



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:54 pm GMT

PDB ID : 2DF7  
Title : Crystal structure of infectious bursal disease virus VP2 subviral particle  
Authors : Ko, T.P.; Lee, C.C.; Wang, M.Y.; Wang, A.H.  
Deposited on : 2006-02-27  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

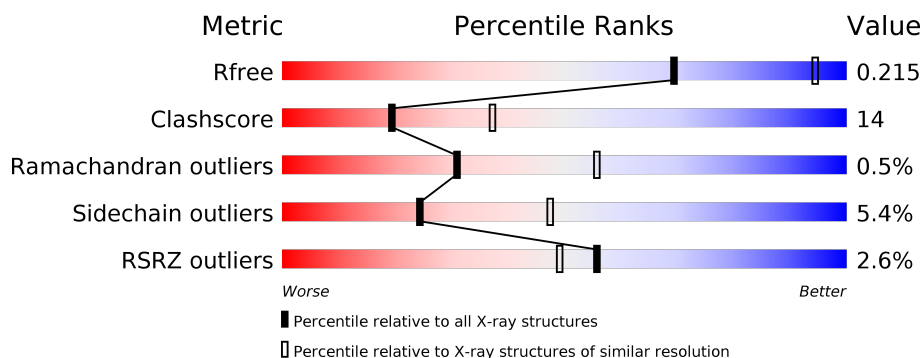
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	458	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	458	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	458	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>20%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	458	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	458	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	458	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	458	
1	H	458	
1	I	458	
1	J	458	
1	K	458	
1	L	458	
1	M	458	
1	N	458	
1	O	458	
1	P	458	
1	Q	458	
1	R	458	
1	S	458	
1	T	458	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 66956 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 structural polyprotein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3162	2006	520	626	10			
1	B	418	Total	C	N	O	S	0	0	0
			3149	1997	518	624	10			
1	C	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	D	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	E	415	Total	C	N	O	S	0	0	0
			3130	1985	515	620	10			
1	F	413	Total	C	N	O	S	0	0	0
			3113	1974	513	616	10			
1	G	412	Total	C	N	O	S	0	0	0
			3110	1971	512	617	10			
1	H	413	Total	C	N	O	S	0	0	0
			3117	1976	513	618	10			
1	I	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	J	411	Total	C	N	O	S	0	0	0
			3102	1965	511	616	10			
1	K	417	Total	C	N	O	S	0	0	0
			3137	1988	517	622	10			
1	L	418	Total	C	N	O	S	0	0	0
			3150	1998	518	624	10			
1	M	412	Total	C	N	O	S	0	0	0
			3110	1971	512	617	10			
1	N	413	Total	C	N	O	S	0	0	0
			3109	1970	513	616	10			
1	O	412	Total	C	N	O	S	0	0	0
			3109	1970	512	617	10			
1	P	417	Total	C	N	O	S	0	0	0
			3138	1989	517	622	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	417	Total	C	N	O	S	0	0	0
			3138	1989	517	622	10			
1	R	411	Total	C	N	O	S	0	0	0
			3101	1966	511	614	10			
1	S	414	Total	C	N	O	S	0	0	0
			3116	1975	514	617	10			
1	T	418	Total	C	N	O	S	0	0	0
			3150	1998	518	624	10			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
A	330	SER	MET	ENGINEERED	UNP Q6S9I7
A	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
A	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
B	330	SER	MET	ENGINEERED	UNP Q6S9I7
B	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
B	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
C	330	SER	MET	ENGINEERED	UNP Q6S9I7
C	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
C	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
D	330	SER	MET	ENGINEERED	UNP Q6S9I7
D	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
D	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
E	330	SER	MET	ENGINEERED	UNP Q6S9I7
E	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
E	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
F	330	SER	MET	ENGINEERED	UNP Q6S9I7
F	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
F	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
G	330	SER	MET	ENGINEERED	UNP Q6S9I7
G	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
G	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
H	330	SER	MET	ENGINEERED	UNP Q6S9I7
H	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
H	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	135	GLU	ASP	ENGINEERED	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	330	SER	MET	ENGINEERED	UNP Q6S9I7
I	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
I	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
J	330	SER	MET	ENGINEERED	UNP Q6S9I7
J	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
J	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
K	330	SER	MET	ENGINEERED	UNP Q6S9I7
K	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
K	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
L	330	SER	MET	ENGINEERED	UNP Q6S9I7
L	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
L	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
M	330	SER	MET	ENGINEERED	UNP Q6S9I7
M	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
M	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
N	330	SER	MET	ENGINEERED	UNP Q6S9I7
N	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
N	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
O	330	SER	MET	ENGINEERED	UNP Q6S9I7
O	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
O	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
P	330	SER	MET	ENGINEERED	UNP Q6S9I7
P	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
P	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
Q	330	SER	MET	ENGINEERED	UNP Q6S9I7
Q	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
Q	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
R	330	SER	MET	ENGINEERED	UNP Q6S9I7
R	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
R	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
S	330	SER	MET	ENGINEERED	UNP Q6S9I7
S	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
S	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
T	330	SER	MET	ENGINEERED	UNP Q6S9I7
T	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
T	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	R	1	Total Cl 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	I	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	R	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	252	Total 252	O 252	0	0
4	B	250	Total 250	O 250	0	0
4	C	204	Total 204	O 204	0	0
4	D	245	Total 245	O 245	0	0
4	E	211	Total 211	O 211	0	0
4	F	235	Total 235	O 235	0	0
4	G	226	Total 226	O 226	0	0
4	H	195	Total 195	O 195	0	0
4	I	202	Total 202	O 202	0	0
4	J	213	Total 213	O 213	0	0
4	K	226	Total 226	O 226	0	0

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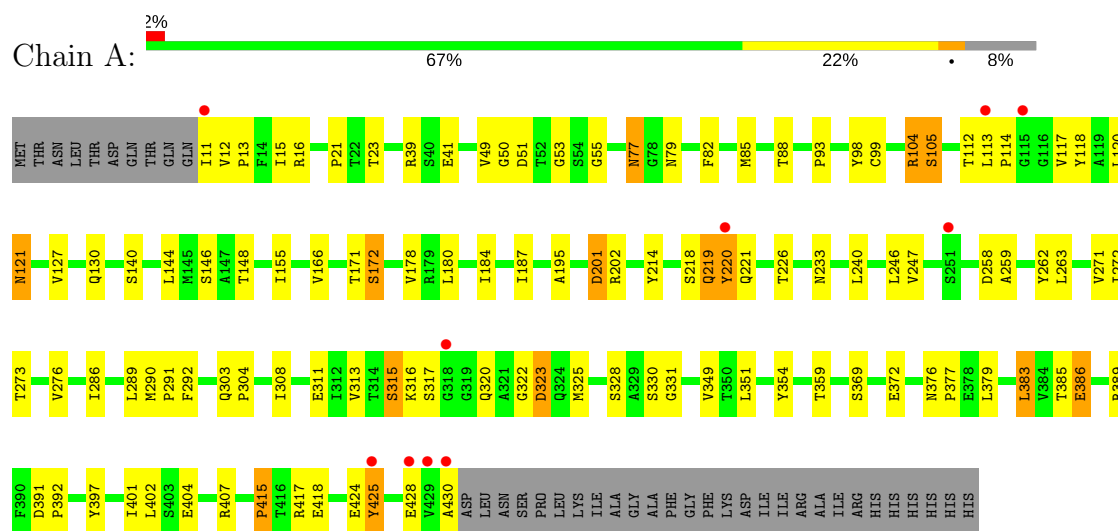
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	234	Total 234	O 234	0	0
4	M	235	Total 235	O 235	0	0
4	N	195	Total 195	O 195	0	0
4	O	216	Total 216	O 216	0	0
4	P	183	Total 183	O 183	0	0
4	Q	201	Total 201	O 201	0	0
4	R	226	Total 226	O 226	0	0
4	S	226	Total 226	O 226	0	0
4	T	270	Total 270	O 270	0	0

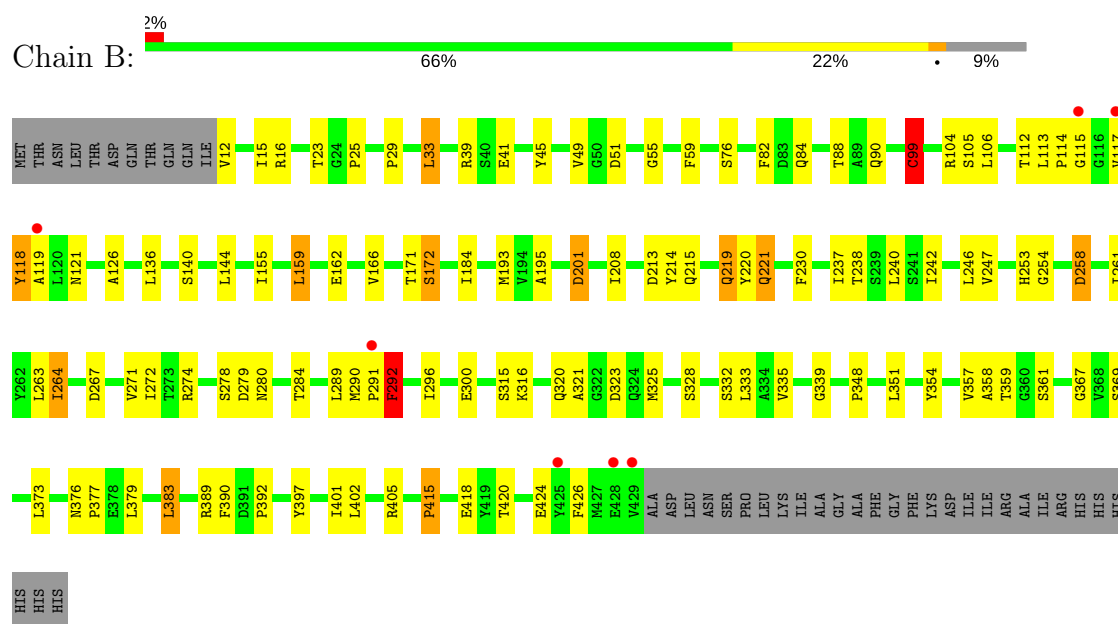
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

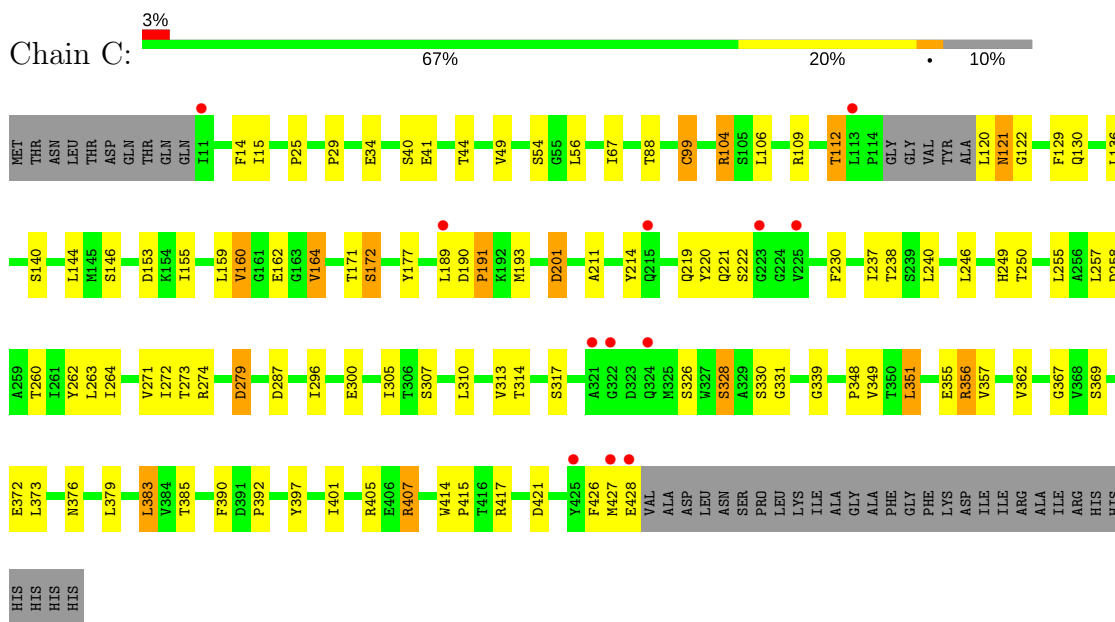
#### • Molecule 1: structural polypeptide VP2



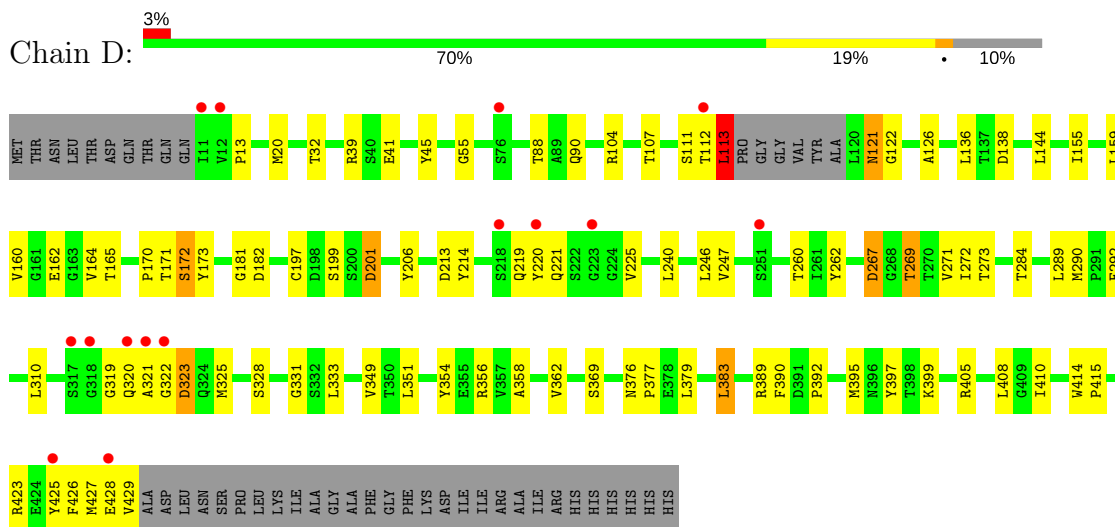
#### • Molecule 1: structural polypeptide VP2



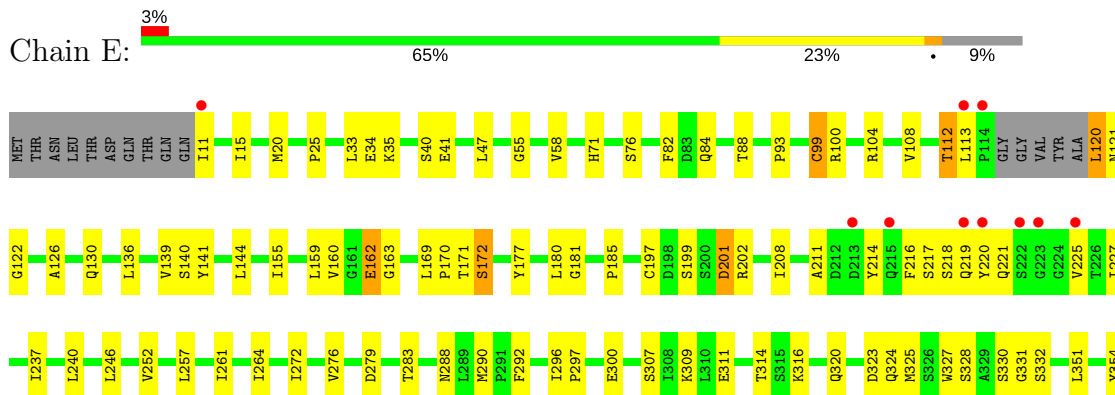
#### • Molecule 1: structural polypeptide VP2

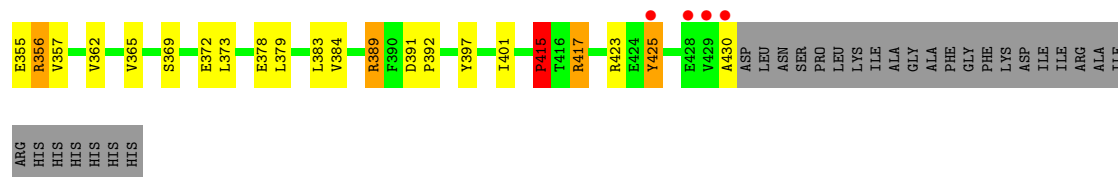


- Molecule 1: structural polyprotein VP2

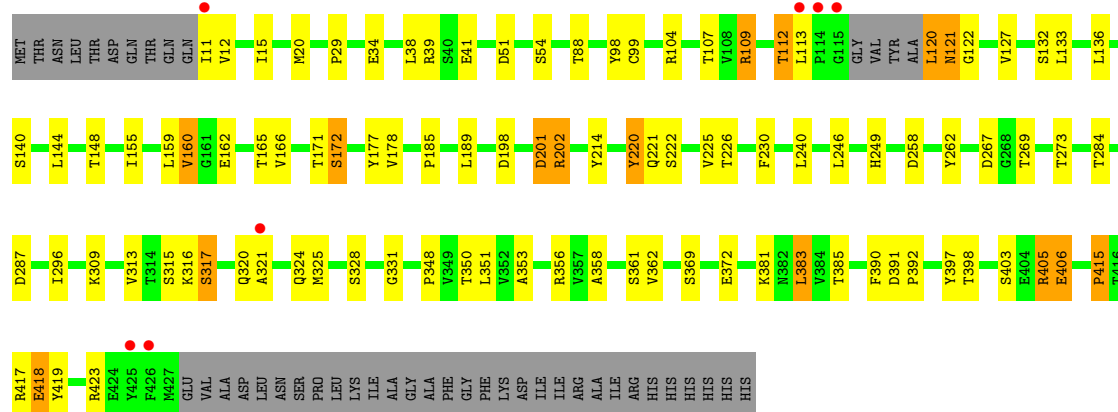


- Molecule 1: structural polyprotein VP2

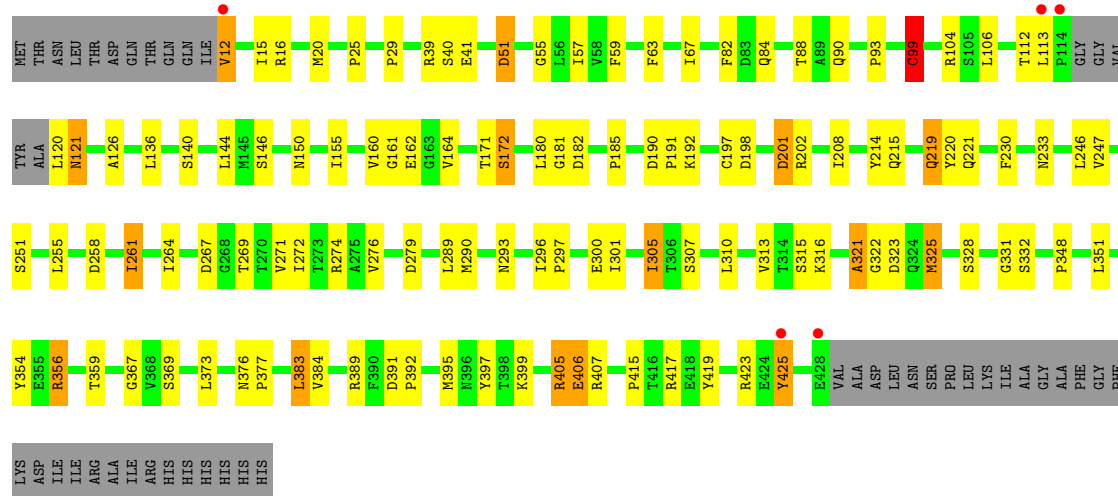




• Molecule 1: structural polypeptide VP2

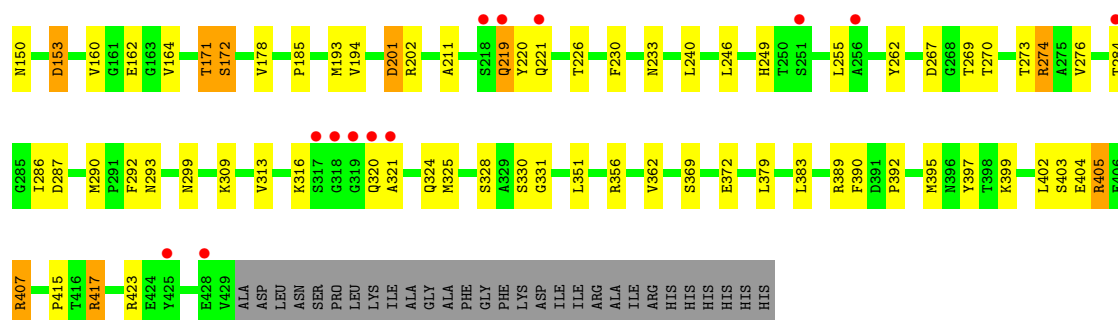


• Molecule 1: structural polypeptide VP2

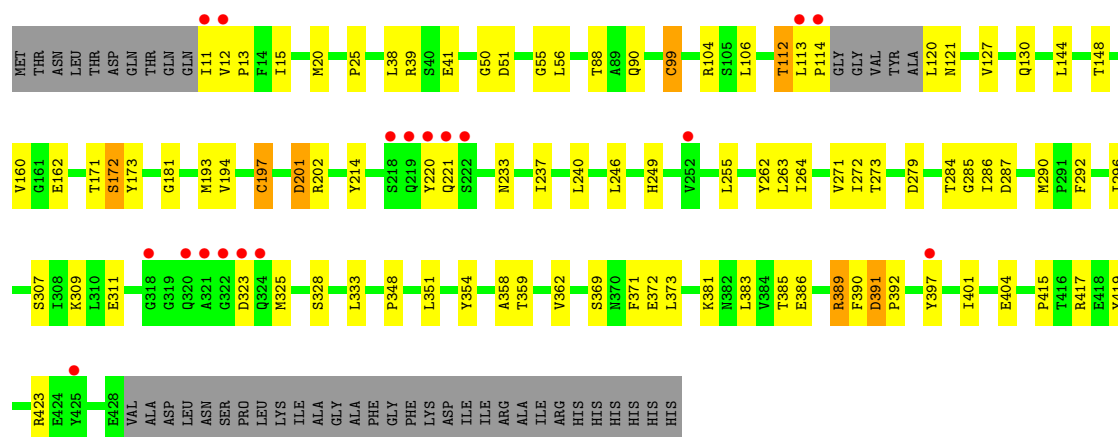


• Molecule 1: structural polypeptide VP2

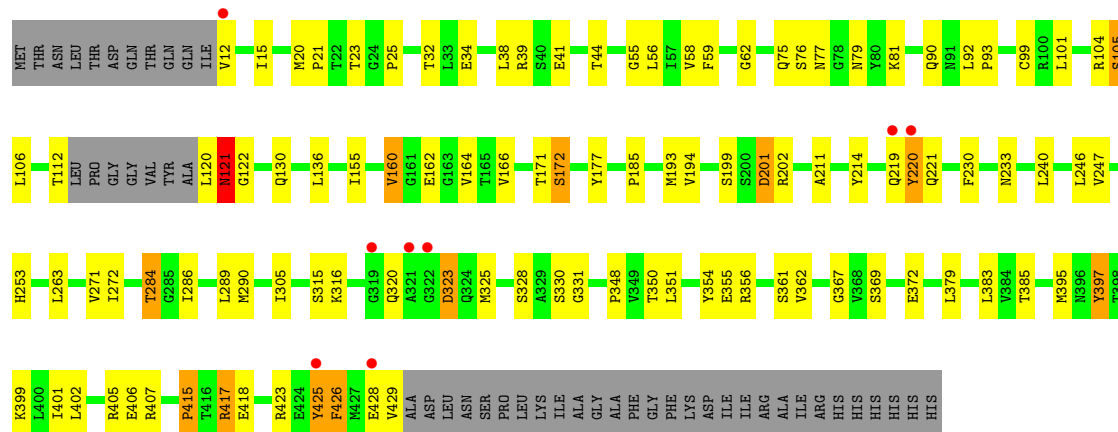




• Molecule 1: structural polypeptide VP2

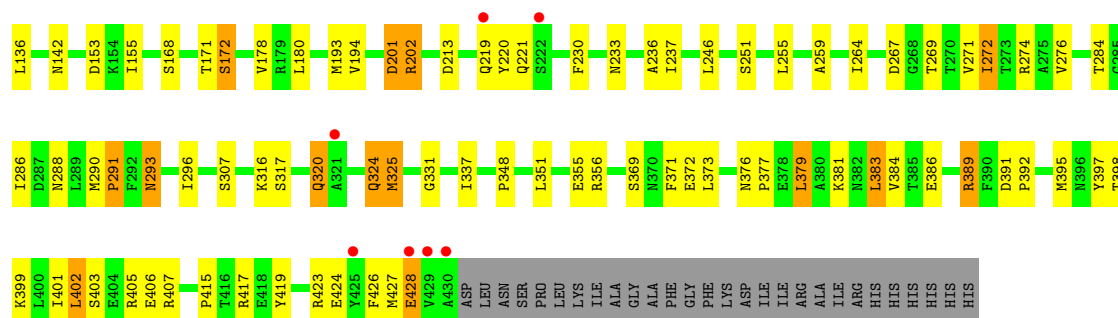


• Molecule 1: structural polypeptide VP2

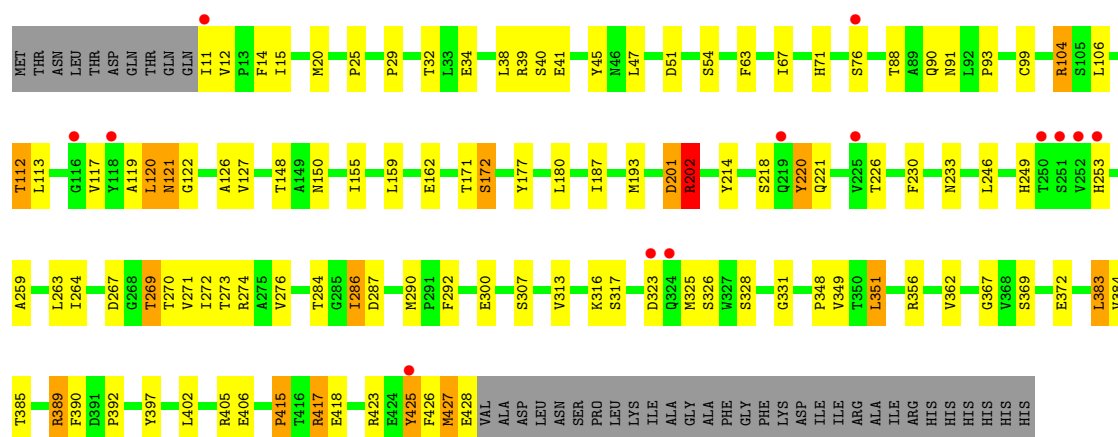


• Molecule 1: structural polypeptide VP2

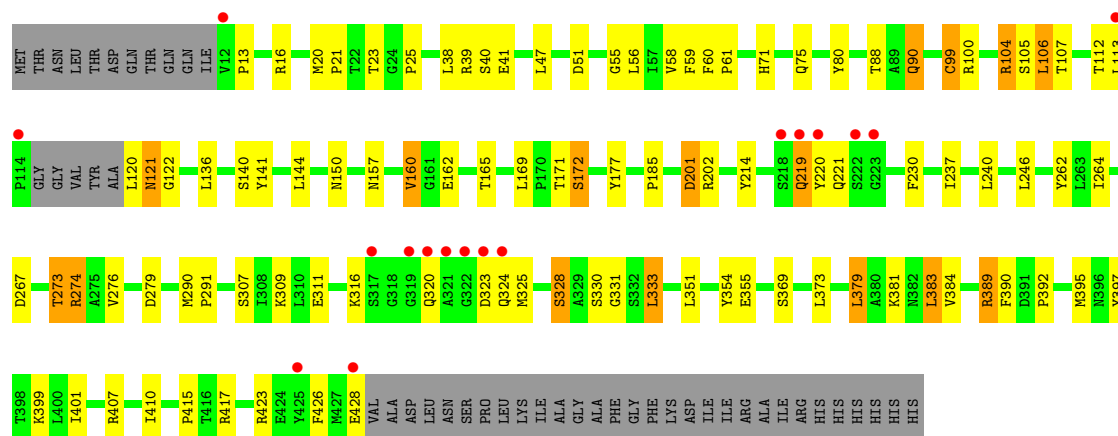




• Molecule 1: structural polypeptide VP2



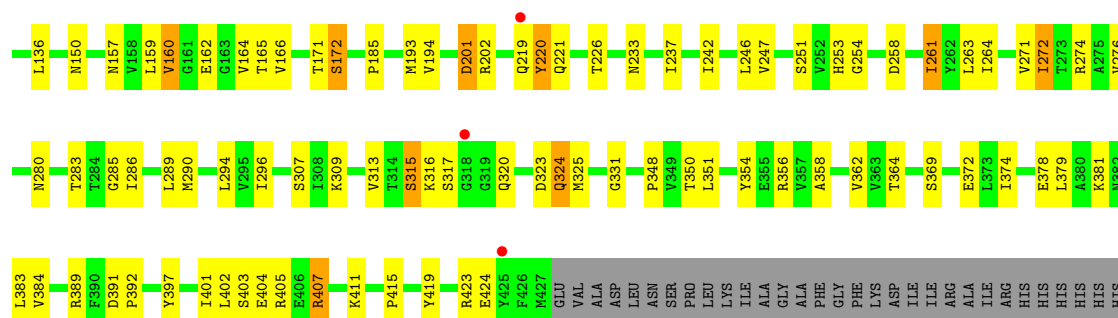
• Molecule 1: structural polypeptide VP2



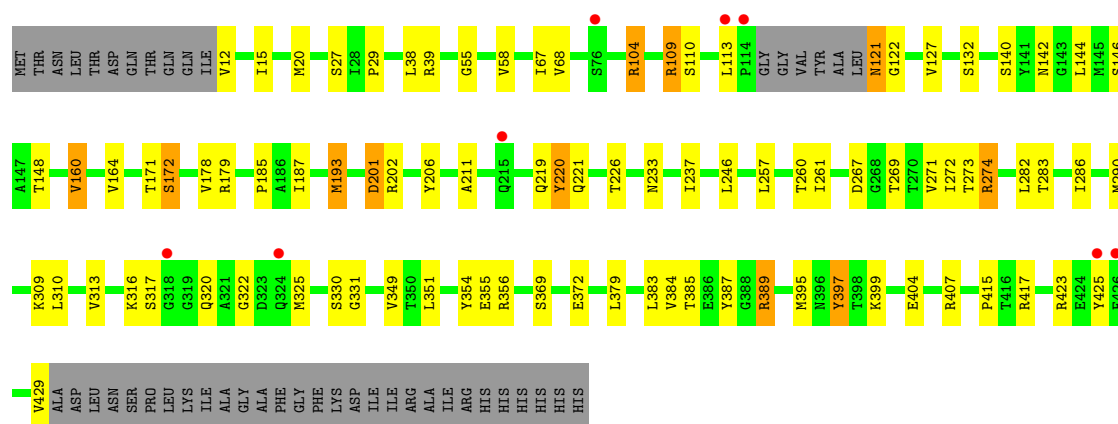
• Molecule 1: structural polypeptide VP2



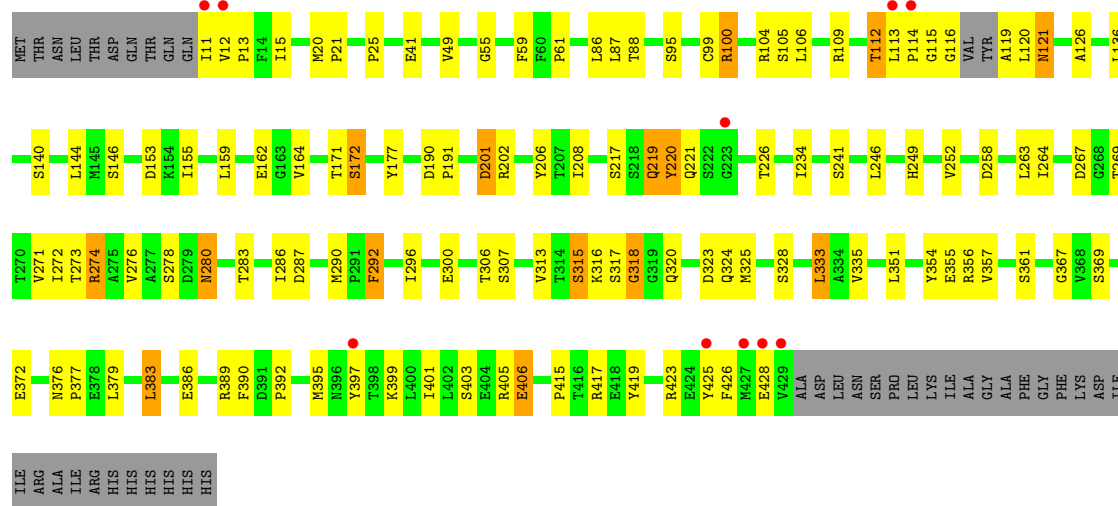




• Molecule 1: structural polypeptide VP2

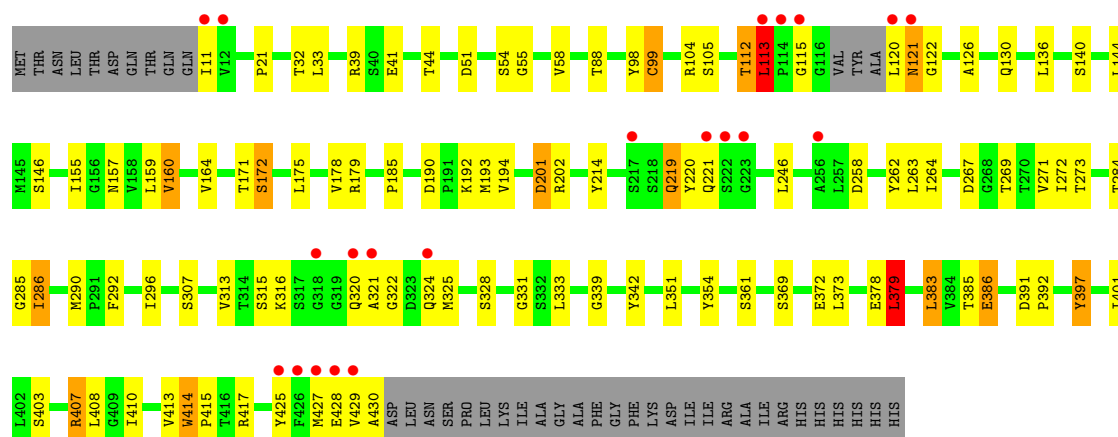


• Molecule 1: structural polypeptide VP2



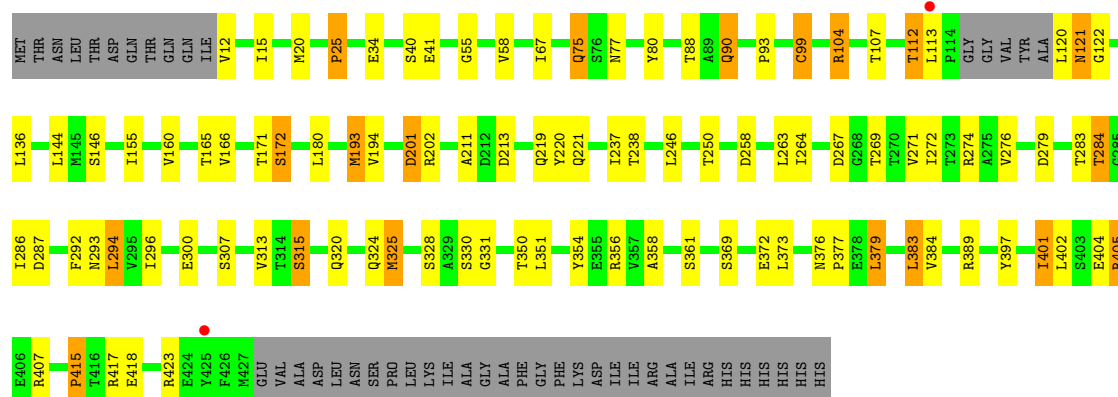
• Molecule 1: structural polypeptide VP2





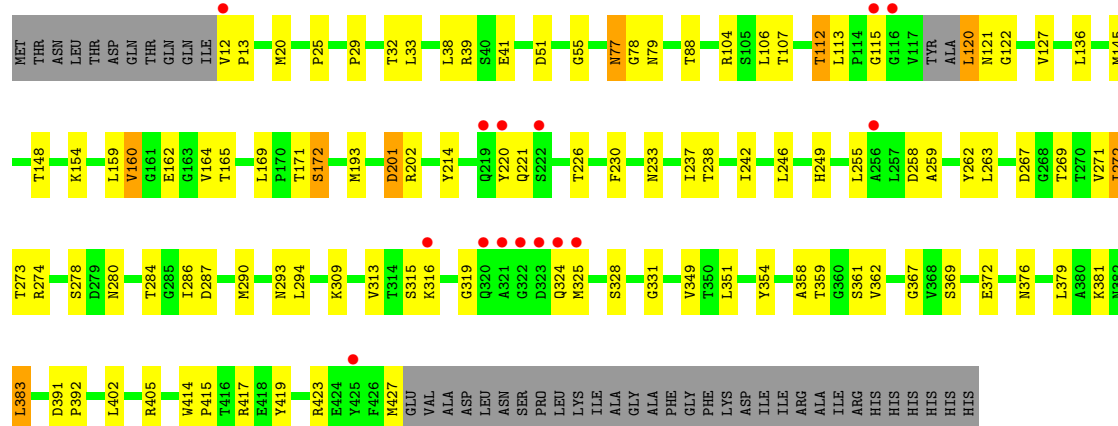
• Molecule 1: structural polyprotein VP2

Chain R: 68% 18% 10%



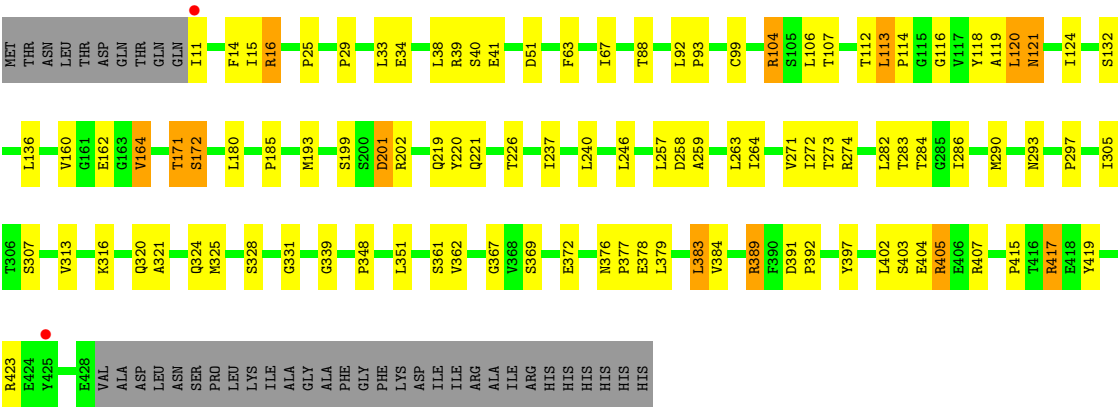
• Molecule 1: structural polyprotein VP2

Chain S: 3% 68% 21% 10%



• Molecule 1: structural polyprotein VP2

Chain T: 69% 20% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	316.41Å 316.41Å 316.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 49.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.6 (40.00-2.60) 89.6 (49.42-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.165 , 0.215 0.166 , 0.215	Depositor DCC
$R_{free}$ test set	14256 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	66956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, CL

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	0.81	1/3226 (0.0%)	0.90	4/4407 (0.1%)
1	B	0.87	2/3213 (0.1%)	0.96	3/4389 (0.1%)
1	C	0.77	0/3180	0.92	5/4342 (0.1%)
1	D	0.81	0/3179	0.94	8/4340 (0.2%)
1	E	0.82	2/3192 (0.1%)	0.94	3/4359 (0.1%)
1	F	0.79	0/3175	0.92	5/4335 (0.1%)
1	G	0.80	1/3172 (0.0%)	0.91	3/4331 (0.1%)
1	H	0.75	0/3179	0.88	5/4341 (0.1%)
1	I	0.74	1/3180 (0.0%)	0.88	3/4342 (0.1%)
1	J	0.76	0/3163	0.88	2/4318 (0.0%)
1	K	0.76	1/3199 (0.0%)	0.89	2/4368 (0.0%)
1	L	0.79	0/3214	0.90	4/4390 (0.1%)
1	M	0.77	0/3172	0.89	3/4331 (0.1%)
1	N	0.79	0/3171	0.91	5/4329 (0.1%)
1	O	0.75	0/3171	0.90	4/4330 (0.1%)
1	P	0.79	0/3200	0.94	2/4369 (0.0%)
1	Q	0.75	1/3200 (0.0%)	0.89	4/4369 (0.1%)
1	R	0.80	0/3163	0.94	4/4319 (0.1%)
1	S	0.79	0/3178	0.92	3/4339 (0.1%)
1	T	0.83	2/3214 (0.1%)	0.93	4/4390 (0.1%)
All	All	0.79	11/63741 (0.0%)	0.91	76/87038 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	3
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1
1	L	0	1
1	O	0	3
1	Q	0	1
All	All	0	11

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	PHE	CB-CG	-8.56	1.36	1.51
1	E	327	TRP	CB-CG	6.17	1.61	1.50
1	T	378	GLU	CG-CD	6.11	1.61	1.51
1	K	99	CYS	CB-SG	-5.85	1.72	1.81
1	G	99	CYS	CB-SG	-5.50	1.72	1.81
1	B	99	CYS	CB-SG	-5.30	1.73	1.81
1	A	99	CYS	CB-SG	-5.23	1.73	1.81
1	T	99	CYS	CB-SG	-5.11	1.73	1.81
1	Q	378	GLU	CG-CD	5.09	1.59	1.51
1	I	197	CYS	CB-SG	-5.05	1.73	1.81
1	E	378	GLU	CG-CD	5.02	1.59	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	120	LEU	CA-CB-CG	7.95	133.57	115.30
1	G	415	PRO	N-CA-C	-7.75	91.94	112.10
1	S	415	PRO	N-CA-C	-7.72	92.03	112.10
1	Q	415	PRO	N-CA-C	-7.60	92.33	112.10
1	K	415	PRO	N-CA-C	-7.60	92.35	112.10
1	T	415	PRO	N-CA-C	-7.52	92.55	112.10
1	J	415	PRO	N-CA-C	-7.46	92.70	112.10
1	O	415	PRO	N-CA-C	-7.42	92.80	112.10
1	D	113	LEU	CA-CB-CG	7.39	132.31	115.30
1	C	415	PRO	N-CA-C	-7.37	92.93	112.10
1	M	333	LEU	CA-CB-CG	7.36	132.22	115.30
1	M	415	PRO	N-CA-C	-7.35	92.99	112.10
1	A	415	PRO	N-CA-C	-7.34	93.01	112.10
1	H	415	PRO	N-CA-C	-7.34	93.03	112.10
1	F	415	PRO	N-CA-C	-7.25	93.26	112.10
1	E	120	LEU	CA-CB-CG	7.17	131.80	115.30
1	B	415	PRO	N-CA-C	-7.13	93.55	112.10
1	D	415	PRO	N-CA-C	-7.04	93.78	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	415	PRO	N-CA-C	-6.99	93.94	112.10
1	I	415	PRO	N-CA-C	-6.98	93.95	112.10
1	P	415	PRO	N-CA-C	-6.97	93.97	112.10
1	L	415	PRO	N-CA-C	-6.95	94.03	112.10
1	A	104	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	E	415	PRO	N-CA-C	-6.73	94.60	112.10
1	C	104	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	T	405	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	N	415	PRO	N-CA-C	-6.63	94.85	112.10
1	F	198	ASP	CB-CG-OD1	6.42	124.08	118.30
1	F	202	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	Q	379	LEU	CA-CB-CG	-6.27	100.88	115.30
1	K	372	GLU	N-CA-C	-6.22	94.20	111.00
1	N	407	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	144	LEU	CA-CB-CG	6.04	129.18	115.30
1	O	372	GLU	N-CA-C	-6.01	94.78	111.00
1	I	372	GLU	N-CA-C	-5.79	95.37	111.00
1	A	372	GLU	N-CA-C	-5.70	95.61	111.00
1	D	405	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	P	372	GLU	N-CA-C	-5.62	95.84	111.00
1	T	372	GLU	N-CA-C	-5.57	95.97	111.00
1	H	153	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	N	372	GLU	N-CA-C	-5.49	96.17	111.00
1	L	104	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	Q	372	GLU	N-CA-C	-5.46	96.25	111.00
1	S	372	GLU	N-CA-C	-5.46	96.26	111.00
1	C	372	GLU	N-CA-C	-5.45	96.28	111.00
1	L	372	GLU	N-CA-C	-5.45	96.30	111.00
1	T	104	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	R	325	MET	CG-SD-CE	-5.39	91.58	100.20
1	Q	113	LEU	CA-CB-CG	5.36	127.63	115.30
1	O	104	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	S	33	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	H	372	GLU	N-CA-C	-5.35	96.56	111.00
1	C	122	GLY	N-CA-C	5.34	126.45	113.10
1	N	51	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	267	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	D	356	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	H	104	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	383	LEU	CA-CB-CG	5.30	127.49	115.30
1	J	372	GLU	N-CA-C	-5.28	96.75	111.00
1	E	372	GLU	N-CA-C	-5.27	96.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	R	104	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	138	ASP	CB-CG-OD1	5.19	122.97	118.30
1	R	372	GLU	N-CA-C	-5.19	96.99	111.00
1	D	414	TRP	CB-CA-C	-5.17	100.06	110.40
1	O	274	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	G	405	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	F	372	GLU	N-CA-C	-5.08	97.30	111.00
1	H	405	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	L	202	ARG	CG-CD-NE	5.07	122.44	111.80
1	G	198	ASP	N-CA-C	5.06	124.67	111.00
1	F	405	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	M	104	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	D	267	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	264	ILE	CG1-CB-CG2	-5.01	100.38	111.40
1	N	356	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	TYR	Sidechain
1	D	206	TYR	Sidechain
1	D	397	TYR	Sidechain
1	D	45	TYR	Sidechain
1	J	397	TYR	Sidechain
1	K	14	PHE	Sidechain
1	L	45	TYR	Sidechain
1	O	206	TYR	Sidechain
1	O	387	TYR	Sidechain
1	O	397	TYR	Sidechain
1	Q	397	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3162	0	3141	111	0
1	B	3149	0	3125	102	0
1	C	3118	0	3097	92	0
1	D	3118	0	3099	62	0
1	E	3130	0	3111	99	0
1	F	3113	0	3094	85	0
1	G	3110	0	3086	111	0
1	H	3117	0	3095	84	0
1	I	3118	0	3097	69	0
1	J	3102	0	3077	89	0
1	K	3137	0	3115	94	0
1	L	3150	0	3127	95	0
1	M	3110	0	3086	88	0
1	N	3109	0	3086	83	0
1	O	3109	0	3084	79	0
1	P	3138	0	3117	102	0
1	Q	3138	0	3117	95	0
1	R	3101	0	3080	107	0
1	S	3116	0	3095	92	0
1	T	3150	0	3127	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	P	1	0	0	0	0
2	R	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
4	A	252	0	0	1	0
4	B	250	0	0	2	0
4	C	204	0	0	3	0
4	D	245	0	0	5	0
4	E	211	0	0	0	0
4	F	235	0	0	4	0
4	G	226	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	195	0	0	7	0
4	I	202	0	0	2	0
4	J	213	0	0	7	0
4	K	226	0	0	10	0
4	L	234	0	0	2	0
4	M	235	0	0	4	0
4	N	195	0	0	4	0
4	O	216	0	0	6	0
4	P	183	0	0	4	0
4	Q	201	0	0	1	0
4	R	226	0	0	4	0
4	S	226	0	0	8	0
4	T	270	0	0	5	0
All	All	66956	0	62056	1715	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1715) 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)
4:J:512:HOH:O	1:P:121:ASN:HB3	1.32	1.23
1:T:417:ARG:HH11	1:T:417:ARG:HB2	1.07	1.15
1:R:379:LEU:HD23	1:R:383:LEU:HD22	1.28	1.14
1:G:279:ASP:HB3	1:K:286:ILE:HD11	1.31	1.12
1:D:379:LEU:HG	1:D:383:LEU:HD12	1.27	1.10
1:T:112:THR:HG21	1:T:362:VAL:H	1.12	1.10
1:O:379:LEU:HG	1:O:383:LEU:HD12	1.13	1.10
1:T:219:GLN:NE2	1:T:324:GLN:HE22	1.52	1.08
1:A:85:MET:HE3	1:A:304:PRO:HD3	1.30	1.07
1:P:246:LEU:HD12	1:P:290:MET:HE2	1.29	1.06
1:F:112:THR:HG22	1:F:362:VAL:H	1.18	1.05
1:K:246:LEU:HD23	1:K:331:GLY:HA3	1.39	1.04
1:T:112:THR:CG2	1:T:362:VAL:H	1.70	1.03
1:A:121:ASN:HD21	1:T:112:THR:HB	1.19	1.03
1:E:136:LEU:HD11	1:E:351:LEU:HD11	1.40	1.02
1:A:13:PRO:HG3	1:A:389:ARG:HH21	1.25	1.01
1:M:13:PRO:HG3	1:R:407:ARG:HH12	1.22	1.01
1:A:113:LEU:HD12	1:B:119:ALA:HB3	1.41	1.00
1:R:276:VAL:HG11	1:R:292:PHE:CD2	1.97	1.00
1:G:279:ASP:CB	1:K:286:ILE:HD11	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:PRO:HB2	1:K:233:ASN:HD22	1.24	0.98
1:K:407:ARG:HH11	1:K:407:ARG:HB2	1.27	0.97
1:M:120:LEU:C	1:M:121:ASN:HD22	1.69	0.95
1:T:112:THR:HG21	1:T:362:VAL:N	1.80	0.95
1:C:120:LEU:HD21	1:R:113:LEU:HD12	1.50	0.93
1:A:233:ASN:HD22	1:F:185:PRO:HB2	1.30	0.93
1:O:379:LEU:HG	1:O:383:LEU:CD1	1.99	0.93
1:N:112:THR:HG22	1:N:362:VAL:H	1.32	0.92
1:D:389:ARG:HG2	4:D:553:HOH:O	1.68	0.92
1:K:407:ARG:NH1	1:K:407:ARG:HB2	1.85	0.92
1:G:316:LYS:HB3	1:G:321:ALA:HB3	1.52	0.92
1:S:246:LEU:HD23	1:S:331:GLY:HA3	1.51	0.91
1:B:219:GLN:NE2	1:B:219:GLN:H	1.67	0.91
1:A:121:ASN:ND2	1:T:112:THR:HB	1.85	0.91
1:S:162:GLU:OE1	1:S:417:ARG:HD2	1.71	0.91
1:T:316:LYS:HB2	1:T:325:MET:HE3	1.52	0.91
1:G:290:MET:HB2	4:G:6083:HOH:O	1.69	0.90
1:H:185:PRO:HB2	1:O:233:ASN:HD22	1.38	0.89
1:A:113:LEU:HD12	1:B:119:ALA:CB	2.02	0.89
1:H:233:ASN:HD22	1:N:185:PRO:HB2	1.35	0.89
1:R:404:GLU:OE2	1:R:407:ARG:HD3	1.70	0.89
1:R:315:SER:HA	1:R:325:MET:HE1	1.51	0.89
1:F:20:MET:HE2	1:F:423:ARG:HE	1.38	0.88
1:O:379:LEU:CG	1:O:383:LEU:HD12	2.02	0.88
1:C:189:LEU:HD12	1:E:227:ILE:HD12	1.55	0.88
1:B:106:LEU:HD23	1:B:367:GLY:HA3	1.53	0.88
1:H:417:ARG:HG2	1:H:417:ARG:HH11	1.38	0.87
1:H:320:GLN:HB3	4:H:5948:HOH:O	1.75	0.87
1:J:112:THR:OG1	4:J:512:HOH:O	1.93	0.87
1:T:417:ARG:CB	1:T:417:ARG:HH11	1.88	0.87
1:F:113:LEU:H	1:S:121:ASN:HD21	1.13	0.87
1:O:246:LEU:HD23	1:O:331:GLY:HA3	1.56	0.86
1:A:379:LEU:HG	1:A:383:LEU:HD12	1.58	0.86
1:P:246:LEU:HD12	1:P:290:MET:CE	2.06	0.85
1:T:112:THR:HG23	1:T:112:THR:O	1.75	0.84
1:T:219:GLN:NE2	1:T:324:GLN:NE2	2.25	0.84
1:O:417:ARG:HB2	1:O:417:ARG:NH1	1.93	0.84
1:I:121:ASN:HD22	1:I:358:ALA:H	1.21	0.84
1:N:246:LEU:HD12	1:N:290:MET:HE1	1.60	0.84
1:O:395:MET:HG3	1:O:399:LYS:HE3	1.60	0.84
1:E:220:TYR:O	1:E:221:GLN:HG3	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ASP:OD1	1:D:269:THR:HB	1.78	0.83
1:H:246:LEU:HD12	1:H:290:MET:CE	2.08	0.83
1:T:417:ARG:NH1	1:T:417:ARG:HB2	1.93	0.83
1:H:274:ARG:HH11	1:H:274:ARG:CG	1.89	0.83
1:N:11:ILE:HG13	1:N:12:VAL:H	1.43	0.83
1:F:112:THR:HG22	1:F:362:VAL:N	1.94	0.83
1:J:106:LEU:HD23	1:J:367:GLY:HA3	1.60	0.82
1:J:379:LEU:HG	1:J:383:LEU:HG	1.62	0.82
1:C:379:LEU:HG	1:C:383:LEU:HG	1.60	0.82
1:P:121:ASN:HD22	1:P:121:ASN:N	1.75	0.82
1:P:226:THR:OG1	1:P:313:VAL:HG22	1.78	0.82
1:F:121:ASN:OD1	1:F:358:ALA:N	2.13	0.82
1:P:292:PHE:HE1	1:P:333:LEU:HD23	1.42	0.82
1:P:120:LEU:HD12	1:P:121:ASN:H	1.45	0.81
1:F:246:LEU:HD23	1:F:331:GLY:HA3	1.62	0.81
1:C:219:GLN:HG3	4:C:6107:HOH:O	1.80	0.81
1:D:104:ARG:HD3	1:D:369:SER:OG	1.81	0.81
1:G:407:ARG:HD3	4:G:6122:HOH:O	1.80	0.80
1:H:246:LEU:HD12	1:H:290:MET:HE1	1.61	0.80
1:J:246:LEU:HD23	1:J:331:GLY:HA3	1.60	0.80
1:P:119:ALA:HA	4:P:5958:HOH:O	1.82	0.80
1:B:113:LEU:HD22	1:B:117:VAL:HB	1.60	0.80
1:J:75:GLN:NE2	1:J:81:LYS:HE3	1.96	0.80
1:E:379:LEU:HG	1:E:383:LEU:HG	1.63	0.80
1:H:12:VAL:N	4:H:6084:HOH:O	2.14	0.80
1:P:271:VAL:HG12	1:P:272:ILE:HD12	1.63	0.79
1:Q:219:GLN:NE2	1:Q:322:GLY:H	1.81	0.79
1:R:379:LEU:HD23	1:R:383:LEU:CD2	2.11	0.79
1:O:283:THR:HB	1:O:286:ILE:HG21	1.62	0.79
1:A:407:ARG:HB2	1:A:407:ARG:NH1	1.96	0.79
1:C:112:THR:OG1	1:N:121:ASN:HA	1.83	0.79
1:E:185:PRO:HB2	1:L:233:ASN:HD22	1.45	0.79
1:L:120:LEU:HD12	1:L:121:ASN:H	1.45	0.79
1:O:355:GLU:HG3	1:O:356:ARG:HG2	1.64	0.79
1:L:405:ARG:HD3	1:L:406:GLU:OE2	1.83	0.79
1:F:113:LEU:H	1:S:121:ASN:ND2	1.80	0.79
1:M:246:LEU:HD23	1:M:331:GLY:HA3	1.65	0.78
1:A:233:ASN:ND2	1:F:185:PRO:HB2	1.98	0.78
1:H:316:LYS:HB2	1:H:325:MET:HE2	1.65	0.78
1:S:269:THR:HG21	4:S:561:HOH:O	1.82	0.78
1:D:246:LEU:HD12	1:D:290:MET:CE	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:ARG:HG3	1:E:356:ARG:HH11	1.48	0.78
4:F:655:HOH:O	1:S:120:LEU:HD13	1.83	0.78
1:P:249:HIS:NE2	1:P:287:ASP:OD1	2.17	0.78
1:P:162:GLU:HG2	1:P:417:ARG:NH1	1.98	0.78
1:K:246:LEU:HD12	1:K:290:MET:HE1	1.66	0.78
1:R:202:ARG:HD2	1:S:201:ASP:OD2	1.83	0.77
1:C:106:LEU:HD23	1:C:367:GLY:HA3	1.66	0.77
1:M:246:LEU:HD12	1:M:290:MET:HE1	1.63	0.77
1:H:246:LEU:HD23	1:H:331:GLY:HA3	1.65	0.77
1:R:112:THR:HG22	1:R:361:SER:HA	1.65	0.77
1:G:192:LYS:HE2	4:K:579:HOH:O	1.84	0.77
1:S:379:LEU:CD2	1:S:383:LEU:HD22	2.15	0.77
1:G:279:ASP:HB3	1:K:286:ILE:CD1	2.13	0.77
1:N:389:ARG:HH11	1:N:389:ARG:HG2	1.49	0.77
1:K:407:ARG:NH2	4:K:485:HOH:O	2.18	0.77
1:M:120:LEU:C	1:M:121:ASN:ND2	2.37	0.77
1:G:104:ARG:HD3	1:G:369:SER:OG	1.85	0.77
1:A:121:ASN:CG	1:T:112:THR:HG1	1.89	0.77
1:H:274:ARG:HH11	1:H:274:ARG:HG3	1.50	0.77
1:N:233:ASN:HD22	1:O:185:PRO:HB2	1.47	0.77
1:D:395:MET:HG3	1:D:399:LYS:HE2	1.66	0.76
1:M:136:LEU:HD13	1:M:351:LEU:HD11	1.65	0.76
1:K:406:GLU:HG2	4:K:519:HOH:O	1.85	0.76
1:D:171:THR:O	1:D:172:SER:HB3	1.86	0.76
1:C:246:LEU:HD23	1:C:331:GLY:HA3	1.67	0.76
1:G:185:PRO:HB2	1:K:233:ASN:ND2	1.99	0.76
1:H:404:GLU:OE1	1:H:407:ARG:HD2	1.85	0.76
1:J:402:LEU:HD12	1:Q:33:LEU:HD13	1.67	0.76
1:I:233:ASN:HB2	1:J:185:PRO:HG2	1.68	0.76
1:R:122:GLY:HA2	1:R:356:ARG:HB2	1.68	0.76
1:I:285:GLY:O	1:I:286:ILE:HD12	1.87	0.76
1:L:316:LYS:HB2	1:L:325:MET:CE	2.15	0.75
1:L:417:ARG:HH11	1:L:417:ARG:HG3	1.51	0.75
1:M:13:PRO:CG	1:R:407:ARG:HH12	1.99	0.75
1:Q:144:LEU:HD22	1:Q:351:LEU:HD12	1.67	0.75
1:C:112:THR:HG22	1:C:362:VAL:H	1.52	0.75
1:H:104:ARG:HD3	1:H:369:SER:OG	1.86	0.75
1:H:120:LEU:HD12	4:I:6019:HOH:O	1.87	0.75
1:O:407:ARG:HB2	1:O:407:ARG:NH1	2.02	0.75
1:R:104:ARG:HD3	1:R:369:SER:OG	1.87	0.75
1:E:246:LEU:HD23	1:E:331:GLY:HA3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:316:LYS:HB2	1:L:325:MET:HE3	1.68	0.75
1:G:395:MET:HG3	1:G:399:LYS:HE3	1.69	0.75
1:H:112:THR:HG22	1:H:362:VAL:H	1.52	0.75
1:L:11:ILE:HD12	1:L:12:VAL:H	1.51	0.75
1:P:112:THR:HG23	1:P:113:LEU:N	2.02	0.75
1:B:292:PHE:CD2	1:B:292:PHE:N	2.48	0.74
1:J:112:THR:HB	1:J:362:VAL:H	1.51	0.74
1:T:119:ALA:O	1:T:120:LEU:HD23	1.87	0.74
1:F:249:HIS:HE1	1:F:287:ASP:OD1	1.71	0.74
1:G:267:ASP:OD1	1:G:269:THR:HB	1.87	0.74
1:K:246:LEU:CD2	1:K:331:GLY:HA3	2.17	0.74
1:N:136:LEU:HD13	1:N:351:LEU:HD11	1.69	0.74
1:G:120:LEU:HB3	4:G:5990:HOH:O	1.85	0.74
1:Q:104:ARG:NH1	4:Q:629:HOH:O	2.19	0.74
1:M:136:LEU:CD1	1:M:351:LEU:HD11	2.18	0.74
1:S:316:LYS:HB2	1:S:325:MET:HE3	1.70	0.74
1:C:263:LEU:HB3	1:C:305:ILE:HD13	1.67	0.74
1:Q:316:LYS:HB2	1:Q:325:MET:HE3	1.70	0.74
1:B:104:ARG:HD3	1:B:369:SER:OG	1.89	0.73
1:O:104:ARG:HD3	1:O:369:SER:OG	1.87	0.73
1:P:144:LEU:HD22	1:P:351:LEU:HD12	1.70	0.73
1:S:77:ASN:ND2	1:S:79:ASN:H	1.86	0.73
1:P:246:LEU:CD1	1:P:290:MET:HE2	2.16	0.73
1:Q:246:LEU:HD23	1:Q:331:GLY:HA3	1.70	0.73
1:I:171:THR:O	1:I:172:SER:HB3	1.87	0.73
1:T:162:GLU:HG2	1:T:417:ARG:NH2	2.04	0.73
1:E:58:VAL:HG22	1:E:351:LEU:HD23	1.69	0.73
1:I:285:GLY:C	1:I:286:ILE:HD12	2.09	0.73
1:H:316:LYS:N	1:H:325:MET:HE3	2.03	0.73
1:K:296:ILE:N	1:K:296:ILE:HD12	2.03	0.73
1:E:136:LEU:CD1	1:E:351:LEU:HD11	2.19	0.73
1:K:356:ARG:HH11	1:K:356:ARG:HG2	1.52	0.73
1:F:171:THR:O	1:F:172:SER:HB3	1.87	0.73
1:N:193:MET:HG2	1:N:194:VAL:N	2.02	0.73
1:G:12:VAL:HG23	4:G:6123:HOH:O	1.89	0.72
1:B:219:GLN:HE21	1:B:219:GLN:H	1.34	0.72
1:S:104:ARG:HD3	1:S:369:SER:OG	1.89	0.72
1:H:233:ASN:ND2	1:N:185:PRO:HB2	2.04	0.72
1:A:39:ARG:NH2	1:A:383:LEU:HD21	2.05	0.72
1:T:246:LEU:HD23	1:T:331:GLY:HA3	1.70	0.72
1:A:11:ILE:HB	1:A:430:ALA:HB1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:246:LEU:HD12	1:I:290:MET:CE	2.20	0.72
1:G:162:GLU:HG2	1:G:417:ARG:HH22	1.54	0.72
1:B:258:ASP:OD1	1:B:278:SER:HA	1.89	0.72
1:Q:262:TYR:CD2	1:Q:273:THR:HG22	2.25	0.72
1:S:20:MET:HB3	1:S:423:ARG:HH12	1.54	0.72
1:E:171:THR:O	1:E:172:SER:HB3	1.89	0.71
1:J:171:THR:O	1:J:172:SER:HB3	1.90	0.71
1:P:171:THR:O	1:P:172:SER:HB3	1.89	0.71
1:R:121:ASN:N	1:R:121:ASN:HD22	1.87	0.71
1:I:249:HIS:NE2	1:I:287:ASP:OD1	2.22	0.71
1:D:428:GLU:O	1:D:429:VAL:HG23	1.90	0.71
1:E:120:LEU:HB2	1:O:113:LEU:HD12	1.72	0.71
1:P:219:GLN:H	1:P:219:GLN:NE2	1.89	0.71
1:R:121:ASN:H	1:R:121:ASN:HD22	1.39	0.71
1:T:112:THR:HG21	1:T:361:SER:CA	2.20	0.71
1:S:271:VAL:HG12	1:S:272:ILE:HD12	1.70	0.71
1:F:267:ASP:OD1	1:F:269:THR:HB	1.91	0.71
1:B:415:PRO:HG2	1:B:418:GLU:HG3	1.71	0.71
1:O:389:ARG:HB2	1:O:389:ARG:HH11	1.55	0.71
1:A:320:GLN:O	1:A:323:ASP:OD2	2.09	0.70
1:S:20:MET:HE3	1:S:423:ARG:CZ	2.21	0.70
1:A:85:MET:CE	1:A:304:PRO:HD3	2.14	0.70
1:A:13:PRO:CG	1:A:389:ARG:HH21	2.02	0.70
1:R:220:TYR:CD1	1:R:325:MET:HE1	2.26	0.70
1:F:415:PRO:HG2	1:F:418:GLU:HB2	1.72	0.70
1:G:120:LEU:HD21	1:G:161:GLY:HA3	1.73	0.70
1:H:379:LEU:HG	1:H:383:LEU:HG	1.74	0.70
1:R:324:GLN:HA	1:R:324:GLN:HE21	1.56	0.70
1:D:246:LEU:HD23	1:D:331:GLY:HA3	1.73	0.70
1:H:389:ARG:HG2	4:H:5965:HOH:O	1.90	0.70
1:A:121:ASN:OD1	1:T:112:THR:OG1	2.04	0.70
1:A:262:TYR:CD2	1:A:273:THR:HG22	2.27	0.70
1:N:112:THR:HG22	1:N:362:VAL:N	2.07	0.70
1:R:294:LEU:HD22	1:R:296:ILE:HD11	1.72	0.70
1:D:383:LEU:HG	1:E:383:LEU:CD2	2.21	0.69
1:G:316:LYS:HB3	1:G:321:ALA:CB	2.21	0.69
1:N:41:GLU:OE1	1:N:90:GLN:HG2	1.92	0.69
1:F:39:ARG:NH2	1:F:383:LEU:HD21	2.06	0.69
1:A:121:ASN:ND2	1:T:112:THR:CB	2.55	0.69
1:E:283:THR:H	1:E:288:ASN:HD21	1.40	0.69
1:D:112:THR:HB	1:D:362:VAL:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:THR:OG1	1:L:121:ASN:ND2	2.25	0.69
1:L:104:ARG:HD3	1:L:369:SER:OG	1.93	0.69
1:P:121:ASN:ND2	1:P:121:ASN:N	2.39	0.69
1:A:15:ILE:HG13	1:A:397:TYR:HD2	1.57	0.69
1:L:417:ARG:HH11	1:L:417:ARG:CG	2.06	0.69
1:J:405:ARG:HD3	1:J:406:GLU:OE2	1.93	0.69
1:J:233:ASN:HD22	1:Q:185:PRO:HB2	1.58	0.69
1:J:246:LEU:CD2	1:J:331:GLY:HA3	2.22	0.69
1:P:121:ASN:ND2	4:P:5955:HOH:O	2.26	0.69
1:S:120:LEU:O	1:S:121:ASN:ND2	2.25	0.69
1:H:162:GLU:HB3	4:H:6004:HOH:O	1.93	0.68
1:O:404:GLU:OE1	1:O:407:ARG:HD2	1.93	0.68
1:P:405:ARG:HD3	1:P:406:GLU:OE2	1.93	0.68
1:G:261:ILE:HD12	1:G:310:LEU:HD13	1.73	0.68
1:O:389:ARG:HB2	1:O:389:ARG:NH1	2.08	0.68
1:O:425:TYR:O	1:O:429:VAL:HG23	1.93	0.68
1:R:415:PRO:HG2	1:R:418:GLU:HB2	1.74	0.68
1:A:349:VAL:HG12	1:A:351:LEU:HD22	1.75	0.68
1:K:379:LEU:HD23	1:K:383:LEU:HB2	1.73	0.68
1:I:11:ILE:HD12	1:I:12:VAL:H	1.57	0.68
1:J:425:TYR:O	1:J:425:TYR:HD2	1.76	0.68
1:N:246:LEU:HD23	1:N:331:GLY:HA3	1.75	0.68
1:K:428:GLU:O	1:K:428:GLU:HG2	1.94	0.68
1:L:417:ARG:NH1	1:L:417:ARG:HG3	2.09	0.68
1:M:121:ASN:HD22	1:M:121:ASN:N	1.91	0.68
1:S:249:HIS:NE2	1:S:287:ASP:OD1	2.22	0.68
1:F:316:LYS:N	1:F:325:MET:HE2	2.09	0.68
1:F:159:LEU:HB2	1:F:162:GLU:HG3	1.75	0.68
1:B:117:VAL:C	1:B:118:TYR:HD2	1.96	0.68
1:N:261:ILE:HD12	1:N:276:VAL:HG21	1.75	0.68
1:Q:379:LEU:CD2	1:Q:383:LEU:HD23	2.24	0.68
1:L:121:ASN:HD22	1:L:122:GLY:H	1.41	0.67
1:R:171:THR:O	1:R:172:SER:HB3	1.93	0.67
1:R:274:ARG:CB	1:R:294:LEU:HD21	2.23	0.67
1:G:219:GLN:HG3	1:G:220:TYR:N	2.07	0.67
1:M:379:LEU:HD23	1:M:383:LEU:HD23	1.76	0.67
1:M:397:TYR:O	1:M:401:ILE:HG12	1.94	0.67
1:S:316:LYS:HD3	1:S:319:GLY:HA3	1.75	0.67
1:E:356:ARG:HH11	1:E:356:ARG:CG	2.08	0.67
1:F:112:THR:CG2	1:F:362:VAL:H	2.02	0.67
1:L:267:ASP:OD1	1:L:269:THR:HB	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:511:HOH:O	1:Q:120:LEU:HD12	1.94	0.67
1:S:269:THR:CG2	4:S:561:HOH:O	2.41	0.67
1:B:15:ILE:HG13	1:B:397:TYR:HD2	1.57	0.67
1:D:112:THR:HG22	1:D:112:THR:O	1.93	0.67
1:P:106:LEU:HD23	1:P:367:GLY:HA3	1.75	0.67
1:E:112:THR:HG23	1:E:113:LEU:N	2.08	0.67
1:G:59:PHE:CE2	1:G:106:LEU:HD13	2.29	0.67
1:J:136:LEU:HD13	1:J:351:LEU:HD11	1.76	0.67
1:P:397:TYR:O	1:P:401:ILE:HG12	1.93	0.67
1:G:182:ASP:OD2	4:G:6063:HOH:O	2.13	0.67
1:K:389:ARG:HG3	1:K:389:ARG:O	1.94	0.67
1:A:407:ARG:HB2	1:A:407:ARG:HH11	1.59	0.67
1:N:246:LEU:HD12	1:N:290:MET:CE	2.24	0.67
1:R:20:MET:CE	1:R:423:ARG:HH21	2.06	0.67
1:C:272:ILE:HD13	1:C:296:ILE:CG2	2.24	0.67
1:Q:58:VAL:HG22	1:Q:351:LEU:HD22	1.76	0.67
1:A:13:PRO:HG3	1:A:389:ARG:NH2	2.06	0.66
1:B:219:GLN:N	1:B:219:GLN:HE21	1.92	0.66
1:M:219:GLN:HA	1:M:324:GLN:NE2	2.10	0.66
1:A:77:ASN:ND2	1:A:79:ASN:H	1.93	0.66
1:M:219:GLN:HG2	1:M:324:GLN:NE2	2.10	0.66
1:S:267:ASP:OD1	1:S:269:THR:HB	1.96	0.66
1:I:104:ARG:HD3	1:I:369:SER:OG	1.95	0.66
1:S:349:VAL:HG12	1:S:351:LEU:HD23	1.76	0.66
1:C:356:ARG:HH11	1:C:356:ARG:HG3	1.59	0.66
1:L:120:LEU:HD12	1:L:121:ASN:N	2.10	0.66
1:T:274:ARG:HH11	1:T:274:ARG:HG3	1.61	0.66
1:J:395:MET:HG3	1:J:399:LYS:HE3	1.77	0.66
1:K:419:TYR:CE2	1:K:423:ARG:HD2	2.31	0.66
1:M:316:LYS:HB2	1:M:325:MET:HE2	1.78	0.66
1:N:136:LEU:CD1	1:N:351:LEU:HD11	2.24	0.66
1:R:276:VAL:HG11	1:R:292:PHE:CE2	2.31	0.66
1:M:13:PRO:HG3	1:R:407:ARG:NH1	2.05	0.66
1:R:246:LEU:HD23	1:R:331:GLY:HA3	1.78	0.65
1:H:316:LYS:HB2	1:H:325:MET:CE	2.27	0.65
1:O:39:ARG:HH21	1:O:383:LEU:HD21	1.60	0.65
1:P:144:LEU:CD2	1:P:351:LEU:HD12	2.26	0.65
1:B:171:THR:HG21	1:B:348:PRO:HD3	1.78	0.65
1:E:240:LEU:HD23	1:E:296:ILE:HB	1.77	0.65
1:J:112:THR:CB	4:J:512:HOH:O	2.43	0.65
1:E:217:SER:HA	1:E:325:MET:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:GLY:O	1:F:160:VAL:HG23	1.97	0.65
1:Q:112:THR:C	1:Q:113:LEU:HD12	2.17	0.65
1:L:246:LEU:HD23	1:L:331:GLY:HA3	1.78	0.65
1:B:315:SER:HA	1:B:325:MET:CE	2.27	0.65
1:H:417:ARG:HG3	4:H:6004:HOH:O	1.95	0.65
1:O:39:ARG:NH2	1:O:383:LEU:HD21	2.12	0.65
1:C:417:ARG:HB2	1:C:417:ARG:NH1	2.11	0.65
1:D:111:SER:C	1:D:113:LEU:HD12	2.17	0.65
1:P:389:ARG:HG2	4:P:5986:HOH:O	1.97	0.65
1:T:324:GLN:HA	1:T:324:GLN:NE2	2.12	0.65
1:T:112:THR:CG2	1:T:361:SER:HB3	2.27	0.65
1:E:240:LEU:CD2	1:E:296:ILE:HB	2.27	0.64
1:B:113:LEU:CD2	1:B:117:VAL:HB	2.28	0.64
1:G:301:ILE:HG23	1:G:305:ILE:HD12	1.79	0.64
1:J:246:LEU:HD12	1:J:290:MET:HE1	1.78	0.64
1:K:193:MET:HG2	1:K:194:VAL:N	2.10	0.64
1:C:383:LEU:CD2	1:O:383:LEU:HG	2.28	0.64
1:E:201:ASP:OD2	1:L:202:ARG:NH1	2.31	0.64
1:G:425:TYR:HD1	4:G:6007:HOH:O	1.79	0.64
1:P:220:TYR:O	1:P:221:GLN:HG2	1.97	0.64
1:R:20:MET:HE2	1:R:423:ARG:HH21	1.62	0.64
1:H:274:ARG:CG	1:H:274:ARG:NH1	2.56	0.64
1:K:112:THR:HG22	1:K:113:LEU:N	2.12	0.64
1:O:417:ARG:HB2	1:O:417:ARG:HH11	1.60	0.64
1:B:215:GLN:OE1	1:B:328:SER:HB3	1.98	0.64
1:I:390:PHE:CE2	1:I:392:PRO:HG3	2.33	0.64
1:N:316:LYS:HB2	1:N:325:MET:HE3	1.80	0.64
1:O:389:ARG:CB	1:O:389:ARG:HH11	2.11	0.64
1:P:246:LEU:HD21	1:P:292:PHE:HZ	1.62	0.64
1:T:324:GLN:HA	1:T:324:GLN:HE21	1.63	0.64
1:A:171:THR:O	1:A:172:SER:HB3	1.98	0.63
1:A:246:LEU:HD12	1:A:290:MET:CE	2.28	0.63
1:T:389:ARG:HG3	1:T:389:ARG:O	1.97	0.63
1:G:162:GLU:HG2	1:G:417:ARG:NH2	2.13	0.63
1:P:120:LEU:HD12	1:P:121:ASN:N	2.13	0.63
1:Q:122:GLY:O	1:Q:160:VAL:HG22	1.98	0.63
1:S:417:ARG:HG3	4:S:646:HOH:O	1.98	0.63
1:H:417:ARG:HG2	1:H:417:ARG:NH1	2.13	0.63
1:E:220:TYR:CG	1:E:221:GLN:N	2.67	0.63
1:G:162:GLU:OE1	4:G:5947:HOH:O	2.16	0.63
1:R:417:ARG:HG3	1:R:417:ARG:HH11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG22	1:A:113:LEU:N	2.14	0.63
1:H:171:THR:O	1:H:172:SER:HB3	1.98	0.63
1:J:155:ILE:HG12	1:J:415:PRO:HD3	1.79	0.63
1:A:316:LYS:N	1:A:325:MET:HE2	2.13	0.63
1:T:171:THR:O	1:T:172:SER:HB3	1.97	0.63
1:F:316:LYS:N	1:F:325:MET:CE	2.62	0.63
1:R:237:ILE:HG22	1:R:238:THR:HG23	1.80	0.63
1:H:59:PHE:CE2	1:H:106:LEU:HD22	2.34	0.63
1:R:315:SER:CA	1:R:325:MET:HE1	2.28	0.63
1:E:246:LEU:HD12	1:E:290:MET:CE	2.29	0.62
1:D:246:LEU:HD12	1:D:290:MET:HE1	1.80	0.62
1:N:220:TYR:CG	1:N:221:GLN:N	2.67	0.62
1:P:379:LEU:HG	1:P:383:LEU:HD23	1.79	0.62
1:R:220:TYR:CD1	1:R:325:MET:CE	2.81	0.62
1:B:118:TYR:N	1:B:118:TYR:CD2	2.67	0.62
1:I:246:LEU:HD12	1:I:290:MET:HE1	1.81	0.62
1:B:136:LEU:HD13	1:B:351:LEU:HD11	1.80	0.62
1:H:233:ASN:HD22	1:N:185:PRO:CB	2.09	0.62
1:N:379:LEU:CD2	1:N:383:LEU:HD22	2.29	0.62
1:Q:316:LYS:HB2	1:Q:325:MET:CE	2.29	0.62
1:E:171:THR:O	1:E:172:SER:CB	2.46	0.62
1:P:112:THR:CG2	1:P:113:LEU:N	2.62	0.62
1:Q:144:LEU:CD2	1:Q:351:LEU:HD12	2.29	0.62
1:L:426:PHE:C	1:L:428:GLU:H	2.02	0.62
1:D:379:LEU:HG	1:D:383:LEU:CD1	2.17	0.62
1:E:276:VAL:HG11	1:E:292:PHE:CE2	2.34	0.62
1:K:201:ASP:OD2	1:M:202:ARG:HD2	1.99	0.62
1:B:155:ILE:HG12	1:B:415:PRO:HD3	1.80	0.62
1:T:316:LYS:HB2	1:T:325:MET:CE	2.27	0.62
1:L:316:LYS:N	1:L:325:MET:HE1	2.14	0.62
1:N:226:THR:OG1	1:N:313:VAL:HG22	2.00	0.62
1:P:104:ARG:HD3	1:P:369:SER:OG	2.00	0.62
1:B:16:ARG:NH1	1:B:23:THR:HB	2.14	0.61
1:B:136:LEU:CD1	1:B:351:LEU:HD11	2.30	0.61
1:M:121:ASN:ND2	4:M:504:HOH:O	2.32	0.61
1:R:267:ASP:OD1	1:R:269:THR:HB	2.00	0.61
1:S:145:MET:O	1:S:154:LYS:HE2	1.99	0.61
1:O:417:ARG:CB	1:O:417:ARG:HH11	2.12	0.61
1:R:293:ASN:HD21	1:T:293:ASN:HD21	1.49	0.61
1:A:121:ASN:HD21	1:T:112:THR:CB	2.03	0.61
1:C:171:THR:O	1:C:172:SER:HB3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:LEU:O	1:G:113:LEU:HD12	2.01	0.61
1:K:389:ARG:HG2	4:K:623:HOH:O	1.99	0.61
1:O:407:ARG:HB2	1:O:407:ARG:HH11	1.65	0.61
1:Q:417:ARG:HB2	1:Q:417:ARG:NH1	2.15	0.61
1:A:155:ILE:HG12	1:A:415:PRO:HD3	1.83	0.61
1:E:397:TYR:O	1:E:401:ILE:HG12	2.00	0.61
1:K:246:LEU:HD12	1:K:290:MET:CE	2.30	0.61
1:L:415:PRO:HG2	1:L:418:GLU:HB2	1.82	0.61
1:M:246:LEU:HD12	1:M:290:MET:CE	2.30	0.61
1:B:15:ILE:HG13	1:B:397:TYR:CD2	2.35	0.61
1:B:415:PRO:HG2	1:B:418:GLU:CG	2.31	0.61
1:G:12:VAL:N	4:G:6123:HOH:O	2.33	0.61
1:G:297:PRO:HG2	1:G:300:GLU:HG3	1.83	0.61
1:L:423:ARG:HH21	1:L:427:MET:HE3	1.65	0.61
1:Q:112:THR:HG22	1:Q:361:SER:HA	1.81	0.61
1:A:12:VAL:HG12	1:A:15:ILE:H	1.66	0.61
1:B:389:ARG:NH1	1:B:389:ARG:HB3	2.16	0.61
1:S:20:MET:HG2	1:S:423:ARG:NH1	2.15	0.61
1:A:247:VAL:HG22	1:A:289:LEU:CD2	2.31	0.61
1:E:20:MET:CE	1:E:423:ARG:HD2	2.31	0.61
1:G:246:LEU:HD23	1:G:331:GLY:HA3	1.83	0.61
1:E:20:MET:HE2	1:E:423:ARG:HD2	1.83	0.61
1:G:220:TYR:CG	1:G:221:GLN:N	2.68	0.61
1:A:407:ARG:CB	1:A:407:ARG:HH11	2.14	0.60
1:C:279:ASP:CG	1:C:279:ASP:O	2.39	0.60
1:N:166:VAL:HG13	1:N:350:THR:HG21	1.81	0.60
1:A:323:ASP:OD2	1:A:323:ASP:N	2.34	0.60
1:N:285:GLY:O	1:N:286:ILE:HD12	2.01	0.60
1:Q:267:ASP:OD1	1:Q:269:THR:HB	2.01	0.60
1:R:120:LEU:HG	4:R:6030:HOH:O	2.01	0.60
1:M:171:THR:O	1:M:172:SER:HB3	2.00	0.60
1:M:316:LYS:N	1:M:325:MET:HE3	2.16	0.60
1:Q:171:THR:O	1:Q:172:SER:HB3	2.02	0.60
1:R:107:THR:HG22	1:R:165:THR:OG1	2.01	0.60
1:S:246:LEU:CD2	1:S:331:GLY:HA3	2.27	0.60
1:J:38:LEU:O	1:J:39:ARG:NH1	2.27	0.60
1:G:185:PRO:CB	1:K:233:ASN:HD22	2.05	0.60
1:M:407:ARG:NH2	1:Q:11:ILE:HG22	2.17	0.60
1:N:324:GLN:OE1	1:N:324:GLN:HA	2.02	0.60
1:C:121:ASN:N	1:C:121:ASN:HD22	2.00	0.60
1:M:273:THR:O	1:M:274:ARG:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:429:VAL:O	1:Q:429:VAL:HG12	2.01	0.60
1:M:320:GLN:O	1:M:323:ASP:HB2	2.02	0.60
1:B:292:PHE:HD2	1:B:292:PHE:N	1.96	0.60
1:H:15:ILE:HG13	1:H:397:TYR:HD2	1.66	0.60
1:K:397:TYR:O	1:K:401:ILE:HG12	2.02	0.60
1:M:104:ARG:HD3	1:M:369:SER:OG	2.01	0.60
1:T:259:ALA:HB3	1:T:290:MET:HE3	1.83	0.60
1:A:219:GLN:NE2	1:A:322:GLY:H	2.00	0.60
1:T:136:LEU:CD1	1:T:351:LEU:HD11	2.32	0.60
1:B:219:GLN:N	1:B:219:GLN:NE2	2.45	0.59
1:F:38:LEU:O	1:F:39:ARG:NH1	2.32	0.59
1:S:379:LEU:HD21	1:S:383:LEU:HD22	1.82	0.59
1:S:379:LEU:HD23	1:S:383:LEU:HD22	1.83	0.59
1:L:226:THR:OG1	1:L:313:VAL:HG22	2.03	0.59
1:S:171:THR:O	1:S:172:SER:HB3	2.00	0.59
1:T:114:PRO:O	1:T:118:TYR:HB2	2.01	0.59
1:N:271:VAL:HG12	1:N:272:ILE:HD12	1.84	0.59
1:S:255:LEU:HD22	1:S:325:MET:HE2	1.84	0.59
1:D:121:ASN:HD21	1:D:358:ALA:H	1.50	0.59
1:F:144:LEU:HD22	1:F:351:LEU:CD1	2.32	0.59
1:H:273:THR:O	1:H:274:ARG:HD3	2.03	0.59
1:P:220:TYR:HB2	1:P:316:LYS:HE2	1.83	0.59
1:N:159:LEU:HB2	1:N:162:GLU:HG3	1.84	0.59
1:T:274:ARG:NH1	1:T:274:ARG:HG3	2.16	0.59
1:C:15:ILE:HG13	1:C:397:TYR:HD2	1.67	0.59
1:H:25:PRO:HD3	1:H:40:SER:OG	2.03	0.59
1:J:315:SER:HA	1:J:325:MET:HE1	1.84	0.59
1:L:155:ILE:HG12	1:L:415:PRO:HD3	1.85	0.59
1:G:417:ARG:HG3	1:G:417:ARG:NH1	2.17	0.59
1:N:389:ARG:HG2	1:N:389:ARG:NH1	2.16	0.59
1:A:146:SER:O	1:F:381:LYS:HG2	2.03	0.59
1:A:219:GLN:HE22	1:A:322:GLY:H	1.49	0.59
1:F:220:TYR:CG	1:F:221:GLN:N	2.70	0.59
1:K:171:THR:O	1:K:172:SER:HB3	2.03	0.59
1:B:390:PHE:CE2	1:B:392:PRO:HG3	2.37	0.59
1:C:356:ARG:HH11	1:C:356:ARG:CG	2.15	0.59
1:M:309:LYS:NZ	4:M:611:HOH:O	2.35	0.59
1:E:316:LYS:N	1:E:325:MET:HE3	2.17	0.58
1:D:39:ARG:NH2	1:D:383:LEU:HD21	2.19	0.58
1:E:216:PHE:CE1	1:E:227:ILE:HG21	2.38	0.58
1:F:249:HIS:CE1	1:F:287:ASP:OD1	2.54	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:246:LEU:HD12	1:I:290:MET:HE2	1.84	0.58
1:Q:417:ARG:HH11	1:Q:417:ARG:HB2	1.69	0.58
1:B:115:GLY:HA2	4:B:6059:HOH:O	2.03	0.58
1:C:249:HIS:NE2	1:C:287:ASP:OD1	2.27	0.58
1:T:383:LEU:C	1:T:383:LEU:HD12	2.24	0.58
1:C:258:ASP:HB2	1:C:313:VAL:HB	1.85	0.58
1:M:274:ARG:CG	1:M:274:ARG:HH11	2.16	0.58
1:T:402:LEU:O	1:T:405:ARG:HB2	2.04	0.58
1:C:390:PHE:CE2	1:C:392:PRO:HG3	2.39	0.58
1:E:216:PHE:HE1	1:E:227:ILE:HG21	1.67	0.58
1:J:171:THR:O	1:J:172:SER:CB	2.52	0.58
1:K:219:GLN:HG2	1:K:324:GLN:HG2	1.84	0.58
1:K:379:LEU:HD21	1:K:383:LEU:HD23	1.85	0.58
1:Q:99:CYS:HB2	1:Q:373:LEU:HD23	1.85	0.58
1:T:112:THR:CG2	1:T:112:THR:O	2.51	0.58
1:G:316:LYS:HD2	1:G:322:GLY:O	2.04	0.58
1:M:141:TYR:CE1	1:M:355:GLU:HG2	2.38	0.58
1:G:112:THR:CG2	1:G:113:LEU:N	2.66	0.58
1:K:356:ARG:NH1	1:K:356:ARG:HG2	2.19	0.58
1:S:159:LEU:HB2	1:S:162:GLU:HG3	1.85	0.58
1:T:419:TYR:CE2	1:T:423:ARG:HD2	2.38	0.58
1:C:220:TYR:CG	1:C:221:GLN:N	2.72	0.58
1:E:252:VAL:CG1	1:E:316:LYS:HE3	2.34	0.58
1:M:390:PHE:CZ	1:M:392:PRO:HG3	2.38	0.58
1:N:171:THR:O	1:N:172:SER:HB3	2.04	0.58
1:J:397:TYR:O	1:J:401:ILE:HG12	2.03	0.58
1:J:41:GLU:OE1	1:J:90:GLN:HG2	2.04	0.58
1:P:201:ASP:O	1:P:202:ARG:HB2	2.03	0.58
1:P:274:ARG:CG	1:P:274:ARG:HH11	2.15	0.58
1:L:41:GLU:OE1	1:L:90:GLN:HG2	2.04	0.58
1:R:324:GLN:HA	1:R:324:GLN:NE2	2.18	0.58
1:G:201:ASP:OD2	1:K:202:ARG:HD2	2.03	0.57
1:O:146:SER:HB2	4:O:616:HOH:O	2.04	0.57
1:I:144:LEU:HD21	1:I:351:LEU:HD12	1.87	0.57
1:K:99:CYS:HB2	1:K:373:LEU:HD23	1.87	0.57
1:A:246:LEU:HD12	1:A:290:MET:HE1	1.86	0.57
1:L:171:THR:O	1:L:172:SER:HB3	2.05	0.57
1:R:315:SER:HA	1:R:325:MET:CE	2.29	0.57
1:A:385:THR:C	1:A:386:GLU:HG2	2.25	0.57
1:P:274:ARG:HG3	1:P:274:ARG:HH11	1.68	0.57
1:L:349:VAL:HG12	1:L:351:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:273:THR:O	1:P:274:ARG:HD3	2.03	0.57
1:Q:21:PRO:HG2	1:Q:105:SER:HB3	1.87	0.57
1:G:417:ARG:HH11	1:G:417:ARG:HG3	1.67	0.57
1:R:296:ILE:N	1:R:296:ILE:HD12	2.19	0.57
1:B:280:ASN:HB3	1:B:290:MET:HE1	1.86	0.57
1:F:112:THR:CG2	1:F:362:VAL:N	2.65	0.57
1:J:220:TYR:CG	1:J:221:GLN:N	2.73	0.57
1:J:379:LEU:HG	1:J:383:LEU:CG	2.34	0.56
4:J:512:HOH:O	1:P:121:ASN:CB	2.12	0.56
1:C:407:ARG:HH11	1:C:407:ARG:HB2	1.69	0.56
1:E:25:PRO:HD3	1:E:40:SER:OG	2.05	0.56
1:G:405:ARG:HD3	1:G:406:GLU:OE2	2.05	0.56
1:K:104:ARG:HD3	1:K:369:SER:OG	2.05	0.56
1:N:11:ILE:HG13	1:N:12:VAL:N	2.16	0.56
1:O:187:ILE:O	1:O:187:ILE:HG13	2.05	0.56
1:Q:271:VAL:HG12	1:Q:272:ILE:HG12	1.87	0.56
1:B:379:LEU:CD2	1:B:383:LEU:HD23	2.35	0.56
1:H:41:GLU:OE1	1:H:90:GLN:HG2	2.05	0.56
1:J:104:ARG:HD3	1:J:369:SER:OG	2.05	0.56
1:J:34:GLU:HG3	1:J:177:TYR:CE1	2.41	0.56
1:M:144:LEU:HD22	1:M:351:LEU:HD12	1.88	0.56
1:O:267:ASP:OD1	1:O:269:THR:HG23	2.04	0.56
1:E:162:GLU:HG3	1:E:163:GLY:N	2.20	0.56
1:E:208:ILE:O	1:E:332:SER:HA	2.05	0.56
1:G:356:ARG:HG3	1:G:356:ARG:HH11	1.70	0.56
1:P:59:PHE:O	1:P:61:PRO:HD3	2.05	0.56
1:C:230:PHE:CD1	1:C:230:PHE:C	2.78	0.56
1:M:58:VAL:HG22	1:M:351:LEU:HD22	1.86	0.56
1:P:315:SER:HA	1:P:325:MET:HE1	1.86	0.56
1:O:171:THR:O	1:O:172:SER:HB3	2.06	0.56
1:B:171:THR:O	1:B:172:SER:CB	2.54	0.56
1:C:262:TYR:CD2	1:C:273:THR:HG22	2.40	0.56
1:J:20:MET:HG2	1:J:423:ARG:HG2	1.86	0.56
1:O:140:SER:O	1:O:144:LEU:HG	2.05	0.56
1:B:112:THR:HG22	1:D:122:GLY:H	1.71	0.56
1:G:279:ASP:OD2	4:G:6118:HOH:O	2.18	0.56
1:I:171:THR:HG21	1:I:348:PRO:HD3	1.88	0.56
1:N:397:TYR:CE2	1:N:401:ILE:HD11	2.40	0.56
1:R:293:ASN:HD21	1:T:293:ASN:ND2	2.04	0.56
1:H:136:LEU:HD13	1:H:351:LEU:HD11	1.86	0.56
1:K:75:GLN:NE2	1:K:81:LYS:HD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:171:THR:O	1:P:172:SER:CB	2.53	0.56
1:S:358:ALA:O	1:S:361:SER:OG	2.20	0.56
1:S:427:MET:C	4:S:532:HOH:O	2.45	0.56
1:K:99:CYS:HB3	1:K:180:LEU:HD21	1.88	0.56
1:P:11:ILE:HD12	1:P:12:VAL:H	1.70	0.56
1:A:13:PRO:CG	1:A:389:ARG:NH2	2.68	0.55
1:F:171:THR:O	1:F:172:SER:CB	2.53	0.55
1:L:20:MET:HG2	1:L:423:ARG:HG2	1.88	0.55
1:N:404:GLU:OE1	1:N:407:ARG:NH1	2.39	0.55
1:R:75:GLN:HB2	1:R:77:ASN:OD1	2.06	0.55
1:T:171:THR:O	1:T:172:SER:CB	2.54	0.55
1:C:250:THR:OG1	1:C:326:SER:O	2.21	0.55
1:E:355:GLU:O	1:E:356:ARG:HB2	2.05	0.55
1:H:395:MET:HG3	1:H:399:LYS:HE3	1.87	0.55
1:I:255:LEU:CD2	1:I:325:MET:HG2	2.36	0.55
1:A:118:TYR:OH	1:L:113:LEU:HD13	2.06	0.55
1:R:201:ASP:OD2	1:T:202:ARG:HD2	2.06	0.55
1:A:379:LEU:CG	1:A:383:LEU:HD12	2.34	0.55
1:B:41:GLU:OE1	1:B:90:GLN:HG2	2.07	0.55
1:H:140:SER:O	1:H:144:LEU:HG	2.05	0.55
1:J:253:HIS:CE1	1:J:284:THR:HG21	2.41	0.55
1:O:395:MET:CG	1:O:399:LYS:HE3	2.35	0.55
1:P:121:ASN:HD22	1:P:121:ASN:H	1.53	0.55
1:Q:428:GLU:C	1:Q:430:ALA:H	2.09	0.55
1:R:274:ARG:NH2	1:R:300:GLU:OE1	2.39	0.55
1:A:417:ARG:NH2	4:A:6077:HOH:O	2.39	0.55
1:B:420:THR:O	1:B:424:GLU:HG3	2.07	0.55
1:D:408:LEU:HB2	1:D:410:ILE:HD12	1.88	0.55
1:F:317:SER:HA	4:F:569:HOH:O	2.04	0.55
1:M:426:PHE:C	1:M:428:GLU:H	2.09	0.55
1:O:220:TYR:CG	1:O:221:GLN:N	2.74	0.55
1:A:118:TYR:HA	1:B:118:TYR:CD1	2.42	0.55
1:B:315:SER:CA	1:B:325:MET:HE2	2.36	0.55
1:D:271:VAL:HG12	1:D:272:ILE:HG12	1.88	0.55
1:G:171:THR:O	1:G:172:SER:HB3	2.07	0.55
1:T:25:PRO:HD3	1:T:40:SER:OG	2.07	0.55
1:B:264:ILE:N	1:B:264:ILE:HD12	2.22	0.55
1:R:12:VAL:CG1	1:R:15:ILE:HG12	2.37	0.55
1:R:15:ILE:HG13	1:R:397:TYR:HD2	1.71	0.55
1:T:112:THR:HG21	1:T:361:SER:HA	1.87	0.55
1:I:56:LEU:HD11	1:I:351:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:THR:HG22	1:K:113:LEU:H	1.72	0.55
1:M:395:MET:HG3	1:M:399:LYS:HD2	1.89	0.55
1:T:11:ILE:HG22	1:T:16:ARG:NH1	2.21	0.55
1:A:104:ARG:HD3	1:A:369:SER:OG	2.07	0.55
1:D:121:ASN:HA	4:D:671:HOH:O	2.06	0.55
1:D:292:PHE:CZ	1:D:333:LEU:HD21	2.42	0.55
1:C:189:LEU:CD1	1:E:227:ILE:HD12	2.32	0.55
1:J:15:ILE:HG13	1:J:397:TYR:HD2	1.72	0.55
1:O:407:ARG:HH11	1:O:407:ARG:CB	2.20	0.55
1:J:211:ALA:O	1:J:330:SER:HA	2.07	0.54
1:K:267:ASP:OD1	1:K:269:THR:HB	2.07	0.54
1:K:63:PHE:CZ	1:K:67:ILE:HD12	2.42	0.54
1:A:397:TYR:O	1:A:401:ILE:HG12	2.05	0.54
1:N:91:ASN:OD1	1:N:93:PRO:HD2	2.08	0.54
1:P:86:LEU:O	1:P:87:LEU:HD23	2.07	0.54
1:C:255:LEU:HB2	4:C:6077:HOH:O	2.08	0.54
1:H:185:PRO:HB2	1:O:233:ASN:ND2	2.16	0.54
1:I:162:GLU:HB3	4:I:5963:HOH:O	2.06	0.54
1:Q:122:GLY:C	1:Q:160:VAL:HG22	2.28	0.54
1:S:220:TYR:CG	1:S:221:GLN:N	2.75	0.54
1:H:121:ASN:HD22	1:H:121:ASN:N	2.04	0.54
1:E:162:GLU:CD	1:E:417:ARG:HD3	2.28	0.54
1:O:144:LEU:HD22	1:O:351:LEU:HD12	1.88	0.54
1:A:233:ASN:HD22	1:F:185:PRO:CB	2.13	0.54
1:B:379:LEU:HD21	1:B:383:LEU:HD23	1.89	0.54
1:L:112:THR:HG22	1:L:362:VAL:H	1.73	0.54
1:L:99:CYS:HB3	1:L:180:LEU:HD21	1.89	0.54
1:R:121:ASN:O	1:R:160:VAL:CG2	2.56	0.54
1:T:93:PRO:HG3	1:T:180:LEU:HB3	1.89	0.54
1:A:118:TYR:HB2	1:B:118:TYR:CE1	2.43	0.54
1:G:264:ILE:HB	1:G:307:SER:OG	2.08	0.54
1:A:219:GLN:HE22	1:A:322:GLY:N	2.06	0.54
1:A:247:VAL:HG22	1:A:289:LEU:HD23	1.89	0.54
1:B:171:THR:O	1:B:172:SER:HB3	2.07	0.54
1:F:155:ILE:HG12	1:F:415:PRO:HD3	1.89	0.54
1:G:106:LEU:HD23	1:G:367:GLY:HA3	1.90	0.54
1:H:417:ARG:CG	4:H:6004:HOH:O	2.54	0.54
1:J:59:PHE:CE2	1:J:106:LEU:HD13	2.42	0.54
1:P:263:LEU:HB2	1:P:272:ILE:HB	1.90	0.54
1:P:280:ASN:C	1:P:280:ASN:HD22	2.11	0.54
1:T:15:ILE:HG13	1:T:397:TYR:HD2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:283:THR:CG2	1:T:286:ILE:HG12	2.37	0.54
1:D:113:LEU:C	1:L:119:ALA:HB1	2.29	0.54
1:M:316:LYS:HB2	1:M:325:MET:CE	2.37	0.54
1:A:112:THR:CG2	1:A:113:LEU:N	2.71	0.53
1:D:121:ASN:ND2	1:D:358:ALA:H	2.06	0.53
1:E:55:GLY:HA3	1:E:354:TYR:CZ	2.43	0.53
1:G:162:GLU:CG	1:G:417:ARG:HH22	2.20	0.53
1:M:38:LEU:O	1:M:39:ARG:NH1	2.35	0.53
1:O:309:LYS:HE2	4:O:605:HOH:O	2.07	0.53
1:I:397:TYR:CE2	1:I:401:ILE:HD11	2.43	0.53
1:S:274:ARG:HH11	1:S:274:ARG:HG3	1.72	0.53
1:S:293:ASN:HD21	1:T:293:ASN:HD21	1.57	0.53
1:A:271:VAL:HG12	1:A:272:ILE:HG13	1.89	0.53
1:C:397:TYR:O	1:C:401:ILE:HG12	2.07	0.53
1:F:262:TYR:CD2	1:F:273:THR:HG22	2.43	0.53
1:S:112:THR:HG22	1:S:361:SER:HA	1.91	0.53
1:C:272:ILE:HD13	1:C:296:ILE:HG23	1.89	0.53
1:C:104:ARG:HD3	1:C:369:SER:OG	2.08	0.53
1:C:41:GLU:HB3	1:C:88:THR:HB	1.90	0.53
1:I:233:ASN:HD22	1:J:185:PRO:CG	2.22	0.53
1:C:383:LEU:HD21	1:O:383:LEU:HG	1.90	0.53
1:Q:428:GLU:HA	1:Q:428:GLU:OE1	2.08	0.53
1:T:121:ASN:HD22	1:T:121:ASN:N	2.05	0.53
1:B:315:SER:HA	1:B:325:MET:HE1	1.88	0.53
1:R:258:ASP:HB2	1:R:313:VAL:HB	1.90	0.53
1:T:324:GLN:HE21	1:T:324:GLN:CA	2.20	0.53
1:D:136:LEU:HD13	1:D:351:LEU:HD11	1.89	0.53
1:E:140:SER:O	1:E:144:LEU:HG	2.08	0.53
1:F:405:ARG:HD3	1:F:406:GLU:OE2	2.08	0.53
1:G:315:SER:HA	1:G:325:MET:HE1	1.89	0.53
1:L:121:ASN:HD22	1:L:122:GLY:N	2.06	0.53
1:A:219:GLN:NE2	1:A:322:GLY:CA	2.72	0.53
1:J:193:MET:HG2	1:J:194:VAL:N	2.24	0.53
1:L:389:ARG:HB3	1:L:389:ARG:NH1	2.23	0.53
1:S:120:LEU:O	1:S:121:ASN:CG	2.46	0.53
1:S:233:ASN:HD22	1:T:185:PRO:HB2	1.73	0.53
1:T:219:GLN:HE21	1:T:324:GLN:HE22	1.51	0.53
1:A:171:THR:O	1:A:172:SER:CB	2.56	0.53
1:F:11:ILE:HD12	1:F:12:VAL:H	1.73	0.53
1:I:50:GLY:O	1:I:359:THR:HG23	2.09	0.53
1:R:121:ASN:O	1:R:160:VAL:HG21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:402:LEU:O	1:R:405:ARG:HB2	2.09	0.53
1:C:120:LEU:HD21	1:R:113:LEU:HB2	1.91	0.53
1:I:121:ASN:ND2	1:I:358:ALA:H	2.00	0.53
1:L:34:GLU:HG3	1:L:177:TYR:CE1	2.44	0.53
1:P:220:TYR:HB2	1:P:316:LYS:CE	2.39	0.53
1:Q:296:ILE:HD12	1:Q:296:ILE:N	2.24	0.53
1:A:415:PRO:HG2	1:A:418:GLU:CG	2.39	0.53
1:B:215:GLN:HE22	1:B:328:SER:CB	2.22	0.53
1:F:390:PHE:CE2	1:F:392:PRO:HG3	2.44	0.53
1:G:15:ILE:HG13	1:G:397:TYR:HD2	1.74	0.53
1:I:15:ILE:HG13	1:I:397:TYR:HD2	1.74	0.53
1:I:404:GLU:OE2	1:I:404:GLU:HA	2.09	0.53
1:J:316:LYS:N	1:J:325:MET:CE	2.72	0.53
1:L:171:THR:O	1:L:172:SER:CB	2.57	0.53
1:P:271:VAL:HG12	1:P:272:ILE:CD1	2.34	0.53
1:Q:171:THR:O	1:Q:172:SER:CB	2.57	0.53
1:B:316:LYS:HB2	1:B:325:MET:HE3	1.91	0.52
1:B:389:ARG:HH11	1:B:389:ARG:CB	2.21	0.52
1:D:260:THR:O	1:D:310:LEU:HD12	2.10	0.52
1:I:144:LEU:CD2	1:I:351:LEU:HD12	2.39	0.52
1:J:320:GLN:O	1:J:323:ASP:OD2	2.28	0.52
1:K:99:CYS:HB2	1:K:373:LEU:CD2	2.40	0.52
1:L:276:VAL:HG21	1:L:292:PHE:CE2	2.43	0.52
1:L:426:PHE:O	1:L:428:GLU:N	2.42	0.52
1:E:155:ILE:CD1	1:E:415:PRO:HD3	2.40	0.52
1:E:159:LEU:HD11	1:O:109:ARG:HH11	1.74	0.52
1:E:425:TYR:HD2	1:E:425:TYR:O	1.92	0.52
1:M:120:LEU:HD12	1:M:121:ASN:N	2.24	0.52
1:N:25:PRO:HD3	1:N:40:SER:OG	2.09	0.52
1:T:121:ASN:HB2	4:T:645:HOH:O	2.09	0.52
1:K:426:PHE:C	1:K:428:GLU:H	2.12	0.52
1:M:279:ASP:CG	1:M:279:ASP:O	2.48	0.52
1:P:21:PRO:CG	1:P:105:SER:HB3	2.40	0.52
1:P:283:THR:O	1:P:286:ILE:HG22	2.09	0.52
1:I:171:THR:O	1:I:172:SER:CB	2.54	0.52
1:J:233:ASN:ND2	1:Q:185:PRO:HB2	2.25	0.52
1:A:120:LEU:HB2	1:T:116:GLY:HA2	1.92	0.52
1:A:415:PRO:HG2	1:A:418:GLU:HG3	1.92	0.52
1:B:315:SER:HA	1:B:325:MET:HE2	1.92	0.52
1:E:384:VAL:HG13	1:L:150:ASN:OD1	2.10	0.52
1:R:219:GLN:H	1:R:219:GLN:NE2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:417:ARG:HH11	1:H:417:ARG:CG	2.17	0.52
1:I:38:LEU:O	1:I:39:ARG:NH1	2.37	0.52
1:J:263:LEU:HB3	1:J:305:ILE:HD13	1.91	0.52
1:G:150:ASN:OD1	1:M:384:VAL:HG13	2.08	0.52
1:P:219:GLN:H	1:P:219:GLN:HE21	1.55	0.52
1:S:349:VAL:HG12	1:S:351:LEU:CD2	2.40	0.52
1:C:121:ASN:O	1:C:160:VAL:HG21	2.09	0.52
1:D:171:THR:O	1:D:172:SER:CB	2.56	0.52
1:E:261:ILE:HG12	1:E:276:VAL:HG21	1.89	0.52
1:F:144:LEU:HD22	1:F:351:LEU:HD12	1.91	0.52
1:I:201:ASP:OD2	1:Q:202:ARG:HD2	2.10	0.52
1:N:296:ILE:N	1:N:296:ILE:HD12	2.25	0.52
1:T:63:PHE:CZ	1:T:67:ILE:HD12	2.44	0.52
1:K:259:ALA:HB3	1:K:276:VAL:CG2	2.40	0.52
1:A:220:TYR:CG	1:A:221:GLN:N	2.78	0.52
1:E:201:ASP:O	1:E:202:ARG:HB2	2.08	0.52
1:E:320:GLN:HB3	1:E:323:ASP:HB2	1.92	0.52
1:F:315:SER:C	1:F:325:MET:HE2	2.30	0.52
1:H:112:THR:HG22	1:H:362:VAL:N	2.22	0.52
1:R:274:ARG:HG3	1:R:294:LEU:HD21	1.92	0.52
1:R:283:THR:HG21	1:R:286:ILE:HD12	1.91	0.52
1:A:246:LEU:HD23	1:A:331:GLY:HA3	1.92	0.52
1:D:262:TYR:CD2	1:D:273:THR:HG22	2.45	0.52
1:E:219:GLN:O	1:E:225:VAL:HG21	2.09	0.51
1:M:107:THR:HG22	1:M:165:THR:OG1	2.10	0.51
1:R:166:VAL:HG13	1:R:350:THR:HG21	1.92	0.51
1:D:225:VAL:HG23	1:D:325:MET:HE1	1.91	0.51
1:D:395:MET:CG	1:D:399:LYS:HE2	2.39	0.51
1:F:127:VAL:CG2	1:F:148:THR:HG22	2.41	0.51
1:I:255:LEU:HD21	1:I:325:MET:HG2	1.90	0.51
1:K:402:LEU:O	1:K:405:ARG:HB2	2.10	0.51
1:L:271:VAL:HG12	1:L:272:ILE:HG12	1.91	0.51
1:E:33:LEU:HD13	1:L:402:LEU:HD12	1.92	0.51
1:P:292:PHE:N	1:P:292:PHE:CD2	2.76	0.51
1:M:121:ASN:HB3	1:Q:112:THR:OG1	2.11	0.51
1:Q:379:LEU:HD23	1:Q:383:LEU:HD23	1.92	0.51
1:A:118:TYR:HB2	1:B:118:TYR:CD1	2.44	0.51
1:D:220:TYR:CG	1:D:221:GLN:N	2.79	0.51
1:C:385:THR:OG1	1:E:130:GLN:NE2	2.43	0.51
1:I:99:CYS:HB2	1:I:373:LEU:HD23	1.92	0.51
1:A:201:ASP:O	1:A:202:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:SER:O	1:E:325:MET:HG3	2.10	0.51
1:F:107:THR:HG22	1:F:165:THR:OG1	2.10	0.51
1:F:34:GLU:HG3	1:F:177:TYR:CE1	2.45	0.51
1:F:51:ASP:OD1	1:F:51:ASP:N	2.40	0.51
1:J:75:GLN:HE22	1:J:81:LYS:HE3	1.73	0.51
1:R:274:ARG:NE	4:R:5961:HOH:O	2.30	0.51
1:T:226:THR:OG1	1:T:313:VAL:HG22	2.11	0.51
1:B:247:VAL:HG13	1:B:289:LEU:HD23	1.92	0.51
1:R:293:ASN:ND2	1:T:293:ASN:HD21	2.08	0.51
1:G:171:THR:O	1:G:172:SER:CB	2.57	0.51
1:J:21:PRO:HG2	1:J:105:SER:HB3	1.91	0.51
1:I:381:LYS:HG2	1:Q:146:SER:O	2.11	0.51
1:A:127:VAL:CG2	1:A:148:THR:HG22	2.41	0.51
1:C:49:VAL:HG21	1:C:357:VAL:HG11	1.93	0.51
1:I:114:PRO:HG2	1:I:114:PRO:O	2.11	0.51
1:I:56:LEU:HD11	1:I:351:LEU:HB3	1.93	0.51
1:J:136:LEU:CD1	1:J:351:LEU:HD11	2.40	0.51
1:L:349:VAL:HG12	1:L:351:LEU:CD2	2.41	0.51
1:N:166:VAL:CG1	1:N:350:THR:HG21	2.41	0.51
1:C:120:LEU:HD21	1:R:113:LEU:CD1	2.30	0.51
1:G:296:ILE:HD12	1:G:296:ILE:N	2.25	0.51
1:G:419:TYR:O	1:G:423:ARG:HG3	2.11	0.51
1:P:220:TYR:CG	1:P:221:GLN:N	2.78	0.51
1:R:220:TYR:CG	1:R:221:GLN:N	2.79	0.51
1:R:279:ASP:CG	1:R:279:ASP:O	2.48	0.51
1:A:214:TYR:O	1:A:328:SER:HA	2.11	0.51
1:J:12:VAL:HG12	1:J:12:VAL:O	2.10	0.51
1:L:112:THR:HB	1:L:362:VAL:HB	1.93	0.51
1:S:316:LYS:HD3	1:S:319:GLY:CA	2.39	0.51
1:T:120:LEU:O	4:T:596:HOH:O	2.19	0.51
1:C:189:LEU:HB3	1:E:214:TYR:CZ	2.46	0.51
1:E:397:TYR:CE2	1:E:401:ILE:HD11	2.45	0.51
1:E:47:LEU:HD13	1:E:71:HIS:CG	2.46	0.51
1:F:220:TYR:O	1:F:221:GLN:HG3	2.11	0.51
1:K:395:MET:HG3	1:K:399:LYS:HE3	1.91	0.51
1:N:419:TYR:CE2	1:N:423:ARG:HD2	2.46	0.51
1:Q:136:LEU:HD13	1:Q:351:LEU:HD11	1.92	0.51
1:C:130:GLN:HE22	1:L:385:THR:HG21	1.76	0.50
1:M:121:ASN:N	1:M:121:ASN:ND2	2.59	0.50
1:M:99:CYS:HB2	1:M:373:LEU:HD23	1.92	0.50
1:C:417:ARG:HH11	1:C:417:ARG:CB	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:VAL:HG22	1:G:289:LEU:CD2	2.42	0.50
1:G:293:ASN:ND2	1:K:291:PRO:HB3	2.26	0.50
1:J:323:ASP:OD2	1:J:323:ASP:N	2.44	0.50
1:L:20:MET:HE2	1:L:423:ARG:NE	2.25	0.50
1:P:12:VAL:HB	1:P:15:ILE:HG12	1.93	0.50
1:T:38:LEU:O	1:T:39:ARG:NH1	2.35	0.50
1:C:159:LEU:HB2	1:C:162:GLU:HG3	1.93	0.50
1:E:201:ASP:OD2	1:L:202:ARG:HG2	2.11	0.50
1:F:122:GLY:C	1:F:160:VAL:CG2	2.80	0.50
1:L:106:LEU:HD23	1:L:367:GLY:HA3	1.93	0.50
1:M:59:PHE:O	1:M:61:PRO:HD3	2.11	0.50
1:S:273:THR:O	1:S:274:ARG:HD3	2.11	0.50
1:T:124:ILE:HD13	1:T:164:VAL:HG22	1.93	0.50
1:B:49:VAL:HG21	1:B:357:VAL:HG11	1.93	0.50
1:H:255:LEU:CD2	1:H:325:MET:HE2	2.41	0.50
1:I:201:ASP:O	1:I:202:ARG:HB2	2.11	0.50
1:J:121:ASN:O	1:J:160:VAL:HG21	2.11	0.50
1:K:20:MET:HG2	1:K:423:ARG:HG2	1.94	0.50
1:N:379:LEU:HG	1:N:383:LEU:HD22	1.94	0.50
1:P:355:GLU:HG3	1:P:356:ARG:HG2	1.94	0.50
1:Q:104:ARG:HD3	1:Q:369:SER:OG	2.12	0.50
1:T:15:ILE:HG13	1:T:397:TYR:CD2	2.46	0.50
1:I:296:ILE:HD12	1:I:296:ILE:N	2.26	0.50
1:L:390:PHE:CE2	1:L:392:PRO:HG3	2.47	0.50
1:B:184:ILE:HD11	1:B:195:ALA:HB1	1.94	0.50
1:B:315:SER:C	1:B:325:MET:HE2	2.32	0.50
1:D:182:ASP:OD2	4:D:499:HOH:O	2.20	0.50
1:D:32:THR:HG22	1:D:32:THR:O	2.11	0.50
1:F:166:VAL:HG13	1:F:350:THR:HG21	1.92	0.50
1:G:279:ASP:O	1:G:279:ASP:CG	2.49	0.50
1:K:142:ASN:ND2	4:K:534:HOH:O	2.45	0.50
1:K:398:THR:O	1:K:402:LEU:HD22	2.11	0.50
1:L:269:THR:CG2	4:L:668:HOH:O	2.59	0.50
1:P:219:GLN:N	1:P:219:GLN:NE2	2.57	0.50
1:A:316:LYS:N	1:A:325:MET:CE	2.74	0.50
1:E:316:LYS:HD3	1:E:323:ASP:OD1	2.12	0.50
1:K:220:TYR:CG	1:K:221:GLN:N	2.80	0.50
1:L:11:ILE:CD1	1:L:12:VAL:H	2.24	0.50
1:P:426:PHE:C	1:P:428:GLU:H	2.14	0.50
1:S:55:GLY:HA3	1:S:354:TYR:CZ	2.47	0.50
1:T:11:ILE:HG22	1:T:16:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ILE:HB	1:C:307:SER:OG	2.12	0.50
1:C:379:LEU:CG	1:C:383:LEU:HG	2.38	0.50
1:F:132:SER:HB2	4:F:503:HOH:O	2.11	0.50
1:M:120:LEU:O	1:M:121:ASN:ND2	2.44	0.50
1:S:127:VAL:CG2	1:S:148:THR:HG22	2.42	0.50
1:S:309:LYS:NZ	4:S:636:HOH:O	2.44	0.50
1:B:220:TYR:CG	1:B:221:GLN:N	2.80	0.50
1:C:171:THR:HG21	1:C:348:PRO:HD3	1.93	0.50
1:D:112:THR:HG23	1:L:121:ASN:OD1	2.12	0.50
1:D:136:LEU:CD1	1:D:351:LEU:HD11	2.42	0.50
1:G:41:GLU:OE1	1:G:90:GLN:HG2	2.12	0.50
1:H:120:LEU:N	1:I:113:LEU:HD12	2.27	0.50
1:S:122:GLY:O	1:S:160:VAL:HG22	2.11	0.50
1:C:171:THR:O	1:C:172:SER:CB	2.60	0.49
1:G:99:CYS:HB2	1:G:373:LEU:HD23	1.94	0.49
1:I:55:GLY:HA3	1:I:354:TYR:CZ	2.46	0.49
1:K:274:ARG:HH11	1:K:274:ARG:HG3	1.77	0.49
1:L:99:CYS:CB	1:L:180:LEU:HD21	2.42	0.49
1:M:55:GLY:HA3	1:M:354:TYR:CZ	2.47	0.49
1:Q:140:SER:O	1:Q:144:LEU:HG	2.11	0.49
1:S:162:GLU:CD	1:S:417:ARG:HD2	2.31	0.49
1:B:390:PHE:CZ	1:B:392:PRO:HG3	2.46	0.49
1:D:390:PHE:CE2	1:D:392:PRO:HD3	2.47	0.49
1:L:246:LEU:HD12	1:L:290:MET:CE	2.41	0.49
1:L:25:PRO:HD3	1:L:40:SER:OG	2.12	0.49
1:B:159:LEU:HB2	1:B:162:GLU:HG3	1.94	0.49
1:E:34:GLU:HG3	1:E:177:TYR:CE1	2.47	0.49
1:H:274:ARG:HG2	1:H:274:ARG:NH1	2.26	0.49
1:M:20:MET:HE2	1:M:423:ARG:HE	1.77	0.49
1:Q:121:ASN:O	1:Q:160:VAL:HG21	2.12	0.49
1:R:193:MET:HG2	1:R:194:VAL:N	2.27	0.49
1:R:67:ILE:HD13	1:R:237:ILE:CG2	2.42	0.49
1:F:122:GLY:HA2	1:F:356:ARG:HB2	1.94	0.49
1:J:417:ARG:HG2	4:J:560:HOH:O	2.11	0.49
1:M:390:PHE:CE2	1:M:392:PRO:HG3	2.46	0.49
1:N:315:SER:C	1:N:325:MET:HE2	2.32	0.49
1:E:356:ARG:NH1	1:E:356:ARG:CG	2.69	0.49
1:F:214:TYR:O	1:F:328:SER:HA	2.11	0.49
1:H:267:ASP:OD1	1:H:269:THR:HB	2.12	0.49
1:H:58:VAL:HG22	1:H:351:LEU:HD22	1.94	0.49
1:K:20:MET:HE1	1:K:427:MET:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:THR:HG21	1:L:348:PRO:HD3	1.94	0.49
1:O:201:ASP:O	1:O:202:ARG:HB2	2.12	0.49
1:B:230:PHE:C	1:B:230:PHE:CD1	2.85	0.49
1:C:237:ILE:HG22	1:C:238:THR:HG23	1.95	0.49
1:J:395:MET:HG3	1:J:399:LYS:CE	2.42	0.49
1:J:415:PRO:HG2	1:J:418:GLU:HB2	1.93	0.49
1:J:77:ASN:HD21	1:J:79:ASN:HD22	1.60	0.49
1:M:112:THR:HG22	1:M:113:LEU:N	2.27	0.49
1:R:271:VAL:C	1:R:272:ILE:HG13	2.32	0.49
1:R:397:TYR:CZ	1:R:401:ILE:HD11	2.48	0.49
1:S:162:GLU:HB3	4:S:646:HOH:O	2.10	0.49
1:C:34:GLU:HG3	1:C:177:TYR:CE1	2.48	0.49
1:D:219:GLN:HE22	1:D:322:GLY:HA2	1.76	0.49
1:G:247:VAL:HG22	1:G:289:LEU:HD23	1.94	0.49
1:J:199:SER:HB3	4:J:473:HOH:O	2.13	0.49
1:J:58:VAL:HG22	1:J:351:LEU:HD22	1.94	0.49
1:K:112:THR:CG2	1:K:113:LEU:N	2.76	0.49
1:N:264:ILE:HB	1:N:307:SER:OG	2.12	0.49
1:Q:193:MET:HE3	1:Q:194:VAL:C	2.33	0.49
1:S:51:ASP:HA	1:S:359:THR:OG1	2.12	0.49
1:M:290:MET:HB2	4:M:660:HOH:O	2.12	0.49
1:N:317:SER:HB3	4:N:640:HOH:O	2.11	0.49
1:T:383:LEU:HD12	1:T:384:VAL:N	2.28	0.49
1:A:424:GLU:O	1:A:428:GLU:HG2	2.12	0.49
1:D:320:GLN:O	1:D:321:ALA:C	2.51	0.49
1:G:120:LEU:N	4:G:5967:HOH:O	2.46	0.49
1:I:51:ASP:HA	1:I:359:THR:CG2	2.43	0.49
1:P:113:LEU:HD21	1:P:120:LEU:CA	2.43	0.49
1:P:13:PRO:HG2	1:P:389:ARG:HH11	1.77	0.49
1:P:390:PHE:CE2	1:P:392:PRO:HG3	2.48	0.49
1:P:419:TYR:CE2	1:P:423:ARG:HD2	2.47	0.49
1:Q:408:LEU:HB2	1:Q:410:ILE:HD13	1.94	0.49
1:S:171:THR:O	1:S:172:SER:CB	2.60	0.49
1:S:136:LEU:CD1	1:S:351:LEU:HD11	2.43	0.49
1:L:201:ASP:OD1	1:L:201:ASP:N	2.46	0.49
1:C:112:THR:HG1	1:N:121:ASN:HA	1.75	0.49
1:D:107:THR:HG22	1:D:165:THR:OG1	2.13	0.48
1:G:261:ILE:CD1	1:G:310:LEU:HD13	2.42	0.48
1:G:20:MET:CE	1:G:423:ARG:HE	2.26	0.48
1:K:284:THR:HG22	4:K:653:HOH:O	2.12	0.48
1:L:349:VAL:CG1	1:L:351:LEU:CD2	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:171:THR:O	1:M:172:SER:CB	2.60	0.48
1:Q:220:TYR:CG	1:Q:221:GLN:N	2.81	0.48
1:S:202:ARG:HD2	1:T:201:ASP:OD2	2.13	0.48
1:T:271:VAL:HG12	1:T:272:ILE:HG12	1.95	0.48
1:A:130:GLN:NE2	1:F:385:THR:OG1	2.47	0.48
1:B:290:MET:N	1:B:291:PRO:HD3	2.29	0.48
1:H:139:VAL:HA	1:H:144:LEU:HD21	1.96	0.48
1:H:112:THR:HG21	1:H:362:VAL:HG23	1.95	0.48
1:I:271:VAL:HG12	1:I:272:ILE:HG12	1.95	0.48
1:J:426:PHE:C	1:J:428:GLU:H	2.16	0.48
4:K:679:HOH:O	1:Q:39:ARG:HD2	2.12	0.48
1:A:77:ASN:HD21	1:A:79:ASN:HB2	1.78	0.48
1:C:211:ALA:O	1:C:330:SER:HA	2.12	0.48
1:H:276:VAL:HG11	1:H:292:PHE:CE2	2.49	0.48
1:L:264:ILE:HB	1:L:307:SER:OG	2.13	0.48
1:M:59:PHE:CE2	1:M:106:LEU:HD13	2.48	0.48
1:P:274:ARG:CG	1:P:274:ARG:NH1	2.75	0.48
1:S:127:VAL:HG23	1:S:148:THR:HG22	1.94	0.48
1:T:246:LEU:CD2	1:T:331:GLY:HA3	2.43	0.48
1:A:219:GLN:NE2	1:A:322:GLY:N	2.61	0.48
1:G:121:ASN:HB3	4:G:6042:HOH:O	2.12	0.48
1:H:262:TYR:CD2	1:H:273:THR:HG22	2.48	0.48
1:L:47:LEU:HD13	1:L:71:HIS:CG	2.49	0.48
1:N:402:LEU:O	1:N:405:ARG:HB2	2.13	0.48
1:O:122:GLY:O	1:O:160:VAL:HG22	2.13	0.48
1:P:100:ARG:HD3	1:P:177:TYR:CD1	2.48	0.48
1:S:106:LEU:HD23	1:S:367:GLY:HA3	1.95	0.48
1:D:323:ASP:OD2	1:D:323:ASP:N	2.45	0.48
1:G:93:PRO:HG3	1:G:180:LEU:HB3	1.94	0.48
1:N:171:THR:O	1:N:172:SER:CB	2.62	0.48
1:T:259:ALA:CB	1:T:290:MET:CE	2.91	0.48
1:T:51:ASP:OD2	1:T:51:ASP:N	2.46	0.48
1:D:20:MET:HG2	1:D:423:ARG:HG2	1.96	0.48
1:J:77:ASN:ND2	1:J:79:ASN:HD22	2.12	0.48
1:M:21:PRO:HG2	1:M:105:SER:HB3	1.96	0.48
1:N:309:LYS:NZ	4:N:627:HOH:O	2.45	0.48
1:R:121:ASN:N	1:R:121:ASN:ND2	2.58	0.48
1:S:77:ASN:HD22	1:S:78:GLY:N	2.12	0.48
1:B:263:LEU:HD11	1:B:296:ILE:HD13	1.96	0.48
1:E:181:GLY:HA2	1:E:197:CYS:O	2.14	0.48
1:J:162:GLU:OE1	1:J:417:ARG:NH1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:384:VAL:HG13	1:M:150:ASN:OD1	2.14	0.48
1:L:126:ALA:HB3	1:L:155:ILE:HG22	1.96	0.48
1:Q:264:ILE:HB	1:Q:307:SER:OG	2.12	0.48
1:A:118:TYR:CE2	1:T:114:PRO:HB3	2.49	0.48
1:C:153:ASP:OD2	1:C:405:ARG:NH2	2.37	0.48
1:C:15:ILE:HG13	1:C:397:TYR:CD2	2.48	0.48
1:D:201:ASP:N	1:D:201:ASP:OD1	2.45	0.48
1:E:272:ILE:HG21	1:E:296:ILE:HD12	1.95	0.48
1:I:127:VAL:CG2	1:I:148:THR:HG22	2.44	0.48
1:K:201:ASP:O	1:K:202:ARG:HB2	2.13	0.48
1:G:233:ASN:HD22	1:M:185:PRO:HB2	1.78	0.48
1:H:34:GLU:OE2	1:O:171:THR:HG23	2.14	0.48
1:P:283:THR:HB	1:P:286:ILE:HG21	1.96	0.48
1:T:104:ARG:HD3	1:T:369:SER:OG	2.13	0.48
1:C:67:ILE:HD13	1:C:237:ILE:CG2	2.43	0.48
1:E:297:PRO:HG2	1:E:300:GLU:HG3	1.96	0.48
1:P:190:ASP:OD1	1:P:191:PRO:HD2	2.14	0.48
1:P:20:MET:HE2	1:P:423:ARG:HE	1.78	0.48
1:F:109:ARG:NH1	1:S:159:LEU:HD11	2.28	0.48
1:C:121:ASN:O	1:C:160:VAL:CG2	2.62	0.48
1:D:126:ALA:HB3	1:D:155:ILE:HG22	1.96	0.48
1:E:283:THR:H	1:E:288:ASN:ND2	2.10	0.48
1:F:201:ASP:O	1:F:202:ARG:HB2	2.14	0.48
1:F:390:PHE:CZ	1:F:392:PRO:HG3	2.49	0.48
1:J:20:MET:CG	1:J:423:ARG:HG2	2.43	0.48
1:M:80:TYR:O	1:M:267:ASP:HB2	2.13	0.48
1:S:259:ALA:HB3	1:S:290:MET:HE3	1.95	0.48
1:T:201:ASP:O	1:T:202:ARG:HB2	2.14	0.48
1:B:214:TYR:O	1:B:328:SER:HA	2.14	0.47
1:F:144:LEU:HD22	1:F:351:LEU:HD13	1.96	0.47
1:J:171:THR:HG21	1:J:348:PRO:HD3	1.96	0.47
1:J:20:MET:HE3	1:J:23:THR:HG21	1.96	0.47
1:N:11:ILE:HG13	1:N:12:VAL:HG23	1.95	0.47
1:R:389:ARG:HB3	1:R:389:ARG:CZ	2.44	0.47
1:S:77:ASN:HD22	1:S:77:ASN:C	2.18	0.47
1:B:320:GLN:O	1:B:323:ASP:HB2	2.14	0.47
1:D:121:ASN:O	1:D:160:VAL:HG11	2.14	0.47
1:H:226:THR:OG1	1:H:313:VAL:HG22	2.14	0.47
1:H:320:GLN:O	1:H:321:ALA:C	2.53	0.47
1:H:390:PHE:CE2	1:H:392:PRO:HG3	2.49	0.47
1:H:402:LEU:O	1:H:405:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:ASN:ND2	1:J:79:ASN:ND2	2.62	0.47
1:K:39:ARG:HH21	1:K:383:LEU:HD21	1.79	0.47
1:D:427:MET:O	1:L:425:TYR:OH	2.31	0.47
1:S:274:ARG:HD3	1:S:274:ARG:HA	1.67	0.47
1:E:15:ILE:HG13	1:E:397:TYR:HD2	1.78	0.47
1:F:104:ARG:HD3	1:F:369:SER:OG	2.14	0.47
1:K:293:ASN:CG	1:M:291:PRO:HB3	2.34	0.47
1:N:171:THR:HG21	1:N:348:PRO:HD3	1.96	0.47
1:C:109:ARG:NH1	1:N:159:LEU:HD11	2.29	0.47
1:H:58:VAL:HG22	1:H:351:LEU:CD2	2.44	0.47
1:J:122:GLY:O	1:J:160:VAL:HG22	2.14	0.47
1:A:114:PRO:O	1:A:117:VAL:HG12	2.14	0.47
1:B:397:TYR:O	1:B:401:ILE:HG12	2.13	0.47
1:C:121:ASN:HD22	1:C:121:ASN:H	1.60	0.47
1:C:417:ARG:HH11	1:C:417:ARG:HB2	1.77	0.47
1:C:427:MET:C	1:C:428:GLU:HG3	2.34	0.47
1:D:214:TYR:O	1:D:328:SER:HA	2.13	0.47
1:I:397:TYR:O	1:I:401:ILE:HG13	2.14	0.47
1:J:55:GLY:HA3	1:J:354:TYR:CZ	2.49	0.47
1:K:271:VAL:HG12	1:K:272:ILE:HD12	1.97	0.47
1:M:122:GLY:O	1:M:160:VAL:HG22	2.14	0.47
1:M:274:ARG:NH1	1:M:274:ARG:CG	2.75	0.47
1:D:13:PRO:HB3	4:D:555:HOH:O	2.13	0.47
1:E:389:ARG:NH1	1:E:389:ARG:HB2	2.29	0.47
1:F:15:ILE:HG13	1:F:397:TYR:HD2	1.80	0.47
1:I:419:TYR:CE2	1:I:423:ARG:HD2	2.50	0.47
1:K:112:THR:CG2	1:K:113:LEU:H	2.28	0.47
1:N:258:ASP:HB2	1:N:313:VAL:HB	1.96	0.47
1:O:67:ILE:HD13	1:O:237:ILE:CG2	2.44	0.47
1:L:286:ILE:HD12	1:L:286:ILE:HA	1.72	0.47
1:Q:58:VAL:HG22	1:Q:351:LEU:CD2	2.43	0.47
1:R:171:THR:O	1:R:172:SER:CB	2.61	0.47
1:A:85:MET:HE3	1:A:303:GLN:HA	1.95	0.47
1:C:272:ILE:HD13	1:C:296:ILE:HG21	1.96	0.47
1:C:99:CYS:HB2	1:C:373:LEU:HD23	1.96	0.47
1:E:122:GLY:O	1:E:160:VAL:HG22	2.14	0.47
1:I:262:TYR:HE1	1:I:311:GLU:HB2	1.80	0.47
1:J:316:LYS:CB	1:J:325:MET:HE3	2.44	0.47
1:J:425:TYR:O	1:J:425:TYR:CD2	2.62	0.47
1:L:214:TYR:O	1:L:328:SER:HA	2.14	0.47
1:N:378:GLU:OE2	1:N:381:LYS:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:20:MET:HE3	1:O:423:ARG:HG2	1.96	0.47
1:P:258:ASP:OD1	1:P:278:SER:HA	2.15	0.47
1:S:202:ARG:CD	1:T:201:ASP:OD2	2.62	0.47
1:C:25:PRO:HD3	1:C:40:SER:OG	2.15	0.47
1:D:395:MET:HG3	1:D:399:LYS:CE	2.42	0.47
1:G:121:ASN:HD22	1:G:121:ASN:N	2.13	0.47
1:G:220:TYR:N	1:G:323:ASP:O	2.47	0.47
1:J:32:THR:HG22	1:J:32:THR:O	2.13	0.47
1:O:178:VAL:HG12	1:O:179:ARG:O	2.15	0.47
1:B:41:GLU:HB3	1:B:88:THR:HB	1.96	0.47
1:E:264:ILE:HB	1:E:307:SER:OG	2.15	0.47
1:F:112:THR:CG2	1:F:361:SER:HA	2.45	0.47
1:G:171:THR:HG21	1:G:348:PRO:HD3	1.97	0.47
1:I:121:ASN:O	1:I:160:VAL:HG21	2.15	0.47
1:J:122:GLY:C	1:J:160:VAL:HG22	2.36	0.47
1:K:264:ILE:HB	1:K:307:SER:OG	2.15	0.47
1:L:316:LYS:N	1:L:325:MET:CE	2.78	0.47
1:M:20:MET:CE	1:M:423:ARG:HE	2.28	0.47
1:A:50:GLY:O	1:A:359:THR:HG23	2.15	0.47
1:G:201:ASP:O	1:G:202:ARG:HB2	2.14	0.47
1:J:112:THR:HG22	1:J:112:THR:O	2.14	0.47
1:K:296:ILE:HD12	1:K:296:ILE:H	1.77	0.47
1:M:219:GLN:HG2	1:M:324:GLN:HE21	1.80	0.47
1:O:283:THR:O	1:O:286:ILE:HG22	2.14	0.47
1:O:55:GLY:HA3	1:O:354:TYR:CZ	2.49	0.47
1:Q:379:LEU:HD22	1:Q:383:LEU:HD23	1.97	0.47
1:R:315:SER:C	1:R:325:MET:CE	2.83	0.47
1:E:112:THR:HG22	1:E:362:VAL:H	1.80	0.46
1:F:320:GLN:O	1:F:321:ALA:C	2.54	0.46
1:H:320:GLN:HG2	1:H:321:ALA:N	2.30	0.46
1:J:201:ASP:O	1:J:202:ARG:HB2	2.15	0.46
1:M:25:PRO:HD3	1:M:40:SER:OG	2.15	0.46
1:N:233:ASN:ND2	1:O:185:PRO:HB2	2.23	0.46
1:P:246:LEU:HG	1:P:292:PHE:CE2	2.50	0.46
1:P:296:ILE:N	1:P:296:ILE:HD12	2.30	0.46
1:P:49:VAL:HG21	1:P:357:VAL:HG11	1.96	0.46
1:R:324:GLN:HE21	1:R:324:GLN:CA	2.18	0.46
1:B:389:ARG:CB	1:B:389:ARG:NH1	2.79	0.46
1:Q:32:THR:O	1:Q:32:THR:HG22	2.15	0.46
1:R:144:LEU:CD2	1:R:351:LEU:HD12	2.46	0.46
1:A:11:ILE:HG13	1:A:12:VAL:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HG13	1:A:397:TYR:CD2	2.45	0.46
1:A:240:LEU:N	1:A:240:LEU:HD23	2.31	0.46
1:B:253:HIS:CG	1:B:254:GLY:N	2.84	0.46
1:H:320:GLN:CG	1:H:321:ALA:N	2.78	0.46
1:H:136:LEU:CD1	1:H:351:LEU:HD11	2.46	0.46
1:L:316:LYS:CB	1:L:325:MET:CE	2.92	0.46
1:Q:286:ILE:HA	1:Q:286:ILE:HD12	1.76	0.46
1:R:315:SER:C	1:R:325:MET:HE2	2.35	0.46
1:A:112:THR:CG2	1:A:113:LEU:H	2.29	0.46
1:B:246:LEU:HG	1:B:292:PHE:HE2	1.80	0.46
1:D:159:LEU:HD12	1:D:162:GLU:OE2	2.15	0.46
1:E:220:TYR:HB3	1:E:320:GLN:O	2.14	0.46
1:J:162:GLU:HB3	4:J:477:HOH:O	2.15	0.46
1:J:271:VAL:C	1:J:272:ILE:HG13	2.36	0.46
1:K:428:GLU:O	1:K:428:GLU:CG	2.63	0.46
1:N:107:THR:HG22	1:N:165:THR:OG1	2.15	0.46
1:P:21:PRO:HG2	1:P:105:SER:HB3	1.96	0.46
1:P:55:GLY:HA3	1:P:354:TYR:CZ	2.50	0.46
1:Q:246:LEU:HD12	1:Q:290:MET:HE1	1.97	0.46
1:R:264:ILE:HB	1:R:307:SER:OG	2.14	0.46
1:T:259:ALA:CB	1:T:290:MET:HE1	2.46	0.46
1:F:296:ILE:N	1:F:296:ILE:HD12	2.30	0.46
1:J:230:PHE:C	1:J:230:PHE:CD1	2.88	0.46
1:L:187:ILE:O	1:L:187:ILE:HG13	2.14	0.46
1:L:316:LYS:HB2	1:L:325:MET:HE1	1.97	0.46
1:N:104:ARG:HD3	1:N:369:SER:OG	2.16	0.46
1:R:12:VAL:HG11	1:R:15:ILE:HG12	1.98	0.46
1:D:39:ARG:HD2	4:D:488:HOH:O	2.15	0.46
1:O:219:GLN:NE2	1:O:322:GLY:H	2.14	0.46
1:R:274:ARG:CG	1:R:294:LEU:HD21	2.46	0.46
1:S:38:LEU:O	1:S:39:ARG:NH1	2.32	0.46
1:F:201:ASP:N	1:F:201:ASP:OD1	2.48	0.46
1:F:220:TYR:HD1	1:F:325:MET:HE3	1.81	0.46
1:G:15:ILE:HG13	1:G:397:TYR:CD2	2.51	0.46
1:J:112:THR:CG2	1:J:361:SER:HA	2.45	0.46
1:L:274:ARG:NH2	1:L:300:GLU:OE1	2.39	0.46
1:M:140:SER:O	1:M:144:LEU:HG	2.16	0.46
1:O:417:ARG:CB	1:O:417:ARG:NH1	2.69	0.46
1:Q:385:THR:C	1:Q:386:GLU:HG2	2.36	0.46
1:R:99:CYS:HB2	1:R:373:LEU:HD23	1.98	0.46
1:B:144:LEU:HD22	1:B:351:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:PRO:HB2	1:L:233:ASN:ND2	2.24	0.46
4:K:567:HOH:O	1:M:399:LYS:HE2	2.15	0.46
1:N:110:SER:HB3	1:N:160:VAL:HG13	1.97	0.46
1:T:92:LEU:HB2	1:T:93:PRO:HD3	1.96	0.46
1:B:272:ILE:CD1	1:B:300:GLU:HB3	2.46	0.46
1:C:140:SER:O	1:C:144:LEU:HG	2.15	0.46
1:E:11:ILE:HB	1:E:430:ALA:HB1	1.97	0.46
1:K:29:PRO:HG2	1:K:395:MET:HE1	1.98	0.46
1:Q:55:GLY:HA3	1:Q:354:TYR:CZ	2.51	0.46
1:Q:379:LEU:HD23	1:Q:383:LEU:HB2	1.98	0.46
1:T:112:THR:HG21	1:T:361:SER:C	2.35	0.46
1:A:55:GLY:HA3	1:A:354:TYR:CZ	2.51	0.46
1:B:121:ASN:CG	1:B:358:ALA:H	2.17	0.46
1:E:58:VAL:HG22	1:E:351:LEU:CD2	2.41	0.46
1:L:20:MET:CE	1:L:423:ARG:HE	2.29	0.46
1:O:38:LEU:O	1:O:39:ARG:NH1	2.40	0.46
1:P:395:MET:HG3	1:P:399:LYS:HE3	1.98	0.46
1:S:237:ILE:HG22	1:S:238:THR:HG23	1.97	0.46
1:S:262:TYR:CD2	1:S:273:THR:HG22	2.51	0.46
1:E:155:ILE:HG12	1:E:415:PRO:HD3	1.99	0.45
1:F:140:SER:O	1:F:144:LEU:HG	2.16	0.45
1:G:261:ILE:HD12	1:G:310:LEU:CD1	2.45	0.45
1:K:60:PHE:CE2	1:K:237:ILE:HD11	2.51	0.45
1:L:220:TYR:CG	1:L:221:GLN:N	2.84	0.45
1:C:44:THR:HB	1:N:157:ASN:ND2	2.31	0.45
1:O:283:THR:HB	1:O:286:ILE:CG2	2.40	0.45
1:A:118:TYR:CB	1:B:118:TYR:CD1	2.99	0.45
1:C:356:ARG:NH1	1:C:356:ARG:CG	2.76	0.45
1:E:93:PRO:HG3	1:E:180:LEU:HB3	1.97	0.45
1:F:315:SER:HA	1:F:325:MET:HE1	1.98	0.45
1:J:121:ASN:N	1:J:121:ASN:HD22	2.14	0.45
1:G:279:ASP:HB2	1:K:286:ILE:HD11	1.91	0.45
1:K:98:TYR:HA	1:K:178:VAL:O	2.16	0.45
1:O:58:VAL:HG22	1:O:351:LEU:HD22	1.98	0.45
1:F:112:THR:OG1	1:S:121:ASN:ND2	2.50	0.45
1:T:106:LEU:HD23	1:T:367:GLY:HA3	1.97	0.45
1:T:171:THR:HG22	4:T:475:HOH:O	2.14	0.45
1:B:215:GLN:HE22	1:B:328:SER:HB3	1.82	0.45
1:E:316:LYS:HB2	1:E:325:MET:HE3	1.98	0.45
1:L:269:THR:HG21	4:L:668:HOH:O	2.15	0.45
1:L:316:LYS:CB	1:L:325:MET:HE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:171:THR:O	1:O:172:SER:CB	2.65	0.45
1:Q:126:ALA:HB3	1:Q:155:ILE:HG22	1.99	0.45
1:R:324:GLN:NE2	1:R:324:GLN:CA	2.77	0.45
1:R:376:ASN:HB2	1:R:377:PRO:CD	2.46	0.45
1:A:118:TYR:CB	1:B:118:TYR:HD1	2.29	0.45
1:E:237:ILE:HG22	1:E:237:ILE:O	2.15	0.45
1:M:274:ARG:HG3	1:M:274:ARG:HH11	1.81	0.45
1:N:55:GLY:HA3	1:N:354:TYR:CZ	2.52	0.45
1:N:379:LEU:HD21	1:N:383:LEU:HD22	1.98	0.45
1:O:142:ASN:ND2	4:O:514:HOH:O	2.49	0.45
1:O:27:SER:HB3	4:O:643:HOH:O	2.15	0.45
1:N:111:SER:HB2	1:Q:159:LEU:HD22	1.99	0.45
1:Q:315:SER:HA	1:Q:325:MET:HE1	1.99	0.45
1:S:259:ALA:CB	1:S:290:MET:HE3	2.46	0.45
1:A:376:ASN:HB2	1:A:377:PRO:CD	2.46	0.45
1:G:201:ASP:OD2	1:K:202:ARG:CD	2.64	0.45
1:G:230:PHE:CD1	1:G:230:PHE:C	2.90	0.45
1:G:301:ILE:HG23	1:G:305:ILE:CD1	2.47	0.45
1:I:181:GLY:HA2	1:I:197:CYS:O	2.16	0.45
1:T:258:ASP:HB2	1:T:313:VAL:HB	1.99	0.45
1:G:120:LEU:HD23	4:G:5990:HOH:O	2.16	0.45
1:G:55:GLY:HA3	1:G:354:TYR:CZ	2.51	0.45
1:G:39:ARG:NH2	1:G:383:LEU:HD21	2.31	0.45
1:Q:201:ASP:O	1:Q:202:ARG:HB2	2.16	0.45
1:T:264:ILE:HB	1:T:307:SER:OG	2.16	0.45
1:A:171:THR:HG23	1:F:34:GLU:OE2	2.17	0.45
1:B:246:LEU:HG	1:B:292:PHE:CE2	2.51	0.45
1:P:153:ASP:CG	1:P:405:ARG:HH22	2.20	0.45
1:R:286:ILE:CG2	1:R:287:ASP:N	2.80	0.45
1:R:55:GLY:HA3	1:R:354:TYR:CZ	2.51	0.45
1:A:226:THR:OG1	1:A:313:VAL:HG22	2.17	0.45
1:C:279:ASP:OD1	1:C:279:ASP:O	2.35	0.45
1:H:171:THR:O	1:H:172:SER:CB	2.62	0.45
1:H:211:ALA:O	1:H:330:SER:HA	2.17	0.45
1:L:41:GLU:HB3	1:L:88:THR:HB	1.99	0.45
1:M:121:ASN:OD1	1:Q:112:THR:OG1	2.30	0.45
1:Q:121:ASN:ND2	1:Q:121:ASN:O	2.49	0.45
1:Q:41:GLU:HB3	1:Q:88:THR:HB	1.99	0.45
1:R:263:LEU:HA	1:R:263:LEU:HD23	1.79	0.45
1:T:273:THR:O	1:T:274:ARG:HD3	2.17	0.45
1:E:99:CYS:HB2	1:E:373:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:LEU:CD2	1:F:351:LEU:HD13	2.47	0.45
1:G:376:ASN:HB2	1:G:377:PRO:CD	2.47	0.45
1:K:171:THR:O	1:K:172:SER:CB	2.64	0.45
1:K:236:ALA:HB2	1:K:337:ILE:HD12	1.99	0.45
1:K:407:ARG:CB	1:K:407:ARG:HH11	2.13	0.45
1:M:220:TYR:CG	1:M:221:GLN:N	2.84	0.45
1:M:379:LEU:CD2	1:M:383:LEU:HD23	2.45	0.45
1:P:121:ASN:HB2	1:P:356:ARG:O	2.17	0.45
1:R:155:ILE:HA	1:R:155:ILE:HD12	1.80	0.45
1:S:20:MET:CB	1:S:423:ARG:HH12	2.27	0.45
1:T:283:THR:HG22	1:T:286:ILE:HG12	1.99	0.45
1:A:407:ARG:CB	1:A:407:ARG:NH1	2.73	0.45
1:C:153:ASP:CG	1:C:405:ARG:HH22	2.19	0.45
1:H:417:ARG:CG	1:H:417:ARG:NH1	2.80	0.45
1:N:201:ASP:O	1:N:202:ARG:HB2	2.17	0.45
1:O:261:ILE:HA	1:O:261:ILE:HD13	1.82	0.45
1:O:271:VAL:O	1:O:272:ILE:HG13	2.16	0.45
1:Q:316:LYS:CB	1:Q:325:MET:HE3	2.42	0.45
1:R:211:ALA:O	1:R:330:SER:HA	2.17	0.45
1:A:201:ASP:N	1:A:201:ASP:OD1	2.49	0.44
1:A:404:GLU:OE1	1:A:407:ARG:NH1	2.51	0.44
1:C:274:ARG:HH21	1:C:300:GLU:CD	2.20	0.44
1:E:272:ILE:HD13	1:E:296:ILE:HG21	2.00	0.44
1:P:126:ALA:HB3	1:P:155:ILE:HG22	1.99	0.44
1:N:364:THR:CG2	1:Q:157:ASN:HB3	2.48	0.44
1:Q:285:GLY:O	1:Q:286:ILE:CD1	2.65	0.44
1:R:41:GLU:HB3	1:R:88:THR:HB	1.99	0.44
1:B:59:PHE:CE2	1:B:106:LEU:HD13	2.52	0.44
1:C:14:PHE:CG	1:C:29:PRO:HD3	2.53	0.44
1:E:122:GLY:C	1:E:160:VAL:HG22	2.37	0.44
1:F:226:THR:OG1	1:F:313:VAL:HG22	2.16	0.44
1:H:153:ASP:CG	1:H:405:ARG:HH22	2.21	0.44
1:J:122:GLY:HA2	1:J:356:ARG:HB2	1.98	0.44
1:M:162:GLU:HB3	4:M:641:HOH:O	2.17	0.44
1:Q:112:THR:CG2	1:Q:361:SER:HA	2.47	0.44
1:B:144:LEU:CD2	1:B:351:LEU:HD12	2.47	0.44
1:B:126:ALA:HB3	1:B:155:ILE:HG22	1.99	0.44
1:C:355:GLU:O	1:C:356:ARG:HB2	2.16	0.44
1:J:62:GLY:HA2	1:J:101:LEU:HD23	1.99	0.44
1:J:246:LEU:HA	1:J:246:LEU:HD23	1.66	0.44
1:L:14:PHE:CG	1:L:29:PRO:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:249:HIS:NE2	1:L:287:ASP:OD1	2.45	0.44
1:P:226:THR:HG1	1:P:313:VAL:HG22	1.81	0.44
1:R:246:LEU:HD23	1:R:246:LEU:HA	1.79	0.44
1:S:226:THR:OG1	1:S:313:VAL:HG22	2.17	0.44
1:A:11:ILE:HD13	1:A:430:ALA:HB2	1.98	0.44
1:B:271:VAL:HG12	1:B:272:ILE:HG12	1.99	0.44
1:D:55:GLY:HA3	1:D:354:TYR:CZ	2.53	0.44
1:F:155:ILE:HA	1:F:155:ILE:HD12	1.88	0.44
1:G:255:LEU:HB2	4:G:6091:HOH:O	2.17	0.44
1:H:230:PHE:CD1	1:H:230:PHE:C	2.91	0.44
1:K:51:ASP:N	1:K:51:ASP:OD1	2.40	0.44
1:L:246:LEU:HD12	1:L:290:MET:HE2	1.98	0.44
1:O:316:LYS:N	1:O:325:MET:HE2	2.33	0.44
1:R:201:ASP:O	1:R:202:ARG:HB2	2.18	0.44
1:T:112:THR:HG21	1:T:361:SER:HB3	1.97	0.44
1:G:120:LEU:HD21	1:G:161:GLY:CA	2.44	0.44
1:G:155:ILE:HD12	1:G:155:ILE:HA	1.86	0.44
1:H:249:HIS:NE2	1:H:287:ASP:OD2	2.45	0.44
1:H:395:MET:CG	1:H:399:LYS:HE3	2.48	0.44
1:L:127:VAL:CG2	1:L:148:THR:HG22	2.47	0.44
1:P:316:LYS:N	1:P:325:MET:CE	2.81	0.44
1:Q:292:PHE:CE1	1:Q:333:LEU:HD21	2.53	0.44
1:R:250:THR:O	1:R:284:THR:HG22	2.18	0.44
1:A:98:TYR:HA	1:A:178:VAL:O	2.17	0.44
1:B:402:LEU:O	1:B:405:ARG:HB2	2.17	0.44
1:C:49:VAL:HG21	1:C:357:VAL:CG1	2.47	0.44
1:H:262:TYR:HB2	1:H:309:LYS:HG2	1.99	0.44
1:P:280:ASN:ND2	1:P:280:ASN:C	2.70	0.44
1:Q:178:VAL:HG12	1:Q:179:ARG:O	2.17	0.44
1:T:391:ASP:HA	1:T:392:PRO:HD2	1.75	0.44
1:B:55:GLY:HA3	1:B:354:TYR:CZ	2.53	0.44
1:H:20:MET:HG2	1:H:423:ARG:HG2	1.98	0.44
1:J:247:VAL:HG22	1:J:289:LEU:HD22	1.99	0.44
1:L:11:ILE:HD12	1:L:12:VAL:N	2.25	0.44
1:N:391:ASP:HA	1:N:392:PRO:HD2	1.76	0.44
1:O:12:VAL:N	4:O:594:HOH:O	2.50	0.44
1:T:107:THR:HG23	4:T:631:HOH:O	2.18	0.44
1:A:263:LEU:HD23	1:A:308:ILE:HG13	2.00	0.44
1:C:274:ARG:HD3	1:C:274:ARG:HA	1.83	0.44
1:C:426:PHE:C	1:C:428:GLU:H	2.20	0.44
1:F:133:LEU:HD12	1:F:136:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:VAL:O	1:G:272:ILE:HG13	2.18	0.44
1:I:130:GLN:HE22	1:J:385:THR:HG21	1.83	0.44
1:I:201:ASP:OD1	1:I:201:ASP:N	2.46	0.44
1:I:264:ILE:HB	1:I:307:SER:OG	2.17	0.44
1:I:389:ARG:HD3	1:I:391:ASP:OD2	2.17	0.44
1:M:169:LEU:HD11	1:M:410:ILE:HG22	2.00	0.44
1:M:201:ASP:OD1	1:M:201:ASP:N	2.50	0.44
1:M:219:GLN:HA	1:M:324:GLN:HE22	1.83	0.44
1:M:41:GLU:HB3	1:M:88:THR:HB	1.99	0.44
1:Q:258:ASP:HB2	1:Q:313:VAL:HB	2.00	0.44
1:S:12:VAL:O	1:S:13:PRO:C	2.55	0.44
1:T:259:ALA:HB3	1:T:290:MET:CE	2.46	0.44
1:A:41:GLU:HB3	1:A:88:THR:HB	1.99	0.44
1:B:114:PRO:HG3	1:B:359:THR:O	2.18	0.44
1:C:121:ASN:O	1:C:121:ASN:ND2	2.51	0.44
1:D:113:LEU:HD12	1:D:113:LEU:H	1.82	0.44
1:E:126:ALA:HB3	1:E:155:ILE:HG22	1.98	0.44
1:F:122:GLY:C	1:F:160:VAL:HG23	2.37	0.44
1:G:113:LEU:HD12	4:G:6120:HOH:O	2.18	0.44
1:I:112:THR:HB	1:I:362:VAL:HB	1.99	0.44
1:K:230:PHE:CD1	1:K:230:PHE:C	2.91	0.44
1:L:276:VAL:HG21	1:L:292:PHE:CD2	2.53	0.44
1:Q:121:ASN:HD22	1:Q:121:ASN:N	2.16	0.44
1:R:272:ILE:HD13	1:R:296:ILE:CG2	2.47	0.44
1:R:136:LEU:HD13	1:R:351:LEU:HD11	2.00	0.44
1:S:280:ASN:HB2	4:S:551:HOH:O	2.18	0.44
1:T:113:LEU:HA	1:T:114:PRO:HD3	1.62	0.44
1:F:120:LEU:HD13	1:F:121:ASN:H	1.82	0.43
1:G:57:ILE:HG21	1:G:59:PHE:CZ	2.53	0.43
1:K:369:SER:HB3	1:K:371:PHE:CZ	2.53	0.43
1:K:41:GLU:HB3	1:K:88:THR:HB	2.00	0.43
1:L:32:THR:O	1:L:32:THR:HG22	2.18	0.43
1:L:402:LEU:O	1:L:405:ARG:HB2	2.17	0.43
1:N:112:THR:HG21	1:N:362:VAL:HG23	2.00	0.43
1:O:226:THR:OG1	1:O:313:VAL:HG22	2.18	0.43
1:P:274:ARG:NH2	1:P:300:GLU:OE1	2.49	0.43
1:S:349:VAL:CG1	1:S:351:LEU:CD2	2.96	0.43
1:T:376:ASN:HB2	1:T:377:PRO:CD	2.48	0.43
1:A:425:TYR:O	1:A:425:TYR:HD1	2.01	0.43
1:A:77:ASN:HD22	1:A:79:ASN:H	1.64	0.43
1:B:140:SER:O	1:B:144:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ILE:HG21	1:B:237:ILE:HD13	1.85	0.43
1:D:383:LEU:HG	1:E:383:LEU:HD23	1.98	0.43
1:J:271:VAL:O	1:J:272:ILE:HG13	2.18	0.43
1:L:270:THR:HG21	1:L:273:THR:HG22	2.00	0.43
1:M:230:PHE:CD1	1:M:230:PHE:C	2.90	0.43
1:O:193:MET:C	1:O:193:MET:HE3	2.38	0.43
1:O:246:LEU:CD2	1:O:331:GLY:HA3	2.37	0.43
1:T:11:ILE:CG2	1:T:16:ARG:NH1	2.81	0.43
1:T:171:THR:HG21	1:T:348:PRO:HD3	1.99	0.43
1:B:105:SER:HA	1:B:166:VAL:O	2.18	0.43
1:D:379:LEU:CG	1:D:383:LEU:HD12	2.21	0.43
1:E:211:ALA:O	1:E:330:SER:HA	2.18	0.43
1:G:41:GLU:HB3	1:G:88:THR:HB	2.01	0.43
1:L:230:PHE:CD1	1:L:230:PHE:C	2.91	0.43
1:N:320:GLN:O	1:N:323:ASP:HB2	2.19	0.43
1:R:146:SER:O	1:S:381:LYS:HG2	2.18	0.43
1:R:25:PRO:HD3	1:R:40:SER:OG	2.19	0.43
1:F:262:TYR:HB2	1:F:309:LYS:HG2	2.00	0.43
1:G:82:PHE:CZ	1:G:84:GLN:HA	2.53	0.43
1:M:157:ASN:ND2	1:Q:44:THR:HB	2.33	0.43
1:T:220:TYR:CG	1:T:221:GLN:N	2.87	0.43
1:F:41:GLU:HB3	1:F:88:THR:HB	2.00	0.43
1:L:389:ARG:HB3	1:L:389:ARG:HH11	1.83	0.43
1:L:426:PHE:C	1:L:428:GLU:N	2.70	0.43
1:N:41:GLU:HB3	1:N:88:THR:HB	2.00	0.43
1:O:257:LEU:CD1	1:O:282:LEU:HD21	2.48	0.43
1:P:41:GLU:HB3	1:P:88:THR:HB	1.99	0.43
1:Q:391:ASP:HA	1:Q:392:PRO:HD2	1.73	0.43
1:S:32:THR:HG22	1:S:32:THR:O	2.18	0.43
1:T:112:THR:HG21	1:T:361:SER:CB	2.48	0.43
1:A:118:TYR:CZ	1:T:114:PRO:HB3	2.53	0.43
1:T:112:THR:HG22	1:T:362:VAL:H	1.69	0.43
1:B:274:ARG:HH11	1:B:274:ARG:HG3	1.83	0.43
1:B:208:ILE:O	1:B:332:SER:HA	2.19	0.43
1:C:164:VAL:HG22	1:C:414:TRP:O	2.19	0.43
1:C:190:ASP:OD1	1:C:191:PRO:N	2.51	0.43
1:G:274:ARG:NH2	1:G:300:GLU:OE1	2.51	0.43
1:H:262:TYR:HD2	1:H:273:THR:HG22	1.83	0.43
1:I:279:ASP:CG	1:I:279:ASP:O	2.57	0.43
1:I:41:GLU:HB3	1:I:88:THR:HB	2.00	0.43
1:P:376:ASN:HB2	1:P:377:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:136:LEU:HD11	1:T:351:LEU:HD11	1.99	0.43
1:A:276:VAL:HG11	1:A:292:PHE:CE2	2.54	0.43
1:D:181:GLY:HA2	1:D:197:CYS:O	2.19	0.43
1:G:25:PRO:HD3	1:G:40:SER:OG	2.18	0.43
1:I:220:TYR:N	1:I:323:ASP:O	2.37	0.43
1:I:292:PHE:CE1	1:I:333:LEU:HD21	2.54	0.43
1:P:112:THR:HG22	1:P:361:SER:HA	2.00	0.43
1:E:141:TYR:CE1	1:E:355:GLU:HG2	2.54	0.43
1:F:98:TYR:HA	1:F:178:VAL:O	2.18	0.43
1:I:220:TYR:CG	1:I:221:GLN:N	2.87	0.43
1:M:214:TYR:O	1:M:328:SER:HA	2.19	0.43
1:N:98:TYR:HB2	1:N:374:ILE:HB	2.01	0.43
1:N:150:ASN:OD1	1:O:384:VAL:HG13	2.19	0.43
1:Q:320:GLN:O	1:Q:321:ALA:C	2.56	0.43
1:Q:315:SER:C	1:Q:325:MET:HE2	2.39	0.43
1:E:391:ASP:HA	1:E:392:PRO:HD2	1.70	0.43
1:F:162:GLU:OE1	1:F:417:ARG:HD2	2.18	0.43
1:G:214:TYR:O	1:G:328:SER:HA	2.19	0.43
1:L:253:HIS:CE1	1:L:284:THR:HG21	2.53	0.43
1:O:429:VAL:O	1:O:429:VAL:HG12	2.19	0.43
1:Q:316:LYS:N	1:Q:325:MET:CE	2.81	0.43
1:J:130:GLN:NE2	1:Q:385:THR:OG1	2.52	0.43
1:Q:425:TYR:O	1:Q:429:VAL:HG23	2.19	0.43
1:R:34:GLU:HB3	4:R:6065:HOH:O	2.17	0.43
1:R:58:VAL:HG22	1:R:351:LEU:CD2	2.49	0.43
1:R:202:ARG:CD	1:S:201:ASP:OD2	2.62	0.43
1:T:171:THR:CG2	4:T:475:HOH:O	2.67	0.43
1:A:315:SER:C	1:A:325:MET:HE2	2.39	0.43
1:D:376:ASN:HB2	1:D:377:PRO:CD	2.48	0.43
1:E:104:ARG:HD3	1:E:369:SER:OG	2.17	0.43
1:F:258:ASP:HB2	1:F:313:VAL:HB	2.01	0.43
1:H:270:THR:HG21	1:H:273:THR:CG2	2.49	0.43
1:L:91:ASN:OD1	1:L:93:PRO:HD2	2.19	0.43
1:M:122:GLY:C	1:M:160:VAL:HG22	2.38	0.43
1:M:389:ARG:HH11	1:M:389:ARG:HB3	1.84	0.43
1:Q:214:TYR:O	1:Q:328:SER:HA	2.19	0.43
1:S:391:ASP:HA	1:S:392:PRO:HD2	1.72	0.43
1:T:162:GLU:HG2	1:T:417:ARG:CZ	2.49	0.43
1:C:189:LEU:HB3	1:E:214:TYR:CE1	2.54	0.42
1:E:82:PHE:CZ	1:E:84:GLN:HA	2.54	0.42
1:G:59:PHE:CD2	1:G:106:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:391:ASP:HA	1:G:392:PRO:HD2	1.84	0.42
1:I:20:MET:HE2	1:I:423:ARG:HH21	1.84	0.42
1:I:99:CYS:HB2	1:I:373:LEU:CD2	2.48	0.42
1:K:246:LEU:HA	1:K:246:LEU:HD23	1.82	0.42
1:M:100:ARG:HG2	1:M:177:TYR:HA	2.01	0.42
1:M:16:ARG:NH2	1:M:23:THR:HB	2.34	0.42
1:I:385:THR:HG21	1:Q:130:GLN:HE22	1.84	0.42
1:R:121:ASN:HB2	1:R:358:ALA:H	1.83	0.42
1:R:155:ILE:HG12	1:R:415:PRO:HD3	2.01	0.42
1:S:263:LEU:HB2	1:S:272:ILE:HB	2.01	0.42
1:C:379:LEU:HD21	1:C:383:LEU:HD11	2.01	0.42
1:F:246:LEU:HA	1:F:246:LEU:HD23	1.74	0.42
1:H:286:ILE:HA	1:H:286:ILE:HD13	1.95	0.42
1:H:246:LEU:CD1	1:H:290:MET:HE1	2.42	0.42
1:I:369:SER:HB3	1:I:371:PHE:CZ	2.54	0.42
1:L:259:ALA:HB3	1:L:276:VAL:HG12	2.01	0.42
1:N:389:ARG:HE	1:Q:407:ARG:HH22	1.67	0.42
1:M:120:LEU:O	1:Q:113:LEU:HD13	2.19	0.42
1:L:383:LEU:HD22	1:R:383:LEU:HD12	1.99	0.42
1:S:165:THR:HG21	1:S:419:TYR:CD2	2.54	0.42
1:A:155:ILE:HA	1:A:155:ILE:HD12	1.95	0.42
1:B:33:LEU:HD23	1:B:33:LEU:N	2.33	0.42
1:E:41:GLU:HB3	1:E:88:THR:HB	2.01	0.42
1:P:315:SER:HA	1:P:325:MET:CE	2.49	0.42
1:S:214:TYR:O	1:S:328:SER:HA	2.19	0.42
1:T:237:ILE:HD13	1:T:237:ILE:HG21	1.89	0.42
1:C:112:THR:HG21	1:C:362:VAL:HG23	2.02	0.42
1:C:129:PHE:HB3	1:C:349:VAL:HG23	2.01	0.42
1:F:144:LEU:HD11	1:F:353:ALA:HB2	2.01	0.42
1:G:146:SER:O	1:M:381:LYS:HG2	2.20	0.42
1:G:356:ARG:CG	1:G:356:ARG:HH11	2.32	0.42
1:G:162:GLU:CD	1:G:417:ARG:NH2	2.73	0.42
1:H:219:GLN:HA	1:H:324:GLN:NE2	2.34	0.42
1:N:39:ARG:HD2	4:N:502:HOH:O	2.19	0.42
1:R:112:THR:HG22	1:R:361:SER:CA	2.42	0.42
1:S:376:ASN:OD1	1:S:376:ASN:C	2.58	0.42
1:A:246:LEU:HD12	1:A:290:MET:HE2	2.00	0.42
1:B:242:ILE:HG23	1:B:335:VAL:HG22	2.01	0.42
1:C:112:THR:HG22	1:C:362:VAL:N	2.25	0.42
1:C:56:LEU:HD11	1:C:351:LEU:HB3	2.00	0.42
1:D:319:GLY:O	1:D:320:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:THR:HG21	1:K:348:PRO:HD3	2.02	0.42
1:L:63:PHE:CZ	1:L:67:ILE:HD12	2.55	0.42
1:N:237:ILE:HD13	1:N:237:ILE:HG21	1.85	0.42
1:P:208:ILE:HB	1:P:333:LEU:CD1	2.50	0.42
1:S:112:THR:HG23	1:S:113:LEU:N	2.33	0.42
1:A:258:ASP:HB2	1:A:313:VAL:HB	2.02	0.42
1:B:12:VAL:HG12	1:B:12:VAL:O	2.19	0.42
1:B:215:GLN:NE2	1:B:328:SER:HB3	2.34	0.42
1:C:257:LEU:HD23	1:C:314:THR:HA	2.01	0.42
1:E:162:GLU:OE2	1:E:417:ARG:HD3	2.19	0.42
1:H:201:ASP:O	1:H:202:ARG:HB2	2.19	0.42
1:H:20:MET:CG	1:H:423:ARG:HG2	2.50	0.42
1:I:263:LEU:HB2	1:I:272:ILE:HB	2.02	0.42
1:K:274:ARG:HD3	1:K:274:ARG:HA	1.81	0.42
1:L:263:LEU:HB2	1:L:272:ILE:HB	2.02	0.42
1:O:67:ILE:HD13	1:O:237:ILE:HG21	2.01	0.42
1:Q:98:TYR:HA	1:Q:178:VAL:O	2.20	0.42
1:S:164:VAL:HG23	1:S:414:TRP:O	2.20	0.42
1:B:320:GLN:O	1:B:321:ALA:C	2.58	0.42
1:C:155:ILE:HA	1:C:155:ILE:HD12	1.86	0.42
1:F:391:ASP:HA	1:F:392:PRO:HD3	1.82	0.42
1:F:417:ARG:HG3	4:F:530:HOH:O	2.19	0.42
1:N:202:ARG:HD2	1:O:201:ASP:OD2	2.20	0.42
1:P:140:SER:O	1:P:144:LEU:HG	2.20	0.42
1:Q:201:ASP:N	1:Q:201:ASP:OD1	2.51	0.42
1:R:112:THR:CG2	1:R:361:SER:HA	2.44	0.42
1:R:93:PRO:HG3	1:R:180:LEU:HB3	2.02	0.42
1:S:242:ILE:HB	1:S:294:LEU:HB2	2.01	0.42
1:T:320:GLN:O	1:T:321:ALA:C	2.57	0.42
1:E:139:VAL:HA	1:E:144:LEU:HD21	2.02	0.42
1:E:257:LEU:HD21	1:E:314:THR:HG23	2.02	0.42
1:G:140:SER:O	1:G:144:LEU:HG	2.20	0.42
1:G:121:ASN:O	1:G:160:VAL:HG11	2.19	0.42
1:K:20:MET:CE	1:K:423:ARG:HG2	2.50	0.42
1:M:47:LEU:HD13	1:M:71:HIS:CG	2.55	0.42
1:N:121:ASN:OD1	1:N:358:ALA:N	2.26	0.42
1:N:92:LEU:N	1:N:93:PRO:CD	2.83	0.42
1:O:121:ASN:HB3	4:O:549:HOH:O	2.20	0.42
1:P:267:ASP:OD1	1:P:269:THR:HB	2.19	0.42
1:P:280:ASN:ND2	4:P:6061:HOH:O	2.52	0.42
1:C:120:LEU:CD2	1:R:113:LEU:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:MET:HG2	1:E:423:ARG:CD	2.50	0.42
1:G:272:ILE:HD13	1:G:296:ILE:HG21	2.01	0.42
1:I:41:GLU:OE1	1:I:90:GLN:HG2	2.20	0.42
1:K:426:PHE:C	1:K:428:GLU:N	2.73	0.42
1:L:15:ILE:HG13	1:L:397:TYR:HD2	1.85	0.42
1:E:159:LEU:CD1	1:O:109:ARG:HH11	2.33	0.42
1:O:274:ARG:HG3	1:O:274:ARG:NH1	2.35	0.42
1:P:21:PRO:HG2	1:P:105:SER:CB	2.50	0.42
1:A:120:LEU:O	1:T:112:THR:HA	2.20	0.42
1:A:391:ASP:HA	1:A:392:PRO:HD2	1.84	0.42
1:B:315:SER:C	1:B:325:MET:CE	2.88	0.42
1:E:121:ASN:O	1:E:121:ASN:CG	2.58	0.42
1:F:419:TYR:CE2	1:F:423:ARG:HD2	2.55	0.42
1:K:133:LEU:HD12	1:K:136:LEU:HD12	2.01	0.42
1:L:390:PHE:CZ	1:L:392:PRO:HG3	2.55	0.42
1:N:130:GLN:NE2	1:O:385:THR:OG1	2.52	0.42
1:P:21:PRO:HG3	1:P:105:SER:HB3	2.01	0.42
1:P:162:GLU:HG2	1:P:417:ARG:HH11	1.79	0.42
1:Q:285:GLY:O	1:Q:286:ILE:HD12	2.20	0.42
1:R:274:ARG:HB2	1:R:294:LEU:HD21	2.00	0.42
1:R:315:SER:CA	1:R:325:MET:CE	2.94	0.42
1:S:402:LEU:O	1:S:405:ARG:HB2	2.20	0.42
1:C:376:ASN:C	1:C:376:ASN:OD1	2.58	0.41
1:D:170:PRO:HB3	1:D:173:TYR:CZ	2.54	0.41
1:D:41:GLU:HB3	1:D:88:THR:HB	2.02	0.41
1:E:257:LEU:HD23	1:E:314:THR:HA	2.02	0.41
1:E:108:VAL:HG22	1:E:365:VAL:HG22	2.01	0.41
1:F:112:THR:HB	1:F:362:VAL:HB	2.02	0.41
1:F:230:PHE:C	1:F:230:PHE:CD1	2.93	0.41
1:G:126:ALA:HB3	1:G:155:ILE:HG22	2.02	0.41
1:P:246:LEU:CD2	1:P:292:PHE:HZ	2.31	0.41
1:N:13:PRO:HG3	1:Q:407:ARG:HH21	1.85	0.41
1:S:169:LEU:HD23	1:S:169:LEU:HA	1.84	0.41
1:S:284:THR:HG22	4:S:641:HOH:O	2.19	0.41
1:T:14:PHE:CG	1:T:29:PRO:HD3	2.55	0.41
1:T:263:LEU:HB3	1:T:305:ILE:HD12	2.02	0.41
1:T:41:GLU:HB3	1:T:88:THR:HB	2.02	0.41
1:A:219:GLN:HE22	1:A:322:GLY:CA	2.33	0.41
1:E:120:LEU:HB2	1:O:113:LEU:CD1	2.46	0.41
1:E:121:ASN:O	1:E:357:VAL:HA	2.20	0.41
1:H:144:LEU:HD22	1:H:351:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:237:ILE:O	1:I:237:ILE:HG22	2.20	0.41
1:I:249:HIS:HB2	1:I:328:SER:OG	2.20	0.41
1:K:259:ALA:HB3	1:K:276:VAL:HG23	2.01	0.41
1:O:274:ARG:HG3	1:O:274:ARG:HH11	1.85	0.41
1:A:140:SER:O	1:A:144:LEU:HG	2.20	0.41
1:F:12:VAL:HG12	1:F:15:ILE:H	1.86	0.41
1:G:246:LEU:HA	1:G:246:LEU:HD23	1.92	0.41
1:G:293:ASN:ND2	1:K:291:PRO:CB	2.83	0.41
1:M:60:PHE:CE2	1:M:237:ILE:HD11	2.55	0.41
1:R:166:VAL:CG1	1:R:350:THR:HG21	2.51	0.41
1:S:112:THR:HG22	1:S:362:VAL:H	1.84	0.41
1:S:325:MET:HB3	1:S:325:MET:HE2	1.88	0.41
1:M:90:GLN:NE2	1:S:381:LYS:HB3	2.35	0.41
1:A:12:VAL:HA	1:A:13:PRO:HD2	1.94	0.41
1:A:21:PRO:HG2	1:A:105:SER:HB3	2.02	0.41
1:A:49:VAL:CG1	1:A:53:GLY:HA2	2.50	0.41
1:K:155:ILE:HG23	1:K:155:ILE:O	2.21	0.41
1:P:114:PRO:O	1:P:116:GLY:N	2.54	0.41
1:P:234:ILE:O	1:P:306:THR:HA	2.20	0.41
1:Q:263:LEU:HB2	1:Q:272:ILE:HB	2.02	0.41
1:R:377:PRO:HD2	4:R:6002:HOH:O	2.19	0.41
1:R:80:TYR:O	1:R:267:ASP:HB2	2.20	0.41
1:S:230:PHE:C	1:S:230:PHE:CD1	2.93	0.41
1:B:215:GLN:HE22	1:B:328:SER:HB2	1.84	0.41
1:B:376:ASN:HB2	1:B:377:PRO:CD	2.50	0.41
1:C:237:ILE:HG21	1:C:237:ILE:HD13	1.82	0.41
1:D:247:VAL:HG22	1:D:289:LEU:CD2	2.50	0.41
1:G:220:TYR:CZ	1:G:221:GLN:O	2.74	0.41
1:I:51:ASP:HA	1:I:359:THR:HG23	2.02	0.41
1:M:56:LEU:HD11	1:M:351:LEU:HB3	2.02	0.41
1:P:264:ILE:HB	1:P:307:SER:OG	2.20	0.41
1:S:162:GLU:OE1	1:S:417:ARG:NH1	2.53	0.41
1:B:114:PRO:HD3	1:B:361:SER:OG	2.20	0.41
1:E:169:LEU:HD23	1:E:169:LEU:HA	1.72	0.41
1:E:35:LYS:HD3	1:L:405:ARG:NH1	2.36	0.41
1:F:171:THR:HG21	1:F:348:PRO:HD3	2.01	0.41
1:G:51:ASP:HA	1:G:359:THR:OG1	2.20	0.41
1:H:193:MET:HG2	1:H:194:VAL:N	2.35	0.41
1:J:426:PHE:C	1:J:428:GLU:N	2.73	0.41
1:J:428:GLU:O	1:J:429:VAL:C	2.58	0.41
1:M:58:VAL:HG22	1:M:351:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:ASN:OD1	1:N:384:VAL:HG13	2.21	0.41
1:P:286:ILE:HD13	1:P:286:ILE:HG21	1.69	0.41
1:S:107:THR:HG22	1:S:165:THR:OG1	2.20	0.41
1:S:274:ARG:NH1	1:S:274:ARG:HG3	2.34	0.41
1:T:324:GLN:NE2	1:T:324:GLN:CA	2.80	0.41
1:A:105:SER:HA	1:A:166:VAL:O	2.21	0.41
1:C:201:ASP:O	1:C:339:GLY:HA2	2.21	0.41
1:J:112:THR:HG21	1:J:361:SER:HA	2.02	0.41
1:K:376:ASN:HB3	4:K:496:HOH:O	2.21	0.41
1:P:252:VAL:HG21	1:P:324:GLN:O	2.20	0.41
1:Q:190:ASP:OD1	1:Q:192:LYS:HB2	2.21	0.41
1:Q:417:ARG:HH11	1:Q:417:ARG:CB	2.31	0.41
1:R:144:LEU:HD22	1:R:351:LEU:HD12	2.03	0.41
1:A:184:ILE:HD11	1:A:195:ALA:HB1	2.03	0.41
1:B:39:ARG:HD2	4:B:5977:HOH:O	2.20	0.41
1:F:189:LEU:HD23	1:F:189:LEU:HA	1.86	0.41
1:G:162:GLU:CG	1:G:417:ARG:NH2	2.81	0.41
1:G:181:GLY:HA2	1:G:197:CYS:O	2.21	0.41
1:G:255:LEU:HD23	1:G:255:LEU:HA	1.75	0.41
1:H:293:ASN:ND2	1:H:293:ASN:N	2.68	0.41
1:I:130:GLN:NE2	1:J:385:THR:OG1	2.54	0.41
1:J:355:GLU:O	1:J:356:ARG:HB2	2.20	0.41
1:O:417:ARG:HB2	1:O:417:ARG:CZ	2.49	0.41
1:Q:164:VAL:HA	1:Q:414:TRP:O	2.21	0.41
1:Q:201:ASP:O	1:Q:339:GLY:HA2	2.21	0.41
1:R:12:VAL:O	1:R:12:VAL:HG12	2.21	0.41
1:T:379:LEU:HD12	1:T:379:LEU:HA	1.86	0.41
1:B:272:ILE:HD11	1:B:300:GLU:O	2.21	0.41
1:C:260:THR:O	1:C:310:LEU:HD12	2.21	0.41
1:F:121:ASN:N	1:F:121:ASN:HD22	2.19	0.41
1:G:208:ILE:O	1:G:332:SER:HA	2.21	0.41
1:H:399:LYS:NZ	4:H:6000:HOH:O	2.54	0.41
1:N:247:VAL:HG22	1:N:289:LEU:HD23	2.03	0.41
1:O:127:VAL:CG2	1:O:148:THR:HG22	2.51	0.41
1:O:15:ILE:HG13	1:O:397:TYR:HD2	1.85	0.41
1:O:246:LEU:HD12	1:O:290:MET:HE1	2.03	0.41
1:Q:175:LEU:HB3	1:Q:342:TYR:OH	2.21	0.41
1:Q:246:LEU:HA	1:Q:246:LEU:HD23	1.77	0.41
1:S:258:ASP:HB2	1:S:313:VAL:HB	2.03	0.41
1:S:171:THR:HA	1:T:34:GLU:HG3	2.01	0.41
1:B:237:ILE:HG22	1:B:238:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:LEU:HD12	1:G:290:MET:SD	2.60	0.41
1:G:258:ASP:HB2	1:G:313:VAL:HB	2.02	0.41
1:H:122:GLY:C	1:H:160:VAL:HG13	2.42	0.41
1:H:220:TYR:CG	1:H:221:GLN:N	2.89	0.41
1:I:173:TYR:HA	1:I:173:TYR:HD2	1.79	0.41
1:I:193:MET:HG2	1:I:194:VAL:N	2.35	0.41
1:J:20:MET:HB2	1:J:20:MET:HE2	1.86	0.41
1:K:41:GLU:OE1	1:K:90:GLN:HG2	2.20	0.41
1:L:246:LEU:HA	1:L:246:LEU:HD23	1.95	0.41
1:M:237:ILE:HD13	1:M:237:ILE:HG21	1.77	0.41
1:O:273:THR:O	1:O:274:ARG:HD3	2.21	0.41
1:T:124:ILE:HG21	1:T:164:VAL:HG21	2.03	0.41
1:A:93:PRO:HG3	1:A:180:LEU:HB3	2.03	0.41
1:B:99:CYS:HB2	1:B:373:LEU:HD23	2.03	0.41
1:B:397:TYR:CZ	1:B:401:ILE:HD11	2.56	0.41
1:B:82:PHE:CZ	1:B:84:GLN:HA	2.56	0.41
1:E:379:LEU:HG	1:E:383:LEU:CG	2.44	0.41
1:G:112:THR:HG22	1:G:113:LEU:N	2.36	0.41
1:J:316:LYS:HB2	1:J:325:MET:CE	2.51	0.41
1:K:320:GLN:HE21	1:K:320:GLN:HB2	1.59	0.41
1:K:355:GLU:O	1:K:356:ARG:HB2	2.20	0.41
1:N:242:ILE:HD12	1:N:294:LEU:HD12	2.03	0.41
1:N:315:SER:CA	1:N:325:MET:HE2	2.51	0.41
1:A:259:ALA:HA	1:A:311:GLU:O	2.21	0.40
1:A:82:PHE:CZ	1:A:85:MET:HE2	2.55	0.40
1:B:315:SER:CA	1:B:325:MET:CE	2.94	0.40
1:C:146:SER:HB2	4:C:6010:HOH:O	2.22	0.40
1:D:219:GLN:HE22	1:D:322:GLY:CA	2.34	0.40
1:F:20:MET:HG2	1:F:423:ARG:HG2	2.03	0.40
1:G:63:PHE:CZ	1:G:67:ILE:HD12	2.56	0.40
1:J:56:LEU:HD11	1:J:351:LEU:HB3	2.04	0.40
1:K:286:ILE:HG22	1:K:288:ASN:ND2	2.36	0.40
1:K:255:LEU:HD21	1:K:325:MET:HB3	2.03	0.40
1:N:253:HIS:CG	1:N:254:GLY:N	2.89	0.40
1:N:77:ASN:OD1	1:N:77:ASN:C	2.60	0.40
1:P:113:LEU:HD21	1:P:120:LEU:HA	2.01	0.40
1:P:220:TYR:CD1	1:P:221:GLN:N	2.87	0.40
1:Q:397:TYR:O	1:Q:401:ILE:HG12	2.21	0.40
1:R:12:VAL:HG12	1:R:15:ILE:H	1.86	0.40
1:R:274:ARG:HG3	1:R:294:LEU:CD2	2.51	0.40
1:R:286:ILE:HG23	1:R:287:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:136:LEU:HD13	1:T:351:LEU:HD11	2.03	0.40
1:B:240:LEU:N	1:B:240:LEU:HD23	2.36	0.40
1:G:383:LEU:HD12	1:G:384:VAL:O	2.20	0.40
1:J:166:VAL:HG13	1:J:350:THR:HG21	2.03	0.40
1:J:92:LEU:N	1:J:93:PRO:CD	2.85	0.40
1:M:262:TYR:HE1	1:M:311:GLU:HB2	1.86	0.40
1:N:263:LEU:HD12	1:N:272:ILE:HG21	2.03	0.40
1:P:206:TYR:HB2	1:P:335:VAL:HB	2.02	0.40
1:P:320:GLN:O	1:P:323:ASP:HB2	2.21	0.40
1:Q:262:TYR:CE2	1:Q:273:THR:HG22	2.55	0.40
1:S:41:GLU:HB3	1:S:88:THR:HB	2.02	0.40
1:A:16:ARG:HH21	1:A:23:THR:HB	1.86	0.40
1:C:129:PHE:CG	1:C:136:LEU:HD21	2.57	0.40
1:C:214:TYR:O	1:C:328:SER:HA	2.21	0.40
1:E:389:ARG:NH1	1:E:389:ARG:CB	2.84	0.40
1:F:15:ILE:HD11	1:F:398:THR:OG1	2.21	0.40
1:G:190:ASP:OD1	1:G:191:PRO:HD2	2.21	0.40
1:G:136:LEU:HD13	1:G:351:LEU:HD11	2.03	0.40
1:H:390:PHE:CZ	1:H:392:PRO:HG3	2.57	0.40
1:K:316:LYS:HB2	1:K:325:MET:CE	2.52	0.40
1:K:153:ASP:CG	1:K:405:ARG:HH22	2.24	0.40
1:N:12:VAL:H	1:N:12:VAL:HG23	1.63	0.40
1:N:274:ARG:HG3	1:N:274:ARG:HH11	1.87	0.40
1:Q:427:MET:O	1:Q:428:GLU:OE1	2.40	0.40
1:R:41:GLU:OE1	1:R:90:GLN:HG3	2.21	0.40
1:T:201:ASP:O	1:T:339:GLY:HA2	2.22	0.40
1:B:41:GLU:CD	1:B:90:GLN:HG2	2.42	0.40
1:C:271:VAL:O	1:C:272:ILE:HG13	2.21	0.40
1:G:395:MET:O	1:G:399:LYS:HG3	2.22	0.40
1:H:98:TYR:HA	1:H:178:VAL:O	2.21	0.40
1:H:356:ARG:HG2	1:H:356:ARG:HH11	1.87	0.40
1:I:12:VAL:O	1:I:13:PRO:C	2.59	0.40
1:I:262:TYR:HB2	1:I:309:LYS:HG2	2.03	0.40
1:K:155:ILE:CG2	1:K:155:ILE:O	2.69	0.40
1:K:14:PHE:CG	1:K:29:PRO:HD3	2.56	0.40
1:K:376:ASN:HB2	1:K:377:PRO:CD	2.51	0.40
1:K:391:ASP:HA	1:K:392:PRO:HD2	1.76	0.40
1:K:417:ARG:HD3	4:K:594:HOH:O	2.22	0.40
1:M:264:ILE:HB	1:M:307:SER:OG	2.22	0.40
1:N:59:PHE:CE2	1:N:106:LEU:HD13	2.56	0.40
1:O:211:ALA:O	1:O:330:SER:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:219:GLN:N	1:P:219:GLN:CD	2.74	0.40
1:P:317:SER:O	1:P:318:GLY:C	2.60	0.40
1:P:95:SER:HA	1:P:376:ASN:ND2	2.36	0.40
1:J:214:TYR:HB2	1:Q:190:ASP:OD2	2.22	0.40
1:A:402:LEU:HA	1:A:402:LEU:HD23	1.70	0.40
1:B:201:ASP:O	1:B:339:GLY:HA2	2.21	0.40
1:H:402:LEU:HD23	1:H:402:LEU:HA	1.92	0.40
1:I:214:TYR:O	1:I:328:SER:HA	2.21	0.40
1:L:38:LEU:O	1:L:39:ARG:NH1	2.41	0.40
1:O:260:THR:O	1:O:310:LEU:HD12	2.22	0.40
1:P:86:LEU:C	1:P:87:LEU:HD23	2.42	0.40
1:Q:104:ARG:HG3	1:Q:105:SER:N	2.37	0.40
1:J:402:LEU:CD1	1:Q:33:LEU:HD13	2.42	0.40
1:T:257:LEU:HD11	1:T:282:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/458 (91%)	397 (95%)	18 (4%)	3 (1%)	24	46
1	B	416/458 (91%)	399 (96%)	16 (4%)	1 (0%)	49	74
1	C	409/458 (89%)	390 (95%)	17 (4%)	2 (0%)	31	56
1	D	409/458 (89%)	387 (95%)	21 (5%)	1 (0%)	49	74
1	E	411/458 (90%)	392 (95%)	18 (4%)	1 (0%)	49	74
1	F	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	24	46
1	G	408/458 (89%)	389 (95%)	17 (4%)	2 (0%)	31	56
1	H	409/458 (89%)	390 (95%)	18 (4%)	1 (0%)	49	74
1	I	409/458 (89%)	388 (95%)	20 (5%)	1 (0%)	49	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	407/458 (89%)	387 (95%)	17 (4%)	3 (1%)	24	46
1	K	413/458 (90%)	391 (95%)	20 (5%)	2 (0%)	31	56
1	L	416/458 (91%)	396 (95%)	17 (4%)	3 (1%)	24	46
1	M	408/458 (89%)	388 (95%)	19 (5%)	1 (0%)	49	74
1	N	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	24	46
1	O	408/458 (89%)	386 (95%)	19 (5%)	3 (1%)	24	46
1	P	413/458 (90%)	388 (94%)	21 (5%)	4 (1%)	17	35
1	Q	413/458 (90%)	394 (95%)	17 (4%)	2 (0%)	31	56
1	R	407/458 (89%)	391 (96%)	15 (4%)	1 (0%)	49	74
1	S	410/458 (90%)	389 (95%)	19 (5%)	2 (0%)	31	56
1	T	416/458 (91%)	392 (94%)	23 (6%)	1 (0%)	49	74
All	All	8218/9160 (90%)	7810 (95%)	368 (4%)	40 (0%)	31	56

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	115	GLY
1	Q	115	GLY
1	A	220	TYR
1	G	321	ALA
1	J	220	TYR
1	L	427	MET
1	N	115	GLY
1	N	220	TYR
1	O	220	TYR
1	P	318	GLY
1	S	115	GLY
1	E	172	SER
1	F	220	TYR
1	G	172	SER
1	I	172	SER
1	J	172	SER
1	L	172	SER
1	Q	172	SER
1	S	172	SER
1	T	172	SER
1	A	172	SER
1	A	317	SER

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Mol	Chain	Res	Type
1	B	172	SER
1	C	172	SER
1	D	172	SER
1	F	172	SER
1	F	317	SER
1	K	172	SER
1	L	220	TYR
1	M	172	SER
1	N	172	SER
1	P	172	SER
1	R	172	SER
1	C	317	SER
1	H	172	SER
1	J	121	ASN
1	K	317	SER
1	O	172	SER
1	P	220	TYR
1	O	317	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/385 (91%)	336 (96%)	16 (4%)	30	56
1	B	351/385 (91%)	330 (94%)	21 (6%)	21	42
1	C	349/385 (91%)	332 (95%)	17 (5%)	27	52
1	D	349/385 (91%)	334 (96%)	15 (4%)	32	58
1	E	350/385 (91%)	332 (95%)	18 (5%)	26	50
1	F	348/385 (90%)	330 (95%)	18 (5%)	25	49
1	G	348/385 (90%)	328 (94%)	20 (6%)	23	45
1	H	349/385 (91%)	332 (95%)	17 (5%)	27	52
1	I	349/385 (91%)	336 (96%)	13 (4%)	37	64
1	J	347/385 (90%)	327 (94%)	20 (6%)	22	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	350/385 (91%)	324 (93%)	26 (7%)	15	30
1	L	351/385 (91%)	326 (93%)	25 (7%)	16	32
1	M	348/385 (90%)	328 (94%)	20 (6%)	23	45
1	N	347/385 (90%)	327 (94%)	20 (6%)	22	44
1	O	348/385 (90%)	335 (96%)	13 (4%)	37	64
1	P	350/385 (91%)	324 (93%)	26 (7%)	15	30
1	Q	350/385 (91%)	331 (95%)	19 (5%)	24	47
1	R	347/385 (90%)	328 (94%)	19 (6%)	24	47
1	S	348/385 (90%)	334 (96%)	14 (4%)	34	61
1	T	351/385 (91%)	329 (94%)	22 (6%)	20	40
All	All	6982/7700 (91%)	6603 (95%)	379 (5%)	24	47

All (379) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	A	77	ASN
1	A	105	SER
1	A	121	ASN
1	A	187	ILE
1	A	201	ASP
1	A	218	SER
1	A	219	GLN
1	A	286	ILE
1	A	291	PRO
1	A	315	SER
1	A	323	ASP
1	A	330	SER
1	A	383	LEU
1	A	386	GLU
1	A	425	TYR
1	B	25	PRO
1	B	29	PRO
1	B	33	LEU
1	B	51	ASP
1	B	76	SER
1	B	99	CYS
1	B	118	TYR

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Mol	Chain	Res	Type
1	B	159	LEU
1	B	193	MET
1	B	201	ASP
1	B	213	ASP
1	B	219	GLN
1	B	221	GLN
1	B	258	ASP
1	B	261	ILE
1	B	279	ASP
1	B	284	THR
1	B	292	PHE
1	B	333	LEU
1	B	383	LEU
1	B	426	PHE
1	C	54	SER
1	C	99	CYS
1	C	112	THR
1	C	121	ASN
1	C	160	VAL
1	C	164	VAL
1	C	191	PRO
1	C	193	MET
1	C	201	ASP
1	C	222	SER
1	C	240	LEU
1	C	279	ASP
1	C	328	SER
1	C	351	LEU
1	C	356	ARG
1	C	407	ARG
1	C	421	ASP
1	D	90	GLN
1	D	113	LEU
1	D	121	ASN
1	D	164	VAL
1	D	199	SER
1	D	201	ASP
1	D	213	ASP
1	D	240	LEU
1	D	269	THR
1	D	284	THR
1	D	323	ASP

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Mol	Chain	Res	Type
1	D	349	VAL
1	D	383	LEU
1	D	425	TYR
1	D	426	PHE
1	E	76	SER
1	E	99	CYS
1	E	100	ARG
1	E	112	THR
1	E	162	GLU
1	E	170	PRO
1	E	199	SER
1	E	201	ASP
1	E	279	ASP
1	E	309	LYS
1	E	311	GLU
1	E	324	GLN
1	E	328	SER
1	E	356	ARG
1	E	389	ARG
1	E	415	PRO
1	E	417	ARG
1	E	425	TYR
1	F	29	PRO
1	F	54	SER
1	F	99	CYS
1	F	109	ARG
1	F	112	THR
1	F	120	LEU
1	F	121	ASN
1	F	160	VAL
1	F	201	ASP
1	F	222	SER
1	F	225	VAL
1	F	240	LEU
1	F	284	THR
1	F	324	GLN
1	F	383	LEU
1	F	403	SER
1	F	406	GLU
1	F	418	GLU
1	G	12	VAL
1	G	16	ARG

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Mol	Chain	Res	Type
1	G	29	PRO
1	G	51	ASP
1	G	99	CYS
1	G	121	ASN
1	G	164	VAL
1	G	201	ASP
1	G	215	GLN
1	G	219	GLN
1	G	251	SER
1	G	261	ILE
1	G	276	VAL
1	G	305	ILE
1	G	325	MET
1	G	356	ARG
1	G	383	LEU
1	G	389	ARG
1	G	406	GLU
1	G	425	TYR
1	H	51	ASP
1	H	112	THR
1	H	121	ASN
1	H	132	SER
1	H	146	SER
1	H	164	VAL
1	H	171	THR
1	H	201	ASP
1	H	219	GLN
1	H	240	LEU
1	H	274	ARG
1	H	284	THR
1	H	299	ASN
1	H	328	SER
1	H	403	SER
1	H	407	ARG
1	H	417	ARG
1	I	25	PRO
1	I	99	CYS
1	I	106	LEU
1	I	112	THR
1	I	201	ASP
1	I	240	LEU
1	I	273	THR

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Mol	Chain	Res	Type
1	I	284	THR
1	I	383	LEU
1	I	386	GLU
1	I	389	ARG
1	I	391	ASP
1	I	417	ARG
1	J	25	PRO
1	J	44	THR
1	J	76	SER
1	J	99	CYS
1	J	105	SER
1	J	120	LEU
1	J	121	ASN
1	J	160	VAL
1	J	164	VAL
1	J	201	ASP
1	J	219	GLN
1	J	240	LEU
1	J	284	THR
1	J	286	ILE
1	J	323	ASP
1	J	328	SER
1	J	407	ARG
1	J	417	ARG
1	J	425	TYR
1	J	426	PHE
1	K	12	VAL
1	K	51	ASP
1	K	54	SER
1	K	99	CYS
1	K	106	LEU
1	K	168	SER
1	K	201	ASP
1	K	202	ARG
1	K	213	ASP
1	K	251	SER
1	K	272	ILE
1	K	291	PRO
1	K	293	ASN
1	K	320	GLN
1	K	324	GLN
1	K	325	MET

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Mol	Chain	Res	Type
1	K	351	LEU
1	K	379	LEU
1	K	381	LYS
1	K	383	LEU
1	K	386	GLU
1	K	389	ARG
1	K	402	LEU
1	K	403	SER
1	K	424	GLU
1	K	428	GLU
1	L	51	ASP
1	L	54	SER
1	L	76	SER
1	L	112	THR
1	L	117	VAL
1	L	120	LEU
1	L	121	ASN
1	L	159	LEU
1	L	162	GLU
1	L	193	MET
1	L	201	ASP
1	L	202	ARG
1	L	218	SER
1	L	269	THR
1	L	286	ILE
1	L	317	SER
1	L	323	ASP
1	L	326	SER
1	L	351	LEU
1	L	356	ARG
1	L	383	LEU
1	L	384	VAL
1	L	389	ARG
1	L	417	ARG
1	L	425	TYR
1	M	51	ASP
1	M	75	GLN
1	M	90	GLN
1	M	99	CYS
1	M	106	LEU
1	M	121	ASN
1	M	160	VAL

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Mol	Chain	Res	Type
1	M	201	ASP
1	M	219	GLN
1	M	240	LEU
1	M	273	THR
1	M	274	ARG
1	M	276	VAL
1	M	328	SER
1	M	330	SER
1	M	333	LEU
1	M	379	LEU
1	M	383	LEU
1	M	389	ARG
1	M	417	ARG
1	N	11	ILE
1	N	29	PRO
1	N	76	SER
1	N	99	CYS
1	N	112	THR
1	N	121	ASN
1	N	160	VAL
1	N	164	VAL
1	N	201	ASP
1	N	219	GLN
1	N	251	SER
1	N	261	ILE
1	N	272	ILE
1	N	280	ASN
1	N	283	THR
1	N	315	SER
1	N	324	GLN
1	N	403	SER
1	N	411	LYS
1	N	424	GLU
1	O	29	PRO
1	O	68	VAL
1	O	109	ARG
1	O	110	SER
1	O	121	ASN
1	O	132	SER
1	O	160	VAL
1	O	164	VAL
1	O	193	MET

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Mol	Chain	Res	Type
1	O	201	ASP
1	O	320	GLN
1	O	349	VAL
1	O	389	ARG
1	P	25	PRO
1	P	99	CYS
1	P	100	ARG
1	P	109	ARG
1	P	112	THR
1	P	121	ASN
1	P	136	LEU
1	P	146	SER
1	P	159	LEU
1	P	164	VAL
1	P	201	ASP
1	P	217	SER
1	P	219	GLN
1	P	241	SER
1	P	274	ARG
1	P	276	VAL
1	P	280	ASN
1	P	292	PHE
1	P	315	SER
1	P	328	SER
1	P	333	LEU
1	P	383	LEU
1	P	386	GLU
1	P	403	SER
1	P	406	GLU
1	P	425	TYR
1	Q	51	ASP
1	Q	54	SER
1	Q	99	CYS
1	Q	112	THR
1	Q	113	LEU
1	Q	121	ASN
1	Q	160	VAL
1	Q	201	ASP
1	Q	219	GLN
1	Q	284	THR
1	Q	286	ILE
1	Q	324	GLN

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Mol	Chain	Res	Type
1	Q	379	LEU
1	Q	383	LEU
1	Q	386	GLU
1	Q	403	SER
1	Q	407	ARG
1	Q	413	VAL
1	Q	414	TRP
1	R	25	PRO
1	R	75	GLN
1	R	90	GLN
1	R	99	CYS
1	R	112	THR
1	R	121	ASN
1	R	193	MET
1	R	201	ASP
1	R	213	ASP
1	R	284	THR
1	R	294	LEU
1	R	315	SER
1	R	320	GLN
1	R	328	SER
1	R	379	LEU
1	R	383	LEU
1	R	384	VAL
1	R	401	ILE
1	R	405	ARG
1	S	25	PRO
1	S	29	PRO
1	S	77	ASN
1	S	112	THR
1	S	120	LEU
1	S	160	VAL
1	S	193	MET
1	S	201	ASP
1	S	272	ILE
1	S	278	SER
1	S	286	ILE
1	S	315	SER
1	S	324	GLN
1	S	383	LEU
1	T	16	ARG
1	T	33	LEU

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Mol	Chain	Res	Type
1	T	113	LEU
1	T	120	LEU
1	T	121	ASN
1	T	132	SER
1	T	160	VAL
1	T	164	VAL
1	T	171	THR
1	T	193	MET
1	T	199	SER
1	T	201	ASP
1	T	240	LEU
1	T	284	THR
1	T	297	PRO
1	T	328	SER
1	T	383	LEU
1	T	389	ARG
1	T	403	SER
1	T	404	GLU
1	T	407	ARG
1	T	417	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	79	ASN
1	A	90	GLN
1	A	121	ASN
1	A	130	GLN
1	A	215	GLN
1	A	219	GLN
1	A	233	ASN
1	B	90	GLN
1	B	219	GLN
1	C	90	GLN
1	C	130	GLN
1	C	219	GLN
1	C	233	ASN
1	D	90	GLN
1	D	121	ASN
1	D	219	GLN
1	D	324	GLN

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Mol	Chain	Res	Type
1	E	90	GLN
1	E	121	ASN
1	E	130	GLN
1	E	233	ASN
1	E	288	ASN
1	E	293	ASN
1	F	90	GLN
1	F	249	HIS
1	F	382	ASN
1	G	130	GLN
1	G	221	GLN
1	G	233	ASN
1	G	293	ASN
1	G	320	GLN
1	G	396	ASN
1	H	90	GLN
1	H	130	GLN
1	H	233	ASN
1	H	293	ASN
1	H	299	ASN
1	H	320	GLN
1	H	324	GLN
1	I	79	ASN
1	I	90	GLN
1	I	121	ASN
1	I	130	GLN
1	I	215	GLN
1	I	219	GLN
1	I	221	GLN
1	I	233	ASN
1	I	324	GLN
1	J	75	GLN
1	J	79	ASN
1	J	130	GLN
1	J	233	ASN
1	K	79	ASN
1	K	90	GLN
1	K	121	ASN
1	K	130	GLN
1	K	233	ASN
1	K	320	GLN
1	L	79	ASN

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Mol	Chain	Res	Type
1	L	90	GLN
1	L	121	ASN
1	L	130	GLN
1	L	233	ASN
1	L	253	HIS
1	L	293	ASN
1	M	90	GLN
1	M	121	ASN
1	M	130	GLN
1	M	324	GLN
1	N	79	ASN
1	N	84	GLN
1	N	90	GLN
1	N	130	GLN
1	N	221	GLN
1	N	233	ASN
1	N	280	ASN
1	O	90	GLN
1	O	130	GLN
1	O	142	ASN
1	O	219	GLN
1	O	233	ASN
1	O	320	GLN
1	P	121	ASN
1	P	219	GLN
1	P	280	ASN
1	Q	90	GLN
1	Q	130	GLN
1	Q	219	GLN
1	Q	324	GLN
1	R	79	ASN
1	R	121	ASN
1	R	130	GLN
1	R	219	GLN
1	R	253	HIS
1	R	320	GLN
1	R	324	GLN
1	R	396	ASN
1	S	77	ASN
1	S	90	GLN
1	S	97	ASN
1	S	121	ASN

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Mol	Chain	Res	Type
1	S	130	GLN
1	S	233	ASN
1	S	293	ASN
1	S	320	GLN
1	S	324	GLN
1	T	121	ASN
1	T	130	GLN
1	T	219	GLN
1	T	233	ASN
1	T	293	ASN
1	T	324	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 ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	420/458 (91%)	-0.49	10 (2%) 59 52	23, 33, 72, 105	0
1	B	418/458 (91%)	-0.62	7 (1%) 70 65	20, 32, 67, 106	0
1	C	413/458 (90%)	-0.48	12 (2%) 51 44	26, 37, 72, 105	0
1	D	413/458 (90%)	-0.44	15 (3%) 42 35	23, 34, 63, 106	0
1	E	415/458 (90%)	-0.35	14 (3%) 45 37	27, 36, 74, 114	0
1	F	413/458 (90%)	-0.53	7 (1%) 70 65	22, 35, 66, 98	0
1	G	412/458 (89%)	-0.58	5 (1%) 79 75	25, 37, 61, 106	0
1	H	413/458 (90%)	-0.43	13 (3%) 49 41	27, 39, 67, 114	0
1	I	413/458 (90%)	-0.37	18 (4%) 34 26	28, 38, 71, 107	0
1	J	411/458 (89%)	-0.43	8 (1%) 66 61	27, 38, 70, 99	0
1	K	417/458 (91%)	-0.42	10 (2%) 59 52	27, 38, 74, 108	0
1	L	418/458 (91%)	-0.35	13 (3%) 49 41	24, 34, 73, 103	0
1	M	412/458 (89%)	-0.34	17 (4%) 37 29	25, 38, 68, 105	0
1	N	413/458 (90%)	-0.48	6 (1%) 73 69	27, 38, 68, 104	0
1	O	412/458 (89%)	-0.53	8 (1%) 66 61	27, 37, 72, 104	0
1	P	417/458 (91%)	-0.54	10 (2%) 59 52	27, 39, 82, 112	0
1	Q	417/458 (91%)	-0.34	21 (5%) 29 22	27, 39, 77, 118	0
1	R	411/458 (89%)	-0.60	2 (0%) 90 89	26, 36, 56, 102	0
1	S	414/458 (90%)	-0.39	15 (3%) 42 35	25, 35, 65, 95	0
1	T	418/458 (91%)	-0.70	2 (0%) 90 89	23, 33, 62, 101	0
All	All	8290/9160 (90%)	-0.47	213 (2%) 56 49	20, 37, 70, 118	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	113	LEU	5.1
1	P	223	GLY	4.9
1	H	425	TYR	4.9
1	N	113	LEU	4.9
1	C	321	ALA	4.7
1	O	114	PRO	4.6
1	B	425	TYR	4.5
1	B	428	GLU	4.5
1	I	114	PRO	4.4
1	E	425	TYR	4.3
1	C	11	ILE	4.1
1	N	425	TYR	4.1
1	P	425	TYR	4.0
1	A	428	GLU	4.0
1	I	425	TYR	3.9
1	R	113	LEU	3.8
1	K	115	GLY	3.8
1	R	425	TYR	3.8
1	Q	428	GLU	3.8
1	M	113	LEU	3.7
1	I	11	ILE	3.7
1	A	429	VAL	3.7
1	P	11	ILE	3.7
1	F	113	LEU	3.7
1	D	428	GLU	3.7
1	I	324	GLN	3.6
1	T	11	ILE	3.6
1	F	114	PRO	3.5
1	D	425	TYR	3.5
1	L	324	GLN	3.5
1	I	322	GLY	3.5
1	C	324	GLN	3.4
1	M	114	PRO	3.4
1	Q	11	ILE	3.4
1	O	426	PHE	3.4
1	B	119	ALA	3.4
1	P	428	GLU	3.4
1	Q	427	MET	3.3
1	N	11	ILE	3.3
1	E	429	VAL	3.3
1	O	425	TYR	3.3
1	Q	114	PRO	3.3
1	C	428	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	425	TYR	3.2
1	H	428	GLU	3.2
1	A	430	ALA	3.2
1	E	114	PRO	3.2
1	P	12	VAL	3.2
1	J	425	TYR	3.2
1	C	425	TYR	3.2
1	C	189	LEU	3.2
1	Q	425	TYR	3.2
1	Q	120	LEU	3.2
1	M	219	GLN	3.2
1	S	220	TYR	3.1
1	E	11	ILE	3.1
1	M	322	GLY	3.1
1	E	113	LEU	3.1
1	G	113	LEU	3.1
1	H	317	SER	3.1
1	D	12	VAL	3.0
1	H	321	ALA	3.0
1	A	425	TYR	3.0
1	T	425	TYR	3.0
1	M	324	GLN	3.0
1	I	321	ALA	3.0
1	M	321	ALA	3.0
1	M	220	TYR	3.0
1	S	425	TYR	3.0
1	B	115	GLY	3.0
1	N	114	PRO	2.9
1	D	11	ILE	2.9
1	M	222	SER	2.9
1	J	219	GLN	2.9
1	K	425	TYR	2.9
1	H	320	GLN	2.9
1	L	323	ASP	2.9
1	S	115	GLY	2.9
1	E	428	GLU	2.9
1	I	113	LEU	2.8
1	E	219	GLN	2.8
1	K	321	ALA	2.8
1	S	321	ALA	2.8
1	G	12	VAL	2.8
1	H	318	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	Q	121	ASN	2.8
1	B	429	VAL	2.8
1	S	320	GLN	2.8
1	Q	426	PHE	2.7
1	Q	429	VAL	2.7
1	S	322	GLY	2.7
1	J	12	VAL	2.7
1	Q	12	VAL	2.7
1	P	113	LEU	2.7
1	G	428	GLU	2.7
1	D	318	GLY	2.7
1	S	323	ASP	2.7
1	I	219	GLN	2.7
1	L	252	VAL	2.6
1	F	115	GLY	2.6
1	I	220	TYR	2.6
1	F	321	ALA	2.6
1	S	219	GLN	2.6
1	P	114	PRO	2.6
1	I	222	SER	2.6
1	H	219	GLN	2.6
1	H	251	SER	2.6
1	B	117	VAL	2.5
1	P	429	VAL	2.5
1	C	322	GLY	2.5
1	M	320	GLN	2.5
1	K	113	LEU	2.5
1	J	321	ALA	2.5
1	M	425	TYR	2.5
1	Q	221	GLN	2.5
1	P	427	MET	2.5
1	M	323	ASP	2.5
1	O	324	GLN	2.5
1	M	218	SER	2.5
1	J	319	GLY	2.5
1	N	318	GLY	2.5
1	D	220	TYR	2.5
1	O	318	GLY	2.4
1	E	222	SER	2.4
1	S	325	MET	2.4
1	A	113	LEU	2.4
1	D	317	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	318	GLY	2.4
1	C	427	MET	2.4
1	C	113	LEU	2.4
1	G	425	TYR	2.4
1	A	318	GLY	2.4
1	S	12	VAL	2.4
1	L	425	TYR	2.4
1	D	320	GLN	2.4
1	M	317	SER	2.4
1	S	116	GLY	2.4
1	H	256	ALA	2.3
1	K	116	GLY	2.3
1	Q	115	GLY	2.3
1	I	12	VAL	2.3
1	I	252	VAL	2.3
1	M	12	VAL	2.3
1	D	112	THR	2.3
1	O	113	LEU	2.3
1	E	215	GLN	2.3
1	O	215	GLN	2.3
1	K	428	GLU	2.3
1	K	222	SER	2.3
1	Q	217	SER	2.3
1	C	225	VAL	2.3
1	E	430	ALA	2.3
1	P	397	TYR	2.3
1	I	323	ASP	2.3
1	A	115	GLY	2.3
1	A	251	SER	2.3
1	J	322	GLY	2.3
1	M	319	GLY	2.3
1	H	319	GLY	2.2
1	I	221	GLN	2.2
1	N	219	GLN	2.2
1	Q	321	ALA	2.2
1	I	397	TYR	2.2
1	F	11	ILE	2.2
1	L	251	SER	2.2
1	E	220	TYR	2.2
1	E	213	ASP	2.2
1	C	223	GLY	2.2
1	E	225	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	324	GLN	2.2
1	D	321	ALA	2.2
1	L	11	ILE	2.2
1	I	218	SER	2.2
1	D	223	GLY	2.2
1	A	11	ILE	2.2
1	D	76	SER	2.2
1	Q	324	GLN	2.2
1	L	116	GLY	2.2
1	Q	256	ALA	2.2
1	L	253	HIS	2.2
1	L	118	TYR	2.1
1	J	428	GLU	2.1
1	Q	222	SER	2.1
1	D	251	SER	2.1
1	Q	320	GLN	2.1
1	K	430	ALA	2.1
1	H	284	THR	2.1
1	I	318	GLY	2.1
1	M	223	GLY	2.1
1	O	76	SER	2.1
1	M	428	GLU	2.1
1	A	220	TYR	2.1
1	K	219	GLN	2.1
1	F	426	PHE	2.1
1	D	322	GLY	2.1
1	Q	223	GLY	2.1
1	L	219	GLN	2.1
1	D	218	SER	2.1
1	L	250	THR	2.1
1	C	215	GLN	2.0
1	S	256	ALA	2.0
1	H	218	SER	2.0
1	S	316	LYS	2.0
1	I	320	GLN	2.0
1	B	291	PRO	2.0
1	K	429	VAL	2.0
1	J	220	TYR	2.0
1	E	223	GLY	2.0
1	L	76	SER	2.0
1	S	222	SER	2.0
1	H	221	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	114	PRO	2.0
1	L	225	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	I	5507	1/1	0.97	0.22	33,33,33,33	0
2	CL	G	5505	1/1	0.98	0.19	33,33,33,33	0
2	CL	B	5501	1/1	0.98	0.17	26,26,26,26	1
2	CL	A	5503	1/1	0.98	0.23	32,32,32,32	0
3	CA	P	5902	1/1	0.98	0.03	40,40,40,40	1
3	CA	C	5904	1/1	0.99	0.04	39,39,39,39	0
3	CA	I	5907	1/1	0.99	0.03	41,41,41,41	0
3	CA	R	5908	1/1	0.99	0.03	36,36,36,36	0
3	CA	H	5906	1/1	0.99	0.03	39,39,39,39	0
2	CL	R	5508	1/1	0.99	0.17	27,27,27,27	0
3	CA	G	5905	1/1	0.99	0.03	45,45,45,45	0
3	CA	A	5903	1/1	0.99	0.03	34,34,34,34	0
2	CL	H	5506	1/1	0.99	0.14	31,31,31,31	0
2	CL	C	5504	1/1	0.99	0.21	30,30,30,30	0
2	CL	P	5502	1/1	1.00	0.13	26,26,26,26	1
3	CA	B	5901	1/1	1.00	0.03	33,33,33,33	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.