



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:18 PM GMT

PDB ID : 1JJK  
Title : Selenomethionine Substitution of Orotidine-5'-monophosphate Decarboxylase from E. coli Causes a Change in Crystal Contacts and Space Group  
Authors : Poulsen, J.-C.N.; Harris, P.; Jensen, K.F.; Larsen, S.  
Deposited on : 2001-07-06  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

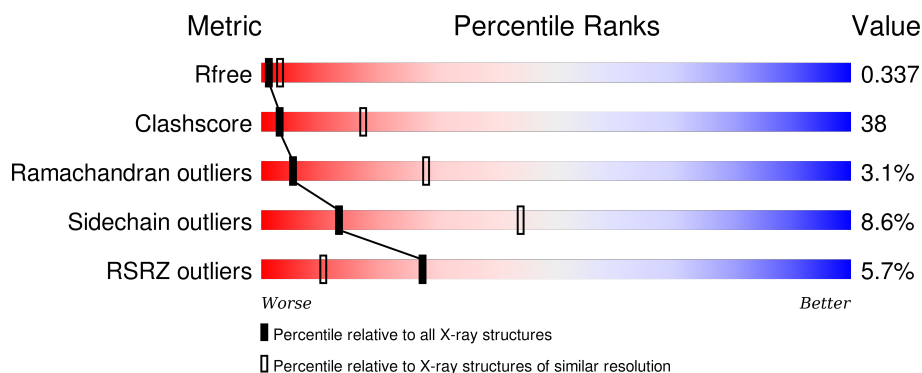
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	245	<div> <div>0%</div> <div> <div>41%</div> <div>46%</div> <div>6% • 6%</div> </div> </div>
1	B	245	<div> <div>2%</div> <div> <div>40%</div> <div>48%</div> <div>6% • 6%</div> </div> </div>
1	C	245	<div> <div>41%</div> <div>47%</div> <div>6% • 6%</div> </div>
1	D	245	<div> <div>2%</div> <div> <div>40%</div> <div>47%</div> <div>6% • 6%</div> </div> </div>
1	E	245	<div> <div>3%</div> <div> <div>41%</div> <div>47%</div> <div>6% • 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	245	
1	G	245	
1	H	245	
1	I	245	
1	J	245	
1	K	245	
1	L	245	
1	M	245	
1	N	245	
1	O	245	
1	P	245	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28336 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 OROTIDINE 5'-PHOSPHATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	B	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	C	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	D	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	E	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	F	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	G	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	H	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	I	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	J	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	K	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	L	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	M	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	N	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	O	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	P	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	133	MSE	MET	MODIFIED RESIDUE	UNP P08244

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Chain	Residue	Modelled	Actual	Comment	Reference
E	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	95	MSE	MET	MODIFIED RESIDUE	UNP P08244

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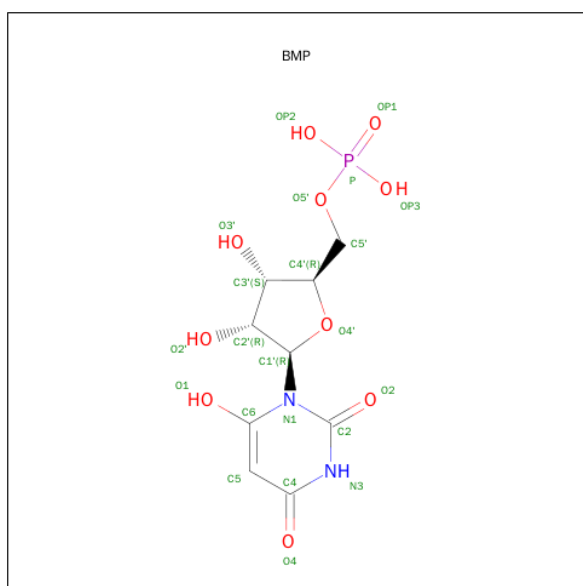
Chain	Residue	Modelled	Actual	Comment	Reference
J	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
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L	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	218	MSE	MET	MODIFIED RESIDUE	UNP P08244

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Chain	Residue	Modelled	Actual	Comment	Reference
O	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	218	MSE	MET	MODIFIED RESIDUE	UNP P08244

- Molecule 2 is 6-HYDROXYURIDINE-5'-PHOSPHATE (three-letter code: BMP) (formula:  $C_9H_{13}N_2O_{10}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	B	1	Total	C	N	O	P	0	0
			22	9	2	10	1		

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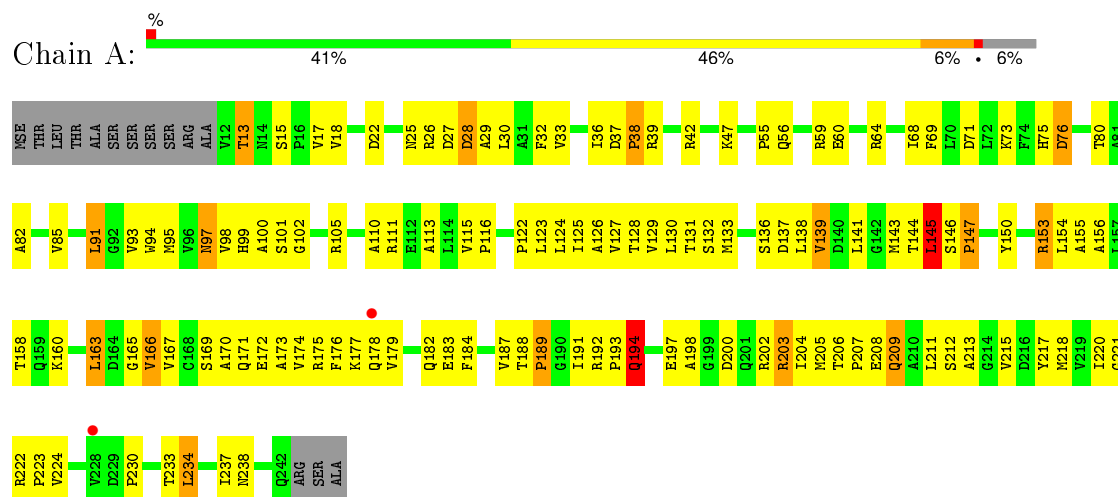
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	D	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	E	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	F	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	G	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	H	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	I	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	J	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	K	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	L	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	M	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	N	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	O	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	P	1	Total 22	C 9	N 2	O 10	P 1	0	0

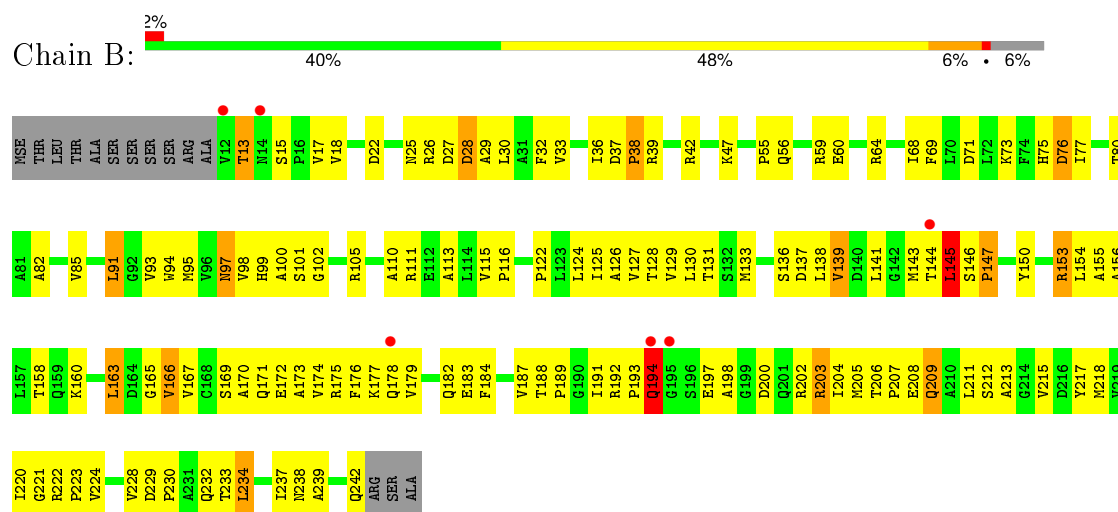
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

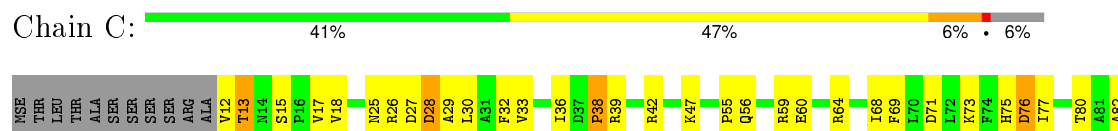
#### • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

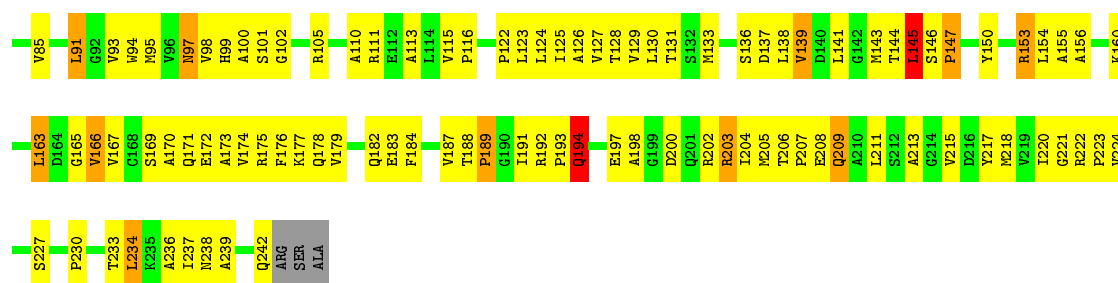


#### • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

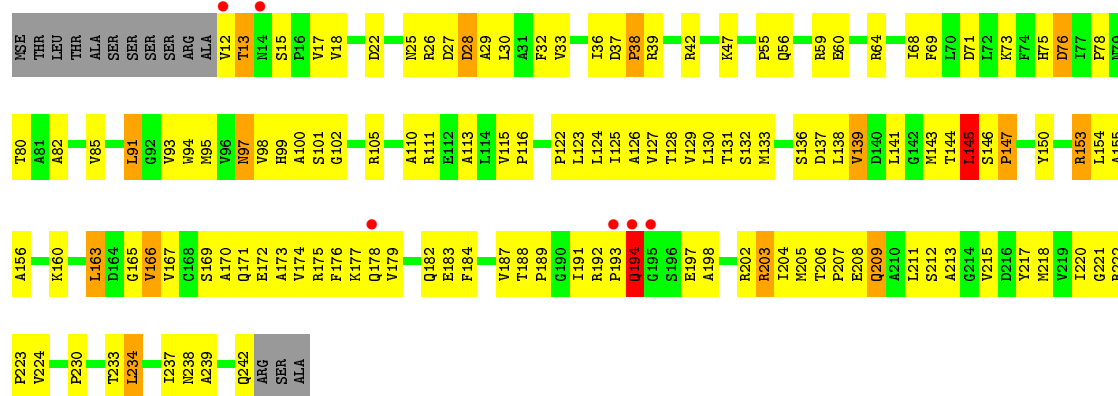


#### • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

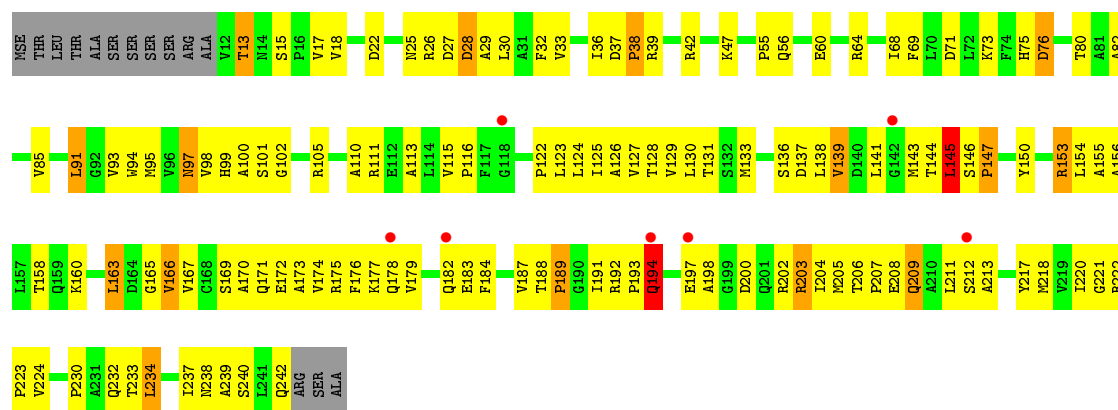




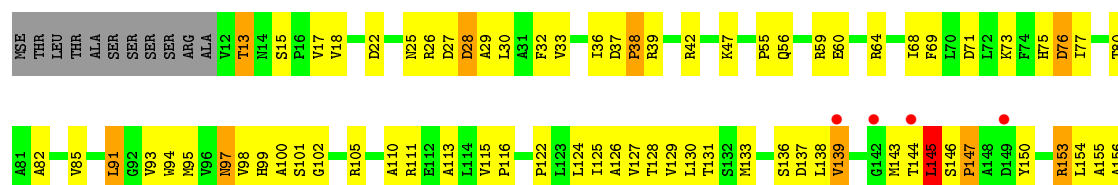
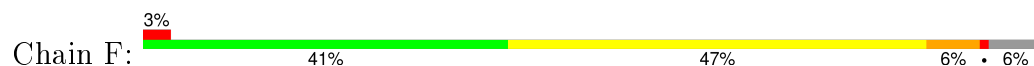
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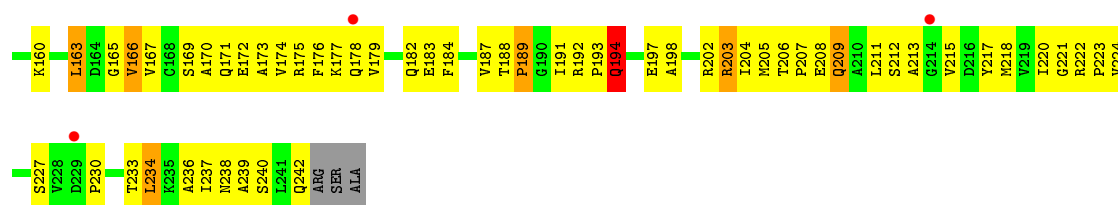


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

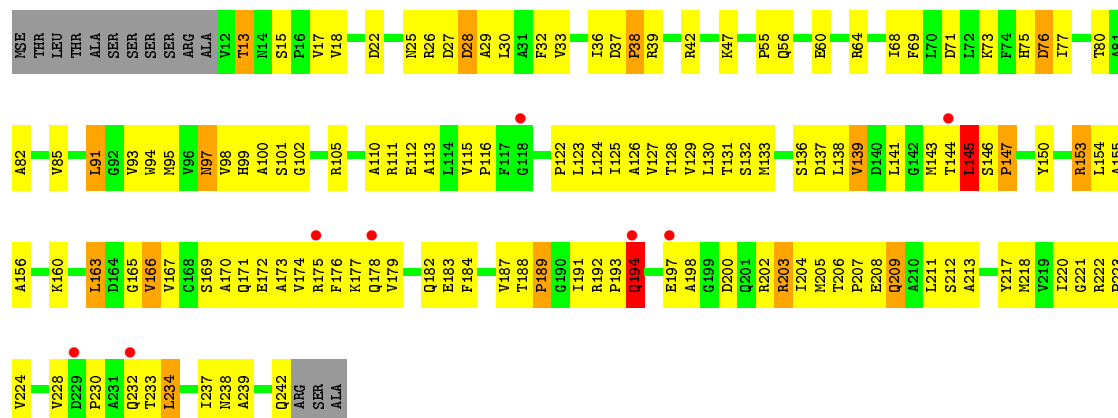


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

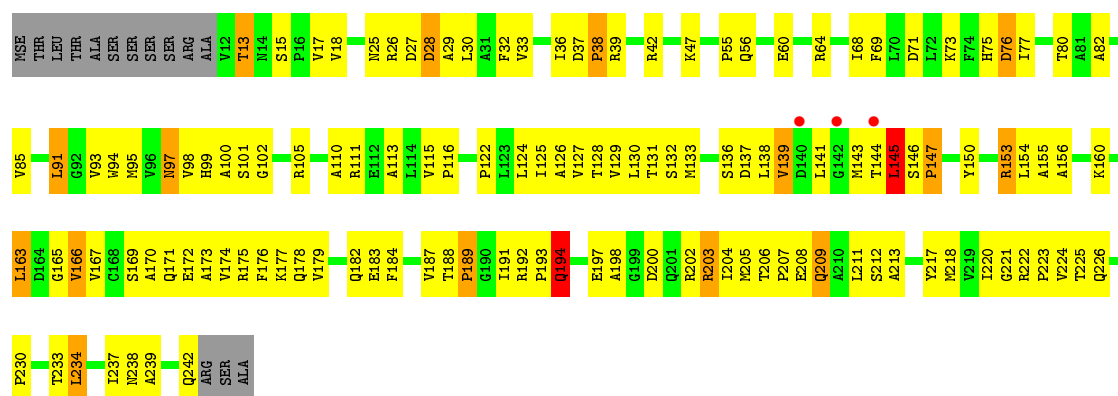




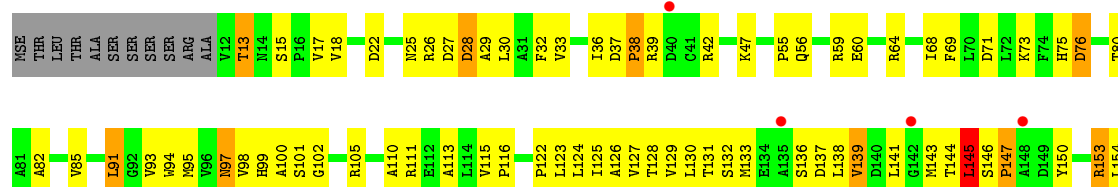
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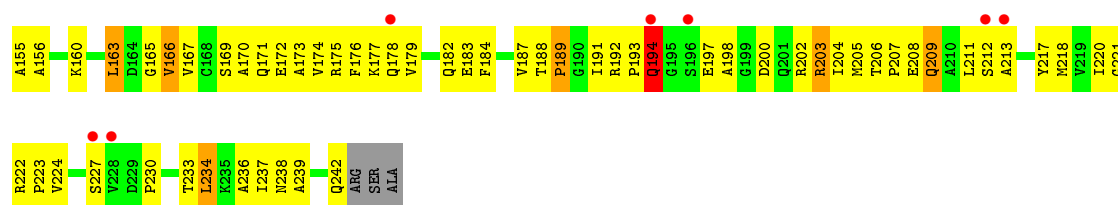


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

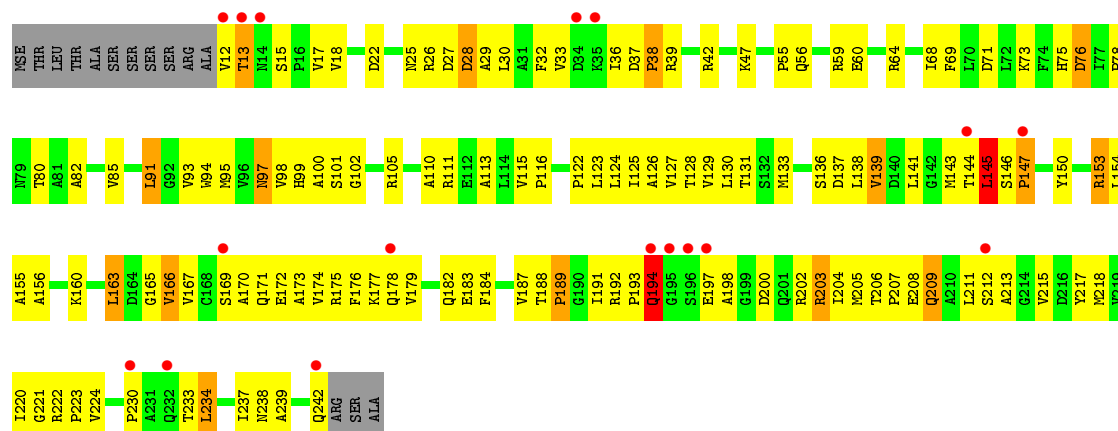


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE





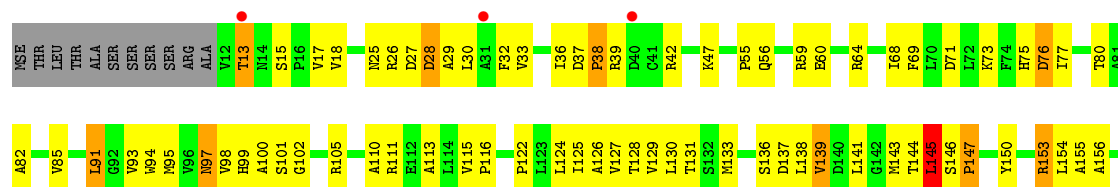
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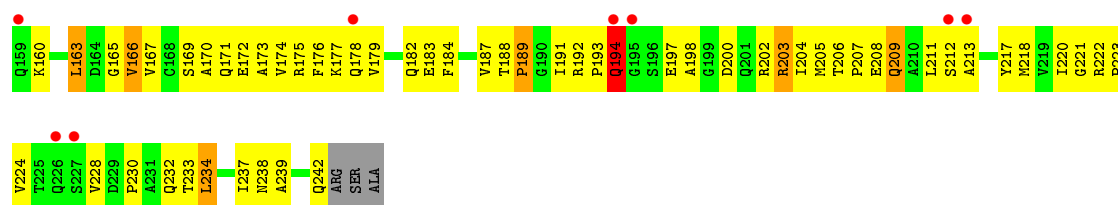


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

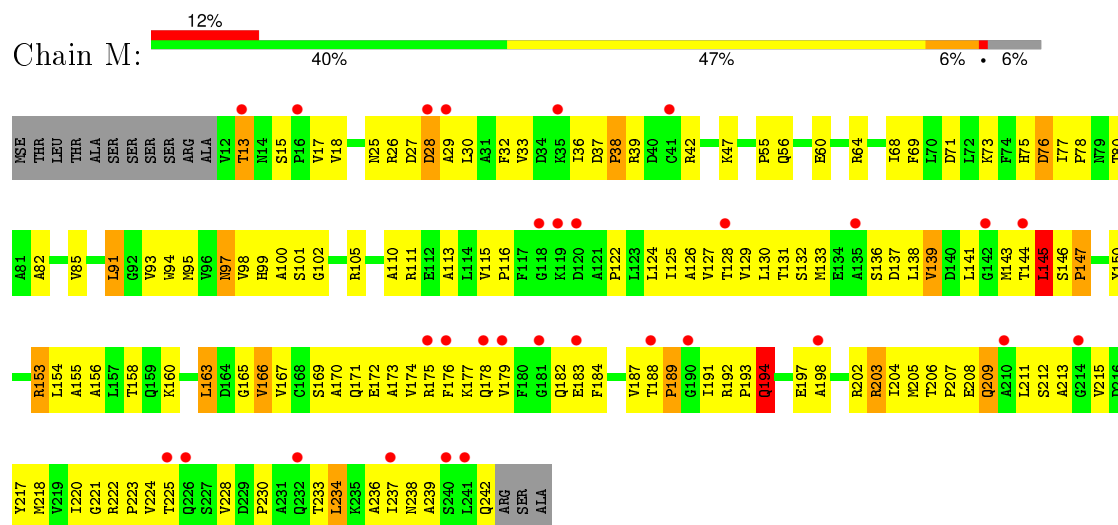


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

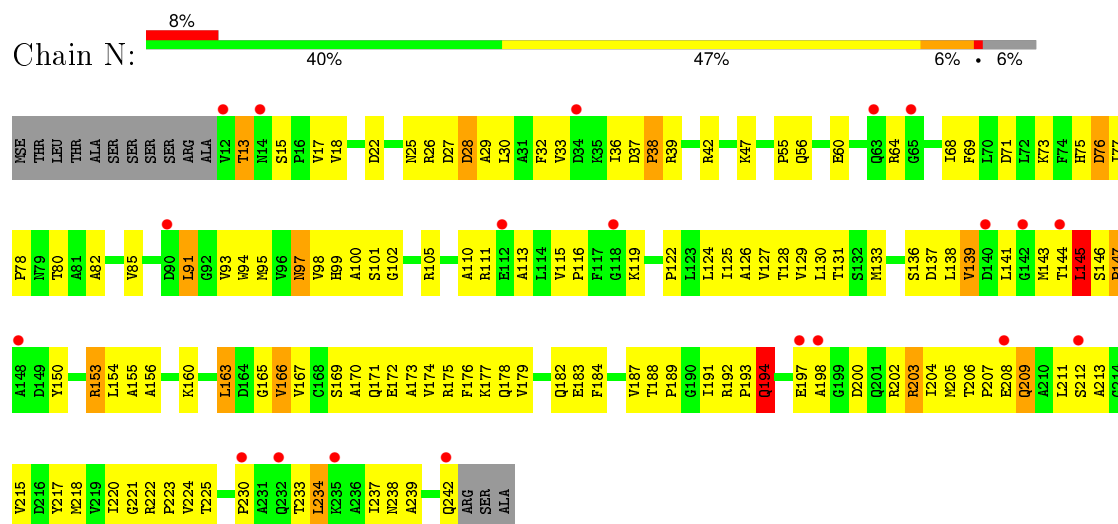




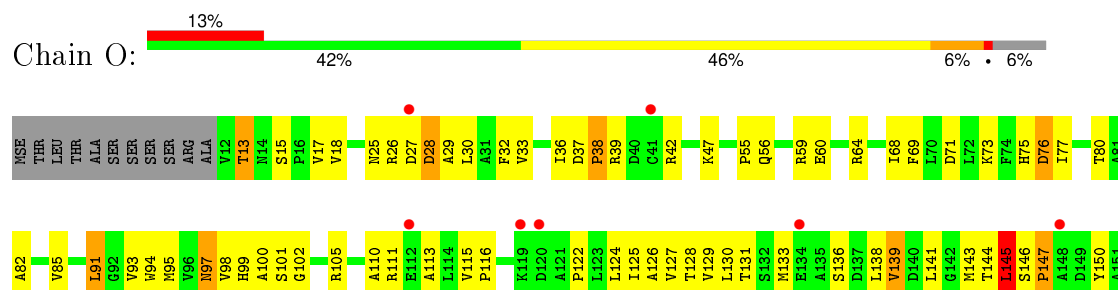
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

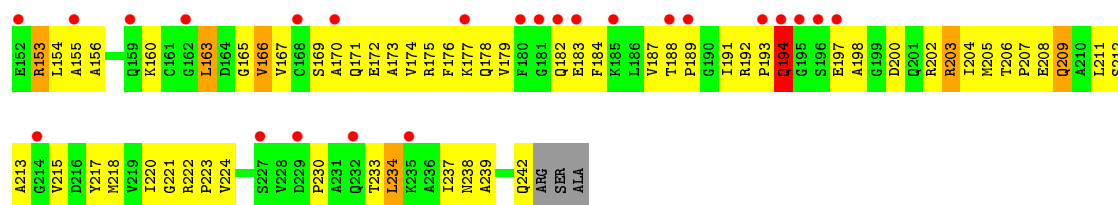


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

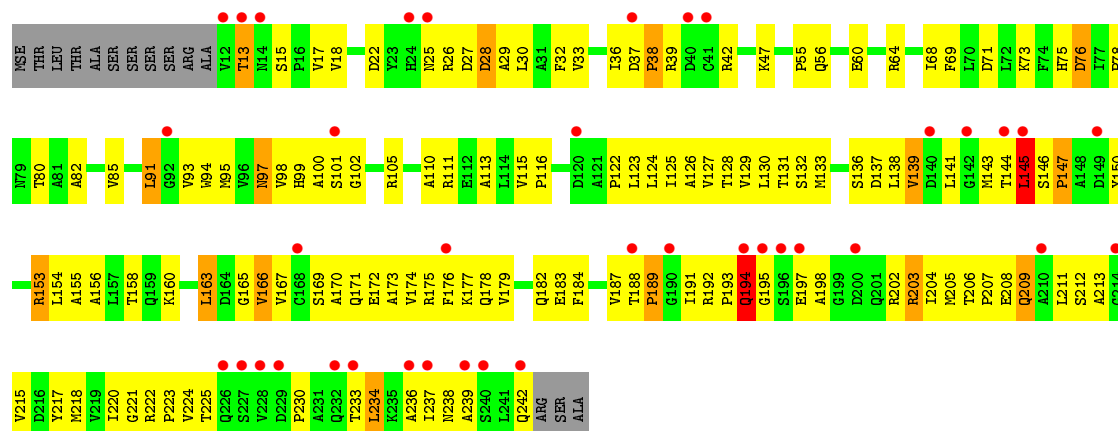


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE





• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.50Å 149.00Å 115.60Å 90.00° 115.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (30.00-3.00) 91.4 (29.82-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.41 (at 3.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.344 , 0.344 0.342 , 0.337	Depositor DCC
$R_{free}$ test set	3274 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.5	EDS
Estimated twinning fraction	0.376 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	3 of 64895 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	28336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1146e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: BMP

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	0.40	0/1772	0.67	0/2392
1	B	0.40	0/1772	0.67	0/2392
1	C	0.40	0/1772	0.67	0/2392
1	D	0.40	0/1772	0.67	0/2392
1	E	0.40	0/1772	0.67	0/2392
1	F	0.40	0/1772	0.67	0/2392
1	G	0.40	0/1772	0.67	0/2392
1	H	0.40	0/1772	0.67	0/2392
1	I	0.40	0/1772	0.67	0/2392
1	J	0.40	0/1772	0.67	0/2392
1	K	0.40	0/1772	0.67	0/2392
1	L	0.40	0/1772	0.67	0/2392
1	M	0.40	0/1772	0.67	0/2392
1	N	0.40	0/1772	0.67	0/2392
1	O	0.40	0/1772	0.67	0/2392
1	P	0.40	0/1772	0.67	0/2392
All	All	0.40	0/28352	0.67	0/38272

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1749	0	1758	139	1
1	B	1749	0	1758	162	0
1	C	1749	0	1758	163	0
1	D	1749	0	1758	141	0
1	E	1749	0	1758	138	3
1	F	1749	0	1758	152	0
1	G	1749	0	1758	155	0
1	H	1749	0	1758	135	1
1	I	1749	0	1758	138	2
1	J	1749	0	1758	148	1
1	K	1749	0	1758	145	2
1	L	1749	0	1758	138	2
1	M	1749	0	1758	144	2
1	N	1749	0	1758	143	0
1	O	1749	0	1758	135	1
1	P	1749	0	1758	141	3
2	A	22	0	11	2	0
2	B	22	0	11	2	0
2	C	22	0	11	2	0
2	D	22	0	11	2	0
2	E	22	0	11	3	0
2	F	22	0	11	2	0
2	G	22	0	11	2	0
2	H	22	0	11	2	0
2	I	22	0	11	2	0
2	J	22	0	11	2	0
2	K	22	0	11	2	0
2	L	22	0	11	2	0
2	M	22	0	11	3	0
2	N	22	0	11	4	0
2	O	22	0	11	2	0
2	P	22	0	11	2	0
All	All	28336	0	28304	2177	9

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 38.

All (2177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLN:HG3	1:J:12:VAL:CG1	1.65	1.26
1:B:232:GLN:NE2	1:C:227:SER:HA	1.53	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:ALA:CB	1:G:228:VAL:HG21	1.77	1.13
1:F:236:ALA:CB	1:G:228:VAL:CG2	2.26	1.11
1:F:236:ALA:HB3	1:G:228:VAL:HG21	1.37	1.04
1:O:218:MSE:HE2	1:O:220:ILE:HD11	1.42	1.02
1:K:218:MSE:HE2	1:K:220:ILE:HD11	1.42	1.02
1:I:218:MSE:HE2	1:I:220:ILE:HD11	1.42	1.01
1:C:182:GLN:HG3	1:J:12:VAL:HG11	1.05	1.01
1:P:218:MSE:HE2	1:P:220:ILE:HD11	1.42	1.01
1:G:218:MSE:HE2	1:G:220:ILE:HD11	1.42	1.01
1:N:218:MSE:HE2	1:N:220:ILE:HD11	1.42	1.01
1:H:218:MSE:HE2	1:H:220:ILE:HD11	1.42	1.01
1:A:218:MSE:HE2	1:A:220:ILE:HD11	1.42	1.00
1:E:218:MSE:HE2	1:E:220:ILE:HD11	1.42	1.00
1:F:218:MSE:HE2	1:F:220:ILE:HD11	1.42	1.00
1:M:218:MSE:HE2	1:M:220:ILE:HD11	1.42	0.99
1:D:218:MSE:HE2	1:D:220:ILE:HD11	1.42	0.99
1:C:218:MSE:HE2	1:C:220:ILE:HD11	1.42	0.99
1:B:218:MSE:HE2	1:B:220:ILE:HD11	1.42	0.98
1:F:227:SER:HA	1:G:232:GLN:NE2	1.78	0.98
1:B:228:VAL:CG2	1:C:236:ALA:CB	2.40	0.98
1:D:12:VAL:HG11	1:K:182:GLN:HG3	1.43	0.98
1:C:182:GLN:CG	1:J:12:VAL:HG11	1.93	0.98
1:J:218:MSE:HE2	1:J:220:ILE:HD11	1.42	0.97
1:L:218:MSE:HE2	1:L:220:ILE:HD11	1.42	0.97
1:D:182:GLN:HG3	1:K:12:VAL:HG11	1.45	0.97
1:B:228:VAL:HG21	1:C:236:ALA:HB3	1.46	0.95
1:B:232:GLN:HE21	1:C:227:SER:HA	1.13	0.94
1:C:182:GLN:CG	1:J:12:VAL:CG1	2.46	0.93
1:F:236:ALA:HB1	1:G:228:VAL:CG2	1.98	0.92
1:M:25:ASN:HD22	1:M:28:ASP:HB2	1.35	0.92
1:B:25:ASN:HD22	1:B:28:ASP:HB2	1.35	0.92
1:N:25:ASN:HD22	1:N:28:ASP:HB2	1.35	0.91
1:I:25:ASN:HD22	1:I:28:ASP:HB2	1.35	0.91
1:D:25:ASN:HD22	1:D:28:ASP:HB2	1.35	0.91
1:O:25:ASN:HD22	1:O:28:ASP:HB2	1.35	0.91
1:E:25:ASN:HD22	1:E:28:ASP:HB2	1.35	0.91
1:J:147:PRO:HB3	1:J:203:ARG:HE	1.36	0.91
1:B:147:PRO:HB3	1:B:203:ARG:HE	1.36	0.91
1:G:25:ASN:HD22	1:G:28:ASP:HB2	1.35	0.91
1:A:25:ASN:HD22	1:A:28:ASP:HB2	1.35	0.91
1:J:25:ASN:HD22	1:J:28:ASP:HB2	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:PRO:HB3	1:F:203:ARG:HE	1.36	0.90
1:O:147:PRO:HB3	1:O:203:ARG:HE	1.36	0.90
1:K:25:ASN:HD22	1:K:28:ASP:HB2	1.35	0.90
1:I:147:PRO:HB3	1:I:203:ARG:HE	1.36	0.90
1:H:25:ASN:HD22	1:H:28:ASP:HB2	1.35	0.90
1:D:147:PRO:HB3	1:D:203:ARG:HE	1.36	0.90
1:P:25:ASN:HD22	1:P:28:ASP:HB2	1.35	0.90
1:L:147:PRO:HB3	1:L:203:ARG:HE	1.36	0.90
1:C:25:ASN:HD22	1:C:28:ASP:HB2	1.35	0.90
1:H:147:PRO:HB3	1:H:203:ARG:HE	1.36	0.90
1:F:25:ASN:HD22	1:F:28:ASP:HB2	1.35	0.90
1:P:25:ASN:ND2	1:P:28:ASP:H	1.71	0.89
1:F:25:ASN:ND2	1:F:28:ASP:H	1.71	0.89
1:L:25:ASN:HD22	1:L:28:ASP:HB2	1.35	0.89
1:M:75:HIS:H	1:N:47:LYS:HZ2	1.17	0.89
1:E:25:ASN:ND2	1:E:28:ASP:H	1.71	0.89
1:G:25:ASN:ND2	1:G:28:ASP:H	1.71	0.89
1:N:25:ASN:ND2	1:N:28:ASP:H	1.71	0.89
1:A:25:ASN:ND2	1:A:28:ASP:H	1.71	0.89
1:M:75:HIS:H	1:N:47:LYS:NZ	1.71	0.89
1:C:25:ASN:ND2	1:C:28:ASP:H	1.71	0.89
1:B:25:ASN:ND2	1:B:28:ASP:H	1.71	0.89
1:D:25:ASN:ND2	1:D:28:ASP:H	1.71	0.89
1:H:25:ASN:ND2	1:H:28:ASP:H	1.71	0.88
1:M:147:PRO:HB3	1:M:203:ARG:HE	1.36	0.88
1:N:147:PRO:HB3	1:N:203:ARG:HE	1.36	0.88
1:A:147:PRO:HB3	1:A:203:ARG:HE	1.36	0.88
1:P:147:PRO:HB3	1:P:203:ARG:HE	1.36	0.88
1:K:147:PRO:HB3	1:K:203:ARG:HE	1.36	0.88
1:K:25:ASN:ND2	1:K:28:ASP:H	1.71	0.88
1:E:147:PRO:HB3	1:E:203:ARG:HE	1.36	0.88
1:C:147:PRO:HB3	1:C:203:ARG:HE	1.36	0.88
1:L:25:ASN:ND2	1:L:28:ASP:H	1.71	0.87
1:G:147:PRO:HB3	1:G:203:ARG:HE	1.36	0.87
1:I:25:ASN:ND2	1:I:28:ASP:H	1.71	0.87
1:O:25:ASN:ND2	1:O:28:ASP:H	1.71	0.87
1:M:25:ASN:ND2	1:M:28:ASP:H	1.71	0.87
1:J:25:ASN:ND2	1:J:28:ASP:H	1.71	0.87
1:B:232:GLN:HE21	1:C:227:SER:CA	1.89	0.86
1:B:228:VAL:HG23	1:C:236:ALA:CB	2.06	0.85
1:B:228:VAL:CG2	1:C:236:ALA:HB3	2.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:204:ILE:HG22	1:O:205:MSE:N	1.93	0.84
1:D:204:ILE:HG22	1:D:205:MSE:N	1.93	0.84
1:F:204:ILE:HG22	1:F:205:MSE:N	1.93	0.84
1:N:192:ARG:HG3	1:N:204:ILE:HD13	1.60	0.84
1:N:204:ILE:HG22	1:N:205:MSE:N	1.93	0.84
1:H:192:ARG:HG3	1:H:204:ILE:HD13	1.60	0.84
1:H:204:ILE:HG22	1:H:205:MSE:N	1.93	0.84
1:M:192:ARG:HG3	1:M:204:ILE:HD13	1.60	0.84
1:F:192:ARG:HG3	1:F:204:ILE:HD13	1.60	0.83
1:J:204:ILE:HG22	1:J:205:MSE:N	1.93	0.83
1:B:204:ILE:HG22	1:B:205:MSE:N	1.93	0.83
1:G:204:ILE:HG22	1:G:205:MSE:N	1.93	0.83
1:P:204:ILE:HG22	1:P:205:MSE:N	1.93	0.83
1:O:192:ARG:HG3	1:O:204:ILE:HD13	1.60	0.83
1:C:204:ILE:HG22	1:C:205:MSE:N	1.93	0.83
1:E:204:ILE:HG22	1:E:205:MSE:N	1.93	0.83
1:E:192:ARG:HG3	1:E:204:ILE:HD13	1.60	0.82
1:K:192:ARG:HG3	1:K:204:ILE:HD13	1.60	0.82
1:A:204:ILE:HG22	1:A:205:MSE:N	1.93	0.82
1:F:236:ALA:CB	1:G:228:VAL:HG23	2.07	0.82
1:P:192:ARG:HG3	1:P:204:ILE:HD13	1.60	0.82
1:K:204:ILE:HG22	1:K:205:MSE:N	1.93	0.82
1:B:192:ARG:HG3	1:B:204:ILE:HD13	1.60	0.82
1:M:204:ILE:HG22	1:M:205:MSE:N	1.93	0.82
1:G:192:ARG:HG3	1:G:204:ILE:HD13	1.60	0.82
1:A:192:ARG:HG3	1:A:204:ILE:HD13	1.60	0.82
1:L:192:ARG:HG3	1:L:204:ILE:HD13	1.60	0.82
1:G:153:ARG:HH11	1:G:153:ARG:HB2	1.45	0.82
1:E:153:ARG:HH11	1:E:153:ARG:HB2	1.45	0.82
1:D:192:ARG:HG3	1:D:204:ILE:HD13	1.60	0.81
1:C:192:ARG:HG3	1:C:204:ILE:HD13	1.60	0.81
1:I:204:ILE:HG22	1:I:205:MSE:N	1.93	0.81
1:J:192:ARG:HG3	1:J:204:ILE:HD13	1.60	0.81
1:L:204:ILE:HG22	1:L:205:MSE:N	1.93	0.81
1:O:153:ARG:HH11	1:O:153:ARG:HB2	1.45	0.81
1:I:192:ARG:HG3	1:I:204:ILE:HD13	1.60	0.81
1:H:153:ARG:HB2	1:H:153:ARG:HH11	1.45	0.81
1:J:153:ARG:HH11	1:J:153:ARG:HB2	1.45	0.81
1:D:153:ARG:HH11	1:D:153:ARG:HB2	1.45	0.81
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.45	0.81
1:B:153:ARG:HH11	1:B:153:ARG:HB2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:ARG:HH11	1:F:153:ARG:HB2	1.45	0.80
1:N:153:ARG:HB2	1:N:153:ARG:HH11	1.45	0.80
1:K:153:ARG:HB2	1:K:153:ARG:HH11	1.45	0.80
1:L:153:ARG:HH11	1:L:153:ARG:HB2	1.45	0.80
1:M:204:ILE:HG22	1:M:205:MSE:H	1.47	0.80
1:B:204:ILE:HG22	1:B:205:MSE:H	1.47	0.80
1:A:204:ILE:HG22	1:A:205:MSE:H	1.47	0.80
1:D:204:ILE:HG22	1:D:205:MSE:H	1.47	0.80
1:I:153:ARG:HB2	1:I:153:ARG:HH11	1.45	0.80
1:C:153:ARG:HB2	1:C:153:ARG:HH11	1.45	0.80
1:I:204:ILE:HG22	1:I:205:MSE:H	1.47	0.79
1:K:204:ILE:HG22	1:K:205:MSE:H	1.47	0.79
1:J:204:ILE:HG22	1:J:205:MSE:H	1.47	0.79
1:A:75:HIS:H	1:B:47:LYS:HZ2	1.31	0.79
1:M:153:ARG:HB2	1:M:153:ARG:HH11	1.45	0.79
1:P:69:PHE:CD2	1:P:95:MSE:HE3	2.18	0.79
1:P:153:ARG:HB2	1:P:153:ARG:HH11	1.45	0.79
1:C:182:GLN:HG3	1:J:12:VAL:HG12	1.65	0.78
1:N:69:PHE:CD2	1:N:95:MSE:HE3	2.18	0.78
1:D:69:PHE:CD2	1:D:95:MSE:HE3	2.18	0.78
1:H:69:PHE:CD2	1:H:95:MSE:HE3	2.19	0.78
1:N:204:ILE:HG22	1:N:205:MSE:H	1.47	0.78
1:B:69:PHE:CD2	1:B:95:MSE:HE3	2.18	0.78
1:G:204:ILE:HG22	1:G:205:MSE:H	1.47	0.78
1:M:69:PHE:CD2	1:M:95:MSE:HE3	2.19	0.78
1:E:204:ILE:HG22	1:E:205:MSE:H	1.47	0.78
1:I:69:PHE:CD2	1:I:95:MSE:HE3	2.18	0.78
1:F:204:ILE:HG22	1:F:205:MSE:H	1.47	0.78
1:F:69:PHE:CD2	1:F:95:MSE:HE3	2.18	0.78
1:H:204:ILE:HG22	1:H:205:MSE:H	1.47	0.78
1:G:69:PHE:CD2	1:G:95:MSE:HE3	2.18	0.78
1:C:204:ILE:HG22	1:C:205:MSE:H	1.47	0.77
1:E:69:PHE:CD2	1:E:95:MSE:HE3	2.19	0.77
1:C:69:PHE:CD2	1:C:95:MSE:HE3	2.18	0.77
1:A:69:PHE:CD2	1:A:95:MSE:HE3	2.18	0.77
1:B:228:VAL:HB	1:C:236:ALA:HB1	1.65	0.77
1:J:69:PHE:CD2	1:J:95:MSE:HE3	2.18	0.77
1:L:204:ILE:HG22	1:L:205:MSE:H	1.47	0.77
1:O:204:ILE:HG22	1:O:205:MSE:H	1.47	0.77
1:K:69:PHE:CD2	1:K:95:MSE:HE3	2.18	0.77
1:O:69:PHE:CD2	1:O:95:MSE:HE3	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:THR:O	1:B:237:ILE:HG13	1.85	0.76
1:P:204:ILE:HG22	1:P:205:MSE:H	1.47	0.76
1:J:233:THR:O	1:J:237:ILE:HG13	1.85	0.76
1:L:69:PHE:CD2	1:L:95:MSE:HE3	2.18	0.76
1:P:233:THR:O	1:P:237:ILE:HG13	1.85	0.76
1:H:233:THR:O	1:H:237:ILE:HG13	1.85	0.76
1:E:47:LYS:NZ	1:F:75:HIS:H	1.83	0.76
1:C:47:LYS:NZ	1:D:75:HIS:H	1.83	0.76
1:K:233:THR:O	1:K:237:ILE:HG13	1.85	0.76
1:N:233:THR:O	1:N:237:ILE:HG13	1.85	0.76
1:F:233:THR:O	1:F:237:ILE:HG13	1.85	0.76
1:M:233:THR:O	1:M:237:ILE:HG13	1.85	0.76
1:A:233:THR:O	1:A:237:ILE:HG13	1.85	0.76
1:I:233:THR:O	1:I:237:ILE:HG13	1.85	0.76
1:G:233:THR:O	1:G:237:ILE:HG13	1.85	0.76
1:F:227:SER:HA	1:G:232:GLN:HE22	1.51	0.76
1:L:124:LEU:HG	1:L:163:LEU:HD13	1.68	0.76
1:D:233:THR:O	1:D:237:ILE:HG13	1.85	0.76
1:D:130:LEU:HB2	1:D:133:MSE:HE2	1.68	0.75
1:B:124:LEU:HG	1:B:163:LEU:HD13	1.68	0.75
1:M:130:LEU:HB2	1:M:133:MSE:HE2	1.68	0.75
1:L:130:LEU:HB2	1:L:133:MSE:HE2	1.68	0.75
1:F:130:LEU:HB2	1:F:133:MSE:HE2	1.68	0.75
1:L:233:THR:O	1:L:237:ILE:HG13	1.85	0.75
1:P:130:LEU:HB2	1:P:133:MSE:HE2	1.68	0.75
1:B:130:LEU:HB2	1:B:133:MSE:HE2	1.68	0.75
1:O:124:LEU:HG	1:O:163:LEU:HD13	1.68	0.75
1:J:124:LEU:HG	1:J:163:LEU:HD13	1.68	0.75
1:I:75:HIS:H	1:J:47:LYS:NZ	1.84	0.75
1:E:233:THR:O	1:E:237:ILE:HG13	1.85	0.75
1:D:124:LEU:HG	1:D:163:LEU:HD13	1.68	0.75
1:H:130:LEU:HB2	1:H:133:MSE:HE2	1.68	0.75
1:O:233:THR:O	1:O:237:ILE:HG13	1.85	0.75
1:C:233:THR:O	1:C:237:ILE:HG13	1.85	0.75
1:I:47:LYS:NZ	1:J:75:HIS:H	1.86	0.74
1:G:130:LEU:HB2	1:G:133:MSE:HE2	1.68	0.74
1:A:124:LEU:HG	1:A:163:LEU:HD13	1.68	0.74
1:K:130:LEU:HB2	1:K:133:MSE:HE2	1.68	0.74
1:G:124:LEU:HG	1:G:163:LEU:HD13	1.68	0.74
1:I:124:LEU:HG	1:I:163:LEU:HD13	1.68	0.74
1:N:130:LEU:HB2	1:N:133:MSE:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HB2	1:A:133:MSE:HE2	1.68	0.74
1:F:124:LEU:HG	1:F:163:LEU:HD13	1.68	0.74
1:C:124:LEU:HG	1:C:163:LEU:HD13	1.68	0.74
1:O:130:LEU:HB2	1:O:133:MSE:HE2	1.68	0.74
1:I:130:LEU:HB2	1:I:133:MSE:HE2	1.68	0.74
1:M:124:LEU:HG	1:M:163:LEU:HD13	1.68	0.74
1:J:130:LEU:HB2	1:J:133:MSE:HE2	1.68	0.74
1:E:130:LEU:HB2	1:E:133:MSE:HE2	1.68	0.74
1:C:130:LEU:HB2	1:C:133:MSE:HE2	1.68	0.73
1:E:124:LEU:HG	1:E:163:LEU:HD13	1.68	0.73
1:N:124:LEU:HG	1:N:163:LEU:HD13	1.68	0.73
1:K:124:LEU:HG	1:K:163:LEU:HD13	1.68	0.73
1:P:124:LEU:HG	1:P:163:LEU:HD13	1.68	0.73
1:H:124:LEU:HG	1:H:163:LEU:HD13	1.68	0.73
1:M:47:LYS:NZ	1:N:75:HIS:H	1.86	0.73
1:M:137:ASP:OD2	1:N:105:ARG:HD3	1.88	0.73
1:B:232:GLN:HE22	1:C:227:SER:HA	1.53	0.73
1:B:69:PHE:CG	1:B:95:MSE:HE3	2.25	0.72
1:E:47:LYS:HZ2	1:F:75:HIS:H	1.36	0.72
1:K:69:PHE:CG	1:K:95:MSE:HE3	2.25	0.72
1:P:69:PHE:CG	1:P:95:MSE:HE3	2.25	0.72
1:M:69:PHE:CG	1:M:95:MSE:HE3	2.25	0.72
1:A:69:PHE:CG	1:A:95:MSE:HE3	2.25	0.72
1:N:69:PHE:CG	1:N:95:MSE:HE3	2.25	0.72
1:D:69:PHE:CG	1:D:95:MSE:HE3	2.25	0.72
1:O:69:PHE:CG	1:O:95:MSE:HE3	2.25	0.72
1:G:69:PHE:CG	1:G:95:MSE:HE3	2.25	0.72
1:C:69:PHE:CG	1:C:95:MSE:HE3	2.25	0.72
1:F:69:PHE:CG	1:F:95:MSE:HE3	2.25	0.72
1:E:69:PHE:CG	1:E:95:MSE:HE3	2.25	0.72
1:E:75:HIS:H	1:F:47:LYS:NZ	1.87	0.72
1:O:191:ILE:HG21	1:O:218:MSE:HE3	1.72	0.71
1:P:191:ILE:HG21	1:P:218:MSE:HE3	1.72	0.71
1:L:191:ILE:HG21	1:L:218:MSE:HE3	1.72	0.71
1:I:69:PHE:CG	1:I:95:MSE:HE3	2.25	0.71
1:F:236:ALA:HB2	1:G:228:VAL:HG23	1.71	0.71
1:H:69:PHE:CG	1:H:95:MSE:HE3	2.25	0.71
1:N:191:ILE:HG21	1:N:218:MSE:HE3	1.72	0.71
1:L:69:PHE:CG	1:L:95:MSE:HE3	2.25	0.71
1:O:47:LYS:NZ	1:P:75:HIS:H	1.88	0.71
1:K:75:HIS:H	1:L:47:LYS:HZ2	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:ILE:HG21	1:K:218:MSE:HE3	1.72	0.71
1:F:191:ILE:HG21	1:F:218:MSE:HE3	1.72	0.71
1:J:25:ASN:HD22	1:J:28:ASP:H	1.39	0.71
1:C:47:LYS:HZ2	1:D:75:HIS:H	1.39	0.71
1:E:191:ILE:HG21	1:E:218:MSE:HE3	1.72	0.71
1:M:191:ILE:HG21	1:M:218:MSE:HE3	1.72	0.71
1:A:75:HIS:H	1:B:47:LYS:NZ	1.89	0.71
1:H:191:ILE:HG21	1:H:218:MSE:HE3	1.72	0.71
1:G:191:ILE:HG21	1:G:218:MSE:HE3	1.72	0.70
1:J:69:PHE:CG	1:J:95:MSE:HE3	2.25	0.70
1:J:191:ILE:HG21	1:J:218:MSE:HE3	1.72	0.70
1:I:25:ASN:HD22	1:I:28:ASP:H	1.39	0.70
1:A:25:ASN:HD22	1:A:28:ASP:H	1.39	0.70
1:M:47:LYS:HZ2	1:N:75:HIS:H	1.36	0.70
1:I:191:ILE:HG21	1:I:218:MSE:HE3	1.72	0.70
1:B:229:ASP:OD1	1:C:227:SER:HB2	1.91	0.70
1:K:207:PRO:HA	1:K:218:MSE:HE1	1.74	0.70
1:A:191:ILE:HG21	1:A:218:MSE:HE3	1.72	0.70
1:G:75:HIS:H	1:H:47:LYS:NZ	1.90	0.70
1:D:191:ILE:HG21	1:D:218:MSE:HE3	1.72	0.70
1:G:25:ASN:HD22	1:G:28:ASP:H	1.39	0.70
1:A:207:PRO:HA	1:A:218:MSE:HE1	1.74	0.70
1:F:207:PRO:HA	1:F:218:MSE:HE1	1.74	0.70
1:C:207:PRO:HA	1:C:218:MSE:HE1	1.74	0.70
1:P:207:PRO:HA	1:P:218:MSE:HE1	1.74	0.69
1:I:207:PRO:HA	1:I:218:MSE:HE1	1.74	0.69
1:N:207:PRO:HA	1:N:218:MSE:HE1	1.74	0.69
1:H:207:PRO:HA	1:H:218:MSE:HE1	1.74	0.69
1:N:25:ASN:HD22	1:N:28:ASP:H	1.39	0.69
1:P:25:ASN:HD22	1:P:28:ASP:H	1.39	0.69
1:L:25:ASN:HD22	1:L:28:ASP:H	1.39	0.69
1:D:25:ASN:HD22	1:D:28:ASP:H	1.39	0.69
1:D:192:ARG:HH22	2:D:304:BMP:P	2.16	0.69
1:F:192:ARG:HH22	2:F:306:BMP:P	2.16	0.69
1:M:192:ARG:HH22	2:M:313:BMP:P	2.15	0.69
1:C:25:ASN:HD22	1:C:28:ASP:H	1.39	0.69
1:H:192:ARG:HH22	2:H:308:BMP:P	2.16	0.69
1:G:192:ARG:HH22	2:G:307:BMP:P	2.15	0.69
1:K:75:HIS:H	1:L:47:LYS:NZ	1.89	0.69
1:O:25:ASN:HD22	1:O:28:ASP:H	1.39	0.69
1:E:25:ASN:HD22	1:E:28:ASP:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ARG:HH22	2:C:303:BMP:P	2.16	0.69
1:C:191:ILE:HG21	1:C:218:MSE:HE3	1.72	0.69
1:B:191:ILE:HG21	1:B:218:MSE:HE3	1.72	0.69
1:B:228:VAL:HG23	1:C:236:ALA:HB2	1.74	0.69
1:N:192:ARG:HH22	2:N:314:BMP:P	2.16	0.69
1:K:192:ARG:HH22	2:K:311:BMP:P	2.16	0.69
1:O:204:ILE:CG2	1:O:205:MSE:H	2.06	0.69
1:M:204:ILE:CG2	1:M:205:MSE:H	2.06	0.69
1:O:207:PRO:HA	1:O:218:MSE:HE1	1.74	0.69
1:B:25:ASN:HD22	1:B:28:ASP:H	1.39	0.69
1:K:25:ASN:HD22	1:K:28:ASP:H	1.39	0.69
1:H:25:ASN:HD22	1:H:28:ASP:H	1.39	0.69
1:F:25:ASN:HD22	1:F:28:ASP:H	1.39	0.69
1:D:204:ILE:CG2	1:D:205:MSE:H	2.06	0.69
1:H:204:ILE:CG2	1:H:205:MSE:H	2.06	0.69
1:B:204:ILE:CG2	1:B:205:MSE:H	2.06	0.69
1:E:192:ARG:HH22	2:E:305:BMP:P	2.15	0.69
1:L:192:ARG:HH22	2:L:312:BMP:P	2.16	0.69
1:G:47:LYS:NZ	1:H:75:HIS:H	1.91	0.69
1:B:228:VAL:CG2	1:C:233:THR:HA	2.23	0.69
1:M:25:ASN:HD22	1:M:28:ASP:H	1.39	0.69
1:J:192:ARG:HH22	2:J:310:BMP:P	2.15	0.69
1:F:204:ILE:CG2	1:F:205:MSE:H	2.06	0.68
1:P:192:ARG:HH22	2:P:316:BMP:P	2.16	0.68
1:I:192:ARG:HH22	2:I:309:BMP:P	2.15	0.68
1:L:207:PRO:HA	1:L:218:MSE:HE1	1.74	0.68
1:B:192:ARG:HH22	2:B:302:BMP:P	2.16	0.68
1:E:207:PRO:HA	1:E:218:MSE:HE1	1.74	0.68
1:O:192:ARG:HH22	2:O:315:BMP:P	2.15	0.68
1:A:204:ILE:CG2	1:A:205:MSE:H	2.06	0.68
1:C:12:VAL:HG11	1:J:182:GLN:HG3	1.75	0.68
1:A:192:ARG:HH22	2:A:301:BMP:P	2.15	0.68
1:A:47:LYS:NZ	1:B:75:HIS:H	1.90	0.68
1:C:182:GLN:CG	1:J:12:VAL:HG12	2.22	0.68
1:C:204:ILE:CG2	1:C:205:MSE:H	2.06	0.68
1:G:207:PRO:HA	1:G:218:MSE:HE1	1.74	0.68
1:K:47:LYS:NZ	1:L:75:HIS:H	1.92	0.68
1:M:207:PRO:HA	1:M:218:MSE:HE1	1.74	0.67
1:J:207:PRO:HA	1:J:218:MSE:HE1	1.74	0.67
1:E:204:ILE:CG2	1:E:205:MSE:H	2.06	0.67
1:I:47:LYS:HZ2	1:J:75:HIS:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:HIS:H	1:F:47:LYS:HZ2	1.43	0.67
1:D:207:PRO:HA	1:D:218:MSE:HE1	1.74	0.67
1:J:204:ILE:CG2	1:J:205:MSE:H	2.06	0.67
1:K:138:LEU:O	1:K:143:MSE:HB3	1.95	0.67
1:N:204:ILE:CG2	1:N:205:MSE:H	2.06	0.67
1:L:204:ILE:CG2	1:L:205:MSE:H	2.06	0.67
1:E:138:LEU:O	1:E:143:MSE:HB3	1.95	0.67
1:P:169:SER:HB3	1:P:172:GLU:OE1	1.95	0.67
1:G:138:LEU:O	1:G:143:MSE:HB3	1.95	0.67
1:O:138:LEU:O	1:O:143:MSE:HB3	1.95	0.67
1:N:169:SER:HB3	1:N:172:GLU:OE1	1.95	0.67
1:G:204:ILE:CG2	1:G:205:MSE:H	2.06	0.67
1:P:204:ILE:CG2	1:P:205:MSE:H	2.06	0.67
1:A:218:MSE:CE	1:A:220:ILE:HD11	2.23	0.67
1:G:169:SER:HB3	1:G:172:GLU:OE1	1.95	0.67
1:K:204:ILE:CG2	1:K:205:MSE:H	2.06	0.67
1:C:138:LEU:O	1:C:143:MSE:HB3	1.95	0.67
1:B:207:PRO:HA	1:B:218:MSE:HE1	1.74	0.67
1:D:169:SER:HB3	1:D:172:GLU:OE1	1.95	0.67
1:I:204:ILE:CG2	1:I:205:MSE:H	2.06	0.67
1:M:218:MSE:CE	1:M:220:ILE:HD11	2.23	0.67
1:N:138:LEU:O	1:N:143:MSE:HB3	1.95	0.67
1:P:138:LEU:O	1:P:143:MSE:HB3	1.95	0.67
1:A:138:LEU:O	1:A:143:MSE:HB3	1.95	0.66
1:I:138:LEU:O	1:I:143:MSE:HB3	1.95	0.66
1:D:138:LEU:O	1:D:143:MSE:HB3	1.95	0.66
1:B:169:SER:HB3	1:B:172:GLU:OE1	1.95	0.66
1:E:169:SER:HB3	1:E:172:GLU:OE1	1.95	0.66
1:G:75:HIS:H	1:H:47:LYS:HZ2	1.43	0.66
1:L:138:LEU:O	1:L:143:MSE:HB3	1.95	0.66
1:C:75:HIS:H	1:D:47:LYS:NZ	1.93	0.66
1:M:138:LEU:O	1:M:143:MSE:HB3	1.95	0.66
1:K:169:SER:HB3	1:K:172:GLU:OE1	1.95	0.66
1:I:75:HIS:H	1:J:47:LYS:HZ2	1.43	0.66
1:J:138:LEU:O	1:J:143:MSE:HB3	1.95	0.66
1:O:169:SER:HB3	1:O:172:GLU:OE1	1.95	0.66
1:H:169:SER:HB3	1:H:172:GLU:OE1	1.95	0.66
1:H:98:VAL:O	1:H:126:ALA:HA	1.96	0.66
1:G:47:LYS:HZ2	1:H:75:HIS:H	1.42	0.66
1:K:98:VAL:O	1:K:126:ALA:HA	1.96	0.66
1:P:206:THR:OG1	1:P:209:GLN:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:O	1:B:143:MSE:HB3	1.95	0.66
1:C:218:MSE:CE	1:C:220:ILE:HD11	2.23	0.66
1:O:206:THR:OG1	1:O:209:GLN:HG2	1.96	0.66
1:M:98:VAL:O	1:M:126:ALA:HA	1.96	0.66
1:C:169:SER:HB3	1:C:172:GLU:OE1	1.95	0.66
1:F:206:THR:OG1	1:F:209:GLN:HG2	1.96	0.66
1:C:206:THR:OG1	1:C:209:GLN:HG2	1.96	0.66
1:K:206:THR:OG1	1:K:209:GLN:HG2	1.96	0.66
1:A:206:THR:OG1	1:A:209:GLN:HG2	1.96	0.66
1:F:98:VAL:O	1:F:126:ALA:HA	1.96	0.66
1:F:138:LEU:O	1:F:143:MSE:HB3	1.95	0.66
1:I:169:SER:HB3	1:I:172:GLU:OE1	1.95	0.65
1:H:206:THR:OG1	1:H:209:GLN:HG2	1.96	0.65
1:F:30:LEU:HD22	1:F:64:ARG:HH21	1.61	0.65
1:M:169:SER:HB3	1:M:172:GLU:OE1	1.95	0.65
1:D:204:ILE:CG2	1:D:205:MSE:N	2.60	0.65
1:C:30:LEU:HD22	1:C:64:ARG:HH21	1.61	0.65
1:I:98:VAL:O	1:I:126:ALA:HA	1.96	0.65
1:H:30:LEU:HD22	1:H:64:ARG:HH21	1.61	0.65
1:J:169:SER:HB3	1:J:172:GLU:OE1	1.95	0.65
1:A:169:SER:HB3	1:A:172:GLU:OE1	1.95	0.65
1:B:204:ILE:CG2	1:B:205:MSE:N	2.60	0.65
1:I:206:THR:OG1	1:I:209:GLN:HG2	1.96	0.65
1:H:138:LEU:O	1:H:143:MSE:HB3	1.95	0.65
1:J:30:LEU:HD22	1:J:64:ARG:HH21	1.61	0.65
1:K:218:MSE:CE	1:K:220:ILE:HD11	2.23	0.65
1:H:218:MSE:CE	1:H:220:ILE:HD11	2.23	0.65
1:F:169:SER:HB3	1:F:172:GLU:OE1	1.95	0.65
1:N:206:THR:OG1	1:N:209:GLN:HG2	1.96	0.65
1:G:98:VAL:O	1:G:126:ALA:HA	1.96	0.65
1:P:30:LEU:HD22	1:P:64:ARG:HH21	1.61	0.65
1:G:30:LEU:HD22	1:G:64:ARG:HH21	1.61	0.65
1:O:105:ARG:HD3	1:P:137:ASP:OD2	1.97	0.65
1:L:204:ILE:CG2	1:L:205:MSE:N	2.60	0.65
1:I:218:MSE:CE	1:I:220:ILE:HD11	2.23	0.65
1:P:218:MSE:CE	1:P:220:ILE:HD11	2.23	0.65
1:A:204:ILE:CG2	1:A:205:MSE:N	2.60	0.65
1:L:30:LEU:HD22	1:L:64:ARG:HH21	1.61	0.65
1:E:98:VAL:O	1:E:126:ALA:HA	1.96	0.65
1:O:204:ILE:CG2	1:O:205:MSE:N	2.60	0.65
1:M:204:ILE:CG2	1:M:205:MSE:N	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:VAL:O	1:L:126:ALA:HA	1.96	0.65
1:L:169:SER:HB3	1:L:172:GLU:OE1	1.95	0.65
1:N:98:VAL:O	1:N:126:ALA:HA	1.96	0.65
1:A:30:LEU:HD22	1:A:64:ARG:HH21	1.61	0.65
1:N:204:ILE:CG2	1:N:205:MSE:N	2.60	0.65
1:C:204:ILE:CG2	1:C:205:MSE:N	2.60	0.65
1:H:69:PHE:CD1	1:H:95:MSE:HG2	2.32	0.65
1:F:69:PHE:CD1	1:F:95:MSE:HG2	2.33	0.65
1:N:30:LEU:HD22	1:N:64:ARG:HH21	1.61	0.65
1:O:218:MSE:CE	1:O:220:ILE:HD11	2.23	0.64
1:H:204:ILE:CG2	1:H:205:MSE:N	2.60	0.64
1:P:204:ILE:CG2	1:P:205:MSE:N	2.60	0.64
1:E:30:LEU:HD22	1:E:64:ARG:HH21	1.61	0.64
1:D:30:LEU:HD22	1:D:64:ARG:HH21	1.61	0.64
1:B:206:THR:OG1	1:B:209:GLN:HG2	1.96	0.64
1:N:69:PHE:CD1	1:N:95:MSE:HG2	2.33	0.64
1:G:69:PHE:CD1	1:G:95:MSE:HG2	2.32	0.64
1:M:206:THR:OG1	1:M:209:GLN:HG2	1.96	0.64
1:J:206:THR:OG1	1:J:209:GLN:HG2	1.96	0.64
1:G:206:THR:OG1	1:G:209:GLN:HG2	1.96	0.64
1:E:69:PHE:CD1	1:E:95:MSE:HG2	2.33	0.64
1:L:69:PHE:CD1	1:L:95:MSE:HG2	2.33	0.64
1:C:98:VAL:O	1:C:126:ALA:HA	1.96	0.64
1:O:98:VAL:O	1:O:126:ALA:HA	1.96	0.64
1:B:30:LEU:HD22	1:B:64:ARG:HH21	1.61	0.64
1:E:206:THR:OG1	1:E:209:GLN:HG2	1.96	0.64
1:O:69:PHE:CD1	1:O:95:MSE:HG2	2.33	0.64
1:A:98:VAL:O	1:A:126:ALA:HA	1.96	0.64
1:K:30:LEU:HD22	1:K:64:ARG:HH21	1.61	0.64
1:P:69:PHE:CD1	1:P:95:MSE:HG2	2.33	0.64
1:G:204:ILE:CG2	1:G:205:MSE:N	2.60	0.64
1:D:69:PHE:CD1	1:D:95:MSE:HG2	2.32	0.64
1:J:98:VAL:O	1:J:126:ALA:HA	1.96	0.64
1:I:69:PHE:CD1	1:I:95:MSE:HG2	2.33	0.64
1:B:98:VAL:O	1:B:126:ALA:HA	1.96	0.64
1:D:206:THR:OG1	1:D:209:GLN:HG2	1.96	0.64
1:J:204:ILE:CG2	1:J:205:MSE:N	2.60	0.64
1:A:69:PHE:CD1	1:A:95:MSE:HG2	2.33	0.64
1:K:69:PHE:CD1	1:K:95:MSE:HG2	2.33	0.64
1:L:206:THR:OG1	1:L:209:GLN:HG2	1.96	0.64
1:B:69:PHE:CD1	1:B:95:MSE:HG2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:VAL:O	1:D:126:ALA:HA	1.96	0.64
1:F:204:ILE:CG2	1:F:205:MSE:N	2.60	0.64
1:M:69:PHE:CD1	1:M:95:MSE:HG2	2.32	0.64
1:J:69:PHE:CD1	1:J:95:MSE:HG2	2.33	0.64
1:O:30:LEU:HD22	1:O:64:ARG:HH21	1.61	0.64
1:P:98:VAL:O	1:P:126:ALA:HA	1.96	0.64
1:G:218:MSE:CE	1:G:220:ILE:HD11	2.23	0.63
1:C:69:PHE:CD1	1:C:95:MSE:HG2	2.33	0.63
1:M:30:LEU:HD22	1:M:64:ARG:HH21	1.61	0.63
1:I:30:LEU:HD22	1:I:64:ARG:HH21	1.61	0.63
1:I:137:ASP:OD2	1:J:105:ARG:HD3	1.99	0.63
1:E:218:MSE:CE	1:E:220:ILE:HD11	2.23	0.63
1:D:182:GLN:HG3	1:K:12:VAL:CG1	2.25	0.63
1:A:47:LYS:HZ2	1:B:75:HIS:H	1.48	0.62
1:D:218:MSE:CE	1:D:220:ILE:HD11	2.23	0.62
1:A:56:GLN:NE2	1:A:56:GLN:HA	2.15	0.62
1:F:227:SER:HA	1:G:232:GLN:HE21	1.60	0.62
1:D:59:ARG:HD3	1:H:28:ASP:OD1	2.00	0.62
1:H:56:GLN:HA	1:H:56:GLN:NE2	2.15	0.62
1:C:56:GLN:HA	1:C:56:GLN:NE2	2.15	0.62
1:K:94:TRP:CZ3	1:K:95:MSE:HE2	2.35	0.62
1:F:56:GLN:HA	1:F:56:GLN:NE2	2.15	0.62
1:P:56:GLN:HA	1:P:56:GLN:NE2	2.15	0.62
1:L:94:TRP:CZ3	1:L:95:MSE:HE2	2.35	0.62
1:L:218:MSE:CE	1:L:220:ILE:HD11	2.23	0.62
1:E:56:GLN:NE2	1:E:56:GLN:HA	2.15	0.62
1:N:218:MSE:CE	1:N:220:ILE:HD11	2.23	0.61
1:I:94:TRP:CZ3	1:I:95:MSE:HE2	2.35	0.61
1:F:94:TRP:CZ3	1:F:95:MSE:HE2	2.35	0.61
1:H:94:TRP:CZ3	1:H:95:MSE:HE2	2.35	0.61
1:C:75:HIS:H	1:D:47:LYS:HZ2	1.48	0.61
1:K:56:GLN:HA	1:K:56:GLN:NE2	2.15	0.61
1:D:71:ASP:OD1	1:D:97:ASN:ND2	2.34	0.61
1:N:56:GLN:NE2	1:N:56:GLN:HA	2.15	0.61
1:N:94:TRP:CZ3	1:N:95:MSE:HE2	2.35	0.61
1:C:71:ASP:OD1	1:C:97:ASN:ND2	2.33	0.61
1:G:56:GLN:HA	1:G:56:GLN:NE2	2.15	0.61
1:B:71:ASP:OD1	1:B:97:ASN:ND2	2.34	0.61
1:O:71:ASP:OD1	1:O:97:ASN:ND2	2.34	0.61
1:F:71:ASP:OD1	1:F:97:ASN:ND2	2.34	0.61
1:O:56:GLN:NE2	1:O:56:GLN:HA	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:GLN:NE2	1:I:56:GLN:HA	2.15	0.61
1:F:236:ALA:HB1	1:G:228:VAL:CB	2.30	0.61
1:E:94:TRP:CZ3	1:E:95:MSE:HE2	2.35	0.61
1:O:94:TRP:CZ3	1:O:95:MSE:HE2	2.35	0.61
1:A:71:ASP:OD1	1:A:97:ASN:ND2	2.34	0.61
1:M:94:TRP:CZ3	1:M:95:MSE:HE2	2.35	0.61
1:B:56:GLN:NE2	1:B:56:GLN:HA	2.15	0.61
1:K:71:ASP:OD1	1:K:97:ASN:ND2	2.34	0.61
1:C:105:ARG:HD3	1:D:137:ASP:OD2	2.00	0.61
1:M:71:ASP:OD1	1:M:97:ASN:ND2	2.34	0.61
1:M:56:GLN:HA	1:M:56:GLN:NE2	2.15	0.61
1:G:94:TRP:CZ3	1:G:95:MSE:HE2	2.35	0.61
1:J:94:TRP:CZ3	1:J:95:MSE:HE2	2.35	0.61
1:P:94:TRP:CZ3	1:P:95:MSE:HE2	2.35	0.61
1:H:71:ASP:OD1	1:H:97:ASN:ND2	2.34	0.61
1:D:94:TRP:CZ3	1:D:95:MSE:HE2	2.35	0.61
1:B:94:TRP:CZ3	1:B:95:MSE:HE2	2.35	0.61
1:O:47:LYS:HZ2	1:P:75:HIS:H	1.49	0.61
1:C:94:TRP:CZ3	1:C:95:MSE:HE2	2.35	0.61
1:A:94:TRP:CZ3	1:A:95:MSE:HE2	2.35	0.61
1:D:56:GLN:HA	1:D:56:GLN:NE2	2.15	0.61
1:F:236:ALA:HB1	1:G:228:VAL:HB	1.83	0.60
1:P:71:ASP:OD1	1:P:97:ASN:ND2	2.34	0.60
1:J:56:GLN:NE2	1:J:56:GLN:HA	2.15	0.60
1:I:71:ASP:OD1	1:I:97:ASN:ND2	2.33	0.60
1:L:56:GLN:HA	1:L:56:GLN:NE2	2.15	0.60
1:B:218:MSE:CE	1:B:220:ILE:HD11	2.23	0.60
1:J:218:MSE:CE	1:J:220:ILE:HD11	2.23	0.60
1:L:71:ASP:OD1	1:L:97:ASN:ND2	2.34	0.60
1:N:71:ASP:OD1	1:N:97:ASN:ND2	2.33	0.60
1:H:192:ARG:HB2	1:H:204:ILE:HG21	1.84	0.60
1:J:71:ASP:OD1	1:J:97:ASN:ND2	2.34	0.60
1:E:71:ASP:OD1	1:E:97:ASN:ND2	2.34	0.60
1:G:71:ASP:OD1	1:G:97:ASN:ND2	2.34	0.60
1:A:192:ARG:HB2	1:A:204:ILE:HG21	1.84	0.60
1:M:130:LEU:HD13	1:N:76:ASP:C	2.22	0.60
1:C:192:ARG:HB2	1:C:204:ILE:HG21	1.84	0.60
1:L:192:ARG:HB2	1:L:204:ILE:HG21	1.84	0.60
1:P:192:ARG:HB2	1:P:204:ILE:HG21	1.84	0.60
1:K:47:LYS:HZ3	1:L:75:HIS:H	1.50	0.60
1:J:192:ARG:HB2	1:J:204:ILE:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:ARG:HB2	1:F:204:ILE:HG21	1.84	0.59
1:B:228:VAL:HG21	1:C:233:THR:HA	1.83	0.59
1:B:169:SER:HB2	1:B:203:ARG:HH11	1.68	0.59
1:I:192:ARG:HB2	1:I:204:ILE:HG21	1.84	0.59
1:E:105:ARG:HD3	1:F:137:ASP:OD2	2.01	0.59
1:D:169:SER:HB2	1:D:203:ARG:HH11	1.68	0.59
1:N:169:SER:HB2	1:N:203:ARG:HH11	1.68	0.59
1:N:175:ARG:O	1:N:179:VAL:HG23	2.03	0.59
1:F:236:ALA:HB2	1:G:228:VAL:CG2	2.26	0.59
1:F:218:MSE:CE	1:F:220:ILE:HD11	2.23	0.59
1:A:169:SER:HB2	1:A:203:ARG:HH11	1.68	0.59
1:K:204:ILE:CG2	1:K:205:MSE:N	2.60	0.59
1:F:175:ARG:O	1:F:179:VAL:HG23	2.03	0.59
1:G:175:ARG:O	1:G:179:VAL:HG23	2.03	0.59
1:O:169:SER:HB2	1:O:203:ARG:HH11	1.68	0.59
1:K:192:ARG:HB2	1:K:204:ILE:HG21	1.84	0.59
1:E:175:ARG:O	1:E:179:VAL:HG23	2.03	0.59
1:J:175:ARG:O	1:J:179:VAL:HG23	2.03	0.59
1:C:169:SER:HB2	1:C:203:ARG:HH11	1.67	0.59
1:O:192:ARG:HB2	1:O:204:ILE:HG21	1.84	0.59
1:D:192:ARG:HB2	1:D:204:ILE:HG21	1.84	0.59
1:A:175:ARG:O	1:A:179:VAL:HG23	2.03	0.59
1:H:175:ARG:O	1:H:179:VAL:HG23	2.03	0.59
1:C:175:ARG:O	1:C:179:VAL:HG23	2.03	0.59
1:M:192:ARG:HB2	1:M:204:ILE:HG21	1.84	0.59
1:B:192:ARG:HB2	1:B:204:ILE:HG21	1.84	0.59
1:K:137:ASP:OD2	1:L:105:ARG:HD3	2.03	0.59
1:A:137:ASP:OD2	1:B:105:ARG:HD3	2.03	0.59
1:K:175:ARG:O	1:K:179:VAL:HG23	2.03	0.59
1:L:175:ARG:O	1:L:179:VAL:HG23	2.03	0.58
1:B:228:VAL:CB	1:C:236:ALA:HB1	2.31	0.58
1:I:169:SER:HB2	1:I:203:ARG:HH11	1.68	0.58
1:K:169:SER:HB2	1:K:203:ARG:HH11	1.68	0.58
1:M:169:SER:HB2	1:M:203:ARG:HH11	1.68	0.58
1:A:234:LEU:HD13	1:A:238:ASN:HD21	1.69	0.58
1:P:175:ARG:O	1:P:179:VAL:HG23	2.03	0.58
1:M:175:ARG:O	1:M:179:VAL:HG23	2.03	0.58
1:C:234:LEU:HD13	1:C:238:ASN:HD21	1.69	0.58
1:D:234:LEU:HD13	1:D:238:ASN:HD21	1.69	0.58
1:F:94:TRP:HZ3	1:F:95:MSE:HE2	1.68	0.58
1:L:94:TRP:HZ3	1:L:95:MSE:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HD13	1:B:238:ASN:HD21	1.69	0.58
1:I:175:ARG:O	1:I:179:VAL:HG23	2.03	0.58
1:C:191:ILE:HG21	1:C:218:MSE:CE	2.34	0.58
1:L:169:SER:HB2	1:L:203:ARG:HH11	1.67	0.58
1:M:132:SER:OG	1:N:78:PRO:HD3	2.04	0.58
1:C:94:TRP:HZ3	1:C:95:MSE:HE2	1.68	0.58
1:O:175:ARG:O	1:O:179:VAL:HG23	2.03	0.58
1:A:191:ILE:HG21	1:A:218:MSE:CE	2.34	0.58
1:J:169:SER:HB2	1:J:203:ARG:HH11	1.68	0.58
1:F:169:SER:HB2	1:F:203:ARG:HH11	1.68	0.58
1:N:192:ARG:HB2	1:N:204:ILE:HG21	1.84	0.58
1:H:94:TRP:HZ3	1:H:95:MSE:HE2	1.68	0.58
1:M:170:ALA:HA	1:M:188:THR:HG21	1.86	0.58
1:K:191:ILE:HG21	1:K:218:MSE:CE	2.34	0.58
1:I:191:ILE:HG21	1:I:218:MSE:CE	2.34	0.58
1:H:169:SER:HB2	1:H:203:ARG:HH11	1.67	0.58
1:G:192:ARG:HB2	1:G:204:ILE:HG21	1.84	0.58
1:E:170:ALA:HA	1:E:188:THR:HG21	1.86	0.58
1:B:170:ALA:HA	1:B:188:THR:HG21	1.86	0.58
1:N:94:TRP:HZ3	1:N:95:MSE:HE2	1.68	0.58
1:D:175:ARG:O	1:D:179:VAL:HG23	2.03	0.58
1:B:175:ARG:O	1:B:179:VAL:HG23	2.03	0.58
1:C:177:LYS:HE3	1:C:182:GLN:HA	1.86	0.58
1:J:177:LYS:HE3	1:J:182:GLN:HA	1.86	0.58
1:M:234:LEU:HD13	1:M:238:ASN:HD21	1.69	0.58
1:G:234:LEU:HD13	1:G:238:ASN:HD21	1.69	0.58
1:O:234:LEU:HD13	1:O:238:ASN:HD21	1.69	0.58
1:I:234:LEU:HD13	1:I:238:ASN:HD21	1.69	0.58
1:M:94:TRP:HZ3	1:M:95:MSE:HE2	1.68	0.57
1:A:94:TRP:HZ3	1:A:95:MSE:HE2	1.68	0.57
1:N:234:LEU:HD13	1:N:238:ASN:HD21	1.69	0.57
1:F:234:LEU:HD13	1:F:238:ASN:HD21	1.69	0.57
1:E:234:LEU:HD13	1:E:238:ASN:HD21	1.69	0.57
1:D:170:ALA:HA	1:D:188:THR:HG21	1.86	0.57
1:E:192:ARG:HB2	1:E:204:ILE:HG21	1.84	0.57
1:B:150:TYR:CE1	1:B:154:LEU:HD11	2.40	0.57
1:G:170:ALA:HA	1:G:188:THR:HG21	1.86	0.57
1:G:169:SER:HB2	1:G:203:ARG:HH11	1.68	0.57
1:E:94:TRP:HZ3	1:E:95:MSE:HE2	1.68	0.57
1:J:94:TRP:HZ3	1:J:95:MSE:HE2	1.68	0.57
1:E:177:LYS:HE3	1:E:182:GLN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:150:TYR:CE1	1:N:154:LEU:HD11	2.40	0.57
1:J:150:TYR:CE1	1:J:154:LEU:HD11	2.39	0.57
1:D:150:TYR:CE1	1:D:154:LEU:HD11	2.40	0.57
1:J:170:ALA:HA	1:J:188:THR:HG21	1.86	0.57
1:B:191:ILE:HG21	1:B:218:MSE:CE	2.34	0.57
1:P:169:SER:HB2	1:P:203:ARG:HH11	1.68	0.57
1:E:169:SER:HB2	1:E:203:ARG:HH11	1.68	0.57
1:C:124:LEU:CG	1:C:163:LEU:HD13	2.35	0.57
1:N:124:LEU:CG	1:N:163:LEU:HD13	2.35	0.57
1:P:234:LEU:HD13	1:P:238:ASN:HD21	1.68	0.57
1:J:234:LEU:HD13	1:J:238:ASN:HD21	1.69	0.57
1:O:170:ALA:HA	1:O:188:THR:HG21	1.86	0.57
1:G:191:ILE:HG21	1:G:218:MSE:CE	2.34	0.57
1:K:177:LYS:HE3	1:K:182:GLN:HA	1.87	0.57
1:K:94:TRP:HZ3	1:K:95:MSE:HE2	1.68	0.57
1:L:124:LEU:CG	1:L:163:LEU:HD13	2.35	0.57
1:L:170:ALA:HA	1:L:188:THR:HG21	1.86	0.57
1:A:177:LYS:HE3	1:A:182:GLN:HA	1.86	0.57
1:I:94:TRP:HZ3	1:I:95:MSE:HE2	1.68	0.57
1:M:150:TYR:CE1	1:M:154:LEU:HD11	2.40	0.57
1:G:177:LYS:HE3	1:G:182:GLN:HA	1.86	0.57
1:A:170:ALA:HA	1:A:188:THR:HG21	1.86	0.57
1:I:177:LYS:HE3	1:I:182:GLN:HA	1.86	0.57
1:K:150:TYR:CE1	1:K:154:LEU:HD11	2.40	0.57
1:O:191:ILE:HG21	1:O:218:MSE:CE	2.34	0.57
1:P:191:ILE:HG21	1:P:218:MSE:CE	2.34	0.57
1:N:191:ILE:HG21	1:N:218:MSE:CE	2.34	0.57
1:E:191:ILE:HG21	1:E:218:MSE:CE	2.34	0.57
1:G:94:TRP:HZ3	1:G:95:MSE:HE2	1.68	0.57
1:O:94:TRP:HZ3	1:O:95:MSE:HE2	1.68	0.57
1:F:124:LEU:CG	1:F:163:LEU:HD13	2.35	0.57
1:A:138:LEU:HB3	1:A:143:MSE:HG2	1.87	0.57
1:L:177:LYS:HE3	1:L:182:GLN:HA	1.86	0.57
1:H:234:LEU:HD13	1:H:238:ASN:HD21	1.69	0.57
1:C:194:GLN:HG3	1:C:194:GLN:O	2.05	0.57
1:A:124:LEU:CG	1:A:163:LEU:HD13	2.35	0.57
1:G:138:LEU:HB3	1:G:143:MSE:HG2	1.87	0.57
1:P:138:LEU:HB3	1:P:143:MSE:HG2	1.87	0.57
1:M:138:LEU:HB3	1:M:143:MSE:HG2	1.87	0.57
1:L:234:LEU:HD13	1:L:238:ASN:HD21	1.69	0.57
1:I:150:TYR:CE1	1:I:154:LEU:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLN:HG3	1:A:194:GLN:O	2.05	0.57
1:H:194:GLN:HG3	1:H:194:GLN:O	2.05	0.57
1:K:234:LEU:HD13	1:K:238:ASN:HD21	1.69	0.57
1:E:150:TYR:CE1	1:E:154:LEU:HD11	2.40	0.57
1:K:170:ALA:HA	1:K:188:THR:HG21	1.86	0.57
1:H:191:ILE:HG21	1:H:218:MSE:CE	2.34	0.57
1:E:138:LEU:HB3	1:E:143:MSE:HG2	1.87	0.57
1:C:138:LEU:HB3	1:C:143:MSE:HG2	1.87	0.57
1:N:138:LEU:HB3	1:N:143:MSE:HG2	1.87	0.57
1:N:177:LYS:HE3	1:N:182:GLN:HA	1.87	0.57
1:C:150:TYR:CE1	1:C:154:LEU:HD11	2.39	0.57
1:M:194:GLN:O	1:M:194:GLN:HG3	2.05	0.57
1:B:177:LYS:HE3	1:B:182:GLN:HA	1.86	0.57
1:F:150:TYR:CE1	1:F:154:LEU:HD11	2.40	0.57
1:F:191:ILE:HG21	1:F:218:MSE:CE	2.34	0.57
1:O:124:LEU:CG	1:O:163:LEU:HD13	2.35	0.57
1:M:124:LEU:CG	1:M:163:LEU:HD13	2.35	0.57
1:P:194:GLN:HG3	1:P:194:GLN:O	2.05	0.57
1:H:150:TYR:CE1	1:H:154:LEU:HD11	2.39	0.57
1:F:194:GLN:O	1:F:194:GLN:HG3	2.05	0.57
1:O:177:LYS:HE3	1:O:182:GLN:HA	1.86	0.56
1:O:150:TYR:CE1	1:O:154:LEU:HD11	2.40	0.56
1:P:150:TYR:CE1	1:P:154:LEU:HD11	2.40	0.56
1:M:191:ILE:HG21	1:M:218:MSE:CE	2.34	0.56
1:P:94:TRP:HZ3	1:P:95:MSE:HE2	1.68	0.56
1:I:194:GLN:O	1:I:194:GLN:HG3	2.05	0.56
1:K:194:GLN:O	1:K:194:GLN:HG3	2.05	0.56
1:E:137:ASP:OD2	1:F:105:ARG:HD3	2.04	0.56
1:L:191:ILE:HG21	1:L:218:MSE:CE	2.34	0.56
1:J:191:ILE:HG21	1:J:218:MSE:CE	2.34	0.56
1:K:124:LEU:CG	1:K:163:LEU:HD13	2.35	0.56
1:D:194:GLN:HG3	1:D:194:GLN:O	2.05	0.56
1:I:170:ALA:HA	1:I:188:THR:HG21	1.86	0.56
1:N:170:ALA:HA	1:N:188:THR:HG21	1.86	0.56
1:C:170:ALA:HA	1:C:188:THR:HG21	1.86	0.56
1:B:194:GLN:HG3	1:B:194:GLN:O	2.05	0.56
1:L:150:TYR:CE1	1:L:154:LEU:HD11	2.40	0.56
1:K:192:ARG:HD2	1:K:198:ALA:HA	1.88	0.56
1:B:94:TRP:HZ3	1:B:95:MSE:HE2	1.68	0.56
1:G:150:TYR:CE1	1:G:154:LEU:HD11	2.40	0.56
1:D:94:TRP:HZ3	1:D:95:MSE:HE2	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:LEU:CG	1:I:163:LEU:HD13	2.35	0.56
1:O:138:LEU:HB3	1:O:143:MSE:HG2	1.87	0.56
1:B:138:LEU:HB3	1:B:143:MSE:HG2	1.87	0.56
1:H:170:ALA:HA	1:H:188:THR:HG21	1.86	0.56
1:P:177:LYS:HE3	1:P:182:GLN:HA	1.86	0.56
1:P:124:LEU:CG	1:P:163:LEU:HD13	2.35	0.56
1:A:150:TYR:CE1	1:A:154:LEU:HD11	2.40	0.56
1:D:191:ILE:HG21	1:D:218:MSE:CE	2.34	0.56
1:D:177:LYS:HE3	1:D:182:GLN:HA	1.86	0.56
1:I:138:LEU:HB3	1:I:143:MSE:HG2	1.87	0.56
1:M:177:LYS:HE3	1:M:182:GLN:HA	1.86	0.56
1:I:192:ARG:HD2	1:I:198:ALA:HA	1.88	0.56
1:K:138:LEU:HB3	1:K:143:MSE:HG2	1.87	0.56
1:D:138:LEU:HB3	1:D:143:MSE:HG2	1.87	0.56
1:J:194:GLN:O	1:J:194:GLN:HG3	2.05	0.56
1:C:192:ARG:HD2	1:C:198:ALA:HA	1.88	0.56
1:J:138:LEU:HB3	1:J:143:MSE:HG2	1.87	0.56
1:G:173:ALA:O	1:G:177:LYS:HB2	2.06	0.56
1:F:170:ALA:HA	1:F:188:THR:HG21	1.86	0.56
1:L:194:GLN:HG3	1:L:194:GLN:O	2.05	0.56
1:N:192:ARG:HD2	1:N:198:ALA:HA	1.88	0.56
1:G:192:ARG:HD2	1:G:198:ALA:HA	1.88	0.56
1:E:192:ARG:HD2	1:E:198:ALA:HA	1.88	0.56
1:L:138:LEU:HB3	1:L:143:MSE:HG2	1.87	0.56
1:F:177:LYS:HE3	1:F:182:GLN:HA	1.86	0.56
1:N:194:GLN:HG3	1:N:194:GLN:O	2.05	0.56
1:H:138:LEU:HB3	1:H:143:MSE:HG2	1.87	0.55
1:M:192:ARG:HD2	1:M:198:ALA:HA	1.88	0.55
1:A:192:ARG:HD2	1:A:198:ALA:HA	1.88	0.55
1:J:124:LEU:CG	1:J:163:LEU:HD13	2.35	0.55
1:G:137:ASP:OD2	1:H:105:ARG:HD3	2.05	0.55
1:E:194:GLN:HG3	1:E:194:GLN:O	2.05	0.55
1:H:177:LYS:HE3	1:H:182:GLN:HA	1.86	0.55
1:J:192:ARG:HD2	1:J:198:ALA:HA	1.88	0.55
1:P:171:GLN:HG2	1:P:205:MSE:CE	2.37	0.55
1:E:173:ALA:O	1:E:177:LYS:HB2	2.06	0.55
1:B:173:ALA:O	1:B:177:LYS:HB2	2.06	0.55
1:M:173:ALA:O	1:M:177:LYS:HB2	2.06	0.55
1:O:194:GLN:O	1:O:194:GLN:HG3	2.05	0.55
1:P:170:ALA:HA	1:P:188:THR:HG21	1.86	0.55
1:E:171:GLN:HG2	1:E:205:MSE:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:ALA:O	1:N:177:LYS:HB2	2.06	0.55
1:O:192:ARG:HD2	1:O:198:ALA:HA	1.88	0.55
1:K:171:GLN:HG2	1:K:205:MSE:CE	2.37	0.55
1:L:192:ARG:HD2	1:L:198:ALA:HA	1.88	0.55
1:B:124:LEU:CG	1:B:163:LEU:HD13	2.35	0.55
1:F:138:LEU:HB3	1:F:143:MSE:HG2	1.87	0.55
1:G:194:GLN:HG3	1:G:194:GLN:O	2.05	0.55
1:D:173:ALA:O	1:D:177:LYS:HB2	2.06	0.55
1:H:192:ARG:HD2	1:H:198:ALA:HA	1.88	0.55
1:I:171:GLN:HG2	1:I:205:MSE:CE	2.37	0.55
1:D:192:ARG:HD2	1:D:198:ALA:HA	1.88	0.55
1:N:171:GLN:HG2	1:N:205:MSE:CE	2.37	0.55
1:G:171:GLN:HG2	1:G:205:MSE:CE	2.37	0.55
1:A:171:GLN:HG2	1:A:205:MSE:CE	2.37	0.55
1:I:105:ARG:HD3	1:J:137:ASP:OD2	2.06	0.55
1:F:192:ARG:HD2	1:F:198:ALA:HA	1.88	0.55
1:L:173:ALA:O	1:L:177:LYS:HB2	2.06	0.55
1:F:227:SER:CB	1:G:232:GLN:HE21	2.19	0.55
1:H:171:GLN:HG2	1:H:205:MSE:CE	2.37	0.55
1:C:171:GLN:HG2	1:C:205:MSE:CE	2.37	0.55
1:E:124:LEU:CG	1:E:163:LEU:HD13	2.35	0.55
1:J:173:ALA:O	1:J:177:LYS:HB2	2.06	0.55
1:A:173:ALA:O	1:A:177:LYS:HB2	2.06	0.55
1:N:125:ILE:HG23	1:N:165:GLY:C	2.28	0.55
1:C:173:ALA:O	1:C:177:LYS:HB2	2.06	0.54
1:O:171:GLN:HG2	1:O:205:MSE:CE	2.37	0.54
1:J:171:GLN:HG2	1:J:205:MSE:CE	2.37	0.54
1:F:173:ALA:O	1:F:177:LYS:HB2	2.06	0.54
1:A:127:VAL:HA	1:A:167:VAL:HB	1.89	0.54
1:L:125:ILE:HG23	1:L:165:GLY:C	2.28	0.54
1:B:228:VAL:CG2	1:C:236:ALA:HB1	2.36	0.54
1:A:125:ILE:HG23	1:A:165:GLY:C	2.28	0.54
1:L:127:VAL:HA	1:L:167:VAL:HB	1.89	0.54
1:P:125:ILE:HG23	1:P:165:GLY:C	2.28	0.54
1:D:205:MSE:HG3	1:D:209:GLN:CD	2.28	0.54
1:F:171:GLN:HG2	1:F:205:MSE:CE	2.37	0.54
1:M:171:GLN:HG2	1:M:205:MSE:CE	2.37	0.54
1:O:173:ALA:O	1:O:177:LYS:HB2	2.06	0.54
1:P:127:VAL:HA	1:P:167:VAL:HB	1.89	0.54
1:M:127:VAL:HA	1:M:167:VAL:HB	1.89	0.54
1:K:127:VAL:HA	1:K:167:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:VAL:HA	1:I:167:VAL:HB	1.89	0.54
1:B:171:GLN:HG2	1:B:205:MSE:CE	2.37	0.54
1:B:192:ARG:HD2	1:B:198:ALA:HA	1.88	0.54
1:B:205:MSE:HG3	1:B:209:GLN:CD	2.28	0.54
1:G:205:MSE:HG3	1:G:209:GLN:CD	2.28	0.54
1:C:205:MSE:HG3	1:C:209:GLN:CD	2.28	0.54
1:I:173:ALA:O	1:I:177:LYS:HB2	2.06	0.54
1:N:127:VAL:HA	1:N:167:VAL:HB	1.89	0.54
1:B:127:VAL:HA	1:B:167:VAL:HB	1.89	0.54
1:D:171:GLN:HG2	1:D:205:MSE:CE	2.37	0.54
1:P:192:ARG:HD2	1:P:198:ALA:HA	1.88	0.54
1:E:205:MSE:HG3	1:E:209:GLN:CD	2.28	0.54
1:A:205:MSE:HG3	1:A:209:GLN:CD	2.28	0.54
1:P:173:ALA:O	1:P:177:LYS:HB2	2.06	0.54
1:H:173:ALA:O	1:H:177:LYS:HB2	2.06	0.54
1:C:127:VAL:HA	1:C:167:VAL:HB	1.90	0.54
1:F:205:MSE:HG3	1:F:209:GLN:CD	2.28	0.54
1:E:204:ILE:CG2	1:E:205:MSE:N	2.60	0.54
1:L:171:GLN:HG2	1:L:205:MSE:CE	2.37	0.54
1:I:205:MSE:HG3	1:I:209:GLN:CD	2.28	0.54
1:D:124:LEU:CG	1:D:163:LEU:HD13	2.35	0.54
1:G:124:LEU:CG	1:G:163:LEU:HD13	2.35	0.54
1:B:125:ILE:HG23	1:B:165:GLY:C	2.28	0.54
1:G:125:ILE:HG23	1:G:165:GLY:C	2.28	0.54
1:J:125:ILE:HG23	1:J:165:GLY:C	2.28	0.54
1:I:207:PRO:CA	1:I:218:MSE:HE1	2.38	0.54
1:M:207:PRO:CA	1:M:218:MSE:HE1	2.38	0.54
1:J:205:MSE:HG3	1:J:209:GLN:CD	2.28	0.54
1:C:125:ILE:HG23	1:C:165:GLY:C	2.28	0.54
1:D:127:VAL:HA	1:D:167:VAL:HB	1.89	0.54
1:D:125:ILE:HG23	1:D:165:GLY:C	2.28	0.54
1:N:205:MSE:HG3	1:N:209:GLN:CD	2.28	0.54
1:K:205:MSE:HG3	1:K:209:GLN:CD	2.28	0.54
1:J:127:VAL:HA	1:J:167:VAL:HB	1.90	0.54
1:H:127:VAL:HA	1:H:167:VAL:HB	1.89	0.54
1:F:125:ILE:HG23	1:F:165:GLY:C	2.28	0.54
1:O:25:ASN:HD22	1:O:28:ASP:CB	2.16	0.54
1:H:147:PRO:HB3	1:H:203:ARG:NE	2.17	0.54
1:E:125:ILE:HG23	1:E:165:GLY:C	2.28	0.54
1:B:232:GLN:HE21	1:C:227:SER:CB	2.20	0.54
1:E:207:PRO:CA	1:E:218:MSE:HE1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:SER:CA	1:G:232:GLN:NE2	2.64	0.54
1:H:205:MSE:HG3	1:H:209:GLN:CD	2.28	0.54
1:P:205:MSE:HG3	1:P:209:GLN:CD	2.28	0.54
1:M:125:ILE:HG23	1:M:165:GLY:C	2.28	0.54
1:G:127:VAL:HA	1:G:167:VAL:HB	1.89	0.54
1:D:12:VAL:HG11	1:K:182:GLN:CG	2.27	0.53
1:H:124:LEU:CG	1:H:163:LEU:HD13	2.35	0.53
1:I:234:LEU:HD13	1:I:238:ASN:ND2	2.24	0.53
1:P:234:LEU:HD13	1:P:238:ASN:ND2	2.24	0.53
1:I:125:ILE:HG23	1:I:165:GLY:C	2.28	0.53
1:G:207:PRO:CA	1:G:218:MSE:HE1	2.38	0.53
1:K:173:ALA:O	1:K:177:LYS:HB2	2.06	0.53
1:C:25:ASN:HD22	1:C:28:ASP:CB	2.16	0.53
1:G:234:LEU:HD13	1:G:238:ASN:ND2	2.24	0.53
1:N:234:LEU:HD13	1:N:238:ASN:ND2	2.24	0.53
1:E:234:LEU:HD13	1:E:238:ASN:ND2	2.24	0.53
1:H:125:ILE:HG23	1:H:165:GLY:C	2.28	0.53
1:F:127:VAL:HA	1:F:167:VAL:HB	1.89	0.53
1:O:127:VAL:HA	1:O:167:VAL:HB	1.89	0.53
1:G:221:GLY:HA3	2:G:307:BMP:OP3	2.09	0.53
1:M:234:LEU:HD13	1:M:238:ASN:ND2	2.24	0.53
1:K:234:LEU:HD13	1:K:238:ASN:ND2	2.24	0.53
1:I:224:VAL:O	1:I:230:PRO:HB3	2.09	0.53
1:N:25:ASN:HD22	1:N:28:ASP:CB	2.16	0.53
1:M:205:MSE:HG3	1:M:209:GLN:CD	2.28	0.53
1:E:221:GLY:HA3	2:E:305:BMP:OP3	2.09	0.53
1:C:207:PRO:CA	1:C:218:MSE:HE1	2.38	0.53
1:C:224:VAL:O	1:C:230:PRO:HB3	2.09	0.53
1:O:205:MSE:HG3	1:O:209:GLN:CD	2.28	0.53
1:L:205:MSE:HG3	1:L:209:GLN:CD	2.28	0.53
1:O:125:ILE:HG23	1:O:165:GLY:C	2.28	0.53
1:P:82:ALA:HB1	1:P:113:ALA:HB2	1.91	0.53
1:P:224:VAL:O	1:P:230:PRO:HB3	2.09	0.53
1:A:224:VAL:O	1:A:230:PRO:HB3	2.09	0.53
1:D:207:PRO:CA	1:D:218:MSE:HE1	2.38	0.53
1:B:207:PRO:CA	1:B:218:MSE:HE1	2.38	0.53
1:N:221:GLY:HA3	2:N:314:BMP:OP3	2.09	0.53
1:O:75:HIS:H	1:P:47:LYS:NZ	2.07	0.53
1:N:224:VAL:O	1:N:230:PRO:HB3	2.09	0.53
1:M:224:VAL:O	1:M:230:PRO:HB3	2.09	0.53
1:L:221:GLY:HA3	2:L:312:BMP:OP3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:234:LEU:HD13	1:O:238:ASN:ND2	2.24	0.53
1:F:234:LEU:HD13	1:F:238:ASN:ND2	2.24	0.53
1:F:221:GLY:HA3	2:F:306:BMP:OP3	2.09	0.53
1:H:221:GLY:HA3	2:H:308:BMP:OP3	2.09	0.53
1:I:221:GLY:HA3	2:I:309:BMP:OP3	2.09	0.53
1:E:127:VAL:HA	1:E:167:VAL:HB	1.89	0.53
1:O:77:ILE:HG22	1:P:132:SER:HB3	1.90	0.53
1:K:224:VAL:O	1:K:230:PRO:HB3	2.09	0.53
1:J:207:PRO:CA	1:J:218:MSE:HE1	2.38	0.53
1:J:221:GLY:HA3	2:J:310:BMP:OP3	2.09	0.53
1:L:73:LYS:H	1:L:97:ASN:HB3	1.74	0.53
1:M:105:ARG:HH22	1:N:200:ASP:HA	1.74	0.53
1:E:82:ALA:HB1	1:E:113:ALA:HB2	1.91	0.53
1:K:207:PRO:CA	1:K:218:MSE:HE1	2.38	0.53
1:P:207:PRO:CA	1:P:218:MSE:HE1	2.38	0.53
1:C:221:GLY:HA3	2:C:303:BMP:OP3	2.09	0.53
1:O:124:LEU:HG	1:O:163:LEU:CD1	2.39	0.53
1:J:73:LYS:H	1:J:97:ASN:HB3	1.74	0.53
1:H:234:LEU:HD13	1:H:238:ASN:ND2	2.24	0.53
1:K:125:ILE:HG23	1:K:165:GLY:C	2.28	0.53
1:A:105:ARG:HD3	1:B:137:ASP:OD2	2.09	0.53
1:G:82:ALA:HB1	1:G:113:ALA:HB2	1.91	0.53
1:G:224:VAL:O	1:G:230:PRO:HB3	2.09	0.52
1:B:224:VAL:O	1:B:230:PRO:HB3	2.09	0.52
1:A:25:ASN:HD22	1:A:28:ASP:CB	2.16	0.52
1:O:221:GLY:HA3	2:O:315:BMP:OP3	2.09	0.52
1:M:221:GLY:HA3	2:M:313:BMP:OP3	2.09	0.52
1:D:234:LEU:HD13	1:D:238:ASN:ND2	2.24	0.52
1:H:82:ALA:HB1	1:H:113:ALA:HB2	1.91	0.52
1:A:207:PRO:CA	1:A:218:MSE:HE1	2.38	0.52
1:F:224:VAL:O	1:F:230:PRO:HB3	2.09	0.52
1:D:221:GLY:HA3	2:D:304:BMP:OP3	2.09	0.52
1:B:73:LYS:H	1:B:97:ASN:HB3	1.74	0.52
1:F:73:LYS:H	1:F:97:ASN:HB3	1.74	0.52
1:D:82:ALA:HB1	1:D:113:ALA:HB2	1.91	0.52
1:A:221:GLY:HA3	2:A:301:BMP:OP3	2.09	0.52
1:N:124:LEU:HG	1:N:163:LEU:CD1	2.39	0.52
1:M:73:LYS:H	1:M:97:ASN:HB3	1.74	0.52
1:I:82:ALA:HB1	1:I:113:ALA:HB2	1.91	0.52
1:E:25:ASN:HD22	1:E:28:ASP:CB	2.16	0.52
1:D:73:LYS:H	1:D:97:ASN:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:73:LYS:H	1:O:97:ASN:HB3	1.74	0.52
1:A:73:LYS:H	1:A:97:ASN:HB3	1.74	0.52
1:K:73:LYS:H	1:K:97:ASN:HB3	1.74	0.52
1:H:73:LYS:H	1:H:97:ASN:HB3	1.74	0.52
1:J:82:ALA:HB1	1:J:113:ALA:HB2	1.91	0.52
1:F:82:ALA:HB1	1:F:113:ALA:HB2	1.91	0.52
1:C:183:GLU:OE1	1:C:183:GLU:HA	2.10	0.52
1:H:224:VAL:O	1:H:230:PRO:HB3	2.09	0.52
1:L:207:PRO:CA	1:L:218:MSE:HE1	2.38	0.52
1:K:221:GLY:HA3	2:K:311:BMP:OP3	2.09	0.52
1:B:82:ALA:HB1	1:B:113:ALA:HB2	1.91	0.52
1:L:82:ALA:HB1	1:L:113:ALA:HB2	1.91	0.52
1:I:183:GLU:HA	1:I:183:GLU:OE1	2.10	0.52
1:M:136:SER:O	1:M:139:VAL:HG12	2.10	0.52
1:O:224:VAL:O	1:O:230:PRO:HB3	2.09	0.52
1:B:221:GLY:HA3	2:B:302:BMP:OP3	2.09	0.52
1:P:221:GLY:HA3	2:P:316:BMP:OP3	2.09	0.52
1:P:124:LEU:HG	1:P:163:LEU:CD1	2.39	0.52
1:C:73:LYS:H	1:C:97:ASN:HB3	1.74	0.52
1:C:234:LEU:HD13	1:C:238:ASN:ND2	2.24	0.52
1:K:82:ALA:HB1	1:K:113:ALA:HB2	1.91	0.52
1:A:183:GLU:HA	1:A:183:GLU:OE1	2.10	0.52
1:E:224:VAL:O	1:E:230:PRO:HB3	2.09	0.52
1:B:131:THR:HA	1:B:203:ARG:NH1	2.25	0.52
1:G:25:ASN:HD22	1:G:28:ASP:CB	2.16	0.52
1:K:25:ASN:HD22	1:K:28:ASP:CB	2.16	0.52
1:N:73:LYS:H	1:N:97:ASN:HB3	1.74	0.52
1:A:234:LEU:HD13	1:A:238:ASN:ND2	2.24	0.52
1:B:234:LEU:HD13	1:B:238:ASN:ND2	2.24	0.52
1:M:128:THR:OG1	1:M:129:VAL:N	2.43	0.52
1:B:136:SER:O	1:B:139:VAL:HG12	2.10	0.52
1:B:183:GLU:HA	1:B:183:GLU:OE1	2.10	0.52
1:J:224:VAL:O	1:J:230:PRO:HB3	2.09	0.52
1:D:131:THR:HA	1:D:203:ARG:NH1	2.25	0.52
1:O:82:ALA:HB1	1:O:113:ALA:HB2	1.91	0.52
1:N:136:SER:O	1:N:139:VAL:HG12	2.10	0.52
1:J:136:SER:O	1:J:139:VAL:HG12	2.10	0.52
1:N:82:ALA:HB1	1:N:113:ALA:HB2	1.91	0.52
1:D:183:GLU:OE1	1:D:183:GLU:HA	2.10	0.52
1:G:183:GLU:OE1	1:G:183:GLU:HA	2.10	0.52
1:D:224:VAL:O	1:D:230:PRO:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:PRO:HB3	1:K:203:ARG:NE	2.17	0.52
1:N:76:ASP:HB3	1:N:80:THR:HB	1.92	0.52
1:M:76:ASP:HB3	1:M:80:THR:HB	1.92	0.52
1:I:136:SER:O	1:I:139:VAL:HG12	2.10	0.52
1:D:136:SER:O	1:D:139:VAL:HG12	2.10	0.52
1:M:183:GLU:OE1	1:M:183:GLU:HA	2.10	0.52
1:N:183:GLU:HA	1:N:183:GLU:OE1	2.10	0.52
1:J:131:THR:HA	1:J:203:ARG:NH1	2.25	0.52
1:J:76:ASP:HB3	1:J:80:THR:HB	1.92	0.52
1:E:73:LYS:H	1:E:97:ASN:HB3	1.74	0.52
1:M:174:VAL:HG22	1:M:213:ALA:HB1	1.92	0.52
1:D:174:VAL:HG22	1:D:213:ALA:HB1	1.92	0.52
1:J:183:GLU:HA	1:J:183:GLU:OE1	2.10	0.52
1:P:211:LEU:HD12	1:P:211:LEU:O	2.10	0.52
1:O:147:PRO:HB3	1:O:203:ARG:NE	2.17	0.51
1:L:131:THR:HA	1:L:203:ARG:NH1	2.25	0.51
1:J:124:LEU:HG	1:J:163:LEU:CD1	2.39	0.51
1:O:174:VAL:HG22	1:O:213:ALA:HB1	1.92	0.51
1:C:136:SER:O	1:C:139:VAL:HG12	2.10	0.51
1:P:136:SER:O	1:P:139:VAL:HG12	2.10	0.51
1:L:136:SER:O	1:L:139:VAL:HG12	2.10	0.51
1:H:211:LEU:O	1:H:211:LEU:HD12	2.10	0.51
1:K:183:GLU:OE1	1:K:183:GLU:HA	2.10	0.51
1:J:211:LEU:O	1:J:211:LEU:HD12	2.11	0.51
1:A:136:SER:O	1:A:139:VAL:HG12	2.10	0.51
1:H:207:PRO:CA	1:H:218:MSE:HE1	2.38	0.51
1:I:131:THR:HA	1:I:203:ARG:NH1	2.25	0.51
1:H:131:THR:HA	1:H:203:ARG:NH1	2.25	0.51
1:E:131:THR:HA	1:E:203:ARG:NH1	2.25	0.51
1:G:73:LYS:H	1:G:97:ASN:HB3	1.74	0.51
1:G:174:VAL:HG22	1:G:213:ALA:HB1	1.92	0.51
1:C:174:VAL:HG22	1:C:213:ALA:HB1	1.92	0.51
1:E:183:GLU:OE1	1:E:183:GLU:HA	2.10	0.51
1:F:207:PRO:CA	1:F:218:MSE:HE1	2.38	0.51
1:L:224:VAL:O	1:L:230:PRO:HB3	2.09	0.51
1:I:25:ASN:HD22	1:I:28:ASP:CB	2.16	0.51
1:O:131:THR:HA	1:O:203:ARG:NH1	2.25	0.51
1:N:131:THR:HA	1:N:203:ARG:NH1	2.25	0.51
1:A:131:THR:HA	1:A:203:ARG:NH1	2.25	0.51
1:H:174:VAL:HG22	1:H:213:ALA:HB1	1.92	0.51
1:K:174:VAL:HG22	1:K:213:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:234:LEU:HD13	1:J:238:ASN:ND2	2.24	0.51
1:L:234:LEU:HD13	1:L:238:ASN:ND2	2.24	0.51
1:A:82:ALA:HB1	1:A:113:ALA:HB2	1.91	0.51
1:L:183:GLU:HA	1:L:183:GLU:OE1	2.10	0.51
1:E:211:LEU:HD12	1:E:211:LEU:O	2.11	0.51
1:L:211:LEU:HD12	1:L:211:LEU:O	2.10	0.51
1:F:211:LEU:HD12	1:F:211:LEU:O	2.10	0.51
1:O:207:PRO:CA	1:O:218:MSE:HE1	2.38	0.51
1:B:228:VAL:HG22	1:C:233:THR:HG23	1.92	0.51
1:P:73:LYS:H	1:P:97:ASN:HB3	1.74	0.51
1:B:174:VAL:HG22	1:B:213:ALA:HB1	1.92	0.51
1:O:136:SER:O	1:O:139:VAL:HG12	2.10	0.51
1:N:211:LEU:HD12	1:N:211:LEU:O	2.10	0.51
1:H:183:GLU:OE1	1:H:183:GLU:HA	2.10	0.51
1:O:183:GLU:OE1	1:O:183:GLU:HA	2.10	0.51
1:N:207:PRO:CA	1:N:218:MSE:HE1	2.38	0.51
1:O:76:ASP:HB3	1:O:80:THR:HB	1.92	0.51
1:B:187:VAL:HG22	1:B:217:TYR:HB2	1.93	0.51
1:A:211:LEU:HD12	1:A:211:LEU:O	2.10	0.51
1:K:131:THR:HA	1:K:203:ARG:NH1	2.25	0.51
1:C:131:THR:HA	1:C:203:ARG:NH1	2.25	0.51
1:G:131:THR:HA	1:G:203:ARG:NH1	2.25	0.51
1:B:128:THR:OG1	1:B:129:VAL:N	2.43	0.51
1:C:82:ALA:HB1	1:C:113:ALA:HB2	1.91	0.51
1:O:128:THR:OG1	1:O:129:VAL:N	2.43	0.51
1:J:128:THR:OG1	1:J:129:VAL:N	2.43	0.51
1:F:183:GLU:OE1	1:F:183:GLU:HA	2.10	0.51
1:A:76:ASP:HB3	1:A:80:THR:HB	1.92	0.51
1:F:131:THR:HA	1:F:203:ARG:NH1	2.25	0.51
1:I:73:LYS:H	1:I:97:ASN:HB3	1.74	0.51
1:P:128:THR:OG1	1:P:129:VAL:N	2.43	0.51
1:D:128:THR:OG1	1:D:129:VAL:N	2.43	0.51
1:K:136:SER:O	1:K:139:VAL:HG12	2.10	0.51
1:I:187:VAL:HG22	1:I:217:TYR:HB2	1.93	0.51
1:M:211:LEU:O	1:M:211:LEU:HD12	2.11	0.51
1:D:187:VAL:HG22	1:D:217:TYR:HB2	1.93	0.51
1:M:187:VAL:HG22	1:M:217:TYR:HB2	1.93	0.51
1:L:76:ASP:HB3	1:L:80:THR:HB	1.92	0.51
1:B:76:ASP:HB3	1:B:80:THR:HB	1.92	0.51
1:E:174:VAL:HG22	1:E:213:ALA:HB1	1.92	0.51
1:I:174:VAL:HG22	1:I:213:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:187:VAL:HG22	1:N:217:TYR:HB2	1.93	0.51
1:E:136:SER:O	1:E:139:VAL:HG12	2.10	0.51
1:M:82:ALA:HB1	1:M:113:ALA:HB2	1.91	0.51
1:G:211:LEU:HD12	1:G:211:LEU:O	2.10	0.51
1:G:136:SER:O	1:G:139:VAL:HG12	2.10	0.51
1:N:25:ASN:ND2	1:N:28:ASP:HB2	2.17	0.51
1:H:25:ASN:HD22	1:H:28:ASP:CB	2.16	0.51
1:M:131:THR:HA	1:M:203:ARG:NH1	2.25	0.51
1:A:124:LEU:HG	1:A:163:LEU:CD1	2.39	0.51
1:K:124:LEU:HG	1:K:163:LEU:CD1	2.39	0.51
1:I:76:ASP:HB3	1:I:80:THR:HB	1.92	0.51
1:C:137:ASP:OD2	1:D:105:ARG:HD3	2.11	0.51
1:L:187:VAL:HG22	1:L:217:TYR:HB2	1.93	0.51
1:L:128:THR:OG1	1:L:129:VAL:N	2.43	0.51
1:P:183:GLU:OE1	1:P:183:GLU:HA	2.10	0.51
1:I:211:LEU:O	1:I:211:LEU:HD12	2.10	0.51
1:C:211:LEU:O	1:C:211:LEU:HD12	2.10	0.51
1:P:220:ILE:HG21	1:P:224:VAL:HG23	1.93	0.51
1:B:220:ILE:HG21	1:B:224:VAL:HG23	1.93	0.51
1:F:227:SER:CA	1:G:232:GLN:HE21	2.21	0.51
1:B:124:LEU:HG	1:B:163:LEU:CD1	2.39	0.51
1:F:76:ASP:HB3	1:F:80:THR:HB	1.92	0.51
1:F:174:VAL:HG22	1:F:213:ALA:HB1	1.92	0.51
1:A:174:VAL:HG22	1:A:213:ALA:HB1	1.92	0.51
1:K:187:VAL:HG22	1:K:217:TYR:HB2	1.93	0.51
1:H:136:SER:O	1:H:139:VAL:HG12	2.10	0.51
1:A:128:THR:OG1	1:A:129:VAL:N	2.43	0.51
1:C:187:VAL:HG22	1:C:217:TYR:HB2	1.93	0.51
1:B:211:LEU:HD12	1:B:211:LEU:O	2.11	0.51
1:O:211:LEU:O	1:O:211:LEU:HD12	2.10	0.51
1:D:220:ILE:HG21	1:D:224:VAL:HG23	1.93	0.50
1:B:228:VAL:CB	1:C:236:ALA:CB	2.89	0.50
1:P:131:THR:HA	1:P:203:ARG:NH1	2.25	0.50
1:H:76:ASP:HB3	1:H:80:THR:HB	1.92	0.50
1:C:124:LEU:HG	1:C:163:LEU:CD1	2.39	0.50
1:A:178:GLN:HG3	1:A:179:VAL:N	2.27	0.50
1:D:125:ILE:HD12	1:D:125:ILE:N	2.27	0.50
1:C:128:THR:OG1	1:C:129:VAL:N	2.43	0.50
1:G:105:ARG:HD3	1:H:137:ASP:OD2	2.10	0.50
1:H:178:GLN:HG3	1:H:179:VAL:N	2.27	0.50
1:O:125:ILE:N	1:O:125:ILE:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ASP:HB3	1:D:80:THR:HB	1.92	0.50
1:A:187:VAL:HG22	1:A:217:TYR:HB2	1.93	0.50
1:F:136:SER:O	1:F:139:VAL:HG12	2.10	0.50
1:D:211:LEU:HD12	1:D:211:LEU:O	2.11	0.50
1:J:220:ILE:HG21	1:J:224:VAL:HG23	1.93	0.50
1:J:174:VAL:HG22	1:J:213:ALA:HB1	1.92	0.50
1:L:174:VAL:HG22	1:L:213:ALA:HB1	1.92	0.50
1:K:125:ILE:N	1:K:125:ILE:HD12	2.27	0.50
1:B:125:ILE:N	1:B:125:ILE:HD12	2.27	0.50
1:J:187:VAL:HG22	1:J:217:TYR:HB2	1.93	0.50
1:G:76:ASP:HB3	1:G:80:THR:HB	1.92	0.50
1:K:220:ILE:HG21	1:K:224:VAL:HG23	1.93	0.50
1:M:25:ASN:HD22	1:M:28:ASP:CB	2.16	0.50
1:C:131:THR:HA	1:C:203:ARG:HH12	1.77	0.50
1:K:178:GLN:HG3	1:K:179:VAL:N	2.27	0.50
1:P:174:VAL:HG22	1:P:213:ALA:HB1	1.92	0.50
1:I:220:ILE:HG21	1:I:224:VAL:HG23	1.93	0.50
1:E:220:ILE:HG21	1:E:224:VAL:HG23	1.93	0.50
1:C:76:ASP:HB3	1:C:80:THR:HB	1.92	0.50
1:F:178:GLN:HG3	1:F:179:VAL:N	2.27	0.50
1:C:178:GLN:HG3	1:C:179:VAL:N	2.27	0.50
1:O:178:GLN:HG3	1:O:179:VAL:N	2.27	0.50
1:N:125:ILE:HD12	1:N:125:ILE:N	2.27	0.50
1:L:125:ILE:N	1:L:125:ILE:HD12	2.27	0.50
1:P:187:VAL:HG22	1:P:217:TYR:HB2	1.93	0.50
1:M:220:ILE:HG21	1:M:224:VAL:HG23	1.93	0.50
1:E:76:ASP:HB3	1:E:80:THR:HB	1.92	0.50
1:N:174:VAL:HG22	1:N:213:ALA:HB1	1.92	0.50
1:N:178:GLN:HG3	1:N:179:VAL:N	2.27	0.50
1:P:178:GLN:HG3	1:P:179:VAL:N	2.27	0.50
1:I:125:ILE:N	1:I:125:ILE:HD12	2.27	0.50
1:P:76:ASP:HB3	1:P:80:THR:HB	1.92	0.50
1:K:76:ASP:HB3	1:K:80:THR:HB	1.92	0.50
1:K:128:THR:OG1	1:K:129:VAL:N	2.43	0.50
1:H:187:VAL:HG22	1:H:217:TYR:HB2	1.93	0.50
1:G:220:ILE:HG21	1:G:224:VAL:HG23	1.93	0.50
1:F:25:ASN:HD22	1:F:28:ASP:CB	2.16	0.50
1:A:131:THR:HA	1:A:203:ARG:HH12	1.77	0.50
1:D:124:LEU:HG	1:D:163:LEU:CD1	2.39	0.50
1:L:178:GLN:HG3	1:L:179:VAL:N	2.27	0.50
1:M:125:ILE:N	1:M:125:ILE:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ILE:HD12	1:G:125:ILE:N	2.27	0.50
1:N:128:THR:OG1	1:N:129:VAL:N	2.43	0.50
1:O:131:THR:HA	1:O:203:ARG:HH12	1.77	0.50
1:P:192:ARG:O	1:P:206:THR:HG22	2.12	0.50
1:J:178:GLN:HG3	1:J:179:VAL:N	2.27	0.50
1:K:105:ARG:HD3	1:L:137:ASP:OD2	2.11	0.50
1:P:25:ASN:HD22	1:P:28:ASP:CB	2.16	0.50
1:L:131:THR:HA	1:L:203:ARG:HH12	1.77	0.50
1:L:124:LEU:HG	1:L:163:LEU:CD1	2.39	0.50
1:A:125:ILE:N	1:A:125:ILE:HD12	2.27	0.50
1:C:125:ILE:HD12	1:C:125:ILE:N	2.27	0.50
1:I:128:THR:OG1	1:I:129:VAL:N	2.43	0.50
1:G:187:VAL:HG22	1:G:217:TYR:HB2	1.93	0.50
1:O:220:ILE:HG21	1:O:224:VAL:HG23	1.93	0.49
1:N:220:ILE:HG21	1:N:224:VAL:HG23	1.93	0.49
1:A:220:ILE:HG21	1:A:224:VAL:HG23	1.93	0.49
1:L:220:ILE:HG21	1:L:224:VAL:HG23	1.93	0.49
1:B:131:THR:HA	1:B:203:ARG:HH12	1.77	0.49
1:L:25:ASN:ND2	1:L:28:ASP:HB2	2.17	0.49
1:M:192:ARG:O	1:M:206:THR:HG22	2.12	0.49
1:E:125:ILE:N	1:E:125:ILE:HD12	2.27	0.49
1:E:187:VAL:HG22	1:E:217:TYR:HB2	1.93	0.49
1:K:211:LEU:O	1:K:211:LEU:HD12	2.10	0.49
1:O:192:ARG:O	1:O:206:THR:HG22	2.12	0.49
1:J:192:ARG:O	1:J:206:THR:HG22	2.12	0.49
1:C:192:ARG:O	1:C:206:THR:HG22	2.12	0.49
1:A:192:ARG:O	1:A:206:THR:HG22	2.12	0.49
1:L:192:ARG:O	1:L:206:THR:HG22	2.12	0.49
1:H:124:LEU:HG	1:H:163:LEU:CD1	2.39	0.49
1:G:128:THR:OG1	1:G:129:VAL:N	2.43	0.49
1:B:192:ARG:O	1:B:206:THR:HG22	2.12	0.49
1:F:187:VAL:HG22	1:F:217:TYR:HB2	1.93	0.49
1:C:25:ASN:ND2	1:C:28:ASP:HB2	2.17	0.49
1:M:202:ARG:O	1:M:204:ILE:N	2.46	0.49
1:P:202:ARG:O	1:P:204:ILE:N	2.46	0.49
1:F:124:LEU:HG	1:F:163:LEU:CD1	2.39	0.49
1:M:178:GLN:HG3	1:M:179:VAL:N	2.27	0.49
1:E:128:THR:OG1	1:E:129:VAL:N	2.43	0.49
1:D:131:THR:HA	1:D:203:ARG:HH12	1.77	0.49
1:O:202:ARG:O	1:O:204:ILE:N	2.46	0.49
1:G:192:ARG:O	1:G:206:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:GLN:HG3	1:I:179:VAL:N	2.27	0.49
1:P:125:ILE:N	1:P:125:ILE:HD12	2.27	0.49
1:J:125:ILE:N	1:J:125:ILE:HD12	2.27	0.49
1:O:187:VAL:HG22	1:O:217:TYR:HB2	1.93	0.49
1:N:131:THR:HA	1:N:203:ARG:HH12	1.77	0.49
1:K:131:THR:HA	1:K:203:ARG:HH12	1.77	0.49
1:F:192:ARG:O	1:F:206:THR:HG22	2.12	0.49
1:N:192:ARG:O	1:N:206:THR:HG22	2.12	0.49
1:D:178:GLN:HG3	1:D:179:VAL:N	2.27	0.49
1:F:125:ILE:HD12	1:F:125:ILE:N	2.27	0.49
1:H:220:ILE:HG21	1:H:224:VAL:HG23	1.93	0.49
1:F:220:ILE:HG21	1:F:224:VAL:HG23	1.93	0.49
1:C:220:ILE:HG21	1:C:224:VAL:HG23	1.93	0.49
1:E:192:ARG:O	1:E:206:THR:HG22	2.12	0.49
1:K:202:ARG:O	1:K:204:ILE:N	2.46	0.49
1:L:202:ARG:O	1:L:204:ILE:N	2.46	0.49
1:B:178:GLN:HG3	1:B:179:VAL:N	2.27	0.49
1:J:202:ARG:O	1:J:204:ILE:N	2.46	0.49
1:O:32:PHE:CE2	1:O:36:ILE:HD13	2.48	0.49
1:J:32:PHE:CE2	1:J:36:ILE:HD13	2.48	0.49
1:I:25:ASN:ND2	1:I:28:ASP:HB2	2.17	0.49
1:O:25:ASN:ND2	1:O:28:ASP:HB2	2.17	0.49
1:I:131:THR:HA	1:I:203:ARG:HH12	1.77	0.49
1:M:131:THR:HA	1:M:203:ARG:HH12	1.77	0.49
1:P:131:THR:HA	1:P:203:ARG:HH12	1.77	0.49
1:D:192:ARG:O	1:D:206:THR:HG22	2.12	0.49
1:G:202:ARG:O	1:G:204:ILE:N	2.46	0.49
1:H:125:ILE:HD12	1:H:125:ILE:N	2.27	0.49
1:K:32:PHE:CE2	1:K:36:ILE:HD13	2.48	0.49
1:L:32:PHE:CE2	1:L:36:ILE:HD13	2.48	0.49
1:I:147:PRO:HB3	1:I:203:ARG:NE	2.17	0.49
1:N:202:ARG:O	1:N:204:ILE:N	2.46	0.49
1:C:206:THR:H	1:C:209:GLN:HG3	1.78	0.49
1:L:193:PRO:O	1:L:194:GLN:O	2.31	0.49
1:A:32:PHE:CE2	1:A:36:ILE:HD13	2.48	0.49
1:H:32:PHE:CE2	1:H:36:ILE:HD13	2.48	0.49
1:C:32:PHE:CE2	1:C:36:ILE:HD13	2.48	0.49
1:G:178:GLN:HG3	1:G:179:VAL:N	2.27	0.48
1:H:193:PRO:O	1:H:194:GLN:O	2.31	0.48
1:E:32:PHE:CE2	1:E:36:ILE:HD13	2.48	0.48
1:B:32:PHE:CE2	1:B:36:ILE:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:PHE:CE2	1:I:36:ILE:HD13	2.48	0.48
1:A:206:THR:H	1:A:209:GLN:HG3	1.79	0.48
1:I:192:ARG:O	1:I:206:THR:HG22	2.12	0.48
1:J:193:PRO:O	1:J:194:GLN:O	2.31	0.48
1:F:32:PHE:CE2	1:F:36:ILE:HD13	2.48	0.48
1:G:32:PHE:CE2	1:G:36:ILE:HD13	2.48	0.48
1:D:32:PHE:CE2	1:D:36:ILE:HD13	2.48	0.48
1:J:131:THR:HA	1:J:203:ARG:HH12	1.77	0.48
1:K:25:ASN:ND2	1:K:28:ASP:HB2	2.17	0.48
1:H:192:ARG:O	1:H:206:THR:HG22	2.12	0.48
1:H:202:ARG:O	1:H:204:ILE:N	2.46	0.48
1:K:192:ARG:O	1:K:206:THR:HG22	2.12	0.48
1:G:124:LEU:HG	1:G:163:LEU:CD1	2.39	0.48
1:N:193:PRO:O	1:N:194:GLN:O	2.31	0.48
1:H:128:THR:OG1	1:H:129:VAL:N	2.43	0.48
1:F:131:THR:HA	1:F:203:ARG:HH12	1.77	0.48
1:M:206:THR:H	1:M:209:GLN:HG3	1.79	0.48
1:L:206:THR:H	1:L:209:GLN:HG3	1.78	0.48
1:I:124:LEU:HG	1:I:163:LEU:CD1	2.39	0.48
1:F:193:PRO:O	1:F:194:GLN:O	2.31	0.48
1:O:200:ASP:HA	1:P:105:ARG:HH22	1.79	0.48
1:F:227:SER:HB2	1:G:232:GLN:HE21	1.76	0.48
1:F:202:ARG:O	1:F:204:ILE:N	2.46	0.48
2:M:313:BMP:O2	1:N:77:ILE:HD13	2.14	0.48
1:G:206:THR:H	1:G:209:GLN:HG3	1.78	0.48
1:I:202:ARG:O	1:I:204:ILE:N	2.46	0.48
1:M:193:PRO:O	1:M:194:GLN:O	2.31	0.48
1:M:32:PHE:CE2	1:M:36:ILE:HD13	2.48	0.48
1:L:115:VAL:N	1:L:116:PRO:CD	2.77	0.48
1:N:115:VAL:N	1:N:116:PRO:CD	2.77	0.48
1:G:115:VAL:N	1:G:116:PRO:CD	2.77	0.48
1:P:206:THR:H	1:P:209:GLN:HG3	1.78	0.48
1:P:193:PRO:O	1:P:194:GLN:O	2.31	0.48
1:E:115:VAL:N	1:E:116:PRO:CD	2.77	0.48
1:M:115:VAL:N	1:M:116:PRO:CD	2.77	0.48
1:B:115:VAL:N	1:B:116:PRO:CD	2.77	0.48
1:F:202:ARG:O	1:F:204:ILE:HG13	2.14	0.48
1:E:178:GLN:HG3	1:E:179:VAL:N	2.27	0.48
1:E:131:THR:HA	1:E:203:ARG:HH12	1.77	0.48
1:H:202:ARG:O	1:H:204:ILE:HG13	2.14	0.48
1:E:206:THR:H	1:E:209:GLN:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:O	1:A:204:ILE:N	2.46	0.48
1:G:193:PRO:O	1:G:194:GLN:O	2.31	0.48
1:C:200:ASP:HA	1:D:105:ARG:HH22	1.78	0.48
1:K:115:VAL:N	1:K:116:PRO:CD	2.77	0.48
1:M:13:THR:CG2	1:M:38:PRO:O	2.62	0.48
1:N:32:PHE:CE2	1:N:36:ILE:HD13	2.48	0.48
1:O:207:PRO:CB	1:O:218:MSE:HE1	2.44	0.48
1:C:202:ARG:O	1:C:204:ILE:N	2.46	0.48
1:I:206:THR:H	1:I:209:GLN:HG3	1.79	0.48
1:A:193:PRO:O	1:A:194:GLN:O	2.31	0.48
1:K:193:PRO:O	1:K:194:GLN:O	2.31	0.48
1:O:193:PRO:O	1:O:194:GLN:O	2.31	0.48
1:I:115:VAL:N	1:I:116:PRO:CD	2.77	0.48
1:C:115:VAL:N	1:C:116:PRO:CD	2.77	0.48
1:D:115:VAL:N	1:D:116:PRO:CD	2.77	0.48
1:A:13:THR:CG2	1:A:38:PRO:O	2.62	0.48
1:P:32:PHE:CE2	1:P:36:ILE:HD13	2.48	0.48
1:I:13:THR:CG2	1:I:38:PRO:O	2.62	0.48
1:F:207:PRO:CB	1:F:218:MSE:HE1	2.44	0.48
1:D:207:PRO:CB	1:D:218:MSE:HE1	2.44	0.48
1:N:206:THR:H	1:N:209:GLN:HG3	1.78	0.48
1:M:202:ARG:O	1:M:204:ILE:HG13	2.14	0.48
1:J:206:THR:H	1:J:209:GLN:HG3	1.78	0.48
1:E:202:ARG:O	1:E:204:ILE:HG13	2.14	0.48
1:E:124:LEU:HG	1:E:163:LEU:CD1	2.39	0.48
1:B:207:PRO:CB	1:B:218:MSE:HE1	2.44	0.47
1:H:131:THR:HA	1:H:203:ARG:HH12	1.77	0.47
1:M:75:HIS:N	1:N:47:LYS:NZ	2.52	0.47
1:P:202:ARG:O	1:P:204:ILE:HG13	2.14	0.47
1:K:202:ARG:O	1:K:204:ILE:HG13	2.14	0.47
1:I:202:ARG:O	1:I:204:ILE:HG13	2.14	0.47
1:N:125:ILE:HG23	1:N:166:VAL:N	2.29	0.47
1:L:125:ILE:HG23	1:L:166:VAL:N	2.29	0.47
1:P:125:ILE:HG23	1:P:166:VAL:N	2.29	0.47
1:M:125:ILE:HG23	1:M:166:VAL:N	2.29	0.47
1:J:115:VAL:N	1:J:116:PRO:CD	2.77	0.47
1:K:13:THR:CG2	1:K:38:PRO:O	2.62	0.47
1:P:13:THR:CG2	1:P:38:PRO:O	2.62	0.47
1:H:115:VAL:N	1:H:116:PRO:CD	2.77	0.47
1:M:207:PRO:CB	1:M:218:MSE:HE1	2.44	0.47
1:O:25:ASN:HB3	1:O:28:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:202:ARG:O	1:O:204:ILE:HG13	2.14	0.47
1:N:202:ARG:O	1:N:204:ILE:HG13	2.14	0.47
1:B:202:ARG:O	1:B:204:ILE:N	2.46	0.47
1:E:202:ARG:O	1:E:204:ILE:N	2.46	0.47
1:L:30:LEU:HA	1:L:30:LEU:HD23	1.73	0.47
1:I:193:PRO:O	1:I:194:GLN:O	2.31	0.47
1:B:193:PRO:O	1:B:194:GLN:O	2.31	0.47
1:P:115:VAL:N	1:P:116:PRO:CD	2.77	0.47
1:I:207:PRO:CB	1:I:218:MSE:HE1	2.44	0.47
1:N:207:PRO:CB	1:N:218:MSE:HE1	2.44	0.47
1:H:207:PRO:CB	1:H:218:MSE:HE1	2.44	0.47
1:G:131:THR:HA	1:G:203:ARG:HH12	1.77	0.47
1:D:202:ARG:O	1:D:204:ILE:N	2.46	0.47
1:G:202:ARG:O	1:G:204:ILE:HG13	2.14	0.47
1:K:206:THR:H	1:K:209:GLN:HG3	1.78	0.47
1:E:193:PRO:O	1:E:194:GLN:O	2.31	0.47
1:E:13:THR:CG2	1:E:38:PRO:O	2.62	0.47
1:N:13:THR:CG2	1:N:38:PRO:O	2.62	0.47
1:J:13:THR:CG2	1:J:38:PRO:O	2.62	0.47
1:K:207:PRO:CB	1:K:218:MSE:HE1	2.44	0.47
1:L:207:PRO:CB	1:L:218:MSE:HE1	2.44	0.47
1:B:27:ASP:CG	1:N:119:LYS:HB2	2.35	0.47
1:J:147:PRO:HB3	1:J:203:ARG:NE	2.17	0.47
1:A:25:ASN:ND2	1:A:28:ASP:HB2	2.17	0.47
1:J:125:ILE:HG23	1:J:166:VAL:N	2.29	0.47
1:H:125:ILE:HG23	1:H:166:VAL:N	2.29	0.47
1:O:125:ILE:HG23	1:O:166:VAL:N	2.29	0.47
1:L:115:VAL:HB	1:L:116:PRO:HD3	1.97	0.47
1:C:13:THR:CG2	1:C:38:PRO:O	2.62	0.47
1:A:115:VAL:N	1:A:116:PRO:CD	2.77	0.47
1:A:207:PRO:CB	1:A:218:MSE:HE1	2.44	0.47
1:M:147:PRO:HB3	1:M:203:ARG:NE	2.17	0.47
1:A:125:ILE:HG23	1:A:166:VAL:N	2.29	0.47
1:F:125:ILE:HG23	1:F:166:VAL:N	2.29	0.47
1:F:115:VAL:N	1:F:116:PRO:CD	2.77	0.47
1:N:25:ASN:HB3	1:N:28:ASP:HB2	1.96	0.47
1:M:141:LEU:O	1:M:143:MSE:N	2.45	0.47
1:K:125:ILE:HG23	1:K:166:VAL:N	2.29	0.47
1:L:13:THR:CG2	1:L:38:PRO:O	2.62	0.47
1:O:115:VAL:N	1:O:116:PRO:CD	2.77	0.47
1:G:13:THR:CG2	1:G:38:PRO:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:THR:CG2	1:B:38:PRO:O	2.62	0.47
1:D:13:THR:CG2	1:D:38:PRO:O	2.62	0.47
1:P:207:PRO:CB	1:P:218:MSE:HE1	2.44	0.47
1:C:207:PRO:CB	1:C:218:MSE:HE1	2.44	0.47
1:C:25:ASN:HB3	1:C:28:ASP:HB2	1.97	0.47
1:C:147:PRO:HB3	1:C:203:ARG:NE	2.17	0.47
1:O:206:THR:H	1:O:209:GLN:HG3	1.78	0.47
1:D:206:THR:H	1:D:209:GLN:HG3	1.78	0.47
1:B:206:THR:H	1:B:209:GLN:HG3	1.78	0.47
1:L:202:ARG:O	1:L:204:ILE:HG13	2.14	0.47
1:M:124:LEU:HG	1:M:163:LEU:CD1	2.39	0.47
1:H:141:LEU:O	1:H:143:MSE:N	2.45	0.47
1:E:188:THR:HA	1:E:189:PRO:HD3	1.75	0.47
1:G:188:THR:HA	1:G:189:PRO:HD3	1.75	0.47
1:C:193:PRO:O	1:C:194:GLN:O	2.31	0.47
1:E:125:ILE:HG23	1:E:166:VAL:N	2.29	0.47
1:J:115:VAL:HB	1:J:116:PRO:HD3	1.97	0.47
1:B:85:VAL:HG21	1:B:110:ALA:HB1	1.97	0.47
1:J:207:PRO:CB	1:J:218:MSE:HE1	2.44	0.47
1:M:25:ASN:HB3	1:M:28:ASP:HB2	1.96	0.47
1:B:27:ASP:OD2	1:N:119:LYS:HB2	2.14	0.47
1:L:141:LEU:O	1:L:143:MSE:N	2.45	0.47
1:G:125:ILE:HG23	1:G:166:VAL:N	2.29	0.47
1:H:115:VAL:HB	1:H:116:PRO:HD3	1.97	0.47
1:F:13:THR:CG2	1:F:38:PRO:O	2.62	0.47
1:D:85:VAL:HG21	1:D:110:ALA:HB1	1.97	0.47
1:M:85:VAL:HG21	1:M:110:ALA:HB1	1.97	0.47
1:K:85:VAL:HG21	1:K:110:ALA:HB1	1.97	0.47
1:F:206:THR:H	1:F:209:GLN:HG3	1.79	0.47
1:I:204:ILE:CG2	1:I:205:MSE:N	2.60	0.47
1:D:193:PRO:O	1:D:194:GLN:O	2.31	0.47
1:I:125:ILE:HG23	1:I:166:VAL:N	2.29	0.47
1:D:115:VAL:HB	1:D:116:PRO:HD3	1.97	0.47
1:G:15:SER:C	1:G:17:VAL:H	2.18	0.47
1:A:15:SER:C	1:A:17:VAL:H	2.18	0.47
1:H:13:THR:CG2	1:H:38:PRO:O	2.62	0.47
1:O:13:THR:CG2	1:O:38:PRO:O	2.62	0.47
1:A:25:ASN:HB3	1:A:28:ASP:HB2	1.97	0.47
1:O:76:ASP:C	1:P:130:LEU:HD13	2.36	0.47
1:B:125:ILE:HG23	1:B:166:VAL:N	2.29	0.47
1:C:125:ILE:HG23	1:C:166:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:SER:C	1:C:17:VAL:H	2.18	0.47
1:D:15:SER:C	1:D:17:VAL:H	2.18	0.47
1:I:25:ASN:HB3	1:I:28:ASP:HB2	1.97	0.46
1:J:25:ASN:HB3	1:J:28:ASP:HB2	1.97	0.46
1:D:202:ARG:O	1:D:204:ILE:HG13	2.14	0.46
1:B:202:ARG:O	1:B:204:ILE:HG13	2.14	0.46
1:C:188:THR:HA	1:C:189:PRO:HD3	1.75	0.46
1:M:105:ARG:HD3	1:N:137:ASP:OD2	2.14	0.46
1:M:115:VAL:HB	1:M:116:PRO:HD3	1.97	0.46
1:B:115:VAL:HB	1:B:116:PRO:HD3	1.97	0.46
1:C:115:VAL:HB	1:C:116:PRO:HD3	1.97	0.46
1:F:115:VAL:HB	1:F:116:PRO:HD3	1.97	0.46
1:I:85:VAL:HG21	1:I:110:ALA:HB1	1.97	0.46
1:P:85:VAL:HG21	1:P:110:ALA:HB1	1.97	0.46
1:B:15:SER:C	1:B:17:VAL:H	2.18	0.46
1:F:85:VAL:HG21	1:F:110:ALA:HB1	1.97	0.46
1:E:207:PRO:CB	1:E:218:MSE:HE1	2.44	0.46
1:B:25:ASN:HB3	1:B:28:ASP:HB2	1.97	0.46
1:E:25:ASN:HB3	1:E:28:ASP:HB2	1.97	0.46
1:C:202:ARG:O	1:C:204:ILE:HG13	2.14	0.46
1:O:73:LYS:HB3	1:O:99:HIS:CD2	2.51	0.46
1:I:73:LYS:HB3	1:I:99:HIS:CD2	2.51	0.46
1:F:179:VAL:O	1:F:179:VAL:HG12	2.15	0.46
1:P:179:VAL:O	1:P:179:VAL:HG12	2.15	0.46
1:O:15:SER:C	1:O:17:VAL:H	2.18	0.46
1:G:207:PRO:CB	1:G:218:MSE:HE1	2.44	0.46
1:D:25:ASN:HB3	1:D:28:ASP:HB2	1.97	0.46
1:K:25:ASN:HB3	1:K:28:ASP:HB2	1.97	0.46
1:P:25:ASN:HB3	1:P:28:ASP:HB2	1.97	0.46
1:C:73:LYS:HB3	1:C:99:HIS:CD2	2.51	0.46
1:K:73:LYS:HB3	1:K:99:HIS:CD2	2.51	0.46
1:H:179:VAL:O	1:H:179:VAL:HG12	2.16	0.46
1:O:85:VAL:HG21	1:O:110:ALA:HB1	1.97	0.46
1:H:85:VAL:HG21	1:H:110:ALA:HB1	1.97	0.46
1:I:15:SER:C	1:I:17:VAL:H	2.18	0.46
1:A:147:PRO:HB3	1:A:203:ARG:NE	2.17	0.46
1:H:206:THR:H	1:H:209:GLN:HG3	1.78	0.46
1:I:75:HIS:H	1:J:47:LYS:HZ3	1.62	0.46
1:C:141:LEU:O	1:C:143:MSE:N	2.45	0.46
1:J:179:VAL:O	1:J:179:VAL:HG12	2.16	0.46
1:D:125:ILE:HG23	1:D:166:VAL:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:VAL:HG21	1:J:110:ALA:HB1	1.97	0.46
1:P:15:SER:C	1:P:17:VAL:H	2.18	0.46
1:E:15:SER:C	1:E:17:VAL:H	2.18	0.46
1:E:30:LEU:HD23	1:E:30:LEU:HA	1.73	0.46
1:B:73:LYS:HB3	1:B:99:HIS:CD2	2.51	0.46
1:N:115:VAL:HB	1:N:116:PRO:HD3	1.97	0.46
1:K:115:VAL:HB	1:K:116:PRO:HD3	1.97	0.46
1:F:25:ASN:HB3	1:F:28:ASP:HB2	1.96	0.46
1:J:202:ARG:O	1:J:204:ILE:HG13	2.14	0.46
1:D:73:LYS:HB3	1:D:99:HIS:CD2	2.51	0.46
1:A:73:LYS:HB3	1:A:99:HIS:CD2	2.51	0.46
1:J:73:LYS:HB3	1:J:99:HIS:CD2	2.51	0.46
1:C:179:VAL:O	1:C:179:VAL:HG12	2.16	0.46
1:I:115:VAL:HB	1:I:116:PRO:HD3	1.97	0.46
1:A:115:VAL:HB	1:A:116:PRO:HD3	1.97	0.46
1:L:85:VAL:HG21	1:L:110:ALA:HB1	1.97	0.46
1:A:85:VAL:HG21	1:A:110:ALA:HB1	1.97	0.46
1:L:25:ASN:HB3	1:L:28:ASP:HB2	1.97	0.46
1:A:202:ARG:O	1:A:204:ILE:HG13	2.14	0.46
1:N:73:LYS:HB3	1:N:99:HIS:CD2	2.51	0.46
1:A:179:VAL:O	1:A:179:VAL:HG12	2.16	0.46
1:B:150:TYR:CZ	1:B:154:LEU:HD11	2.51	0.46
1:J:150:TYR:CZ	1:J:154:LEU:HD11	2.51	0.46
1:D:150:TYR:CZ	1:D:154:LEU:HD11	2.51	0.46
1:E:150:TYR:CZ	1:E:154:LEU:HD11	2.51	0.46
1:G:150:TYR:CZ	1:G:154:LEU:HD11	2.51	0.46
1:O:115:VAL:HB	1:O:116:PRO:HD3	1.97	0.46
1:G:85:VAL:HG21	1:G:110:ALA:HB1	1.97	0.46
1:M:25:ASN:ND2	1:M:28:ASP:HB2	2.17	0.46
1:H:25:ASN:HB3	1:H:28:ASP:HB2	1.97	0.46
1:O:176:PHE:C	1:O:178:GLN:N	2.69	0.46
1:L:150:TYR:CZ	1:L:154:LEU:HD11	2.51	0.46
1:P:115:VAL:HB	1:P:116:PRO:HD3	1.97	0.46
1:O:179:VAL:HG12	1:O:179:VAL:O	2.16	0.46
1:M:78:PRO:HD2	1:N:200:ASP:OD2	2.16	0.46
1:H:15:SER:C	1:H:17:VAL:H	2.18	0.46
1:G:25:ASN:HB3	1:G:28:ASP:HB2	1.97	0.46
1:P:163:LEU:N	1:P:163:LEU:HD23	2.31	0.46
1:A:141:LEU:O	1:A:143:MSE:N	2.45	0.46
1:P:73:LYS:HB3	1:P:99:HIS:CD2	2.51	0.46
1:E:179:VAL:O	1:E:179:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:TYR:CZ	1:K:154:LEU:HD11	2.51	0.46
1:M:93:VAL:O	1:M:122:PRO:HB3	2.16	0.46
1:L:93:VAL:O	1:L:122:PRO:HB3	2.17	0.46
1:E:73:LYS:HB3	1:E:99:HIS:CD2	2.51	0.45
1:I:179:VAL:O	1:I:179:VAL:HG12	2.16	0.45
1:M:150:TYR:CZ	1:M:154:LEU:HD11	2.51	0.45
1:A:150:TYR:CZ	1:A:154:LEU:HD11	2.51	0.45
1:I:166:VAL:HG13	1:I:167:VAL:N	2.32	0.45
1:E:115:VAL:HB	1:E:116:PRO:HD3	1.97	0.45
1:E:85:VAL:HG21	1:E:110:ALA:HB1	1.97	0.45
1:P:25:ASN:ND2	1:P:28:ASP:HB2	2.17	0.45
1:C:192:ARG:HD2	1:C:197:GLU:O	2.17	0.45
1:B:163:LEU:N	1:B:163:LEU:HD23	2.31	0.45
1:O:141:LEU:O	1:O:143:MSE:N	2.45	0.45
1:P:166:VAL:HG13	1:P:167:VAL:N	2.32	0.45
1:L:15:SER:C	1:L:17:VAL:H	2.18	0.45
1:D:26:ARG:NH1	1:D:60:GLU:OE2	2.49	0.45
1:F:192:ARG:HD2	1:F:197:GLU:O	2.17	0.45
1:C:163:LEU:N	1:C:163:LEU:HD23	2.31	0.45
1:N:163:LEU:HD23	1:N:163:LEU:N	2.32	0.45
1:K:179:VAL:HG12	1:K:179:VAL:O	2.16	0.45
1:L:179:VAL:O	1:L:179:VAL:HG12	2.16	0.45
1:N:150:TYR:CZ	1:N:154:LEU:HD11	2.51	0.45
1:H:150:TYR:CZ	1:H:154:LEU:HD11	2.51	0.45
1:O:166:VAL:HG13	1:O:167:VAL:N	2.32	0.45
1:G:115:VAL:HB	1:G:116:PRO:HD3	1.97	0.45
1:B:93:VAL:O	1:B:122:PRO:HB3	2.16	0.45
1:P:192:ARG:HD2	1:P:197:GLU:O	2.17	0.45
1:L:192:ARG:HD2	1:L:197:GLU:O	2.17	0.45
1:O:163:LEU:N	1:O:163:LEU:HD23	2.31	0.45
1:D:163:LEU:N	1:D:163:LEU:HD23	2.31	0.45
1:K:130:LEU:H	1:K:133:MSE:CE	2.30	0.45
1:E:163:LEU:N	1:E:163:LEU:HD23	2.31	0.45
1:P:141:LEU:O	1:P:143:MSE:N	2.45	0.45
1:G:30:LEU:HA	1:G:30:LEU:HD23	1.73	0.45
1:L:73:LYS:HB3	1:L:99:HIS:CD2	2.51	0.45
1:G:179:VAL:O	1:G:179:VAL:HG12	2.16	0.45
1:M:188:THR:HA	1:M:189:PRO:HD3	1.75	0.45
1:F:150:TYR:CZ	1:F:154:LEU:HD11	2.51	0.45
1:P:150:TYR:CZ	1:P:154:LEU:HD11	2.51	0.45
1:A:166:VAL:HG13	1:A:167:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:THR:O	1:G:145:LEU:O	2.35	0.45
1:F:93:VAL:O	1:F:122:PRO:HB3	2.16	0.45
1:N:93:VAL:O	1:N:122:PRO:HB3	2.16	0.45
1:M:15:SER:C	1:M:17:VAL:H	2.18	0.45
1:J:93:VAL:O	1:J:122:PRO:HB3	2.16	0.45
1:N:85:VAL:HG21	1:N:110:ALA:HB1	1.97	0.45
1:D:93:VAL:O	1:D:122:PRO:HB3	2.16	0.45
1:H:192:ARG:HD2	1:H:197:GLU:O	2.17	0.45
1:A:192:ARG:HD2	1:A:197:GLU:O	2.17	0.45
1:I:192:ARG:HD2	1:I:197:GLU:O	2.17	0.45
1:A:163:LEU:HD23	1:A:163:LEU:N	2.31	0.45
1:M:163:LEU:HD23	1:M:163:LEU:N	2.31	0.45
1:E:141:LEU:O	1:E:143:MSE:N	2.45	0.45
1:M:176:PHE:C	1:M:178:GLN:N	2.69	0.45
1:M:179:VAL:HG12	1:M:179:VAL:O	2.16	0.45
1:I:150:TYR:CZ	1:I:154:LEU:HD11	2.51	0.45
1:N:166:VAL:HG13	1:N:167:VAL:N	2.31	0.45
1:J:166:VAL:HG13	1:J:167:VAL:N	2.31	0.45
1:F:15:SER:C	1:F:17:VAL:H	2.18	0.45
1:B:144:THR:O	1:B:145:LEU:O	2.35	0.45
1:C:85:VAL:HG21	1:C:110:ALA:HB1	1.97	0.45
1:E:26:ARG:NH1	1:E:60:GLU:OE2	2.49	0.45
1:B:26:ARG:NH1	1:B:60:GLU:OE2	2.49	0.45
1:E:144:THR:O	1:E:145:LEU:O	2.35	0.45
1:O:192:ARG:HD2	1:O:197:GLU:O	2.17	0.45
1:M:192:ARG:HD2	1:M:197:GLU:O	2.17	0.45
1:J:192:ARG:HD2	1:J:197:GLU:O	2.17	0.45
1:G:163:LEU:HD23	1:G:163:LEU:N	2.31	0.45
1:I:163:LEU:N	1:I:163:LEU:HD23	2.31	0.45
1:I:130:LEU:HD13	1:J:76:ASP:C	2.36	0.45
1:J:176:PHE:C	1:J:178:GLN:N	2.69	0.45
1:C:150:TYR:CZ	1:C:154:LEU:HD11	2.51	0.45
1:B:166:VAL:HG13	1:B:167:VAL:N	2.32	0.45
1:A:144:THR:O	1:A:145:LEU:O	2.35	0.45
1:C:77:ILE:HG22	1:D:132:SER:HB3	1.98	0.45
1:K:93:VAL:O	1:K:122:PRO:HB3	2.16	0.45
1:E:93:VAL:O	1:E:122:PRO:HB3	2.16	0.45
1:K:144:THR:O	1:K:145:LEU:O	2.35	0.45
1:G:26:ARG:NH1	1:G:60:GLU:OE2	2.49	0.45
1:J:111:ARG:HG2	1:J:111:ARG:HH11	1.82	0.45
1:O:224:VAL:O	1:O:230:PRO:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:VAL:O	1:G:230:PRO:CB	2.65	0.45
1:E:224:VAL:O	1:E:230:PRO:CB	2.65	0.45
1:L:224:VAL:O	1:L:230:PRO:CB	2.65	0.45
1:I:206:THR:HG23	1:I:209:GLN:OE1	2.17	0.45
1:C:130:LEU:H	1:C:133:MSE:CE	2.30	0.45
1:K:163:LEU:N	1:K:163:LEU:HD23	2.32	0.45
1:M:137:ASP:OD2	1:N:105:ARG:CD	2.61	0.45
1:D:141:LEU:O	1:D:143:MSE:N	2.45	0.45
1:F:73:LYS:HB3	1:F:99:HIS:CD2	2.51	0.45
1:G:93:VAL:O	1:G:122:PRO:HB3	2.16	0.45
1:H:93:VAL:O	1:H:122:PRO:HB3	2.16	0.45
1:P:26:ARG:NH1	1:P:60:GLU:OE2	2.49	0.45
1:I:144:THR:O	1:I:145:LEU:O	2.35	0.45
1:I:111:ARG:HG2	1:I:111:ARG:HH11	1.82	0.45
1:L:111:ARG:HG2	1:L:111:ARG:HH11	1.82	0.45
1:F:111:ARG:HH11	1:F:111:ARG:HG2	1.82	0.45
1:I:224:VAL:O	1:I:230:PRO:CB	2.65	0.45
1:N:224:VAL:O	1:N:230:PRO:CB	2.65	0.45
1:C:224:VAL:O	1:C:230:PRO:CB	2.65	0.45
1:B:147:PRO:HB3	1:B:203:ARG:NE	2.17	0.45
1:P:147:PRO:HB3	1:P:203:ARG:NE	2.17	0.45
1:N:192:ARG:HD2	1:N:197:GLU:O	2.17	0.45
1:C:206:THR:HG23	1:C:209:GLN:OE1	2.17	0.45
1:L:163:LEU:HD23	1:L:163:LEU:N	2.31	0.45
1:J:163:LEU:HD23	1:J:163:LEU:N	2.31	0.45
1:I:130:LEU:H	1:I:133:MSE:CE	2.30	0.45
1:K:141:LEU:O	1:K:143:MSE:N	2.45	0.45
1:M:73:LYS:HB3	1:M:99:HIS:CD2	2.51	0.45
1:G:73:LYS:HB3	1:G:99:HIS:CD2	2.51	0.45
1:D:179:VAL:O	1:D:179:VAL:HG12	2.15	0.45
1:O:150:TYR:CZ	1:O:154:LEU:HD11	2.51	0.45
1:L:26:ARG:NH1	1:L:60:GLU:OE2	2.49	0.45
1:D:144:THR:O	1:D:145:LEU:O	2.35	0.45
1:K:15:SER:C	1:K:17:VAL:H	2.18	0.45
1:J:15:SER:C	1:J:17:VAL:H	2.18	0.45
1:A:111:ARG:HH11	1:A:111:ARG:HG2	1.82	0.45
1:P:224:VAL:O	1:P:230:PRO:CB	2.65	0.45
1:P:130:LEU:H	1:P:133:MSE:CE	2.30	0.45
1:A:130:LEU:H	1:A:133:MSE:CE	2.30	0.45
1:H:73:LYS:HB3	1:H:99:HIS:CD2	2.51	0.45
1:P:176:PHE:C	1:P:178:GLN:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:VAL:HG13	1:F:167:VAL:N	2.32	0.45
1:A:93:VAL:O	1:A:122:PRO:HB3	2.16	0.45
1:N:15:SER:C	1:N:17:VAL:H	2.18	0.45
1:O:111:ARG:HH11	1:O:111:ARG:HG2	1.82	0.45
1:D:224:VAL:O	1:D:230:PRO:CB	2.65	0.45
1:B:224:VAL:O	1:B:230:PRO:CB	2.65	0.45
1:H:25:ASN:ND2	1:H:28:ASP:HB2	2.17	0.45
1:M:77:ILE:CD1	2:N:314:BMP:H2'	2.47	0.45
1:M:206:THR:HG23	1:M:209:GLN:OE1	2.17	0.45
1:A:206:THR:HG23	1:A:209:GLN:OE1	2.17	0.45
1:C:76:ASP:C	1:D:130:LEU:HD13	2.37	0.45
1:N:130:LEU:H	1:N:133:MSE:CE	2.30	0.45
1:L:176:PHE:C	1:L:178:GLN:N	2.69	0.45
1:J:188:THR:HA	1:J:189:PRO:HD3	1.75	0.45
1:J:26:ARG:NH1	1:J:60:GLU:OE2	2.49	0.45
1:O:93:VAL:O	1:O:122:PRO:HB3	2.16	0.45
1:C:144:THR:O	1:C:145:LEU:O	2.35	0.45
1:P:144:THR:O	1:P:145:LEU:O	2.35	0.45
1:C:111:ARG:HG2	1:C:111:ARG:HH11	1.82	0.45
1:K:111:ARG:HH11	1:K:111:ARG:HG2	1.82	0.45
1:D:147:PRO:HB3	1:D:203:ARG:NE	2.17	0.44
1:B:206:THR:HG23	1:B:209:GLN:OE1	2.17	0.44
1:B:141:LEU:O	1:B:143:MSE:N	2.45	0.44
1:H:176:PHE:C	1:H:178:GLN:N	2.69	0.44
1:B:179:VAL:O	1:B:179:VAL:HG12	2.15	0.44
1:C:166:VAL:HG13	1:C:167:VAL:N	2.32	0.44
1:D:192:ARG:HD2	1:D:197:GLU:O	2.17	0.44
1:F:130:LEU:H	1:F:133:MSE:CE	2.30	0.44
1:J:130:LEU:H	1:J:133:MSE:CE	2.30	0.44
1:H:163:LEU:N	1:H:163:LEU:HD23	2.31	0.44
1:C:12:VAL:CG1	1:J:182:GLN:HG3	2.45	0.44
1:M:166:VAL:HG13	1:M:167:VAL:N	2.32	0.44
1:K:166:VAL:HG13	1:K:167:VAL:N	2.32	0.44
1:I:132:SER:OG	1:J:78:PRO:HD3	2.17	0.44
1:C:93:VAL:O	1:C:122:PRO:HB3	2.16	0.44
1:P:93:VAL:O	1:P:122:PRO:HB3	2.16	0.44
1:M:55:PRO:CB	1:M:91:LEU:HD11	2.48	0.44
1:K:192:ARG:HD2	1:K:197:GLU:O	2.17	0.44
1:K:206:THR:HG23	1:K:209:GLN:OE1	2.17	0.44
1:D:130:LEU:H	1:D:133:MSE:CE	2.30	0.44
1:L:130:LEU:H	1:L:133:MSE:CE	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:LEU:N	1:F:163:LEU:HD23	2.31	0.44
1:I:30:LEU:HA	1:I:30:LEU:HD23	1.73	0.44
1:B:176:PHE:C	1:B:178:GLN:N	2.69	0.44
1:H:55:PRO:CB	1:H:91:LEU:HD11	2.48	0.44
1:D:111:ARG:HG2	1:D:111:ARG:HH11	1.82	0.44
1:K:224:VAL:O	1:K:230:PRO:CB	2.65	0.44
1:A:224:VAL:O	1:A:230:PRO:CB	2.65	0.44
1:M:224:VAL:O	1:M:230:PRO:CB	2.65	0.44
1:D:206:THR:HG23	1:D:209:GLN:OE1	2.17	0.44
1:F:206:THR:HG23	1:F:209:GLN:OE1	2.17	0.44
1:H:130:LEU:H	1:H:133:MSE:CE	2.30	0.44
1:O:47:LYS:HZ3	1:P:75:HIS:H	1.61	0.44
1:G:141:LEU:O	1:G:143:MSE:N	2.45	0.44
1:M:30:LEU:HA	1:M:30:LEU:HD23	1.73	0.44
1:N:179:VAL:HG12	1:N:179:VAL:O	2.16	0.44
1:K:176:PHE:C	1:K:178:GLN:N	2.69	0.44
1:D:176:PHE:C	1:D:178:GLN:N	2.69	0.44
1:L:166:VAL:HG13	1:L:167:VAL:N	2.32	0.44
1:H:166:VAL:HG13	1:H:167:VAL:N	2.32	0.44
1:I:145:LEU:H	1:I:145:LEU:CD2	2.31	0.44
1:D:55:PRO:CB	1:D:91:LEU:HD11	2.48	0.44
1:N:144:THR:O	1:N:145:LEU:O	2.35	0.44
1:H:144:THR:O	1:H:145:LEU:O	2.35	0.44
1:H:145:LEU:H	1:H:145:LEU:CD2	2.31	0.44
1:F:145:LEU:H	1:F:145:LEU:CD2	2.31	0.44
1:J:224:VAL:O	1:J:230:PRO:CB	2.65	0.44
1:O:206:THR:HG23	1:O:209:GLN:OE1	2.17	0.44
1:P:206:THR:HG23	1:P:209:GLN:OE1	2.17	0.44
1:N:176:PHE:C	1:N:178:GLN:N	2.69	0.44
1:G:176:PHE:C	1:G:178:GLN:N	2.69	0.44
1:I:176:PHE:C	1:I:178:GLN:N	2.69	0.44
1:D:166:VAL:HG13	1:D:167:VAL:N	2.32	0.44
1:F:144:THR:O	1:F:145:LEU:O	2.35	0.44
1:I:93:VAL:O	1:I:122:PRO:HB3	2.16	0.44
1:K:26:ARG:NH1	1:K:60:GLU:OE2	2.49	0.44
1:J:145:LEU:H	1:J:145:LEU:CD2	2.31	0.44
1:K:55:PRO:CB	1:K:91:LEU:HD11	2.48	0.44
1:B:55:PRO:CB	1:B:91:LEU:HD11	2.48	0.44
1:B:111:ARG:HG2	1:B:111:ARG:HH11	1.82	0.44
1:I:55:PRO:CB	1:I:91:LEU:HD11	2.48	0.44
1:L:147:PRO:HB3	1:L:203:ARG:NE	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:171:GLN:HG2	1:O:205:MSE:HE3	2.00	0.44
1:C:171:GLN:HG2	1:C:205:MSE:HE3	2.00	0.44
1:A:171:GLN:HG2	1:A:205:MSE:HE3	2.00	0.44
1:O:153:ARG:HH11	1:O:153:ARG:CB	2.25	0.44
1:E:130:LEU:H	1:E:133:MSE:CE	2.30	0.44
1:F:176:PHE:C	1:F:178:GLN:N	2.69	0.44
1:A:145:LEU:CD2	1:A:145:LEU:H	2.31	0.44
1:C:145:LEU:H	1:C:145:LEU:CD2	2.31	0.44
1:J:55:PRO:CB	1:J:91:LEU:HD11	2.47	0.44
1:L:145:LEU:H	1:L:145:LEU:CD2	2.31	0.44
1:F:55:PRO:CB	1:F:91:LEU:HD11	2.48	0.44
1:H:111:ARG:HG2	1:H:111:ARG:HH11	1.82	0.44
1:J:25:ASN:HD22	1:J:28:ASP:CB	2.16	0.44
1:D:146:SER:O	1:D:147:PRO:C	2.56	0.44
1:M:146:SER:O	1:M:147:PRO:C	2.56	0.44
1:N:147:PRO:HB3	1:N:203:ARG:NE	2.17	0.44
1:E:192:ARG:HD2	1:E:197:GLU:O	2.17	0.44
1:B:130:LEU:H	1:B:133:MSE:CE	2.30	0.44
1:O:130:LEU:H	1:O:133:MSE:CE	2.30	0.44
1:I:141:LEU:O	1:I:143:MSE:N	2.45	0.44
1:N:145:LEU:CD2	1:N:145:LEU:H	2.31	0.44
1:L:144:THR:O	1:L:145:LEU:O	2.35	0.44
1:M:144:THR:O	1:M:145:LEU:O	2.35	0.44
1:I:222:ARG:O	1:I:223:PRO:C	2.56	0.44
1:O:144:THR:O	1:O:145:LEU:O	2.35	0.44
1:F:128:THR:OG1	1:F:129:VAL:N	2.43	0.44
1:A:26:ARG:NH1	1:A:60:GLU:OE2	2.49	0.44
1:F:222:ARG:O	1:F:223:PRO:C	2.56	0.44
1:N:171:GLN:HG2	1:N:205:MSE:HE3	2.00	0.44
1:G:192:ARG:HD2	1:G:197:GLU:O	2.17	0.44
1:M:130:LEU:H	1:M:133:MSE:CE	2.30	0.44
1:G:130:LEU:H	1:G:133:MSE:CE	2.30	0.44
1:E:176:PHE:C	1:E:178:GLN:N	2.69	0.44
1:G:200:ASP:HA	1:H:105:ARG:HH22	1.83	0.44
1:B:25:ASN:HD22	1:B:28:ASP:CB	2.16	0.44
1:K:222:ARG:O	1:K:223:PRO:C	2.56	0.44
1:A:222:ARG:O	1:A:223:PRO:C	2.56	0.44
1:C:176:PHE:C	1:C:178:GLN:N	2.69	0.44
1:G:145:LEU:H	1:G:145:LEU:CD2	2.31	0.44
1:D:55:PRO:HB3	1:D:91:LEU:HD11	2.00	0.44
1:J:144:THR:O	1:J:145:LEU:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PRO:HB3	1:B:91:LEU:HD11	2.00	0.44
1:O:55:PRO:CB	1:O:91:LEU:HD11	2.48	0.44
1:N:55:PRO:HB3	1:N:91:LEU:HD11	2.00	0.44
1:L:55:PRO:CB	1:L:91:LEU:HD11	2.48	0.44
1:N:111:ARG:HG2	1:N:111:ARG:HH11	1.82	0.44
1:C:55:PRO:CB	1:C:91:LEU:HD11	2.48	0.44
1:A:169:SER:HB2	1:A:203:ARG:NH1	2.33	0.43
1:F:171:GLN:HG2	1:F:205:MSE:HE3	2.00	0.43
1:H:206:THR:HG23	1:H:209:GLN:OE1	2.17	0.43
1:B:192:ARG:HD2	1:B:197:GLU:O	2.17	0.43
1:C:222:ARG:O	1:C:223:PRO:C	2.56	0.43
1:L:206:THR:HG23	1:L:209:GLN:OE1	2.17	0.43
1:M:76:ASP:OD1	1:N:73:LYS:NZ	2.51	0.43
1:E:200:ASP:HA	1:F:105:ARG:HH22	1.83	0.43
1:E:145:LEU:CD2	1:E:145:LEU:H	2.31	0.43
1:O:55:PRO:HB3	1:O:91:LEU:HD11	2.00	0.43
1:N:55:PRO:CB	1:N:91:LEU:HD11	2.48	0.43
1:A:55:PRO:HB3	1:A:91:LEU:HD11	2.00	0.43
1:E:111:ARG:HG2	1:E:111:ARG:HH11	1.82	0.43
1:C:169:SER:HB2	1:C:203:ARG:NH1	2.33	0.43
1:G:171:GLN:HG2	1:G:205:MSE:HE3	2.00	0.43
1:P:222:ARG:O	1:P:223:PRO:C	2.56	0.43
1:E:76:ASP:C	1:F:130:LEU:HD13	2.39	0.43
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.73	0.43
1:M:145:LEU:CD2	1:M:145:LEU:H	2.31	0.43
1:H:222:ARG:O	1:H:223:PRO:C	2.56	0.43
1:M:111:ARG:HH11	1:M:111:ARG:HG2	1.82	0.43
1:H:224:VAL:O	1:H:230:PRO:CB	2.65	0.43
1:F:224:VAL:O	1:F:230:PRO:CB	2.65	0.43
1:J:146:SER:O	1:J:147:PRO:C	2.56	0.43
1:N:206:THR:HG23	1:N:209:GLN:OE1	2.17	0.43
1:G:206:THR:HG23	1:G:209:GLN:OE1	2.17	0.43
1:P:171:GLN:HG2	1:P:205:MSE:HE3	2.00	0.43
1:E:206:THR:HG23	1:E:209:GLN:OE1	2.17	0.43
1:I:171:GLN:HG2	1:I:205:MSE:HE3	2.00	0.43
1:C:55:PRO:HB3	1:C:91:LEU:HD11	2.00	0.43
1:G:55:PRO:HB3	1:G:91:LEU:HD11	2.00	0.43
1:E:55:PRO:HB3	1:E:91:LEU:HD11	2.00	0.43
1:P:55:PRO:CB	1:P:91:LEU:HD11	2.48	0.43
1:M:222:ARG:O	1:M:223:PRO:C	2.56	0.43
1:G:111:ARG:HG2	1:G:111:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:SER:HB2	1:E:203:ARG:NH1	2.33	0.43
1:H:171:GLN:HG2	1:H:205:MSE:HE3	2.00	0.43
1:J:206:THR:HG23	1:J:209:GLN:OE1	2.17	0.43
1:J:56:GLN:HE21	1:J:56:GLN:HA	1.84	0.43
1:M:55:PRO:HB3	1:M:91:LEU:HD11	2.00	0.43
1:A:55:PRO:CB	1:A:91:LEU:HD11	2.48	0.43
1:P:55:PRO:HB3	1:P:91:LEU:HD11	2.00	0.43
1:O:222:ARG:O	1:O:223:PRO:C	2.56	0.43
1:P:111:ARG:HH11	1:P:111:ARG:HG2	1.82	0.43
1:M:171:GLN:HG2	1:M:205:MSE:HE3	2.00	0.43
1:A:176:PHE:C	1:A:178:GLN:N	2.69	0.43
1:K:145:LEU:CD2	1:K:145:LEU:H	2.31	0.43
1:K:55:PRO:HB3	1:K:91:LEU:HD11	2.00	0.43
1:G:55:PRO:CB	1:G:91:LEU:HD11	2.48	0.43
1:E:55:PRO:CB	1:E:91:LEU:HD11	2.48	0.43
1:C:26:ARG:NH1	1:C:60:GLU:OE2	2.49	0.43
1:F:26:ARG:NH1	1:F:60:GLU:OE2	2.49	0.43
1:H:26:ARG:NH1	1:H:60:GLU:OE2	2.49	0.43
1:I:26:ARG:NH1	1:I:60:GLU:OE2	2.49	0.43
1:M:169:SER:HB2	1:M:203:ARG:NH1	2.33	0.43
1:N:146:SER:O	1:N:147:PRO:C	2.56	0.43
1:P:169:SER:HB2	1:P:203:ARG:NH1	2.33	0.43
1:B:171:GLN:HG2	1:B:205:MSE:HE3	2.00	0.43
1:N:141:LEU:O	1:N:143:MSE:N	2.45	0.43
1:L:188:THR:HA	1:L:189:PRO:HD3	1.75	0.43
1:G:166:VAL:HG13	1:G:167:VAL:N	2.32	0.43
1:O:145:LEU:CD2	1:O:145:LEU:H	2.31	0.43
1:O:26:ARG:NH1	1:O:60:GLU:OE2	2.49	0.43
1:F:147:PRO:HB3	1:F:203:ARG:NE	2.17	0.43
1:O:169:SER:HB2	1:O:203:ARG:NH1	2.33	0.43
1:D:169:SER:HB2	1:D:203:ARG:NH1	2.33	0.43
1:L:25:ASN:HD22	1:L:28:ASP:CB	2.16	0.43
1:J:171:GLN:HG2	1:J:205:MSE:HE3	2.00	0.43
1:E:166:VAL:HG13	1:E:167:VAL:N	2.32	0.43
1:O:200:ASP:OD2	1:P:78:PRO:HD2	2.18	0.43
1:B:145:LEU:CD2	1:B:145:LEU:H	2.31	0.43
1:M:26:ARG:NH1	1:M:60:GLU:OE2	2.49	0.43
1:L:153:ARG:HH11	1:L:153:ARG:CB	2.25	0.43
1:P:145:LEU:H	1:P:145:LEU:CD2	2.31	0.43
1:A:156:ALA:O	1:A:160:LYS:HG3	2.19	0.43
1:N:26:ARG:NH1	1:N:60:GLU:OE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:HB2	1:B:203:ARG:NH1	2.33	0.43
1:G:146:SER:O	1:G:147:PRO:C	2.56	0.43
1:F:202:ARG:HA	1:F:202:ARG:HD3	1.89	0.43
1:O:75:HIS:H	1:P:47:LYS:HZ2	1.66	0.43
1:F:55:PRO:HB3	1:F:91:LEU:HD11	2.01	0.43
1:N:222:ARG:O	1:N:223:PRO:C	2.56	0.43
1:G:156:ALA:O	1:G:160:LYS:HG3	2.19	0.43
1:B:156:ALA:O	1:B:160:LYS:HG3	2.19	0.43
1:C:146:SER:O	1:C:147:PRO:C	2.56	0.43
1:E:171:GLN:HG2	1:E:205:MSE:HE3	2.00	0.43
1:N:30:LEU:HA	1:N:30:LEU:HD23	1.73	0.43
1:H:56:GLN:HA	1:H:56:GLN:HE21	1.84	0.43
1:C:156:ALA:O	1:C:160:LYS:HG3	2.19	0.43
1:E:156:ALA:O	1:E:160:LYS:HG3	2.19	0.43
1:G:25:ASN:HD22	1:G:28:ASP:N	2.13	0.42
1:F:25:ASN:ND2	1:F:28:ASP:HB2	2.17	0.42
1:L:56:GLN:HA	1:L:56:GLN:HE21	1.84	0.42
1:H:55:PRO:HB3	1:H:91:LEU:HD11	2.00	0.42
1:K:29:ALA:O	1:K:33:VAL:HG23	2.19	0.42
1:N:156:ALA:O	1:N:160:LYS:HG3	2.19	0.42
1:E:146:SER:O	1:E:147:PRO:C	2.56	0.42
1:G:206:THR:H	1:G:209:GLN:CG	2.33	0.42
1:N:56:GLN:HE21	1:N:56:GLN:HA	1.84	0.42
1:D:155:ALA:HA	1:D:166:VAL:HG21	2.02	0.42
1:I:55:PRO:HB3	1:I:91:LEU:HD11	2.00	0.42
1:J:55:PRO:HB3	1:J:91:LEU:HD11	2.00	0.42
1:L:156:ALA:O	1:L:160:LYS:HG3	2.19	0.42
1:F:29:ALA:O	1:F:33:VAL:HG23	2.20	0.42
1:M:100:ALA:C	1:M:102:GLY:H	2.23	0.42
1:O:146:SER:O	1:O:147:PRO:C	2.57	0.42
1:K:146:SER:O	1:K:147:PRO:C	2.56	0.42
1:E:147:PRO:HB3	1:E:203:ARG:NE	2.17	0.42
1:H:206:THR:H	1:H:209:GLN:CG	2.33	0.42
1:E:206:THR:H	1:E:209:GLN:CG	2.33	0.42
1:K:171:GLN:HG2	1:K:205:MSE:HE3	2.00	0.42
1:K:202:ARG:HD3	1:K:202:ARG:HA	1.89	0.42
1:L:222:ARG:O	1:L:223:PRO:C	2.56	0.42
1:D:30:LEU:HA	1:D:30:LEU:HD23	1.73	0.42
1:O:56:GLN:HA	1:O:56:GLN:HE21	1.84	0.42
1:O:174:VAL:O	1:O:178:GLN:HB3	2.20	0.42
1:K:155:ALA:HA	1:K:166:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:HA	1:B:166:VAL:HG21	2.02	0.42
1:E:155:ALA:HA	1:E:166:VAL:HG21	2.02	0.42
1:D:145:LEU:H	1:D:145:LEU:CD2	2.31	0.42
1:A:29:ALA:O	1:A:33:VAL:HG23	2.19	0.42
1:F:100:ALA:C	1:F:102:GLY:H	2.23	0.42
1:H:100:ALA:C	1:H:102:GLY:H	2.23	0.42
1:H:29:ALA:O	1:H:33:VAL:HG23	2.19	0.42
1:B:29:ALA:O	1:B:33:VAL:HG23	2.20	0.42
1:J:156:ALA:O	1:J:160:LYS:HG3	2.19	0.42
1:G:112:GLU:CD	1:K:160:LYS:NZ	2.73	0.42
1:B:25:ASN:ND2	1:B:28:ASP:HB2	2.17	0.42
1:D:25:ASN:HD22	1:D:28:ASP:CB	2.16	0.42
1:D:171:GLN:HG2	1:D:205:MSE:HE3	2.00	0.42
1:F:206:THR:H	1:F:209:GLN:CG	2.33	0.42
1:B:206:THR:H	1:B:209:GLN:CG	2.33	0.42
1:L:206:THR:H	1:L:209:GLN:CG	2.33	0.42
1:A:130:LEU:HD13	1:B:76:ASP:C	2.40	0.42
1:I:188:THR:HA	1:I:189:PRO:HD3	1.75	0.42
1:N:155:ALA:HA	1:N:166:VAL:HG21	2.01	0.42
1:O:77:ILE:CG2	1:P:132:SER:HB3	2.49	0.42
1:L:55:PRO:HB3	1:L:91:LEU:HD11	2.00	0.42
1:K:156:ALA:O	1:K:160:LYS:HG3	2.19	0.42
1:M:156:ALA:O	1:M:160:LYS:HG3	2.19	0.42
1:D:156:ALA:O	1:D:160:LYS:HG3	2.19	0.42
1:B:228:VAL:HB	1:C:236:ALA:CB	2.42	0.42
1:P:25:ASN:HD22	1:P:28:ASP:N	2.13	0.42
1:D:206:THR:H	1:D:209:GLN:CG	2.33	0.42
1:H:202:ARG:HA	1:H:202:ARG:HD3	1.89	0.42
1:H:68:ILE:O	1:H:94:TRP:HB3	2.20	0.42
1:G:68:ILE:O	1:G:94:TRP:HB3	2.20	0.42
1:E:68:ILE:O	1:E:94:TRP:HB3	2.20	0.42
1:C:68:ILE:O	1:C:94:TRP:HB3	2.20	0.42
1:A:68:ILE:O	1:A:94:TRP:HB3	2.20	0.42
1:K:68:ILE:O	1:K:94:TRP:HB3	2.20	0.42
1:L:174:VAL:O	1:L:178:GLN:HB3	2.20	0.42
1:P:155:ALA:HA	1:P:166:VAL:HG21	2.02	0.42
1:G:155:ALA:HA	1:G:166:VAL:HG21	2.02	0.42
1:D:29:ALA:O	1:D:33:VAL:HG23	2.19	0.42
1:G:18:VAL:HA	1:G:42:ARG:O	2.20	0.42
1:C:29:ALA:O	1:C:33:VAL:HG23	2.19	0.42
1:I:29:ALA:O	1:I:33:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:VAL:HA	1:D:42:ARG:O	2.20	0.42
1:J:29:ALA:O	1:J:33:VAL:HG23	2.19	0.42
1:M:25:ASN:HD21	1:M:27:ASP:HB2	1.85	0.42
1:O:25:ASN:HD21	1:O:27:ASP:HB2	1.85	0.42
1:I:169:SER:HB2	1:I:203:ARG:NH1	2.33	0.42
1:L:146:SER:O	1:L:147:PRO:C	2.56	0.42
1:C:25:ASN:HD21	1:C:27:ASP:HB2	1.85	0.42
1:M:68:ILE:O	1:M:94:TRP:HB3	2.20	0.42
1:F:68:ILE:O	1:F:94:TRP:HB3	2.20	0.42
1:E:174:VAL:O	1:E:178:GLN:HB3	2.19	0.42
1:A:174:VAL:O	1:A:178:GLN:HB3	2.20	0.42
1:P:100:ALA:C	1:P:102:GLY:H	2.23	0.42
1:B:222:ARG:O	1:B:223:PRO:C	2.56	0.42
1:K:18:VAL:HA	1:K:42:ARG:O	2.20	0.42
1:M:29:ALA:O	1:M:33:VAL:HG23	2.20	0.42
1:O:156:ALA:O	1:O:160:LYS:HG3	2.19	0.42
1:C:18:VAL:HA	1:C:42:ARG:O	2.20	0.42
1:E:18:VAL:HA	1:E:42:ARG:O	2.20	0.42
1:O:18:VAL:HA	1:O:42:ARG:O	2.20	0.42
1:F:146:SER:O	1:F:147:PRO:C	2.56	0.42
1:O:206:THR:H	1:O:209:GLN:CG	2.33	0.42
1:M:206:THR:H	1:M:209:GLN:CG	2.33	0.42
1:J:222:ARG:O	1:J:223:PRO:C	2.56	0.42
1:P:30:LEU:HA	1:P:30:LEU:HD23	1.73	0.42
1:J:174:VAL:O	1:J:178:GLN:HB3	2.20	0.42
1:M:155:ALA:HA	1:M:166:VAL:HG21	2.02	0.42
1:F:156:ALA:O	1:F:160:LYS:HG3	2.19	0.42
1:L:18:VAL:HA	1:L:42:ARG:O	2.20	0.42
1:D:222:ARG:O	1:D:223:PRO:C	2.56	0.42
1:P:29:ALA:O	1:P:33:VAL:HG23	2.19	0.42
1:G:25:ASN:HD21	1:G:27:ASP:HB2	1.85	0.42
1:A:25:ASN:HD21	1:A:27:ASP:HB2	1.85	0.42
1:G:147:PRO:HB3	1:G:203:ARG:NE	2.17	0.42
1:L:171:GLN:HG2	1:L:205:MSE:HE3	2.00	0.42
1:F:56:GLN:HA	1:F:56:GLN:HE21	1.84	0.42
1:C:174:VAL:O	1:C:178:GLN:HB3	2.19	0.42
1:L:155:ALA:HA	1:L:166:VAL:HG21	2.02	0.42
1:I:100:ALA:C	1:I:102:GLY:H	2.23	0.42
1:G:77:ILE:HG22	1:H:132:SER:HB3	2.02	0.42
1:G:100:ALA:C	1:G:102:GLY:H	2.23	0.42
1:B:25:ASN:HD21	1:B:27:ASP:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:ASN:HD21	1:I:27:ASP:HB2	1.85	0.42
1:E:25:ASN:HD21	1:E:27:ASP:HB2	1.85	0.42
1:E:25:ASN:HD22	1:E:28:ASP:N	2.13	0.42
1:K:25:ASN:HD21	1:K:27:ASP:HB2	1.85	0.42
1:L:169:SER:HB2	1:L:203:ARG:NH1	2.33	0.42
1:A:146:SER:O	1:A:147:PRO:C	2.56	0.42
1:J:206:THR:H	1:J:209:GLN:CG	2.33	0.42
1:K:206:THR:H	1:K:209:GLN:CG	2.33	0.42
1:J:141:LEU:O	1:J:143:MSE:N	2.45	0.42
1:D:174:VAL:O	1:D:178:GLN:HB3	2.20	0.42
1:K:188:THR:HA	1:K:189:PRO:HD3	1.75	0.42
1:J:155:ALA:HA	1:J:166:VAL:HG21	2.01	0.42
1:J:18:VAL:HA	1:J:42:ARG:O	2.20	0.42
1:D:100:ALA:C	1:D:102:GLY:H	2.23	0.42
1:H:156:ALA:O	1:H:160:LYS:HG3	2.19	0.42
1:I:18:VAL:HA	1:I:42:ARG:O	2.20	0.42
1:O:29:ALA:O	1:O:33:VAL:HG23	2.19	0.42
1:C:182:GLN:HG2	1:J:12:VAL:HG12	2.00	0.42
1:J:169:SER:HB2	1:J:203:ARG:NH1	2.33	0.42
1:J:205:MSE:HG3	1:J:209:GLN:CG	2.50	0.42
1:E:56:GLN:HE21	1:E:56:GLN:HA	1.84	0.42
1:B:174:VAL:O	1:B:178:GLN:HB3	2.20	0.42
1:I:37:ASP:CG	1:I:38:PRO:HD2	2.41	0.42
1:L:37:ASP:CG	1:L:38:PRO:HD2	2.41	0.42
1:L:29:ALA:O	1:L:33:VAL:HG23	2.19	0.42
1:B:18:VAL:HA	1:B:42:ARG:O	2.20	0.42
1:I:156:ALA:O	1:I:160:LYS:HG3	2.19	0.42
1:A:18:VAL:HA	1:A:42:ARG:O	2.20	0.42
1:J:25:ASN:HD21	1:J:27:ASP:HB2	1.85	0.41
1:I:146:SER:O	1:I:147:PRO:C	2.56	0.41
1:P:25:ASN:HD21	1:P:27:ASP:HB2	1.85	0.41
1:H:146:SER:O	1:H:147:PRO:C	2.56	0.41
1:A:206:THR:H	1:A:209:GLN:CG	2.33	0.41
1:E:153:ARG:HH11	1:E:153:ARG:CB	2.25	0.41
1:L:68:ILE:O	1:L:94:TRP:HB3	2.20	0.41
1:K:56:GLN:HE21	1:K:56:GLN:HA	1.84	0.41
1:F:174:VAL:O	1:F:178:GLN:HB3	2.20	0.41
1:G:174:VAL:O	1:G:178:GLN:HB3	2.20	0.41
1:I:155:ALA:HA	1:I:166:VAL:HG21	2.02	0.41
1:K:105:ARG:HH22	1:L:200:ASP:HA	1.84	0.41
1:H:37:ASP:CG	1:H:38:PRO:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:N	1:A:145:LEU:CD2	2.83	0.41
1:F:145:LEU:N	1:F:145:LEU:CD2	2.83	0.41
1:E:100:ALA:C	1:E:102:GLY:H	2.23	0.41
1:G:29:ALA:O	1:G:33:VAL:HG23	2.20	0.41
1:N:18:VAL:HA	1:N:42:ARG:O	2.20	0.41
1:P:156:ALA:O	1:P:160:LYS:HG3	2.19	0.41
1:P:18:VAL:HA	1:P:42:ARG:O	2.20	0.41
1:A:25:ASN:HD22	1:A:28:ASP:N	2.13	0.41
1:L:25:ASN:HD21	1:L:27:ASP:HB2	1.85	0.41
1:N:206:THR:H	1:N:209:GLN:CG	2.33	0.41
1:P:68:ILE:O	1:P:94:TRP:HB3	2.20	0.41
1:I:68:ILE:O	1:I:94:TRP:HB3	2.20	0.41
1:F:155:ALA:HA	1:F:166:VAL:HG21	2.01	0.41
1:P:37:ASP:CG	1:P:38:PRO:HD2	2.41	0.41
1:J:37:ASP:CG	1:J:38:PRO:HD2	2.40	0.41
1:G:145:LEU:N	1:G:145:LEU:CD2	2.83	0.41
1:C:145:LEU:N	1:C:145:LEU:CD2	2.83	0.41
1:O:145:LEU:CD2	1:O:145:LEU:N	2.84	0.41
1:F:18:VAL:HA	1:F:42:ARG:O	2.20	0.41
1:B:100:ALA:C	1:B:102:GLY:H	2.23	0.41
1:O:100:ALA:C	1:O:102:GLY:H	2.23	0.41
1:B:25:ASN:HD22	1:B:28:ASP:N	2.13	0.41
1:N:169:SER:HB2	1:N:203:ARG:NH1	2.33	0.41
1:K:169:SER:HB2	1:K:203:ARG:NH1	2.34	0.41
1:M:205:MSE:HG3	1:M:209:GLN:CG	2.50	0.41
1:B:205:MSE:HG3	1:B:209:GLN:CG	2.50	0.41
1:P:206:THR:H	1:P:209:GLN:CG	2.33	0.41
1:I:206:THR:H	1:I:209:GLN:CG	2.33	0.41
1:O:68:ILE:O	1:O:94:TRP:HB3	2.20	0.41
1:E:130:LEU:HD13	1:F:76:ASP:C	2.41	0.41
1:K:30:LEU:HD23	1:K:30:LEU:HA	1.73	0.41
1:P:174:VAL:O	1:P:178:GLN:HB3	2.20	0.41
1:F:188:THR:HA	1:F:189:PRO:HD3	1.75	0.41
1:G:105:ARG:HH22	1:H:200:ASP:HA	1.85	0.41
1:M:37:ASP:CG	1:M:38:PRO:HD2	2.41	0.41
1:K:37:ASP:CG	1:K:38:PRO:HD2	2.41	0.41
1:N:37:ASP:CG	1:N:38:PRO:HD2	2.41	0.41
1:O:37:ASP:CG	1:O:38:PRO:HD2	2.41	0.41
1:E:145:LEU:CD2	1:E:145:LEU:N	2.83	0.41
1:E:222:ARG:O	1:E:223:PRO:C	2.56	0.41
1:D:25:ASN:HD22	1:D:28:ASP:N	2.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:MSE:HG3	1:D:209:GLN:CG	2.50	0.41
1:F:209:GLN:O	1:F:212:SER:HB2	2.21	0.41
1:N:205:MSE:HG3	1:N:209:GLN:CG	2.50	0.41
1:H:209:GLN:O	1:H:212:SER:HB2	2.21	0.41
1:C:206:THR:H	1:C:209:GLN:CG	2.33	0.41
1:K:209:GLN:O	1:K:212:SER:HB2	2.20	0.41
1:A:205:MSE:HG3	1:A:209:GLN:CG	2.50	0.41
1:L:205:MSE:HG3	1:L:209:GLN:CG	2.50	0.41
1:F:153:ARG:HH11	1:F:153:ARG:CB	2.25	0.41
1:B:68:ILE:O	1:B:94:TRP:HB3	2.20	0.41
1:J:30:LEU:HD23	1:J:30:LEU:HA	1.73	0.41
1:I:200:ASP:HA	1:J:105:ARG:HH22	1.85	0.41
1:K:174:VAL:O	1:K:178:GLN:HB3	2.20	0.41
1:C:155:ALA:HA	1:C:166:VAL:HG21	2.02	0.41
1:A:105:ARG:HH22	1:B:200:ASP:HA	1.85	0.41
1:F:37:ASP:CG	1:F:38:PRO:HD2	2.41	0.41
1:I:145:LEU:N	1:I:145:LEU:CD2	2.84	0.41
1:H:145:LEU:N	1:H:145:LEU:CD2	2.83	0.41
1:L:145:LEU:N	1:L:145:LEU:CD2	2.83	0.41
1:M:18:VAL:HA	1:M:42:ARG:O	2.20	0.41
1:N:29:ALA:O	1:N:33:VAL:HG23	2.19	0.41
1:H:25:ASN:HD21	1:H:27:ASP:HB2	1.85	0.41
1:C:25:ASN:HD22	1:C:28:ASP:N	2.13	0.41
1:F:25:ASN:HD21	1:F:27:ASP:HB2	1.85	0.41
1:I:205:MSE:HG3	1:I:209:GLN:CG	2.50	0.41
1:O:69:PHE:CE2	1:O:95:MSE:HE3	2.55	0.41
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.73	0.41
1:D:56:GLN:HA	1:D:56:GLN:HE21	1.84	0.41
1:H:174:VAL:O	1:H:178:GLN:HB3	2.20	0.41
1:M:174:VAL:O	1:M:178:GLN:HB3	2.20	0.41
1:I:174:VAL:O	1:I:178:GLN:HB3	2.20	0.41
1:N:145:LEU:N	1:N:145:LEU:CD2	2.83	0.41
1:A:100:ALA:C	1:A:102:GLY:H	2.23	0.41
1:D:25:ASN:HD21	1:D:27:ASP:HB2	1.85	0.41
1:L:209:GLN:O	1:L:212:SER:HB2	2.20	0.41
1:D:68:ILE:O	1:D:94:TRP:HB3	2.20	0.41
1:G:130:LEU:HD13	1:H:76:ASP:C	2.41	0.41
1:K:130:LEU:HD13	1:L:76:ASP:C	2.40	0.41
1:G:56:GLN:HA	1:G:56:GLN:HE21	1.84	0.41
1:P:123:LEU:HB3	1:P:125:ILE:HD11	2.03	0.41
1:H:155:ALA:HA	1:H:166:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ASP:CG	1:D:38:PRO:HD2	2.41	0.41
1:B:145:LEU:CD2	1:B:145:LEU:N	2.84	0.41
1:G:222:ARG:O	1:G:223:PRO:C	2.56	0.41
1:N:25:ASN:HD21	1:N:27:ASP:HB2	1.85	0.41
1:D:209:GLN:O	1:D:212:SER:HB2	2.21	0.41
1:N:209:GLN:O	1:N:212:SER:HB2	2.20	0.41
1:P:205:MSE:HG3	1:P:209:GLN:CG	2.50	0.41
1:C:205:MSE:HG3	1:C:209:GLN:CG	2.50	0.41
1:I:202:ARG:HA	1:I:202:ARG:HD3	1.89	0.41
1:E:69:PHE:CE2	1:E:95:MSE:HE3	2.55	0.41
1:B:56:GLN:HE21	1:B:56:GLN:HA	1.84	0.41
1:G:37:ASP:CG	1:G:38:PRO:HD2	2.41	0.41
1:P:145:LEU:N	1:P:145:LEU:CD2	2.84	0.41
1:E:29:ALA:O	1:E:33:VAL:HG23	2.20	0.41
1:O:209:GLN:O	1:O:212:SER:HB2	2.21	0.41
1:M:132:SER:HB3	1:N:77:ILE:HG22	2.03	0.41
1:M:209:GLN:O	1:M:212:SER:HB2	2.21	0.41
1:J:209:GLN:O	1:J:212:SER:HB2	2.21	0.41
1:B:209:GLN:O	1:B:212:SER:HB2	2.21	0.41
1:K:205:MSE:HG3	1:K:209:GLN:CG	2.50	0.41
1:J:69:PHE:CE2	1:J:95:MSE:HE3	2.55	0.41
1:L:56:GLN:NE2	1:L:59:ARG:HH11	2.19	0.41
1:A:188:THR:HA	1:A:189:PRO:HD3	1.75	0.41
1:E:37:ASP:CG	1:E:38:PRO:HD2	2.41	0.41
1:B:37:ASP:CG	1:B:38:PRO:HD2	2.41	0.41
1:K:100:ALA:C	1:K:102:GLY:H	2.23	0.41
1:N:100:ALA:C	1:N:102:GLY:H	2.23	0.41
1:N:22:ASP:OD1	1:N:22:ASP:N	2.54	0.41
1:L:239:ALA:HA	1:L:242:GLN:NE2	2.36	0.41
1:F:239:ALA:HA	1:F:242:GLN:NE2	2.36	0.41
1:A:132:SER:HB3	1:B:77:ILE:HG22	2.03	0.41
1:L:25:ASN:HD22	1:L:28:ASP:N	2.13	0.41
1:O:205:MSE:HG3	1:O:209:GLN:CG	2.50	0.41
1:H:205:MSE:HG3	1:H:209:GLN:CG	2.50	0.41
1:I:209:GLN:O	1:I:212:SER:HB2	2.21	0.41
1:B:153:ARG:HH11	1:B:153:ARG:CB	2.25	0.41
1:N:68:ILE:O	1:N:94:TRP:HB3	2.20	0.41
1:G:69:PHE:CE2	1:G:95:MSE:HE3	2.55	0.41
1:J:68:ILE:O	1:J:94:TRP:HB3	2.20	0.41
1:L:141:LEU:C	1:L:143:MSE:H	2.24	0.41
1:I:56:GLN:NE2	1:I:59:ARG:HH11	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:VAL:HG22	1:J:213:ALA:CB	2.51	0.41
1:H:174:VAL:HG22	1:H:213:ALA:CB	2.51	0.41
1:M:174:VAL:HG22	1:M:213:ALA:CB	2.51	0.41
1:P:188:THR:HA	1:P:189:PRO:HD3	1.75	0.41
1:A:155:ALA:HA	1:A:166:VAL:HG21	2.02	0.41
1:M:158:THR:HG21	1:M:166:VAL:HG23	2.03	0.41
1:C:123:LEU:HB3	1:C:125:ILE:HD11	2.03	0.41
1:E:123:LEU:HB3	1:E:125:ILE:HD11	2.03	0.41
1:K:145:LEU:N	1:K:145:LEU:CD2	2.84	0.41
1:M:239:ALA:HA	1:M:242:GLN:NE2	2.36	0.41
1:J:100:ALA:C	1:J:102:GLY:H	2.23	0.41
1:N:239:ALA:HA	1:N:242:GLN:NE2	2.36	0.41
1:N:239:ALA:HA	1:N:242:GLN:HE21	1.86	0.41
1:O:239:ALA:HA	1:O:242:GLN:NE2	2.36	0.41
1:P:239:ALA:HA	1:P:242:GLN:NE2	2.36	0.41
1:H:18:VAL:HA	1:H:42:ARG:O	2.20	0.41
1:B:239:ALA:HA	1:B:242:GLN:NE2	2.36	0.41
1:E:239:ALA:HA	1:E:242:GLN:HE21	1.86	0.41
1:B:22:ASP:N	1:B:22:ASP:OD1	2.54	0.41
1:P:146:SER:O	1:P:147:PRO:C	2.56	0.41
1:G:169:SER:HB2	1:G:203:ARG:NH1	2.33	0.41
1:F:205:MSE:HG3	1:F:209:GLN:CG	2.50	0.41
1:M:77:ILE:HD13	2:N:314:BMP:H2'	2.03	0.41
2:E:305:BMP:H2'	1:F:77:ILE:CD1	2.52	0.41
1:P:153:ARG:HH11	1:P:153:ARG:CB	2.25	0.41
1:N:174:VAL:O	1:N:178:GLN:HB3	2.20	0.41
1:F:174:VAL:HG22	1:F:213:ALA:CB	2.51	0.41
1:A:200:ASP:HA	1:B:105:ARG:HH22	1.85	0.41
1:L:174:VAL:HG22	1:L:213:ALA:CB	2.51	0.41
1:H:188:THR:HA	1:H:189:PRO:HD3	1.75	0.41
1:K:158:THR:HG21	1:K:166:VAL:HG23	2.03	0.41
1:I:123:LEU:HB3	1:I:125:ILE:HD11	2.03	0.41
1:J:145:LEU:N	1:J:145:LEU:CD2	2.83	0.41
1:M:145:LEU:CD2	1:M:145:LEU:N	2.84	0.41
1:N:222:ARG:HA	1:N:225:THR:OG1	2.21	0.41
1:H:239:ALA:HA	1:H:242:GLN:NE2	2.36	0.41
1:I:239:ALA:HA	1:I:242:GLN:NE2	2.36	0.41
1:L:100:ALA:C	1:L:102:GLY:H	2.23	0.41
1:B:228:VAL:CG2	1:C:233:THR:HG23	2.50	0.40
1:M:25:ASN:HD22	1:M:28:ASP:N	2.13	0.40
1:E:205:MSE:HG3	1:E:209:GLN:CG	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:ARG:HH21	1:L:223:PRO:CD	2.35	0.40
1:M:69:PHE:CE2	1:M:95:MSE:HE3	2.55	0.40
1:A:56:GLN:NE2	1:A:59:ARG:HH11	2.19	0.40
1:I:56:GLN:HE21	1:I:56:GLN:HA	1.84	0.40
1:A:174:VAL:HG22	1:A:213:ALA:CB	2.51	0.40
1:K:200:ASP:HA	1:L:105:ARG:HH22	1.86	0.40
1:P:158:THR:HG21	1:P:166:VAL:HG23	2.03	0.40
1:G:132:SER:HB3	1:H:77:ILE:HG22	2.02	0.40
1:C:100:ALA:C	1:C:102:GLY:H	2.23	0.40
1:G:239:ALA:HA	1:G:242:GLN:HE21	1.86	0.40
1:D:239:ALA:HA	1:D:242:GLN:NE2	2.36	0.40
1:F:22:ASP:N	1:F:22:ASP:OD1	2.54	0.40
1:K:173:ALA:CB	1:K:215:VAL:HG12	2.52	0.40
1:A:192:ARG:HH21	1:A:223:PRO:CD	2.35	0.40
1:D:64:ARG:HG2	1:D:64:ARG:HH11	1.87	0.40
1:I:64:ARG:HG2	1:I:64:ARG:HH11	1.86	0.40
1:C:56:GLN:NE2	1:C:59:ARG:HH11	2.19	0.40
1:N:174:VAL:HG22	1:N:213:ALA:CB	2.51	0.40
1:N:173:ALA:CB	1:N:215:VAL:HG12	2.52	0.40
1:A:22:ASP:OD1	1:A:22:ASP:N	2.54	0.40
1:P:22:ASP:OD1	1:P:22:ASP:N	2.54	0.40
1:E:240:SER:HG	1:E:240:SER:H	1.66	0.40
1:D:173:ALA:CB	1:D:215:VAL:HG12	2.52	0.40
1:B:146:SER:O	1:B:147:PRO:C	2.56	0.40
1:G:209:GLN:O	1:G:212:SER:HB2	2.21	0.40
1:P:209:GLN:O	1:P:212:SER:HB2	2.21	0.40
1:E:209:GLN:O	1:E:212:SER:HB2	2.21	0.40
1:F:56:GLN:NE2	1:F:59:ARG:HH11	2.19	0.40
1:O:56:GLN:NE2	1:O:59:ARG:HH11	2.19	0.40
1:K:174:VAL:HG22	1:K:213:ALA:CB	2.51	0.40
1:B:174:VAL:HG22	1:B:213:ALA:CB	2.51	0.40
1:A:173:ALA:CB	1:A:215:VAL:HG12	2.52	0.40
1:B:173:ALA:CB	1:B:215:VAL:HG12	2.52	0.40
1:I:105:ARG:HH22	1:J:200:ASP:HA	1.86	0.40
1:K:123:LEU:HB3	1:K:125:ILE:HD11	2.03	0.40
1:B:158:THR:HG21	1:B:166:VAL:HG23	2.03	0.40
1:G:123:LEU:HB3	1:G:125:ILE:HD11	2.03	0.40
1:D:123:LEU:HB3	1:D:125:ILE:HD11	2.03	0.40
1:E:158:THR:HG21	1:E:166:VAL:HG23	2.03	0.40
1:A:37:ASP:CG	1:A:38:PRO:HD2	2.41	0.40
1:D:145:LEU:CD2	1:D:145:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ALA:HA	1:G:242:GLN:NE2	2.36	0.40
1:J:239:ALA:HA	1:J:242:GLN:HE21	1.86	0.40
1:K:239:ALA:HA	1:K:242:GLN:NE2	2.36	0.40
1:J:22:ASP:N	1:J:22:ASP:OD1	2.54	0.40
1:G:22:ASP:N	1:G:22:ASP:OD1	2.54	0.40
1:C:173:ALA:CB	1:C:215:VAL:HG12	2.52	0.40
1:J:192:ARG:HH21	1:J:223:PRO:CD	2.35	0.40
1:C:192:ARG:HH21	1:C:223:PRO:CD	2.35	0.40
1:K:192:ARG:HH21	1:K:223:PRO:CD	2.34	0.40
1:G:153:ARG:CB	1:G:153:ARG:HH11	2.25	0.40
1:D:69:PHE:CE2	1:D:95:MSE:HE3	2.55	0.40
1:J:173:ALA:CB	1:J:215:VAL:HG12	2.52	0.40
1:A:47:LYS:HZ3	1:B:75:HIS:H	1.69	0.40
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.87	0.40
1:M:64:ARG:HH11	1:M:64:ARG:HG2	1.86	0.40
1:B:56:GLN:NE2	1:B:59:ARG:HH11	2.19	0.40
1:J:56:GLN:NE2	1:J:59:ARG:HH11	2.19	0.40
1:E:174:VAL:HG22	1:E:213:ALA:CB	2.51	0.40
1:C:174:VAL:HG22	1:C:213:ALA:CB	2.51	0.40
1:O:173:ALA:CB	1:O:215:VAL:HG12	2.52	0.40
1:M:173:ALA:CB	1:M:215:VAL:HG12	2.52	0.40
1:F:173:ALA:CB	1:F:215:VAL:HG12	2.52	0.40
1:A:123:LEU:HB3	1:A:125:ILE:HD11	2.03	0.40
1:O:155:ALA:HA	1:O:166:VAL:HG21	2.02	0.40
1:M:222:ARG:HA	1:M:225:THR:OG1	2.21	0.40
1:K:239:ALA:HA	1:K:242:GLN:HE21	1.86	0.40
1:C:239:ALA:HA	1:C:242:GLN:NE2	2.36	0.40
1:K:132:SER:HB3	1:L:77:ILE:HG22	2.02	0.40
1:I:22:ASP:OD1	1:I:22:ASP:N	2.54	0.40
1:P:192:ARG:HH21	1:P:223:PRO:CD	2.35	0.40
1:P:222:ARG:HA	1:P:225:THR:OG1	2.22	0.40
1:A:209:GLN:O	1:A:212:SER:HB2	2.21	0.40
1:G:64:ARG:HG2	1:G:64:ARG:HH11	1.86	0.40
1:K:56:GLN:NE2	1:K:59:ARG:HH11	2.19	0.40
1:P:174:VAL:HG22	1:P:213:ALA:CB	2.51	0.40
1:P:173:ALA:CB	1:P:215:VAL:HG12	2.52	0.40
1:A:158:THR:HG21	1:A:166:VAL:HG23	2.03	0.40
1:J:123:LEU:HB3	1:J:125:ILE:HD11	2.03	0.40
1:C:200:ASP:OD2	1:D:78:PRO:HD2	2.21	0.40
1:H:222:ARG:HA	1:H:225:THR:OG1	2.22	0.40
1:D:22:ASP:N	1:D:22:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:SER:HG	1:F:240:SER:H	1.66	0.40
1:E:22:ASP:N	1:E:22:ASP:OD1	2.54	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:OE1	1:O:242:GLN:OE1[2_545]	1.39	0.81
1:E:242:GLN:OE1	1:K:178:GLN:OE1[1_454]	1.53	0.67
1:M:228:VAL:CG2	1:P:236:ALA:CB[1_455]	1.84	0.36
1:J:56:GLN:NE2	1:P:27:ASP:CB[2_646]	2.01	0.19
1:M:236:ALA:CB	1:P:195:GLY:O[1_455]	2.07	0.13
1:I:227:SER:CA	1:L:232:GLN:NE2[1_556]	2.10	0.10
1:E:242:GLN:OE1	1:K:178:GLN:CD[1_454]	2.14	0.06
1:I:236:ALA:CB	1:L:228:VAL:CG2[1_556]	2.16	0.04
1:E:232:GLN:NE2	1:H:226:GLN:O[1_454]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	B	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	C	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	D	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	E	229/245 (94%)	185 (81%)	37 (16%)	7 (3%)	5	28
1	F	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	G	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	H	229/245 (94%)	183 (80%)	39 (17%)	7 (3%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	J	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	K	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	L	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	M	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	N	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	O	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
1	P	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	5	28
All	All	3664/3920 (94%)	2944 (80%)	608 (17%)	112 (3%)	5	28

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	LEU
1	A	194	GLN
1	B	145	LEU
1	B	194	GLN
1	C	145	LEU
1	C	194	GLN
1	D	145	LEU
1	D	194	GLN
1	E	145	LEU
1	E	194	GLN
1	F	145	LEU
1	F	194	GLN
1	G	145	LEU
1	G	194	GLN
1	H	145	LEU
1	H	194	GLN
1	I	145	LEU
1	I	194	GLN
1	J	145	LEU
1	J	194	GLN
1	K	145	LEU
1	K	194	GLN
1	L	145	LEU
1	L	194	GLN
1	M	145	LEU
1	M	194	GLN

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Mol	Chain	Res	Type
1	N	145	LEU
1	N	194	GLN
1	O	145	LEU
1	O	194	GLN
1	P	145	LEU
1	P	194	GLN
1	A	147	PRO
1	B	147	PRO
1	C	147	PRO
1	D	147	PRO
1	E	147	PRO
1	F	147	PRO
1	G	147	PRO
1	H	147	PRO
1	I	147	PRO
1	J	147	PRO
1	K	147	PRO
1	L	147	PRO
1	M	147	PRO
1	N	147	PRO
1	O	147	PRO
1	P	147	PRO
1	A	208	GLU
1	B	208	GLU
1	C	208	GLU
1	D	208	GLU
1	E	208	GLU
1	F	208	GLU
1	G	208	GLU
1	H	208	GLU
1	I	208	GLU
1	J	208	GLU
1	K	208	GLU
1	L	208	GLU
1	M	208	GLU
1	N	208	GLU
1	O	208	GLU
1	P	208	GLU
1	A	203	ARG
1	B	203	ARG
1	C	203	ARG
1	D	203	ARG

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Mol	Chain	Res	Type
1	E	203	ARG
1	F	203	ARG
1	G	203	ARG
1	H	203	ARG
1	I	203	ARG
1	J	203	ARG
1	K	203	ARG
1	L	203	ARG
1	M	203	ARG
1	N	203	ARG
1	O	203	ARG
1	P	203	ARG
1	A	189	PRO
1	B	189	PRO
1	C	189	PRO
1	D	189	PRO
1	E	189	PRO
1	F	189	PRO
1	G	189	PRO
1	H	189	PRO
1	I	189	PRO
1	J	189	PRO
1	K	189	PRO
1	L	189	PRO
1	M	189	PRO
1	N	189	PRO
1	O	189	PRO
1	P	189	PRO
1	A	38	PRO
1	B	38	PRO
1	C	38	PRO
1	D	38	PRO
1	E	38	PRO
1	F	38	PRO
1	G	38	PRO
1	H	38	PRO
1	I	38	PRO
1	J	38	PRO
1	K	38	PRO
1	L	38	PRO
1	M	38	PRO
1	N	38	PRO

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Mol	Chain	Res	Type
1	O	38	PRO
1	P	38	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	B	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	C	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	D	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	E	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	F	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	G	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	H	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	I	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	J	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	K	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	L	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	M	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	N	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	O	185/187 (99%)	169 (91%)	16 (9%)	13	44
1	P	185/187 (99%)	169 (91%)	16 (9%)	13	44
All	All	2960/2992 (99%)	2704 (91%)	256 (9%)	13	44

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	28	ASP

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Mol	Chain	Res	Type
1	A	39	ARG
1	A	76	ASP
1	A	91	LEU
1	A	97	ASN
1	A	101	SER
1	A	139	VAL
1	A	145	LEU
1	A	153	ARG
1	A	163	LEU
1	A	166	VAL
1	A	184	PHE
1	A	194	GLN
1	A	209	GLN
1	A	234	LEU
1	B	13	THR
1	B	28	ASP
1	B	39	ARG
1	B	76	ASP
1	B	91	LEU
1	B	97	ASN
1	B	101	SER
1	B	139	VAL
1	B	145	LEU
1	B	153	ARG
1	B	163	LEU
1	B	166	VAL
1	B	184	PHE
1	B	194	GLN
1	B	209	GLN
1	B	234	LEU
1	C	13	THR
1	C	28	ASP
1	C	39	ARG
1	C	76	ASP
1	C	91	LEU
1	C	97	ASN
1	C	101	SER
1	C	139	VAL
1	C	145	LEU
1	C	153	ARG
1	C	163	LEU
1	C	166	VAL

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Mol	Chain	Res	Type
1	C	184	PHE
1	C	194	GLN
1	C	209	GLN
1	C	234	LEU
1	D	13	THR
1	D	28	ASP
1	D	39	ARG
1	D	76	ASP
1	D	91	LEU
1	D	97	ASN
1	D	101	SER
1	D	139	VAL
1	D	145	LEU
1	D	153	ARG
1	D	163	LEU
1	D	166	VAL
1	D	184	PHE
1	D	194	GLN
1	D	209	GLN
1	D	234	LEU
1	E	13	THR
1	E	28	ASP
1	E	39	ARG
1	E	76	ASP
1	E	91	LEU
1	E	97	ASN
1	E	101	SER
1	E	139	VAL
1	E	145	LEU
1	E	153	ARG
1	E	163	LEU
1	E	166	VAL
1	E	184	PHE
1	E	194	GLN
1	E	209	GLN
1	E	234	LEU
1	F	13	THR
1	F	28	ASP
1	F	39	ARG
1	F	76	ASP
1	F	91	LEU
1	F	97	ASN

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Mol	Chain	Res	Type
1	F	101	SER
1	F	139	VAL
1	F	145	LEU
1	F	153	ARG
1	F	163	LEU
1	F	166	VAL
1	F	184	PHE
1	F	194	GLN
1	F	209	GLN
1	F	234	LEU
1	G	13	THR
1	G	28	ASP
1	G	39	ARG
1	G	76	ASP
1	G	91	LEU
1	G	97	ASN
1	G	101	SER
1	G	139	VAL
1	G	145	LEU
1	G	153	ARG
1	G	163	LEU
1	G	166	VAL
1	G	184	PHE
1	G	194	GLN
1	G	209	GLN
1	G	234	LEU
1	H	13	THR
1	H	28	ASP
1	H	39	ARG
1	H	76	ASP
1	H	91	LEU
1	H	97	ASN
1	H	101	SER
1	H	139	VAL
1	H	145	LEU
1	H	153	ARG
1	H	163	LEU
1	H	166	VAL
1	H	184	PHE
1	H	194	GLN
1	H	209	GLN
1	H	234	LEU

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Mol	Chain	Res	Type
1	I	13	THR
1	I	28	ASP
1	I	39	ARG
1	I	76	ASP
1	I	91	LEU
1	I	97	ASN
1	I	101	SER
1	I	139	VAL
1	I	145	LEU
1	I	153	ARG
1	I	163	LEU
1	I	166	VAL
1	I	184	PHE
1	I	194	GLN
1	I	209	GLN
1	I	234	LEU
1	J	13	THR
1	J	28	ASP
1	J	39	ARG
1	J	76	ASP
1	J	91	LEU
1	J	97	ASN
1	J	101	SER
1	J	139	VAL
1	J	145	LEU
1	J	153	ARG
1	J	163	LEU
1	J	166	VAL
1	J	184	PHE
1	J	194	GLN
1	J	209	GLN
1	J	234	LEU
1	K	13	THR
1	K	28	ASP
1	K	39	ARG
1	K	76	ASP
1	K	91	LEU
1	K	97	ASN
1	K	101	SER
1	K	139	VAL
1	K	145	LEU
1	K	153	ARG

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Mol	Chain	Res	Type
1	K	163	LEU
1	K	166	VAL
1	K	184	PHE
1	K	194	GLN
1	K	209	GLN
1	K	234	LEU
1	L	13	THR
1	L	28	ASP
1	L	39	ARG
1	L	76	ASP
1	L	91	LEU
1	L	97	ASN
1	L	101	SER
1	L	139	VAL
1	L	145	LEU
1	L	153	ARG
1	L	163	LEU
1	L	166	VAL
1	L	184	PHE
1	L	194	GLN
1	L	209	GLN
1	L	234	LEU
1	M	13	THR
1	M	28	ASP
1	M	39	ARG
1	M	76	ASP
1	M	91	LEU
1	M	97	ASN
1	M	101	SER
1	M	139	VAL
1	M	145	LEU
1	M	153	ARG
1	M	163	LEU
1	M	166	VAL
1	M	184	PHE
1	M	194	GLN
1	M	209	GLN
1	M	234	LEU
1	N	13	THR
1	N	28	ASP
1	N	39	ARG
1	N	76	ASP

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Mol	Chain	Res	Type
1	N	91	LEU
1	N	97	ASN
1	N	101	SER
1	N	139	VAL
1	N	145	LEU
1	N	153	ARG
1	N	163	LEU
1	N	166	VAL
1	N	184	PHE
1	N	194	GLN
1	N	209	GLN
1	N	234	LEU
1	O	13	THR
1	O	28	ASP
1	O	39	ARG
1	O	76	ASP
1	O	91	LEU
1	O	97	ASN
1	O	101	SER
1	O	139	VAL
1	O	145	LEU
1	O	153	ARG
1	O	163	LEU
1	O	166	VAL
1	O	184	PHE
1	O	194	GLN
1	O	209	GLN
1	O	234	LEU
1	P	13	THR
1	P	28	ASP
1	P	39	ARG
1	P	76	ASP
1	P	91	LEU
1	P	97	ASN
1	P	101	SER
1	P	139	VAL
1	P	145	LEU
1	P	153	ARG
1	P	163	LEU
1	P	166	VAL
1	P	184	PHE
1	P	194	GLN

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Mol	Chain	Res	Type
1	P	209	GLN
1	P	234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	56	GLN
1	A	62	GLN
1	A	83	HIS
1	A	159	GLN
1	A	171	GLN
1	A	194	GLN
1	A	226	GLN
1	A	238	ASN
1	A	242	GLN
1	B	25	ASN
1	B	56	GLN
1	B	62	GLN
1	B	83	HIS
1	B	159	GLN
1	B	171	GLN
1	B	194	GLN
1	B	226	GLN
1	B	232	GLN
1	B	238	ASN
1	B	242	GLN
1	C	25	ASN
1	C	56	GLN
1	C	62	GLN
1	C	83	HIS
1	C	159	GLN
1	C	171	GLN
1	C	194	GLN
1	C	226	GLN
1	C	238	ASN
1	C	242	GLN
1	D	25	ASN
1	D	56	GLN
1	D	62	GLN
1	D	83	HIS
1	D	159	GLN

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Mol	Chain	Res	Type
1	D	171	GLN
1	D	194	GLN
1	D	226	GLN
1	D	238	ASN
1	D	242	GLN
1	E	25	ASN
1	E	56	GLN
1	E	62	GLN
1	E	83	HIS
1	E	159	GLN
1	E	171	GLN
1	E	194	GLN
1	E	226	GLN
1	E	238	ASN
1	E	242	GLN
1	F	25	ASN
1	F	56	GLN
1	F	62	GLN
1	F	83	HIS
1	F	159	GLN
1	F	171	GLN
1	F	194	GLN
1	F	226	GLN
1	F	238	ASN
1	F	242	GLN
1	G	25	ASN
1	G	56	GLN
1	G	62	GLN
1	G	83	HIS
1	G	159	GLN
1	G	171	GLN
1	G	194	GLN
1	G	226	GLN
1	G	232	GLN
1	G	238	ASN
1	G	242	GLN
1	H	25	ASN
1	H	56	GLN
1	H	62	GLN
1	H	83	HIS
1	H	159	GLN
1	H	171	GLN

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Mol	Chain	Res	Type
1	H	194	GLN
1	H	226	GLN
1	H	238	ASN
1	H	242	GLN
1	I	25	ASN
1	I	56	GLN
1	I	62	GLN
1	I	83	HIS
1	I	159	GLN
1	I	171	GLN
1	I	194	GLN
1	I	226	GLN
1	I	238	ASN
1	I	242	GLN
1	J	25	ASN
1	J	56	GLN
1	J	62	GLN
1	J	83	HIS
1	J	159	GLN
1	J	171	GLN
1	J	194	GLN
1	J	226	GLN
1	J	238	ASN
1	J	242	GLN
1	K	25	ASN
1	K	56	GLN
1	K	62	GLN
1	K	83	HIS
1	K	159	GLN
1	K	171	GLN
1	K	194	GLN
1	K	226	GLN
1	K	238	ASN
1	K	242	GLN
1	L	25	ASN
1	L	56	GLN
1	L	62	GLN
1	L	83	HIS
1	L	159	GLN
1	L	171	GLN
1	L	194	GLN
1	L	226	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	L	238	ASN
1	L	242	GLN
1	M	25	ASN
1	M	56	GLN
1	M	62	GLN
1	M	83	HIS
1	M	159	GLN
1	M	171	GLN
1	M	194	GLN
1	M	226	GLN
1	M	238	ASN
1	M	242	GLN
1	N	25	ASN
1	N	56	GLN
1	N	62	GLN
1	N	83	HIS
1	N	159	GLN
1	N	171	GLN
1	N	194	GLN
1	N	226	GLN
1	N	238	ASN
1	N	242	GLN
1	O	25	ASN
1	O	56	GLN
1	O	62	GLN
1	O	83	HIS
1	O	159	GLN
1	O	171	GLN
1	O	194	GLN
1	O	226	GLN
1	O	238	ASN
1	O	242	GLN
1	P	25	ASN
1	P	56	GLN
1	P	62	GLN
1	P	83	HIS
1	P	159	GLN
1	P	171	GLN
1	P	194	GLN
1	P	226	GLN
1	P	238	ASN
1	P	242	GLN

### 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 ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	BMP	A	301	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	6 (31%)
2	BMP	B	302	-	16,23,23	2.38	6 (37%)	19,35,35	2.57	5 (26%)
2	BMP	C	303	-	16,23,23	2.36	6 (37%)	19,35,35	2.56	6 (31%)
2	BMP	D	304	-	16,23,23	2.38	6 (37%)	19,35,35	2.57	6 (31%)
2	BMP	E	305	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	6 (31%)
2	BMP	F	306	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	6 (31%)
2	BMP	G	307	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	5 (26%)
2	BMP	H	308	-	16,23,23	2.37	6 (37%)	19,35,35	2.58	6 (31%)
2	BMP	I	309	-	16,23,23	2.37	6 (37%)	19,35,35	2.56	5 (26%)
2	BMP	J	310	-	16,23,23	2.37	6 (37%)	19,35,35	2.56	5 (26%)
2	BMP	K	311	-	16,23,23	2.37	6 (37%)	19,35,35	2.58	6 (31%)
2	BMP	L	312	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	6 (31%)
2	BMP	M	313	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	5 (26%)
2	BMP	N	314	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMP	O	315	-	16,23,23	2.38	6 (37%)	19,35,35	2.57	6 (31%)
2	BMP	P	316	-	16,23,23	2.37	6 (37%)	19,35,35	2.57	6 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMP	A	301	-	-	0/6/26/26	0/2/2/2
2	BMP	B	302	-	-	0/6/26/26	0/2/2/2
2	BMP	C	303	-	-	0/6/26/26	0/2/2/2
2	BMP	D	304	-	-	0/6/26/26	0/2/2/2
2	BMP	E	305	-	-	0/6/26/26	0/2/2/2
2	BMP	F	306	-	-	0/6/26/26	0/2/2/2
2	BMP	G	307	-	-	0/6/26/26	0/2/2/2
2	BMP	H	308	-	-	0/6/26/26	0/2/2/2
2	BMP	I	309	-	-	0/6/26/26	0/2/2/2
2	BMP	J	310	-	-	0/6/26/26	0/2/2/2
2	BMP	K	311	-	-	0/6/26/26	0/2/2/2
2	BMP	L	312	-	-	0/6/26/26	0/2/2/2
2	BMP	M	313	-	-	0/6/26/26	0/2/2/2
2	BMP	N	314	-	-	0/6/26/26	0/2/2/2
2	BMP	O	315	-	-	0/6/26/26	0/2/2/2
2	BMP	P	316	-	-	0/6/26/26	0/2/2/2

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	308	BMP	C6-N1	-5.74	1.29	1.38
2	B	302	BMP	C6-N1	-5.73	1.29	1.38
2	M	313	BMP	C6-N1	-5.71	1.29	1.38
2	D	304	BMP	C6-N1	-5.71	1.29	1.38
2	O	315	BMP	C6-N1	-5.71	1.29	1.38
2	P	316	BMP	C6-N1	-5.70	1.29	1.38
2	E	305	BMP	C6-N1	-5.70	1.29	1.38
2	A	301	BMP	C6-N1	-5.69	1.29	1.38
2	L	312	BMP	C6-N1	-5.68	1.29	1.38
2	J	310	BMP	C6-N1	-5.68	1.29	1.38
2	N	314	BMP	C6-N1	-5.67	1.29	1.38
2	I	309	BMP	C6-N1	-5.66	1.29	1.38
2	C	303	BMP	C6-N1	-5.66	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	307	BMP	C6-N1	-5.66	1.29	1.38
2	K	311	BMP	C6-N1	-5.66	1.29	1.38
2	F	306	BMP	C6-N1	-5.64	1.29	1.38
2	B	302	BMP	O2'-C2'	-2.41	1.37	1.43
2	E	305	BMP	O2'-C2'	-2.41	1.37	1.43
2	I	309	BMP	O2'-C2'	-2.41	1.37	1.43
2	P	316	BMP	O2'-C2'	-2.41	1.37	1.43
2	D	304	BMP	O2'-C2'	-2.40	1.37	1.43
2	L	312	BMP	O2'-C2'	-2.40	1.37	1.43
2	G	307	BMP	O2'-C2'	-2.40	1.37	1.43
2	J	310	BMP	O2'-C2'	-2.39	1.37	1.43
2	A	301	BMP	O2'-C2'	-2.39	1.37	1.43
2	K	311	BMP	O2'-C2'	-2.39	1.37	1.43
2	O	315	BMP	O2'-C2'	-2.39	1.37	1.43
2	N	314	BMP	O2'-C2'	-2.38	1.37	1.43
2	F	306	BMP	O2'-C2'	-2.38	1.37	1.43
2	M	313	BMP	O2'-C2'	-2.37	1.37	1.43
2	C	303	BMP	O2'-C2'	-2.37	1.37	1.43
2	H	308	BMP	O2'-C2'	-2.36	1.37	1.43
2	C	303	BMP	O3'-C3'	2.17	1.48	1.43
2	E	305	BMP	O3'-C3'	2.17	1.48	1.43
2	D	304	BMP	O3'-C3'	2.18	1.48	1.43
2	P	316	BMP	O3'-C3'	2.18	1.48	1.43
2	N	314	BMP	O3'-C3'	2.19	1.48	1.43
2	J	310	BMP	O3'-C3'	2.19	1.48	1.43
2	O	315	BMP	O3'-C3'	2.19	1.48	1.43
2	M	313	BMP	O3'-C3'	2.19	1.48	1.43
2	H	308	BMP	O3'-C3'	2.20	1.48	1.43
2	A	301	BMP	O3'-C3'	2.20	1.48	1.43
2	I	309	BMP	O3'-C3'	2.20	1.48	1.43
2	L	312	BMP	O3'-C3'	2.21	1.48	1.43
2	G	307	BMP	O3'-C3'	2.21	1.48	1.43
2	B	302	BMP	O3'-C3'	2.21	1.48	1.43
2	K	311	BMP	O3'-C3'	2.21	1.48	1.43
2	F	306	BMP	O3'-C3'	2.22	1.48	1.43
2	E	305	BMP	C4-N3	2.53	1.37	1.33
2	G	307	BMP	C4-N3	2.55	1.37	1.33
2	I	309	BMP	C4-N3	2.55	1.37	1.33
2	H	308	BMP	C4-N3	2.55	1.37	1.33
2	J	310	BMP	C4-N3	2.56	1.37	1.33
2	F	306	BMP	C4-N3	2.57	1.37	1.33
2	A	301	BMP	C4-N3	2.57	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	314	BMP	C4-N3	2.57	1.37	1.33
2	C	303	BMP	C4-N3	2.57	1.37	1.33
2	P	316	BMP	C4-N3	2.58	1.37	1.33
2	M	313	BMP	C4-N3	2.58	1.37	1.33
2	B	302	BMP	C4-N3	2.59	1.37	1.33
2	L	312	BMP	C4-N3	2.59	1.37	1.33
2	K	311	BMP	C4-N3	2.59	1.37	1.33
2	D	304	BMP	C4-N3	2.60	1.37	1.33
2	O	315	BMP	C4-N3	2.61	1.37	1.33
2	H	308	BMP	O4'-C1'	3.52	1.45	1.41
2	L	312	BMP	O4'-C1'	3.55	1.45	1.41
2	B	302	BMP	O4'-C1'	3.59	1.45	1.41
2	P	316	BMP	O4'-C1'	3.59	1.45	1.41
2	O	315	BMP	O4'-C1'	3.59	1.45	1.41
2	I	309	BMP	O4'-C1'	3.59	1.45	1.41
2	K	311	BMP	O4'-C1'	3.59	1.45	1.41
2	C	303	BMP	O4'-C1'	3.60	1.45	1.41
2	G	307	BMP	O4'-C1'	3.60	1.45	1.41
2	A	301	BMP	O4'-C1'	3.60	1.45	1.41
2	E	305	BMP	O4'-C1'	3.61	1.45	1.41
2	N	314	BMP	O4'-C1'	3.61	1.45	1.41
2	D	304	BMP	O4'-C1'	3.61	1.45	1.41
2	M	313	BMP	O4'-C1'	3.61	1.45	1.41
2	F	306	BMP	O4'-C1'	3.63	1.45	1.41
2	J	310	BMP	O4'-C1'	3.63	1.45	1.41
2	P	316	BMP	O4'-C4'	4.52	1.55	1.45
2	L	312	BMP	O4'-C4'	4.52	1.55	1.45
2	J	310	BMP	O4'-C4'	4.53	1.55	1.45
2	M	313	BMP	O4'-C4'	4.53	1.55	1.45
2	E	305	BMP	O4'-C4'	4.53	1.55	1.45
2	B	302	BMP	O4'-C4'	4.53	1.55	1.45
2	C	303	BMP	O4'-C4'	4.53	1.55	1.45
2	N	314	BMP	O4'-C4'	4.53	1.55	1.45
2	D	304	BMP	O4'-C4'	4.54	1.55	1.45
2	G	307	BMP	O4'-C4'	4.55	1.55	1.45
2	H	308	BMP	O4'-C4'	4.55	1.55	1.45
2	K	311	BMP	O4'-C4'	4.55	1.55	1.45
2	A	301	BMP	O4'-C4'	4.55	1.55	1.45
2	I	309	BMP	O4'-C4'	4.56	1.55	1.45
2	F	306	BMP	O4'-C4'	4.57	1.55	1.45
2	O	315	BMP	O4'-C4'	4.57	1.55	1.45

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	311	BMP	C5-C4-N3	-4.40	118.72	124.05
2	H	308	BMP	C5-C4-N3	-4.39	118.73	124.05
2	L	312	BMP	C5-C4-N3	-4.38	118.74	124.05
2	O	315	BMP	C5-C4-N3	-4.38	118.75	124.05
2	N	314	BMP	C5-C4-N3	-4.37	118.76	124.05
2	P	316	BMP	C5-C4-N3	-4.37	118.76	124.05
2	D	304	BMP	C5-C4-N3	-4.36	118.76	124.05
2	M	313	BMP	C5-C4-N3	-4.36	118.77	124.05
2	A	301	BMP	C5-C4-N3	-4.36	118.77	124.05
2	B	302	BMP	C5-C4-N3	-4.35	118.78	124.05
2	G	307	BMP	C5-C4-N3	-4.34	118.79	124.05
2	E	305	BMP	C5-C4-N3	-4.34	118.79	124.05
2	F	306	BMP	C5-C4-N3	-4.34	118.79	124.05
2	I	309	BMP	C5-C4-N3	-4.33	118.80	124.05
2	J	310	BMP	C5-C4-N3	-4.33	118.80	124.05
2	C	303	BMP	C5-C4-N3	-4.30	118.84	124.05
2	J	310	BMP	C4'-O4'-C1'	-4.25	105.05	109.72
2	O	315	BMP	C4'-O4'-C1'	-4.24	105.06	109.72
2	I	309	BMP	C4'-O4'-C1'	-4.24	105.06	109.72
2	F	306	BMP	C4'-O4'-C1'	-4.23	105.07	109.72
2	A	301	BMP	C4'-O4'-C1'	-4.22	105.09	109.72
2	E	305	BMP	C4'-O4'-C1'	-4.22	105.09	109.72
2	M	313	BMP	C4'-O4'-C1'	-4.21	105.09	109.72
2	K	311	BMP	C4'-O4'-C1'	-4.21	105.09	109.72
2	N	314	BMP	C4'-O4'-C1'	-4.21	105.09	109.72
2	C	303	BMP	C4'-O4'-C1'	-4.21	105.09	109.72
2	D	304	BMP	C4'-O4'-C1'	-4.21	105.10	109.72
2	P	316	BMP	C4'-O4'-C1'	-4.20	105.10	109.72
2	B	302	BMP	C4'-O4'-C1'	-4.20	105.10	109.72
2	G	307	BMP	C4'-O4'-C1'	-4.19	105.12	109.72
2	H	308	BMP	C4'-O4'-C1'	-4.18	105.12	109.72
2	L	312	BMP	C4'-O4'-C1'	-4.17	105.13	109.72
2	C	303	BMP	C5'-C4'-C3'	2.00	123.15	115.21
2	K	311	BMP	C5'-C4'-C3'	2.00	123.15	115.21
2	F	306	BMP	C5'-C4'-C3'	2.00	123.15	115.21
2	N	314	BMP	C5'-C4'-C3'	2.00	123.16	115.21
2	P	316	BMP	C5'-C4'-C3'	2.00	123.16	115.21
2	H	308	BMP	C5'-C4'-C3'	2.00	123.16	115.21
2	A	301	BMP	C5'-C4'-C3'	2.00	123.16	115.21
2	E	305	BMP	C5'-C4'-C3'	2.00	123.16	115.21
2	D	304	BMP	C5'-C4'-C3'	2.00	123.17	115.21
2	L	312	BMP	C5'-C4'-C3'	2.01	123.17	115.21
2	O	315	BMP	C5'-C4'-C3'	2.01	123.20	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	311	BMP	O5'-C5'-C4'	2.49	118.30	109.12
2	N	314	BMP	O5'-C5'-C4'	2.49	118.31	109.12
2	P	316	BMP	O5'-C5'-C4'	2.50	118.32	109.12
2	L	312	BMP	O5'-C5'-C4'	2.50	118.32	109.12
2	J	310	BMP	O5'-C5'-C4'	2.50	118.34	109.12
2	I	309	BMP	O5'-C5'-C4'	2.50	118.34	109.12
2	O	315	BMP	O5'-C5'-C4'	2.50	118.34	109.12
2	H	308	BMP	O5'-C5'-C4'	2.50	118.34	109.12
2	A	301	BMP	O5'-C5'-C4'	2.50	118.35	109.12
2	M	313	BMP	O5'-C5'-C4'	2.50	118.35	109.12
2	F	306	BMP	O5'-C5'-C4'	2.50	118.35	109.12
2	D	304	BMP	O5'-C5'-C4'	2.51	118.36	109.12
2	E	305	BMP	O5'-C5'-C4'	2.51	118.36	109.12
2	G	307	BMP	O5'-C5'-C4'	2.51	118.38	109.12
2	B	302	BMP	O5'-C5'-C4'	2.51	118.38	109.12
2	C	303	BMP	O5'-C5'-C4'	2.51	118.39	109.12
2	J	310	BMP	O4'-C1'-N1	2.56	111.22	108.29
2	I	309	BMP	O4'-C1'-N1	2.57	111.23	108.29
2	K	311	BMP	O4'-C1'-N1	2.57	111.23	108.29
2	D	304	BMP	O4'-C1'-N1	2.58	111.23	108.29
2	O	315	BMP	O4'-C1'-N1	2.58	111.24	108.29
2	C	303	BMP	O4'-C1'-N1	2.58	111.24	108.29
2	F	306	BMP	O4'-C1'-N1	2.59	111.25	108.29
2	A	301	BMP	O4'-C1'-N1	2.59	111.25	108.29
2	E	305	BMP	O4'-C1'-N1	2.60	111.26	108.29
2	N	314	BMP	O4'-C1'-N1	2.60	111.26	108.29
2	B	302	BMP	O4'-C1'-N1	2.61	111.27	108.29
2	G	307	BMP	O4'-C1'-N1	2.62	111.28	108.29
2	H	308	BMP	O4'-C1'-N1	2.62	111.28	108.29
2	L	312	BMP	O4'-C1'-N1	2.62	111.28	108.29
2	M	313	BMP	O4'-C1'-N1	2.63	111.29	108.29
2	P	316	BMP	O4'-C1'-N1	2.63	111.30	108.29
2	C	303	BMP	C4-N3-C2	7.49	121.56	114.14
2	P	316	BMP	C4-N3-C2	7.51	121.58	114.14
2	I	309	BMP	C4-N3-C2	7.51	121.58	114.14
2	J	310	BMP	C4-N3-C2	7.51	121.58	114.14
2	B	302	BMP	C4-N3-C2	7.52	121.59	114.14
2	D	304	BMP	C4-N3-C2	7.52	121.59	114.14
2	O	315	BMP	C4-N3-C2	7.52	121.59	114.14
2	A	301	BMP	C4-N3-C2	7.53	121.60	114.14
2	L	312	BMP	C4-N3-C2	7.53	121.60	114.14
2	F	306	BMP	C4-N3-C2	7.53	121.60	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	314	BMP	C4-N3-C2	7.53	121.60	114.14
2	M	313	BMP	C4-N3-C2	7.53	121.60	114.14
2	G	307	BMP	C4-N3-C2	7.54	121.61	114.14
2	E	305	BMP	C4-N3-C2	7.55	121.62	114.14
2	K	311	BMP	C4-N3-C2	7.57	121.64	114.14
2	H	308	BMP	C4-N3-C2	7.59	121.66	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	BMP	2	0
2	B	302	BMP	2	0
2	C	303	BMP	2	0
2	D	304	BMP	2	0
2	E	305	BMP	3	0
2	F	306	BMP	2	0
2	G	307	BMP	2	0
2	H	308	BMP	2	0
2	I	309	BMP	2	0
2	J	310	BMP	2	0
2	K	311	BMP	2	0
2	L	312	BMP	2	0
2	M	313	BMP	3	0
2	N	314	BMP	4	0
2	O	315	BMP	2	0
2	P	316	BMP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	223/245 (91%)	0.17	2 (0%) 85 64	1, 23, 44, 59	0
1	B	223/245 (91%)	0.28	6 (2%) 58 28	1, 23, 44, 59	0
1	C	223/245 (91%)	0.10	0 100 100	1, 23, 44, 59	0
1	D	223/245 (91%)	0.23	6 (2%) 58 28	1, 23, 44, 59	0
1	E	223/245 (91%)	0.36	7 (3%) 52 24	1, 23, 44, 59	0
1	F	223/245 (91%)	0.45	7 (3%) 52 24	1, 23, 44, 59	0
1	G	223/245 (91%)	0.40	8 (3%) 46 20	1, 23, 44, 59	0
1	H	223/245 (91%)	0.33	3 (1%) 79 53	1, 23, 44, 59	0
1	I	223/245 (91%)	0.38	11 (4%) 33 13	1, 23, 44, 59	0
1	J	223/245 (91%)	0.55	17 (7%) 17 6	1, 23, 44, 59	0
1	K	223/245 (91%)	0.46	6 (2%) 58 28	1, 23, 44, 59	0
1	L	223/245 (91%)	0.48	11 (4%) 33 13	1, 23, 44, 59	0
1	M	223/245 (91%)	1.01	30 (13%) 4 1	1, 23, 44, 59	0
1	N	223/245 (91%)	0.79	20 (8%) 12 4	1, 23, 44, 59	0
1	O	223/245 (91%)	1.00	31 (13%) 4 1	1, 23, 44, 59	0
1	P	223/245 (91%)	1.12	38 (17%) 2 1	1, 23, 44, 59	0
All	All	3568/3920 (91%)	0.51	203 (5%) 27 10	1, 23, 45, 59	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	162	GLY	5.0
1	M	178	GLN	4.1
1	H	144	THR	4.1
1	P	196	SER	4.0
1	P	227	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	P	144	THR	4.0
1	O	182	GLN	3.9
1	N	14	ASN	3.7
1	J	12	VAL	3.7
1	M	28	ASP	3.6
1	I	213	ALA	3.6
1	P	190	GLY	3.5
1	M	214	GLY	3.5
1	O	119	LYS	3.5
1	I	178	GLN	3.5
1	P	194	GLN	3.5
1	J	144	THR	3.4
1	P	214	GLY	3.4
1	F	139	VAL	3.4
1	L	194	GLN	3.3
1	I	142	GLY	3.3
1	P	226	GLN	3.2
1	P	120	ASP	3.2
1	O	168	CYS	3.2
1	N	208	GLU	3.2
1	F	142	GLY	3.2
1	N	198	ALA	3.1
1	P	200	ASP	3.1
1	O	229	ASP	3.1
1	P	197	GLU	3.1
1	I	227	SER	3.1
1	M	198	ALA	3.1
1	K	12	VAL	3.1
1	P	237	ILE	3.0
1	O	148	ALA	3.0
1	M	241	LEU	3.0
1	P	140	ASP	3.0
1	M	35	LYS	3.0
1	N	212	SER	3.0
1	M	118	GLY	3.0
1	O	197	GLU	3.0
1	P	40	ASP	3.0
1	L	178	GLN	3.0
1	P	195	GLY	3.0
1	P	242	GLN	2.9
1	B	194	GLN	2.9
1	A	228	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	35	LYS	2.9
1	J	195	GLY	2.9
1	F	214	GLY	2.9
1	J	212	SER	2.9
1	L	195	GLY	2.8
1	N	118	GLY	2.8
1	O	170	ALA	2.8
1	O	155	ALA	2.8
1	P	239	ALA	2.8
1	P	240	SER	2.8
1	O	188	THR	2.8
1	E	212	SER	2.8
1	N	142	GLY	2.8
1	P	41	CYS	2.7
1	O	177	LYS	2.7
1	M	120	ASP	2.7
1	H	142	GLY	2.7
1	M	128	THR	2.7
1	P	145	LEU	2.7
1	M	240	SER	2.7
1	A	178	GLN	2.7
1	O	194	GLN	2.7
1	N	12	VAL	2.7
1	D	194	GLN	2.6
1	L	212	SER	2.6
1	F	144	THR	2.6
1	P	229	ASP	2.6
1	E	182	GLN	2.6
1	P	24	HIS	2.6
1	M	13	THR	2.6
1	M	226	GLN	2.6
1	N	144	THR	2.6
1	N	34	ASP	2.6
1	J	13	THR	2.6
1	M	176	PHE	2.6
1	I	194	GLN	2.5
1	M	237	ILE	2.5
1	L	31	ALA	2.5
1	O	193	PRO	2.5
1	O	27	ASP	2.5
1	O	120	ASP	2.5
1	M	181	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	144	THR	2.5
1	P	210	ALA	2.5
1	O	180	PHE	2.5
1	J	242	GLN	2.5
1	K	178	GLN	2.5
1	J	34	ASP	2.5
1	B	195	GLY	2.5
1	B	178	GLN	2.5
1	M	142	GLY	2.5
1	M	135	ALA	2.4
1	O	189	PRO	2.4
1	H	140	ASP	2.4
1	O	41	CYS	2.4
1	P	12	VAL	2.4
1	P	228	VAL	2.4
1	D	195	GLY	2.4
1	J	232	GLN	2.4
1	O	134	GLU	2.4
1	M	232	GLN	2.4
1	P	232	GLN	2.4
1	M	179	VAL	2.4
1	I	135	ALA	2.4
1	K	15	SER	2.4
1	O	152	GLU	2.4
1	J	194	GLN	2.4
1	F	149	ASP	2.4
1	O	232	GLN	2.4
1	E	194	GLN	2.4
1	E	197	GLU	2.4
1	M	188	THR	2.4
1	M	29	ALA	2.4
1	N	65	GLY	2.3
1	G	144	THR	2.3
1	P	236	ALA	2.3
1	B	12	VAL	2.3
1	L	159	GLN	2.3
1	O	112	GLU	2.3
1	E	118	GLY	2.3
1	L	13	THR	2.3
1	L	40	ASP	2.3
1	I	196	SER	2.3
1	J	169	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	226	GLN	2.3
1	L	213	ALA	2.3
1	D	178	GLN	2.3
1	M	16	PRO	2.3
1	N	197	GLU	2.3
1	O	185	LYS	2.3
1	D	12	VAL	2.3
1	L	227	SER	2.3
1	I	228	VAL	2.3
1	G	197	GLU	2.3
1	P	188	THR	2.3
1	I	40	ASP	2.2
1	F	178	GLN	2.2
1	M	225	THR	2.2
1	O	196	SER	2.2
1	J	197	GLU	2.2
1	O	183	GLU	2.2
1	P	25	ASN	2.2
1	G	194	GLN	2.2
1	N	242	GLN	2.2
1	J	178	GLN	2.2
1	K	39	ARG	2.2
1	N	140	ASP	2.2
1	N	230	PRO	2.2
1	M	183	GLU	2.2
1	J	230	PRO	2.2
1	D	193	PRO	2.2
1	E	142	GLY	2.2
1	I	212	SER	2.2
1	J	196	SER	2.2
1	J	14	ASN	2.2
1	O	195	GLY	2.2
1	G	232	GLN	2.2
1	O	181	GLY	2.2
1	P	13	THR	2.2
1	M	175	ARG	2.2
1	O	214	GLY	2.1
1	B	144	THR	2.1
1	P	14	ASN	2.1
1	K	63	GLN	2.1
1	N	232	GLN	2.1
1	G	178	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	37	ASP	2.1
1	P	149	ASP	2.1
1	B	14	ASN	2.1
1	M	210	ALA	2.1
1	M	119	LYS	2.1
1	P	92	GLY	2.1
1	D	14	ASN	2.1
1	P	233	THR	2.1
1	J	147	PRO	2.1
1	M	41	CYS	2.1
1	P	142	GLY	2.1
1	E	178	GLN	2.1
1	N	235	LYS	2.1
1	O	235	LYS	2.1
1	P	176	PHE	2.1
1	P	168	CYS	2.1
1	M	190	GLY	2.1
1	N	148	ALA	2.1
1	G	118	GLY	2.0
1	N	112	GLU	2.0
1	N	90	ASP	2.0
1	N	63	GLN	2.0
1	O	159	GLN	2.0
1	P	101	SER	2.0
1	G	175	ARG	2.0
1	K	228	VAL	2.0
1	F	229	ASP	2.0
1	G	229	ASP	2.0
1	O	227	SER	2.0
1	I	148	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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(Å <sup>2</sup> )	Q<0.9
2	BMP	L	312	22/22	0.86	0.26	0.34	6,8,12,13	0
2	BMP	E	305	22/22	0.88	0.26	0.16	6,8,12,13	0
2	BMP	J	310	22/22	0.89	0.24	0.08	6,8,12,13	0
2	BMP	N	314	22/22	0.86	0.28	-0.04	6,8,12,13	0
2	BMP	O	315	22/22	0.84	0.29	-0.12	6,8,12,13	0
2	BMP	B	302	22/22	0.90	0.23	-0.14	6,8,12,13	0
2	BMP	D	304	22/22	0.91	0.22	-0.22	6,8,12,13	0
2	BMP	A	301	22/22	0.93	0.21	-0.23	6,8,12,13	0
2	BMP	G	307	22/22	0.87	0.25	-0.24	6,8,12,13	0
2	BMP	P	316	22/22	0.83	0.30	-0.34	6,8,12,13	0
2	BMP	M	313	22/22	0.80	0.30	-0.36	6,8,12,13	0
2	BMP	C	303	22/22	0.94	0.21	-0.38	6,8,12,13	0
2	BMP	K	311	22/22	0.92	0.22	-0.41	6,8,12,13	0
2	BMP	I	309	22/22	0.92	0.22	-0.49	6,8,12,13	0
2	BMP	F	306	22/22	0.92	0.20	-0.71	6,8,12,13	0
2	BMP	H	308	22/22	0.94	0.18	-1.36	6,8,12,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.