C:128:TYR:CE2	1:C:216:THR:HB	2.53	0.43
1:H:55:TYR:CE2	1:H:314:TYR:CE2	3.06	0.43
1:H:194:LEU:HD23	1:H:194:LEU:HA	1.26	0.43
1:H:213:PHE:CD1	1:H:213:PHE:C	2.91	0.43
1:C:178:ILE:O	1:C:178:ILE:HG22	2.18	0.43
1:D:331:GLY:O	1:D:334:LEU:HB2	2.17	0.43
1:F:36:ALA:HA	2:F:348:FAB:N3A	2.33	0.43
2:A:348:FAB:O2'	2:A:348:FAB:H9	2.18	0.43
1:C:55:TYR:CE2	1:C:314:TYR:CE2	3.06	0.43
1:B:151:ARG:HH21	1:B:154:GLU:CD	2.21	0.43
1:H:246:ASN:OD1	1:H:246:ASN:C	2.56	0.43
1:A:254:GLN:NE2	1:A:254:GLN:H	2.15	0.43
1:G:331:GLY:O	1:G:334:LEU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:TRP:CA	1:C:110:MET:HG3	2.48	0.43
2:F:348:FAB:HM71	2:F:348:FAB:HM82	1.76	0.43
2:B:348:FAB:H9	2:B:348:FAB:O2'	2.18	0.43
1:D:161:LEU:HD13	1:D:161:LEU:HA	1.68	0.43
1:B:236:VAL:CG1	1:B:237:THR:N	2.81	0.43
1:C:236:VAL:CG1	1:C:237:THR:N	2.81	0.43
1:D:192:ASP:OD1	1:D:194:LEU:HB2	2.18	0.43
1:H:61:ASN:OD1	1:H:63:GLN:HB2	2.18	0.43
1:H:145:LEU:HD23	1:H:145:LEU:HA	1.77	0.43
1:F:112:LEU:HD23	1:F:112:LEU:HA	1.82	0.43
1:F:76:LEU:HD23	1:F:76:LEU:HA	1.61	0.43
1:C:331:GLY:O	1:C:334:LEU:HB2	2.17	0.43
1:H:331:GLY:O	1:H:334:LEU:HB2	2.17	0.43
1:G:167:PHE:CE1	1:G:189:LEU:CB	2.88	0.43
1:F:17:LEU:HD12	1:F:17:LEU:HA	1.47	0.43
1:B:107:TRP:CA	1:B:110:MET:HG3	2.48	0.43
1:G:39:PHE:HE2	1:G:161:LEU:HA	1.83	0.43
1:B:36:ALA:HA	2:B:348:FAB:N3A	2.33	0.43
1:F:55:TYR:CE2	1:F:314:TYR:CE2	3.06	0.43
1:G:68:ASN:OD1	1:G:318:ILE:HB	2.19	0.43
1:F:192:ASP:OD1	1:F:194:LEU:HB2	2.18	0.43
1:H:315:GLY:O	1:H:319:HIS:HB3	2.18	0.43
1:H:180:ASN:C	1:H:180:ASN:ND2	2.72	0.43
1:F:331:GLY:O	1:F:334:LEU:HB2	2.17	0.43
1:B:252:ASN:HD21	1:B:255:ASP:CB	2.31	0.43
1:D:55:TYR:CE2	1:D:314:TYR:CE2	3.06	0.43
1:C:68:ASN:OD1	1:C:318:ILE:HB	2.19	0.43
1:E:238:LEU:HA	1:E:238:LEU:HD12	1.50	0.43
1:A:265:ARG:O	1:A:265:ARG:HG2	2.18	0.43
1:E:252:ASN:HD21	1:E:255:ASP:CB	2.31	0.43
1:H:286:ARG:HG3	1:H:287:PRO:HD2	1.98	0.43
1:D:36:ALA:HA	2:D:348:FAB:N3A	2.33	0.43
1:B:55:TYR:CE2	1:B:314:TYR:CE2	3.06	0.43
1:C:151:ARG:HH21	1:C:154:GLU:CD	2.21	0.43
1:B:151:ARG:NH2	1:B:154:GLU:OE1	2.40	0.43
1:A:213:PHE:CD1	1:A:213:PHE:C	2.91	0.43
1:H:148:LEU:HA	1:H:148:LEU:HD23	1.76	0.43
1:D:142:ARG:NH1	1:D:142:ARG:CG	2.69	0.43
1:G:89:LEU:HA	1:G:138:ILE:O	2.17	0.43
1:G:252:ASN:HD21	1:G:255:ASP:CB	2.31	0.43
1:D:167:PHE:HE1	1:D:189:LEU:HB3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:PRO:HG2	1:H:107:TRP:CG	2.52	0.43
1:B:170:VAL:CG1	1:B:178:ILE:HD11	2.48	0.43
1:D:78:HIS:CD2	1:D:87:MET:HE3	2.54	0.43
1:B:10:VAL:CG1	1:B:11:ILE:N	2.82	0.43
1:A:10:VAL:CG1	1:A:11:ILE:N	2.82	0.43
1:H:68:ASN:OD1	1:H:318:ILE:HB	2.19	0.43
1:C:192:ASP:OD1	1:C:194:LEU:HB2	2.18	0.43
1:B:335:GLU:O	1:B:338:ASN:N	2.43	0.43
1:C:145:LEU:HD23	1:C:145:LEU:HA	1.77	0.43
1:D:62:PRO:CD	1:D:63:GLN:H	2.30	0.43
1:B:168:GLU:O	1:B:169:GLU:C	2.57	0.43
1:E:195:LEU:HA	1:E:195:LEU:HD12	1.63	0.43
1:D:10:VAL:CG1	1:D:11:ILE:N	2.82	0.43
1:D:236:VAL:CG1	1:D:237:THR:N	2.81	0.43
1:E:270:LEU:HD23	1:E:270:LEU:HA	1.54	0.43
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.82	0.43
1:E:148:LEU:HA	1:E:148:LEU:HD23	1.76	0.43
1:A:252:ASN:HD21	1:A:255:ASP:CB	2.31	0.43
1:H:168:GLU:O	1:H:172:ARG:HG3	2.18	0.43
1:A:101:ALA:CA	1:A:130:TYR:CD2	2.96	0.43
1:F:286:ARG:HG3	1:F:287:PRO:HD2	1.98	0.43
1:B:286:ARG:HA	1:B:287:PRO:HD3	1.84	0.43
1:G:179:ILE:CD1	1:G:179:ILE:N	2.77	0.43
1:G:61:ASN:CG	1:G:63:GLN:HB2	2.39	0.43
1:D:293:ARG:HD3	1:D:293:ARG:HH11	1.61	0.43
1:H:236:VAL:CG1	1:H:237:THR:N	2.81	0.43
1:C:151:ARG:NH2	1:C:154:GLU:OE1	2.40	0.43
1:E:151:ARG:HH21	1:E:154:GLU:CD	2.21	0.43
1:A:151:ARG:HH21	1:A:154:GLU:CD	2.21	0.43
1:B:192:ASP:OD1	1:B:194:LEU:HB2	2.18	0.43
1:B:213:PHE:CD1	1:B:213:PHE:C	2.91	0.43
1:B:233:LEU:O	1:F:208:PRO:HB2	2.18	0.43
1:H:251:ASN:HA	1:H:280:THR:CG2	2.48	0.43
1:F:10:VAL:CG1	1:F:11:ILE:N	2.82	0.43
1:A:68:ASN:OD1	1:A:318:ILE:HB	2.19	0.43
1:G:192:ASP:OD1	1:G:194:LEU:HB2	2.18	0.43
1:D:40:THR:OG1	1:D:46:ASP:OD1	2.18	0.42
1:E:54:PRO:HG2	1:E:107:TRP:CG	2.52	0.42
1:D:286:ARG:HG3	1:D:287:PRO:HD2	1.98	0.42
1:A:54:PRO:HG2	1:A:107:TRP:CG	2.52	0.42
1:E:265:ARG:O	1:E:266:LEU:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PHE:O	1:A:160:PHE:CD1	2.72	0.42
1:H:216:THR:OG1	1:H:226:SER:HB3	2.19	0.42
1:A:192:ASP:OD1	1:A:194:LEU:HB2	2.18	0.42
1:C:170:VAL:O	1:C:175:ALA:HB2	2.18	0.42
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.77	0.42
1:B:279:TYR:CD1	1:B:279:TYR:N	2.87	0.42
1:E:63:GLN:HG2	1:E:63:GLN:H	1.13	0.42
1:E:286:ARG:CG	1:E:287:PRO:CD	2.92	0.42
2:G:348:FAB:HM71	2:G:348:FAB:HM82	1.76	0.42
1:C:216:THR:OG1	1:C:226:SER:HB3	2.20	0.42
1:E:68:ASN:OD1	1:E:318:ILE:HB	2.19	0.42
1:F:315:GLY:O	1:F:319:HIS:HB3	2.18	0.42
1:F:279:TYR:CD1	1:F:279:TYR:N	2.87	0.42
1:C:10:VAL:CG1	1:C:11:ILE:N	2.82	0.42
1:D:324:LEU:HA	1:D:324:LEU:HD23	1.68	0.42
1:D:68:ASN:OD1	1:D:318:ILE:HB	2.19	0.42
1:E:216:THR:OG1	1:E:226:SER:HB3	2.20	0.42
1:D:250:ILE:HD12	1:D:250:ILE:HG23	1.43	0.42
1:A:253:ILE:CG2	1:A:254:GLN:N	2.82	0.42
1:B:17:LEU:HA	1:B:17:LEU:HD12	1.47	0.42
1:A:52:TRP:CE2	1:A:317:THR:HG23	2.55	0.42
1:G:61:ASN:HD21	1:G:63:GLN:HG3	1.83	0.42
1:D:52:TRP:CE2	1:D:317:THR:HG23	2.55	0.42
1:C:251:ASN:HA	1:C:280:THR:CG2	2.48	0.42
1:C:78:HIS:CD2	1:C:87:MET:HE3	2.54	0.42
1:D:124:MET:HB2	1:D:125:PHE:CD1	2.54	0.42
1:F:3:VAL:HG12	1:F:4:VAL:N	2.35	0.42
1:F:68:ASN:OD1	1:F:318:ILE:HB	2.19	0.42
1:F:216:THR:OG1	1:F:226:SER:HB3	2.20	0.42
1:G:216:THR:OG1	1:G:226:SER:HB3	2.20	0.42
1:E:89:LEU:HA	1:E:89:LEU:HD23	1.88	0.42
1:B:286:ARG:CG	1:B:287:PRO:CD	2.92	0.42
1:B:52:TRP:CE2	1:B:317:THR:HG23	2.55	0.42
1:B:270:LEU:O	1:B:271:LYS:C	2.58	0.42
1:E:3:VAL:HG12	1:E:4:VAL:N	2.35	0.42
1:A:128:TYR:OH	1:A:216:THR:HB	2.19	0.42
1:D:88:GLY:HA2	1:D:233:LEU:HD11	2.02	0.42
1:G:213:PHE:CD1	1:G:213:PHE:C	2.91	0.42
1:G:279:TYR:N	1:G:279:TYR:CD1	2.87	0.42
1:B:88:GLY:HA2	1:B:233:LEU:HD11	2.02	0.42
1:C:142:ARG:O	1:C:146:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HG3	1:A:287:PRO:HD2	1.98	0.42
1:F:54:PRO:HG2	1:F:107:TRP:CG	2.52	0.42
1:C:286:ARG:HD3	1:C:288:GLN:O	2.20	0.42
1:H:52:TRP:CE2	1:H:317:THR:HG23	2.55	0.42
1:C:55:TYR:CD1	1:C:223:ILE:HD13	2.55	0.42
1:B:179:ILE:HD12	1:B:179:ILE:HG23	1.55	0.42
1:B:216:THR:OG1	1:B:226:SER:HB3	2.20	0.42
1:G:88:GLY:HA2	1:G:233:LEU:HD11	2.02	0.42
1:E:52:TRP:CE2	1:E:317:THR:HG23	2.55	0.42
1:F:236:VAL:CG1	1:F:237:THR:N	2.81	0.42
1:B:55:TYR:CD1	1:B:223:ILE:HD13	2.55	0.42
1:A:55:TYR:CE2	1:A:314:TYR:CE2	3.06	0.42
1:E:55:TYR:CE2	1:E:314:TYR:CE2	3.06	0.42
1:H:324:LEU:HD23	1:H:324:LEU:HA	1.68	0.42
1:A:216:THR:OG1	1:A:226:SER:HB3	2.20	0.42
1:H:151:ARG:HH21	1:H:154:GLU:CD	2.21	0.42
1:H:218:ASP:HB3	1:H:221:ARG:HB2	2.02	0.42
1:F:88:GLY:HA2	1:F:233:LEU:HD11	2.02	0.42
1:E:218:ASP:HB3	1:E:221:ARG:HB2	2.02	0.42
1:A:279:TYR:N	1:A:279:TYR:CD1	2.87	0.42
1:D:89:LEU:HD23	1:D:89:LEU:HA	1.88	0.42
1:G:170:VAL:O	1:G:171:ALA:C	2.57	0.42
1:B:161:LEU:HA	1:B:161:LEU:HD12	1.54	0.42
1:F:251:ASN:HA	1:F:280:THR:CG2	2.48	0.42
1:B:267:GLU:C	1:B:267:GLU:OE1	2.58	0.42
1:C:3:VAL:HG12	1:C:4:VAL:N	2.35	0.42
1:G:151:ARG:HH21	1:G:154:GLU:CD	2.21	0.42
1:G:218:ASP:HB3	1:G:221:ARG:HB2	2.02	0.42
1:H:279:TYR:N	1:H:279:TYR:CD1	2.87	0.42
1:G:53:GLN:HA	1:G:54:PRO:HD2	1.94	0.42
1:H:142:ARG:O	1:H:146:GLN:HG3	2.20	0.42
1:D:118:THR:H	1:D:118:THR:HG23	1.36	0.42
1:G:286:ARG:HA	1:G:287:PRO:HD3	1.84	0.42
1:A:178:ILE:HB	1:A:305:VAL:HG22	2.01	0.42
1:C:97:LEU:HD11	1:C:125:PHE:CD2	2.55	0.42
1:E:10:VAL:CG1	1:E:11:ILE:N	2.82	0.42
1:A:269:THR:H	1:A:269:THR:HG23	1.45	0.42
1:F:55:TYR:CD1	1:F:223:ILE:HD13	2.55	0.42
1:H:151:ARG:NH2	1:H:154:GLU:OE1	2.40	0.42
1:B:218:ASP:HB3	1:B:221:ARG:HB2	2.02	0.42
1:C:218:ASP:HB3	1:C:221:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:HE1	1:E:177:VAL:CG2	2.50	0.42
1:B:112:LEU:HA	1:B:112:LEU:HD23	1.82	0.42
1:C:129:ARG:HE	1:C:129:ARG:HB3	1.55	0.42
1:A:142:ARG:O	1:A:146:GLN:HG3	2.20	0.42
1:G:142:ARG:O	1:G:146:GLN:HG3	2.20	0.42
1:F:142:ARG:O	1:F:146:GLN:HG3	2.20	0.42
1:F:52:TRP:CE2	1:F:317:THR:HG23	2.55	0.42
1:C:52:TRP:CE2	1:C:317:THR:HG23	2.55	0.42
1:B:168:GLU:O	1:B:171:ALA:N	2.53	0.42
1:G:195:LEU:HA	1:G:195:LEU:HD12	1.63	0.42
1:D:195:LEU:HD12	1:D:195:LEU:HA	1.63	0.42
1:H:10:VAL:CG1	1:H:11:ILE:N	2.82	0.42
1:G:55:TYR:CE2	1:G:314:TYR:CE2	3.06	0.42
1:D:279:TYR:CD1	1:D:279:TYR:N	2.87	0.42
1:C:279:TYR:CD1	1:C:279:TYR:N	2.87	0.42
1:D:256:HIS:HD1	1:D:278:GLU:CD	2.12	0.41
1:C:53:GLN:HA	1:C:54:PRO:HD2	1.94	0.41
1:F:190:GLN:HA	1:F:191:PRO:HD3	1.74	0.41
1:G:52:TRP:CE2	1:G:317:THR:HG23	2.55	0.41
1:H:130:TYR:C	1:H:130:TYR:CD1	2.93	0.41
1:G:10:VAL:CG1	1:G:11:ILE:N	2.82	0.41
1:E:55:TYR:CD1	1:E:223:ILE:HD13	2.55	0.41
1:D:230:ILE:HA	1:D:231:PRO:HD3	1.83	0.41
1:E:98:PHE:O	1:E:128:TYR:HB3	2.20	0.41
1:B:18:CYS:SG	1:B:324:LEU:HD23	2.60	0.41
1:A:18:CYS:SG	1:A:324:LEU:HD23	2.60	0.41
1:H:55:TYR:CD1	1:H:223:ILE:HD13	2.55	0.41
1:B:68:ASN:OD1	1:B:318:ILE:HB	2.19	0.41
1:E:65:ALA:CB	1:E:106:TYR:CE2	3.03	0.41
1:A:88:GLY:HA2	1:A:233:LEU:HD11	2.02	0.41
1:G:3:VAL:CG1	1:G:179:ILE:HD11	2.50	0.41
1:G:63:GLN:O	1:G:64:GLU:C	2.59	0.41
1:G:49:ALA:HB3	2:G:348:FAB:O4	2.21	0.41
1:B:49:ALA:HB3	2:B:348:FAB:O4	2.21	0.41
1:A:78:HIS:CD2	1:A:87:MET:HE3	2.55	0.41
1:E:18:CYS:SG	1:E:324:LEU:HD23	2.60	0.41
1:A:3:VAL:HG12	1:A:4:VAL:N	2.35	0.41
1:E:159:PHE:C	1:E:160:PHE:CD1	2.93	0.41
1:E:88:GLY:HA2	1:E:233:LEU:HD11	2.02	0.41
1:A:130:TYR:CD1	1:A:131:GLY:N	2.89	0.41
1:F:107:TRP:HB3	1:F:110:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ALA:HB3	2:F:348:FAB:O4	2.21	0.41
1:A:49:ALA:HB3	2:A:348:FAB:O4	2.21	0.41
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.63	0.41
1:B:138:ILE:HG21	1:B:138:ILE:HD13	1.82	0.41
1:D:142:ARG:O	1:D:146:GLN:HG3	2.20	0.41
1:B:97:LEU:HB3	1:B:128:TYR:CD2	2.55	0.41
1:B:142:ARG:O	1:B:146:GLN:HG3	2.20	0.41
1:B:159:PHE:CD1	1:B:159:PHE:N	2.88	0.41
1:F:7:GLY:HA2	2:F:348:FAB:H1B	2.03	0.41
1:G:61:ASN:HD22	1:G:63:GLN:H	1.64	0.41
1:E:49:ALA:CB	2:E:348:FAB:H3'	2.48	0.41
1:F:18:CYS:SG	1:F:324:LEU:HD23	2.60	0.41
1:C:18:CYS:SG	1:C:324:LEU:HD23	2.60	0.41
1:D:3:VAL:HG12	1:D:4:VAL:N	2.35	0.41
1:H:3:VAL:HG12	1:H:4:VAL:N	2.35	0.41
1:F:238:LEU:HD12	1:F:238:LEU:HA	1.49	0.41
1:A:337:ARG:O	1:A:338:ASN:HB2	2.21	0.41
1:C:246:ASN:OD1	1:C:247:TRP:N	2.54	0.41
1:B:246:ASN:OD1	1:B:247:TRP:N	2.54	0.41
1:F:246:ASN:OD1	1:F:247:TRP:N	2.54	0.41
1:B:2:ARG:O	1:B:176:ASP:HB2	2.19	0.41
1:E:75:LEU:HD23	1:E:75:LEU:HA	1.92	0.41
1:E:142:ARG:O	1:E:146:GLN:HG3	2.20	0.41
1:G:61:ASN:ND2	1:G:63:GLN:CB	2.81	0.41
1:C:86:ASN:HD21	1:G:271:LYS:HE2	1.86	0.41
1:C:195:LEU:HA	1:C:195:LEU:HD12	1.63	0.41
1:D:269:THR:C	1:D:271:LYS:N	2.74	0.41
1:D:55:TYR:CD1	1:D:223:ILE:HD13	2.55	0.41
1:D:216:THR:OG1	1:D:226:SER:HB3	2.20	0.41
1:B:23:TYR:O	1:B:24:HIS:C	2.59	0.41
1:C:88:GLY:HA2	1:C:233:LEU:HD11	2.02	0.41
1:A:286:ARG:HA	1:A:287:PRO:HD3	1.84	0.41
1:B:162:ARG:O	2:B:348:FAB:H2A	2.21	0.41
1:B:7:GLY:HA2	2:B:348:FAB:H1B	2.03	0.41
1:F:170:VAL:H	1:F:170:VAL:HG23	1.70	0.41
1:H:18:CYS:SG	1:H:324:LEU:HD23	2.60	0.41
1:F:151:ARG:NH2	1:F:154:GLU:OE1	2.40	0.41
1:G:337:ARG:O	1:G:338:ASN:HB2	2.21	0.41
1:G:76:LEU:HD23	1:G:76:LEU:HA	1.61	0.41
1:G:97:LEU:HB3	1:G:128:TYR:CG	2.54	0.41
1:D:142:ARG:HD2	1:D:142:ARG:C	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ARG:C	1:C:142:ARG:HD2	2.42	0.41
1:A:207:ALA:HA	1:A:208:PRO:HD3	1.79	0.41
1:E:84:ALA:O	1:E:89:LEU:HB2	2.21	0.41
1:D:138:ILE:HG21	1:D:138:ILE:HD13	1.81	0.41
1:A:84:ALA:O	1:A:89:LEU:HB2	2.21	0.41
1:H:138:ILE:HD13	1:H:138:ILE:HG21	1.81	0.41
1:D:61:ASN:N	1:D:61:ASN:ND2	2.63	0.41
1:B:107:TRP:HB3	1:B:110:MET:HE3	2.03	0.41
1:A:101:ALA:C	1:A:102:VAL:HG23	2.42	0.41
1:G:179:ILE:H	1:G:179:ILE:HD12	1.79	0.41
1:E:7:GLY:HA2	2:E:348:FAB:H1B	2.03	0.41
1:H:101:ALA:C	1:H:102:VAL:HG23	2.42	0.41
1:D:7:GLY:HA2	2:D:348:FAB:H1B	2.03	0.41
1:G:251:ASN:HA	1:G:280:THR:CG2	2.48	0.41
1:A:251:ASN:HA	1:A:280:THR:CG2	2.48	0.41
1:B:210:LEU:CD1	1:B:270:LEU:HD21	2.50	0.41
1:H:195:LEU:HA	1:H:195:LEU:HD12	1.63	0.41
1:C:1:MET:HG3	1:C:176:ASP:HB2	2.01	0.41
1:D:101:ALA:C	1:D:102:VAL:HG23	2.41	0.41
1:E:101:ALA:C	1:E:102:VAL:HG23	2.42	0.41
1:D:18:CYS:SG	1:D:324:LEU:HD23	2.60	0.41
1:A:55:TYR:CD1	1:A:223:ILE:HD13	2.55	0.41
1:G:18:CYS:SG	1:G:324:LEU:HD23	2.60	0.41
1:G:55:TYR:CD1	1:G:223:ILE:HD13	2.55	0.41
1:B:3:VAL:HG12	1:B:4:VAL:N	2.35	0.41
1:E:170:VAL:HG12	1:E:178:ILE:CD1	2.51	0.41
1:G:246:ASN:OD1	1:G:247:TRP:N	2.54	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.26	0.41
1:B:58:GLU:CG	1:B:59:PRO:HD2	2.51	0.41
1:D:218:ASP:HB3	1:D:221:ARG:HB2	2.02	0.41
1:B:167:PHE:CE1	1:B:189:LEU:HD13	2.56	0.41
1:C:23:TYR:O	1:C:24:HIS:C	2.59	0.41
1:H:142:ARG:C	1:H:142:ARG:HD2	2.41	0.41
1:H:166:SER:O	1:H:167:PHE:C	2.54	0.41
1:G:84:ALA:O	1:G:89:LEU:HB2	2.21	0.41
1:C:84:ALA:O	1:C:89:LEU:HB2	2.21	0.41
1:H:84:ALA:O	1:H:89:LEU:HB2	2.21	0.41
1:D:1:MET:CE	1:D:177:VAL:HG23	2.51	0.41
1:A:170:VAL:HG23	1:A:170:VAL:H	1.52	0.41
1:E:49:ALA:HB3	2:E:348:FAB:O4	2.21	0.41
1:G:101:ALA:C	1:G:102:VAL:HG23	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:VAL:CG1	1:E:237:THR:N	2.81	0.41
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.68	0.41
1:D:318:ILE:HD13	1:D:318:ILE:HG21	1.75	0.41
1:H:337:ARG:O	1:H:338:ASN:HB2	2.21	0.41
1:E:246:ASN:OD1	1:E:247:TRP:N	2.54	0.41
1:F:171:ALA:O	1:F:174:GLY:N	2.54	0.41
1:D:157:VAL:HG12	1:D:158:LYS:N	2.36	0.41
1:G:43:THR:HG23	1:G:43:THR:H	1.66	0.41
1:E:145:LEU:HD23	1:E:145:LEU:HA	1.77	0.41
1:A:218:ASP:HB3	1:A:221:ARG:HB2	2.02	0.41
1:F:175:ALA:HB1	1:F:177:VAL:O	2.21	0.40
1:B:256:HIS:HB2	1:E:42:PHE:HZ	1.87	0.40
1:C:101:ALA:C	1:C:102:VAL:HG23	2.42	0.40
1:F:84:ALA:O	1:F:89:LEU:HB2	2.21	0.40
1:A:17:LEU:HA	1:A:152:LEU:HD21	2.03	0.40
1:D:17:LEU:HA	1:D:152:LEU:HD21	2.03	0.40
1:C:64:GLU:O	1:C:67:TRP:N	2.54	0.40
1:G:3:VAL:HG12	1:G:4:VAL:N	2.35	0.40
1:G:7:GLY:HA2	2:G:348:FAB:H1B	2.03	0.40
1:E:49:ALA:HB1	1:E:230:ILE:HD12	2.03	0.40
1:A:7:GLY:HA2	2:A:348:FAB:H1B	2.03	0.40
1:D:49:ALA:HB3	2:D:348:FAB:O4	2.21	0.40
1:H:49:ALA:CB	2:H:348:FAB:H3'	2.48	0.40
1:G:78:HIS:CD2	1:G:87:MET:HE3	2.55	0.40
1:G:324:LEU:HD23	1:G:324:LEU:HA	1.68	0.40
1:F:337:ARG:O	1:F:338:ASN:HB2	2.21	0.40
1:C:268:PRO:C	1:C:270:LEU:H	2.25	0.40
1:E:142:ARG:HD2	1:E:142:ARG:C	2.42	0.40
1:D:84:ALA:O	1:D:89:LEU:HB2	2.21	0.40
1:H:267:GLU:HA	1:H:268:PRO:HD2	1.69	0.40
1:D:49:ALA:HB1	1:D:230:ILE:HD12	2.04	0.40
1:D:251:ASN:HA	1:D:280:THR:CG2	2.48	0.40
1:B:293:ARG:NH2	1:B:336:GLU:CD	2.74	0.40
1:E:269:THR:C	1:E:271:LYS:H	2.24	0.40
1:D:246:ASN:OD1	1:D:247:TRP:N	2.54	0.40
1:E:159:PHE:N	1:E:159:PHE:CD1	2.89	0.40
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.82	0.40
1:E:286:ARG:HA	1:E:287:PRO:HD3	1.84	0.40
1:C:190:GLN:HA	1:C:191:PRO:HD3	1.74	0.40
1:A:166:SER:O	1:A:170:VAL:HG23	2.22	0.40
1:H:49:ALA:HB1	1:H:230:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:ARG:HH11	1:H:293:ARG:HD3	1.61	0.40
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.76	0.40
1:D:148:LEU:HA	1:D:148:LEU:HD23	1.76	0.40
1:F:207:ALA:HA	1:F:208:PRO:HD3	1.79	0.40
1:F:17:LEU:HA	1:F:152:LEU:HD21	2.03	0.40
1:H:107:TRP:O	1:H:108:LYS:C	2.60	0.40
1:F:49:ALA:HB1	1:F:230:ILE:HD12	2.04	0.40
1:C:49:ALA:HB3	2:C:348:FAB:O4	2.21	0.40
1:D:193:PRO:HG2	1:F:73:ASN:HB3	2.04	0.40
1:B:117:LEU:HD23	1:B:133:PHE:HB2	2.04	0.40
1:C:337:ARG:O	1:C:338:ASN:HB2	2.21	0.40
1:F:218:ASP:HB3	1:F:221:ARG:HB2	2.02	0.40
1:H:76:LEU:HA	1:H:76:LEU:HD23	1.61	0.40
1:D:215:ILE:HG21	1:D:215:ILE:HD13	1.90	0.40
1:F:138:ILE:HG21	1:F:138:ILE:HD13	1.82	0.40
1:H:118:THR:H	1:H:118:THR:HG23	1.36	0.40
1:E:107:TRP:O	1:E:108:LYS:C	2.60	0.40
1:A:107:TRP:O	1:A:108:LYS:C	2.60	0.40
1:H:286:ARG:HA	1:H:287:PRO:HD3	1.84	0.40
1:C:208:PRO:HB2	1:G:233:LEU:O	2.21	0.40
1:H:7:GLY:HA2	2:H:348:FAB:H1B	2.03	0.40
1:H:36:ALA:O	1:H:161:LEU:HA	2.22	0.40
1:F:324:LEU:HA	1:F:324:LEU:HD23	1.68	0.40
1:H:75:LEU:HA	1:H:75:LEU:HD23	1.92	0.40

All (5) 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:G:73:ASN:OD1	1:H:2:ARG:NH2[4_565]	1.42	0.78
1:C:2:ARG:NH2	1:D:73:ASN:OD1[3_655]	1.78	0.42
1:C:162:ARG:NH2	1:H:123:ASP:OD1[3_655]	2.01	0.19
1:C:123:ASP:OD1	1:H:162:ARG:NH2[4_565]	2.07	0.13
1:E:247:TRP:NE1	1:F:247:TRP:NE1[7_555]	2.12	0.08



## 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	337/347 (97%)	311 (92%)	23 (7%)	3 (1%)	21	67
1	B	337/347 (97%)	308 (91%)	26 (8%)	3 (1%)	21	67
1	C	337/347 (97%)	306 (91%)	28 (8%)	3 (1%)	21	67
1	D	337/347 (97%)	310 (92%)	24 (7%)	3 (1%)	21	67
1	E	337/347 (97%)	311 (92%)	23 (7%)	3 (1%)	21	67
1	F	337/347 (97%)	312 (93%)	21 (6%)	4 (1%)	16	60
1	G	337/347 (97%)	310 (92%)	24 (7%)	3 (1%)	21	67
1	H	337/347 (97%)	308 (91%)	25 (7%)	4 (1%)	16	60
All	All	2696/2776 (97%)	2476 (92%)	194 (7%)	26 (1%)	19	65

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	B	30	LEU
1	C	30	LEU
1	D	30	LEU
1	E	30	LEU
1	F	30	LEU
1	G	30	LEU
1	H	30	LEU
1	A	240	GLY
1	B	240	GLY
1	C	240	GLY
1	D	240	GLY
1	E	240	GLY
1	F	240	GLY
1	G	240	GLY
1	H	240	GLY
1	H	173	GLY

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Mol	Chain	Res	Type
1	F	174	GLY
1	C	28	GLN
1	F	28	GLN
1	A	28	GLN
1	B	28	GLN
1	D	28	GLN
1	E	28	GLN
1	G	28	GLN
1	H	28	GLN

### 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	290/298 (97%)	267 (92%)	23 (8%)	15	53
1	B	290/298 (97%)	261 (90%)	29 (10%)	9	37
1	C	290/298 (97%)	264 (91%)	26 (9%)	12	43
1	D	290/298 (97%)	265 (91%)	25 (9%)	13	46
1	E	290/298 (97%)	266 (92%)	24 (8%)	14	49
1	F	290/298 (97%)	265 (91%)	25 (9%)	13	46
1	G	290/298 (97%)	269 (93%)	21 (7%)	18	57
1	H	290/298 (97%)	268 (92%)	22 (8%)	16	55
All	All	2320/2384 (97%)	2125 (92%)	195 (8%)	14	48

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	76	LEU
1	A	81	SER
1	A	115	ARG
1	A	118	THR
1	A	135	THR

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Mol	Chain	Res	Type
1	A	142	ARG
1	A	151	ARG
1	A	157	VAL
1	A	159	PHE
1	A	184	VAL
1	A	205	VAL
1	A	221	ARG
1	A	226	SER
1	A	238	LEU
1	A	242	PHE
1	A	252	ASN
1	A	253	ILE
1	A	254	GLN
1	A	258	THR
1	A	267	GLU
1	A	280	THR
1	A	291	LEU
1	B	31	ASP
1	B	56	THR
1	B	58	GLU
1	B	62	PRO
1	B	76	LEU
1	B	81	SER
1	B	115	ARG
1	B	118	THR
1	B	129	ARG
1	B	135	THR
1	B	142	ARG
1	B	151	ARG
1	B	160	PHE
1	B	161	LEU
1	B	169	GLU
1	B	176	ASP
1	B	180	ASN
1	B	184	VAL
1	B	205	VAL
1	B	221	ARG
1	B	226	SER
1	B	238	LEU
1	B	242	PHE
1	B	252	ASN
1	B	253	ILE

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Mol	Chain	Res	Type
1	B	258	THR
1	B	267	GLU
1	B	280	THR
1	B	291	LEU
1	C	31	ASP
1	C	56	THR
1	C	76	LEU
1	C	81	SER
1	C	115	ARG
1	C	118	THR
1	C	126	PRO
1	C	135	THR
1	C	142	ARG
1	C	151	ARG
1	C	157	VAL
1	C	161	LEU
1	C	162	ARG
1	C	184	VAL
1	C	205	VAL
1	C	221	ARG
1	C	226	SER
1	C	238	LEU
1	C	242	PHE
1	C	252	ASN
1	C	253	ILE
1	C	258	THR
1	C	269	THR
1	C	280	THR
1	C	288	GLN
1	C	291	LEU
1	D	31	ASP
1	D	57	SER
1	D	61	ASN
1	D	76	LEU
1	D	81	SER
1	D	115	ARG
1	D	118	THR
1	D	127	ASP
1	D	130	TYR
1	D	135	THR
1	D	142	ARG
1	D	151	ARG

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Mol	Chain	Res	Type
1	D	161	LEU
1	D	162	ARG
1	D	184	VAL
1	D	205	VAL
1	D	221	ARG
1	D	226	SER
1	D	238	LEU
1	D	242	PHE
1	D	252	ASN
1	D	253	ILE
1	D	258	THR
1	D	280	THR
1	D	291	LEU
1	E	31	ASP
1	E	57	SER
1	E	58	GLU
1	E	63	GLN
1	E	76	LEU
1	E	81	SER
1	E	115	ARG
1	E	118	THR
1	E	125	PHE
1	E	135	THR
1	E	142	ARG
1	E	151	ARG
1	E	161	LEU
1	E	184	VAL
1	E	205	VAL
1	E	221	ARG
1	E	226	SER
1	E	238	LEU
1	E	242	PHE
1	E	252	ASN
1	E	253	ILE
1	E	258	THR
1	E	280	THR
1	E	291	LEU
1	F	31	ASP
1	F	57	SER
1	F	58	GLU
1	F	76	LEU
1	F	81	SER

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Mol	Chain	Res	Type
1	F	115	ARG
1	F	118	THR
1	F	126	PRO
1	F	135	THR
1	F	142	ARG
1	F	151	ARG
1	F	184	VAL
1	F	205	VAL
1	F	221	ARG
1	F	226	SER
1	F	238	LEU
1	F	242	PHE
1	F	252	ASN
1	F	253	ILE
1	F	258	THR
1	F	268	PRO
1	F	269	THR
1	F	280	THR
1	F	288	GLN
1	F	291	LEU
1	G	31	ASP
1	G	61	ASN
1	G	76	LEU
1	G	81	SER
1	G	115	ARG
1	G	118	THR
1	G	127	ASP
1	G	135	THR
1	G	142	ARG
1	G	151	ARG
1	G	184	VAL
1	G	205	VAL
1	G	221	ARG
1	G	226	SER
1	G	238	LEU
1	G	242	PHE
1	G	252	ASN
1	G	253	ILE
1	G	258	THR
1	G	280	THR
1	G	291	LEU
1	H	31	ASP

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Mol	Chain	Res	Type
1	H	57	SER
1	H	76	LEU
1	H	81	SER
1	H	115	ARG
1	H	118	THR
1	H	135	THR
1	H	142	ARG
1	H	151	ARG
1	H	161	LEU
1	H	180	ASN
1	H	184	VAL
1	H	205	VAL
1	H	221	ARG
1	H	226	SER
1	H	238	LEU
1	H	242	PHE
1	H	252	ASN
1	H	253	ILE
1	H	258	THR
1	H	280	THR
1	H	291	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	53	GLN
1	A	61	ASN
1	A	78	HIS
1	A	96	ASN
1	A	134	ASN
1	A	180	ASN
1	A	190	GLN
1	A	217	HIS
1	A	252	ASN
1	A	254	GLN
1	A	307	HIS
1	B	24	HIS
1	B	53	GLN
1	B	78	HIS
1	B	96	ASN
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	180	ASN
1	B	190	GLN
1	B	217	HIS
1	B	307	HIS
1	C	24	HIS
1	C	53	GLN
1	C	78	HIS
1	C	86	ASN
1	C	96	ASN
1	C	134	ASN
1	C	180	ASN
1	C	190	GLN
1	C	217	HIS
1	C	252	ASN
1	C	307	HIS
1	D	24	HIS
1	D	53	GLN
1	D	61	ASN
1	D	63	GLN
1	D	78	HIS
1	D	86	ASN
1	D	96	ASN
1	D	134	ASN
1	D	190	GLN
1	D	217	HIS
1	D	252	ASN
1	D	254	GLN
1	D	288	GLN
1	D	307	HIS
1	E	24	HIS
1	E	53	GLN
1	E	63	GLN
1	E	78	HIS
1	E	86	ASN
1	E	96	ASN
1	E	134	ASN
1	E	190	GLN
1	E	217	HIS
1	E	252	ASN
1	E	254	GLN
1	E	307	HIS
1	F	24	HIS

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Mol	Chain	Res	Type
1	F	53	GLN
1	F	78	HIS
1	F	96	ASN
1	F	134	ASN
1	F	180	ASN
1	F	190	GLN
1	F	217	HIS
1	F	252	ASN
1	F	288	GLN
1	F	307	HIS
1	G	24	HIS
1	G	53	GLN
1	G	61	ASN
1	G	63	GLN
1	G	78	HIS
1	G	96	ASN
1	G	134	ASN
1	G	180	ASN
1	G	190	GLN
1	G	217	HIS
1	G	307	HIS
1	H	24	HIS
1	H	53	GLN
1	H	78	HIS
1	H	96	ASN
1	H	134	ASN
1	H	180	ASN
1	H	190	GLN
1	H	217	HIS
1	H	252	ASN
1	H	307	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAB	A	348	-	48,63,63	1.33	3 (6%)	54,97,97	3.28	17 (31%)
2	FAB	B	348	-	48,63,63	1.32	3 (6%)	54,97,97	3.28	17 (31%)
2	FAB	C	348	-	48,63,63	1.33	3 (6%)	54,97,97	3.28	17 (31%)
2	FAB	D	348	-	48,63,63	1.33	3 (6%)	54,97,97	3.28	16 (29%)
2	FAB	E	348	-	48,63,63	1.32	3 (6%)	54,97,97	3.29	18 (33%)
2	FAB	F	348	-	48,63,63	1.32	3 (6%)	54,97,97	3.28	17 (31%)
2	FAB	G	348	-	48,63,63	1.32	3 (6%)	54,97,97	3.29	17 (31%)
2	FAB	H	348	-	48,63,63	1.33	3 (6%)	54,97,97	3.29	17 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAB	A	348	-	-	0/34/58/58	0/6/6/6
2	FAB	B	348	-	-	0/34/58/58	0/6/6/6
2	FAB	C	348	-	-	0/34/58/58	0/6/6/6
2	FAB	D	348	-	-	0/34/58/58	0/6/6/6
2	FAB	E	348	-	-	0/34/58/58	0/6/6/6
2	FAB	F	348	-	-	0/34/58/58	0/6/6/6
2	FAB	G	348	-	-	0/34/58/58	0/6/6/6
2	FAB	H	348	-	-	0/34/58/58	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	348	FAB	C10-N10	-2.95	1.35	1.39
2	A	348	FAB	C10-N10	-2.95	1.35	1.39
2	F	348	FAB	C10-N10	-2.93	1.35	1.39
2	G	348	FAB	C10-N10	-2.93	1.35	1.39
2	E	348	FAB	C10-N10	-2.92	1.35	1.39
2	C	348	FAB	C10-N10	-2.89	1.35	1.39
2	B	348	FAB	C10-N10	-2.88	1.35	1.39
2	H	348	FAB	C10-N10	-2.87	1.35	1.39
2	D	348	FAB	C4-N3	3.40	1.39	1.33
2	G	348	FAB	C4-N3	3.44	1.39	1.33
2	F	348	FAB	C4-N3	3.45	1.39	1.33
2	A	348	FAB	C4-N3	3.46	1.39	1.33
2	E	348	FAB	C4-N3	3.46	1.39	1.33
2	B	348	FAB	C4-N3	3.47	1.39	1.33
2	H	348	FAB	C4-N3	3.48	1.39	1.33
2	C	348	FAB	C4-N3	3.48	1.39	1.33
2	E	348	FAB	C3'-C2'	6.41	1.63	1.52
2	B	348	FAB	C3'-C2'	6.43	1.63	1.52
2	G	348	FAB	C3'-C2'	6.46	1.63	1.52
2	F	348	FAB	C3'-C2'	6.47	1.63	1.52
2	H	348	FAB	C3'-C2'	6.47	1.63	1.52
2	A	348	FAB	C3'-C2'	6.48	1.63	1.52
2	D	348	FAB	C3'-C2'	6.49	1.63	1.52
2	C	348	FAB	C3'-C2'	6.53	1.63	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	348	FAB	C4X-C10-N10	-9.79	114.75	120.52
2	E	348	FAB	C4X-C10-N10	-9.78	114.75	120.52
2	H	348	FAB	C4X-C10-N10	-9.77	114.76	120.52
2	B	348	FAB	C4X-C10-N10	-9.76	114.77	120.52
2	C	348	FAB	C4X-C10-N10	-9.76	114.77	120.52
2	G	348	FAB	C4X-C10-N10	-9.75	114.78	120.52
2	G	348	FAB	C4X-N5-C5X	-9.73	109.08	121.64
2	A	348	FAB	C4X-C10-N10	-9.71	114.80	120.52
2	F	348	FAB	C4X-N5-C5X	-9.70	109.12	121.64
2	A	348	FAB	C4X-N5-C5X	-9.70	109.12	121.64
2	D	348	FAB	C4X-C10-N10	-9.69	114.81	120.52
2	H	348	FAB	C4X-N5-C5X	-9.69	109.14	121.64
2	E	348	FAB	C4X-N5-C5X	-9.68	109.15	121.64
2	D	348	FAB	C4X-N5-C5X	-9.67	109.16	121.64
2	B	348	FAB	C4X-N5-C5X	-9.67	109.16	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	348	FAB	C4X-N5-C5X	-9.66	109.17	121.64
2	E	348	FAB	C4X-C4-N3	-7.25	113.68	123.59
2	H	348	FAB	C4X-C4-N3	-7.24	113.69	123.59
2	G	348	FAB	C4X-C4-N3	-7.24	113.69	123.59
2	B	348	FAB	C4X-C4-N3	-7.24	113.69	123.59
2	D	348	FAB	C4X-C4-N3	-7.23	113.71	123.59
2	A	348	FAB	C4X-C4-N3	-7.22	113.72	123.59
2	F	348	FAB	C4X-C4-N3	-7.22	113.72	123.59
2	C	348	FAB	C4X-C4-N3	-7.21	113.73	123.59
2	D	348	FAB	C7M-C7-C8	-4.87	110.04	120.73
2	C	348	FAB	C7M-C7-C8	-4.86	110.04	120.73
2	A	348	FAB	C7M-C7-C8	-4.86	110.05	120.73
2	G	348	FAB	C7M-C7-C8	-4.86	110.06	120.73
2	H	348	FAB	C7M-C7-C8	-4.86	110.06	120.73
2	B	348	FAB	C7M-C7-C8	-4.85	110.07	120.73
2	E	348	FAB	C7M-C7-C8	-4.85	110.08	120.73
2	F	348	FAB	C7M-C7-C8	-4.84	110.09	120.73
2	H	348	FAB	P-O3P-PA	-3.09	124.04	132.73
2	C	348	FAB	P-O3P-PA	-3.09	124.06	132.73
2	A	348	FAB	P-O3P-PA	-3.08	124.07	132.73
2	B	348	FAB	P-O3P-PA	-3.08	124.09	132.73
2	E	348	FAB	P-O3P-PA	-3.08	124.09	132.73
2	F	348	FAB	P-O3P-PA	-3.07	124.10	132.73
2	G	348	FAB	P-O3P-PA	-3.07	124.12	132.73
2	D	348	FAB	P-O3P-PA	-3.06	124.14	132.73
2	H	348	FAB	O3P-P-O5'	-3.02	94.93	102.94
2	B	348	FAB	O3P-P-O5'	-3.02	94.93	102.94
2	E	348	FAB	O3P-P-O5'	-3.00	94.97	102.94
2	A	348	FAB	O3P-P-O5'	-3.00	94.97	102.94
2	G	348	FAB	O3P-P-O5'	-3.00	94.97	102.94
2	C	348	FAB	O3P-P-O5'	-3.00	94.98	102.94
2	F	348	FAB	O3P-P-O5'	-3.00	94.98	102.94
2	D	348	FAB	O3P-P-O5'	-2.99	95.01	102.94
2	F	348	FAB	C5'-C3'-C4'	-2.41	101.09	111.90
2	E	348	FAB	C5'-C3'-C4'	-2.41	101.10	111.90
2	A	348	FAB	C5'-C3'-C4'	-2.40	101.12	111.90
2	B	348	FAB	C5'-C3'-C4'	-2.40	101.12	111.90
2	D	348	FAB	C5'-C3'-C4'	-2.40	101.13	111.90
2	C	348	FAB	C5'-C3'-C4'	-2.40	101.14	111.90
2	H	348	FAB	C5'-C3'-C4'	-2.40	101.16	111.90
2	G	348	FAB	C5'-C3'-C4'	-2.39	101.17	111.90
2	D	348	FAB	O3P-PA-O5B	-2.12	97.32	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	348	FAB	O3P-PA-O5B	-2.10	97.35	102.94
2	B	348	FAB	O2'-C2D-C1'	-2.10	104.78	109.94
2	A	348	FAB	O3P-PA-O5B	-2.10	97.37	102.94
2	H	348	FAB	O2'-C2D-C1'	-2.10	104.79	109.94
2	C	348	FAB	O3P-PA-O5B	-2.10	97.37	102.94
2	B	348	FAB	O3P-PA-O5B	-2.10	97.37	102.94
2	F	348	FAB	O3P-PA-O5B	-2.10	97.38	102.94
2	D	348	FAB	O2'-C2D-C1'	-2.09	104.80	109.94
2	E	348	FAB	O3P-PA-O5B	-2.09	97.39	102.94
2	H	348	FAB	O3P-PA-O5B	-2.09	97.40	102.94
2	E	348	FAB	O2'-C2D-C1'	-2.09	104.82	109.94
2	G	348	FAB	O2'-C2D-C1'	-2.09	104.82	109.94
2	C	348	FAB	O2'-C2D-C1'	-2.08	104.82	109.94
2	A	348	FAB	O2'-C2D-C1'	-2.08	104.83	109.94
2	F	348	FAB	O2'-C2D-C1'	-2.06	104.88	109.94
2	F	348	FAB	O3B-C3B-C2B	-2.02	105.24	111.83
2	B	348	FAB	O3B-C3B-C2B	-2.01	105.28	111.83
2	A	348	FAB	O3B-C3B-C2B	-2.01	105.29	111.83
2	E	348	FAB	C1B-N9A-C4A	-2.01	123.91	126.94
2	H	348	FAB	O3B-C3B-C2B	-2.01	105.30	111.83
2	G	348	FAB	O3B-C3B-C2B	-2.01	105.30	111.83
2	C	348	FAB	O3B-C3B-C2B	-2.00	105.31	111.83
2	E	348	FAB	O3B-C3B-C2B	-2.00	105.31	111.83
2	E	348	FAB	C4A-C5A-N7A	2.09	111.41	109.48
2	C	348	FAB	C4A-C5A-N7A	2.11	111.42	109.48
2	H	348	FAB	C4A-C5A-N7A	2.11	111.42	109.48
2	B	348	FAB	C4A-C5A-N7A	2.12	111.43	109.48
2	D	348	FAB	C4A-C5A-N7A	2.13	111.44	109.48
2	A	348	FAB	C4A-C5A-N7A	2.14	111.44	109.48
2	G	348	FAB	C4A-C5A-N7A	2.15	111.46	109.48
2	E	348	FAB	C2B-C1B-N9A	2.16	117.59	114.29
2	B	348	FAB	C2B-C1B-N9A	2.17	117.60	114.29
2	H	348	FAB	C2B-C1B-N9A	2.17	117.61	114.29
2	F	348	FAB	C4A-C5A-N7A	2.17	111.47	109.48
2	G	348	FAB	C2B-C1B-N9A	2.17	117.61	114.29
2	C	348	FAB	C2B-C1B-N9A	2.17	117.61	114.29
2	A	348	FAB	C2B-C1B-N9A	2.18	117.62	114.29
2	D	348	FAB	C2B-C1B-N9A	2.18	117.62	114.29
2	F	348	FAB	C2B-C1B-N9A	2.18	117.63	114.29
2	C	348	FAB	C6-C5X-C9A	2.33	121.42	119.06
2	D	348	FAB	C6-C5X-C9A	2.37	121.46	119.06
2	F	348	FAB	C6-C5X-C9A	2.38	121.47	119.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	348	FAB	C6-C5X-C9A	2.39	121.48	119.06
2	H	348	FAB	C6-C5X-C9A	2.40	121.49	119.06
2	A	348	FAB	C6-C5X-C9A	2.41	121.50	119.06
2	G	348	FAB	C6-C5X-C9A	2.41	121.50	119.06
2	E	348	FAB	C6-C5X-C9A	2.44	121.53	119.06
2	F	348	FAB	C7M-C7-C6	2.65	127.49	120.28
2	C	348	FAB	C7M-C7-C6	2.67	127.52	120.28
2	E	348	FAB	C7M-C7-C6	2.67	127.53	120.28
2	A	348	FAB	C7M-C7-C6	2.67	127.53	120.28
2	H	348	FAB	C7M-C7-C6	2.67	127.53	120.28
2	B	348	FAB	C7M-C7-C6	2.68	127.56	120.28
2	G	348	FAB	C7M-C7-C6	2.68	127.57	120.28
2	B	348	FAB	C9-C9A-C5X	2.69	121.78	119.06
2	D	348	FAB	C7M-C7-C6	2.69	127.59	120.28
2	G	348	FAB	C9-C9A-C5X	2.70	121.79	119.06
2	A	348	FAB	C9-C9A-C5X	2.71	121.80	119.06
2	F	348	FAB	C9-C9A-C5X	2.73	121.82	119.06
2	D	348	FAB	C9-C9A-C5X	2.73	121.82	119.06
2	E	348	FAB	C9-C9A-C5X	2.73	121.82	119.06
2	H	348	FAB	C9-C9A-C5X	2.74	121.83	119.06
2	C	348	FAB	C9-C9A-C5X	2.77	121.86	119.06
2	F	348	FAB	C4'-C3'-C2'	4.68	118.08	109.39
2	C	348	FAB	C4'-C3'-C2'	4.68	118.08	109.39
2	G	348	FAB	C4'-C3'-C2'	4.70	118.11	109.39
2	B	348	FAB	C4'-C3'-C2'	4.70	118.11	109.39
2	H	348	FAB	C4'-C3'-C2'	4.70	118.12	109.39
2	A	348	FAB	C4'-C3'-C2'	4.70	118.12	109.39
2	D	348	FAB	C4'-C3'-C2'	4.71	118.12	109.39
2	E	348	FAB	C4'-C3'-C2'	4.71	118.13	109.39
2	C	348	FAB	C4-N3-C2	13.36	126.80	115.25
2	B	348	FAB	C4-N3-C2	13.41	126.84	115.25
2	F	348	FAB	C4-N3-C2	13.42	126.85	115.25
2	G	348	FAB	C4-N3-C2	13.45	126.88	115.25
2	E	348	FAB	C4-N3-C2	13.46	126.88	115.25
2	A	348	FAB	C4-N3-C2	13.46	126.89	115.25
2	H	348	FAB	C4-N3-C2	13.47	126.89	115.25
2	D	348	FAB	C4-N3-C2	13.48	126.90	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	348	FAB	6	0
2	B	348	FAB	7	0
2	C	348	FAB	5	0
2	D	348	FAB	6	0
2	E	348	FAB	7	0
2	F	348	FAB	7	0
2	G	348	FAB	7	0
2	H	348	FAB	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	338/347 (97%)	-0.78	0 100 100	2, 15, 63, 100	24 (7%)
1	B	338/347 (97%)	-0.64	7 (2%) 67 52	1, 16, 69, 100	26 (7%)
1	C	338/347 (97%)	-0.66	6 (1%) 71 58	2, 15, 64, 100	27 (7%)
1	D	338/347 (97%)	-0.71	6 (1%) 71 58	2, 15, 64, 100	24 (7%)
1	E	338/347 (97%)	-0.70	5 (1%) 76 63	2, 15, 64, 100	26 (7%)
1	F	338/347 (97%)	-0.74	3 (0%) 85 78	2, 15, 63, 100	27 (7%)
1	G	338/347 (97%)	-0.61	6 (1%) 71 58	2, 16, 65, 100	28 (8%)
1	H	338/347 (97%)	-0.68	8 (2%) 62 47	2, 15, 65, 100	27 (7%)
All	All	2704/2776 (97%)	-0.69	41 (1%) 76 63	1, 15, 65, 100	209 (7%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	VAL	4.9
1	D	301	SER	4.9
1	C	300	SER	4.8
1	G	300	SER	4.6
1	H	300	SER	4.6
1	B	302	ASN	4.1
1	B	301	SER	4.1
1	B	300	SER	4.1
1	C	25	SER	3.8
1	E	300	SER	3.8
1	D	302	ASN	3.8
1	C	339	LEU	3.7
1	D	299	GLY	3.5
1	G	301	SER	3.5
1	H	28	GLN	3.5
1	F	26	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	25	SER	3.3
1	G	299	GLY	3.2
1	D	300	SER	3.1
1	C	338	ASN	3.1
1	E	26	VAL	3.1
1	H	26	VAL	3.0
1	B	299	GLY	3.0
1	G	28	GLN	2.9
1	G	27	LEU	2.8
1	D	338	ASN	2.8
1	E	299	GLY	2.8
1	H	339	LEU	2.7
1	H	302	ASN	2.7
1	B	28	GLN	2.5
1	C	302	ASN	2.5
1	E	220	GLU	2.5
1	H	301	SER	2.4
1	F	25	SER	2.3
1	B	339	LEU	2.3
1	E	339	LEU	2.2
1	H	299	GLY	2.2
1	H	27	LEU	2.2
1	D	26	VAL	2.1
1	F	300	SER	2.1
1	B	172	ARG	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAB	D	348	58/58	0.97	0.13	-0.20	1,6,21,24	0
2	FAB	E	348	58/58	0.97	0.13	-0.38	1,6,21,24	0
2	FAB	H	348	58/58	0.97	0.12	-0.44	1,6,21,24	0
2	FAB	F	348	58/58	0.97	0.13	-0.49	1,6,21,24	0
2	FAB	B	348	58/58	0.97	0.12	-0.54	1,6,21,24	0
2	FAB	A	348	58/58	0.97	0.12	-0.61	1,6,21,24	0
2	FAB	G	348	58/58	0.97	0.11	-0.76	1,6,21,24	0
2	FAB	C	348	58/58	0.97	0.10	-0.86	1,6,21,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.