



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:15 AM EDT

PDB ID : 2DF7 / pdb\_00002df7  
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.

The types of validation reports are described at

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

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

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

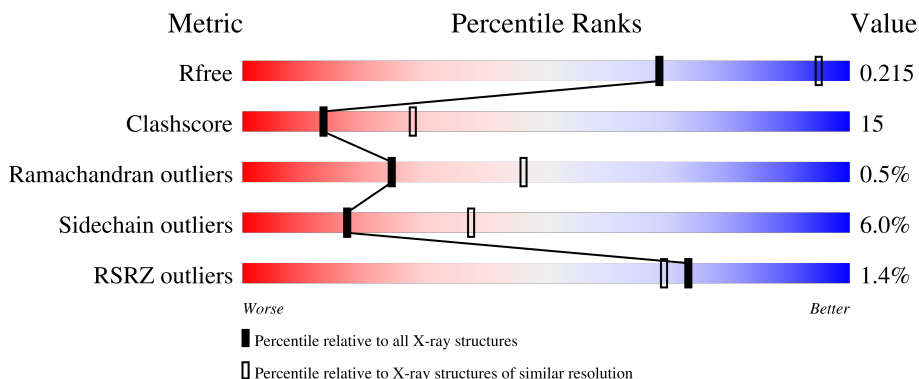
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	458	
1	B	458	
1	C	458	
1	D	458	
1	E	458	

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Mol	Chain	Length	Quality of chain
1	F	458	 64% 20% 5% 10%
1	G	458	 61% 25% 5% 10%
1	H	458	 66% 22% 5% 10%
1	I	458	 67% 21% 5% 10%
1	J	458	 65% 22% 5% 10%
1	K	458	 64% 22% 5% 9%
1	L	458	 63% 23% 5% 9%
1	M	458	 64% 22% 5% 10%
1	N	458	 62% 25% 5% 10%
1	O	458	 65% 22% 5% 10%
1	P	458	 59% 28% 5% 9%
1	Q	458	 65% 21% 5% 9%
1	R	458	 65% 20% 5% 10%
1	S	458	 64% 23% 5% 10%
1	T	458	 66% 22% 5% 9%

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

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

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	GLU	ASP	engineered mutation	UNP Q6S9I7
A	330	SER	MET	engineered mutation	UNP Q6S9I7
A	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
B	330	SER	MET	engineered mutation	UNP Q6S9I7
B	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
C	330	SER	MET	engineered mutation	UNP Q6S9I7
C	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
D	330	SER	MET	engineered mutation	UNP Q6S9I7
D	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
E	330	SER	MET	engineered mutation	UNP Q6S9I7
E	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
F	330	SER	MET	engineered mutation	UNP Q6S9I7
F	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
G	330	SER	MET	engineered mutation	UNP Q6S9I7
G	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
H	330	SER	MET	engineered mutation	UNP Q6S9I7
H	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	330	SER	MET	engineered mutation	UNP Q6S9I7
I	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
J	330	SER	MET	engineered mutation	UNP Q6S9I7
J	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
K	330	SER	MET	engineered mutation	UNP Q6S9I7
K	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
L	330	SER	MET	engineered mutation	UNP Q6S9I7
L	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
M	330	SER	MET	engineered mutation	UNP Q6S9I7
M	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
N	330	SER	MET	engineered mutation	UNP Q6S9I7
N	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
O	330	SER	MET	engineered mutation	UNP Q6S9I7
O	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
P	330	SER	MET	engineered mutation	UNP Q6S9I7
P	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
Q	330	SER	MET	engineered mutation	UNP Q6S9I7
Q	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
R	330	SER	MET	engineered mutation	UNP Q6S9I7
R	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
S	330	SER	MET	engineered mutation	UNP Q6S9I7
S	331	GLY	TRP	engineered mutation	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 mutation	UNP Q6S9I7
T	330	SER	MET	engineered mutation	UNP Q6S9I7
T	331	GLY	TRP	engineered mutation	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 (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

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

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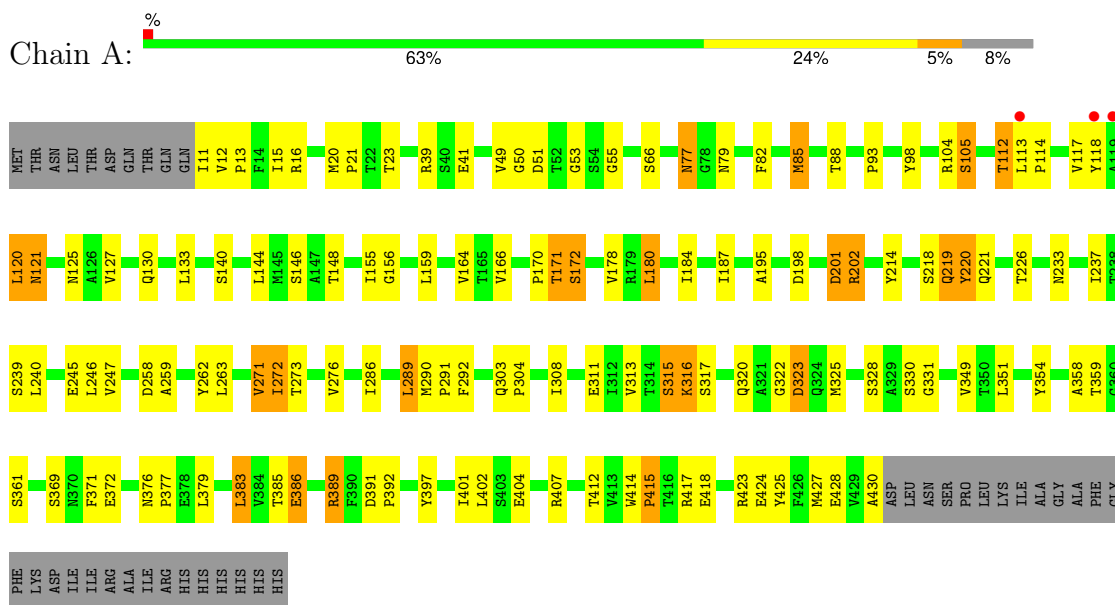
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	L	234	Total 234	O 234	0	0
4	M	235	Total 235	O 235	0	0
4	N	195	Total 195	O 195	0	0
4	O	216	Total 216	O 216	0	0
4	P	183	Total 183	O 183	0	0
4	Q	201	Total 201	O 201	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

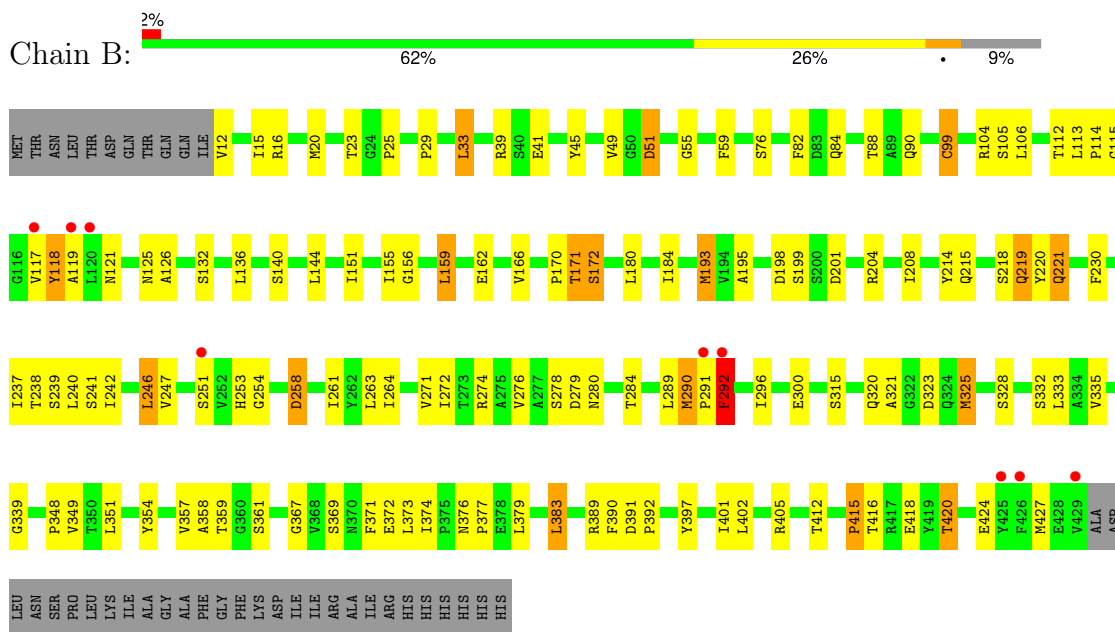
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

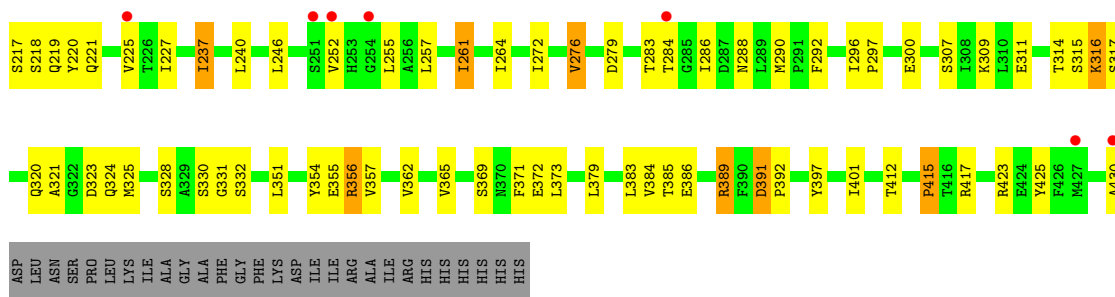
#### • Molecule 1: structural polyprotein VP2



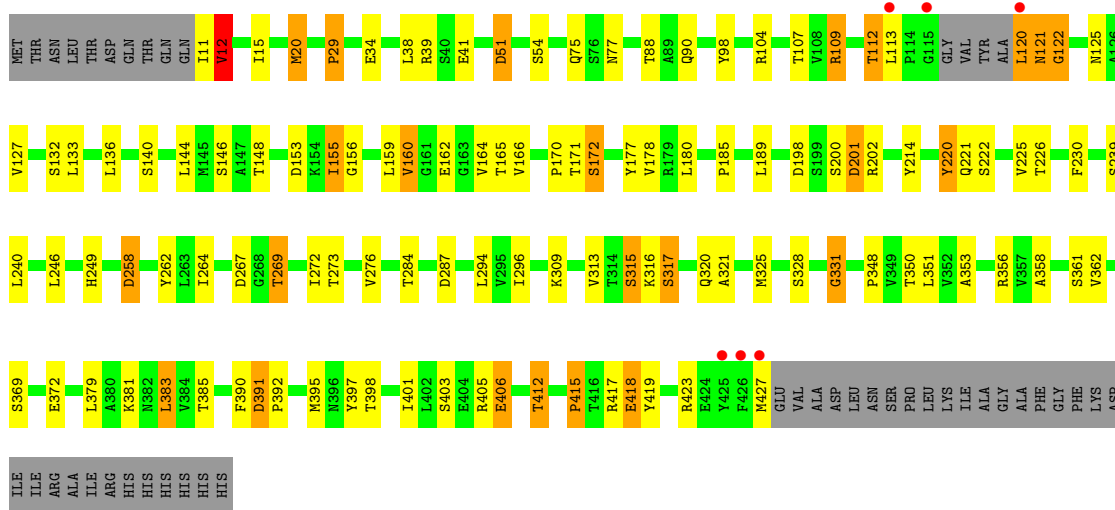
#### • Molecule 1: structural polyprotein VP2



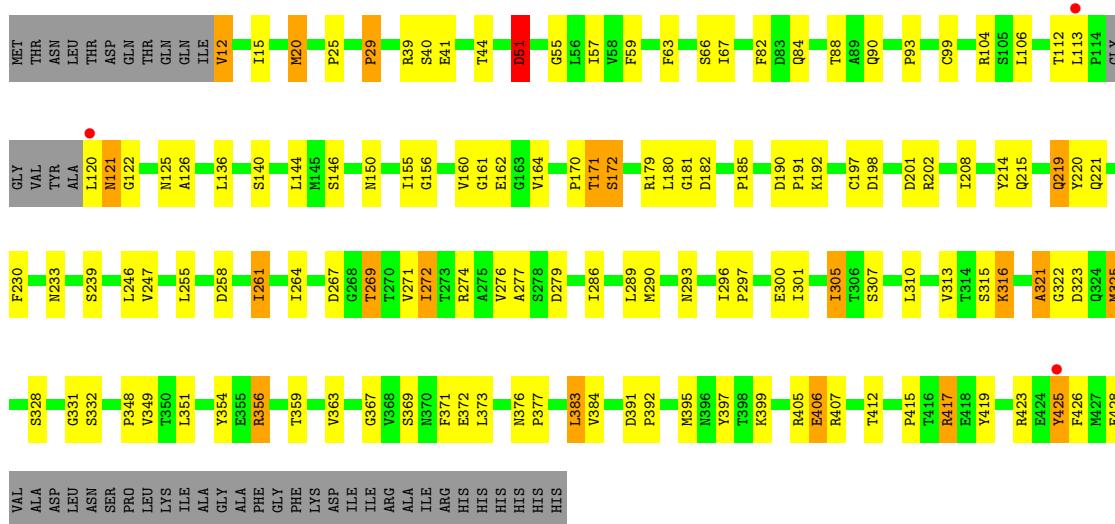




• Molecule 1: structural polypeptide VP2



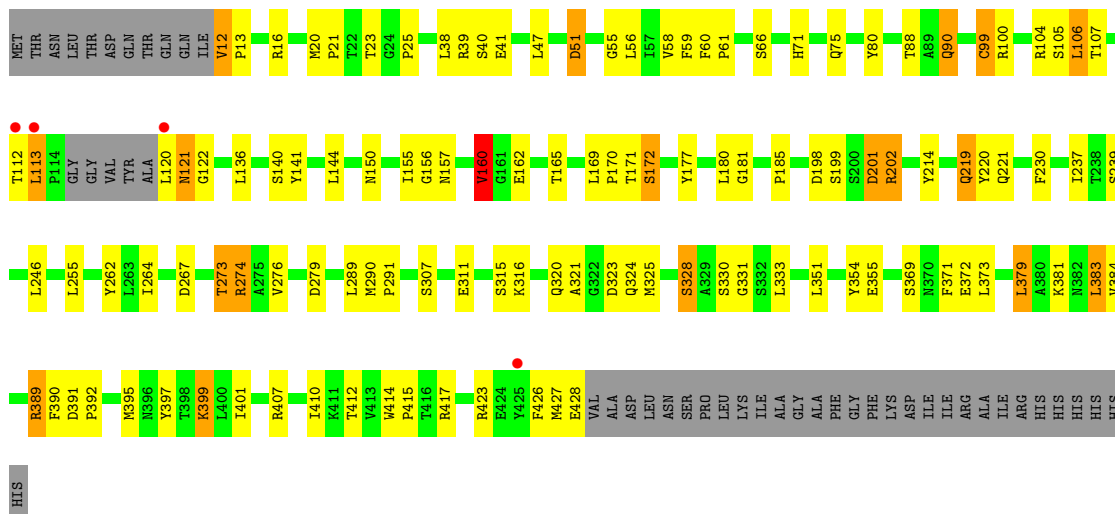
• Molecule 1: structural polypeptide VP2



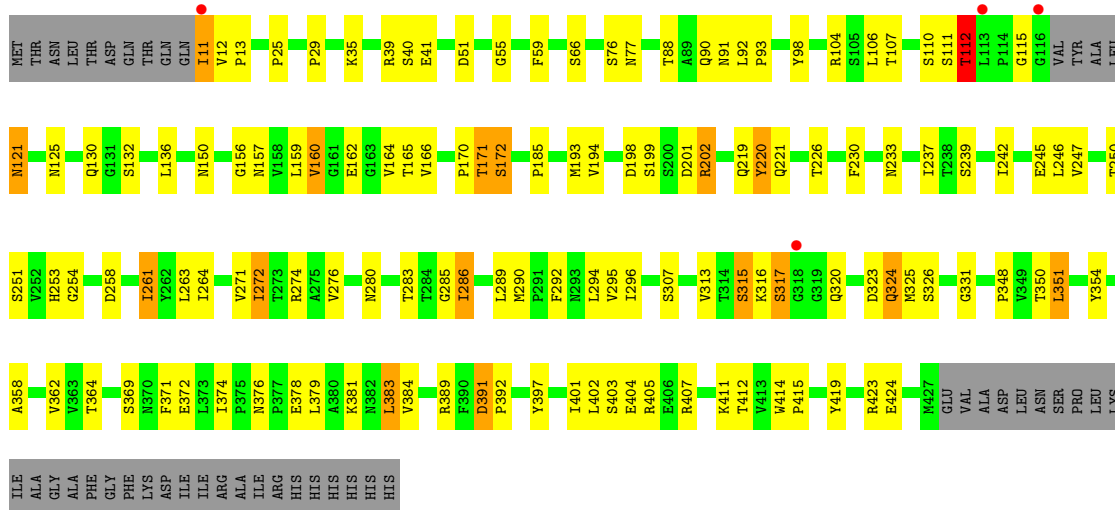
• Molecule 1: structural polypeptide VP2



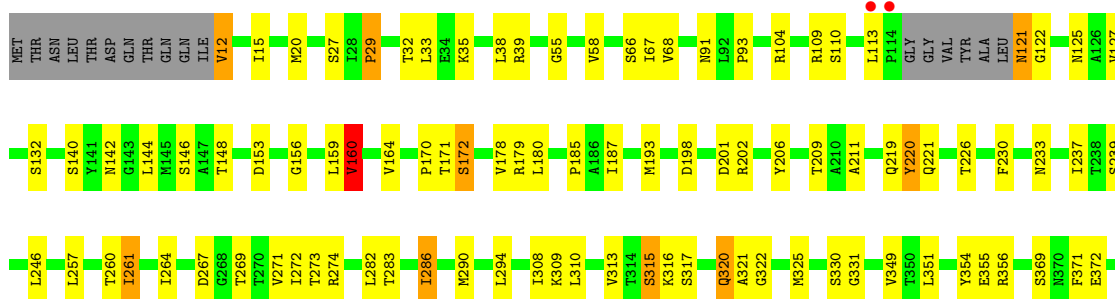




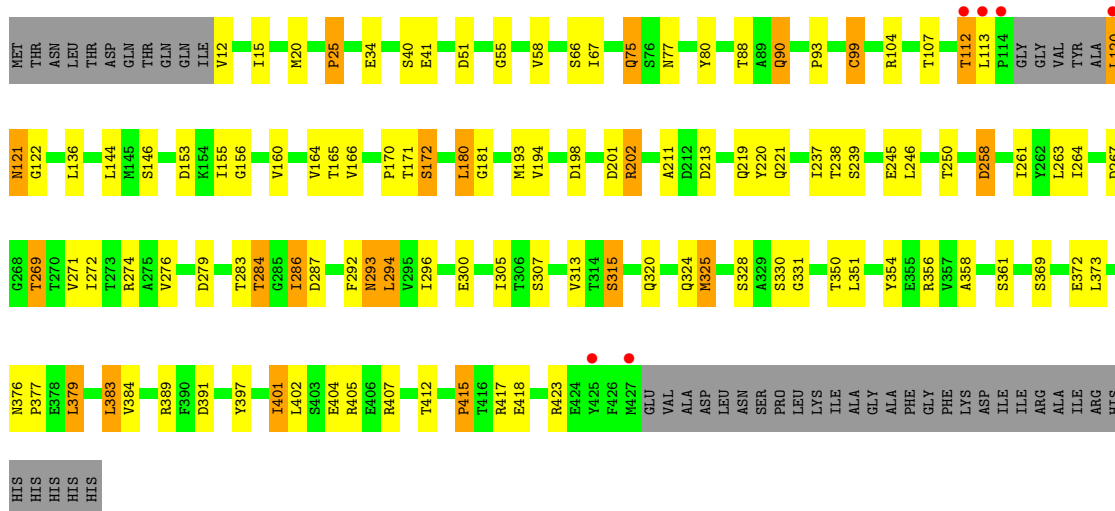
- Molecule 1: structural polypeptide VP2



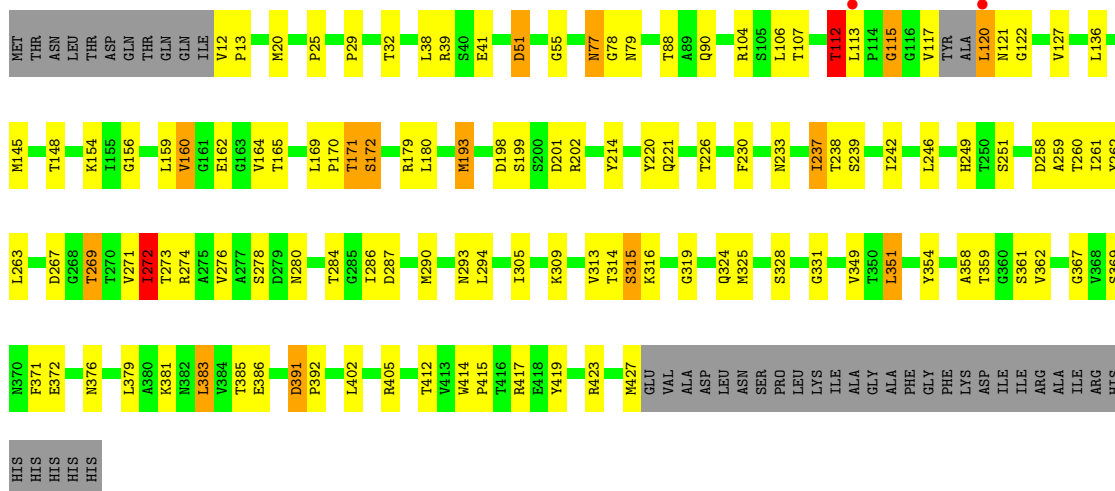
- Molecule 1: structural polypeptide VP2



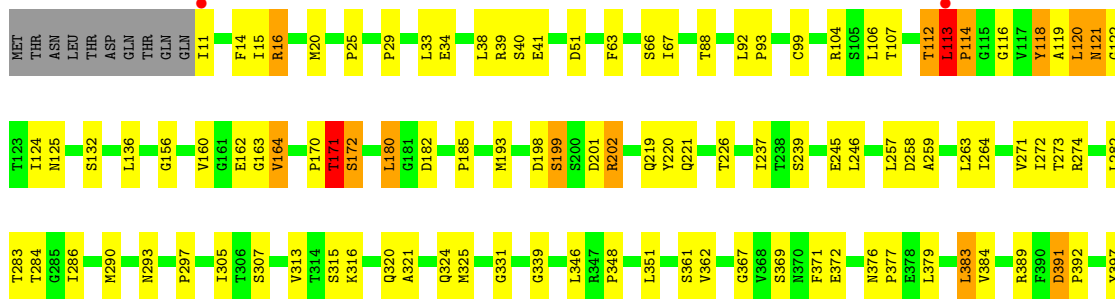


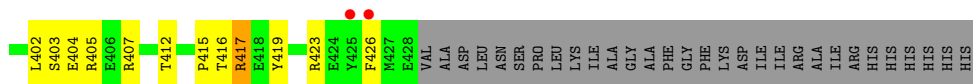


• Molecule 1: structural polyprotein VP2



• Molecule 1: structural polyprotein VP2





## 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 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.6 (40.00-2.60) 89.6 (40.00-2.60)	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)	Xtrriage
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	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.008 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	66956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage'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 i

### 5.1 Standard geometry i

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	0.95	2/3226 (0.1%)	1.19	23/4407 (0.5%)
1	B	1.01	4/3213 (0.1%)	1.24	21/4389 (0.5%)
1	C	0.90	1/3180 (0.0%)	1.17	17/4342 (0.4%)
1	D	0.94	1/3179 (0.0%)	1.20	20/4340 (0.5%)
1	E	0.94	1/3192 (0.0%)	1.20	22/4359 (0.5%)
1	F	0.93	3/3175 (0.1%)	1.18	20/4335 (0.5%)
1	G	0.94	1/3172 (0.0%)	1.18	15/4331 (0.3%)
1	H	0.89	2/3179 (0.1%)	1.17	22/4341 (0.5%)
1	I	0.88	2/3180 (0.1%)	1.13	15/4342 (0.3%)
1	J	0.87	0/3163	1.15	16/4318 (0.4%)
1	K	0.87	1/3199 (0.0%)	1.18	20/4368 (0.5%)
1	L	0.92	0/3214	1.18	23/4390 (0.5%)
1	M	0.90	1/3172 (0.0%)	1.18	22/4331 (0.5%)
1	N	0.90	1/3171 (0.0%)	1.18	19/4329 (0.4%)
1	O	0.89	2/3171 (0.1%)	1.18	20/4330 (0.5%)
1	P	0.94	3/3200 (0.1%)	1.24	24/4369 (0.5%)
1	Q	0.88	3/3200 (0.1%)	1.16	19/4369 (0.4%)
1	R	0.97	1/3163 (0.0%)	1.19	15/4319 (0.3%)
1	S	0.92	1/3178 (0.0%)	1.18	22/4339 (0.5%)
1	T	0.97	0/3214	1.23	29/4390 (0.7%)
All	All	0.92	30/63741 (0.0%)	1.19	404/87038 (0.5%)

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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	325	MET	SD-CE	-10.06	1.54	1.79
1	P	20	MET	SD-CE	8.34	2.00	1.79
1	A	85	MET	SD-CE	-7.72	1.60	1.79
1	B	325	MET	SD-CE	-6.83	1.62	1.79
1	H	325	MET	SD-CE	-6.78	1.62	1.79
1	B	374	ILE	CA-CB	-6.77	1.48	1.54
1	Q	401	ILE	CA-CB	6.23	1.60	1.54
1	C	20	MET	SD-CE	6.05	1.94	1.79
1	B	292	PHE	CB-CG	-6.02	1.36	1.50
1	I	12	VAL	CA-CB	5.94	1.59	1.53
1	I	113	LEU	CA-C	5.82	1.57	1.52
1	G	20	MET	SD-CE	5.76	1.94	1.79
1	Q	139	VAL	CA-CB	5.75	1.60	1.54
1	N	415	PRO	CA-C	5.70	1.58	1.52
1	Q	410	ILE	CA-CB	5.61	1.60	1.53
1	H	20	MET	SD-CE	5.59	1.93	1.79
1	P	145	MET	SD-CE	-5.55	1.65	1.79
1	K	349	VAL	CA-CB	5.53	1.62	1.54
1	O	32	THR	CA-CB	5.53	1.59	1.52
1	F	401	ILE	CA-CB	5.50	1.60	1.54
1	F	12	VAL	CA-CB	5.38	1.61	1.54
1	S	272	ILE	CA-CB	5.34	1.62	1.54
1	O	209	THR	CA-CB	5.33	1.59	1.53
1	F	20	MET	SD-CE	5.29	1.92	1.79
1	P	325	MET	SD-CE	-5.18	1.66	1.79
1	B	349	VAL	CA-CB	5.12	1.62	1.54
1	M	113	LEU	CA-C	5.10	1.58	1.53
1	A	358	ALA	CA-CB	-5.05	1.45	1.53
1	E	113	LEU	CA-C	5.03	1.59	1.52
1	D	12	VAL	CA-CB	5.01	1.60	1.54

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	415	PRO	N-CA-C	-12.01	92.33	111.19
1	G	415	PRO	N-CA-C	-11.41	91.94	110.55
1	S	415	PRO	N-CA-C	-11.36	92.03	110.55
1	C	122	GLY	N-CA-C	11.25	126.45	111.72
1	K	415	PRO	N-CA-C	-11.17	92.35	110.55
1	T	415	PRO	N-CA-C	-11.04	92.55	110.55
1	J	415	PRO	N-CA-C	-10.95	92.70	110.55
1	O	415	PRO	N-CA-C	-10.89	92.80	110.55
1	C	415	PRO	N-CA-C	-10.81	92.93	110.55
1	M	415	PRO	N-CA-C	-10.78	92.99	110.55
1	A	415	PRO	N-CA-C	-10.76	93.01	110.55
1	H	415	PRO	N-CA-C	-10.75	93.03	110.55
1	F	415	PRO	N-CA-C	-10.61	93.26	110.55
1	B	415	PRO	N-CA-C	-10.43	93.55	110.55
1	D	415	PRO	N-CA-C	-10.29	93.78	110.55
1	R	415	PRO	N-CA-C	-10.19	93.94	110.55
1	I	415	PRO	N-CA-C	-10.18	93.95	110.55
1	P	415	PRO	N-CA-C	-10.17	93.97	110.55
1	L	415	PRO	N-CA-C	-10.13	94.03	110.55
1	Q	122	GLY	N-CA-C	10.07	123.56	112.29
1	P	122	GLY	N-CA-C	9.93	121.39	111.95
1	E	415	PRO	N-CA-C	-9.78	94.60	110.55
1	N	415	PRO	N-CA-C	-9.63	94.85	110.55
1	K	372	GLU	N-CA-C	-9.23	94.20	109.07
1	G	198	ASP	N-CA-C	9.19	124.67	110.42
1	K	429	VAL	N-CA-C	-9.17	102.69	113.42
1	T	113	LEU	CA-C-N	9.17	130.61	119.98
1	T	113	LEU	C-N-CA	9.17	130.61	119.98
1	J	180	LEU	N-CA-C	9.16	124.29	113.20
1	P	112	THR	N-CA-C	8.96	122.68	109.07
1	K	198	ASP	N-CA-C	8.93	123.73	110.52
1	O	372	GLU	N-CA-C	-8.88	94.78	109.07
1	H	122	GLY	N-CA-C	8.82	123.28	111.72
1	B	290	MET	CA-C-N	8.65	128.98	119.90
1	B	290	MET	C-N-CA	8.65	128.98	119.90
1	I	372	GLU	N-CA-C	-8.51	95.37	109.07
1	E	198	ASP	N-CA-C	8.47	123.55	110.42
1	N	198	ASP	N-CA-C	8.46	123.04	110.52
1	R	198	ASP	N-CA-C	8.41	123.46	110.42
1	T	113	LEU	N-CA-C	8.41	121.82	109.62
1	A	372	GLU	N-CA-C	-8.36	95.61	109.07
1	A	237	ILE	N-CA-C	-8.25	105.19	112.12
1	H	391	ASP	CA-C-N	8.25	130.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	391	ASP	C-N-CA	8.25	130.15	119.84
1	P	372	GLU	N-CA-C	-8.22	95.84	109.24
1	C	198	ASP	N-CA-C	8.21	122.67	110.52
1	T	372	GLU	N-CA-C	-8.14	95.97	109.07
1	Q	198	ASP	N-CA-C	8.07	122.47	110.52
1	N	372	GLU	N-CA-C	-8.01	96.17	109.07
1	L	412	THR	N-CA-C	-7.97	103.70	113.50
1	Q	372	GLU	N-CA-C	-7.96	96.25	109.07
1	S	372	GLU	N-CA-C	-7.96	96.26	109.07
1	C	372	GLU	N-CA-C	-7.94	96.28	109.07
1	H	237	ILE	N-CA-C	-7.94	105.45	112.12
1	L	372	GLU	N-CA-C	-7.93	96.30	109.07
1	T	198	ASP	N-CA-C	7.92	122.24	110.52
1	L	198	ASP	N-CA-C	7.87	122.17	110.52
1	M	198	ASP	N-CA-C	7.86	122.61	110.42
1	O	198	ASP	N-CA-C	7.81	122.53	110.42
1	H	372	GLU	N-CA-C	-7.78	96.56	109.24
1	B	198	ASP	N-CA-C	7.75	121.99	110.52
1	J	372	GLU	N-CA-C	-7.65	96.75	109.07
1	E	372	GLU	N-CA-C	-7.64	96.77	109.07
1	Q	180	LEU	N-CA-C	7.55	122.33	113.20
1	R	372	GLU	N-CA-C	-7.51	96.99	109.24
1	D	198	ASP	N-CA-C	7.51	121.63	110.52
1	M	391	ASP	CA-C-N	7.47	129.18	119.84
1	M	391	ASP	C-N-CA	7.47	129.18	119.84
1	Q	237	ILE	N-CA-C	-7.45	105.86	112.12
1	S	239	SER	N-CA-C	7.44	120.77	110.35
1	E	316	LYS	N-CA-C	-7.35	98.34	110.17
1	F	372	GLU	N-CA-C	-7.33	97.30	109.24
1	P	180	LEU	N-CA-C	7.31	122.22	113.16
1	Q	391	ASP	CA-C-N	7.29	128.95	119.84
1	Q	391	ASP	C-N-CA	7.29	128.95	119.84
1	H	239	SER	N-CA-C	7.27	120.53	110.35
1	T	239	SER	N-CA-C	7.21	120.44	110.35
1	R	180	LEU	N-CA-C	7.19	122.07	113.16
1	P	121	ASN	N-CA-C	7.18	119.48	108.42
1	A	198	ASP	N-CA-C	7.12	121.46	110.42
1	M	239	SER	N-CA-C	7.12	119.49	110.24
1	O	239	SER	N-CA-C	7.12	119.50	110.24
1	K	180	LEU	N-CA-C	7.11	121.97	113.16
1	K	122	GLY	N-CA-C	7.09	120.23	112.29
1	G	372	GLU	N-CA-C	-7.09	97.69	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	239	SER	N-CA-C	7.08	120.22	110.24
1	N	171	THR	N-CA-C	-7.06	99.86	109.54
1	A	171	THR	N-CA-C	-7.06	99.87	109.54
1	P	391	ASP	CA-C-N	7.06	128.66	119.84
1	P	391	ASP	C-N-CA	7.06	128.66	119.84
1	I	198	ASP	N-CA-C	7.04	121.34	110.42
1	O	66	SER	N-CA-C	6.95	121.59	113.18
1	T	180	LEU	N-CA-C	6.95	121.78	113.16
1	D	239	SER	N-CA-C	6.93	119.25	110.24
1	G	412	THR	N-CA-C	-6.93	104.96	113.41
1	S	180	LEU	N-CA-C	6.92	121.75	113.16
1	L	180	LEU	N-CA-C	6.91	121.54	113.18
1	Q	170	PRO	N-CA-C	6.91	122.06	111.15
1	R	170	PRO	N-CA-C	6.87	122.03	111.11
1	F	198	ASP	N-CA-C	6.85	121.04	110.42
1	H	412	THR	N-CA-C	-6.81	105.12	113.50
1	C	170	PRO	N-CA-C	6.80	121.93	111.11
1	D	372	GLU	N-CA-C	-6.77	98.20	109.24
1	S	112	THR	N-CA-C	6.74	119.42	109.24
1	O	391	ASP	CA-C-N	6.74	128.26	119.84
1	O	391	ASP	C-N-CA	6.74	128.26	119.84
1	P	198	ASP	N-CA-C	6.72	120.84	110.42
1	A	239	SER	N-CA-C	6.72	119.71	110.24
1	H	428	GLU	N-CA-C	-6.71	104.11	112.90
1	D	237	ILE	N-CA-C	-6.69	106.50	112.12
1	G	156	GLY	N-CA-C	6.69	122.88	111.04
1	D	170	PRO	N-CA-C	6.69	121.72	111.15
1	M	372	GLU	N-CA-C	-6.69	98.34	109.24
1	K	239	SER	N-CA-C	6.68	119.66	110.24
1	M	160	VAL	CB-CA-C	-6.68	103.29	112.04
1	K	391	ASP	CA-C-N	6.67	128.18	119.84
1	K	391	ASP	C-N-CA	6.67	128.18	119.84
1	S	198	ASP	N-CA-C	6.67	120.76	110.42
1	N	66	SER	N-CA-C	6.67	121.25	113.18
1	F	180	LEU	N-CA-C	6.65	121.24	113.20
1	E	391	ASP	CA-C-N	6.65	128.15	119.84
1	E	391	ASP	C-N-CA	6.65	128.15	119.84
1	I	170	PRO	N-CA-C	6.64	121.50	111.14
1	H	180	LEU	N-CA-C	6.63	121.38	113.16
1	A	170	PRO	N-CA-C	6.63	121.65	111.11
1	T	171	THR	N-CA-C	-6.61	100.48	109.54
1	J	51	ASP	N-CA-C	6.59	120.58	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	GLU	N-CA-C	-6.58	98.52	109.24
1	M	180	LEU	N-CA-C	6.57	121.15	113.20
1	L	391	ASP	CA-C-N	6.55	128.03	119.84
1	L	391	ASP	C-N-CA	6.55	128.03	119.84
1	Q	160	VAL	CB-CA-C	-6.54	102.50	112.05
1	N	51	ASP	N-CA-C	6.52	121.07	113.18
1	S	170	PRO	N-CA-C	6.52	121.46	111.15
1	S	391	ASP	CA-C-N	6.50	127.96	119.84
1	S	391	ASP	C-N-CA	6.50	127.96	119.84
1	I	391	ASP	CA-C-N	6.48	127.94	119.84
1	I	391	ASP	C-N-CA	6.48	127.94	119.84
1	B	51	ASP	N-CA-C	6.47	120.44	112.54
1	T	346	LEU	N-CA-C	-6.47	107.25	114.62
1	P	371	PHE	N-CA-C	6.46	119.53	109.52
1	L	239	SER	N-CA-C	6.44	119.32	110.24
1	T	66	SER	N-CA-C	6.41	120.95	113.20
1	A	412	THR	N-CA-C	-6.39	105.64	113.50
1	F	391	ASP	CA-C-N	6.39	127.83	119.84
1	F	391	ASP	C-N-CA	6.39	127.83	119.84
1	I	239	SER	N-CA-C	6.37	119.27	110.35
1	M	156	GLY	N-CA-C	6.37	122.31	111.04
1	M	170	PRO	N-CA-C	6.37	121.21	111.15
1	A	180	LEU	N-CA-C	6.37	120.90	113.20
1	J	239	SER	N-CA-C	6.35	119.19	110.24
1	B	251	SER	N-CA-C	-6.30	105.91	113.97
1	F	51	ASP	N-CA-C	6.29	120.22	112.54
1	F	239	SER	N-CA-C	6.29	119.11	110.24
1	B	199	SER	N-CA-C	-6.27	100.62	109.96
1	C	391	ASP	CA-C-N	6.27	127.67	119.84
1	C	391	ASP	C-N-CA	6.27	127.67	119.84
1	T	391	ASP	CA-C-N	6.24	127.63	119.84
1	T	391	ASP	C-N-CA	6.24	127.63	119.84
1	N	412	THR	N-CA-C	-6.23	105.83	113.50
1	C	160	VAL	CB-CA-C	-6.22	102.51	112.16
1	M	289	LEU	N-CA-C	6.22	118.85	108.96
1	G	171	THR	N-CA-C	-6.21	101.03	109.54
1	S	171	THR	N-CA-C	-6.21	101.03	109.54
1	K	412	THR	N-CA-C	-6.21	105.87	113.50
1	I	171	THR	N-CA-C	-6.19	101.05	109.54
1	C	133	LEU	N-CA-C	6.19	118.54	111.11
1	S	305	ILE	CB-CA-C	-6.19	103.24	110.91
1	G	239	SER	N-CA-C	6.19	118.96	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	SER	N-CA-C	6.18	120.65	113.18
1	T	125	ASN	N-CA-C	-6.17	99.34	109.40
1	R	239	SER	N-CA-C	6.17	118.98	110.35
1	M	371	PHE	N-CA-C	6.16	119.06	109.52
1	I	156	GLY	N-CA-C	6.15	121.93	111.04
1	N	112	THR	N-CA-C	6.15	118.12	108.96
1	T	412	THR	N-CA-C	-6.13	105.96	113.50
1	F	170	PRO	N-CA-C	6.13	120.96	111.21
1	N	125	ASN	N-CA-C	-6.13	99.41	109.40
1	R	66	SER	N-CA-C	6.12	120.59	113.18
1	J	171	THR	N-CA-C	-6.12	101.16	109.54
1	L	264	ILE	N-CA-C	6.11	117.81	108.71
1	R	391	ASP	CA-C-N	6.11	127.47	119.84
1	R	391	ASP	C-N-CA	6.11	127.47	119.84
1	O	170	PRO	N-CA-C	6.09	120.78	111.15
1	S	51	ASP	N-CA-C	6.09	120.32	113.01
1	N	391	ASP	CA-C-N	6.08	127.44	119.84
1	N	391	ASP	C-N-CA	6.08	127.44	119.84
1	T	371	PHE	N-CA-C	6.07	118.93	109.52
1	L	170	PRO	N-CA-C	6.06	120.73	111.15
1	J	391	ASP	CA-C-N	6.06	127.42	119.84
1	J	391	ASP	C-N-CA	6.06	127.42	119.84
1	M	155	ILE	CA-C-N	-6.06	117.91	122.33
1	M	155	ILE	C-N-CA	-6.06	117.91	122.33
1	B	391	ASP	CA-C-N	6.05	127.40	119.84
1	B	391	ASP	C-N-CA	6.05	127.40	119.84
1	D	414	TRP	CB-CA-C	-6.03	100.06	109.22
1	K	170	PRO	N-CA-C	6.02	120.78	111.21
1	F	122	GLY	N-CA-C	6.02	117.67	111.95
1	D	371	PHE	N-CA-C	6.01	118.84	109.52
1	N	239	SER	N-CA-C	6.01	118.76	110.35
1	Q	239	SER	N-CA-C	6.00	118.75	110.35
1	M	412	THR	N-CA-C	-5.98	106.15	113.50
1	M	66	SER	N-CA-C	5.95	120.38	113.18
1	I	412	THR	N-CA-C	-5.92	106.22	113.50
1	Q	412	THR	N-CA-C	-5.91	106.23	113.50
1	E	171	THR	N-CA-C	-5.89	101.47	109.54
1	J	170	PRO	N-CA-C	5.89	120.58	111.21
1	C	66	SER	N-CA-C	5.89	120.30	113.18
1	E	317	SER	N-CA-C	5.88	118.64	111.82
1	D	180	LEU	N-CA-C	5.87	120.30	113.20
1	P	24	GLY	CA-C-N	5.87	126.33	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	24	GLY	C-N-CA	5.87	126.33	120.52
1	A	389	ARG	N-CA-C	5.87	118.99	110.42
1	P	51	ASP	N-CA-C	5.86	120.04	113.01
1	B	239	SER	N-CA-C	5.85	117.85	110.24
1	G	122	GLY	N-CA-C	5.85	117.50	111.95
1	T	199	SER	N-CA-C	-5.84	101.25	109.96
1	H	170	PRO	N-CA-C	5.84	120.39	111.11
1	O	264	ILE	N-CA-C	5.83	117.40	108.71
1	T	182	ASP	CA-C-N	-5.83	114.26	120.03
1	T	182	ASP	C-N-CA	-5.83	114.26	120.03
1	E	371	PHE	N-CA-C	5.83	118.04	109.24
1	C	371	PHE	N-CA-C	5.81	118.53	109.52
1	T	114	PRO	N-CA-C	5.81	120.36	110.95
1	A	125	ASN	N-CA-C	-5.79	99.97	109.40
1	B	156	GLY	N-CA-C	5.78	121.28	111.04
1	D	391	ASP	CA-C-N	5.78	127.06	119.84
1	D	391	ASP	C-N-CA	5.78	127.06	119.84
1	J	198	ASP	N-CA-C	5.77	119.37	110.42
1	R	412	THR	N-CA-C	-5.77	106.41	113.50
1	S	237	ILE	N-CA-C	-5.76	107.28	112.12
1	C	412	THR	N-CA-C	-5.76	106.42	113.50
1	L	125	ASN	N-CA-C	-5.76	100.02	109.40
1	L	416	THR	N-CA-C	5.75	118.29	111.33
1	E	156	GLY	N-CA-C	5.74	121.20	111.04
1	T	170	PRO	N-CA-C	5.73	120.22	111.11
1	G	51	ASP	N-CA-C	5.72	119.52	112.54
1	K	156	GLY	N-CA-C	5.71	121.15	111.04
1	H	198	ASP	N-CA-C	5.71	119.27	110.42
1	R	156	GLY	N-CA-C	5.71	121.14	111.04
1	K	371	PHE	N-CA-C	5.70	118.36	109.52
1	J	160	VAL	CB-CA-C	-5.70	103.73	112.05
1	O	33	LEU	N-CA-C	5.70	118.95	108.58
1	Q	305	ILE	CB-CA-C	-5.69	103.86	110.91
1	F	125	ASN	N-CA-C	-5.68	100.15	109.40
1	A	272	ILE	N-CA-C	5.67	116.85	108.45
1	B	170	PRO	N-CA-C	5.67	120.22	111.21
1	J	66	SER	N-CA-C	5.67	120.06	113.20
1	C	156	GLY	N-CA-C	5.66	121.06	111.04
1	L	156	GLY	N-CA-C	5.66	121.05	111.04
1	E	412	THR	N-CA-C	-5.65	106.55	113.50
1	B	171	THR	N-CA-C	-5.64	99.19	108.49
1	M	12	VAL	CA-C-N	5.62	125.08	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	12	VAL	C-N-CA	5.62	125.08	119.24
1	P	170	PRO	N-CA-C	5.62	120.02	111.15
1	L	199	SER	N-CA-C	-5.61	101.60	109.96
1	F	156	GLY	N-CA-C	5.61	121.28	111.46
1	O	412	THR	N-CA-C	-5.61	106.61	113.50
1	A	371	PHE	N-CA-C	5.59	117.68	109.24
1	R	305	ILE	CB-CA-C	-5.59	103.98	110.91
1	K	125	ASN	N-CA-C	-5.58	100.31	109.40
1	M	199	SER	N-CA-C	-5.57	101.67	109.96
1	G	170	PRO	N-CA-C	5.57	119.96	111.11
1	B	371	PHE	N-CA-C	5.56	118.14	109.52
1	N	170	PRO	N-CA-C	5.56	120.05	111.21
1	S	412	THR	N-CA-C	-5.56	106.63	113.41
1	L	171	THR	N-CA-C	-5.56	99.32	108.49
1	A	120	LEU	N-CA-C	-5.55	102.27	110.48
1	G	125	ASN	N-CA-C	-5.55	100.36	109.40
1	P	416	THR	N-CA-C	5.54	118.03	111.33
1	N	245	GLU	N-CA-C	5.52	116.91	108.52
1	H	171	THR	N-CA-C	-5.52	99.38	108.49
1	L	66	SER	N-CA-C	5.52	119.86	113.18
1	O	12	VAL	CA-C-N	5.50	125.60	119.32
1	O	12	VAL	C-N-CA	5.50	125.60	119.32
1	A	133	LEU	N-CA-C	5.50	120.44	111.37
1	D	66	SER	N-CA-C	5.49	119.82	113.18
1	P	412	THR	N-CA-C	-5.48	106.76	113.50
1	R	51	ASP	N-CA-C	5.48	119.59	113.01
1	Q	199	SER	N-CA-C	-5.48	101.80	109.96
1	G	66	SER	N-CA-C	5.46	119.78	113.18
1	F	412	THR	N-CA-C	-5.45	106.79	113.50
1	E	125	ASN	N-CA-C	-5.45	100.51	109.40
1	T	163	GLY	N-CA-C	5.44	120.87	112.81
1	D	305	ILE	CB-CA-C	-5.44	104.17	110.91
1	G	363	VAL	N-CA-C	-5.44	100.05	107.99
1	K	179	ARG	N-CA-C	-5.44	101.61	110.20
1	E	180	LEU	N-CA-C	5.43	119.90	113.28
1	S	237	ILE	CB-CA-C	-5.43	105.59	110.91
1	D	121	ASN	N-CA-CB	-5.43	105.28	111.79
1	H	66	SER	N-CA-C	5.42	119.74	113.18
1	G	371	PHE	N-CA-C	5.41	117.91	109.52
1	A	112	THR	N-CA-C	5.41	117.20	109.14
1	O	294	LEU	N-CA-C	5.41	118.63	109.76
1	I	199	SER	N-CA-C	-5.40	101.92	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	276	VAL	N-CA-C	-5.39	107.57	112.96
1	M	51	ASP	N-CA-C	5.39	119.11	112.54
1	L	121	ASN	N-CA-C	5.38	117.27	108.76
1	K	199	SER	N-CA-C	-5.38	101.94	109.96
1	D	289	LEU	N-CA-C	5.38	118.39	109.46
1	P	125	ASN	N-CA-C	-5.38	100.63	109.40
1	F	264	ILE	N-CA-C	5.38	116.72	108.71
1	O	371	PHE	N-CA-C	5.37	117.85	109.52
1	K	33	LEU	N-CA-C	5.37	118.11	108.17
1	K	171	THR	N-CA-C	-5.37	102.18	109.54
1	N	371	PHE	N-CA-C	5.37	117.84	109.52
1	I	180	LEU	N-CA-C	5.37	119.81	113.16
1	A	271	VAL	N-CA-C	-5.35	107.21	111.81
1	T	156	GLY	N-CA-C	5.35	120.50	111.04
1	E	66	SER	N-CA-C	5.34	119.66	113.20
1	H	157	ASN	N-CA-C	5.34	118.76	111.39
1	T	99	CYS	N-CA-C	5.34	117.20	108.76
1	B	218	SER	N-CA-C	5.34	116.96	108.79
1	A	414	TRP	N-CA-C	5.33	118.28	109.58
1	E	237	ILE	CB-CA-C	-5.32	102.56	111.29
1	S	156	GLY	N-CA-C	5.32	120.50	111.19
1	O	180	LEU	N-CA-C	5.32	119.75	113.16
1	T	112	THR	N-CA-C	-5.32	101.05	108.54
1	A	237	ILE	CB-CA-C	-5.31	105.71	110.91
1	H	156	GLY	N-CA-C	5.31	120.44	111.04
1	E	199	SER	N-CA-C	-5.30	101.80	109.59
1	N	199	SER	N-CA-C	-5.30	101.79	109.59
1	C	414	TRP	CB-CA-C	-5.30	101.16	109.22
1	S	199	SER	N-CA-C	-5.30	102.06	109.96
1	S	179	ARG	N-CA-C	-5.30	102.44	110.28
1	Q	204	ARG	N-CA-C	-5.30	101.07	109.76
1	T	118	TYR	N-CA-C	5.30	117.38	109.59
1	J	412	THR	N-CA-C	-5.27	107.01	113.50
1	T	416	THR	N-CA-C	5.27	117.71	111.33
1	F	331	GLY	N-CA-C	5.27	118.17	111.37
1	F	258	ASP	N-CA-C	-5.26	99.87	108.76
1	I	276	VAL	N-CA-C	-5.25	107.71	112.96
1	N	414	TRP	CB-CA-C	-5.25	100.74	108.87
1	P	122	GLY	CA-C-O	5.25	125.63	122.22
1	Q	125	ASN	N-CA-C	-5.24	100.86	109.40
1	E	197	CYS	N-CA-C	-5.24	99.99	108.52
1	D	156	GLY	N-CA-C	5.23	120.62	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	340	GLY	N-CA-C	5.23	119.21	112.83
1	A	245	GLU	N-CA-C	5.23	117.02	108.76
1	H	35	LYS	N-CA-C	-5.22	101.45	109.76
1	I	66	SER	N-CA-C	5.22	119.50	113.18
1	C	35	LYS	N-CA-C	-5.21	101.27	109.25
1	K	66	SER	N-CA-C	5.21	119.49	113.18
1	G	179	ARG	N-CA-C	-5.21	102.57	110.28
1	H	197	CYS	N-CA-C	-5.21	100.03	108.52
1	C	171	THR	N-CA-C	-5.21	99.90	108.49
1	H	125	ASN	N-CA-C	-5.20	100.92	109.40
1	Q	237	ILE	CB-CA-C	-5.20	105.81	110.91
1	O	125	ASN	N-CA-C	-5.20	100.93	109.40
1	P	254	GLY	N-CA-C	5.19	122.78	115.30
1	T	245	GLU	N-CA-C	5.19	116.97	108.76
1	N	35	LYS	N-CA-C	-5.18	102.19	109.96
1	Q	329	ALA	N-CA-C	5.18	117.26	109.23
1	D	412	THR	N-CA-C	-5.18	107.13	113.50
1	S	115	GLY	N-CA-C	5.18	125.45	113.18
1	E	155	ILE	CA-C-N	-5.17	118.56	122.33
1	E	155	ILE	C-N-CA	-5.17	118.56	122.33
1	D	125	ASN	N-CA-C	-5.17	100.97	109.40
1	L	181	GLY	N-CA-C	-5.17	105.97	114.76
1	M	414	TRP	CB-CA-C	-5.17	101.36	109.22
1	S	371	PHE	N-CA-C	5.17	117.04	109.24
1	L	289	LEU	N-CA-C	5.16	118.02	109.46
1	A	289	LEU	N-CA-C	5.15	117.64	109.24
1	C	222	SER	N-CA-C	-5.15	102.43	110.10
1	H	237	ILE	CB-CA-C	-5.14	105.87	110.91
1	P	237	ILE	N-CA-C	-5.14	107.80	112.12
1	P	156	GLY	N-CA-C	5.14	120.13	111.04
1	Q	66	SER	N-CA-C	5.13	119.52	113.16
1	H	133	LEU	N-CA-C	5.13	119.83	111.37
1	K	121	ASN	N-CA-C	5.13	116.39	107.93
1	L	363	VAL	N-CA-C	-5.13	100.50	107.99
1	D	199	SER	N-CA-C	-5.13	102.32	109.96
1	J	199	SER	N-CA-C	-5.12	102.33	109.96
1	E	276	VAL	N-CA-C	-5.12	107.84	112.96
1	B	412	THR	N-CA-C	-5.11	107.21	113.50
1	O	35	LYS	N-CA-C	-5.11	102.07	109.59
1	S	260	THR	N-CA-C	5.11	117.78	109.24
1	L	51	ASP	N-CA-C	5.10	118.76	112.54
1	E	122	GLY	N-CA-C	5.09	125.25	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ASP	N-CA-C	5.09	118.75	112.54
1	R	258	ASP	N-CA-C	-5.09	101.11	109.40
1	J	112	THR	CA-C-O	-5.08	112.16	120.80
1	P	363	VAL	N-CA-C	-5.08	100.57	107.99
1	D	35	LYS	N-CA-C	-5.08	101.69	109.76
1	R	181	GLY	N-CA-C	-5.08	106.12	114.76
1	M	181	GLY	N-CA-C	-5.08	106.13	114.76
1	F	155	ILE	CA-C-N	-5.08	118.20	121.65
1	F	155	ILE	C-N-CA	-5.08	118.20	121.65
1	O	160	VAL	CB-CA-C	-5.07	104.31	112.16
1	B	204	ARG	N-CA-C	-5.06	101.44	109.59
1	L	157	ASN	N-CA-C	5.06	118.38	111.39
1	F	294	LEU	N-CA-C	5.06	118.05	109.76
1	A	156	GLY	N-CA-C	5.05	119.98	111.04
1	T	122	GLY	N-CA-C	5.05	118.44	112.33
1	B	180	LEU	N-CA-C	5.04	119.41	113.16
1	B	416	THR	N-CA-C	5.04	117.42	111.33
1	N	156	GLY	N-CA-C	5.04	120.27	111.46
1	F	200	SER	N-CA-C	5.03	119.86	113.18
1	O	156	GLY	N-CA-C	5.03	119.94	111.04
1	B	125	ASN	N-CA-C	-5.02	101.21	109.40
1	J	35	LYS	N-CA-C	-5.02	101.78	109.76
1	P	179	ARG	N-CA-C	-5.01	102.86	110.28
1	S	251	SER	N-CA-C	-5.01	107.56	113.97
1	H	33	LEU	N-CA-C	5.00	117.42	108.17

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 [i](#)

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	118	0
1	B	3149	0	3125	107	0
1	C	3118	0	3097	95	0
1	D	3118	0	3099	65	0
1	E	3130	0	3111	106	0
1	F	3113	0	3094	91	0
1	G	3110	0	3086	116	0
1	H	3117	0	3095	96	0
1	I	3118	0	3097	72	0
1	J	3102	0	3077	91	0
1	K	3137	0	3115	103	0
1	L	3150	0	3127	102	0
1	M	3110	0	3086	98	0
1	N	3109	0	3086	96	0
1	O	3109	0	3084	85	0
1	P	3138	0	3117	107	0
1	Q	3138	0	3117	97	0
1	R	3101	0	3080	112	0
1	S	3116	0	3095	106	0
1	T	3150	0	3127	111	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	11	0
4	L	234	0	0	2	0
4	M	235	0	0	3	0
4	N	195	0	0	3	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	9	0
4	T	270	0	0	5	0
All	All	66956	0	62056	1843	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 15.

All (1843) 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:B:315:SER:HA	1:B:325:MET:HE1	1.38	1.05
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:H:316:LYS:HB2	1:H:325:MET:HE3	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:LEU:HD11	1:E:351:LEU:HD11	1.40	1.02
1:A:85:MET:HE1	1:A:304:PRO:HD3	1.35	1.02
1:P:246:LEU:HD12	1:P:290:MET:HE2	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:M:120:LEU:C	1:M:121:ASN:HD22	1.69	0.99
1:G:279:ASP:CB	1:K:286:ILE:HD11	1.93	0.98
1:R:315:SER:HA	1:R:325:MET:HE1	1.42	0.98
1:G:185:PRO:HB2	1:K:233:ASN:HD22	1.24	0.98
1:K:407:ARG:HB2	1:K:407:ARG:HH11	1.27	0.97
1:L:316:LYS:HB2	1:L:325:MET:HE3	1.48	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:HB2	1:K:407:ARG:NH1	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:G:20:MET:HE3	1:G:423:ARG:HE	1.35	0.91
1:S:162:GLU:OE1	1:S:417:ARG:HD2	1.71	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:M:316:LYS:HB2	1:M:325:MET:HE3	1.53	0.89
1:H:233:ASN:HD22	1:N:185:PRO:HB2	1.35	0.89
1:L:20:MET:HE3	1:L:423:ARG:HE	1.35	0.89
1:R:404:GLU:OE2	1:R:407:ARG:HD3	1.70	0.89
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:HH11	1:T:417:ARG:CB	1.88	0.87
1:E:20:MET:HE3	1:E:423:ARG:HD2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:246:LEU:HD12	1:I:290:MET:HE2	1.58	0.85
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:NH1	1:O:417:ARG:HB2	1.93	0.84
1:I:121:ASN:HD22	1:I:358:ALA:H	1.21	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
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:HB2	1:T:417:ARG:NH1	1.93	0.83
1:H:274:ARG:CG	1:H:274:ARG:HH11	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:A:121:ASN:CG	1:T:112:THR:HG1	1.89	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:M:120:LEU:C	1:M:121:ASN:ND2	2.37	0.81
1:G:407:ARG:HD3	4:G:6122:HOH:O	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:276:VAL:HG11	1:Q:290:MET:HE3	1.61	0.79
1:A:407:ARG:NH1	1:A:407:ARG:HB2	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:T:316:LYS:HB2	1:T:325:MET:HE3	1.62	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: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
1:E:356:ARG:HH11	1:E:356:ARG:HG3	1.48	0.78
4:F:655:HOH:O	1:S:120:LEU:HD13	1.83	0.78
1:P:162:GLU:HG2	1:P:417:ARG:NH1	1.98	0.78
1:P:249:HIS:NE2	1:P:287:ASP:OD1	2.17	0.78
1:I:285:GLY:C	1:I:286:ILE:HD12	2.09	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: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:G:315:SER:HA	1:G:325:MET:HE1	1.67	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:HG2	1:N:389:ARG:HH11	1.49	0.77
1:K:407:ARG:NH2	4:K:485:HOH:O	2.18	0.77
1:R:315:SER:CA	1:R:325:MET:HE1	2.15	0.77
1:G:104:ARG:HD3	1:G:369:SER:OG	1.85	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:N:315:SER:HA	1:N:325:MET:HE1	1.67	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:L:246:LEU:HD12	1:L:290:MET:HE2	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:O:407:ARG:HB2	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
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:N	1:B:292:PHE:CD2	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:A:85:MET:CE	1:A:304:PRO:HD3	2.14	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:L:20:MET:HE1	1:L:427:MET:HE3	1.70	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:C:263:LEU:HB3	1:C:305:ILE:HD13	1.67	0.74
1:L:316:LYS:N	1:L:325:MET:HE1	2.02	0.74
1:B:117:VAL:C	1:B:118:TYR:HD2	1.96	0.73
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: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:H:246:LEU:HD12	1:H:290:MET:HE2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:316:LYS:HB2	1:S:325:MET:HE3	1.70	0.73
1:E:58:VAL:HG22	1:E:351:LEU:HD23	1.69	0.73
1:K:296:ILE:HD12	1:K:296:ILE:N	2.03	0.73
1:E:136:LEU:CD1	1:E:351:LEU:HD11	2.19	0.73
1:K:356:ARG:HG2	1:K:356:ARG:HH11	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:E:316:LYS:HB2	1:E:325:MET:HE3	1.70	0.72
1:B:219:GLN:H	1:B:219:GLN:HE21	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:R:20:MET:HE3	1:R:423:ARG:HH21	1.53	0.72
1:T:246:LEU:HD23	1:T:331:GLY:HA3	1.70	0.72
1:M:20:MET:HE3	1:M:423:ARG:HE	1.54	0.72
1:A:11:ILE:HB	1:A:430:ALA:HB1	1.71	0.72
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:Q:276:VAL:CG1	1:Q:290:MET:HE3	2.19	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:P:171:THR:O	1:P:172:SER:HB3	1.89	0.71
1:R:121:ASN:HD22	1:R:121:ASN:N	1.87	0.71
1:L:20:MET:HE3	1:L:423:ARG:NE	2.05	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:NE2	1:P:219:GLN:H	1.89	0.71
1:R:121:ASN:HD22	1:R:121:ASN:H	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:H:316:LYS:CB	1:H:325:MET:HE3	2.15	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:J:171:THR:O	1:J:172:SER:HB3	1.90	0.70
1:S:20:MET:HE2	1:S:423:ARG:NH2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PRO:CG	1:A:389:ARG:HH21	2.02	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:Q:112:THR:C	1:Q:113:LEU:HD12	2.17	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:H:255:LEU:HD22	1:H:325:MET:HE2	1.74	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:O:29:PRO:HG2	1:O:395:MET:HE2	1.74	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
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:L:316:LYS:CB	1:L:325:MET:HE3	2.22	0.69
1:P:121:ASN:N	1:P:121:ASN:ND2	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:D:111:SER:C	1:D:113:LEU:HD12	2.17	0.69
1:J:405:ARG:HD3	1:J:406:GLU:OE2	1.93	0.69
1:B:315:SER:CA	1:B:325:MET:HE1	2.17	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:T:315:SER:HA	1:T:325:MET:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:K:428:GLU:O	1.94	0.68
1:L:417:ARG:HG3	1:L:417:ARG:NH1	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:B:280:ASN:CG	1:B:290:MET:HE2	2.17	0.68
1:F:159:LEU:HB2	1:F:162:GLU:HG3	1.75	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
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:T:259:ALA:CB	1:T:290:MET:HE1	2.25	0.67
1:B:15:ILE:HG13	1:B:397:TYR:HD2	1.57	0.67
1:D:112:THR:O	1:D:112:THR:HG22	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:O	1:K:389:ARG:HG3	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:L:426:PHE:C	1:L:428:GLU:H	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:B:219:GLN:N	1.92	0.66
1:L:20:MET:CE	1:L:427:MET:HE3	2.26	0.66
1:M:219:GLN:HA	1:M:324:GLN:NE2	2.10	0.66
1:M:315:SER:C	1:M:325:MET:HE1	2.20	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: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:C:279:ASP:CG	1:C:279:ASP:O	2.39	0.65
1:H:315:SER:C	1:H:325:MET:HE1	2.21	0.65
1:Q:315:SER:HA	1:Q:325:MET:HE1	1.76	0.65
1:R:246:LEU:HD23	1:R:331:GLY:HA3	1.78	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:R:20:MET:HE3	1:R:423:ARG:HE	1.61	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
1:F:122:GLY:O	1:F:160:VAL:HG23	1.97	0.65
1:L:246:LEU:HD23	1:L:331:GLY:HA3	1.78	0.65
1:A:246:LEU:HD12	1:A:290:MET:HE2	1.78	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:T:316:LYS:HB2	1:T:325:MET:CE	2.27	0.65
1:C:417:ARG:HB2	1:C:417:ARG:NH1	2.11	0.65
1:P:389:ARG:HG2	4:P:5986:HOH:O	1.97	0.65
1:T:324:GLN:NE2	1:T:324:GLN:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:20:MET:HE1	1:P:427:MET:SD	2.37	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: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:H:274:ARG:CG	1:H:274:ARG:NH1	2.56	0.64
1:F:316:LYS:N	1:F:325:MET:HE2	2.13	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:O:389:ARG:HH11	1:O:389:ARG:CB	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:J:315:SER:HA	1:J:325:MET:HE1	1.80	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:K:246:LEU:HD12	1:K:290:MET:HE2	1.80	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:G:162:GLU:OE1	4:G:5947:HOH:O	2.16	0.63
1:R:417:ARG:HH11	1:R:417:ARG:HG3	1.63	0.63
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:L:315:SER:C	1:L:325:MET:HE1	2.23	0.63
1:T:383:LEU:C	1:T:383:LEU:HD12	2.24	0.63
1:J:155:ILE:HG12	1:J:415:PRO:HD3	1.79	0.63
1:K:112:THR:HG22	1:K:113:LEU:N	2.12	0.63
1:R:220:TYR:CD1	1:R:325:MET:CE	2.81	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:E:246:LEU:HB2	1:E:290:MET:HE2	1.81	0.62
1:E:246:LEU:HD12	1:E:290:MET:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:379:LEU:HG	1:P:383:LEU:HD23	1.79	0.62
1:B:118:TYR:CD2	1:B:118:TYR:N	2.67	0.62
1:M:316:LYS:CB	1:M:325:MET:HE3	2.29	0.62
1:Q:316:LYS:HB2	1:Q:325:MET:CE	2.29	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: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:A:385:THR:C	1:A:386:GLU:HG2	2.25	0.62
1:N:246:LEU:HB2	1:N:290:MET:HE2	1.82	0.62
1:S:315:SER:C	1:S:325:MET:HE1	2.23	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:E:315:SER:C	1:E:325:MET:HE1	2.24	0.62
1:K:201:ASP:OD2	1:M:202:ARG:HD2	1.99	0.62
1:M:246:LEU:HB2	1:M:290:MET:HE2	1.81	0.62
1:A:82:PHE:CE1	1:A:85:MET:HE2	2.34	0.62
1:B:155:ILE:HG12	1:B:415:PRO:HD3	1.80	0.62
1:N:220:TYR:CG	1:N:221:GLN:N	2.67	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:HH11	1:O:417:ARG:CB	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
1:G:113:LEU:HD12	1:G:113:LEU:O	2.01	0.61
1:K:246:LEU:HD12	1:K:290:MET:CE	2.30	0.61
1:K:389:ARG:HG2	4:K:623:HOH:O	1.99	0.61
1:N:315:SER:CA	1:N:325:MET:HE1	2.30	0.61
1:O:407:ARG:HB2	1:O:407:ARG:HH11	1.65	0.61
1:Q:417:ARG:NH1	1:Q:417:ARG:HB2	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:L:415:PRO:HG2	1:L:418:GLU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:315:SER:HA	1:F:325:MET:HE1	1.83	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: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:HB3	1:B:389:ARG:NH1	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:C:230:PHE:C	1:C:230:PHE:CD1	2.78	0.61
1:G:246:LEU:HD23	1:G:331:GLY:HA3	1.83	0.61
1:M:20:MET:HE1	1:M:427:MET:SD	2.40	0.61
1:G:220:TYR:CG	1:G:221:GLN:N	2.68	0.61
1:H:255:LEU:CD2	1:H:325:MET:HE2	2.30	0.61
1:A:407:ARG:HH11	1:A:407:ARG:CB	2.14	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:S:427:MET:C	4:S:532:HOH:O	2.45	0.60
1:F:20:MET:HE1	1:F:427:MET:HE3	1.82	0.60
1:M:171:THR:O	1:M:172:SER:HB3	2.00	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:G:185:PRO:CB	1:K:233:ASN:HD22	2.05	0.60
1:J:38:LEU:O	1:J:39:ARG:NH1	2.27	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:HD22	1:C:121:ASN:N	2.00	0.60
1:M:273:THR:O	1:M:274:ARG:HD3	2.01	0.60
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:M:426:PHE:C	1:M:428:GLU:H	2.09	0.60
1:B:292:PHE:N	1:B:292:PHE:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLN:NE2	1:A:322:GLY:H	2.00	0.60
1:Q:428:GLU:C	1:Q:430:ALA:H	2.09	0.60
1:T:136:LEU:CD1	1:T:351:LEU:HD11	2.32	0.60
1:B:219:GLN:NE2	1:B:219:GLN:N	2.45	0.59
1:F:38:LEU:O	1:F:39:ARG:NH1	2.32	0.59
1:S:379:LEU:HD23	1:S:383:LEU:HD22	1.83	0.59
1:S:379:LEU:HD21	1:S:383:LEU:HD22	1.82	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:C:220:TYR:HA	1:C:325:MET:HE2	1.84	0.59
1:F:29:PRO:HG2	1:F:395:MET:HE2	1.84	0.59
1:N:271:VAL:HG12	1:N:272:ILE:HD12	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:Q:122:GLY:C	1:Q:160:VAL:HG22	2.28	0.59
1:N:159:LEU:HB2	1:N:162:GLU:HG3	1.84	0.59
1:T:274:ARG:HG3	1:T:274:ARG:NH1	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:L:155:ILE:HG12	1:L:415:PRO:HD3	1.85	0.59
1:P:280:ASN:HD22	1:P:280:ASN:C	2.11	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:E:162:GLU:CD	1:E:417:ARG:HD3	2.28	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:D:39:ARG:NH2	1:D:383:LEU:HD21	2.19	0.58
1:D:246:LEU:HD12	1:D:290:MET:HE2	1.82	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
1:P:20:MET:HE3	1:P:423:ARG:HE	1.68	0.58
1:Q:417:ARG:HB2	1:Q:417:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ASP:HB2	1:C:313:VAL:HB	1.85	0.58
1:D:113:LEU:C	1:L:119:ALA:HB1	2.29	0.58
1:E:20:MET:CE	1:E:423:ARG:HD2	2.31	0.58
1:M:274:ARG:HH11	1:M:274:ARG:CG	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:P:315:SER:HA	1:P:325:MET:HE1	1.84	0.58
1:G:112:THR:CG2	1:G:113:LEU:N	2.66	0.58
1:K:356:ARG:HG2	1:K:356:ARG:NH1	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:315:SER:HA	1:M:325:MET:HE1	1.85	0.58
1:M:390:PHE:CZ	1:M:392:PRO:HG3	2.38	0.58
1:M:423:ARG:HB3	1:M:427:MET:HE2	1.85	0.58
1:N:171:THR:O	1:N:172:SER:HB3	2.04	0.58
1:J:41:GLU:OE1	1:J:90:GLN:HG2	2.04	0.58
1:J:397:TYR:O	1:J:401:ILE:HG12	2.03	0.58
1:P:201:ASP:O	1:P:202:ARG:HB2	2.03	0.58
1:P:274:ARG:HH11	1:P:274:ARG:CG	2.15	0.58
1:E:220:TYR:CG	1:E:221:GLN:N	2.67	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:A:85:MET:HE3	1:A:303:GLN:HA	1.86	0.57
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:S:120:LEU:O	1:S:121:ASN:CG	2.46	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:S:423:ARG:HB3	1:S:427:MET:HE2	1.86	0.57
1:A:316:LYS:HB2	1:A:325:MET:HE2	1.85	0.57
1:L:171:THR:O	1:L:172:SER:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:274:ARG:HH11	1:P:274:ARG:HG3	1.68	0.57
1:R:20:MET:HE3	1:R:423:ARG:NH2	2.20	0.57
1:L:349:VAL:HG12	1:L:351:LEU:HD23	1.86	0.57
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:HG3	1:G:417:ARG:HH11	1.67	0.57
1:R:296:ILE:N	1:R:296:ILE:HD12	2.19	0.57
1:M:279:ASP:CG	1:M:279:ASP:O	2.48	0.57
1:K:426:PHE:C	1:K:428:GLU:H	2.12	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:HB2	1:C:407:ARG:HH11	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:F:220:TYR:HD1	1:F:325:MET:HE3	1.69	0.56
1:H:41:GLU:OE1	1:H:90:GLN:HG2	2.05	0.56
1:J:34:GLU:HG3	1:J:177:TYR:CE1	2.41	0.56
1:J:104:ARG:HD3	1:J:369:SER:OG	2.05	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:HH11	1:G:356:ARG:HG3	1.70	0.56
1:P:59:PHE:O	1:P:61:PRO:HD3	2.05	0.56
1:R:315:SER:C	1:R:325:MET:HE1	2.30	0.56
1:S:20:MET:HE2	1:S:423:ARG:CZ	2.36	0.56
1:M:58:VAL:HG22	1:M:351:LEU:HD22	1.86	0.56
1:M:315:SER:CA	1:M:325:MET:HE1	2.35	0.56
1:A:85:MET:HE1	1:A:304:PRO:CD	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:255:LEU:CD2	1:E:325:MET:HE2	2.36	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
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: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:R:279:ASP:CG	1:R:279:ASP:O	2.48	0.55
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:316:LYS:HB2	1:Q:325:MET:HE2	1.89	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:122:GLY:C	1:F:160:VAL:CG2	2.80	0.55
1:F:317:SER:HA	4:F:569:HOH:O	2.04	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:D:271:VAL:HG12	1:D:272:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:279:ASP:O	1:G:279:ASP:CG	2.49	0.55
1:I:56:LEU:HD11	1:I:351:LEU:HD13	1.88	0.55
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:C:189:LEU:CD1	1:E:227:ILE:HD12	2.32	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:J:15:ILE:HG13	1:J:397:TYR:HD2	1.72	0.55
1:N:290:MET:HE3	1:N:292:PHE:CZ	2.42	0.55
1:O:407:ARG:HH11	1:O:407:ARG:CB	2.20	0.55
1:P:423:ARG:HB3	1:P:427:MET:HE2	1.88	0.55
1:J:211:ALA:O	1:J:330:SER:HA	2.07	0.54
1:K:63:PHE:CZ	1:K:67:ILE:HD12	2.42	0.54
1:K:267:ASP:OD1	1:K:269:THR:HB	2.07	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:426:PHE:C	1:P:428:GLU:H	2.14	0.54
1:P:86:LEU:O	1:P:87:LEU:HD23	2.07	0.54
1:S:162:GLU:CD	1:S:417:ARG:HD2	2.31	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: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:O:144:LEU:HD22	1:O:351:LEU:HD12	1.88	0.54
1:R:271:VAL:C	1:R:272:ILE:HG13	2.32	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:99:CYS:HB3	1:L:180:LEU:HD21	1.89	0.54
1:L:112:THR:HG22	1:L:362:VAL:H	1.73	0.54
1:N:316:LYS:HB2	1:N:325:MET:HE3	1.89	0.54
1:O:20:MET:HE3	1:O:423:ARG:HG2	1.88	0.54
1:R:121:ASN:O	1:R:160:VAL:CG2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:230:PHE:CD1	1:B:230:PHE:C	2.85	0.54
1:G:264:ILE:HB	1:G:307:SER:OG	2.08	0.54
1:A:82:PHE:CZ	1:A:85:MET:HE2	2.43	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:T:15:ILE:HG13	1:T:397:TYR:HD2	1.73	0.54
1:T:283:THR:CG2	1:T:286:ILE:HG12	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:D:320:GLN:O	1:D:321:ALA:C	2.51	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:N:315:SER:C	1:N:325:MET:HE1	2.32	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:HG3	1:S:274:ARG:HH11	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:A:316:LYS:N	1:A:325:MET:HE2	2.22	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:A:20:MET:HE3	1:A:423:ARG:HG2	1.90	0.53
1:C:41:GLU:HB3	1:C:88:THR:HB	1.90	0.53
1:C:104:ARG:HD3	1:C:369:SER:OG	2.08	0.53
1:C:272:ILE:HD13	1:C:296:ILE:HG23	1.89	0.53
1:C:383:LEU:HD21	1:O:383:LEU:HG	1.90	0.53
1:I:233:ASN:HD22	1:J:185:PRO:CG	2.22	0.53
1:Q:428:GLU:OE1	1:Q:428:GLU:HA	2.08	0.53
1:T:121:ASN:HD22	1:T:121:ASN:N	2.05	0.53
1:R:220:TYR:CD1	1:R:325:MET:HE1	2.42	0.53
1:R:258:ASP:HB2	1:R:313:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:246:LEU:HD12	1:M:290:MET:HE2	1.91	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
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:S:315:SER:CA	1:S:325:MET:HE1	2.39	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:HA	1:I:404:GLU:OE2	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:389:ARG:CB	1:B:389:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:TYR:O	1:E:425:TYR:HD2	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:H:320:GLN:O	1:H:321:ALA:C	2.53	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:S:77:ASN:C	1:S:77:ASN:HD22	2.18	0.52
1:A:120:LEU:HB2	1:T:116:GLY:HA2	1.92	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:J:426:PHE:C	1:J:428:GLU:H	2.16	0.52
1:S:276:VAL:HG12	1:S:290:MET:HE3	1.90	0.52
1:A:415:PRO:HG2	1:A:418:GLU:HG3	1.92	0.52
1:E:384:VAL:HG13	1:L:150:ASN:OD1	2.10	0.52
1:H:316:LYS:HB2	1:H:325:MET:CE	2.27	0.52
1:K:293:ASN:CG	1:M:291:PRO:HB3	2.34	0.52
1:R:219:GLN:NE2	1:R:219:GLN:H	2.07	0.52
1:G:150:ASN:OD1	1:M:384:VAL:HG13	2.08	0.52
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:N:246:LEU:HD12	1:N:290:MET:HE2	1.90	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:C:427:MET:C	1:C:428:GLU:HG3	2.34	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:HD12	1:N:296:ILE:N	2.25	0.52
1:S:193:MET:HE2	1:S:193:MET:O	2.09	0.52
1:T:63:PHE:CZ	1:T:67:ILE:HD12	2.44	0.52
1:F:20:MET:HE3	1:F:423:ARG:HE	1.74	0.52
1:H:246:LEU:HB2	1:H:290:MET:HE2	1.90	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:H:112:THR:HG22	1:H:362:VAL:N	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:315:SER:C	1:R:325:MET:CE	2.83	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:S:193:MET:HE2	1:S:193:MET:C	2.35	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:395:MET:CG	1:D:399:LYS:HE2	2.39	0.51
1:E:33:LEU:HD13	1:L:402:LEU:HD12	1.92	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:J:20:MET:HE3	1:J:23:THR:HG21	1.91	0.51
1:J:122:GLY:C	1:J:160:VAL:HG22	2.36	0.51
1:J:246:LEU:HB2	1:J:290:MET:HE2	1.93	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:M:121:ASN:HB3	1:Q:112:THR:OG1	2.11	0.51
1:P:292:PHE:N	1:P:292:PHE:CD2	2.76	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:C:385:THR:OG1	1:E:130:GLN:NE2	2.43	0.51
1:D:220:TYR:CG	1:D:221:GLN:N	2.79	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
1:B:280:ASN:OD1	1:B:290:MET:HE2	2.11	0.51
1:E:218:SER:O	1:E:325:MET:HG3	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:F:107:THR:HG22	1:F:165:THR:OG1	2.10	0.51
1:F:320:GLN:O	1:F:321:ALA:C	2.54	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:H:316:LYS:N	1:H:325:MET:HE1	2.26	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:I:381:LYS:HG2	1:Q:146:SER:O	2.11	0.51
1:J:21:PRO:HG2	1:J:105:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:246:LEU:HD12	1:N:290:MET:HE1	1.91	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:56:LEU:HD11	1:I:351:LEU:HB3	1.93	0.51
1:I:114:PRO:HG2	1:I:114:PRO:O	2.11	0.51
1:J:136:LEU:CD1	1:J:351:LEU:HD11	2.40	0.51
1:J:271:VAL:C	1:J:272:ILE:HG13	2.36	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:N	1:G:296:ILE:HD12	2.25	0.51
1:G:419:TYR:O	1:G:423:ARG:HG3	2.11	0.51
1:J:230:PHE:CD1	1:J:230:PHE:C	2.88	0.51
1:P:220:TYR:CG	1:P:221:GLN:N	2.78	0.51
1:P:246:LEU:CD1	1:P:290:MET:HE2	2.27	0.51
1:R:220:TYR:CG	1:R:221:GLN:N	2.79	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:47:LEU:HD13	1:E:71:HIS:CG	2.46	0.51
1:E:397:TYR:CE2	1:E:401:ILE:HD11	2.45	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:99:CYS:HB2	1:M:373:LEU:HD23	1.92	0.50
1:C:417:ARG:CB	1:C:417:ARG:HH11	2.24	0.50
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:P:12:VAL:HB	1:P:15:ILE:HG12	1.93	0.50
1:R:358:ALA:O	1:R:361:SER:OG	2.26	0.50
1:T:38:LEU:O	1:T:39:ARG:NH1	2.35	0.50
1:T:112:THR:HG21	1:T:361:SER:C	2.35	0.50
1:A:316:LYS:N	1:A:325:MET:CE	2.74	0.50
1:B:121:ASN:CG	1:B:358:ALA:H	2.17	0.50
1:C:159:LEU:HB2	1:C:162:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ASP:OD2	1:L:202:ARG:HG2	2.11	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: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:K:20:MET:HE1	1:K:427:MET:HG3	1.93	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:B:117:VAL:C	1:B:118:TYR:CD2	2.83	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:D:182:ASP:OD2	4:D:499:HOH:O	2.20	0.50
1:F:166:VAL:HG13	1:F:350:THR:HG21	1.92	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:NE2	1:P:219:GLN:N	2.57	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:Q:385:THR:C	1:Q:386:GLU:HG2	2.36	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
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:G:230:PHE:CD1	1:G:230:PHE:C	2.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:153:ASP:CG	1:C:405:ARG:HH22	2.19	0.49
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:H:20:MET:CE	1:H:427:MET:HE2	2.42	0.49
1:I:55:GLY:HA3	1:I:354:TYR:CZ	2.46	0.49
1:K:274:ARG:HG3	1:K:274:ARG:HH11	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:P:153:ASP:CG	1:P:405:ARG:HH22	2.20	0.49
1:Q:140:SER:O	1:Q:144:LEU:HG	2.11	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:H:20:MET:HE3	1:H:427:MET:HE2	1.94	0.49
1:L:25:PRO:HD3	1:L:40:SER:OG	2.12	0.49
1:B:20:MET:HE1	1:B:427:MET:HE2	1.93	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:NH1	1:H:274:ARG:HG2	2.26	0.49
1:Q:121:ASN:O	1:Q:160:VAL:HG21	2.12	0.49
1:R:67:ILE:HD13	1:R:237:ILE:CG2	2.42	0.49
1:R:193:MET:HG2	1:R:194:VAL:N	2.27	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:Q:316:LYS:HB2	1:Q:325:MET:HE3	1.94	0.49
1:E:356:ARG:CG	1:E:356:ARG:NH1	2.69	0.49
1:F:214:TYR:O	1:F:328:SER:HA	2.11	0.49
1:G:315:SER:CA	1:G:325:MET:HE1	2.41	0.49
1:H:58:VAL:HG22	1:H:351:LEU:HD22	1.94	0.49
1:H:267:ASP:OD1	1:H:269:THR:HB	2.12	0.49
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:C:237:ILE:HG22	1:C:238:THR:HG23	1.95	0.49
1:E:122:GLY:C	1:E:160:VAL:HG22	2.37	0.49
1:H:153:ASP:CG	1:H:405:ARG:HH22	2.21	0.49
1:J:77:ASN:HD21	1:J:79:ASN:HD22	1.60	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:M:112:THR:HG22	1:M:113:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:VAL:HG22	1:J:351:LEU:HD22	1.94	0.49
1:J:199:SER:HB3	4:J:473:HOH:O	2.13	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:S:51:ASP:HA	1:S:359:THR:OG1	2.12	0.49
1:C:274:ARG:HH21	1:C:300:GLU:CD	2.20	0.49
1:H:230:PHE:CD1	1:H:230:PHE:C	2.91	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: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:13:PRO:HG2	1:P:389:ARG:HH11	1.77	0.49
1:P:113:LEU:HD21	1:P:120:LEU:CA	2.43	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:136:LEU:CD1	1:S:351:LEU:HD11	2.43	0.49
1:S:171:THR:O	1:S:172:SER:CB	2.60	0.49
1:C:112:THR:HG1	1:N:121:ASN:HA	1.75	0.49
1:D:32:THR:HG22	1:D:32:THR:O	2.11	0.49
1:L:201:ASP:OD1	1:L:201:ASP:N	2.46	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:K:284:THR:HG22	4:K:653:HOH:O	2.12	0.48
1:L:246:LEU:HD12	1:L:290:MET:CE	2.41	0.48
1:L:349:VAL:CG1	1:L:351:LEU:CD2	2.90	0.48
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:C:426:PHE:C	1:C:428:GLU:H	2.20	0.48
1:H:112:THR:HG21	1:H:362:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:VAL:HA	1:H:144:LEU:HD21	1.96	0.48
1:I:271:VAL:HG12	1:I:272:ILE:HG12	1.95	0.48
4:K:679:HOH:O	1:Q:39:ARG:HD2	2.12	0.48
1:S:309:LYS:NZ	4:S:636:HOH:O	2.44	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:F:122:GLY:C	1:F:160:VAL:HG23	2.37	0.48
1:H:276:VAL:HG11	1:H:292:PHE:CE2	2.49	0.48
1:K:20:MET:CE	1:K:427:MET:HE3	2.43	0.48
1:K:230:PHE:C	1:K:230:PHE:CD1	2.91	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:Q:193:MET:HE3	1:Q:194:VAL:C	2.38	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:K:29:PRO:O	1:K:395:MET:HE2	2.13	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:20:MET:HE3	1:S:423:ARG:HB3	1.94	0.48
1:S:106:LEU:HD23	1:S:367:GLY:HA3	1.95	0.48
1:G:93:PRO:HG3	1:G:180:LEU:HB3	1.94	0.48
1:M:230:PHE:CD1	1:M:230:PHE:C	2.90	0.48
1:N:171:THR:O	1:N:172:SER:CB	2.62	0.48
1:T:51:ASP:OD2	1:T:51:ASP:N	2.46	0.48
1:T:259:ALA:CB	1:T:290:MET:CE	2.91	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:L:230:PHE:CD1	1:L:230:PHE:C	2.91	0.48
1:M:21:PRO:HG2	1:M:105:SER:HB3	1.96	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:A:118:TYR:CE2	1:T:114:PRO:HB3	2.49	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:R:20:MET:HE3	1:R:423:ARG:NE	2.26	0.48
1:C:15:ILE:HG13	1:C:397:TYR:CD2	2.48	0.48
1:C:153:ASP:OD2	1:C:405:ARG:NH2	2.37	0.48
1:D:201:ASP:OD1	1:D:201:ASP:N	2.45	0.48
1:E:272:ILE:HG21	1:E:296:ILE:HD12	1.95	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: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: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:F:109:ARG:NH1	1:S:159:LEU:HD11	2.28	0.48
1:I:279:ASP:CG	1:I:279:ASP:O	2.57	0.48
1:P:190:ASP:OD1	1:P:191:PRO:HD2	2.14	0.48
1:T:20:MET:HE2	1:T:426:PHE:CD1	2.49	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:Q:320:GLN:O	1:Q:321:ALA:C	2.56	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: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: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:E:246:LEU:HD12	1:E:290:MET:HE1	1.96	0.47
1:H:226:THR:OG1	1:H:313:VAL:HG22	2.14	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
1:J:77:ASN:ND2	1:J:79:ASN:ND2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:16:ARG:NH2	1:K:427:MET:HE2	2.29	0.47
1:K:39:ARG:HH21	1:K:383:LEU:HD21	1.79	0.47
1:S:274:ARG:HD3	1:S:274:ARG:HA	1.67	0.47
1:S:314:THR:HG22	1:S:325:MET:HE2	1.96	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:M:122:GLY:C	1:M:160:VAL:HG22	2.38	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:D:323:ASP:OD2	1:D:323:ASP:N	2.45	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:HB2	1:C:417:ARG:HH11	1.77	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:CG	1:M:274:ARG:NH1	2.75	0.47
1:S:20:MET:HE1	1:S:427:MET:SD	2.54	0.47
1:A:20:MET:HE1	1:A:427:MET:HE2	1.95	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:G:162:GLU:CD	1:G:417:ARG:NH2	2.73	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:B:315:SER:HA	1:B:325:MET:CE	2.27	0.47
1:C:99:CYS:HB2	1:C:373:LEU:HD23	1.96	0.47
1:C:272:ILE:HD13	1:C:296:ILE:HG21	1.96	0.47
1:D:427:MET:O	1:L:425:TYR:OH	2.31	0.47
1:E:122:GLY:O	1:E:160:VAL:HG22	2.14	0.47
1:E:316:LYS:N	1:E:325:MET:HE1	2.28	0.47
1:I:262:TYR:HE1	1:I:311:GLU:HB2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:286:ILE:HD12	1:L:286:ILE:HA	1.72	0.47
1:N:378:GLU:OE2	1:N:381:LYS:HD2	2.15	0.47
1:P:258:ASP:OD1	1:P:278:SER:HA	2.15	0.47
1:P:280:ASN:C	1:P:280:ASN:ND2	2.70	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:R:315:SER:HA	1:R:325:MET:CE	2.29	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:O	1:J:32:THR:HG22	2.13	0.47
1:O:178:VAL:HG12	1:O:179:ARG:O	2.15	0.47
1:O:246:LEU:HD12	1:O:290:MET:HE2	1.96	0.47
1:R:220:TYR:CD1	1:R:325:MET:HE3	2.49	0.47
1:S:376:ASN:C	1:S:376:ASN:OD1	2.58	0.47
1:T:320:GLN:O	1:T:321:ALA:C	2.57	0.47
1:B:41:GLU:HB3	1:B:88:THR:HB	1.96	0.47
1:B:320:GLN:O	1:B:321:ALA:C	2.58	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:K:264:ILE:HB	1:K:307:SER:OG	2.15	0.47
1:Q:193:MET:C	1:Q:193:MET:HE2	2.40	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:O	1:J:112:THR:HG22	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:55:GLY:HA3	1:O:354:TYR:CZ	2.49	0.47
1:O:283:THR:O	1:O:286:ILE:HG22	2.14	0.47
1:Q:379:LEU:HD22	1:Q:383:LEU:HD23	1.97	0.47
1:E:112:THR:HG22	1:E:362:VAL:H	1.80	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:K:426:PHE:C	1:K:428:GLU:N	2.73	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:49:VAL:HG21	1:P:357:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:324:GLN:HE21	1:R:324:GLN:CA	2.18	0.46
1:B:389:ARG:NH1	1:B:389:ARG:CB	2.79	0.46
1:E:121:ASN:CG	1:E:121:ASN:O	2.58	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
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:C:376:ASN:C	1:C:376:ASN:OD1	2.58	0.46
1:F:230:PHE:CD1	1:F:230:PHE:C	2.93	0.46
1:H:136:LEU:CD1	1:H:351:LEU:HD11	2.46	0.46
1:H:320:GLN:CG	1:H:321:ALA:N	2.78	0.46
1:Q:286:ILE:HD12	1:Q:286:ILE:HA	1.76	0.46
1:S:12:VAL:O	1:S:13:PRO:C	2.55	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:B:315:SER:C	1:B:325:MET:CE	2.88	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:426:PHE:C	1:J:428:GLU:N	2.73	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:R:264:ILE:HB	1:R:307:SER:OG	2.14	0.46
1:F:296:ILE:HD12	1:F:296:ILE:N	2.30	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:S:230:PHE:C	1:S:230:PHE:CD1	2.93	0.46
1:F:20:MET:CE	1:F:423:ARG:HE	2.29	0.46
1:F:201:ASP:OD1	1:F:201:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:140:SER:O	1:M:144:LEU:HG	2.16	0.46
1:O:417:ARG:NH1	1:O:417:ARG:CB	2.69	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
1:E:185:PRO:HB2	1:L:233:ASN:ND2	2.24	0.46
1:J:428:GLU:O	1:J:429:VAL:C	2.58	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:E:315:SER:CA	1:E:325:MET:HE1	2.46	0.46
1:P:219:GLN:N	1:P:219:GLN:CD	2.74	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:A:55:GLY:HA3	1:A:354:TYR:CZ	2.51	0.46
1:E:58:VAL:HG22	1:E:351:LEU:CD2	2.41	0.46
1:F:315:SER:C	1:F:325:MET:HE2	2.40	0.46
1:H:315:SER:CA	1:H:325:MET:HE1	2.46	0.46
1:K:16:ARG:HH22	1:K:427:MET:HE2	1.81	0.46
1:L:187:ILE:O	1:L:187:ILE:HG13	2.14	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:C:44:THR:HB	1:N:157:ASN:ND2	2.31	0.45
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:K:246:LEU:HB2	1:K:290:MET:HE2	1.97	0.45
1:L:220:TYR:CG	1:L:221:GLN:N	2.84	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:CG	1:C:356:ARG:NH1	2.76	0.45
1:E:93:PRO:HG3	1:E:180:LEU:HB3	1.97	0.45
1:F:112:THR:OG1	1:S:121:ASN:ND2	2.50	0.45
1:G:279:ASP:HB2	1:K:286:ILE:HD11	1.91	0.45
1:H:122:GLY:C	1:H:160:VAL:HG13	2.42	0.45
1:J:121:ASN:N	1:J:121:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:32:THR:HG22	1:Q:32:THR:O	2.15	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:L:269:THR:HG21	4:L:668:HOH:O	2.15	0.45
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:D:246:LEU:HB2	1:D:290:MET:HE2	1.98	0.45
1:E:237:ILE:O	1:E:237:ILE:HG22	2.15	0.45
1:M:274:ARG:HH11	1:M:274:ARG:HG3	1.81	0.45
1:N:55:GLY:HA3	1:N:354:TYR:CZ	2.52	0.45
1:N:77:ASN:C	1:N:77:ASN:OD1	2.60	0.45
1:N:111:SER:HB2	1:Q:159:LEU:HD22	1.99	0.45
1:N:316:LYS:N	1:N:325:MET:HE1	2.32	0.45
1:N:379:LEU:HD21	1:N:383:LEU:HD22	1.98	0.45
1:O:27:SER:HB3	4:O:643:HOH:O	2.15	0.45
1:O:142:ASN:ND2	4:O:514:HOH:O	2.49	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: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:J:41:GLU:CD	1:J:90:GLN:HG2	2.42	0.45
1:K:153:ASP:CG	1:K:405:ARG:HH22	2.24	0.45
1:T:258:ASP:HB2	1:T:313:VAL:HB	1.99	0.45
1:G:39:ARG:NH2	1:G:383:LEU:HD21	2.31	0.45
1:G:55:GLY:HA3	1:G:354:TYR:CZ	2.51	0.45
1:G:120:LEU:HD23	4:G:5990:HOH:O	2.16	0.45
1:Q:201:ASP:O	1:Q:202:ARG:HB2	2.16	0.45
1:T:259:ALA:HB3	1:T:290:MET:CE	2.46	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:K:255:LEU:CD2	1:K:325:MET:HE2	2.47	0.45
1:R:55:GLY:HA3	1:R:354:TYR:CZ	2.51	0.45
1:R:286:ILE:CG2	1:R:287:ASP:N	2.80	0.45
1:A:226:THR:OG1	1:A:313:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLU:CD	1:B:90:GLN:HG2	2.42	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:H:246:LEU:HD12	1:H:290:MET:HE1	1.93	0.45
1:K:117:VAL:C	4:K:660:HOH:O	2.59	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:M:246:LEU:HD12	1:M:290:MET:HE1	1.99	0.45
1:P:86:LEU:C	1:P:87:LEU:HD23	2.42	0.45
1:Q:41:GLU:HB3	1:Q:88:THR:HB	1.99	0.45
1:Q:121:ASN:O	1:Q:121:ASN:ND2	2.49	0.45
1:R:263:LEU:HD23	1:R:263:LEU:HA	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
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:HH11	1:K:407:ARG:CB	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:HD12	1:R:155:ILE:HA	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:NH1	1:A:407:ARG:CB	2.73	0.45
1:H:417:ARG:NH1	1:H:417:ARG:CG	2.80	0.45
1:I:376:ASN:C	1:I:376:ASN:OD1	2.60	0.45
1:M:255:LEU:HD22	1:M:325:MET:HE2	1.99	0.45
1:M:426:PHE:C	1:M:428:GLU:N	2.74	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:R:211:ALA:O	1:R:330:SER:HA	2.17	0.45
1:A:201:ASP:OD1	1:A:201:ASP:N	2.49	0.44
1:A:315:SER:HA	1:A:325:MET:HE1	1.99	0.44
1:A:404:GLU:OE1	1:A:407:ARG:NH1	2.51	0.44
1:E:272:ILE:HD13	1:E:296:ILE:HG21	2.00	0.44
1:N:364:THR:CG2	1:Q:157:ASN:HB3	2.48	0.44
1:P:126:ALA:HB3	1:P:155:ILE:HG22	1.99	0.44
1:Q:285:GLY:O	1:Q:286:ILE:CD1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:225:VAL:HG23	1:D:325:MET:HE1	1.99	0.44
1:F:226:THR:OG1	1:F:313:VAL:HG22	2.16	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:126:ALA:HB3	1:B:155:ILE:HG22	1.99	0.44
1:B:144:LEU:CD2	1:B:351:LEU:HD12	2.47	0.44
1:C:279:ASP:O	1:C:279:ASP:OD1	2.35	0.44
1:C:355:GLU:O	1:C:356:ARG:HB2	2.16	0.44
1:F:77:ASN:C	1:F:77:ASN:OD1	2.58	0.44
1:J:62:GLY:HA2	1:J:101:LEU:HD23	1.99	0.44
1:J:246:LEU:HD23	1:J:246:LEU:HA	1.66	0.44
1:L:14:PHE:CG	1:L:29:PRO:HD3	2.53	0.44
1:L:249:HIS:NE2	1:L:287:ASP:OD1	2.45	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:HD12	1:F:155:ILE:HA	1.88	0.44
1:G:255:LEU:HB2	4:G:6091:HOH:O	2.17	0.44
1:J:316:LYS:CB	1:J:325:MET:HE3	2.47	0.44
1:K:51:ASP:OD1	1:K:51:ASP:N	2.40	0.44
1:O:320:GLN:O	1:O:321:ALA:C	2.60	0.44
1:P:271:VAL:C	1:P:272:ILE:HD12	2.42	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:N:121:ASN:O	1:N:121:ASN:CG	2.59	0.44
1:N:295:VAL:C	1:N:296:ILE:HD12	2.42	0.44
1:O:315:SER:HA	1:O:325:MET:HE1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:315:SER:CA	1:T:325:MET:HE1	2.46	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:L:316:LYS:N	1:L:325:MET:CE	2.78	0.44
1:N:376:ASN:C	1:N:376:ASN:OD1	2.61	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:HA	1:C:274:ARG:HD3	1.83	0.44
1:F:133:LEU:HD12	1:F:136:LEU:HD12	2.00	0.44
1:G:271:VAL:O	1:G:272:ILE:HG13	2.18	0.44
1:I:12:VAL:O	1:I:13:PRO:C	2.59	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:41:GLU:HB3	1:M:88:THR:HB	1.99	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:Q:258:ASP:HB2	1:Q:313:VAL:HB	2.00	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: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:L:276:VAL:HG21	1:L:292:PHE:CD2	2.53	0.44
1:N:230:PHE:CD1	1:N:230:PHE:C	2.96	0.44
1:O:91:ASN:CG	1:O:93:PRO:HD2	2.43	0.44
1:Q:121:ASN:HD22	1:Q:121:ASN:N	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:136:LEU:HD13	1:R:351:LEU:HD11	2.00	0.44
1:R:272:ILE:HD13	1:R:296:ILE:CG2	2.47	0.44
1:S:280:ASN:HB2	4:S:551:HOH:O	2.18	0.44
1:S:385:THR:C	1:S:386:GLU:HG2	2.42	0.44
1:T:113:LEU:HA	1:T:114:PRO:HD3	1.62	0.44
1:D:319:GLY:C	1:D:320:GLN:HG3	2.42	0.43
1:E:320:GLN:O	1:E:321:ALA:C	2.61	0.43
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:41:GLU:HB3	1:K:88:THR:HB	2.00	0.43
1:K:320:GLN:O	1:K:321:ALA:C	2.59	0.43
1:K:369:SER:HB3	1:K:371:PHE:CZ	2.53	0.43
1:L:32:THR:O	1:L:32:THR:HG22	2.18	0.43
1:L:389:ARG:HH22	1:L:391:ASP:CG	2.25	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:P:317:SER:O	1:P:318:GLY:C	2.60	0.43
1:S:77:ASN:ND2	1:S:77:ASN:C	2.76	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:77:ASN:HD22	1:A:79:ASN:H	1.64	0.43
1:A:425:TYR:O	1:A:425:TYR:HD1	2.01	0.43
1:B:140:SER:O	1:B:144:LEU:HG	2.17	0.43
1:B:237:ILE:HD13	1:B:237:ILE:HG21	1.85	0.43
1:D:383:LEU:HG	1:E:383:LEU:HD23	1.98	0.43
1:J:121:ASN:O	1:J:121:ASN:CG	2.61	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: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:M:315:SER:C	1:M:325:MET:CE	2.91	0.43
1:N:320:GLN:O	1:N:323:ASP:HB2	2.19	0.43
1:R:25:PRO:HD3	1:R:40:SER:OG	2.19	0.43
1:R:146:SER:O	1:S:381:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:118:TYR:CZ	1:T:114:PRO:HB3	2.53	0.43
1:B:215:GLN:CD	1:B:328:SER:HB3	2.43	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: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:O:316:LYS:N	1:O:325:MET:HE2	2.33	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:O	1:S:32:THR:HG22	2.18	0.43
1:T:112:THR:HG21	1:T:361:SER:CB	2.48	0.43
1:T:112:THR:HG22	1:T:362:VAL:H	1.69	0.43
1:B:208:ILE:O	1:B:332:SER:HA	2.19	0.43
1:B:274:ARG:HH11	1:B:274:ARG:HG3	1.83	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: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
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:50:GLY:C	1:I:359:THR:HG23	2.44	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:L:255:LEU:HD22	1:L:325:MET:HE2	2.00	0.43
1:P:112:THR:HG22	1:P:361:SER:HA	2.00	0.43
1:S:41:GLU:CD	1:S:90:GLN:HG2	2.44	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:L:193:MET:HE3	1:L:193:MET:C	2.44	0.43
1:L:358:ALA:O	1:L:361:SER:OG	2.33	0.43
1:M:214:TYR:O	1:M:328:SER:HA	2.19	0.43
1:M:320:GLN:O	1:M:321:ALA:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:193:MET:HE2	1:B:193:MET:HB3	1.83	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:J:130:GLN:NE2	1:Q:385:THR:OG1	2.52	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: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:20:MET:HE3	1:A:423:ARG:CG	2.49	0.43
1:B:315:SER:C	1:B:325:MET:HE1	2.44	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:G:41:GLU:CD	1:G:90:GLN:HG2	2.44	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:L:383:LEU:C	1:L:383:LEU:HD12	2.44	0.43
1:M:389:ARG:HB3	1:M:389:ARG:HH11	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
1:G:391:ASP:HA	1:G:392:PRO:HD2	1.84	0.42
1:I:99:CYS:HB2	1:I:373:LEU:CD2	2.48	0.42
1:I:385:THR:HG21	1:Q:130:GLN:HE22	1.84	0.42
1:K:246:LEU:HD23	1:K:246:LEU:HA	1.82	0.42
1:M:16:ARG:NH2	1:M:23:THR:HB	2.34	0.42
1:M:100:ARG:HG2	1:M:177:TYR:HA	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:LEU:HD23	1:F:246:LEU:HA	1.74	0.42
1:G:29:PRO:HG2	1:G:395:MET:HE2	2.01	0.42
1:H:286:ILE:HD13	1:H:286:ILE:HA	1.95	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:L:383:LEU:HD22	1:R:383:LEU:HD12	1.99	0.42
1:M:120:LEU:O	1:Q:113:LEU:HD13	2.19	0.42
1:N:316:LYS:HB2	1:N:325:MET:CE	2.49	0.42
1:N:389:ARG:HE	1:Q:407:ARG:HH22	1.67	0.42
1:S:165:THR:HG21	1:S:419:TYR:CD2	2.54	0.42
1:A:155:ILE:HD12	1:A:155:ILE:HA	1.95	0.42
1:B:33:LEU:N	1:B:33:LEU:HD23	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:HH11	1:G:356:ARG:CG	2.32	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:B:242:ILE:HG23	1:B:335:VAL:HG22	2.01	0.42
1:C:56:LEU:HD11	1:C:351:LEU:HB3	2.00	0.42
1:C:112:THR:HG22	1:C:362:VAL:N	2.25	0.42
1:D:319:GLY:O	1:D:320:GLN:HG3	2.19	0.42
1:H:426:PHE:CD1	1:H:426:PHE:C	2.97	0.42
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:O	1:B:12:VAL:HG12	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:20:MET:CG	1:H:423:ARG:HG2	2.50	0.42
1:H:201:ASP:O	1:H:202:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:316:LYS:N	1:H:325:MET:CE	2.83	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:N:250:THR:OG1	1:N:326:SER:O	2.37	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: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:OD1	1:Q:201:ASP:N	2.51	0.42
1:R:93:PRO:HG3	1:R:180:LEU:HB3	2.02	0.42
1:R:112:THR:CG2	1:R:361:SER:HA	2.44	0.42
1:S:242:ILE:HB	1:S:294:LEU:HB2	2.01	0.42
1:A:82:PHE:HE1	1:A:85:MET:HE2	1.84	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:121:ASN:O	1:G:160:VAL:HG11	2.19	0.42
1:G:140:SER:O	1:G:144:LEU:HG	2.20	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:92:LEU:N	1:N:93:PRO:CD	2.83	0.42
1:N:121:ASN:OD1	1:N:358:ALA:N	2.26	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:A:120:LEU:O	1:T:112:THR:HA	2.20	0.42
1:C:120:LEU:CD2	1:R:113:LEU:HB2	2.50	0.42
1:E:20:MET:HG2	1:E:423:ARG:CD	2.50	0.42
1:E:159:LEU:CD1	1:O:109:ARG:HH11	2.33	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:L:15:ILE:HG13	1:L:397:TYR:HD2	1.85	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:391:ASP:HA	1:A:392:PRO:HD2	1.84	0.42
1:F:419:TYR:CE2	1:F:423:ARG:HD2	2.55	0.42
1:I:230:PHE:CD1	1:I:230:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:280:ASN:C	1:N:280:ASN:HD22	2.28	0.42
1:N:315:SER:C	1:N:325:MET:CE	2.92	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:S:402:LEU:O	1:S:405:ARG:HB2	2.20	0.42
1:D:41:GLU:HB3	1:D:88:THR:HB	2.02	0.41
1:D:170:PRO:HB3	1:D:173:TYR:CZ	2.54	0.41
1:E:108:VAL:HG22	1:E:365:VAL:HG22	2.01	0.41
1:E:257:LEU:HD23	1:E:314:THR:HA	2.02	0.41
1:F:112:THR:HB	1:F:362:VAL:HB	2.02	0.41
1:G:126:ALA:HB3	1:G:155:ILE:HG22	2.02	0.41
1:M:316:LYS:HB2	1:M:325:MET:CE	2.37	0.41
1:N:13:PRO:HG3	1:Q:407:ARG:HH21	1.85	0.41
1:P:246:LEU:CD2	1:P:292:PHE:HZ	2.31	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:41:GLU:HB3	1:T:88:THR:HB	2.02	0.41
1:T:263:LEU:HB3	1:T:305:ILE:HD12	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
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:L:41:GLU:CD	1:L:90:GLN:HG2	2.45	0.41
1:O:193:MET:C	1:O:193:MET:CE	2.93	0.41
1:O:274:ARG:HG3	1:O:274:ARG:HH11	1.85	0.41
1:P:426:PHE:C	1:P:428:GLU:N	2.76	0.41
1:A:140:SER:O	1:A:144:LEU:HG	2.20	0.41
1:C:12:VAL:O	1:C:13:PRO:C	2.61	0.41
1:F:12:VAL:HG12	1:F:15:ILE:H	1.86	0.41
1:G:246:LEU:HD23	1:G:246:LEU:HA	1.92	0.41
1:G:293:ASN:ND2	1:K:291:PRO:CB	2.83	0.41
1:H:290:MET:HE3	1:H:292:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:60:PHE:CE2	1:M:237:ILE:HD11	2.55	0.41
1:M:90:GLN:NE2	1:S:381:LYS:HB3	2.35	0.41
1:M:316:LYS:N	1:M:325:MET:HE1	2.35	0.41
1:O:153:ASP:CG	1:O:405:ARG:HH22	2.28	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: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:C:427:MET:HE3	1:C:427:MET:HB2	1.80	0.41
1:G:277:ALA:CB	1:G:290:MET:HE2	2.50	0.41
1:K:155:ILE:O	1:K:155:ILE:HG23	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:P:320:GLN:O	1:P:321:ALA:C	2.63	0.41
1:P:428:GLU:O	1:P:429:VAL:C	2.63	0.41
1:Q:263:LEU:HB2	1:Q:272:ILE:HB	2.02	0.41
1:R:80:TYR:O	1:R:267:ASP:HB2	2.20	0.41
1:R:377:PRO:HD2	4:R:6002:HOH:O	2.19	0.41
1:T:316:LYS:CB	1:T:325:MET:HE3	2.42	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:HD13	1:C:237:ILE:HG21	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:Q:315:SER:CA	1:Q:325:MET:HE1	2.48	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:B:263:LEU:C	1:B:264:ILE:HD12	2.46	0.41
1:E:35:LYS:HD3	1:L:405:ARG:NH1	2.36	0.41
1:E:169:LEU:HD23	1:E:169:LEU:HA	1.72	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:150:ASN:OD1	1:N:384:VAL:HG13	2.21	0.41
1:K:138:ASP:OD1	1:K:138:ASP:C	2.63	0.41
1:L:316:LYS:CB	1:L:325:MET:CE	2.92	0.41
1:M:20:MET:CE	1:M:423:ARG:HE	2.28	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:P:286:ILE:HG21	1:P:286:ILE:HD13	1.69	0.41
1:S:107:THR:HG22	1:S:165:THR:OG1	2.20	0.41
1:S:274:ARG:HG3	1:S:274:ARG:NH1	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:H:121:ASN:CG	1:H:121:ASN:O	2.63	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:77:ASN:HD22	1:A:77:ASN:C	2.28	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:193:MET:HG2	1:H:194:VAL:N	2.35	0.41
1:H:293:ASN:N	1:H:293:ASN:ND2	2.68	0.41
1:I:130:GLN:NE2	1:J:385:THR:OG1	2.54	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:237:ILE:HG22	1:B:238:THR:HG23	2.03	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:HD22	1:F:121:ASN:N	2.19	0.41
1:G:208:ILE:O	1:G:332:SER:HA	2.21	0.41
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:220:TYR:CG	1:H:221:GLN:N	2.89	0.41
1:H:399:LYS:NZ	4:H:6000:HOH:O	2.54	0.41
1:I:173:TYR:HD2	1:I:173:TYR:HA	1.79	0.41
1:I:193:MET:HG2	1:I:194:VAL:N	2.35	0.41
1:J:246:LEU:HD12	1:J:290:MET:CE	2.51	0.41
1:K:20:MET:HE1	1:K:427:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:41:GLU:OE1	1:K:90:GLN:HG2	2.20	0.41
1:L:246:LEU:HD23	1:L:246:LEU:HA	1.95	0.41
1:M:237:ILE:HG21	1:M:237:ILE:HD13	1.77	0.41
1:N:41:GLU:CD	1:N:90:GLN:HG2	2.45	0.41
1:N:247:VAL:HG22	1:N:289:LEU:HD23	2.03	0.41
1:O:15:ILE:HG13	1:O:397:TYR:HD2	1.85	0.41
1:O:127:VAL:CG2	1:O:148:THR:HG22	2.51	0.41
1:O:273:THR:O	1:O:274:ARG:HD3	2.21	0.41
1:Q:175:LEU:HB3	1:Q:342:TYR:OH	2.21	0.41
1:Q:246:LEU:HD23	1:Q:246:LEU:HA	1.77	0.41
1:R:153:ASP:CG	1:R:405:ARG:HH22	2.28	0.41
1:S:171:THR:HA	1:T:34:GLU:HG3	2.01	0.41
1:S:258:ASP:HB2	1:S:313:VAL:HB	2.03	0.41
1:T:124:ILE:HG21	1:T:164:VAL:HG21	2.03	0.41
1:T:259:ALA:HB1	1:T:290:MET:HE1	2.02	0.41
1:A:93:PRO:HG3	1:A:180:LEU:HB3	2.03	0.41
1:B:82:PHE:CZ	1:B:84:GLN:HA	2.56	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: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:A:259:ALA:HA	1:A:311:GLU:O	2.21	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:H:20:MET:HE3	1:H:423:ARG:HE	1.86	0.40
1:I:20:MET:HE1	1:I:427:MET:SD	2.60	0.40
1:J:56:LEU:HD11	1:J:351:LEU:HB3	2.04	0.40
1:K:255:LEU:HD21	1:K:325:MET:HB3	2.03	0.40
1:K:286:ILE:HG22	1:K:288:ASN:ND2	2.36	0.40
1:N:253:HIS:CG	1:N:254:GLY:N	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:S:20:MET:HE1	1:S:427:MET:CG	2.50	0.40
1:S:122:GLY:C	1:S:160:VAL:HG22	2.46	0.40
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:F:41:GLU:CD	1:F:90:GLN:HG2	2.46	0.40
1:F:153:ASP:OD2	1:F:412:THR:OG1	2.35	0.40
1:G:383:LEU:HD12	1:G:384:VAL:O	2.20	0.40
1:J:92:LEU:N	1:J:93:PRO:CD	2.85	0.40
1:J:166:VAL:HG13	1:J:350:THR:HG21	2.03	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:S:117:VAL:C	4:S:648:HOH:O	2.64	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:136:LEU:HD13	1:G:351:LEU:HD11	2.03	0.40
1:G:190:ASP:OD1	1:G:191:PRO:HD2	2.21	0.40
1:H:390:PHE:CZ	1:H:392:PRO:HG3	2.57	0.40
1:I:121:ASN:O	1:I:121:ASN:CG	2.65	0.40
1:K:316:LYS:HB2	1:K:325:MET:CE	2.52	0.40
1:L:426:PHE:C	1:L:426:PHE:CD1	2.99	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:O:230:PHE:CD1	1:O:230:PHE:C	3.00	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:S:259:ALA:CB	1:S:290:MET:HE1	2.52	0.40
1:T:201:ASP:O	1:T:339:GLY:HA2	2.22	0.40
1:B:20:MET:CE	1:B:427:MET:HE2	2.51	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:G:426:PHE:C	1:G:428:GLU:H	2.29	0.40
1:H:98:TYR:HA	1:H:178:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:356:ARG:HG2	1:H:356:ARG:HH11	1.87	0.40
1:I:262:TYR:HB2	1:I:309:LYS:HG2	2.03	0.40
1:J:214:TYR:HB2	1:Q:190:ASP:OD2	2.22	0.40
1:K:14:PHE:CG	1:K:29:PRO:HD3	2.56	0.40
1:K:155:ILE:O	1:K:155:ILE:CG2	2.69	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
1:P:95:SER:HA	1:P:376:ASN:ND2	2.36	0.40
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.70	0.40
1:B:201:ASP:O	1:B:339:GLY:HA2	2.21	0.40
1:D:20:MET:HE1	1:D:427:MET:SD	2.62	0.40
1:E:385:THR:C	1:E:386:GLU:HG2	2.47	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:J:376:ASN:OD1	1:J:376:ASN:C	2.64	0.40
1:J:402:LEU:CD1	1:Q:33:LEU:HD13	2.42	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:Q:104:ARG:HG3	1:Q:105:SER:N	2.37	0.40
1:S:20:MET:CE	1:S:423:ARG:CZ	3.00	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%)	18 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	416/458 (91%)	399 (96%)	16 (4%)	1 (0%)	43	66
1	C	409/458 (89%)	390 (95%)	17 (4%)	2 (0%)	24	46
1	D	409/458 (89%)	387 (95%)	21 (5%)	1 (0%)	43	66
1	E	411/458 (90%)	392 (95%)	18 (4%)	1 (0%)	43	66
1	F	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	18	38
1	G	408/458 (89%)	389 (95%)	17 (4%)	2 (0%)	24	46
1	H	409/458 (89%)	390 (95%)	18 (4%)	1 (0%)	43	66
1	I	409/458 (89%)	388 (95%)	20 (5%)	1 (0%)	43	66
1	J	407/458 (89%)	387 (95%)	17 (4%)	3 (1%)	18	38
1	K	413/458 (90%)	391 (95%)	20 (5%)	2 (0%)	24	46
1	L	416/458 (91%)	396 (95%)	17 (4%)	3 (1%)	18	38
1	M	408/458 (89%)	388 (95%)	19 (5%)	1 (0%)	43	66
1	N	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	18	38
1	O	408/458 (89%)	386 (95%)	19 (5%)	3 (1%)	18	38
1	P	413/458 (90%)	388 (94%)	21 (5%)	4 (1%)	12	28
1	Q	413/458 (90%)	394 (95%)	17 (4%)	2 (0%)	24	46
1	R	407/458 (89%)	391 (96%)	15 (4%)	1 (0%)	43	66
1	S	410/458 (90%)	389 (95%)	19 (5%)	2 (0%)	24	46
1	T	416/458 (91%)	392 (94%)	23 (6%)	1 (0%)	43	66
All	All	8218/9160 (90%)	7810 (95%)	368 (4%)	40 (0%)	24	46

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

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Mol	Chain	Res	Type
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
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 [i](#)

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%)	332 (94%)	20 (6%)	18	40
1	B	351/385 (91%)	327 (93%)	24 (7%)	14	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	349/385 (91%)	330 (95%)	19 (5%)	20	42
1	D	349/385 (91%)	333 (95%)	16 (5%)	24	49
1	E	350/385 (91%)	330 (94%)	20 (6%)	18	40
1	F	348/385 (90%)	323 (93%)	25 (7%)	13	30
1	G	348/385 (90%)	326 (94%)	22 (6%)	16	36
1	H	349/385 (91%)	329 (94%)	20 (6%)	18	40
1	I	349/385 (91%)	335 (96%)	14 (4%)	28	55
1	J	347/385 (90%)	330 (95%)	17 (5%)	22	47
1	K	350/385 (91%)	324 (93%)	26 (7%)	13	29
1	L	351/385 (91%)	326 (93%)	25 (7%)	13	31
1	M	348/385 (90%)	326 (94%)	22 (6%)	16	36
1	N	347/385 (90%)	324 (93%)	23 (7%)	15	34
1	O	348/385 (90%)	332 (95%)	16 (5%)	24	49
1	P	350/385 (91%)	322 (92%)	28 (8%)	11	25
1	Q	350/385 (91%)	327 (93%)	23 (7%)	15	34
1	R	347/385 (90%)	323 (93%)	24 (7%)	14	32
1	S	348/385 (90%)	332 (95%)	16 (5%)	24	49
1	T	351/385 (91%)	332 (95%)	19 (5%)	20	42
All	All	6982/7700 (91%)	6563 (94%)	419 (6%)	17	37

All (419) 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	159	LEU
1	A	164	VAL
1	A	187	ILE
1	A	201	ASP
1	A	202	ARG
1	A	218	SER
1	A	219	GLN
1	A	286	ILE
1	A	291	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	315	SER
1	A	316	LYS
1	A	323	ASP
1	A	330	SER
1	A	361	SER
1	A	383	LEU
1	A	386	GLU
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
1	B	132	SER
1	B	151	ILE
1	B	159	LEU
1	B	193	MET
1	B	219	GLN
1	B	221	GLN
1	B	241	SER
1	B	246	LEU
1	B	258	ASP
1	B	261	ILE
1	B	276	VAL
1	B	279	ASP
1	B	284	THR
1	B	292	PHE
1	B	333	LEU
1	B	383	LEU
1	B	420	THR
1	C	54	SER
1	C	95	SER
1	C	99	CYS
1	C	100	ARG
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	219	GLN
1	C	222	SER
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	113	LEU
1	D	120	LEU
1	D	164	VAL
1	D	199	SER
1	D	201	ASP
1	D	202	ARG
1	D	213	ASP
1	D	269	THR
1	D	284	THR
1	D	296	ILE
1	D	313	VAL
1	D	315	SER
1	D	323	ASP
1	D	349	VAL
1	D	383	LEU
1	D	425	TYR
1	E	76	SER
1	E	99	CYS
1	E	100	ARG
1	E	112	THR
1	E	132	SER
1	E	162	GLU
1	E	164	VAL
1	E	170	PRO
1	E	193	MET
1	E	199	SER
1	E	261	ILE
1	E	279	ASP
1	E	284	THR
1	E	286	ILE
1	E	309	LYS
1	E	311	GLU
1	E	324	GLN
1	E	328	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	356	ARG
1	E	389	ARG
1	F	12	VAL
1	F	29	PRO
1	F	54	SER
1	F	75	GLN
1	F	109	ARG
1	F	112	THR
1	F	120	LEU
1	F	121	ASN
1	F	146	SER
1	F	160	VAL
1	F	164	VAL
1	F	201	ASP
1	F	222	SER
1	F	225	VAL
1	F	240	LEU
1	F	269	THR
1	F	272	ILE
1	F	276	VAL
1	F	284	THR
1	F	315	SER
1	F	379	LEU
1	F	383	LEU
1	F	403	SER
1	F	406	GLU
1	F	418	GLU
1	G	12	VAL
1	G	29	PRO
1	G	44	THR
1	G	51	ASP
1	G	121	ASN
1	G	164	VAL
1	G	215	GLN
1	G	219	GLN
1	G	261	ILE
1	G	269	THR
1	G	272	ILE
1	G	276	VAL
1	G	286	ILE
1	G	305	ILE
1	G	316	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	325	MET
1	G	349	VAL
1	G	356	ARG
1	G	383	LEU
1	G	406	GLU
1	G	417	ARG
1	G	425	TYR
1	H	51	ASP
1	H	81	LYS
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	274	ARG
1	H	284	THR
1	H	286	ILE
1	H	293	ASN
1	H	299	ASN
1	H	328	SER
1	H	386	GLU
1	H	403	SER
1	H	407	ARG
1	H	417	ARG
1	I	25	PRO
1	I	99	CYS
1	I	112	THR
1	I	159	LEU
1	I	201	ASP
1	I	273	THR
1	I	284	THR
1	I	286	ILE
1	I	363	VAL
1	I	383	LEU
1	I	386	GLU
1	I	389	ARG
1	I	391	ASP
1	I	417	ARG
1	J	25	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	44	THR
1	J	76	SER
1	J	100	ARG
1	J	105	SER
1	J	120	LEU
1	J	121	ASN
1	J	160	VAL
1	J	164	VAL
1	J	219	GLN
1	J	225	VAL
1	J	284	THR
1	J	286	ILE
1	J	323	ASP
1	J	328	SER
1	J	417	ARG
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	202	ARG
1	K	213	ASP
1	K	269	THR
1	K	272	ILE
1	K	286	ILE
1	K	291	PRO
1	K	293	ASN
1	K	320	GLN
1	K	324	GLN
1	K	325	MET
1	K	351	LEU
1	K	379	LEU
1	K	381	LYS
1	K	383	LEU
1	K	386	GLU
1	K	402	LEU
1	K	403	SER
1	K	407	ARG
1	K	424	GLU
1	K	428	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	51	ASP
1	L	54	SER
1	L	76	SER
1	L	106	LEU
1	L	112	THR
1	L	113	LEU
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	269	THR
1	L	276	VAL
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	M	12	VAL
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
1	M	201	ASP
1	M	202	ARG
1	M	219	GLN
1	M	273	THR
1	M	274	ARG
1	M	276	VAL
1	M	328	SER
1	M	330	SER
1	M	333	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	379	LEU
1	M	383	LEU
1	M	389	ARG
1	M	399	LYS
1	M	417	ARG
1	N	11	ILE
1	N	29	PRO
1	N	76	SER
1	N	112	THR
1	N	121	ASN
1	N	132	SER
1	N	160	VAL
1	N	164	VAL
1	N	202	ARG
1	N	219	GLN
1	N	251	SER
1	N	261	ILE
1	N	272	ILE
1	N	283	THR
1	N	286	ILE
1	N	315	SER
1	N	317	SER
1	N	324	GLN
1	N	351	LEU
1	N	383	LEU
1	N	403	SER
1	N	411	LYS
1	N	424	GLU
1	O	29	PRO
1	O	68	VAL
1	O	110	SER
1	O	121	ASN
1	O	132	SER
1	O	159	LEU
1	O	160	VAL
1	O	164	VAL
1	O	261	ILE
1	O	286	ILE
1	O	308	ILE
1	O	315	SER
1	O	320	GLN
1	O	349	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	383	LEU
1	O	389	ARG
1	P	25	PRO
1	P	34	GLU
1	P	67	ILE
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	219	GLN
1	P	226	THR
1	P	241	SER
1	P	270	THR
1	P	272	ILE
1	P	274	ARG
1	P	276	VAL
1	P	286	ILE
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	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	159	LEU
1	Q	160	VAL
1	Q	164	VAL
1	Q	193	MET
1	Q	202	ARG
1	Q	219	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Q	276	VAL
1	Q	284	THR
1	Q	286	ILE
1	Q	324	GLN
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	120	LEU
1	R	121	ASN
1	R	164	VAL
1	R	202	ARG
1	R	213	ASP
1	R	245	GLU
1	R	261	ILE
1	R	269	THR
1	R	284	THR
1	R	286	ILE
1	R	293	ASN
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	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

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Mol	Chain	Res	Type
1	S	261	ILE
1	S	269	THR
1	S	272	ILE
1	S	278	SER
1	S	286	ILE
1	S	315	SER
1	S	324	GLN
1	S	351	LEU
1	S	383	LEU
1	T	16	ARG
1	T	33	LEU
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	202	ARG
1	T	284	THR
1	T	297	PRO
1	T	383	LEU
1	T	403	SER
1	T	404	GLU
1	T	407	ARG
1	T	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	79	ASN
1	A	130	GLN
1	A	142	ASN
1	A	215	GLN
1	A	219	GLN
1	A	233	ASN
1	A	253	HIS
1	B	90	GLN
1	B	142	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	152	ASN
1	B	219	GLN
1	B	303	GLN
1	C	90	GLN
1	C	97	ASN
1	C	130	GLN
1	C	219	GLN
1	C	233	ASN
1	C	299	ASN
1	D	46	ASN
1	D	90	GLN
1	D	121	ASN
1	D	142	ASN
1	D	152	ASN
1	D	219	GLN
1	D	324	GLN
1	E	90	GLN
1	E	130	GLN
1	E	152	ASN
1	E	253	HIS
1	E	288	ASN
1	F	90	GLN
1	F	142	ASN
1	F	249	HIS
1	F	299	ASN
1	F	338	HIS
1	F	382	ASN
1	G	130	GLN
1	G	142	ASN
1	G	221	GLN
1	G	233	ASN
1	G	293	ASN
1	G	299	ASN
1	G	320	GLN
1	H	90	GLN
1	H	130	GLN
1	H	215	GLN
1	H	233	ASN
1	H	293	ASN
1	H	320	GLN
1	H	324	GLN
1	I	75	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	90	GLN
1	I	121	ASN
1	I	130	GLN
1	I	142	ASN
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	221	GLN
1	J	233	ASN
1	J	299	ASN
1	J	324	GLN
1	K	79	ASN
1	K	90	GLN
1	K	121	ASN
1	K	130	GLN
1	K	233	ASN
1	K	293	ASN
1	K	320	GLN
1	L	79	ASN
1	L	121	ASN
1	L	130	GLN
1	L	233	ASN
1	L	303	GLN
1	L	382	ASN
1	M	90	GLN
1	M	121	ASN
1	M	130	GLN
1	M	152	ASN
1	M	324	GLN
1	N	79	ASN
1	N	84	GLN
1	N	97	ASN
1	N	130	GLN
1	N	142	ASN
1	N	221	GLN
1	N	233	ASN
1	N	280	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	N	382	ASN
1	N	396	ASN
1	O	79	ASN
1	O	90	GLN
1	O	121	ASN
1	O	142	ASN
1	O	219	GLN
1	O	233	ASN
1	O	280	ASN
1	O	320	GLN
1	P	90	GLN
1	P	121	ASN
1	P	219	GLN
1	P	233	ASN
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	215	GLN
1	R	219	GLN
1	R	233	ASN
1	R	303	GLN
1	R	320	GLN
1	R	324	GLN
1	R	382	ASN
1	S	77	ASN
1	S	90	GLN
1	S	97	ASN
1	S	121	ASN
1	S	130	GLN
1	S	233	ASN
1	S	320	GLN
1	S	324	GLN
1	T	75	GLN
1	T	84	GLN
1	T	121	ASN
1	T	130	GLN
1	T	219	GLN

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Mol	Chain	Res	Type
1	T	233	ASN
1	T	293	ASN
1	T	324	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	420/458 (91%)	-0.61	3 (0%) 84 82	23, 33, 72, 105	0
1	B	418/458 (91%)	-0.56	9 (2%) 62 57	20, 32, 67, 106	0
1	C	413/458 (90%)	-0.52	7 (1%) 69 64	26, 37, 72, 105	0
1	D	413/458 (90%)	-0.64	5 (1%) 76 73	23, 34, 63, 106	0
1	E	415/458 (90%)	-0.39	12 (2%) 53 48	27, 36, 74, 114	0
1	F	413/458 (90%)	-0.63	6 (1%) 72 68	22, 35, 66, 98	0
1	G	412/458 (89%)	-0.59	3 (0%) 84 82	25, 37, 61, 106	0
1	H	413/458 (90%)	-0.50	6 (1%) 72 68	27, 39, 67, 114	0
1	I	413/458 (90%)	-0.52	5 (1%) 76 73	28, 38, 71, 107	0
1	J	411/458 (89%)	-0.53	5 (1%) 76 73	27, 38, 70, 99	0
1	K	417/458 (91%)	-0.52	6 (1%) 73 69	27, 38, 74, 108	0
1	L	418/458 (91%)	-0.58	4 (0%) 79 76	24, 34, 73, 103	0
1	M	412/458 (89%)	-0.53	4 (0%) 79 76	25, 38, 68, 105	0
1	N	413/458 (90%)	-0.49	4 (0%) 79 76	27, 38, 68, 104	0
1	O	412/458 (89%)	-0.56	4 (0%) 79 76	27, 37, 72, 104	0
1	P	417/458 (91%)	-0.37	11 (2%) 57 51	27, 39, 82, 112	0
1	Q	417/458 (91%)	-0.45	10 (2%) 59 54	27, 39, 77, 118	0
1	R	411/458 (89%)	-0.56	6 (1%) 72 68	26, 36, 56, 102	0
1	S	414/458 (90%)	-0.61	2 (0%) 87 85	25, 35, 65, 95	0
1	T	418/458 (91%)	-0.65	4 (0%) 79 76	23, 33, 62, 101	0
All	All	8290/9160 (90%)	-0.54	116 (1%) 73 69	20, 37, 70, 118	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	117	VAL	4.5
1	R	113	LEU	4.4
1	F	113	LEU	4.3
1	Q	113	LEU	4.3
1	N	113	LEU	4.1
1	Q	120	LEU	4.1
1	B	119	ALA	4.0
1	H	113	LEU	4.0
1	P	113	LEU	3.6
1	B	426	PHE	3.6
1	E	113	LEU	3.6
1	M	113	LEU	3.4
1	I	113	LEU	3.4
1	Q	427	MET	3.4
1	H	120	LEU	3.3
1	I	120	LEU	3.3
1	E	430	ALA	3.3
1	Q	425	TYR	3.2
1	P	223	GLY	3.2
1	B	120	LEU	3.1
1	C	426	PHE	3.1
1	D	429	VAL	3.1
1	C	425	TYR	3.0
1	C	11	ILE	3.0
1	P	425	TYR	3.0
1	R	425	TYR	3.0
1	C	223	GLY	3.0
1	M	112	THR	3.0
1	K	430	ALA	3.0
1	M	120	LEU	3.0
1	O	113	LEU	2.9
1	P	429	VAL	2.9
1	A	113	LEU	2.9
1	K	120	LEU	2.9
1	D	425	TYR	2.9
1	B	117	VAL	2.9
1	C	120	LEU	2.8
1	S	113	LEU	2.8
1	C	113	LEU	2.8
1	F	425	TYR	2.8
1	E	252	VAL	2.8
1	G	113	LEU	2.7
1	B	429	VAL	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	N	318	GLY	2.7
1	B	292	PHE	2.7
1	D	426	PHE	2.7
1	O	426	PHE	2.7
1	I	114	PRO	2.7
1	P	11	ILE	2.6
1	L	120	LEU	2.6
1	E	11	ILE	2.6
1	H	425	TYR	2.6
1	I	427	MET	2.6
1	L	11	ILE	2.6
1	G	120	LEU	2.6
1	K	113	LEU	2.6
1	F	427	MET	2.5
1	E	254	GLY	2.5
1	E	121	ASN	2.5
1	F	120	LEU	2.5
1	Q	114	PRO	2.5
1	A	119	ALA	2.5
1	C	321	ALA	2.5
1	P	220	TYR	2.5
1	N	116	GLY	2.5
1	Q	116	GLY	2.5
1	K	429	VAL	2.5
1	Q	430	ALA	2.5
1	E	251	SER	2.5
1	A	118	TYR	2.5
1	D	11	ILE	2.4
1	R	427	MET	2.4
1	H	429	VAL	2.4
1	J	426	PHE	2.4
1	N	11	ILE	2.4
1	P	119	ALA	2.4
1	R	114	PRO	2.3
1	P	319	GLY	2.3
1	P	120	LEU	2.3
1	O	425	TYR	2.3
1	T	425	TYR	2.3
1	H	121	ASN	2.3
1	J	425	TYR	2.3
1	E	427	MET	2.3
1	Q	115	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	426	PHE	2.3
1	J	120	LEU	2.3
1	T	113	LEU	2.3
1	O	114	PRO	2.2
1	F	115	GLY	2.2
1	F	426	PHE	2.2
1	J	112	THR	2.2
1	H	114	PRO	2.2
1	E	284	THR	2.2
1	B	291	PRO	2.2
1	E	111	SER	2.2
1	B	251	SER	2.2
1	E	225	VAL	2.1
1	P	426	PHE	2.1
1	Q	426	PHE	2.1
1	T	426	PHE	2.1
1	D	112	THR	2.1
1	B	425	TYR	2.1
1	M	425	TYR	2.1
1	R	120	LEU	2.1
1	R	112	THR	2.1
1	E	120	LEU	2.1
1	L	425	TYR	2.1
1	T	11	ILE	2.1
1	J	429	VAL	2.1
1	S	120	LEU	2.0
1	I	11	ILE	2.0
1	P	292	PHE	2.0
1	K	114	PRO	2.0
1	Q	429	VAL	2.0
1	G	425	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
2	CL	I	5507	1/1	0.97	0.04	33,33,33,33	0
2	CL	G	5505	1/1	0.98	0.05	33,33,33,33	0
2	CL	H	5506	1/1	0.98	0.05	31,31,31,31	0
2	CL	B	5501	1/1	0.98	0.03	26,26,26,26	1
2	CL	R	5508	1/1	0.98	0.03	27,27,27,27	0
2	CL	A	5503	1/1	0.99	0.03	32,32,32,32	0
2	CL	P	5502	1/1	0.99	0.03	26,26,26,26	1
2	CL	C	5504	1/1	0.99	0.02	30,30,30,30	0
3	CA	P	5902	1/1	0.99	0.07	40,40,40,40	1
3	CA	B	5901	1/1	1.00	0.06	33,33,33,33	1
3	CA	C	5904	1/1	1.00	0.09	39,39,39,39	0
3	CA	G	5905	1/1	1.00	0.09	45,45,45,45	0
3	CA	H	5906	1/1	1.00	0.06	39,39,39,39	0
3	CA	I	5907	1/1	1.00	0.07	41,41,41,41	0
3	CA	A	5903	1/1	1.00	0.05	34,34,34,34	0
3	CA	R	5908	1/1	1.00	0.06	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.