



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:44 PM GMT

PDB ID : 1YEW  
Title : Crystal structure of particulate methane monooxygenase  
Authors : Lieberman, R.L.; Rosenzweig, A.C.  
Deposited on : 2004-12-28  
Resolution : 2.80 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

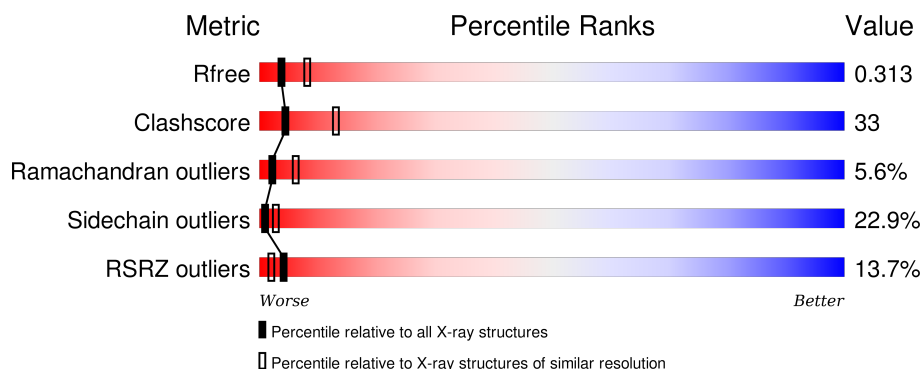
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	382	<div> <div>8%</div> <div>56%</div> <div>31%</div> <div>12%</div> <div>.</div> </div>
1	E	382	<div> <div>8%</div> <div>56%</div> <div>30%</div> <div>13%</div> <div>.</div> </div>
1	I	382	<div> <div>9%</div> <div>54%</div> <div>34%</div> <div>12%</div> <div>.</div> </div>
2	B	247	<div> <div>13%</div> <div>36%</div> <div>37%</div> <div>16%</div> <div>7%</div> <div>.</div> </div>
2	F	247	<div> <div>14%</div> <div>34%</div> <div>38%</div> <div>19%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	247	<div><div></div><div></div><div></div><div></div><div></div></div> <div><div>15%</div><div>34%</div><div>40%</div><div>16%</div><div>6%</div><div></div></div>
3	C	289	<div><div></div><div></div><div></div><div></div><div></div></div> <div><div>11%</div><div>27%</div><div>25%</div><div>11%</div><div></div><div>35%</div></div>
3	G	289	<div><div></div><div></div><div></div><div></div><div></div></div> <div><div>19%</div><div>28%</div><div>24%</div><div>12%</div><div></div><div>35%</div></div>
3	K	289	<div><div></div><div></div><div></div><div></div><div></div></div> <div><div>15%</div><div>29%</div><div>22%</div><div>12%</div><div></div><div>35%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19772 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 particulate methane monooxygenase, B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3018	1938	513	552	15			
1	E	382	Total	C	N	O	S	0	0	0
			3018	1938	513	552	15			
1	I	382	Total	C	N	O	S	0	0	0
			3018	1938	513	552	15			

- Molecule 2 is a protein called particulate methane monooxygenase, A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1955	1317	311	316	11			
2	F	238	Total	C	N	O	S	0	0	0
			1955	1317	311	316	11			
2	J	238	Total	C	N	O	S	0	0	0
			1955	1317	311	316	11			

- Molecule 3 is a protein called particulate methane monooxygenase subunit C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	188	Total	C	N	O	S	0	0	0
			1612	1101	244	264	3			
3	G	188	Total	C	N	O	S	0	0	0
			1612	1101	244	264	3			
3	K	188	Total	C	N	O	S	0	0	0
			1612	1101	244	264	3			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	3	Total	Zn	0	0
			3	3		

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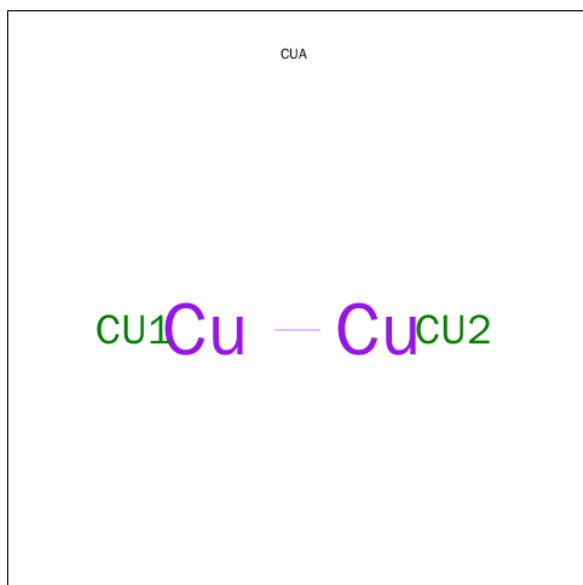
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0
4	C	2	Total 2	Zn 2	0	0
4	K	1	Total 1	Zn 1	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	Cu 1	0	0
5	A	1	Total 1	Cu 1	0	0
5	E	1	Total 1	Cu 1	0	0

- Molecule 6 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 2	Cu 2	0	0
6	E	1	Total 2	Cu 2	0	0

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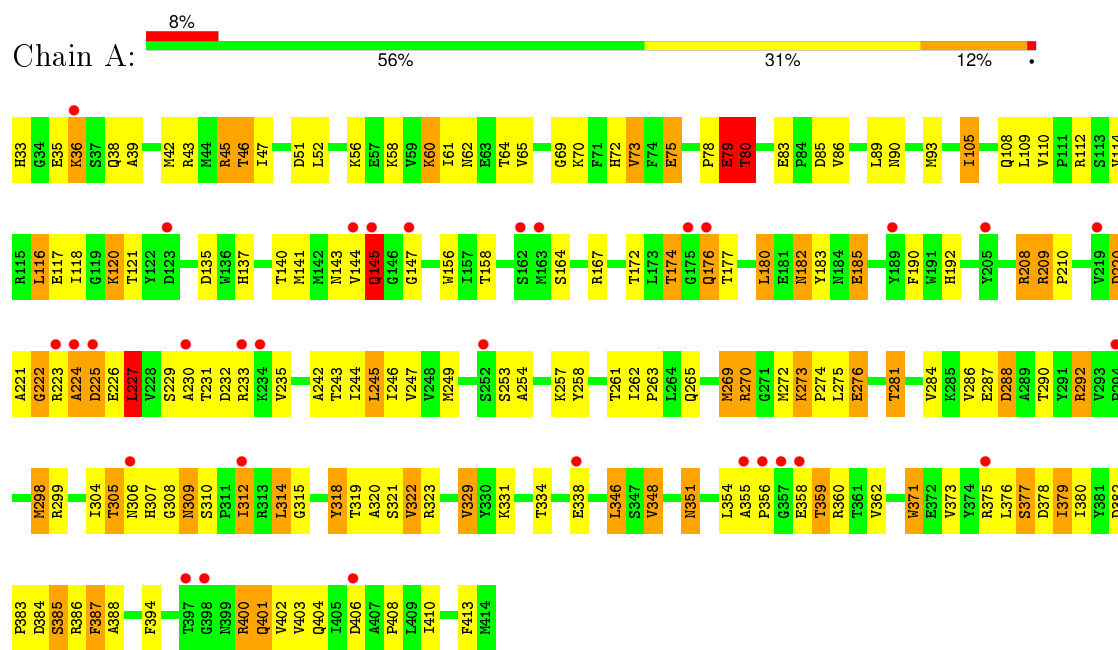
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Cu	0	0
			2	2		

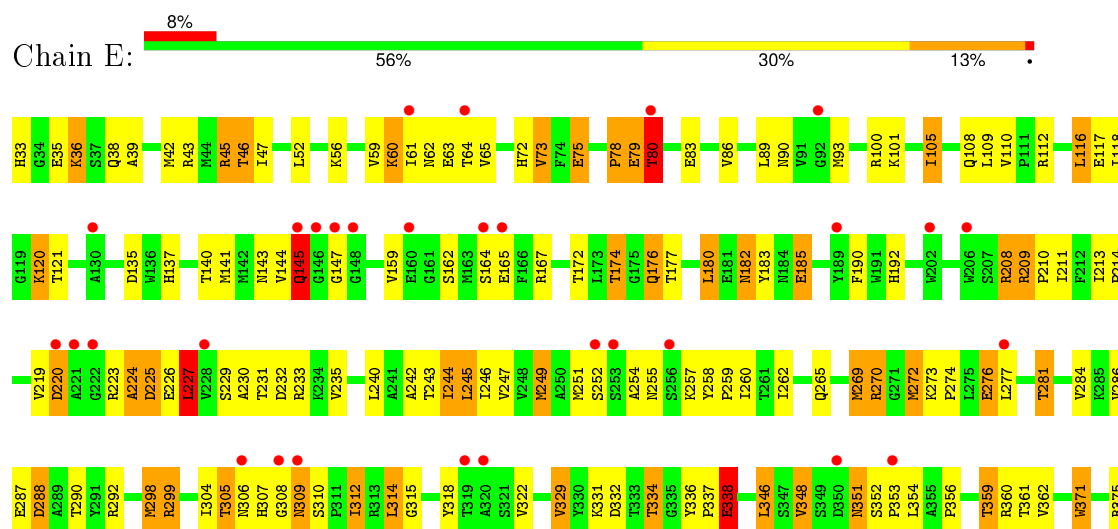
### 3 Residue-property plots

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: particulate methane monooxygenase, B subunit

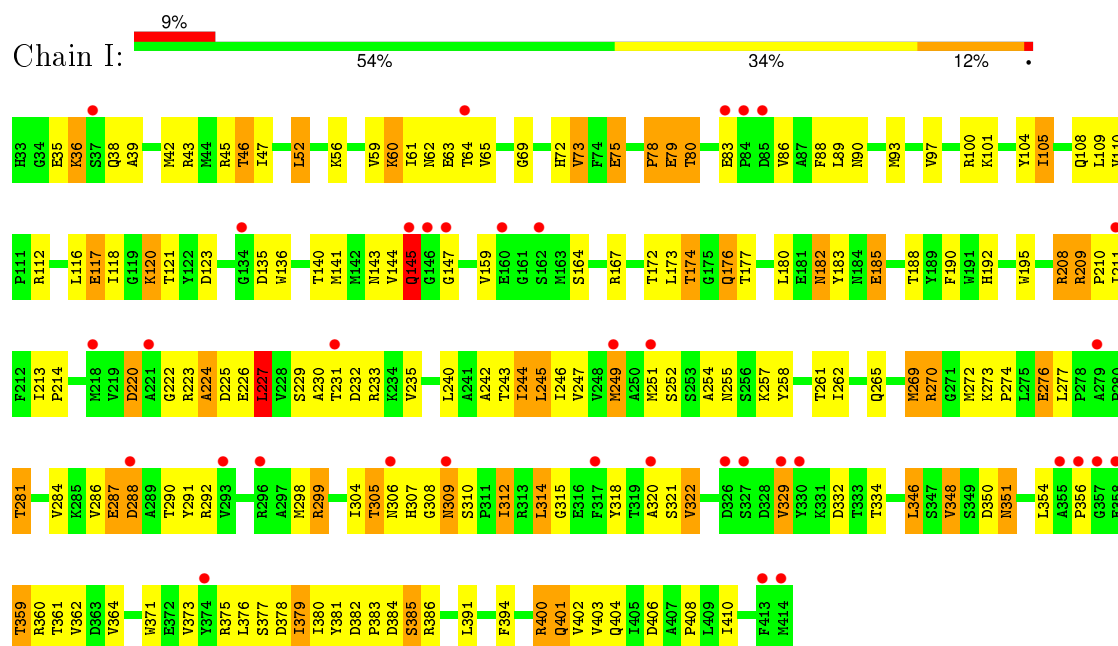


- Molecule 1: particulate methane monooxygenase, B subunit

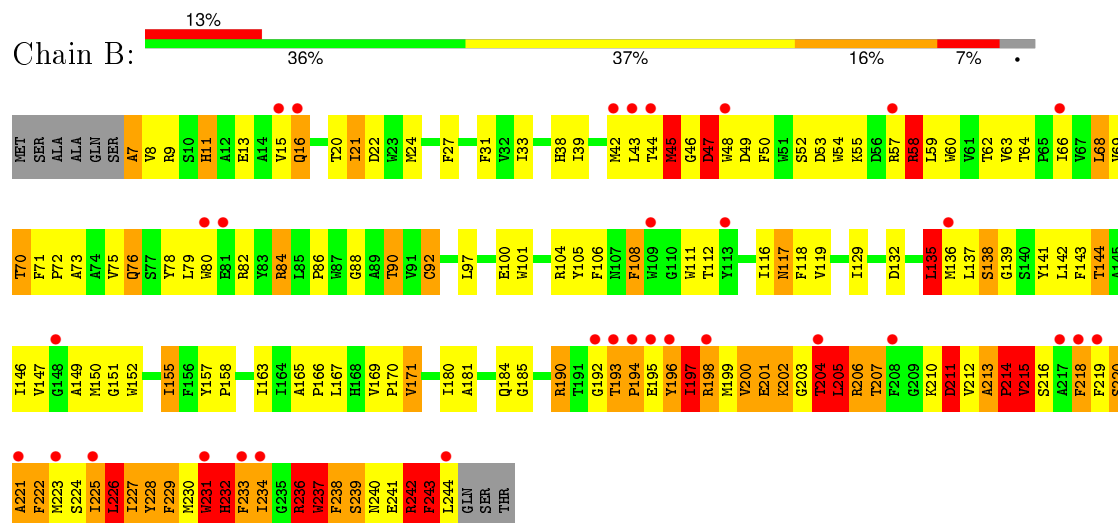




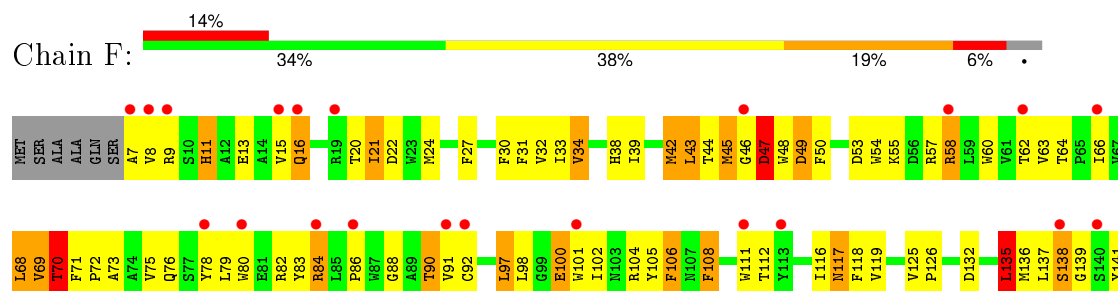
- Molecule 1: particulate methane monooxygenase, B subunit



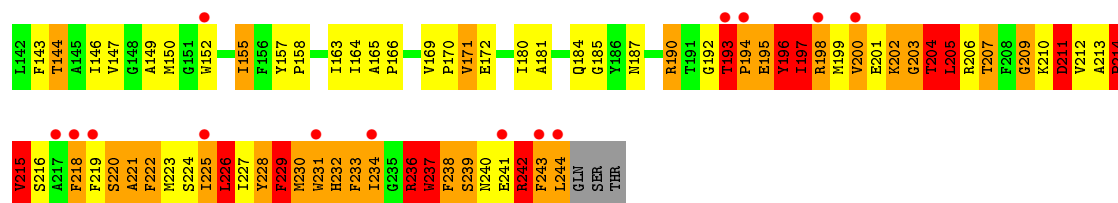
- Molecule 2: particulate methane monooxygenase, A subunit



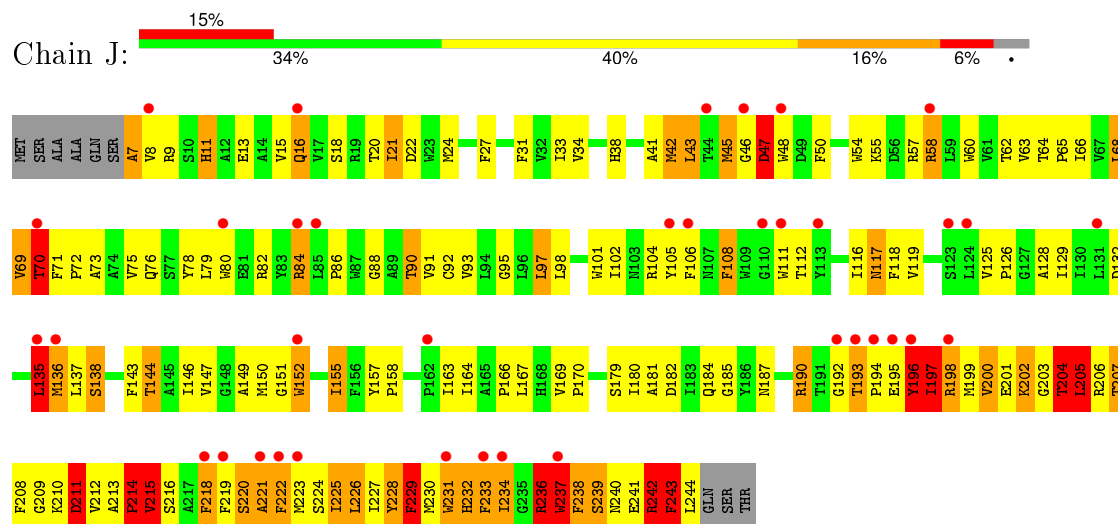
- Molecule 2: particulate methane monooxygenase, A subunit



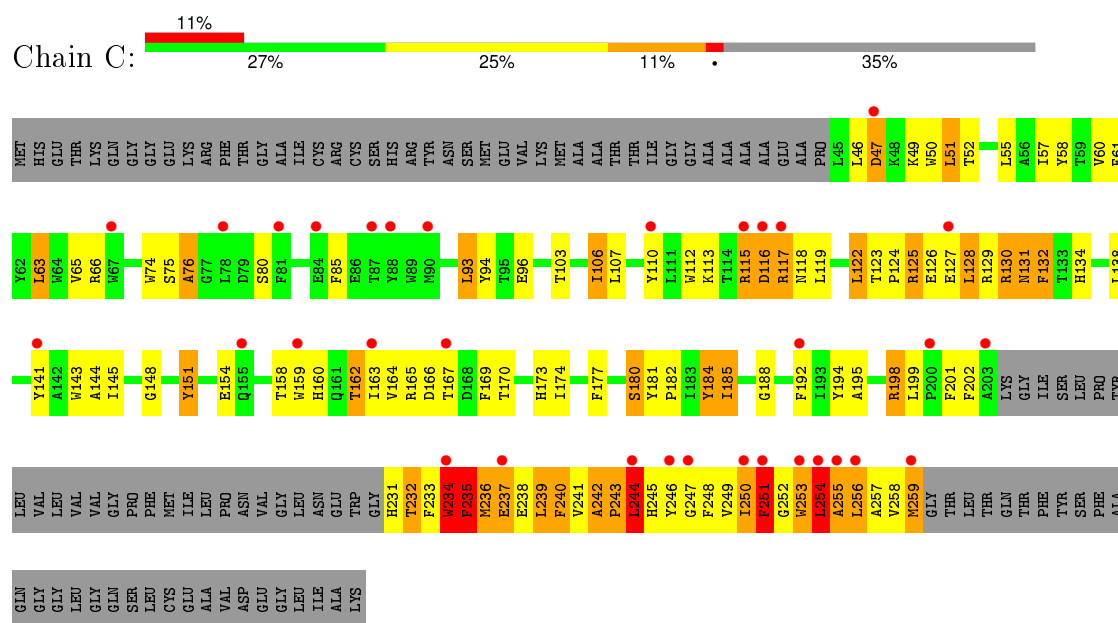




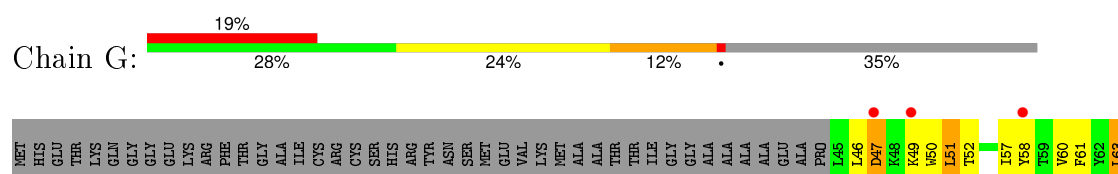
- Molecule 2: particulate methane monooxygenase, A subunit

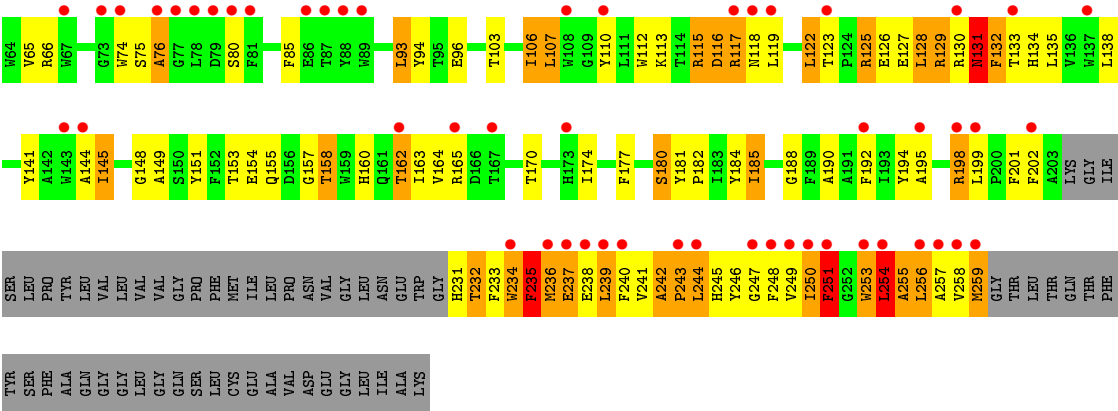


- Molecule 3: particulate methane monooxygenase subunit C2

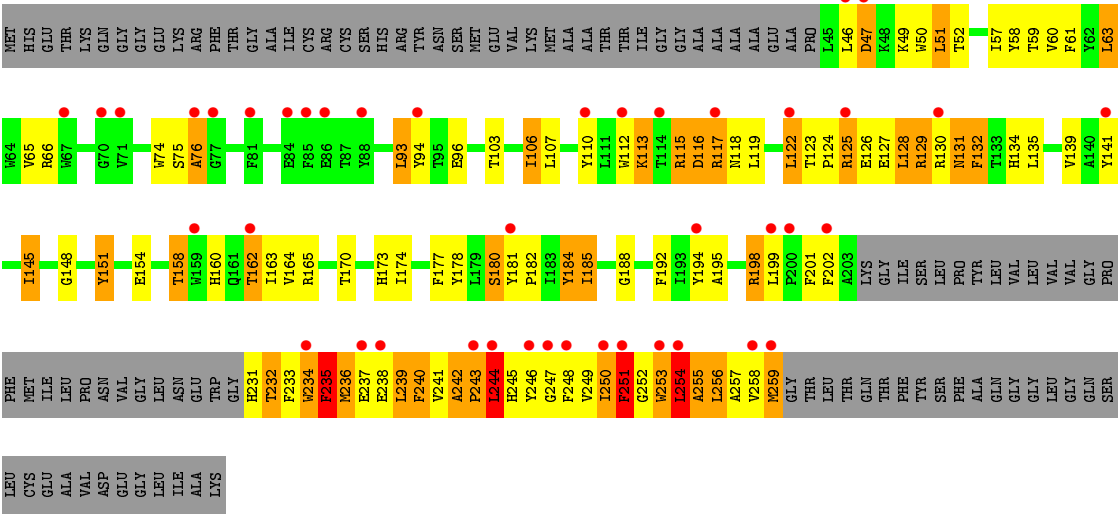
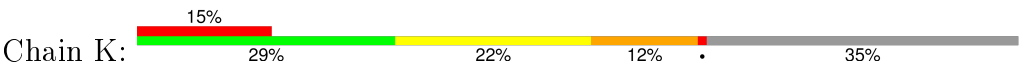


- Molecule 3: particulate methane monooxygenase subunit C2





● Molecule 3: particulate methane monooxygenase subunit C2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.14 Å   264.14 Å   150.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.55 – 2.80 29.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.55-2.80) 91.2 (29.46-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.272   ,   0.302 0.289   ,   0.313	Depositor DCC
$R_{free}$ test set	5932 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 118193 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	19772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: ZN, CUA, CU

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	0.98	4/3100 (0.1%)	0.98	7/4215 (0.2%)
1	E	0.98	3/3100 (0.1%)	0.97	2/4215 (0.0%)
1	I	0.92	2/3100 (0.1%)	0.93	3/4215 (0.1%)
2	B	1.16	10/2031 (0.5%)	1.09	9/2780 (0.3%)
2	F	1.07	7/2031 (0.3%)	1.06	13/2780 (0.5%)
2	J	1.12	7/2031 (0.3%)	1.08	9/2780 (0.3%)
3	C	0.89	1/1680 (0.1%)	0.92	4/2302 (0.2%)
3	G	0.80	1/1680 (0.1%)	0.87	3/2302 (0.1%)
3	K	0.86	1/1680 (0.1%)	0.89	4/2302 (0.2%)
All	All	0.99	36/20433 (0.2%)	0.98	54/27891 (0.2%)

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	3
1	E	0	4
1	I	0	4
2	B	0	11
2	F	0	9
2	J	0	10
3	C	0	3
3	G	0	3
3	K	0	3
All	All	0	50

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	241	GLU	CG-CD	9.72	1.66	1.51
2	B	241	GLU	CG-CD	9.53	1.66	1.51
2	F	241	GLU	CG-CD	8.57	1.64	1.51
2	B	242	ARG	CB-CG	7.37	1.72	1.52
1	I	117	GLU	CG-CD	7.27	1.62	1.51
3	C	251	PHE	CB-CG	7.05	1.63	1.51
2	F	242	ARG	CB-CG	7.04	1.71	1.52
1	E	338	GLU	CG-CD	7.02	1.62	1.51
2	J	242	ARG	CB-CG	7.01	1.71	1.52
1	A	288	ASP	CB-CG	6.85	1.66	1.51
2	B	237	TRP	CE3-CZ3	6.49	1.49	1.38
2	F	200	VAL	CA-CB	6.43	1.68	1.54
2	J	200	VAL	CA-CB	6.41	1.68	1.54
2	B	200	VAL	CA-CB	6.32	1.68	1.54
1	E	288	ASP	CB-CG	6.20	1.64	1.51
2	B	231	TRP	CE3-CZ3	6.17	1.49	1.38
3	K	251	PHE	CB-CG	6.03	1.61	1.51
2	B	231	TRP	CE2-CZ2	5.98	1.50	1.39
2	B	100	GLU	CG-CD	5.97	1.60	1.51
2	J	241	GLU	CB-CG	5.97	1.63	1.52
2	F	237	TRP	CE3-CZ3	5.95	1.48	1.38
2	F	195	GLU	CB-CG	5.68	1.62	1.52
2	J	242	ARG	CG-CD	5.61	1.66	1.51
3	G	251	PHE	CB-CG	5.56	1.60	1.51
2	B	92	CYS	CB-SG	-5.52	1.72	1.81
2	J	237	TRP	CE3-CZ3	5.52	1.47	1.38
1	I	288	ASP	CB-CG	5.46	1.63	1.51
2	F	242	ARG	CG-CD	5.43	1.65	1.51
1	A	371	TRP	CG-CD1	5.38	1.44	1.36
1	E	371	TRP	CG-CD1	5.37	1.44	1.36
1	A	338	GLU	CG-CD	5.14	1.59	1.51
2	B	241	GLU	CB-CG	5.11	1.61	1.52
1	A	387	PHE	CE1-CZ	5.07	1.47	1.37
2	J	208	PHE	CB-CG	5.07	1.59	1.51
2	B	242	ARG	CG-CD	5.07	1.64	1.51
2	F	100	GLU	CG-CD	5.01	1.59	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	47	ASP	N-CA-C	8.38	133.62	111.00
2	J	47	ASP	N-CA-C	8.32	133.48	111.00
2	B	47	ASP	N-CA-C	7.97	132.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	135	LEU	CA-CB-CG	7.36	132.23	115.30
3	G	51	LEU	CA-CB-CG	6.82	130.98	115.30
3	C	51	LEU	CA-CB-CG	6.80	130.93	115.30
2	B	135	LEU	CA-CB-CG	6.69	130.68	115.30
3	K	254	LEU	CA-CB-CG	-6.48	100.39	115.30
2	F	244	LEU	CA-CB-CG	6.48	130.20	115.30
1	E	45	ARG	NE-CZ-NH2	-6.47	117.06	120.30
2	F	232	HIS	CA-C-N	-6.36	103.20	117.20
2	B	232	HIS	CA-C-N	-6.33	103.27	117.20
3	K	51	LEU	CA-CB-CG	6.23	129.63	115.30
3	C	244	LEU	CB-CG-CD1	6.15	121.46	111.00
2	F	212	VAL	N-CA-C	-6.11	94.50	111.00
2	B	212	VAL	N-CA-C	-6.06	94.64	111.00
2	J	135	LEU	CA-CB-CG	6.03	129.17	115.30
2	J	242	ARG	NE-CZ-NH1	6.02	123.31	120.30
3	C	254	LEU	CA-CB-CG	-6.01	101.49	115.30
2	J	212	VAL	N-CA-C	-5.95	94.94	111.00
2	J	232	HIS	CA-C-N	-5.86	104.31	117.20
2	F	226	LEU	CB-CG-CD1	5.80	120.86	111.00
1	E	227	LEU	CA-CB-CG	5.75	128.52	115.30
3	K	251	PHE	N-CA-C	-5.74	95.50	111.00
3	G	254	LEU	CA-CB-CG	-5.73	102.13	115.30
3	G	251	PHE	N-CA-C	-5.69	95.64	111.00
3	C	251	PHE	N-CA-C	-5.66	95.73	111.00
2	B	45	MET	CG-SD-CE	5.65	109.24	100.20
3	K	244	LEU	CB-CG-CD1	5.61	120.53	111.00
2	F	232	HIS	CB-CA-C	5.58	121.56	110.40
2	F	215	VAL	N-CA-C	5.54	125.96	111.00
2	F	216	SER	N-CA-C	5.51	125.88	111.00
2	F	193	THR	C-N-CD	-5.47	108.56	120.60
1	A	79	GLU	C-N-CA	5.44	135.31	121.70
2	J	196	TYR	N-CA-C	5.42	125.64	111.00
1	A	227	LEU	CA-CB-CG	5.42	127.75	115.30
1	A	323	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	F	242	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	I	227	LEU	CA-CB-CG	5.32	127.54	115.30
2	J	244	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	45	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	B	226	LEU	CB-CG-CD1	5.22	119.88	111.00
1	A	79	GLU	N-CA-C	5.19	125.02	111.00
2	B	216	SER	N-CA-C	5.18	124.98	111.00
1	I	123	ASP	CB-CG-OD1	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CB-CG-OD1	5.17	122.95	118.30
2	B	215	VAL	N-CA-C	5.16	124.93	111.00
2	F	196	TYR	N-CA-C	5.16	124.92	111.00
2	B	58	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	I	173	LEU	CB-CG-CD1	-5.11	102.32	111.00
2	J	216	SER	N-CA-C	5.08	124.71	111.00
2	J	232	HIS	CB-CA-C	5.08	120.55	110.40
1	A	288	ASP	CB-CG-OD1	5.03	122.83	118.30
2	F	193	THR	C-N-CA	5.02	143.09	122.00

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	VAL	Peptide
1	A	79	GLU	Peptide
1	A	80	THR	Peptide
2	B	193	THR	Peptide
2	B	204	THR	Peptide
2	B	211	ASP	Peptide
2	B	213	ALA	Peptide
2	B	215	VAL	Peptide
2	B	221	ALA	Peptide
2	B	226	LEU	Peptide
2	B	227	ILE	Peptide
2	B	232	HIS	Peptide
2	B	46	GLY	Peptide
2	B	7	ALA	Peptide
3	C	243	PRO	Peptide
3	C	244	LEU	Peptide
3	C	253	TRP	Peptide
1	E	144	VAL	Peptide
1	E	78	PRO	Peptide
1	E	79	GLU	Peptide
1	E	80	THR	Peptide
2	F	193	THR	Peptide
2	F	204	THR	Peptide
2	F	211	ASP	Peptide
2	F	213	ALA	Peptide
2	F	215	VAL	Peptide
2	F	221	ALA	Peptide
2	F	226	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	F	46	GLY	Peptide
2	F	7	ALA	Peptide
3	G	243	PRO	Peptide
3	G	244	LEU	Peptide
3	G	253	TRP	Peptide
1	I	144	VAL	Peptide
1	I	287	GLU	Peptide
1	I	78	PRO	Peptide
1	I	79	GLU	Peptide
2	J	193	THR	Peptide
2	J	204	THR	Peptide
2	J	211	ASP	Peptide
2	J	213	ALA	Peptide
2	J	215	VAL	Peptide
2	J	221	ALA	Peptide
2	J	226	LEU	Peptide
2	J	46	GLY	Peptide
2	J	47	ASP	Peptide
2	J	7	ALA	Peptide
3	K	243	PRO	Peptide
3	K	244	LEU	Peptide
3	K	253	TRP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3018	0	2980	142	1
1	E	3018	0	2980	138	1
1	I	3018	0	2980	148	0
2	B	1955	0	1916	207	2
2	F	1955	0	1916	209	0
2	J	1955	0	1916	218	0
3	C	1612	0	1541	135	0
3	G	1612	0	1541	137	0
3	K	1612	0	1541	126	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	0	0
4	G	1	0	0	0	0
4	K	1	0	0	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
6	A	2	0	0	0	0
6	E	2	0	0	0	0
6	I	2	0	0	0	0
All	All	19772	0	19311	1278	3

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 33.

All (1278) 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)
2:B:70:THR:CG2	2:B:227:ILE:HD11	1.47	1.42
2:J:70:THR:CG2	2:J:227:ILE:HD11	1.54	1.34
2:B:70:THR:HG22	2:B:227:ILE:CD1	1.57	1.33
2:F:195:GLU:HG2	3:G:160:HIS:CE1	1.65	1.30
2:F:70:THR:CG2	2:F:227:ILE:HD11	1.61	1.29
2:F:62:THR:HA	2:F:236:ARG:NH1	1.49	1.26
2:J:70:THR:HG22	2:J:227:ILE:CD1	1.65	1.26
2:J:62:THR:HA	2:J:236:ARG:NH1	1.48	1.26
2:F:70:THR:HG22	2:F:227:ILE:CD1	1.66	1.24
2:B:62:THR:HA	2:B:236:ARG:NH1	1.49	1.24
1:A:112:ARG:HB2	1:A:269:MET:CE	1.70	1.21
2:J:236:ARG:NH2	2:J:237:TRP:HA	1.56	1.19
2:F:236:ARG:NH2	2:F:237:TRP:HA	1.59	1.17
1:I:112:ARG:HB2	1:I:269:MET:CE	1.76	1.16
2:B:236:ARG:NH2	2:B:237:TRP:HA	1.62	1.13
2:F:112:THR:HG21	3:G:162:THR:HG21	1.25	1.10
2:B:195:GLU:HG2	3:C:160:HIS:CE1	1.90	1.06
1:E:79:GLU:HB3	1:E:80:THR:HG23	1.38	1.06
2:J:112:THR:HG21	3:K:162:THR:HG21	1.31	1.06
1:E:112:ARG:HB2	1:E:269:MET:CE	1.85	1.05
2:F:222:PHE:HA	3:G:256:LEU:HB2	1.34	1.05
2:F:70:THR:HG22	2:F:227:ILE:HD11	1.15	1.04
2:J:70:THR:HG22	2:J:227:ILE:HD11	1.10	1.04
3:C:231:HIS:HA	3:C:233:PHE:H	1.24	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PHE:HA	3:C:256:LEU:HB2	1.39	1.02
2:B:70:THR:HG22	2:B:227:ILE:HD11	1.06	1.02
2:F:8:VAL:HG23	3:G:125:ARG:HH22	1.20	1.02
1:I:79:GLU:HB3	1:I:80:THR:HG23	1.38	1.01
2:F:236:ARG:HE	2:F:236:ARG:C	1.61	1.01
2:B:112:THR:HG21	3:C:162:THR:HG21	1.38	1.01
2:J:8:VAL:HG23	3:K:125:ARG:HH22	1.24	1.01
2:J:195:GLU:HG2	3:K:160:HIS:CE1	1.94	1.00
2:B:230:MET:O	2:B:232:HIS:N	1.94	1.00
2:B:236:ARG:HE	2:B:236:ARG:C	1.64	1.00
2:J:62:THR:HA	2:J:236:ARG:HH12	0.85	1.00
2:B:62:THR:CA	2:B:236:ARG:HH12	1.75	1.00
2:F:230:MET:O	2:F:232:HIS:N	1.94	1.00
1:A:105:ILE:HG23	1:A:110:VAL:HG21	1.42	1.00
2:J:222:PHE:HA	3:K:256:LEU:HB2	1.42	0.99
2:F:62:THR:CA	2:F:236:ARG:HH12	1.76	0.98
1:I:35:GLU:O	1:I:36:LYS:HB2	1.63	0.98
2:J:236:ARG:C	2:J:236:ARG:HE	1.66	0.97
2:F:195:GLU:CG	3:G:160:HIS:CE1	2.47	0.97
3:K:231:HIS:HA	3:K:233:PHE:H	1.28	0.97
1:I:105:ILE:HG23	1:I:110:VAL:HG21	1.44	0.97
2:J:62:THR:CA	2:J:236:ARG:HH12	1.76	0.97
1:A:35:GLU:O	1:A:36:LYS:HB2	1.63	0.96
3:C:254:LEU:O	3:C:257:ALA:HB3	1.65	0.96
2:B:62:THR:HA	2:B:236:ARG:HH12	0.80	0.95
3:G:231:HIS:HA	3:G:233:PHE:H	1.29	0.94
1:A:145:GLN:HE21	1:A:145:GLN:HA	1.30	0.94
2:B:90:THR:HG23	2:B:132:ASP:OD1	1.67	0.94
1:E:272:MET:HA	1:E:272:MET:CE	1.98	0.94
1:A:112:ARG:HB2	1:A:269:MET:HE1	1.51	0.93
2:B:70:THR:HG23	2:B:227:ILE:HD11	1.48	0.93
2:J:236:ARG:CZ	2:J:237:TRP:HA	1.99	0.93
1:A:79:GLU:HB3	1:A:80:THR:HG23	1.49	0.93
2:J:225:ILE:HD13	2:J:225:ILE:O	1.67	0.93
2:J:70:THR:HG23	2:J:227:ILE:HD11	1.51	0.92
2:J:230:MET:O	2:J:232:HIS:N	2.01	0.92
2:F:236:ARG:NE	2:F:236:ARG:C	2.23	0.92
2:B:214:PRO:O	2:B:215:VAL:HG23	1.69	0.92
2:F:236:ARG:CZ	2:F:237:TRP:HA	2.00	0.92
2:B:219:PHE:O	2:B:219:PHE:HD1	1.53	0.91
3:G:254:LEU:O	3:G:257:ALA:HB3	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ARG:CZ	2:B:237:TRP:HA	2.00	0.90
2:B:239:SER:O	2:B:242:ARG:HB3	1.71	0.90
1:E:145:GLN:HA	1:E:145:GLN:HE21	1.33	0.90
2:J:236:ARG:HH21	2:J:237:TRP:HA	1.33	0.90
2:F:214:PRO:O	2:F:215:VAL:HG23	1.72	0.89
2:B:236:ARG:NH2	2:B:240:ASN:H	1.71	0.89
2:J:90:THR:HG23	2:J:132:ASP:OD1	1.73	0.89
1:E:35:GLU:O	1:E:36:LYS:HB2	1.73	0.89
3:C:131:ASN:HB3	3:C:199:LEU:HD21	1.54	0.89
2:J:202:LYS:HA	2:J:202:LYS:NZ	1.87	0.89
3:C:66:ARG:HD3	3:C:151:TYR:OH	1.74	0.88
2:B:8:VAL:HG23	3:C:125:ARG:HH22	1.36	0.88
3:K:66:ARG:HD3	3:K:151:TYR:OH	1.73	0.88
2:F:90:THR:HG23	2:F:132:ASP:OD1	1.73	0.88
2:B:236:ARG:NE	2:B:236:ARG:C	2.26	0.88
2:B:236:ARG:HH21	2:B:237:TRP:HA	1.35	0.87
2:J:214:PRO:O	2:J:215:VAL:HG23	1.75	0.87
1:I:145:GLN:HA	1:I:145:GLN:HE21	1.38	0.87
3:G:131:ASN:HB3	3:G:199:LEU:HD21	1.55	0.87
1:I:112:ARG:HB2	1:I:269:MET:HE3	1.53	0.87
1:E:105:ILE:HG23	1:E:110:VAL:HG21	1.54	0.87
1:E:73:VAL:CG2	1:E:118:ILE:HA	2.04	0.87
2:F:219:PHE:O	2:F:219:PHE:HD1	1.57	0.87
2:B:70:THR:HG22	2:B:227:ILE:HD12	1.52	0.87
1:A:112:ARG:HB2	1:A:269:MET:HE3	1.54	0.86
3:C:234:TRP:HA	3:C:237:GLU:CG	2.05	0.86
3:C:181:TYR:O	3:C:185:ILE:HG23	1.75	0.86
1:E:309:ASN:ND2	1:E:309:ASN:H	1.73	0.86
1:I:112:ARG:HB2	1:I:269:MET:HE1	1.55	0.86
1:I:110:VAL:O	1:I:110:VAL:HG12	1.75	0.86
2:B:8:VAL:HG22	2:B:8:VAL:O	1.76	0.86
1:A:90:ASN:HD22	1:A:143:ASN:HD21	1.24	0.86
2:F:195:GLU:HG2	3:G:160:HIS:HE1	1.38	0.86
2:F:236:ARG:NH2	2:F:240:ASN:H	1.73	0.86
2:J:236:ARG:C	2:J:236:ARG:NE	2.28	0.86
1:I:73:VAL:CG2	1:I:118:ILE:HA	2.05	0.85
2:J:219:PHE:HD1	2:J:219:PHE:O	1.59	0.85
2:F:236:ARG:HH21	2:F:237:TRP:HA	1.36	0.85
1:E:110:VAL:HG12	1:E:110:VAL:O	1.77	0.85
2:J:228:TYR:C	2:J:228:TYR:HD1	1.79	0.85
1:E:112:ARG:HB2	1:E:269:MET:HE1	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:PHE:O	2:B:219:PHE:CD1	2.30	0.85
2:F:70:THR:HG22	2:F:227:ILE:HD12	1.59	0.84
2:J:236:ARG:NH2	2:J:240:ASN:H	1.75	0.84
1:A:110:VAL:HG12	1:A:110:VAL:O	1.77	0.84
2:F:62:THR:HA	2:F:236:ARG:HH12	0.79	0.84
2:F:70:THR:HG23	2:F:227:ILE:HD11	1.59	0.84
2:J:135:LEU:HB2	2:J:144:THR:HG21	1.59	0.84
3:C:234:TRP:HA	3:C:237:GLU:HG3	1.58	0.83
2:J:70:THR:HG22	2:J:227:ILE:HD12	1.60	0.83
3:G:232:THR:HG22	3:G:235:PHE:H	1.42	0.83
3:K:254:LEU:O	3:K:257:ALA:HB3	1.79	0.83
3:K:232:THR:HG22	3:K:235:PHE:H	1.44	0.83
2:B:70:THR:CG2	2:B:227:ILE:CD1	2.31	0.82
2:F:219:PHE:O	2:F:219:PHE:CD1	2.31	0.82
2:B:236:ARG:NE	2:B:239:SER:HB3	1.94	0.82
1:A:72:HIS:CE1	1:A:75:GLU:OE1	2.33	0.82
2:F:58:ARG:HH21	2:F:58:ARG:HG2	1.43	0.82
3:G:66:ARG:HD3	3:G:151:TYR:OH	1.80	0.81
2:F:225:ILE:O	2:F:225:ILE:HD13	1.80	0.81
2:B:228:TYR:HD1	2:B:228:TYR:C	1.83	0.81
2:B:206:ARG:HG2	3:C:184:TYR:CE2	2.16	0.81
3:C:231:HIS:HA	3:C:233:PHE:N	1.96	0.80
2:J:219:PHE:CD1	2:J:219:PHE:O	2.34	0.80
1:A:73:VAL:CG2	1:A:118:ILE:HA	2.10	0.80
2:J:239:SER:O	2:J:242:ARG:HB3	1.82	0.80
2:B:58:ARG:HH21	2:B:58:ARG:HG2	1.47	0.79
1:I:272:MET:HA	1:I:272:MET:CE	2.12	0.79
3:C:254:LEU:O	3:C:255:ALA:O	1.99	0.79
2:B:199:MET:O	2:B:202:LYS:N	2.15	0.79
2:J:228:TYR:C	2:J:228:TYR:CD1	2.51	0.79
1:I:72:HIS:CE1	1:I:75:GLU:OE1	2.35	0.79
2:F:58:ARG:HH12	2:F:237:TRP:HH2	1.28	0.79
3:G:231:HIS:HA	3:G:233:PHE:N	1.98	0.79
2:B:228:TYR:CD1	2:B:228:TYR:C	2.55	0.79
1:E:35:GLU:HA	1:E:38:GLN:HG2	1.66	0.78
1:I:254:ALA:O	1:I:257:LYS:O	2.01	0.78
2:B:135:LEU:HB2	2:B:144:THR:HG21	1.66	0.78
1:E:315:GLY:HA2	1:E:329:VAL:HG22	1.65	0.78
1:A:315:GLY:HA2	1:A:329:VAL:HG22	1.66	0.78
2:F:206:ARG:HG2	3:G:184:TYR:CE2	2.18	0.77
1:E:272:MET:HA	1:E:272:MET:HE2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:ILE:O	2:B:225:ILE:HD13	1.83	0.77
2:J:199:MET:O	2:J:202:LYS:N	2.17	0.77
1:A:265:GLN:HE22	1:I:385:SER:H	1.33	0.77
2:F:228:TYR:C	2:F:228:TYR:HD1	1.87	0.77
2:B:11:HIS:H	2:B:11:HIS:CD2	2.03	0.77
2:F:190:ARG:HH11	2:F:190:ARG:HG2	1.49	0.77
2:J:206:ARG:HG2	3:K:184:TYR:CE2	2.18	0.77
2:F:199:MET:O	2:F:202:LYS:N	2.16	0.76
1:E:254:ALA:O	1:E:257:LYS:O	2.03	0.76
2:B:202:LYS:NZ	2:B:202:LYS:HA	2.01	0.76
1:E:262:ILE:HG12	2:F:170:PRO:HB3	1.67	0.76
2:J:62:THR:CA	2:J:236:ARG:NH1	2.41	0.76
1:E:112:ARG:HB2	1:E:269:MET:HE3	1.65	0.76
3:C:232:THR:HG22	3:C:235:PHE:H	1.51	0.76
3:K:231:HIS:HA	3:K:233:PHE:N	2.00	0.75
3:G:234:TRP:HA	3:G:237:GLU:HG3	1.66	0.75
3:G:234:TRP:HA	3:G:237:GLU:CG	2.16	0.75
1:I:315:GLY:HA2	1:I:329:VAL:HG22	1.68	0.75
2:J:58:ARG:HH12	2:J:237:TRP:HH2	1.33	0.75
3:K:234:TRP:HA	3:K:237:GLU:HG3	1.67	0.75
1:I:72:HIS:HE1	1:I:75:GLU:OE1	1.70	0.75
2:F:202:LYS:HA	2:F:202:LYS:NZ	2.02	0.74
1:E:90:ASN:HD22	1:E:143:ASN:HD21	1.31	0.74
1:A:46:THR:HG22	1:A:47:ILE:H	1.52	0.74
3:G:115:ARG:HD2	3:G:117:ARG:HH22	1.52	0.74
3:K:131:ASN:HB3	3:K:199:LEU:HD21	1.69	0.74
1:E:145:GLN:HA	1:E:145:GLN:NE2	2.03	0.74
1:E:309:ASN:N	1:E:309:ASN:HD22	1.85	0.73
2:F:104:ARG:HA	2:F:108:PHE:HB2	1.71	0.73
1:A:62:ASN:HD21	1:A:167:ARG:H	1.36	0.73
2:J:38:HIS:HE2	3:K:154:GLU:CD	1.92	0.73
2:B:58:ARG:HH12	2:B:237:TRP:HH2	1.34	0.73
2:B:234:ILE:HD11	2:J:199:MET:CG	2.19	0.73
1:I:35:GLU:HA	1:I:38:GLN:HG2	1.70	0.73
1:A:145:GLN:NE2	1:A:145:GLN:HA	2.03	0.73
2:J:210:LYS:HD3	3:K:141:TYR:HE2	1.53	0.73
3:K:181:TYR:O	3:K:185:ILE:HG23	1.88	0.73
1:I:230:ALA:HB2	1:I:233:ARG:HG2	1.70	0.73
3:G:254:LEU:O	3:G:255:ALA:O	2.06	0.73
2:F:8:VAL:HG23	3:G:125:ARG:NH2	2.00	0.72
2:J:8:VAL:HG22	2:J:8:VAL:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:234:TRP:HA	3:K:237:GLU:CG	2.18	0.72
2:B:90:THR:HG21	2:B:129:ILE:HD12	1.72	0.72
3:C:131:ASN:HD22	3:C:131:ASN:H	1.36	0.72
1:A:315:GLY:HA2	1:A:329:VAL:CG2	2.19	0.72
2:F:222:PHE:HA	3:G:256:LEU:CB	2.16	0.72
2:J:58:ARG:HH21	2:J:58:ARG:HG2	1.53	0.72
1:I:46:THR:CG2	1:I:47:ILE:N	2.52	0.72
1:E:315:GLY:HA2	1:E:329:VAL:CG2	2.19	0.72
1:I:315:GLY:HA2	1:I:329:VAL:CG2	2.19	0.72
2:J:104:ARG:NH1	3:K:154:GLU:OE1	2.23	0.71
2:F:62:THR:CA	2:F:236:ARG:NH1	2.44	0.71
2:B:224:SER:HB3	3:C:256:LEU:HD12	1.73	0.71
1:A:272:MET:CE	1:A:272:MET:HA	2.19	0.71
3:K:130:ARG:HE	3:K:198:ARG:HG3	1.56	0.71
1:A:245:LEU:HD13	1:A:249:MET:HG3	1.73	0.71
1:A:224:ALA:O	1:A:226:GLU:N	2.23	0.71
1:A:90:ASN:ND2	1:A:143:ASN:HD21	1.88	0.71
2:F:228:TYR:C	2:F:228:TYR:CD1	2.58	0.70
1:E:79:GLU:CB	1:E:80:THR:HG23	2.19	0.70
2:J:20:THR:O	2:J:24:MET:HG3	1.91	0.70
2:F:227:ILE:HG12	2:F:230:MET:HB2	1.73	0.70
2:B:38:HIS:HE2	3:C:154:GLU:CD	1.93	0.70
1:A:384:ASP:OD1	1:E:112:ARG:NH2	2.24	0.70
2:B:222:PHE:HA	3:C:256:LEU:CB	2.18	0.70
2:F:195:GLU:HG2	3:G:160:HIS:NE2	2.06	0.70
1:I:46:THR:HG22	1:I:47:ILE:H	1.56	0.70
2:B:199:MET:HG3	2:F:234:ILE:HD11	1.72	0.70
1:A:230:ALA:HB2	1:A:233:ARG:HG2	1.73	0.70
1:E:272:MET:HA	1:E:272:MET:HE3	1.73	0.69
1:E:182:ASN:C	1:E:182:ASN:HD22	1.95	0.69
1:A:42:MET:O	1:A:46:THR:HB	1.92	0.69
1:E:332:ASP:OD2	1:E:334:THR:HG23	1.91	0.69
2:F:224:SER:HB3	3:G:256:LEU:HD12	1.73	0.69
2:J:202:LYS:HA	2:J:202:LYS:HZ2	1.54	0.69
2:F:199:MET:HG3	2:J:234:ILE:HD11	1.74	0.69
1:E:73:VAL:HG23	1:E:118:ILE:HA	1.73	0.69
3:G:47:ASP:OD1	3:G:47:ASP:C	2.30	0.69
1:E:192:HIS:CD2	2:F:101:TRP:HE1	2.10	0.69
2:J:227:ILE:HG12	2:J:230:MET:HB2	1.73	0.69
3:K:254:LEU:O	3:K:255:ALA:O	2.09	0.69
3:G:130:ARG:HE	3:G:198:ARG:HG3	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:236:ARG:NE	2:J:239:SER:HB3	2.07	0.69
2:F:135:LEU:HB2	2:F:144:THR:HG21	1.74	0.69
2:B:227:ILE:HG12	2:B:230:MET:HB2	1.75	0.69
2:B:79:LEU:HD12	2:B:88:GLY:HA2	1.75	0.69
3:G:201:PHE:HE2	3:G:248:PHE:HB3	1.57	0.69
3:K:131:ASN:H	3:K:131:ASN:HD22	1.41	0.69
2:B:210:LYS:HD3	3:C:141:TYR:HE2	1.56	0.68
1:E:309:ASN:N	1:E:309:ASN:ND2	2.35	0.68
1:I:62:ASN:HD21	1:I:167:ARG:H	1.41	0.68
1:I:230:ALA:CB	1:I:233:ARG:HG2	2.22	0.68
2:F:239:SER:O	2:F:242:ARG:HB3	1.93	0.68
3:C:131:ASN:ND2	3:C:131:ASN:H	1.91	0.68
1:E:75:GLU:OE1	1:E:404:GLN:NE2	2.26	0.68
2:B:234:ILE:HD11	2:J:199:MET:HG3	1.72	0.68
3:C:201:PHE:HE2	3:C:248:PHE:HB3	1.57	0.68
1:A:35:GLU:HA	1:A:38:GLN:HG2	1.76	0.68
2:F:112:THR:CG2	3:G:162:THR:HG21	2.15	0.68
1:I:247:VAL:HG21	2:J:155:ILE:HD11	1.76	0.68
2:J:222:PHE:HA	3:K:256:LEU:CB	2.19	0.68
2:J:228:TYR:O	2:J:228:TYR:HD1	1.76	0.68
2:F:228:TYR:HD1	2:F:228:TYR:O	1.76	0.68
1:A:220:ASP:OD1	2:B:82:ARG:NH1	2.27	0.68
1:I:220:ASP:OD1	2:J:82:ARG:NH1	2.26	0.68
1:A:72:HIS:HE1	1:A:75:GLU:OE1	1.75	0.68
2:J:104:ARG:HA	2:J:108:PHE:HB2	1.76	0.68
2:F:236:ARG:NE	2:F:239:SER:HB3	2.07	0.67
2:B:206:ARG:HG2	3:C:184:TYR:CZ	2.28	0.67
1:E:72:HIS:CE1	1:E:75:GLU:OE1	2.47	0.67
2:J:8:VAL:HG23	3:K:125:ARG:NH2	2.04	0.67
1:A:120:LYS:HG3	1:A:274:PRO:HB3	1.76	0.67
3:C:254:LEU:O	3:C:255:ALA:C	2.33	0.67
1:I:145:GLN:HA	1:I:145:GLN:NE2	2.09	0.67
1:E:276:GLU:OE2	1:E:276:GLU:HA	1.94	0.67
2:J:224:SER:HB3	3:K:256:LEU:HD12	1.76	0.67
1:I:243:THR:O	1:I:247:VAL:HG23	1.94	0.67
2:J:210:LYS:HD3	3:K:141:TYR:CE2	2.29	0.67
1:E:247:VAL:HG21	2:F:155:ILE:HD11	1.76	0.67
3:K:131:ASN:H	3:K:131:ASN:ND2	1.93	0.67
2:B:228:TYR:O	2:B:228:TYR:HD1	1.76	0.67
1:E:230:ALA:HB2	1:E:233:ARG:HG2	1.76	0.67
1:I:120:LYS:HG3	1:I:274:PRO:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:231:HIS:CA	3:G:233:PHE:H	2.06	0.67
1:I:192:HIS:CD2	2:J:101:TRP:HE1	2.13	0.67
2:F:210:LYS:HD3	3:G:141:TYR:HE2	1.59	0.67
1:A:112:ARG:CB	1:A:269:MET:CE	2.63	0.67
3:G:181:TYR:O	3:G:185:ILE:HG23	1.95	0.66
1:I:272:MET:HA	1:I:272:MET:HE3	1.77	0.66
1:A:46:THR:CG2	1:A:47:ILE:N	2.58	0.66
1:E:385:SER:H	1:I:265:GLN:HE22	1.41	0.66
2:F:79:LEU:HD12	2:F:88:GLY:HA2	1.76	0.66
2:F:105:TYR:HD2	2:F:106:PHE:CE2	2.13	0.66
1:A:379:ILE:HA	1:A:382:ASP:OD2	1.96	0.66
2:F:220:SER:HB2	2:F:222:PHE:HB3	1.77	0.66
1:A:230:ALA:CB	1:A:233:ARG:HG2	2.26	0.66
2:B:104:ARG:HA	2:B:108:PHE:HB2	1.76	0.66
2:B:195:GLU:HG2	3:C:160:HIS:NE2	2.11	0.66
2:F:181:ALA:O	2:F:184:GLN:HB2	1.95	0.66
2:J:206:ARG:HG2	3:K:184:TYR:CZ	2.30	0.66
1:E:46:THR:HG22	1:E:47:ILE:H	1.60	0.66
2:F:47:ASP:HB3	2:F:50:PHE:H	1.60	0.66
2:B:86:PRO:HB3	2:B:136:MET:HG3	1.78	0.65
1:I:73:VAL:HG23	1:I:118:ILE:HA	1.78	0.65
1:E:379:ILE:HA	1:E:382:ASP:OD2	1.96	0.65
3:C:130:ARG:HE	3:C:198:ARG:HG3	1.60	0.65
1:E:120:LYS:HG3	1:E:274:PRO:HB3	1.79	0.65
2:B:20:THR:O	2:B:24:MET:HG3	1.95	0.65
1:E:220:ASP:OD1	2:F:82:ARG:NH1	2.29	0.65
2:F:206:ARG:HD3	3:G:185:ILE:HG22	1.78	0.65
1:I:245:LEU:HD13	1:I:249:MET:HG3	1.77	0.65
3:C:231:HIS:CA	3:C:233:PHE:H	2.07	0.65
1:E:110:VAL:CG1	1:E:110:VAL:O	2.45	0.65
2:B:210:LYS:HD3	3:C:141:TYR:CE2	2.31	0.65
1:A:243:THR:O	1:A:247:VAL:HG23	1.96	0.65
2:B:211:ASP:CG	2:B:211:ASP:O	2.34	0.65
2:F:222:PHE:CA	3:G:256:LEU:HB2	2.22	0.65
1:E:83:GLU:OE1	1:I:270:ARG:NH2	2.30	0.65
2:F:44:THR:O	2:F:45:MET:HG2	1.95	0.65
2:J:79:LEU:HD12	2:J:88:GLY:HA2	1.79	0.65
3:K:47:ASP:C	3:K:47:ASP:OD1	2.35	0.65
1:I:42:MET:O	1:I:46:THR:HB	1.97	0.65
1:E:61:ILE:O	1:E:62:ASN:HB2	1.96	0.65
2:F:205:LEU:O	2:F:207:THR:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:61:PHE:O	3:K:65:VAL:HG23	1.97	0.65
3:K:201:PHE:HE2	3:K:248:PHE:HB3	1.60	0.65
2:F:38:HIS:HE2	3:G:154:GLU:CD	1.99	0.64
1:E:62:ASN:HD21	1:E:167:ARG:H	1.44	0.64
1:A:385:SER:H	1:E:265:GLN:HE22	1.44	0.64
2:F:146:ILE:O	2:F:150:MET:HB2	1.97	0.64
2:B:62:THR:CA	2:B:236:ARG:NH1	2.43	0.64
2:J:90:THR:HG21	2:J:129:ILE:HD12	1.79	0.64
1:E:46:THR:CG2	1:E:47:ILE:N	2.60	0.64
2:F:210:LYS:HD3	3:G:141:TYR:CE2	2.32	0.64
1:I:182:ASN:HD22	1:I:182:ASN:C	2.00	0.64
3:C:231:HIS:N	3:C:233:PHE:CD2	2.66	0.64
2:F:206:ARG:HG2	3:G:184:TYR:CZ	2.32	0.64
1:A:83:GLU:OE1	1:E:270:ARG:NH2	2.31	0.64
2:B:220:SER:HB2	2:B:222:PHE:HB3	1.79	0.63
1:E:46:THR:CG2	1:E:47:ILE:H	2.12	0.63
1:I:79:GLU:CB	1:I:80:THR:HG23	2.21	0.63
1:A:247:VAL:HG21	2:B:155:ILE:HD11	1.80	0.63
2:J:64:THR:O	2:J:68:LEU:HB2	1.98	0.63
2:J:195:GLU:HG2	3:K:160:HIS:NE2	2.12	0.63
1:I:213:ILE:HD11	2:J:21:ILE:HD13	1.80	0.63
1:E:224:ALA:O	1:E:226:GLU:N	2.32	0.63
2:J:105:TYR:HD2	2:J:106:PHE:CE2	2.15	0.63
3:G:239:LEU:C	3:G:243:PRO:HG2	2.18	0.63
2:F:202:LYS:HZ3	2:F:202:LYS:HA	1.64	0.63
2:F:8:VAL:O	2:F:8:VAL:HG22	1.98	0.63
3:G:242:ALA:N	3:G:243:PRO:CD	2.62	0.63
2:F:73:ALA:HB1	2:F:229:PHE:HB3	1.79	0.62
3:G:131:ASN:ND2	3:G:131:ASN:H	1.97	0.62
1:A:272:MET:HA	1:A:272:MET:HE2	1.81	0.62
2:J:220:SER:HB2	2:J:222:PHE:HB3	1.81	0.62
3:C:131:ASN:HD22	3:C:131:ASN:N	1.95	0.62
1:I:110:VAL:O	1:I:110:VAL:CG1	2.47	0.62
3:G:115:ARG:CZ	3:G:117:ARG:HH12	2.13	0.62
2:F:117:ASN:HD22	2:F:184:GLN:NE2	1.97	0.62
2:F:13:GLU:O	2:F:16:GLN:HB2	2.00	0.62
2:J:42:MET:HG2	2:J:198:ARG:HH21	1.63	0.62
2:B:202:LYS:HA	2:B:202:LYS:HZ1	1.63	0.62
2:B:222:PHE:CA	3:C:256:LEU:HB2	2.23	0.62
2:J:135:LEU:HB2	2:J:144:THR:CG2	2.30	0.62
3:G:234:TRP:C	3:G:236:MET:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:TRP:HA	3:C:237:GLU:HG2	1.81	0.61
1:E:230:ALA:CB	1:E:233:ARG:HG2	2.29	0.61
1:E:233:ARG:HH12	2:F:137:LEU:HA	1.63	0.61
3:G:258:VAL:O	3:G:259:MET:HB3	1.99	0.61
1:E:172:THR:C	1:E:174:THR:H	2.02	0.61
1:E:371:TRP:CH2	1:E:377:SER:HA	2.35	0.61
2:B:146:ILE:O	2:B:150:MET:HB2	2.01	0.61
2:J:211:ASP:CG	2:J:211:ASP:O	2.39	0.61
1:A:46:THR:CG2	1:A:47:ILE:H	2.13	0.61
3:K:239:LEU:C	3:K:243:PRO:HG2	2.21	0.61
3:C:248:PHE:O	3:C:248:PHE:CG	2.53	0.61
1:A:309:ASN:H	1:A:309:ASN:ND2	1.96	0.61
1:I:309:ASN:ND2	1:I:309:ASN:H	1.98	0.61
2:J:228:TYR:O	2:J:231:TRP:N	2.34	0.61
3:C:234:TRP:O	3:C:237:GLU:HG3	2.01	0.61
3:G:131:ASN:OD1	3:G:244:LEU:HB3	2.00	0.61
1:A:90:ASN:HB2	1:A:143:ASN:ND2	2.15	0.61
1:A:112:ARG:CB	1:A:269:MET:HE3	2.27	0.61
2:J:205:LEU:O	2:J:207:THR:N	2.34	0.61
2:J:206:ARG:HD3	3:K:185:ILE:HG22	1.82	0.61
3:C:234:TRP:C	3:C:236:MET:H	2.04	0.61
3:C:131:ASN:HB3	3:C:199:LEU:CD2	2.29	0.61
2:J:163:ILE:O	2:J:166:PRO:HD2	2.01	0.61
2:B:7:ALA:HB3	3:C:124:PRO:HG2	1.81	0.61
3:G:170:THR:O	3:G:174:ILE:HG12	2.01	0.61
3:G:131:ASN:HD22	3:G:131:ASN:H	1.47	0.61
2:F:149:ALA:CB	2:F:232:HIS:HB2	2.31	0.60
1:E:290:THR:HA	1:E:410:ILE:O	2.01	0.60
2:B:105:TYR:HD2	2:B:106:PHE:CE2	2.19	0.60
1:A:192:HIS:CD2	2:B:101:TRP:HE1	2.19	0.60
3:G:131:ASN:HB3	3:G:199:LEU:CD2	2.30	0.60
2:B:228:TYR:O	2:B:228:TYR:CD1	2.54	0.60
3:G:49:LYS:HB2	3:G:52:THR:OG1	2.01	0.60
2:J:214:PRO:HD3	2:J:220:SER:HB3	1.83	0.60
3:C:242:ALA:N	3:C:243:PRO:CD	2.64	0.60
2:J:202:LYS:HA	2:J:202:LYS:HZ3	1.67	0.60
1:A:182:ASN:C	1:A:182:ASN:HD22	2.05	0.60
2:F:86:PRO:HB3	2:F:136:MET:HG3	1.82	0.60
2:F:221:ALA:C	2:F:223:MET:H	2.04	0.60
3:C:117:ARG:HA	3:C:117:ARG:HH21	1.67	0.60
3:G:254:LEU:O	3:G:255:ALA:C	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:MET:CG	2:J:234:ILE:HD11	2.32	0.60
3:K:242:ALA:N	3:K:243:PRO:CD	2.65	0.60
2:J:143:PHE:CZ	2:J:147:VAL:HG21	2.37	0.60
2:J:221:ALA:C	2:J:223:MET:H	2.05	0.60
2:F:190:ARG:HG2	2:F:190:ARG:NH1	2.12	0.60
2:B:53:ASP:OD2	2:B:190:ARG:NH2	2.35	0.60
1:E:42:MET:O	1:E:46:THR:HB	2.00	0.60
3:K:195:ALA:HB1	3:K:202:PHE:CE1	2.37	0.60
1:E:281:THR:HG23	1:E:307:HIS:O	2.01	0.60
2:J:13:GLU:O	2:J:16:GLN:HB2	2.02	0.60
2:B:202:LYS:HD3	3:C:181:TYR:CE2	2.37	0.60
2:B:236:ARG:NH2	2:B:240:ASN:N	2.47	0.59
3:K:131:ASN:HD22	3:K:131:ASN:N	1.99	0.59
2:F:20:THR:O	2:F:24:MET:HG3	2.01	0.59
2:J:228:TYR:O	2:J:228:TYR:CD1	2.53	0.59
2:F:236:ARG:O	2:F:236:ARG:NE	2.23	0.59
2:F:112:THR:HG21	3:G:162:THR:CG2	2.18	0.59
3:C:239:LEU:C	3:C:243:PRO:HG2	2.22	0.59
1:E:90:ASN:ND2	1:E:143:ASN:HD21	1.99	0.59
1:I:281:THR:HG23	1:I:307:HIS:O	2.02	0.59
2:B:117:ASN:HD22	2:B:184:GLN:NE2	2.00	0.59
2:B:214:PRO:HD3	2:B:220:SER:HB3	1.83	0.59
3:G:119:LEU:HA	3:G:122:LEU:HD12	1.83	0.59
2:F:228:TYR:CD1	2:F:228:TYR:O	2.54	0.59
1:E:72:HIS:HE1	1:E:75:GLU:OE1	1.84	0.59
1:A:249:MET:HA	1:A:249:MET:CE	2.32	0.59
1:E:174:THR:CG2	1:E:174:THR:O	2.50	0.59
2:B:13:GLU:O	2:B:16:GLN:HB2	2.03	0.59
2:F:64:THR:O	2:F:68:LEU:HB2	2.03	0.59
3:G:158:THR:O	3:G:162:THR:HG22	2.03	0.59
2:B:64:THR:O	2:B:68:LEU:HB2	2.03	0.59
2:J:236:ARG:HH21	2:J:237:TRP:CA	2.13	0.59
1:I:224:ALA:O	1:I:226:GLU:N	2.36	0.59
2:J:222:PHE:CA	3:K:256:LEU:HB2	2.26	0.59
1:E:384:ASP:CG	1:I:112:ARG:HH22	2.06	0.59
1:A:145:GLN:CA	1:A:145:GLN:HE21	2.06	0.59
3:C:131:ASN:OD1	3:C:244:LEU:HB3	2.02	0.59
1:I:145:GLN:CA	1:I:145:GLN:HE21	2.14	0.59
3:C:201:PHE:CE2	3:C:248:PHE:HB3	2.37	0.58
3:K:117:ARG:HH21	3:K:117:ARG:HA	1.68	0.58
3:K:116:ASP:OD1	3:K:122:LEU:HD13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:231:HIS:CA	3:K:233:PHE:H	2.11	0.58
2:J:146:ILE:O	2:J:150:MET:HB2	2.03	0.58
3:K:131:ASN:OD1	3:K:244:LEU:HB3	2.03	0.58
2:J:149:ALA:CB	2:J:232:HIS:HB2	2.33	0.58
3:G:117:ARG:HA	3:G:117:ARG:HH21	1.66	0.58
2:B:236:ARG:HH21	2:B:237:TRP:C	2.06	0.58
1:A:309:ASN:N	1:A:309:ASN:ND2	2.50	0.58
2:B:62:THR:O	2:B:66:ILE:HG13	2.04	0.58
1:I:112:ARG:CB	1:I:269:MET:HE3	2.29	0.58
3:C:195:ALA:HB1	3:C:202:PHE:CE1	2.38	0.58
3:K:254:LEU:O	3:K:255:ALA:C	2.41	0.58
1:A:315:GLY:CA	1:A:329:VAL:CG2	2.81	0.58
1:I:309:ASN:ND2	1:I:309:ASN:N	2.50	0.58
2:J:190:ARG:HH11	2:J:190:ARG:HG2	1.69	0.58
2:J:47:ASP:HB3	2:J:50:PHE:H	1.69	0.58
2:B:199:MET:CG	2:F:234:ILE:HD11	2.32	0.58
2:B:229:PHE:HD2	2:B:229:PHE:O	1.87	0.58
2:J:70:THR:CG2	2:J:227:ILE:CD1	2.39	0.58
1:E:281:THR:H	1:E:401:GLN:HG2	1.68	0.58
3:G:195:ALA:HB1	3:G:202:PHE:CE1	2.39	0.58
2:J:224:SER:O	2:J:227:ILE:HG22	2.04	0.57
1:A:75:GLU:OE1	1:A:404:GLN:NE2	2.34	0.57
3:G:201:PHE:CE2	3:G:248:PHE:HB3	2.38	0.57
1:I:270:ARG:HH11	1:I:270:ARG:HG2	1.68	0.57
2:B:167:LEU:O	2:B:180:ILE:HB	2.04	0.57
1:I:90:ASN:HD22	1:I:143:ASN:HD21	1.52	0.57
2:F:236:ARG:NH2	2:F:240:ASN:N	2.48	0.57
3:C:119:LEU:HA	3:C:122:LEU:HD12	1.86	0.57
2:J:236:ARG:NH2	2:J:237:TRP:CA	2.50	0.57
3:G:234:TRP:O	3:G:236:MET:N	2.37	0.57
2:B:206:ARG:HD3	3:C:185:ILE:HG22	1.86	0.57
1:I:272:MET:HA	1:I:272:MET:HE2	1.86	0.57
2:F:104:ARG:NH1	3:G:154:GLU:OE1	2.37	0.57
2:J:7:ALA:HB3	3:K:124:PRO:HG2	1.86	0.57
1:E:384:ASP:CG	1:I:112:ARG:NH2	2.58	0.57
1:I:211:ILE:HD12	2:J:22:ASP:HB3	1.85	0.57
3:C:61:PHE:O	3:C:65:VAL:HG23	2.03	0.57
1:A:110:VAL:CG1	1:A:110:VAL:O	2.51	0.57
3:K:201:PHE:CE2	3:K:248:PHE:HB3	2.40	0.57
1:I:190:PHE:CD1	1:I:190:PHE:C	2.77	0.57
2:J:202:LYS:HD3	3:K:181:TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:O	1:A:232:ASP:N	2.28	0.57
3:C:49:LYS:HB2	3:C:52:THR:OG1	2.04	0.56
2:F:224:SER:O	2:F:227:ILE:HG22	2.06	0.56
2:F:70:THR:CG2	2:F:227:ILE:CD1	2.42	0.56
2:F:214:PRO:HD3	2:F:220:SER:HB3	1.88	0.56
2:F:197:ILE:O	2:F:199:MET:N	2.39	0.56
2:B:206:ARG:O	2:B:206:ARG:HG3	2.05	0.56
1:I:90:ASN:HB3	1:I:141:MET:HG3	1.87	0.56
1:I:172:THR:C	1:I:174:THR:H	2.08	0.56
1:A:290:THR:HA	1:A:410:ILE:O	2.06	0.56
2:F:88:GLY:O	2:F:91:VAL:HG12	2.05	0.56
1:A:276:GLU:HA	1:A:276:GLU:OE2	2.05	0.56
3:K:234:TRP:C	3:K:236:MET:H	2.08	0.56
1:I:249:MET:HA	1:I:249:MET:CE	2.35	0.56
3:G:231:HIS:N	3:G:233:PHE:CD2	2.74	0.56
1:I:306:ASN:ND2	1:I:312:ILE:HD13	2.21	0.56
1:A:262:ILE:HG12	2:B:170:PRO:HB3	1.86	0.56
3:K:192:PHE:HD1	3:K:251:PHE:CZ	2.24	0.56
2:F:211:ASP:CG	2:F:211:ASP:O	2.44	0.56
2:J:196:TYR:C	2:J:196:TYR:CD2	2.79	0.56
2:B:149:ALA:CB	2:B:232:HIS:HB2	2.36	0.56
2:B:197:ILE:O	2:B:197:ILE:HG12	2.05	0.56
1:E:245:LEU:HD13	1:E:249:MET:HG3	1.87	0.56
2:B:236:ARG:NH2	2:B:237:TRP:CA	2.53	0.56
2:F:204:THR:HG22	2:F:205:LEU:N	2.21	0.56
2:J:86:PRO:HB3	2:J:136:MET:HG3	1.87	0.56
2:F:238:PHE:C	2:F:238:PHE:HD1	2.09	0.56
3:K:231:HIS:N	3:K:233:PHE:CD2	2.74	0.56
2:F:204:THR:O	2:F:206:ARG:N	2.39	0.56
1:I:108:GLN:HG3	1:I:109:LEU:N	2.21	0.56
2:J:231:TRP:CD1	2:J:231:TRP:O	2.59	0.55
1:I:108:GLN:HG3	1:I:109:LEU:O	2.07	0.55
3:C:234:TRP:O	3:C:236:MET:N	2.39	0.55
3:K:119:LEU:HA	3:K:122:LEU:HD12	1.87	0.55
2:F:238:PHE:CD1	2:F:238:PHE:C	2.80	0.55
2:B:90:THR:CG2	2:B:129:ILE:HD12	2.37	0.55
2:F:105:TYR:HD2	2:F:106:PHE:CD2	2.24	0.55
2:F:98:LEU:O	2:F:102:ILE:HG13	2.06	0.55
2:F:236:ARG:HH21	2:F:237:TRP:C	2.10	0.55
2:F:204:THR:CG2	2:F:205:LEU:N	2.69	0.55
1:I:75:GLU:OE1	1:I:404:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:61:ILE:O	1:I:62:ASN:HB2	2.07	0.55
2:F:143:PHE:CZ	2:F:147:VAL:HG21	2.41	0.55
2:B:236:ARG:NE	2:B:237:TRP:HA	2.21	0.55
2:F:80:TRP:CZ3	2:F:84:ARG:HG3	2.42	0.55
2:B:105:TYR:HD2	2:B:106:PHE:CD2	2.24	0.55
2:J:86:PRO:CB	2:J:136:MET:HG3	2.37	0.55
2:J:55:LYS:HD2	2:J:60:TRP:CE2	2.41	0.55
1:A:386:ARG:HG2	1:A:408:PRO:HA	1.87	0.55
2:B:238:PHE:HD1	2:B:238:PHE:C	2.10	0.55
3:C:236:MET:HG3	3:C:237:GLU:N	2.21	0.55
2:B:205:LEU:O	2:B:207:THR:N	2.37	0.55
3:G:248:PHE:O	3:G:248:PHE:CG	2.59	0.55
3:C:258:VAL:O	3:C:259:MET:HB3	2.07	0.55
2:F:69:VAL:HG13	2:F:152:TRP:NE1	2.22	0.55
1:I:90:ASN:ND2	1:I:143:ASN:HD21	2.05	0.55
1:E:249:MET:HA	1:E:249:MET:CE	2.37	0.55
2:B:78:TYR:CD1	3:C:253:TRP:CE3	2.94	0.55
1:I:174:THR:O	1:I:174:THR:CG2	2.54	0.55
2:B:143:PHE:CZ	2:B:147:VAL:HG21	2.42	0.55
2:B:238:PHE:CD1	2:B:238:PHE:C	2.81	0.54
2:F:206:ARG:NH2	3:G:188:GLY:HA3	2.23	0.54
1:I:315:GLY:CA	1:I:329:VAL:CG2	2.84	0.54
2:B:8:VAL:O	2:B:8:VAL:CG2	2.51	0.54
2:F:196:TYR:C	2:F:196:TYR:CD2	2.80	0.54
2:B:27:PHE:CE2	2:B:31:PHE:CE2	2.95	0.54
2:F:236:ARG:HH21	2:F:237:TRP:CA	2.15	0.54
1:A:305:THR:HB	1:A:359:THR:CB	2.37	0.54
3:K:234:TRP:O	3:K:236:MET:N	2.40	0.54
2:F:71:PHE:O	2:F:72:PRO:C	2.45	0.54
2:J:204:THR:CG2	2:J:205:LEU:N	2.71	0.54
2:B:199:MET:HA	2:B:202:LYS:HB2	1.88	0.54
1:I:46:THR:HG23	1:I:47:ILE:N	2.23	0.54
3:K:112:TRP:O	3:K:115:ARG:HB3	2.07	0.54
1:A:182:ASN:O	1:A:185:GLU:HB2	2.06	0.54
2:F:243:PHE:O	2:F:243:PHE:CD1	2.61	0.54
1:I:394:PHE:CD1	1:I:400:ARG:HB3	2.42	0.54
3:G:115:ARG:CD	3:G:117:ARG:HH22	2.19	0.54
2:F:165:ALA:HB3	2:F:166:PRO:HD3	1.90	0.54
2:F:86:PRO:CB	2:F:136:MET:HG3	2.38	0.54
2:B:43:LEU:HG	2:B:196:TYR:OH	2.06	0.54
3:K:248:PHE:CG	3:K:248:PHE:O	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:ASN:O	1:I:185:GLU:HB2	2.08	0.54
3:C:47:ASP:C	3:C:47:ASP:OD1	2.45	0.54
3:G:131:ASN:HA	3:G:134:HIS:HB3	1.90	0.54
2:F:45:MET:HB2	2:F:47:ASP:OD1	2.08	0.54
1:A:371:TRP:CH2	1:A:377:SER:HA	2.43	0.54
2:J:157:TYR:HB3	2:J:158:PRO:CD	2.38	0.54
2:J:11:HIS:H	2:J:11:HIS:CD2	2.24	0.54
3:C:254:LEU:O	3:C:257:ALA:CB	2.49	0.54
2:J:204:THR:HG22	2:J:205:LEU:N	2.23	0.54
3:K:131:ASN:HB3	3:K:199:LEU:CD2	2.38	0.54
2:B:181:ALA:O	2:B:184:GLN:HB2	2.08	0.54
2:B:72:PRO:O	2:B:76:GLN:HB2	2.08	0.54
2:F:206:ARG:HD3	3:G:185:ILE:CG2	2.37	0.54
3:G:47:ASP:OD1	3:G:47:ASP:O	2.26	0.54
2:F:230:MET:C	2:F:232:HIS:H	2.09	0.53
1:A:145:GLN:CA	1:A:145:GLN:NE2	2.69	0.53
3:G:131:ASN:N	3:G:131:ASN:HD22	2.03	0.53
2:B:135:LEU:HB2	2:B:144:THR:CG2	2.37	0.53
3:G:117:ARG:NH2	3:G:117:ARG:HA	2.23	0.53
2:B:230:MET:C	2:B:232:HIS:H	2.11	0.53
1:E:243:THR:O	1:E:247:VAL:HG23	2.07	0.53
2:J:45:MET:HB2	2:J:47:ASP:OD1	2.07	0.53
2:B:118:PHE:CZ	2:B:185:GLY:HA2	2.43	0.53
2:J:236:ARG:HH21	2:J:237:TRP:C	2.11	0.53
3:G:158:THR:O	3:G:162:THR:CG2	2.57	0.53
2:B:73:ALA:HB1	2:B:229:PHE:HB3	1.89	0.53
3:C:116:ASP:OD1	3:C:122:LEU:HD13	2.07	0.53
1:A:281:THR:HG23	1:A:307:HIS:O	2.09	0.53
1:E:299:ARG:CB	1:E:299:ARG:HH11	2.21	0.53
3:C:249:VAL:HG12	3:C:249:VAL:O	2.08	0.53
2:B:234:ILE:HD11	2:J:199:MET:HG2	1.89	0.53
3:G:126:GLU:C	3:G:128:LEU:H	2.12	0.53
3:C:192:PHE:HD1	3:C:251:PHE:CZ	2.25	0.53
1:I:262:ILE:HG12	2:J:170:PRO:HB3	1.91	0.53
1:I:291:TYR:HD2	1:I:371:TRP:HH2	1.56	0.53
2:F:157:TYR:N	2:F:158:PRO:HD2	2.22	0.53
2:F:42:MET:HG2	2:F:198:ARG:HH21	1.73	0.53
2:J:105:TYR:HD2	2:J:106:PHE:CD2	2.27	0.53
2:F:48:TRP:HA	2:F:54:TRP:HB3	1.90	0.53
3:G:116:ASP:OD1	3:G:122:LEU:HD13	2.08	0.53
3:C:126:GLU:C	3:C:128:LEU:H	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:TYR:O	2:B:231:TRP:N	2.42	0.53
3:K:148:GLY:HA2	3:K:180:SER:OG	2.08	0.53
2:B:236:ARG:O	2:B:238:PHE:N	2.42	0.53
2:F:221:ALA:HB3	3:G:253:TRP:CD1	2.44	0.53
1:I:309:ASN:HA	1:I:356:PRO:HB3	1.91	0.53
1:A:183:TYR:HE1	2:B:166:PRO:O	1.92	0.53
2:B:11:HIS:CE1	3:C:237:GLU:OE2	2.62	0.53
1:E:145:GLN:CA	1:E:145:GLN:HE21	2.11	0.53
2:J:21:ILE:HG22	2:J:22:ASP:N	2.22	0.53
2:B:69:VAL:HG13	2:B:152:TRP:NE1	2.23	0.53
1:I:90:ASN:HB2	1:I:143:ASN:ND2	2.24	0.53
2:J:43:LEU:HG	2:J:196:TYR:OH	2.08	0.53
3:C:233:PHE:O	3:C:236:MET:HB3	2.08	0.53
2:F:75:VAL:HA	3:G:253:TRP:CH2	2.44	0.53
2:J:206:ARG:HD3	3:K:185:ILE:CG2	2.39	0.53
3:K:132:PHE:O	3:K:135:LEU:N	2.42	0.53
2:J:243:PHE:CD1	2:J:243:PHE:O	2.62	0.52
2:B:233:PHE:O	2:B:237:TRP:N	2.29	0.52
2:B:236:ARG:HH21	2:B:237:TRP:CA	2.13	0.52
1:A:380:ILE:O	1:A:380:ILE:HG13	2.07	0.52
2:F:203:GLY:HA3	2:J:234:ILE:CD1	2.39	0.52
2:F:202:LYS:HD3	3:G:181:TYR:CE2	2.44	0.52
1:A:73:VAL:HG21	1:A:118:ILE:HA	1.91	0.52
3:K:117:ARG:NH2	3:K:117:ARG:HA	2.24	0.52
3:K:75:SER:O	3:K:76:ALA:CB	2.58	0.52
3:K:126:GLU:C	3:K:128:LEU:H	2.12	0.52
3:G:75:SER:O	3:G:76:ALA:CB	2.57	0.52
2:B:86:PRO:CB	2:B:136:MET:HG3	2.39	0.52
3:K:47:ASP:O	3:K:47:ASP:OD1	2.28	0.52
1:E:211:ILE:HD12	2:F:22:ASP:HB3	1.91	0.52
1:I:379:ILE:HA	1:I:382:ASP:OD2	2.09	0.52
2:J:222:PHE:CG	2:J:222:PHE:O	2.63	0.52
2:J:238:PHE:C	2:J:238:PHE:HD1	2.13	0.52
2:F:8:VAL:CG2	3:G:125:ARG:HH22	2.09	0.52
2:F:72:PRO:O	2:F:76:GLN:HB2	2.08	0.52
1:A:265:GLN:HA	1:I:383:PRO:O	2.10	0.52
1:E:383:PRO:O	1:I:265:GLN:HA	2.09	0.52
1:E:174:THR:O	1:E:174:THR:HG23	2.08	0.52
1:I:90:ASN:HB3	1:I:141:MET:CG	2.40	0.52
1:A:314:LEU:HD13	1:A:346:LEU:HD11	1.92	0.52
1:I:35:GLU:HB2	1:I:43:ARG:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:ILE:HD13	3:C:184:TYR:CE2	2.45	0.52
1:A:270:ARG:NH2	1:I:83:GLU:OE1	2.42	0.52
2:F:229:PHE:O	2:F:229:PHE:HD2	1.92	0.52
2:B:8:VAL:HG23	3:C:125:ARG:NH2	2.16	0.52
1:A:245:LEU:HD13	1:A:249:MET:CG	2.39	0.52
1:A:35:GLU:HB2	1:A:43:ARG:HD3	1.92	0.52
1:E:174:THR:HG22	1:E:176:GLN:HG3	1.92	0.52
1:A:172:THR:C	1:A:174:THR:H	2.11	0.52
2:F:11:HIS:CD2	2:F:11:HIS:H	2.26	0.52
1:A:309:ASN:HA	1:A:356:PRO:HB3	1.91	0.52
2:J:149:ALA:CB	2:J:232:HIS:CB	2.88	0.52
2:F:8:VAL:HB	3:G:125:ARG:HH12	1.74	0.52
1:A:70:LYS:HE3	1:A:275:LEU:HD21	1.92	0.52
2:B:224:SER:O	2:B:227:ILE:HG22	2.08	0.52
1:I:174:THR:O	1:I:174:THR:HG23	2.09	0.52
3:K:192:PHE:HD1	3:K:251:PHE:HZ	1.57	0.52
1:E:242:ALA:O	1:E:246:ILE:HG13	2.09	0.52
3:G:93:LEU:O	3:G:96:GLU:HG2	2.09	0.52
2:J:66:ILE:HG23	2:J:233:PHE:HB2	1.91	0.51
2:B:11:HIS:ND1	3:C:237:GLU:OE2	2.43	0.51
3:C:66:ARG:HD3	3:C:151:TYR:HH	1.75	0.51
2:B:231:TRP:CD1	2:B:231:TRP:O	2.63	0.51
2:B:104:ARG:NH1	3:C:154:GLU:OE1	2.43	0.51
1:I:281:THR:H	1:I:401:GLN:HG2	1.75	0.51
1:I:291:TYR:CD2	1:I:371:TRP:HH2	2.28	0.51
1:I:350:ASP:OD2	1:I:350:ASP:C	2.46	0.51
2:J:238:PHE:C	2:J:238:PHE:CD1	2.83	0.51
3:C:115:ARG:HD2	3:C:117:ARG:HH22	1.74	0.51
3:C:250:ILE:C	3:C:253:TRP:H	2.13	0.51
2:B:38:HIS:NE2	3:C:154:GLU:CD	2.62	0.51
1:E:299:ARG:HB3	1:E:299:ARG:HH11	1.74	0.51
2:J:73:ALA:HB1	2:J:229:PHE:HB3	1.91	0.51
3:G:232:THR:HG22	3:G:235:PHE:N	2.20	0.51
3:C:231:HIS:CE1	3:C:234:TRP:CD1	2.98	0.51
3:C:131:ASN:HA	3:C:134:HIS:HB3	1.92	0.51
2:B:47:ASP:HB3	2:B:50:PHE:H	1.76	0.51
2:F:149:ALA:CB	2:F:232:HIS:CB	2.89	0.51
2:J:57:ARG:O	2:J:240:ASN:ND2	2.44	0.51
2:J:71:PHE:O	2:J:72:PRO:C	2.49	0.51
1:E:182:ASN:O	1:E:185:GLU:HB2	2.10	0.51
2:F:195:GLU:CG	3:G:160:HIS:NE2	2.70	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:181:TYR:CD1	3:G:184:TYR:HE1	2.28	0.51
3:G:145:ILE:HD13	3:G:184:TYR:CE2	2.46	0.51
2:J:229:PHE:O	2:J:229:PHE:HD2	1.94	0.51
3:K:250:ILE:C	3:K:253:TRP:H	2.14	0.51
1:E:73:VAL:HG21	1:E:118:ILE:HA	1.90	0.51
2:F:38:HIS:CE1	3:G:154:GLU:HB2	2.45	0.51
1:A:371:TRP:CD1	1:A:376:LEU:HD12	2.45	0.51
1:E:284:VAL:HG13	1:E:403:VAL:HG21	1.92	0.51
2:F:236:ARG:NH2	2:F:237:TRP:CA	2.52	0.51
2:J:38:HIS:NE2	3:K:154:GLU:CD	2.61	0.51
1:E:209:ARG:HB2	1:E:210:PRO:HD2	1.93	0.51
2:F:118:PHE:CZ	2:F:185:GLY:HA2	2.46	0.51
1:I:276:GLU:HA	1:I:276:GLU:OE2	2.10	0.51
2:B:233:PHE:HA	2:B:236:ARG:HB3	1.93	0.51
1:I:213:ILE:CD1	2:J:21:ILE:HD13	2.40	0.51
3:K:115:ARG:HD2	3:K:117:ARG:HH22	1.75	0.51
3:K:158:THR:O	3:K:162:THR:HG22	2.11	0.51
1:I:332:ASP:OD2	1:I:334:THR:HG23	2.11	0.51
1:E:348:VAL:HG22	1:E:351:ASN:HB2	1.93	0.51
2:B:78:TYR:OH	3:C:249:VAL:HG12	2.11	0.50
3:G:144:ALA:HB1	3:G:184:TYR:CB	2.39	0.50
2:F:137:LEU:O	2:F:138:SER:C	2.48	0.50
3:K:115:ARG:CZ	3:K:117:ARG:HH12	2.24	0.50
1:I:380:ILE:HG13	1:I:380:ILE:O	2.10	0.50
2:B:236:ARG:NE	2:B:236:ARG:O	2.26	0.50
1:A:242:ALA:O	1:A:246:ILE:HG13	2.11	0.50
3:K:170:THR:O	3:K:174:ILE:HG12	2.12	0.50
2:F:231:TRP:CD1	2:F:231:TRP:O	2.64	0.50
3:G:194:TYR:O	3:G:198:ARG:HB2	2.11	0.50
3:G:192:PHE:HD1	3:G:251:PHE:CZ	2.30	0.50
1:A:375:ARG:O	1:A:378:ASP:HB2	2.11	0.50
2:F:111:TRP:CD1	3:G:74:TRP:HZ3	2.28	0.50
2:J:199:MET:HA	2:J:202:LYS:HB2	1.94	0.50
2:J:221:ALA:HB3	3:K:253:TRP:CD1	2.47	0.50
1:E:105:ILE:HD11	1:E:116:LEU:HD11	1.93	0.50
3:C:234:TRP:C	3:C:236:MET:N	2.65	0.50
3:K:234:TRP:O	3:K:237:GLU:HG3	2.11	0.50
3:G:234:TRP:C	3:G:236:MET:N	2.64	0.50
3:G:234:TRP:HA	3:G:237:GLU:HG2	1.94	0.50
2:J:190:ARG:HG2	2:J:190:ARG:NH1	2.27	0.50
3:K:258:VAL:O	3:K:259:MET:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ARG:CZ	3:C:117:ARG:HH12	2.25	0.50
1:I:299:ARG:HH11	1:I:299:ARG:CB	2.24	0.50
2:F:149:ALA:HB3	2:F:232:HIS:CB	2.41	0.50
2:F:236:ARG:CD	2:F:236:ARG:C	2.80	0.50
3:C:117:ARG:HA	3:C:117:ARG:NH2	2.27	0.50
1:I:371:TRP:CH2	1:I:377:SER:HA	2.47	0.50
1:I:214:PRO:HD3	2:J:18:SER:OG	2.12	0.50
2:J:33:ILE:HG21	2:J:92:CYS:HA	1.94	0.50
1:A:284:VAL:HG13	1:A:403:VAL:HG21	1.94	0.50
2:B:149:ALA:HB3	2:B:232:HIS:CB	2.42	0.50
2:F:233:PHE:O	2:F:237:TRP:N	2.32	0.50
3:G:141:TYR:CD1	3:G:188:GLY:HA2	2.47	0.50
2:J:206:ARG:HD3	3:K:185:ILE:HB	1.94	0.50
2:F:135:LEU:HB2	2:F:144:THR:CG2	2.39	0.50
1:I:183:TYR:HE1	2:J:166:PRO:O	1.95	0.50
2:J:58:ARG:HH22	2:J:237:TRP:HZ3	1.56	0.49
3:K:131:ASN:HA	3:K:134:HIS:HB3	1.94	0.49
3:C:170:THR:O	3:C:174:ILE:HG12	2.12	0.49
1:A:394:PHE:CD1	1:A:400:ARG:HB3	2.46	0.49
2:B:135:LEU:HD22	2:B:135:LEU:O	2.11	0.49
1:I:305:THR:HB	1:I:359:THR:HB	1.93	0.49
1:E:108:GLN:HG3	1:E:109:LEU:O	2.12	0.49
1:E:252:SER:HA	1:E:255:ASN:HB2	1.95	0.49
2:B:149:ALA:HB3	2:B:232:HIS:HB2	1.93	0.49
1:I:233:ARG:HH12	2:J:137:LEU:HA	1.76	0.49
2:B:165:ALA:HB3	2:B:166:PRO:HD3	1.93	0.49
2:B:196:TYR:C	2:B:196:TYR:CD2	2.86	0.49
2:F:21:ILE:HG22	2:F:22:ASP:N	2.27	0.49
2:B:195:GLU:CG	3:C:160:HIS:CE1	2.81	0.49
2:F:163:ILE:O	2:F:166:PRO:HD2	2.12	0.49
1:A:305:THR:HB	1:A:359:THR:HB	1.93	0.49
3:K:49:LYS:HB2	3:K:52:THR:OG1	2.12	0.49
1:A:108:GLN:HG3	1:A:109:LEU:N	2.28	0.49
2:B:57:ARG:O	2:B:240:ASN:ND2	2.45	0.49
2:B:221:ALA:HB3	3:C:253:TRP:CD1	2.46	0.49
1:E:315:GLY:CA	1:E:329:VAL:CG2	2.89	0.49
1:I:309:ASN:HD22	1:I:309:ASN:N	2.09	0.49
3:K:173:HIS:CD2	3:K:177:PHE:CE1	3.00	0.49
1:E:385:SER:H	1:I:265:GLN:NE2	2.10	0.49
1:A:383:PRO:O	1:E:265:GLN:HA	2.12	0.49
2:F:236:ARG:NE	2:F:237:TRP:HA	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:TYR:CD1	3:C:188:GLY:HA2	2.48	0.49
3:G:132:PHE:O	3:G:135:LEU:N	2.46	0.49
2:F:233:PHE:HA	2:F:236:ARG:HB3	1.95	0.49
3:G:234:TRP:O	3:G:237:GLU:HG3	2.12	0.49
1:I:320:ALA:O	1:I:321:SER:HB2	2.12	0.49
2:F:206:ARG:HG3	2:F:206:ARG:O	2.12	0.49
3:G:75:SER:O	3:G:76:ALA:HB3	2.13	0.49
3:G:148:GLY:HA2	3:G:180:SER:OG	2.13	0.49
2:B:80:TRP:CZ3	2:B:84:ARG:HG3	2.48	0.49
2:F:222:PHE:CG	2:F:222:PHE:O	2.65	0.49
2:B:243:PHE:CD1	2:B:243:PHE:O	2.66	0.49
3:K:231:HIS:CE1	3:K:234:TRP:CD1	3.01	0.49
3:G:231:HIS:CE1	3:G:234:TRP:CD1	3.01	0.49
1:A:108:GLN:HG3	1:A:109:LEU:O	2.13	0.49
1:E:375:ARG:O	1:E:378:ASP:HB2	2.12	0.49
1:I:386:ARG:HG2	1:I:408:PRO:HA	1.93	0.48
3:G:250:ILE:C	3:G:253:TRP:H	2.16	0.48
3:G:250:ILE:O	3:G:254:LEU:N	2.46	0.48
2:B:204:THR:O	2:B:206:ARG:N	2.46	0.48
3:C:126:GLU:C	3:C:128:LEU:N	2.65	0.48
2:J:48:TRP:HA	2:J:54:TRP:HB3	1.95	0.48
1:A:254:ALA:O	1:A:257:LYS:O	2.30	0.48
3:G:181:TYR:HA	3:G:184:TYR:CE1	2.47	0.48
3:K:250:ILE:O	3:K:254:LEU:N	2.46	0.48
1:E:90:ASN:HB2	1:E:143:ASN:ND2	2.28	0.48
2:B:222:PHE:CG	2:B:222:PHE:O	2.65	0.48
2:F:240:ASN:C	2:F:242:ARG:N	2.63	0.48
2:J:90:THR:CG2	2:J:129:ILE:HD12	2.42	0.48
2:F:171:VAL:HG23	2:F:172:GLU:N	2.28	0.48
2:J:236:ARG:NE	2:J:237:TRP:HA	2.27	0.48
2:B:71:PHE:O	2:B:75:VAL:HG13	2.13	0.48
2:J:72:PRO:O	2:J:76:GLN:HB2	2.12	0.48
2:J:75:VAL:HA	3:K:253:TRP:CH2	2.47	0.48
2:J:38:HIS:CD2	2:J:42:MET:CE	2.96	0.48
2:B:45:MET:HB2	2:B:47:ASP:OD1	2.13	0.48
1:E:305:THR:HB	1:E:359:THR:CB	2.44	0.48
1:I:60:LYS:O	1:I:63:GLU:HB2	2.12	0.48
1:I:36:LYS:HE2	1:I:373:VAL:O	2.13	0.48
3:G:181:TYR:HD1	3:G:184:TYR:HE1	1.61	0.48
3:K:253:TRP:CE3	3:K:253:TRP:O	2.67	0.48
2:B:204:THR:CG2	2:B:205:LEU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LYS:HA	1:E:120:LYS:HD3	1.53	0.48
3:K:75:SER:O	3:K:76:ALA:HB3	2.13	0.48
3:K:249:VAL:O	3:K:249:VAL:HG12	2.14	0.48
1:I:59:VAL:O	1:I:159:VAL:HA	2.14	0.48
2:J:149:ALA:HB3	2:J:232:HIS:CB	2.43	0.48
3:K:236:MET:HG3	3:K:237:GLU:N	2.28	0.48
2:B:71:PHE:O	2:B:72:PRO:C	2.51	0.48
1:A:306:ASN:ND2	1:A:312:ILE:HD13	2.28	0.48
2:B:21:ILE:HG22	2:B:22:ASP:N	2.28	0.48
2:F:106:PHE:CD2	2:F:106:PHE:N	2.82	0.48
2:F:55:LYS:HD2	2:F:60:TRP:CE2	2.48	0.48
2:J:233:PHE:HA	2:J:236:ARG:HB3	1.95	0.48
2:J:236:ARG:O	2:J:238:PHE:N	2.47	0.48
2:F:53:ASP:OD2	2:F:190:ARG:NH2	2.46	0.48
1:E:90:ASN:HB3	1:E:141:MET:CG	2.44	0.48
1:I:209:ARG:HB2	1:I:210:PRO:HD2	1.94	0.48
1:I:290:THR:HA	1:I:410:ILE:O	2.14	0.48
2:J:111:TRP:O	3:K:74:TRP:CH2	2.66	0.48
2:F:149:ALA:HB3	2:F:232:HIS:HB2	1.94	0.48
3:C:232:THR:HG22	3:C:235:PHE:N	2.26	0.48
2:F:199:MET:HA	2:F:202:LYS:HB2	1.96	0.48
1:A:90:ASN:HB3	1:A:141:MET:HG3	1.96	0.48
2:J:135:LEU:O	2:J:135:LEU:HD22	2.13	0.48
2:F:106:PHE:HD2	2:F:106:PHE:N	2.12	0.48
2:F:30:PHE:O	2:F:34:VAL:HG23	2.13	0.48
2:F:58:ARG:CG	2:F:58:ARG:HH21	2.21	0.48
2:J:236:ARG:NH2	2:J:240:ASN:N	2.54	0.48
2:J:204:THR:O	2:J:206:ARG:N	2.47	0.48
1:A:79:GLU:CB	1:A:80:THR:HG23	2.34	0.47
2:B:165:ALA:O	2:B:167:LEU:N	2.47	0.47
2:F:58:ARG:HH22	2:F:237:TRP:HZ3	1.56	0.47
3:C:192:PHE:HD1	3:C:251:PHE:HZ	1.60	0.47
3:C:57:ILE:HG23	3:C:58:TYR:CD1	2.50	0.47
2:J:230:MET:C	2:J:232:HIS:H	2.14	0.47
2:B:82:ARG:HH22	2:B:219:PHE:HZ	1.62	0.47
2:J:76:GLN:NE2	2:J:229:PHE:CZ	2.82	0.47
3:K:232:THR:HG22	3:K:235:PHE:N	2.22	0.47
2:B:42:MET:HG2	2:B:198:ARG:HH21	1.80	0.47
3:K:93:LEU:O	3:K:96:GLU:HG2	2.14	0.47
3:G:249:VAL:O	3:G:249:VAL:HG12	2.14	0.47
2:B:149:ALA:CB	2:B:232:HIS:CB	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:205:LEU:C	2:F:207:THR:H	2.16	0.47
1:E:105:ILE:HG21	1:E:105:ILE:HD13	1.58	0.47
1:A:73:VAL:HG23	1:A:118:ILE:HA	1.91	0.47
1:E:182:ASN:HD22	1:E:183:TYR:N	2.11	0.47
1:I:322:VAL:HG11	1:I:376:LEU:HD11	1.96	0.47
1:E:60:LYS:O	1:E:63:GLU:HB2	2.14	0.47
3:C:131:ASN:ND2	3:C:131:ASN:N	2.56	0.47
2:J:55:LYS:HD2	2:J:60:TRP:CZ2	2.50	0.47
2:B:141:TYR:O	2:B:142:LEU:C	2.52	0.47
3:C:148:GLY:HA2	3:C:180:SER:OG	2.14	0.47
2:J:181:ALA:O	2:J:184:GLN:HB2	2.14	0.47
2:F:32:VAL:HG11	3:G:254:LEU:HG	1.96	0.47
1:I:174:THR:HG22	1:I:176:GLN:HG3	1.96	0.47
2:J:147:VAL:O	2:J:150:MET:HB3	2.14	0.47
2:J:230:MET:C	2:J:232:HIS:N	2.67	0.47
2:J:42:MET:SD	3:K:154:GLU:HG3	2.54	0.47
3:C:194:TYR:O	3:C:198:ARG:HB2	2.14	0.47
1:A:258:TYR:CE2	2:B:166:PRO:HG3	2.50	0.47
3:K:59:THR:O	3:K:63:LEU:HB2	2.15	0.47
1:E:145:GLN:CA	1:E:145:GLN:NE2	2.72	0.47
1:I:306:ASN:HD21	1:I:312:ILE:HD13	1.79	0.47
2:J:243:PHE:CD1	2:J:243:PHE:C	2.87	0.47
2:F:206:ARG:HD3	3:G:185:ILE:HB	1.95	0.47
1:A:320:ALA:O	1:A:321:SER:HB2	2.14	0.47
2:B:224:SER:HB3	3:C:256:LEU:CD1	2.44	0.47
1:E:305:THR:HB	1:E:359:THR:HB	1.96	0.47
2:J:117:ASN:HD22	2:J:184:GLN:NE2	2.13	0.47
3:C:75:SER:O	3:C:76:ALA:CB	2.63	0.47
1:A:387:PHE:CD2	1:A:388:ALA:N	2.83	0.47
2:B:137:LEU:O	2:B:138:SER:C	2.52	0.46
3:G:61:PHE:O	3:G:65:VAL:HG23	2.15	0.46
2:F:236:ARG:HH21	2:F:240:ASN:H	1.58	0.46
2:B:38:HIS:CE1	3:C:154:GLU:HB2	2.51	0.46
2:B:143:PHE:O	2:B:147:VAL:HG22	2.15	0.46
3:C:167:THR:HB	3:C:169:PHE:H	1.80	0.46
3:K:158:THR:O	3:K:162:THR:CG2	2.63	0.46
3:C:144:ALA:HB1	3:C:184:TYR:CB	2.45	0.46
1:E:394:PHE:CD1	1:E:400:ARG:HB3	2.50	0.46
2:J:58:ARG:HA	2:J:240:ASN:ND2	2.29	0.46
2:B:190:ARG:HH11	2:B:190:ARG:HG2	1.80	0.46
2:B:157:TYR:N	2:B:158:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:ALA:O	1:I:246:ILE:HG13	2.15	0.46
3:C:243:PRO:O	3:C:244:LEU:HB2	2.16	0.46
1:I:245:LEU:HD13	1:I:249:MET:CG	2.45	0.46
3:C:254:LEU:HA	3:C:254:LEU:HD13	1.34	0.46
3:K:242:ALA:N	3:K:243:PRO:HD3	2.29	0.46
2:B:163:ILE:O	2:B:166:PRO:HD2	2.16	0.46
2:B:204:THR:HG22	2:B:205:LEU:N	2.30	0.46
2:F:43:LEU:HG	2:F:196:TYR:OH	2.15	0.46
1:E:272:MET:CE	1:E:272:MET:CA	2.80	0.46
2:J:205:LEU:C	2:J:207:THR:H	2.16	0.46
1:E:59:VAL:O	1:E:159:VAL:HA	2.16	0.46
2:F:57:ARG:O	2:F:240:ASN:ND2	2.48	0.46
2:J:62:THR:O	2:J:66:ILE:HG13	2.15	0.46
2:B:236:ARG:CD	2:B:236:ARG:C	2.83	0.46
2:B:58:ARG:HH22	2:B:237:TRP:HZ3	1.62	0.46
1:E:309:ASN:HA	1:E:356:PRO:HB3	1.96	0.46
1:A:61:ILE:O	1:A:62:ASN:HB2	2.15	0.46
1:I:314:LEU:HD13	1:I:346:LEU:HD11	1.98	0.46
1:A:231:THR:O	1:A:235:VAL:HG23	2.16	0.46
2:J:8:VAL:HB	3:K:125:ARG:HH12	1.79	0.46
3:K:234:TRP:C	3:K:236:MET:N	2.69	0.46
3:K:198:ARG:HB3	3:K:199:LEU:HD12	1.98	0.46
2:J:97:LEU:HD12	2:J:97:LEU:HA	1.56	0.46
2:J:224:SER:HB3	3:K:256:LEU:CD1	2.46	0.45
2:F:224:SER:HB3	3:G:256:LEU:CD1	2.44	0.45
2:F:222:PHE:HD2	3:G:256:LEU:HD23	1.79	0.45
3:C:112:TRP:O	3:C:115:ARG:HB3	2.16	0.45
1:A:306:ASN:HD21	1:A:312:ILE:HD13	1.81	0.45
1:A:112:ARG:NH2	1:I:384:ASP:CG	2.70	0.45
2:J:90:THR:HA	2:J:128:ALA:HB1	1.97	0.45
3:G:241:VAL:N	3:G:243:PRO:HD2	2.31	0.45
2:B:206:ARG:HD3	3:C:185:ILE:CG2	2.46	0.45
3:G:126:GLU:O	3:G:130:ARG:HB2	2.16	0.45
1:A:174:THR:HG22	1:A:176:GLN:HG3	1.97	0.45
2:J:71:PHE:O	2:J:75:VAL:HG13	2.17	0.45
2:B:205:LEU:C	2:B:207:THR:H	2.19	0.45
3:C:248:PHE:O	3:C:248:PHE:CD1	2.69	0.45
2:J:88:GLY:O	2:J:91:VAL:HG12	2.17	0.45
1:I:182:ASN:HD22	1:I:183:TYR:N	2.13	0.45
1:A:174:THR:O	1:A:174:THR:CG2	2.64	0.45
1:I:45:ARG:O	1:I:78:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ARG:HD2	1:E:208:ARG:HA	1.66	0.45
2:B:240:ASN:C	2:B:242:ARG:N	2.67	0.45
3:C:253:TRP:O	3:C:253:TRP:CE3	2.69	0.45
2:F:38:HIS:CD2	2:F:42:MET:CE	3.00	0.45
1:A:281:THR:H	1:A:401:GLN:HG2	1.81	0.45
2:B:50:PHE:O	2:B:119:VAL:HA	2.16	0.45
2:B:58:ARG:CG	2:B:58:ARG:HH21	2.25	0.45
1:A:233:ARG:HH12	2:B:137:LEU:HA	1.81	0.45
1:A:318:TYR:C	1:A:318:TYR:CD1	2.90	0.45
3:K:234:TRP:HA	3:K:237:GLU:HG2	1.96	0.45
1:E:182:ASN:C	1:E:182:ASN:ND2	2.67	0.45
1:A:309:ASN:HD22	1:A:309:ASN:N	2.14	0.45
1:A:190:PHE:CD1	1:A:190:PHE:C	2.89	0.45
2:J:69:VAL:O	2:J:70:THR:C	2.55	0.45
2:F:206:ARG:HD3	3:G:185:ILE:CB	2.46	0.45
3:C:241:VAL:N	3:C:243:PRO:HD2	2.32	0.45
2:F:100:GLU:O	2:F:104:ARG:HG2	2.17	0.45
2:F:38:HIS:NE2	3:G:154:GLU:CD	2.68	0.45
1:I:46:THR:HG22	1:I:47:ILE:N	2.22	0.45
3:C:194:TYR:CZ	3:C:198:ARG:HG2	2.51	0.45
1:A:401:GLN:HB2	1:A:401:GLN:HE21	1.43	0.45
3:G:177:PHE:O	3:G:182:PRO:HD3	2.17	0.45
2:J:149:ALA:HB3	2:J:232:HIS:HB2	1.99	0.45
2:J:137:LEU:O	2:J:138:SER:C	2.55	0.45
2:F:157:TYR:HB3	2:F:158:PRO:CD	2.46	0.45
3:G:131:ASN:CB	3:G:199:LEU:HD21	2.38	0.45
2:B:197:ILE:O	2:B:199:MET:N	2.49	0.45
1:I:272:MET:CA	1:I:272:MET:CE	2.90	0.45
3:G:112:TRP:O	3:G:115:ARG:HB3	2.17	0.45
2:J:118:PHE:CZ	2:J:185:GLY:HA2	2.51	0.45
1:I:298:MET:HB2	1:I:298:MET:HE2	1.80	0.45
1:A:413:PHE:CE2	1:E:260:ILE:HG21	2.52	0.45
3:C:242:ALA:N	3:C:243:PRO:HD3	2.32	0.45
2:J:78:TYR:CD1	3:K:253:TRP:CE3	3.05	0.45
3:G:242:ALA:N	3:G:243:PRO:HD3	2.31	0.45
3:G:192:PHE:HD1	3:G:251:PHE:HZ	1.65	0.45
1:E:386:ARG:HG2	1:E:408:PRO:HA	1.99	0.45
2:F:125:VAL:O	2:F:126:PRO:C	2.56	0.45
2:F:66:ILE:HG23	2:F:233:PHE:HB2	1.99	0.44
2:F:62:THR:O	2:F:66:ILE:HG13	2.17	0.44
2:B:236:ARG:HH21	2:B:240:ASN:H	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:ILE:O	3:C:254:LEU:N	2.50	0.44
1:E:46:THR:HG23	1:E:47:ILE:N	2.31	0.44
3:K:126:GLU:C	3:K:128:LEU:N	2.70	0.44
1:E:314:LEU:H	1:E:351:ASN:HD21	1.65	0.44
1:E:318:TYR:CD1	1:E:318:TYR:C	2.90	0.44
2:B:149:ALA:O	2:B:150:MET:C	2.55	0.44
3:K:254:LEU:HA	3:K:254:LEU:HD13	1.30	0.44
1:E:306:ASN:ND2	1:E:312:ILE:HD13	2.32	0.44
2:B:48:TRP:HA	2:B:54:TRP:HB3	2.00	0.44
1:I:100:ARG:O	2:J:187:ASN:ND2	2.49	0.44
2:B:221:ALA:C	2:B:223:MET:H	2.20	0.44
3:C:253:TRP:HA	3:C:255:ALA:HB3	1.99	0.44
3:C:239:LEU:O	3:C:240:PHE:CD2	2.70	0.44
1:A:227:LEU:HD22	1:A:227:LEU:H	1.81	0.44
1:I:258:TYR:CE2	2:J:166:PRO:HG3	2.52	0.44
2:F:33:ILE:HG22	2:F:34:VAL:N	2.31	0.44
1:A:208:ARG:HD2	1:A:208:ARG:HA	1.51	0.44
2:J:27:PHE:CE1	3:K:139:VAL:HG13	2.52	0.44
2:J:27:PHE:CE2	2:J:31:PHE:CE2	3.04	0.44
2:F:32:VAL:HG11	3:G:254:LEU:CD1	2.47	0.44
3:K:253:TRP:HA	3:K:255:ALA:HB3	2.00	0.44
2:B:206:ARG:HG2	3:C:184:TYR:OH	2.17	0.44
3:G:126:GLU:C	3:G:128:LEU:N	2.70	0.44
1:A:174:THR:HG23	1:A:174:THR:O	2.17	0.44
1:E:231:THR:O	1:E:235:VAL:HG23	2.17	0.44
2:B:206:ARG:HD3	3:C:185:ILE:HB	2.00	0.44
1:I:304:ILE:HG22	1:I:354:LEU:HD23	1.99	0.44
3:C:80:SER:HA	3:C:85:PHE:CG	2.52	0.44
3:K:106:ILE:O	3:K:110:TYR:HB2	2.17	0.44
3:C:173:HIS:CD2	3:C:177:PHE:CE1	3.05	0.44
3:C:132:PHE:HA	3:C:132:PHE:HD1	1.73	0.44
2:J:143:PHE:CE1	2:J:147:VAL:HG21	2.53	0.44
2:J:143:PHE:O	2:J:147:VAL:HG22	2.17	0.44
2:J:149:ALA:O	2:J:150:MET:C	2.56	0.44
2:B:42:MET:SD	3:C:154:GLU:HG3	2.58	0.44
1:A:120:LYS:HD3	1:A:120:LYS:HA	1.43	0.44
2:J:106:PHE:HD2	2:J:106:PHE:N	2.16	0.44
1:E:304:ILE:HG22	1:E:354:LEU:HD23	2.00	0.44
1:I:101:LYS:HD2	1:I:101:LYS:HA	1.78	0.44
2:F:228:TYR:O	2:F:231:TRP:N	2.50	0.44
1:E:272:MET:CA	1:E:272:MET:HE3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:210:LYS:HE3	3:K:254:LEU:HB3	2.00	0.44
1:A:249:MET:HA	1:A:249:MET:HE3	1.99	0.44
1:A:172:THR:HA	2:B:171:VAL:HB	2.00	0.44
3:C:75:SER:O	3:C:76:ALA:HB3	2.18	0.44
2:F:141:TYR:HB3	2:F:226:LEU:HD21	1.99	0.44
1:A:51:ASP:O	1:A:69:GLY:HA2	2.17	0.44
1:E:395:ASP:C	1:E:395:ASP:OD2	2.55	0.44
1:E:352:SER:HB2	1:E:353:PRO:HD2	1.99	0.44
2:F:204:THR:HG22	2:F:205:LEU:H	1.82	0.44
2:B:206:ARG:NH2	3:C:188:GLY:HA3	2.33	0.44
2:J:82:ARG:HH22	2:J:219:PHE:HZ	1.66	0.44
1:I:230:ALA:HB2	1:I:233:ARG:CG	2.43	0.44
1:E:386:ARG:HA	1:E:408:PRO:HA	1.99	0.44
1:E:180:LEU:HD11	2:F:180:ILE:HG23	1.99	0.44
2:B:33:ILE:HG21	2:B:92:CYS:HA	2.00	0.44
1:A:105:ILE:HD11	1:A:116:LEU:HD11	2.00	0.44
3:G:254:LEU:O	3:G:257:ALA:CB	2.53	0.44
3:C:131:ASN:CB	3:C:199:LEU:HD21	2.37	0.44
1:I:120:LYS:HA	1:I:120:LYS:HD3	1.63	0.44
2:B:44:THR:O	2:B:45:MET:HG2	2.17	0.44
3:K:246:TYR:O	3:K:249:VAL:N	2.46	0.44
1:A:319:THR:HG23	1:A:320:ALA:N	2.33	0.44
1:I:304:ILE:HG22	1:I:354:LEU:CD2	2.47	0.44
1:E:101:LYS:HD2	1:E:101:LYS:HA	1.80	0.44
2:J:236:ARG:HH21	2:J:240:ASN:H	1.61	0.43
1:I:145:GLN:CA	1:I:145:GLN:NE2	2.76	0.43
2:F:38:HIS:CD2	2:F:42:MET:HE2	2.53	0.43
3:G:246:TYR:O	3:G:247:GLY:C	2.55	0.43
1:I:252:SER:HA	1:I:255:ASN:HB2	1.99	0.43
1:A:180:LEU:HA	1:A:180:LEU:HD12	1.63	0.43
2:B:75:VAL:HA	3:C:253:TRP:CH2	2.53	0.43
2:F:135:LEU:O	2:F:139:GLY:HA2	2.19	0.43
2:B:151:GLY:O	2:B:155:ILE:HG22	2.18	0.43
1:E:213:ILE:N	1:E:214:PRO:HD2	2.33	0.43
1:I:346:LEU:HD21	1:I:364:VAL:HG13	1.99	0.43
2:F:97:LEU:HD12	2:F:97:LEU:HA	1.67	0.43
3:C:63:LEU:HA	3:C:63:LEU:HD12	1.85	0.43
1:A:273:LYS:HB2	1:A:273:LYS:HZ2	1.81	0.43
1:A:298:MET:HE2	1:A:298:MET:HB2	1.76	0.43
2:J:206:ARG:HD2	2:J:206:ARG:HA	1.57	0.43
3:G:243:PRO:O	3:G:244:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG11	1:A:376:LEU:HD11	2.00	0.43
1:E:190:PHE:C	1:E:190:PHE:CD1	2.91	0.43
2:J:228:TYR:C	2:J:230:MET:N	2.72	0.43
3:C:232:THR:HG22	3:C:234:TRP:CB	2.49	0.43
2:F:204:THR:O	2:F:205:LEU:C	2.57	0.43
2:J:197:ILE:O	2:J:199:MET:N	2.51	0.43
2:J:206:ARG:O	2:J:206:ARG:HG3	2.18	0.43
1:I:272:MET:CA	1:I:272:MET:HE3	2.46	0.43
1:A:183:TYR:CE1	2:B:166:PRO:O	2.71	0.43
3:C:177:PHE:O	3:C:182:PRO:HD3	2.17	0.43
2:J:236:ARG:C	2:J:236:ARG:CD	2.87	0.43
2:F:210:LYS:HE3	3:G:254:LEU:HB3	2.01	0.43
2:B:206:ARG:NH2	2:B:210:LYS:HA	2.34	0.43
2:F:143:PHE:O	2:F:147:VAL:HG22	2.17	0.43
1:E:108:GLN:HG3	1:E:109:LEU:N	2.33	0.43
3:K:177:PHE:O	3:K:182:PRO:HD3	2.18	0.43
2:B:58:ARG:HG2	2:B:58:ARG:NH2	2.23	0.43
2:J:195:GLU:CG	3:K:160:HIS:CE1	2.84	0.43
2:B:206:ARG:HA	2:B:206:ARG:HD2	1.69	0.43
3:C:181:TYR:HA	3:C:184:TYR:CE1	2.54	0.43
1:A:304:ILE:HG22	1:A:354:LEU:CD2	2.49	0.43
2:J:65:PRO:HG2	2:J:236:ARG:HD3	2.00	0.43
2:B:236:ARG:CD	2:B:239:SER:HB3	2.48	0.43
2:J:38:HIS:CE1	3:K:154:GLU:HB2	2.53	0.43
3:K:178:TYR:O	3:K:182:PRO:HG2	2.19	0.43
1:E:229:SER:O	1:E:232:ASP:N	2.34	0.43
3:G:144:ALA:HB1	3:G:184:TYR:HB2	2.01	0.43
1:I:243:THR:OG1	2:J:129:ILE:HG21	2.19	0.43
1:E:35:GLU:HB2	1:E:43:ARG:HD3	2.00	0.43
2:B:202:LYS:HD3	3:C:181:TYR:CD2	2.54	0.43
3:C:141:TYR:CE1	3:C:188:GLY:CA	3.02	0.43
1:E:90:ASN:HB3	1:E:141:MET:HG3	2.00	0.43
2:B:39:ILE:O	2:B:43:LEU:HB2	2.18	0.43
2:F:33:ILE:HG21	2:F:92:CYS:HA	2.00	0.43
2:B:141:TYR:HB3	2:B:226:LEU:HD21	1.99	0.43
1:A:137:HIS:CD2	1:A:156:TRP:CE2	3.06	0.43
2:B:222:PHE:HD2	3:C:256:LEU:HD23	1.84	0.43
2:F:228:TYR:C	2:F:230:MET:N	2.71	0.43
2:J:207:THR:O	2:J:209:GLY:N	2.49	0.43
3:K:241:VAL:N	3:K:243:PRO:HD2	2.34	0.43
2:B:106:PHE:CD2	2:B:106:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:243:PHE:O	2:F:244:LEU:C	2.57	0.43
1:I:195:TRP:HB3	2:J:125:VAL:HB	2.00	0.43
2:B:238:PHE:O	2:B:240:ASN:N	2.52	0.43
3:G:144:ALA:CB	3:G:184:TYR:HB2	2.48	0.43
3:G:254:LEU:HD13	3:G:254:LEU:HA	1.43	0.43
2:J:93:VAL:HG21	2:J:128:ALA:HB2	2.01	0.43
1:I:104:TYR:HA	1:I:108:GLN:O	2.19	0.43
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.91	0.43
2:J:111:TRP:CD1	3:K:74:TRP:HZ3	2.36	0.43
1:I:318:TYR:CD1	1:I:318:TYR:C	2.93	0.43
3:K:125:ARG:HG2	3:K:129:ARG:HH12	1.84	0.42
2:J:204:THR:HG22	2:J:205:LEU:H	1.84	0.42
3:K:243:PRO:O	3:K:244:LEU:HB2	2.19	0.42
1:A:225:ASP:O	1:A:226:GLU:C	2.57	0.42
3:K:115:ARG:HE	3:K:115:ARG:HB3	1.58	0.42
3:C:80:SER:OG	3:C:166:ASP:HB3	2.19	0.42
3:G:155:GLN:C	3:G:157:GLY:N	2.71	0.42
1:I:240:LEU:O	1:I:244:ILE:HG23	2.18	0.42
2:J:236:ARG:O	2:J:239:SER:N	2.51	0.42
3:C:250:ILE:C	3:C:252:GLY:N	2.70	0.42
1:A:315:GLY:CA	1:A:329:VAL:HG21	2.49	0.42
2:F:42:MET:HE3	3:G:153:THR:HG22	2.00	0.42
2:J:106:PHE:CD2	2:J:106:PHE:N	2.85	0.42
2:J:125:VAL:O	2:J:126:PRO:C	2.57	0.42
1:A:45:ARG:O	1:A:78:PRO:HD3	2.19	0.42
1:A:114:VAL:HG23	1:A:114:VAL:O	2.18	0.42
2:J:206:ARG:HD3	3:K:185:ILE:CB	2.49	0.42
3:C:181:TYR:CD1	3:C:184:TYR:HE1	2.37	0.42
2:J:21:ILE:HD11	3:K:244:LEU:HD21	2.02	0.42
1:E:219:VAL:HG22	1:E:224:ALA:HB2	2.01	0.42
2:J:50:PHE:O	2:J:119:VAL:HA	2.20	0.42
2:J:41:ALA:O	2:J:45:MET:HG2	2.18	0.42
2:B:157:TYR:HB3	2:B:158:PRO:CD	2.50	0.42
1:A:263:PRO:HG3	1:I:381:TYR:O	2.19	0.42
1:E:336:TYR:CD1	1:E:337:PRO:HD2	2.54	0.42
3:C:144:ALA:HB1	3:C:184:TYR:HB2	1.99	0.42
1:A:272:MET:HA	1:A:272:MET:HE3	2.01	0.42
2:F:47:ASP:CG	2:F:49:ASP:H	2.23	0.42
2:B:167:LEU:HB3	2:B:181:ALA:HB2	2.01	0.42
3:C:143:TRP:HA	3:C:143:TRP:CE3	2.54	0.42
1:I:375:ARG:O	1:I:378:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:PHE:O	2:F:119:VAL:HA	2.20	0.42
3:C:93:LEU:O	3:C:96:GLU:HG2	2.19	0.42
1:A:221:ALA:O	1:A:222:GLY:O	2.37	0.42
3:G:125:ARG:HG2	3:G:129:ARG:HH12	1.85	0.42
3:G:131:ASN:HB2	3:G:244:LEU:HD12	2.01	0.42
3:K:194:TYR:CZ	3:K:198:ARG:HG2	2.55	0.42
2:B:38:HIS:CD2	2:B:42:MET:CE	3.03	0.42
1:I:188:THR:HA	2:J:163:ILE:HG23	2.01	0.42
1:A:137:HIS:CD2	1:A:156:TRP:CD1	3.07	0.42
1:I:231:THR:O	1:I:235:VAL:HG23	2.19	0.42
2:B:111:TRP:CZ3	3:C:159:TRP:CE3	3.08	0.42
1:I:183:TYR:CE1	2:J:166:PRO:O	2.71	0.42
2:B:68:LEU:HA	2:B:68:LEU:HD12	1.78	0.42
1:A:270:ARG:HH11	1:A:270:ARG:HG2	1.84	0.42
3:K:63:LEU:HD12	3:K:63:LEU:HA	1.84	0.42
2:J:98:LEU:O	2:J:102:ILE:HG13	2.19	0.42
1:A:355:ALA:HB3	1:A:358:GLU:OE1	2.19	0.42
1:E:258:TYR:N	1:E:259:PRO:CD	2.82	0.42
2:J:222:PHE:HD2	3:K:256:LEU:HD23	1.85	0.42
2:F:206:ARG:HA	2:F:206:ARG:HD2	1.67	0.42
3:K:250:ILE:C	3:K:252:GLY:N	2.69	0.42
1:I:320:ALA:C	1:I:322:VAL:H	2.22	0.42
2:J:80:TRP:CZ3	2:J:84:ARG:HG3	2.55	0.42
1:A:209:ARG:HB2	1:A:210:PRO:HD2	2.01	0.42
1:E:162:SER:O	1:E:165:GLU:HB2	2.20	0.42
2:F:39:ILE:HG13	3:G:149:ALA:HB1	2.01	0.42
2:F:194:PRO:HD3	3:G:160:HIS:HB3	2.00	0.42
2:F:78:TYR:CD1	3:G:253:TRP:CE3	3.08	0.42
3:K:145:ILE:HD13	3:K:184:TYR:CE2	2.54	0.42
2:F:83:TYR:OH	3:G:246:TYR:HE2	2.03	0.42
3:G:106:ILE:O	3:G:110:TYR:HB2	2.20	0.42
2:J:167:LEU:O	2:J:180:ILE:HB	2.19	0.42
2:B:8:VAL:HB	3:C:125:ARG:HH12	1.84	0.42
1:E:183:TYR:HE1	2:F:166:PRO:O	2.03	0.42
1:I:245:LEU:O	1:I:249:MET:HG2	2.20	0.42
3:K:248:PHE:O	3:K:248:PHE:CD1	2.73	0.42
1:E:172:THR:C	1:E:174:THR:N	2.71	0.42
1:A:182:ASN:C	1:A:182:ASN:ND2	2.73	0.42
2:F:143:PHE:CE1	2:F:147:VAL:HG21	2.55	0.42
3:C:234:TRP:CA	3:C:237:GLU:HG3	2.38	0.41
1:E:314:LEU:HD13	1:E:346:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:LYS:HD2	2:F:60:TRP:CZ2	2.55	0.41
2:B:55:LYS:HD2	2:B:60:TRP:CZ2	2.55	0.41
1:I:52:LEU:HD22	1:I:69:GLY:HA3	2.02	0.41
1:I:386:ARG:HA	1:I:408:PRO:HA	2.02	0.41
2:J:207:THR:C	2:J:209:GLY:H	2.19	0.41
1:A:230:ALA:HB2	1:A:233:ARG:CG	2.45	0.41
1:E:45:ARG:O	1:E:78:PRO:HD3	2.19	0.41
1:A:292:ARG:HA	1:A:292:ARG:HD2	1.84	0.41
2:F:68:LEU:HB3	2:F:152:TRP:HZ2	1.84	0.41
2:J:240:ASN:O	2:J:243:PHE:HD1	2.03	0.41
2:B:194:PRO:HD3	3:C:160:HIS:HB3	2.01	0.41
2:J:151:GLY:O	2:J:155:ILE:HG22	2.20	0.41
3:G:131:ASN:ND2	3:G:131:ASN:N	2.62	0.41
1:A:120:LYS:HG3	1:A:274:PRO:CB	2.48	0.41
3:K:195:ALA:HB1	3:K:202:PHE:CD1	2.55	0.41
1:E:213:ILE:HD11	2:F:21:ILE:HD13	2.01	0.41
1:A:348:VAL:HG22	1:A:351:ASN:HB2	2.03	0.41
1:I:97:VAL:HG21	1:I:136:TRP:CG	2.55	0.41
2:B:240:ASN:O	2:B:243:PHE:HD1	2.04	0.41
2:B:66:ILE:HG23	2:B:233:PHE:HB2	2.02	0.41
3:G:181:TYR:HA	3:G:184:TYR:CD1	2.56	0.41
2:J:202:LYS:NZ	2:J:206:ARG:HB3	2.36	0.41
3:K:194:TYR:O	3:K:198:ARG:HB2	2.20	0.41
1:I:401:GLN:HE21	1:I:401:GLN:HB2	1.46	0.41
2:F:243:PHE:C	2:F:243:PHE:CD1	2.89	0.41
1:A:314:LEU:H	1:A:351:ASN:HD21	1.67	0.41
1:E:378:ASP:C	1:E:380:ILE:N	2.73	0.41
1:I:314:LEU:HA	1:I:314:LEU:HD23	1.90	0.41
2:B:55:LYS:HD2	2:B:60:TRP:CE2	2.55	0.41
2:F:71:PHE:O	2:F:75:VAL:HG13	2.20	0.41
3:G:141:TYR:CE1	3:G:188:GLY:CA	3.03	0.41
2:J:206:ARG:NH2	3:K:188:GLY:HA3	2.35	0.41
3:K:239:LEU:O	3:K:240:PHE:CD2	2.74	0.41
3:K:246:TYR:O	3:K:247:GLY:C	2.59	0.41
3:C:106:ILE:O	3:C:110:TYR:HB2	2.20	0.41
3:C:55:LEU:HA	3:C:55:LEU:HD23	1.77	0.41
2:B:243:PHE:O	2:B:244:LEU:C	2.59	0.41
2:J:221:ALA:C	2:J:223:MET:N	2.72	0.41
1:A:281:THR:HB	1:A:401:GLN:OE1	2.21	0.41
2:F:27:PHE:CE2	2:F:31:PHE:CE2	3.09	0.41
2:J:231:TRP:HD1	2:J:231:TRP:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:ARG:HG2	2:J:58:ARG:NH2	2.27	0.41
2:B:243:PHE:C	2:B:243:PHE:CD1	2.88	0.41
3:C:115:ARG:HE	3:C:115:ARG:HB3	1.57	0.41
1:E:336:TYR:CG	1:E:337:PRO:HD2	2.56	0.41
1:E:100:ARG:O	2:F:187:ASN:ND2	2.52	0.41
3:G:57:ILE:HG23	3:G:58:TYR:CD1	2.56	0.41
2:J:69:VAL:HG13	2:J:152:TRP:NE1	2.35	0.41
1:A:36:LYS:HE2	1:A:373:VAL:O	2.20	0.41
3:C:134:HIS:CE1	3:C:195:ALA:HB2	2.56	0.41
2:B:197:ILE:O	2:B:197:ILE:CG1	2.67	0.41
2:B:43:LEU:HA	2:B:43:LEU:HD12	1.78	0.41
1:A:58:LYS:HG3	1:A:158:THR:HB	2.03	0.41
1:E:298:MET:HE2	1:E:298:MET:HB2	1.75	0.41
3:G:80:SER:HA	3:G:85:PHE:CG	2.55	0.41
1:I:391:LEU:HB2	1:I:403:VAL:HG22	2.03	0.41
1:A:269:MET:HG3	1:I:386:ARG:NH1	2.34	0.41
2:F:207:THR:C	2:F:209:GLY:H	2.24	0.41
3:K:181:TYR:CD1	3:K:184:TYR:HE1	2.39	0.41
3:K:141:TYR:CD1	3:K:188:GLY:HA2	2.55	0.41
2:B:202:LYS:NZ	2:B:206:ARG:HB3	2.36	0.41
1:I:88:PHE:HD2	1:I:143:ASN:HD22	1.69	0.41
1:I:305:THR:HB	1:I:359:THR:CB	2.50	0.41
1:I:348:VAL:HG22	1:I:351:ASN:HB2	2.03	0.41
2:J:179:SER:OG	2:J:182:ASP:OD1	2.33	0.41
3:G:107:LEU:CD1	3:G:190:ALA:HB2	2.50	0.41
1:E:225:ASP:C	1:E:227:LEU:N	2.73	0.41
1:I:208:ARG:HA	1:I:208:ARG:HD2	1.65	0.41
2:F:58:ARG:NH2	2:F:58:ARG:HG2	2.21	0.41
2:J:221:ALA:O	2:J:223:MET:N	2.53	0.41
1:A:272:MET:CE	1:A:272:MET:CA	2.97	0.41
3:G:132:PHE:O	3:G:133:THR:C	2.60	0.41
3:G:63:LEU:HA	3:G:63:LEU:HD12	1.89	0.41
2:J:240:ASN:C	2:J:242:ARG:N	2.73	0.40
3:G:236:MET:HG3	3:G:237:GLU:N	2.36	0.40
1:A:225:ASP:C	1:A:227:LEU:N	2.71	0.40
2:B:68:LEU:HB3	2:B:152:TRP:HZ2	1.87	0.40
2:J:34:VAL:HG22	2:J:95:GLY:CA	2.51	0.40
3:K:57:ILE:HG23	3:K:58:TYR:CD1	2.56	0.40
3:C:246:TYR:O	3:C:247:GLY:C	2.59	0.40
1:E:240:LEU:O	1:E:244:ILE:HG23	2.21	0.40
1:I:227:LEU:HD22	1:I:227:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:GLN:NE2	2:F:229:PHE:CZ	2.90	0.40
3:G:253:TRP:HA	3:G:255:ALA:HB3	2.03	0.40
2:B:135:LEU:O	2:B:139:GLY:HA2	2.21	0.40
2:J:38:HIS:CD2	2:J:42:MET:HE2	2.56	0.40
1:I:270:ARG:NH1	1:I:270:ARG:HG2	2.36	0.40
1:E:249:MET:HE3	1:E:249:MET:HA	2.03	0.40
1:A:384:ASP:CG	1:E:112:ARG:NH2	2.74	0.40
2:F:42:MET:SD	3:G:154:GLU:HG3	2.61	0.40
2:J:42:MET:HG2	2:J:198:ARG:NH2	2.31	0.40
1:E:304:ILE:HG22	1:E:354:LEU:CD2	2.52	0.40
3:K:113:LYS:HE3	3:K:113:LYS:HA	2.04	0.40
2:F:69:VAL:O	2:F:70:THR:C	2.59	0.40
1:A:112:ARG:NH2	1:I:384:ASP:OD1	2.54	0.40
2:B:201:GLU:O	2:B:206:ARG:N	2.46	0.40
1:E:120:LYS:HG3	1:E:274:PRO:CB	2.49	0.40
1:E:245:LEU:HD13	1:E:249:MET:CG	2.52	0.40
2:B:52:SER:HG	2:B:118:PHE:HD1	1.68	0.40
1:I:229:SER:O	1:I:232:ASP:N	2.35	0.40
2:F:207:THR:O	2:F:210:LYS:N	2.53	0.40
2:F:210:LYS:HD2	2:F:210:LYS:HA	1.92	0.40
2:J:207:THR:O	2:J:210:LYS:N	2.51	0.40
2:B:106:PHE:HD2	2:B:106:PHE:N	2.20	0.40
2:J:33:ILE:HG22	2:J:34:VAL:N	2.37	0.40
2:B:111:TRP:O	3:C:74:TRP:CH2	2.75	0.40

All (3) 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)
2:B:11:HIS:CE1	2:B:11:HIS:NE2[7_556]	2.03	0.17
2:B:11:HIS:NE2	2:B:11:HIS:NE2[7_556]	2.14	0.06
1:A:60:LYS:NZ	1:E:338:GLU:OE2[4_455]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/382 (100%)	334 (88%)	34 (9%)	12 (3%)	5	17
1	E	380/382 (100%)	336 (88%)	33 (9%)	11 (3%)	6	19
1	I	380/382 (100%)	327 (86%)	42 (11%)	11 (3%)	6	19
2	B	236/247 (96%)	173 (73%)	42 (18%)	21 (9%)	1	2
2	F	236/247 (96%)	168 (71%)	44 (19%)	24 (10%)	1	1
2	J	236/247 (96%)	166 (70%)	48 (20%)	22 (9%)	1	1
3	C	184/289 (64%)	147 (80%)	25 (14%)	12 (6%)	1	4
3	G	184/289 (64%)	146 (79%)	27 (15%)	11 (6%)	2	5
3	K	184/289 (64%)	145 (79%)	28 (15%)	11 (6%)	2	5
All	All	2400/2754 (87%)	1942 (81%)	323 (14%)	135 (6%)	2	6

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	220	ASP
1	A	224	ALA
1	A	225	ASP
1	A	288	ASP
2	B	45	MET
2	B	194	PRO
2	B	196	TYR
2	B	197	ILE
2	B	200	VAL
2	B	205	LEU
2	B	214	PRO
2	B	215	VAL
2	B	218	PHE
2	B	222	PHE
2	B	231	TRP
3	C	46	LEU
3	C	76	ALA
3	C	255	ALA
1	E	220	ASP
1	E	224	ALA
1	E	225	ASP
1	E	288	ASP

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Mol	Chain	Res	Type
2	F	45	MET
2	F	194	PRO
2	F	196	TYR
2	F	197	ILE
2	F	200	VAL
2	F	205	LEU
2	F	214	PRO
2	F	215	VAL
2	F	218	PHE
2	F	222	PHE
2	F	231	TRP
3	G	46	LEU
3	G	76	ALA
3	G	255	ALA
1	I	36	LYS
1	I	220	ASP
1	I	224	ALA
1	I	225	ASP
1	I	288	ASP
2	J	45	MET
2	J	194	PRO
2	J	196	TYR
2	J	197	ILE
2	J	200	VAL
2	J	205	LEU
2	J	214	PRO
2	J	215	VAL
2	J	218	PHE
2	J	222	PHE
2	J	231	TRP
3	K	46	LEU
3	K	76	ALA
3	K	255	ALA
1	A	145	GLN
1	A	147	GLY
1	A	308	GLY
2	B	192	GLY
2	B	239	SER
3	C	235	PHE
1	E	36	LYS
1	E	145	GLN
1	E	147	GLY

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Mol	Chain	Res	Type
2	F	192	GLY
2	F	239	SER
3	G	116	ASP
3	G	123	THR
3	G	127	GLU
3	G	235	PHE
3	G	240	PHE
1	I	145	GLN
1	I	147	GLY
1	I	308	GLY
2	J	239	SER
3	K	235	PHE
3	K	240	PHE
1	A	39	ALA
1	A	222	GLY
2	B	9	ARG
2	B	236	ARG
3	C	116	ASP
3	C	240	PHE
2	F	70	THR
2	F	236	ARG
2	F	237	TRP
3	G	117	ARG
2	J	9	ARG
2	J	229	PHE
2	J	236	ARG
2	J	237	TRP
3	K	116	ASP
3	K	123	THR
1	A	377	SER
2	B	237	TRP
3	C	117	ARG
3	C	127	GLU
1	E	39	ALA
1	E	308	GLY
2	F	9	ARG
2	F	42	MET
3	G	131	ASN
1	I	39	ALA
2	J	70	THR
2	J	192	GLY
3	K	127	GLU

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Mol	Chain	Res	Type
3	K	151	TYR
2	B	206	ARG
2	B	243	PHE
1	E	377	SER
2	F	229	PHE
2	F	230	MET
1	I	310	SER
2	J	42	MET
3	K	117	ARG
3	C	123	THR
3	C	151	TYR
3	C	234	TRP
1	E	310	SER
2	F	34	VAL
2	F	209	GLY
2	J	243	PHE
2	B	193	THR
2	B	203	GLY
2	B	213	ALA
3	C	242	ALA
1	I	222	GLY
2	J	193	THR
2	F	193	THR
3	G	242	ALA
3	K	242	ALA
2	F	203	GLY
2	J	203	GLY
1	A	310	SER

### 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	323/323 (100%)	256 (79%)	67 (21%)	1	4
1	E	323/323 (100%)	251 (78%)	72 (22%)	1	3
1	I	323/323 (100%)	257 (80%)	66 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	203/210 (97%)	157 (77%)	46 (23%)	1	3
2	F	203/210 (97%)	155 (76%)	48 (24%)	1	2
2	J	203/210 (97%)	156 (77%)	47 (23%)	1	3
3	C	161/237 (68%)	118 (73%)	43 (27%)	0	1
3	G	161/237 (68%)	119 (74%)	42 (26%)	0	1
3	K	161/237 (68%)	120 (74%)	41 (26%)	1	2
All	All	2061/2310 (89%)	1589 (77%)	472 (23%)	1	3

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	46	THR
1	A	52	LEU
1	A	56	LYS
1	A	60	LYS
1	A	64	THR
1	A	65	VAL
1	A	73	VAL
1	A	75	GLU
1	A	80	THR
1	A	86	VAL
1	A	89	LEU
1	A	93	MET
1	A	105	ILE
1	A	116	LEU
1	A	117	GLU
1	A	120	LYS
1	A	121	THR
1	A	135	ASP
1	A	140	THR
1	A	145	GLN
1	A	164	SER
1	A	174	THR
1	A	176	GLN
1	A	177	THR
1	A	180	LEU
1	A	182	ASN
1	A	185	GLU
1	A	208	ARG

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Mol	Chain	Res	Type
1	A	209	ARG
1	A	223	ARG
1	A	227	LEU
1	A	244	ILE
1	A	245	LEU
1	A	253	SER
1	A	261	THR
1	A	269	MET
1	A	270	ARG
1	A	273	LYS
1	A	276	GLU
1	A	281	THR
1	A	286	VAL
1	A	287	GLU
1	A	292	ARG
1	A	298	MET
1	A	299	ARG
1	A	305	THR
1	A	309	ASN
1	A	312	ILE
1	A	314	LEU
1	A	318	TYR
1	A	322	VAL
1	A	329	VAL
1	A	331	LYS
1	A	334	THR
1	A	346	LEU
1	A	348	VAL
1	A	351	ASN
1	A	359	THR
1	A	360	ARG
1	A	362	VAL
1	A	379	ILE
1	A	385	SER
1	A	400	ARG
1	A	401	GLN
1	A	402	VAL
1	A	406	ASP
2	B	11	HIS
2	B	15	VAL
2	B	16	GLN
2	B	21	ILE

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Mol	Chain	Res	Type
2	B	47	ASP
2	B	49	ASP
2	B	58	ARG
2	B	59	LEU
2	B	63	VAL
2	B	68	LEU
2	B	70	THR
2	B	76	GLN
2	B	84	ARG
2	B	90	THR
2	B	97	LEU
2	B	108	PHE
2	B	116	ILE
2	B	117	ASN
2	B	135	LEU
2	B	138	SER
2	B	144	THR
2	B	155	ILE
2	B	169	VAL
2	B	171	VAL
2	B	190	ARG
2	B	197	ILE
2	B	198	ARG
2	B	201	GLU
2	B	202	LYS
2	B	204	THR
2	B	205	LEU
2	B	207	THR
2	B	211	ASP
2	B	214	PRO
2	B	218	PHE
2	B	220	SER
2	B	225	ILE
2	B	226	LEU
2	B	228	TYR
2	B	229	PHE
2	B	233	PHE
2	B	234	ILE
2	B	236	ARG
2	B	238	PHE
2	B	242	ARG
2	B	243	PHE

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Mol	Chain	Res	Type
3	C	47	ASP
3	C	50	TRP
3	C	51	LEU
3	C	60	VAL
3	C	63	LEU
3	C	93	LEU
3	C	94	TYR
3	C	103	THR
3	C	106	ILE
3	C	107	LEU
3	C	113	LYS
3	C	115	ARG
3	C	118	ASN
3	C	122	LEU
3	C	125	ARG
3	C	128	LEU
3	C	129	ARG
3	C	130	ARG
3	C	131	ASN
3	C	132	PHE
3	C	138	LEU
3	C	158	THR
3	C	162	THR
3	C	163	ILE
3	C	164	VAL
3	C	165	ARG
3	C	180	SER
3	C	184	TYR
3	C	185	ILE
3	C	198	ARG
3	C	232	THR
3	C	234	TRP
3	C	235	PHE
3	C	236	MET
3	C	237	GLU
3	C	238	GLU
3	C	239	LEU
3	C	245	HIS
3	C	250	ILE
3	C	251	PHE
3	C	254	LEU
3	C	256	LEU

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Mol	Chain	Res	Type
3	C	259	MET
1	E	33	HIS
1	E	46	THR
1	E	52	LEU
1	E	56	LYS
1	E	60	LYS
1	E	64	THR
1	E	65	VAL
1	E	73	VAL
1	E	75	GLU
1	E	80	THR
1	E	86	VAL
1	E	89	LEU
1	E	93	MET
1	E	105	ILE
1	E	116	LEU
1	E	117	GLU
1	E	120	LYS
1	E	121	THR
1	E	135	ASP
1	E	137	HIS
1	E	140	THR
1	E	145	GLN
1	E	164	SER
1	E	174	THR
1	E	176	GLN
1	E	177	THR
1	E	180	LEU
1	E	182	ASN
1	E	185	GLU
1	E	208	ARG
1	E	209	ARG
1	E	223	ARG
1	E	227	LEU
1	E	244	ILE
1	E	245	LEU
1	E	249	MET
1	E	251	MET
1	E	269	MET
1	E	270	ARG
1	E	272	MET
1	E	273	LYS

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Mol	Chain	Res	Type
1	E	276	GLU
1	E	277	LEU
1	E	281	THR
1	E	286	VAL
1	E	287	GLU
1	E	292	ARG
1	E	298	MET
1	E	299	ARG
1	E	305	THR
1	E	309	ASN
1	E	312	ILE
1	E	314	LEU
1	E	322	VAL
1	E	329	VAL
1	E	331	LYS
1	E	334	THR
1	E	338	GLU
1	E	346	LEU
1	E	348	VAL
1	E	351	ASN
1	E	359	THR
1	E	360	ARG
1	E	361	THR
1	E	362	VAL
1	E	379	ILE
1	E	385	SER
1	E	400	ARG
1	E	401	GLN
1	E	402	VAL
1	E	403	VAL
1	E	406	ASP
2	F	11	HIS
2	F	15	VAL
2	F	16	GLN
2	F	21	ILE
2	F	43	LEU
2	F	47	ASP
2	F	49	ASP
2	F	58	ARG
2	F	63	VAL
2	F	68	LEU
2	F	69	VAL

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Mol	Chain	Res	Type
2	F	70	THR
2	F	84	ARG
2	F	90	THR
2	F	97	LEU
2	F	106	PHE
2	F	108	PHE
2	F	116	ILE
2	F	117	ASN
2	F	135	LEU
2	F	138	SER
2	F	144	THR
2	F	155	ILE
2	F	164	ILE
2	F	169	VAL
2	F	171	VAL
2	F	190	ARG
2	F	197	ILE
2	F	198	ARG
2	F	201	GLU
2	F	202	LYS
2	F	204	THR
2	F	205	LEU
2	F	207	THR
2	F	211	ASP
2	F	214	PRO
2	F	218	PHE
2	F	220	SER
2	F	225	ILE
2	F	226	LEU
2	F	228	TYR
2	F	229	PHE
2	F	233	PHE
2	F	234	ILE
2	F	236	ARG
2	F	238	PHE
2	F	242	ARG
2	F	243	PHE
3	G	47	ASP
3	G	50	TRP
3	G	51	LEU
3	G	60	VAL
3	G	63	LEU

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Mol	Chain	Res	Type
3	G	93	LEU
3	G	94	TYR
3	G	103	THR
3	G	106	ILE
3	G	107	LEU
3	G	113	LYS
3	G	115	ARG
3	G	118	ASN
3	G	122	LEU
3	G	125	ARG
3	G	128	LEU
3	G	129	ARG
3	G	131	ASN
3	G	132	PHE
3	G	138	LEU
3	G	145	ILE
3	G	158	THR
3	G	162	THR
3	G	163	ILE
3	G	164	VAL
3	G	165	ARG
3	G	180	SER
3	G	185	ILE
3	G	198	ARG
3	G	232	THR
3	G	234	TRP
3	G	235	PHE
3	G	236	MET
3	G	237	GLU
3	G	238	GLU
3	G	239	LEU
3	G	245	HIS
3	G	250	ILE
3	G	251	PHE
3	G	254	LEU
3	G	256	LEU
3	G	259	MET
1	I	46	THR
1	I	52	LEU
1	I	56	LYS
1	I	60	LYS
1	I	64	THR

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Mol	Chain	Res	Type
1	I	65	VAL
1	I	73	VAL
1	I	75	GLU
1	I	80	THR
1	I	86	VAL
1	I	89	LEU
1	I	93	MET
1	I	105	ILE
1	I	116	LEU
1	I	117	GLU
1	I	120	LYS
1	I	121	THR
1	I	135	ASP
1	I	140	THR
1	I	145	GLN
1	I	164	SER
1	I	174	THR
1	I	176	GLN
1	I	177	THR
1	I	180	LEU
1	I	182	ASN
1	I	185	GLU
1	I	208	ARG
1	I	209	ARG
1	I	223	ARG
1	I	227	LEU
1	I	244	ILE
1	I	245	LEU
1	I	249	MET
1	I	251	MET
1	I	261	THR
1	I	269	MET
1	I	270	ARG
1	I	273	LYS
1	I	276	GLU
1	I	277	LEU
1	I	281	THR
1	I	284	VAL
1	I	286	VAL
1	I	287	GLU
1	I	292	ARG
1	I	299	ARG

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Mol	Chain	Res	Type
1	I	305	THR
1	I	309	ASN
1	I	312	ILE
1	I	314	LEU
1	I	322	VAL
1	I	329	VAL
1	I	346	LEU
1	I	348	VAL
1	I	351	ASN
1	I	359	THR
1	I	360	ARG
1	I	361	THR
1	I	362	VAL
1	I	379	ILE
1	I	385	SER
1	I	400	ARG
1	I	401	GLN
1	I	402	VAL
1	I	406	ASP
2	J	11	HIS
2	J	15	VAL
2	J	16	GLN
2	J	21	ILE
2	J	43	LEU
2	J	47	ASP
2	J	58	ARG
2	J	63	VAL
2	J	68	LEU
2	J	69	VAL
2	J	70	THR
2	J	84	ARG
2	J	90	THR
2	J	97	LEU
2	J	108	PHE
2	J	116	ILE
2	J	117	ASN
2	J	135	LEU
2	J	136	MET
2	J	138	SER
2	J	144	THR
2	J	152	TRP
2	J	155	ILE

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Mol	Chain	Res	Type
2	J	164	ILE
2	J	169	VAL
2	J	190	ARG
2	J	197	ILE
2	J	198	ARG
2	J	201	GLU
2	J	202	LYS
2	J	204	THR
2	J	205	LEU
2	J	207	THR
2	J	211	ASP
2	J	214	PRO
2	J	218	PHE
2	J	220	SER
2	J	225	ILE
2	J	226	LEU
2	J	228	TYR
2	J	229	PHE
2	J	233	PHE
2	J	234	ILE
2	J	236	ARG
2	J	238	PHE
2	J	242	ARG
2	J	243	PHE
3	K	47	ASP
3	K	50	TRP
3	K	51	LEU
3	K	60	VAL
3	K	63	LEU
3	K	93	LEU
3	K	94	TYR
3	K	103	THR
3	K	106	ILE
3	K	107	LEU
3	K	113	LYS
3	K	115	ARG
3	K	118	ASN
3	K	122	LEU
3	K	125	ARG
3	K	128	LEU
3	K	129	ARG
3	K	131	ASN

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Mol	Chain	Res	Type
3	K	132	PHE
3	K	145	ILE
3	K	158	THR
3	K	162	THR
3	K	163	ILE
3	K	164	VAL
3	K	165	ARG
3	K	180	SER
3	K	184	TYR
3	K	185	ILE
3	K	198	ARG
3	K	232	THR
3	K	234	TRP
3	K	235	PHE
3	K	236	MET
3	K	238	GLU
3	K	239	LEU
3	K	245	HIS
3	K	250	ILE
3	K	251	PHE
3	K	254	LEU
3	K	256	LEU
3	K	259	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	143	ASN
1	A	145	GLN
1	A	182	ASN
1	A	192	HIS
1	A	265	GLN
1	A	306	ASN
1	A	309	ASN
1	A	351	ASN
1	A	401	GLN
2	B	103	ASN
2	B	117	ASN
3	C	131	ASN
1	E	62	ASN
1	E	137	HIS

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Mol	Chain	Res	Type
1	E	143	ASN
1	E	145	GLN
1	E	182	ASN
1	E	192	HIS
1	E	265	GLN
1	E	306	ASN
1	E	309	ASN
1	E	351	ASN
1	E	401	GLN
2	F	103	ASN
2	F	117	ASN
3	G	131	ASN
3	G	231	HIS
1	I	62	ASN
1	I	143	ASN
1	I	145	GLN
1	I	182	ASN
1	I	192	HIS
1	I	265	GLN
1	I	306	ASN
1	I	309	ASN
1	I	351	ASN
1	I	401	GLN
2	J	103	ASN
2	J	117	ASN
3	K	131	ASN
3	K	231	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
6	CUA	A	3	1	0,1,1	0.00	-	0,0,0	0.00	-
6	CUA	E	500	1	0,1,1	0.00	-	0,0,0	0.00	-
6	CUA	I	600	1	0,1,1	0.00	-	0,0,0	0.00	-

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
6	CUA	A	3	1	-	0/0/0/0	0/0/0/0
6	CUA	E	500	1	-	0/0/0/0	0/0/0/0
6	CUA	I	600	1	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	382/382 (100%)	0.49	31 (8%) 15 7	65, 70, 73, 76	0
1	E	382/382 (100%)	0.46	31 (8%) 15 7	66, 70, 73, 76	0
1	I	382/382 (100%)	0.49	36 (9%) 11 5	66, 70, 73, 76	0
2	B	238/247 (96%)	0.96	32 (13%) 4 2	66, 70, 74, 78	0
2	F	238/247 (96%)	1.10	35 (14%) 3 2	66, 70, 74, 78	0
2	J	238/247 (96%)	0.95	37 (15%) 3 1	66, 70, 74, 78	0
3	C	188/289 (65%)	1.17	33 (17%) 2 1	67, 70, 72, 73	0
3	G	188/289 (65%)	1.41	55 (29%) 1 0	67, 70, 72, 73	0
3	K	188/289 (65%)	1.24	42 (22%) 1 1	67, 70, 72, 73	0
All	All	2424/2754 (88%)	0.82	332 (13%) 4 2	65, 70, 73, 78	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	194	PRO	23.6
2	J	194	PRO	14.3
2	B	194	PRO	10.2
3	K	84	GLU	9.4
3	G	87	THR	8.8
3	K	76	ALA	8.3
2	J	231	TRP	7.8
3	C	87	THR	7.8
3	C	234	TRP	7.7
2	B	218	PHE	7.3
3	C	259	MET	7.2
3	K	88	TYR	7.2
2	B	225	ILE	7.0
2	J	237	TRP	6.9
3	G	259	MET	6.9

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Mol	Chain	Res	Type	RSRZ
2	F	7	ALA	6.8
3	K	81	PHE	6.6
2	F	218	PHE	6.6
1	A	357	GLY	6.4
1	A	225	ASP	6.1
3	G	73	GLY	6.1
3	G	88	TYR	6.0
2	B	198	ARG	6.0
1	A	145	GLN	6.0
2	B	195	GLU	5.9
2	F	193	THR	5.8
1	A	398	GLY	5.8
2	B	231	TRP	5.6
2	B	193	THR	5.4
2	F	113	TYR	5.3
2	J	105	TYR	5.3
3	K	259	MET	5.3
2	J	233	PHE	5.1
1	E	222	GLY	5.1
2	F	231	TRP	5.1
3	K	234	TRP	5.0
3	G	238	GLU	5.0
2	F	138	SER	5.0
2	B	192	GLY	4.9
3	C	117	ARG	4.9
3	K	248	PHE	4.8
1	E	61	ILE	4.8
1	I	221	ALA	4.8
1	E	309	ASN	4.8
3	K	244	LEU	4.8
1	A	358	GLU	4.7
2	J	223	MET	4.7
1	A	147	GLY	4.6
3	C	115	ARG	4.6
3	K	77	GLY	4.6
1	E	147	GLY	4.5
1	I	330	TYR	4.5
3	G	237	GLU	4.5
3	C	127	GLU	4.5
3	C	256	LEU	4.4
1	E	165	GLU	4.4
1	E	221	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	J	193	THR	4.3
3	G	123	THR	4.3
2	B	44	THR	4.3
1	E	220	ASP	4.3
3	K	47	ASP	4.3
1	I	279	ALA	4.3
3	K	202	PHE	4.3
2	F	8	VAL	4.2
2	J	198	ARG	4.2
3	G	119	LEU	4.2
3	G	247	GLY	4.2
3	G	80	SER	4.2
1	A	175	GLY	4.1
3	G	243	PRO	4.1
1	A	306	ASN	4.1
3	C	253	TRP	4.1
1	I	147	GLY	4.1
3	C	244	LEU	4.0
3	G	81	PHE	4.0
2	F	111	TRP	3.9
3	K	85	PHE	3.9
1	I	329	VAL	3.9
3	K	112	TRP	3.9
2	F	234	ILE	3.9
3	K	251	PHE	3.8
3	C	84	GLU	3.8
1	E	145	GLN	3.8
1	E	148	GLY	3.8
3	G	118	ASN	3.7
3	K	71	VAL	3.7
3	K	247	GLY	3.7
3	K	67	TRP	3.7
3	C	47	ASP	3.7
1	I	231	THR	3.6
3	C	251	PHE	3.6
1	I	306	ASN	3.6
2	B	208	PHE	3.6
1	E	80	THR	3.6
2	J	136	MET	3.6
2	F	219	PHE	3.6
1	I	85	ASP	3.6
2	J	218	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	326	ASP	3.5
3	G	47	ASP	3.5
3	G	133	THR	3.5
3	C	81	PHE	3.5
3	G	239	LEU	3.5
2	F	92	CYS	3.5
2	J	195	GLU	3.4
3	G	117	ARG	3.4
2	B	244	LEU	3.4
3	G	250	ILE	3.4
2	J	106	PHE	3.4
3	G	256	LEU	3.4
2	J	192	GLY	3.3
2	F	80	TRP	3.3
2	J	48	TRP	3.3
2	F	241	GLU	3.3
2	J	222	PHE	3.3
2	F	9	ARG	3.2
1	E	350	ASP	3.2
1	E	189	TYR	3.2
3	G	86	GLU	3.2
3	G	74	TRP	3.2
1	I	414	MET	3.2
2	B	113	TYR	3.2
3	C	163	ILE	3.2
3	K	254	LEU	3.2
2	B	15	VAL	3.1
2	F	15	VAL	3.1
3	K	117	ARG	3.1
3	C	255	ALA	3.1
2	B	196	TYR	3.1
2	F	62	THR	3.1
3	K	122	LEU	3.1
2	J	46	GLY	3.1
1	E	252	SER	3.1
2	B	43	LEU	3.1
1	A	234	LYS	3.1
3	G	137	TRP	3.1
3	K	258	VAL	3.0
1	E	206	TRP	3.0
3	K	253	TRP	3.0
1	I	249	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	251	MET	3.0
3	G	236	MET	3.0
3	G	244	LEU	3.0
1	I	413	PHE	3.0
3	K	243	PRO	3.0
3	G	234	TRP	3.0
1	A	294	PRO	3.0
3	G	251	PHE	3.0
3	K	162	THR	3.0
1	I	357	GLY	3.0
3	G	67	TRP	3.0
3	K	250	ILE	3.0
3	K	237	GLU	3.0
2	B	221	ALA	2.9
1	A	205	TYR	2.9
2	J	135	LEU	2.9
2	J	110	GLY	2.9
2	F	66	ILE	2.9
1	I	296	ARG	2.9
2	J	58	ARG	2.9
3	C	88	TYR	2.9
1	I	84	PRO	2.9
1	E	414	MET	2.9
2	J	162	PRO	2.8
3	C	90	MET	2.8
3	K	159	TRP	2.8
3	C	250	ILE	2.8
1	E	202	TRP	2.8
2	F	200	VAL	2.8
1	A	397	THR	2.8
1	E	320	ALA	2.8
1	I	320	ALA	2.8
1	I	134	GLY	2.8
3	G	258	VAL	2.8
1	A	233	ARG	2.8
2	F	46	GLY	2.8
3	G	253	TRP	2.8
1	A	355	ALA	2.8
1	E	256	SER	2.7
2	J	84	ARG	2.7
3	G	202	PHE	2.7
2	J	80	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
3	K	125	ARG	2.7
3	C	247	GLY	2.7
3	C	237	GLU	2.7
3	K	94	TYR	2.7
2	F	19	ARG	2.7
1	A	176	GLN	2.7
2	B	217	ALA	2.7
1	A	144	VAL	2.7
1	I	309	ASN	2.7
2	J	8	VAL	2.7
1	A	123	ASP	2.7
2	B	48	TRP	2.7
3	G	144	ALA	2.7
1	A	338	GLU	2.6
3	G	167	THR	2.6
2	B	57	ARG	2.6
2	B	136	MET	2.6
3	G	79	ASP	2.6
3	C	78	LEU	2.6
1	I	374	TYR	2.6
3	G	58	TYR	2.6
1	E	164	SER	2.6
3	G	257	ALA	2.6
2	J	70	THR	2.6
3	C	254	LEU	2.6
1	E	64	THR	2.5
1	E	146	GLY	2.5
1	E	160	GLU	2.5
3	K	200	PRO	2.5
1	I	146	GLY	2.5
2	J	16	GLN	2.5
2	J	85	LEU	2.5
3	G	89	TRP	2.5
3	G	198	ARG	2.5
1	I	211	ILE	2.5
3	C	155	GLN	2.5
2	F	78	TYR	2.5
2	F	244	LEU	2.5
3	K	181	TYR	2.5
1	A	224	ALA	2.5
1	A	219	VAL	2.5
1	I	218	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	16	GLN	2.5
3	G	249	VAL	2.5
2	J	131	LEU	2.4
3	G	162	THR	2.4
2	B	81	GLU	2.4
3	K	238	GLU	2.4
1	E	306	ASN	2.4
3	K	246	TYR	2.4
2	F	91	VAL	2.4
2	B	109	TRP	2.4
3	C	67	TRP	2.4
3	C	159	TRP	2.4
3	K	86	GLU	2.4
2	B	204	THR	2.4
1	I	358	GLU	2.4
2	B	80	TRP	2.4
3	K	199	LEU	2.4
3	C	200	PRO	2.4
3	C	192	PHE	2.4
2	J	234	ILE	2.4
1	A	189	TYR	2.4
1	I	64	THR	2.4
2	J	113	TYR	2.4
1	I	83	GLU	2.4
3	G	78	LEU	2.4
2	F	225	ILE	2.4
3	G	49	LYS	2.4
3	K	110	TYR	2.4
3	G	248	PHE	2.4
3	C	110	TYR	2.4
1	A	163	MET	2.3
1	I	145	GLN	2.3
2	J	221	ALA	2.3
3	C	246	TYR	2.3
3	C	167	THR	2.3
1	A	406	ASP	2.3
1	A	230	ALA	2.3
3	K	70	GLY	2.3
1	A	312	ILE	2.3
2	F	84	ARG	2.3
2	J	44	THR	2.3
1	I	327	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	110	TYR	2.3
2	B	16	GLN	2.3
2	B	42	MET	2.3
1	A	36	LYS	2.3
1	I	37	SER	2.3
2	J	152	TRP	2.3
1	A	356	PRO	2.3
2	B	66	ILE	2.2
1	I	293	VAL	2.2
1	E	308	GLY	2.2
1	I	162	SER	2.2
3	G	173	HIS	2.2
2	F	152	TRP	2.2
3	G	165	ARG	2.2
3	G	195	ALA	2.2
1	E	253	SER	2.2
3	G	143	TRP	2.2
1	I	356	PRO	2.2
3	G	108	TRP	2.2
2	J	196	TYR	2.2
3	K	141	TYR	2.2
3	G	192	PHE	2.2
2	F	198	ARG	2.2
3	K	114	THR	2.2
2	J	124	LEU	2.2
1	I	355	ALA	2.2
2	B	148	GLY	2.1
1	E	130	ALA	2.1
3	C	203	ALA	2.1
3	G	76	ALA	2.1
1	I	160	GLU	2.1
2	B	219	PHE	2.1
2	J	219	PHE	2.1
3	C	141	TYR	2.1
1	A	162	SER	2.1
2	B	234	ILE	2.1
1	A	375	ARG	2.1
2	B	223	MET	2.1
1	A	223	ARG	2.1
1	A	252	SER	2.1
3	G	199	LEU	2.1
2	F	243	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	130	ARG	2.1
2	F	101	TRP	2.1
2	B	233	PHE	2.1
1	I	288	ASP	2.1
1	I	317	PHE	2.0
3	K	130	ARG	2.1
3	C	116	ASP	2.0
1	E	277	LEU	2.0
2	F	58	ARG	2.0
3	G	77	GLY	2.0
1	E	319	THR	2.0
3	K	46	LEU	2.0
1	E	353	PRO	2.0
2	F	86	PRO	2.0
2	J	123	SER	2.0
2	J	111	TRP	2.0
1	E	228	VAL	2.0
3	G	254	LEU	2.0
3	K	194	TYR	2.0
1	E	92	GLY	2.0
2	F	217	ALA	2.0
3	G	240	PHE	2.0
2	F	140	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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
5	CU	A	4	1/1	0.99	0.24	0.55	61,61,61,61	0
4	ZN	E	702	1/1	0.81	0.22	0.06	213,213,213,213	0
6	CUA	I	600	2/2	0.98	0.19	-0.11	76,76,76,82	0
4	ZN	G	662	1/1	0.99	0.33	-0.14	46,46,46,46	0
5	CU	I	601	1/1	0.99	0.18	-0.72	61,61,61,61	0
6	CUA	A	3	2/2	0.91	0.19	-0.85	74,74,74,82	0
4	ZN	C	661	1/1	0.96	0.18	-0.95	73,73,73,73	0
4	ZN	K	663	1/1	0.99	0.18	-1.03	60,60,60,60	0
4	ZN	E	900	1/1	0.99	0.13	-1.07	76,76,76,76	0
6	CUA	E	500	2/2	0.90	0.15	-1.27	75,75,75,82	0
5	CU	E	501	1/1	0.99	0.15	-1.63	61,61,61,61	0
4	ZN	A	800	1/1	0.99	0.12	-	77,77,77,77	0
4	ZN	C	700	1/1	0.98	0.27	-	46,46,46,46	1
4	ZN	E	701	1/1	0.82	0.22	-	55,55,55,55	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.