



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 AM GMT

PDB ID : 2FHH
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome in complex with
a peptidyl boronate inhibitor MLN-273
Authors : Li, H.
Deposited on : 2005-12-23
Resolution : 2.99 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

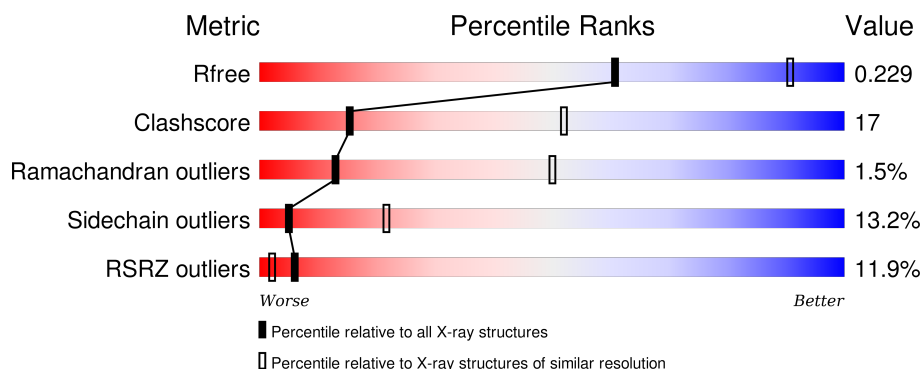
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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



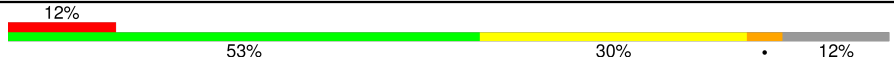




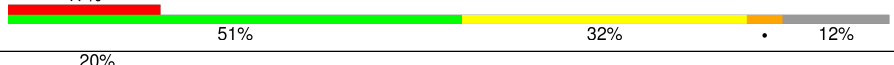
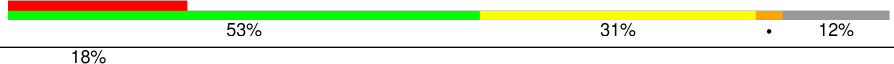

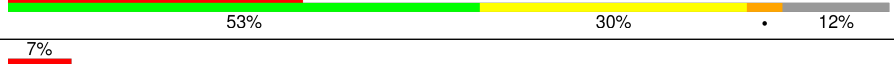


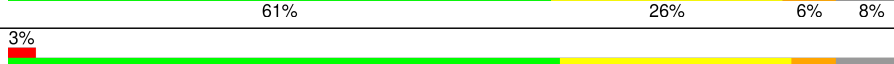

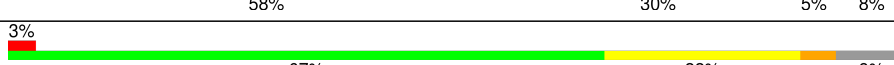

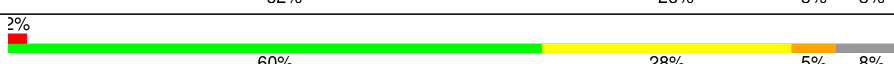
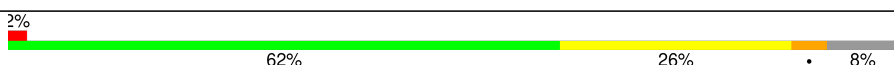
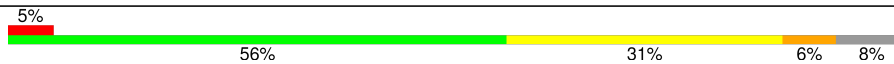
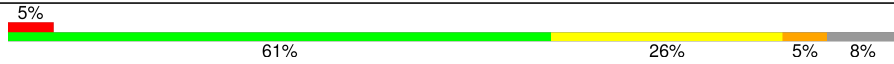




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	1	251	<div> <div>23%</div> <div>54%</div> <div>30%</div> <div>•</div> <div>12%</div> </div>
1	A	251	<div> <div>6%</div> <div>55%</div> <div>29%</div> <div>•</div> <div>12%</div> </div>
1	B	251	<div> <div>12%</div> <div>53%</div> <div>30%</div> <div>•</div> <div>12%</div> </div>
1	D	251	<div> <div>18%</div> <div>54%</div> <div>30%</div> <div>•</div> <div>12%</div> </div>
1	F	251	<div> <div>15%</div> <div>53%</div> <div>29%</div> <div>5%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	251	
1	K	251	
1	M	251	
1	O	251	
1	Q	251	
1	S	251	
1	U	251	
1	W	251	
1	Y	251	
2	2	240	
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	M1N	2	273	-	-	-	X
3	M1N	T	273	-	-	-	X
3	M1N	V	273	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47389 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 20S proteasome, alpha and beta subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	B	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	D	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	F	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	I	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	K	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	M	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	O	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	Q	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	S	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	U	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	W	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	Y	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0
1	1	220	Total 1692	C 1058	N 309	O 322	S 3	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	INITIATING METHIONINE	GB 76783992

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	CLONING ARTIFACT	GB 76783992
A	0	SER	-	CLONING ARTIFACT	GB 76783992
A	1	SER	-	CLONING ARTIFACT	GB 76783992
B	-2	MET	-	INITIATING METHIONINE	GB 76783992
B	-1	ASN	-	CLONING ARTIFACT	GB 76783992
B	0	SER	-	CLONING ARTIFACT	GB 76783992
B	1	SER	-	CLONING ARTIFACT	GB 76783992
D	-2	MET	-	INITIATING METHIONINE	GB 76783992
D	-1	ASN	-	CLONING ARTIFACT	GB 76783992
D	0	SER	-	CLONING ARTIFACT	GB 76783992
D	1	SER	-	CLONING ARTIFACT	GB 76783992
F	-2	MET	-	INITIATING METHIONINE	GB 76783992
F	-1	ASN	-	CLONING ARTIFACT	GB 76783992
F	0	SER	-	CLONING ARTIFACT	GB 76783992
F	1	SER	-	CLONING ARTIFACT	GB 76783992
I	-2	MET	-	INITIATING METHIONINE	GB 76783992
I	-1	ASN	-	CLONING ARTIFACT	GB 76783992
I	0	SER	-	CLONING ARTIFACT	GB 76783992
I	1	SER	-	CLONING ARTIFACT	GB 76783992
K	-2	MET	-	INITIATING METHIONINE	GB 76783992
K	-1	ASN	-	CLONING ARTIFACT	GB 76783992
K	0	SER	-	CLONING ARTIFACT	GB 76783992
K	1	SER	-	CLONING ARTIFACT	GB 76783992
M	-2	MET	-	INITIATING METHIONINE	GB 76783992
M	-1	ASN	-	CLONING ARTIFACT	GB 76783992
M	0	SER	-	CLONING ARTIFACT	GB 76783992
M	1	SER	-	CLONING ARTIFACT	GB 76783992
O	-2	MET	-	INITIATING METHIONINE	GB 76783992
O	-1	ASN	-	CLONING ARTIFACT	GB 76783992
O	0	SER	-	CLONING ARTIFACT	GB 76783992
O	1	SER	-	CLONING ARTIFACT	GB 76783992
Q	-2	MET	-	INITIATING METHIONINE	GB 76783992
Q	-1	ASN	-	CLONING ARTIFACT	GB 76783992
Q	0	SER	-	CLONING ARTIFACT	GB 76783992
Q	1	SER	-	CLONING ARTIFACT	GB 76783992
S	-2	MET	-	INITIATING METHIONINE	GB 76783992
S	-1	ASN	-	CLONING ARTIFACT	GB 76783992
S	0	SER	-	CLONING ARTIFACT	GB 76783992
S	1	SER	-	CLONING ARTIFACT	GB 76783992
U	-2	MET	-	INITIATING METHIONINE	GB 76783992
U	-1	ASN	-	CLONING ARTIFACT	GB 76783992
U	0	SER	-	CLONING ARTIFACT	GB 76783992

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Chain	Residue	Modelled	Actual	Comment	Reference
U	1	SER	-	CLONING ARTIFACT	GB 76783992
W	-2	MET	-	INITIATING METHIONINE	GB 76783992
W	-1	ASN	-	CLONING ARTIFACT	GB 76783992
W	0	SER	-	CLONING ARTIFACT	GB 76783992
W	1	SER	-	CLONING ARTIFACT	GB 76783992
Y	-2	MET	-	INITIATING METHIONINE	GB 76783992
Y	-1	ASN	-	CLONING ARTIFACT	GB 76783992
Y	0	SER	-	CLONING ARTIFACT	GB 76783992
Y	1	SER	-	CLONING ARTIFACT	GB 76783992
1	-2	MET	-	INITIATING METHIONINE	GB 76783992
1	-1	ASN	-	CLONING ARTIFACT	GB 76783992
1	0	SER	-	CLONING ARTIFACT	GB 76783992
1	1	SER	-	CLONING ARTIFACT	GB 76783992

- Molecule 2 is a protein called proteasome, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	C	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	E	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	L	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	N	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	P	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	R	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	T	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	V	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	X	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	Z	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	535	HIS	-	EXPRESSION TAG	GB 13881852
H	536	HIS	-	EXPRESSION TAG	GB 13881852
H	537	HIS	-	EXPRESSION TAG	GB 13881852
H	538	HIS	-	EXPRESSION TAG	GB 13881852
H	539	HIS	-	EXPRESSION TAG	GB 13881852
H	540	HIS	-	EXPRESSION TAG	GB 13881852
C	535	HIS	-	EXPRESSION TAG	GB 13881852
C	536	HIS	-	EXPRESSION TAG	GB 13881852
C	537	HIS	-	EXPRESSION TAG	GB 13881852
C	538	HIS	-	EXPRESSION TAG	GB 13881852
C	539	HIS	-	EXPRESSION TAG	GB 13881852
C	540	HIS	-	EXPRESSION TAG	GB 13881852
E	535	HIS	-	EXPRESSION TAG	GB 13881852
E	536	HIS	-	EXPRESSION TAG	GB 13881852
E	537	HIS	-	EXPRESSION TAG	GB 13881852
E	538	HIS	-	EXPRESSION TAG	GB 13881852
E	539	HIS	-	EXPRESSION TAG	GB 13881852
E	540	HIS	-	EXPRESSION TAG	GB 13881852
G	535	HIS	-	EXPRESSION TAG	GB 13881852
G	536	HIS	-	EXPRESSION TAG	GB 13881852
G	537	HIS	-	EXPRESSION TAG	GB 13881852
G	538	HIS	-	EXPRESSION TAG	GB 13881852
G	539	HIS	-	EXPRESSION TAG	GB 13881852
G	540	HIS	-	EXPRESSION TAG	GB 13881852
J	535	HIS	-	EXPRESSION TAG	GB 13881852
J	536	HIS	-	EXPRESSION TAG	GB 13881852
J	537	HIS	-	EXPRESSION TAG	GB 13881852
J	538	HIS	-	EXPRESSION TAG	GB 13881852
J	539	HIS	-	EXPRESSION TAG	GB 13881852
J	540	HIS	-	EXPRESSION TAG	GB 13881852
L	535	HIS	-	EXPRESSION TAG	GB 13881852
L	536	HIS	-	EXPRESSION TAG	GB 13881852
L	537	HIS	-	EXPRESSION TAG	GB 13881852
L	538	HIS	-	EXPRESSION TAG	GB 13881852
L	539	HIS	-	EXPRESSION TAG	GB 13881852
L	540	HIS	-	EXPRESSION TAG	GB 13881852

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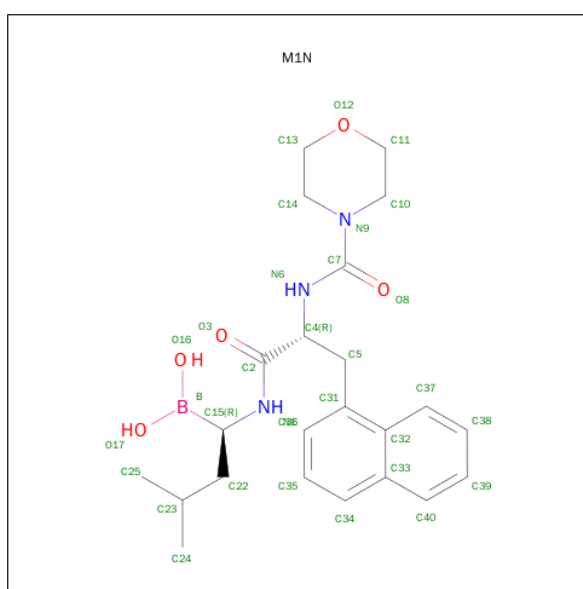
Chain	Residue	Modelled	Actual	Comment	Reference
N	535	HIS	-	EXPRESSION TAG	GB 13881852
N	536	HIS	-	EXPRESSION TAG	GB 13881852
N	537	HIS	-	EXPRESSION TAG	GB 13881852
N	538	HIS	-	EXPRESSION TAG	GB 13881852
N	539	HIS	-	EXPRESSION TAG	GB 13881852
N	540	HIS	-	EXPRESSION TAG	GB 13881852
P	535	HIS	-	EXPRESSION TAG	GB 13881852
P	536	HIS	-	EXPRESSION TAG	GB 13881852
P	537	HIS	-	EXPRESSION TAG	GB 13881852
P	538	HIS	-	EXPRESSION TAG	GB 13881852
P	539	HIS	-	EXPRESSION TAG	GB 13881852
P	540	HIS	-	EXPRESSION TAG	GB 13881852
R	535	HIS	-	EXPRESSION TAG	GB 13881852
R	536	HIS	-	EXPRESSION TAG	GB 13881852
R	537	HIS	-	EXPRESSION TAG	GB 13881852
R	538	HIS	-	EXPRESSION TAG	GB 13881852
R	539	HIS	-	EXPRESSION TAG	GB 13881852
R	540	HIS	-	EXPRESSION TAG	GB 13881852
T	535	HIS	-	EXPRESSION TAG	GB 13881852
T	536	HIS	-	EXPRESSION TAG	GB 13881852
T	537	HIS	-	EXPRESSION TAG	GB 13881852
T	538	HIS	-	EXPRESSION TAG	GB 13881852
T	539	HIS	-	EXPRESSION TAG	GB 13881852
T	540	HIS	-	EXPRESSION TAG	GB 13881852
V	535	HIS	-	EXPRESSION TAG	GB 13881852
V	536	HIS	-	EXPRESSION TAG	GB 13881852
V	537	HIS	-	EXPRESSION TAG	GB 13881852
V	538	HIS	-	EXPRESSION TAG	GB 13881852
V	539	HIS	-	EXPRESSION TAG	GB 13881852
V	540	HIS	-	EXPRESSION TAG	GB 13881852
X	535	HIS	-	EXPRESSION TAG	GB 13881852
X	536	HIS	-	EXPRESSION TAG	GB 13881852
X	537	HIS	-	EXPRESSION TAG	GB 13881852
X	538	HIS	-	EXPRESSION TAG	GB 13881852
X	539	HIS	-	EXPRESSION TAG	GB 13881852
X	540	HIS	-	EXPRESSION TAG	GB 13881852
Z	535	HIS	-	EXPRESSION TAG	GB 13881852
Z	536	HIS	-	EXPRESSION TAG	GB 13881852
Z	537	HIS	-	EXPRESSION TAG	GB 13881852
Z	538	HIS	-	EXPRESSION TAG	GB 13881852
Z	539	HIS	-	EXPRESSION TAG	GB 13881852
Z	540	HIS	-	EXPRESSION TAG	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
2	535	HIS	-	EXPRESSION TAG	GB 13881852
2	536	HIS	-	EXPRESSION TAG	GB 13881852
2	537	HIS	-	EXPRESSION TAG	GB 13881852
2	538	HIS	-	EXPRESSION TAG	GB 13881852
2	539	HIS	-	EXPRESSION TAG	GB 13881852
2	540	HIS	-	EXPRESSION TAG	GB 13881852

- Molecule 3 is (1R)-3-METHYL-1-{{[N-(MORPHOLIN-4-YLCARBONYL)-3-(1-NAPHTHYL)-D-ALANYL]AMINO}BUTYLBORONIC ACID (three-letter code: M1N) (formula: $C_{23}H_{32}BN_3O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	C	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	E	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	G	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	J	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	L	1	Total	B	C	N	O	0	0
			32	1	23	3	5		
3	N	1	Total	B	C	N	O	0	0
			32	1	23	3	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	P	1	Total 32	B 1	C 23	N 3	O 5	0	0
3	R	1	Total 32	B 1	C 23	N 3	O 5	0	0
3	T	1	Total 32	B 1	C 23	N 3	O 5	0	0
3	V	1	Total 32	B 1	C 23	N 3	O 5	0	0
3	X	1	Total 32	B 1	C 23	N 3	O 5	0	0
3	Z	1	Total 32	B 1	C 23	N 3	O 5	0	0
3	2	1	Total 32	B 1	C 23	N 3	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	6	Total 6	O 6	0	0
4	2	21	Total 21	O 21	0	0
4	A	10	Total 10	O 10	0	0
4	B	10	Total 10	O 10	0	0
4	C	20	Total 20	O 20	0	0
4	D	4	Total 4	O 4	0	0
4	E	10	Total 10	O 10	0	0
4	F	7	Total 7	O 7	0	0
4	G	16	Total 16	O 16	0	0
4	H	16	Total 16	O 16	0	0
4	I	11	Total 11	O 11	0	0
4	J	13	Total 13	O 13	0	0

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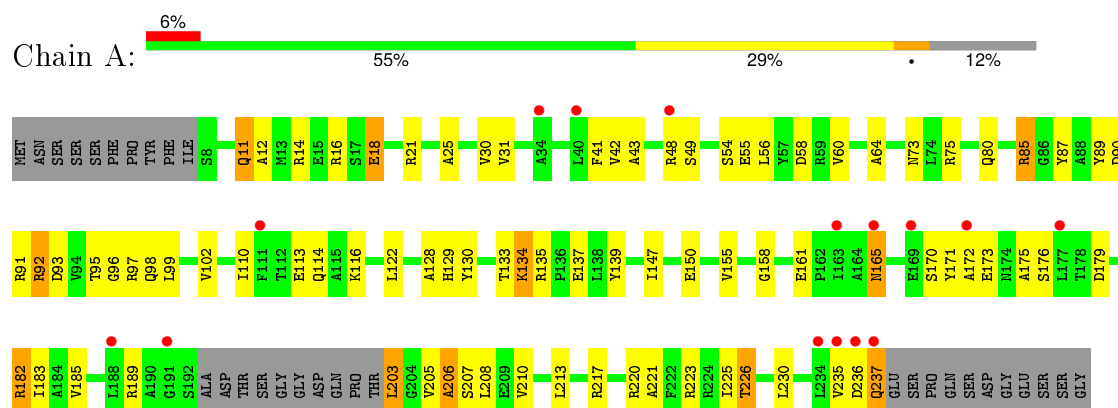
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	9	Total O 9 9	0	0
4	L	14	Total O 14 14	0	0
4	M	13	Total O 13 13	0	0
4	N	12	Total O 12 12	0	0
4	O	15	Total O 15 15	0	0
4	P	15	Total O 15 15	0	0
4	Q	6	Total O 6 6	0	0
4	R	12	Total O 12 12	0	0
4	S	5	Total O 5 5	0	0
4	T	8	Total O 8 8	0	0
4	U	2	Total O 2 2	0	0
4	V	20	Total O 20 20	0	0
4	W	7	Total O 7 7	0	0
4	X	20	Total O 20 20	0	0
4	Y	11	Total O 11 11	0	0
4	Z	8	Total O 8 8	0	0

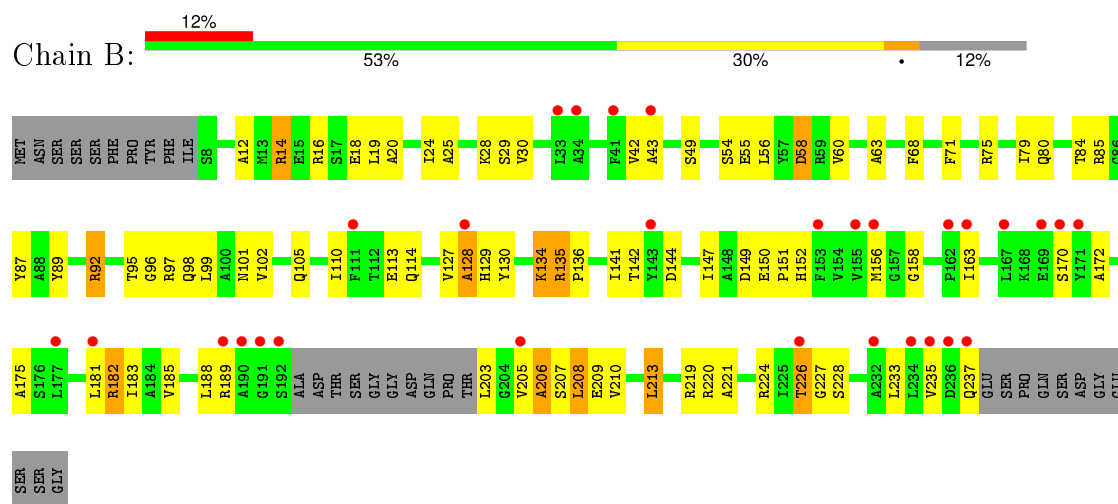
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

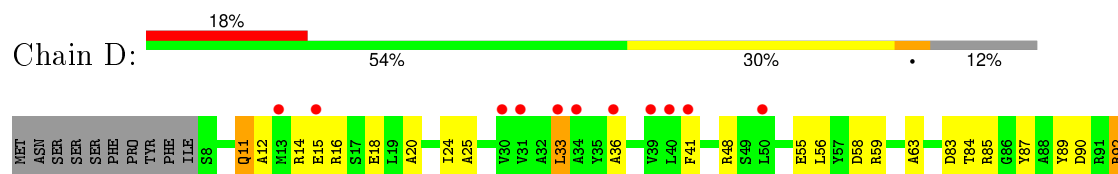
- Molecule 1: 20S proteasome, alpha and beta subunits

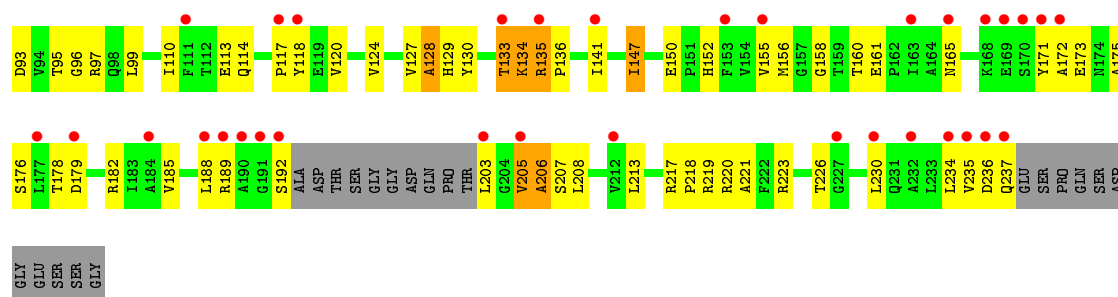


- Molecule 1: 20S proteasome, alpha and beta subunits

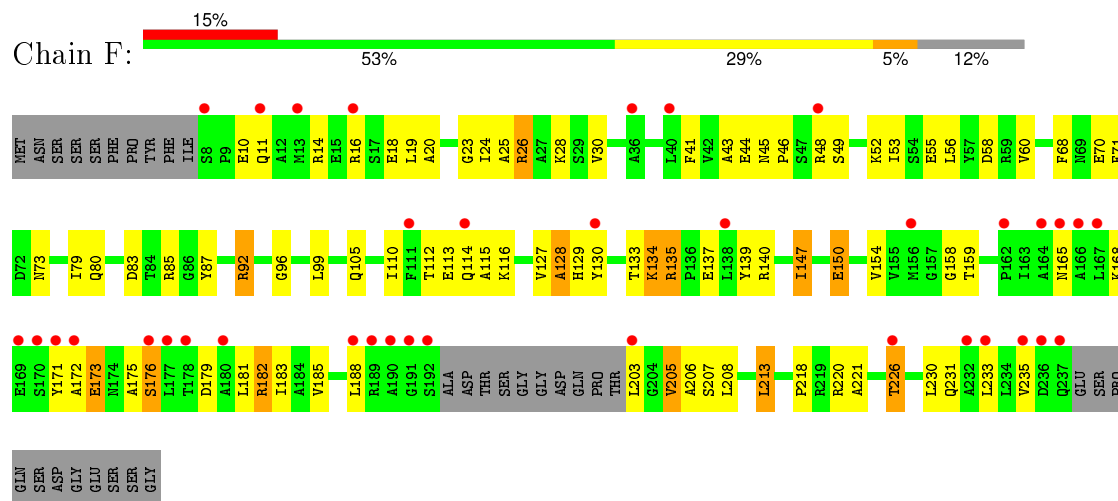


- Molecule 1: 20S proteasome, alpha and beta subunits

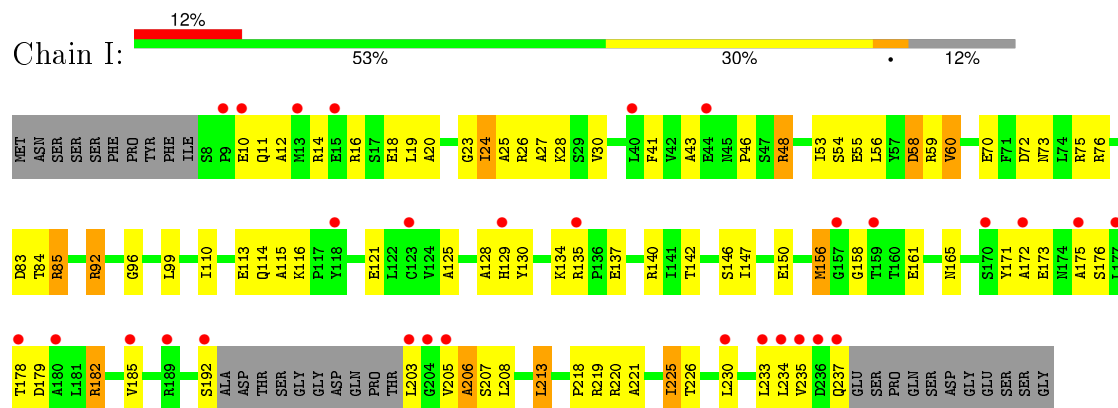




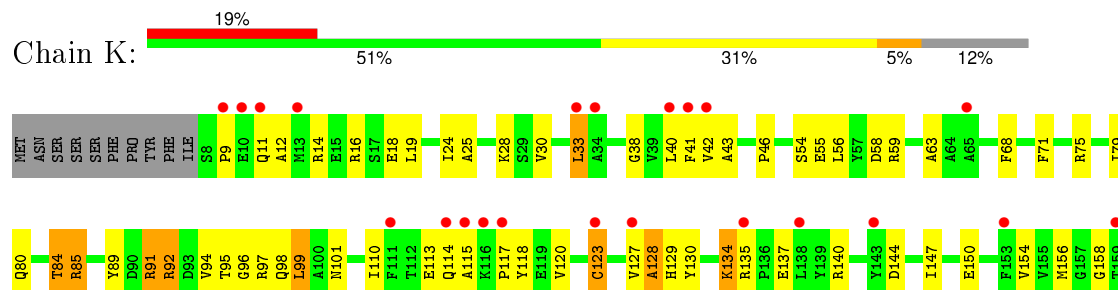
- Molecule 1: 20S proteasome, alpha and beta subunits



- Molecule 1: 20S proteasome, alpha and beta subunits



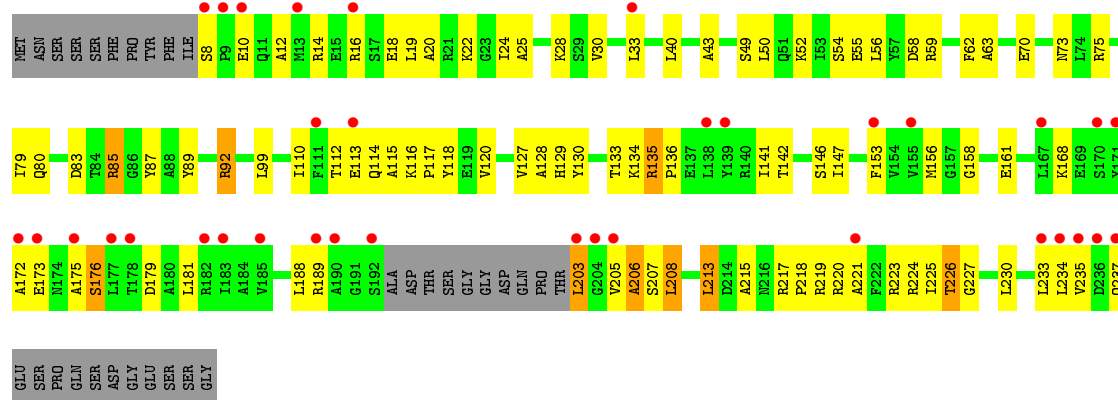
- Molecule 1: 20S proteasome, alpha and beta subunits

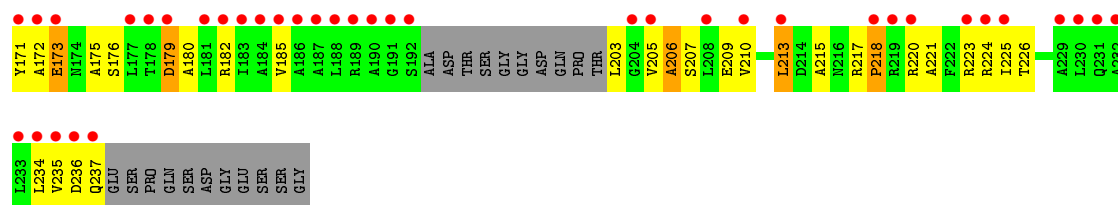




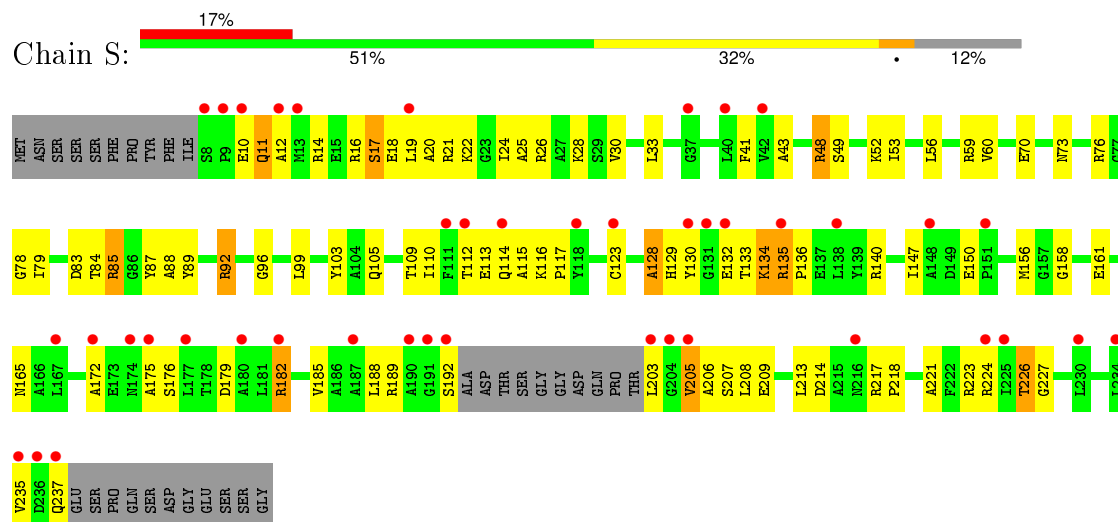
- Molecule 1: 20S proteasome, alpha and beta subunits

Chain M: 14% 51% 33% 12%

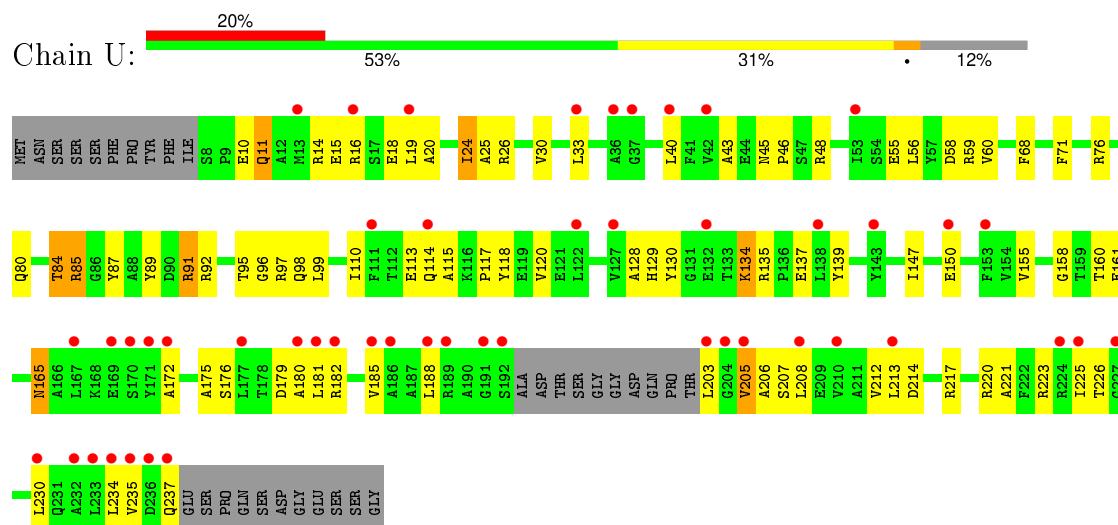




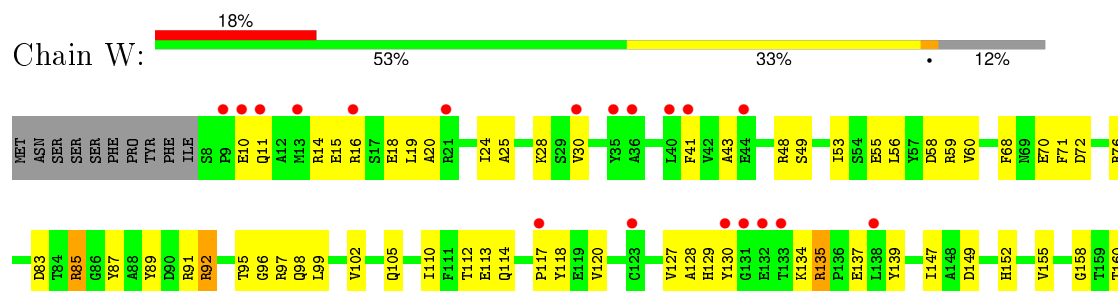
- Molecule 1: 20S proteasome, alpha and beta subunits

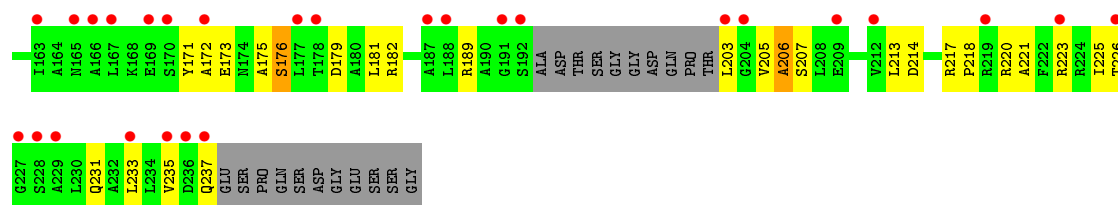


- Molecule 1: 20S proteasome, alpha and beta subunits

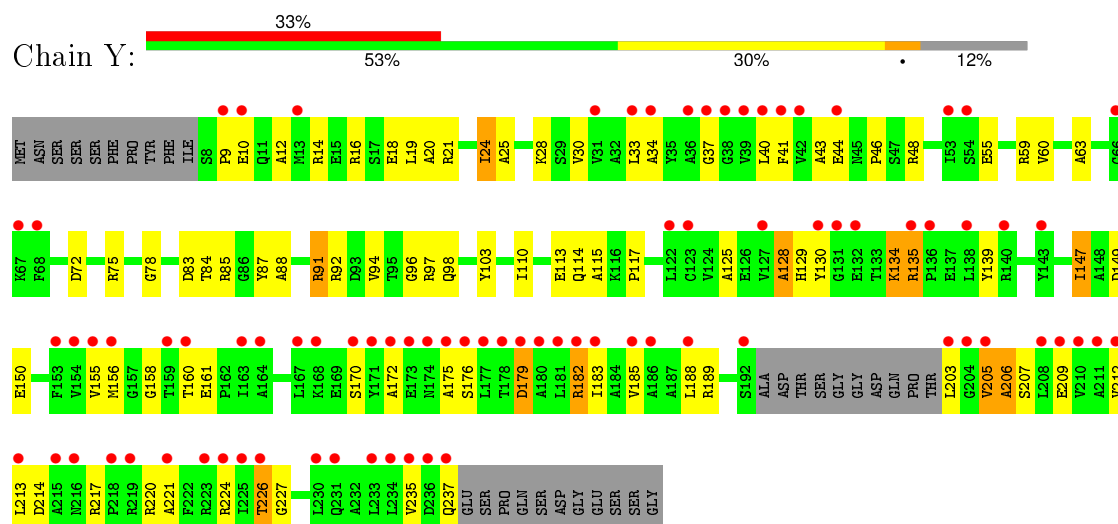


- Molecule 1: 20S proteasome, alpha and beta subunits

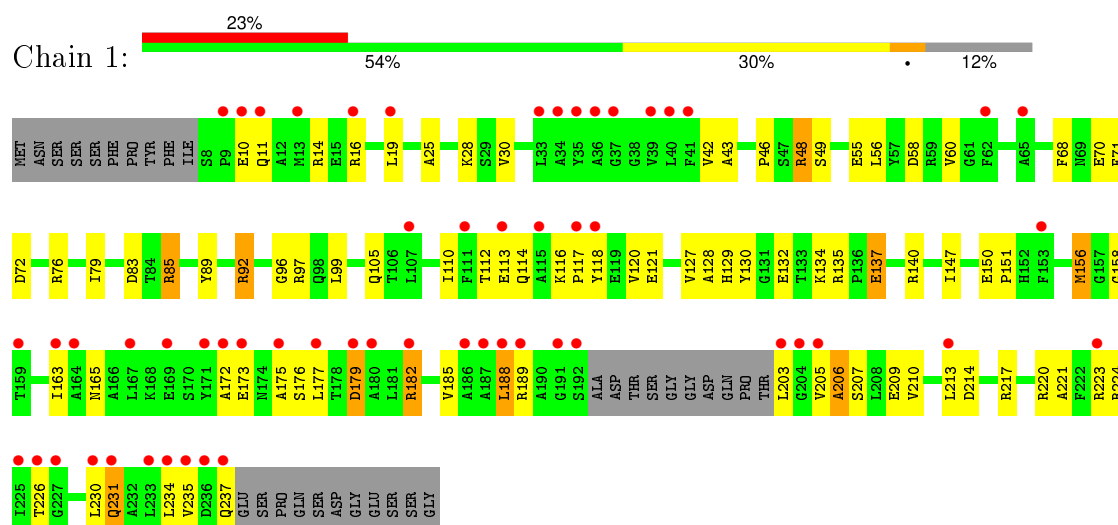




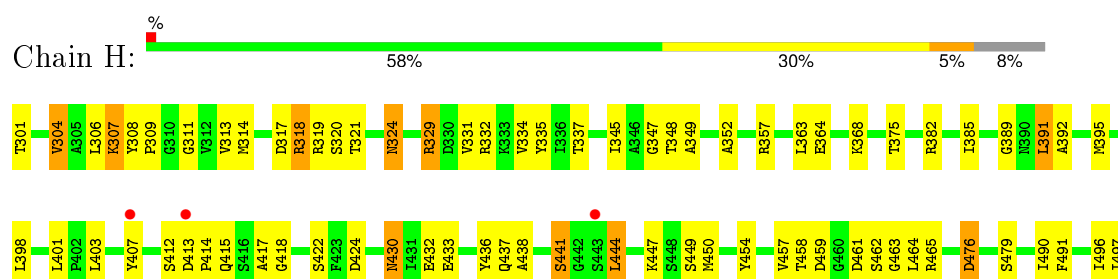
- Molecule 1: 20S proteasome, alpha and beta subunits



- Molecule 1: 20S proteasome, alpha and beta subunits

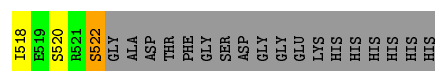
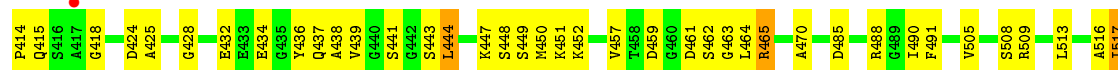
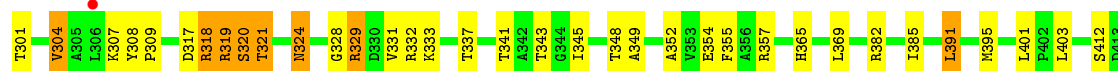


- Molecule 2: proteasome, beta subunit

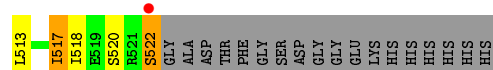
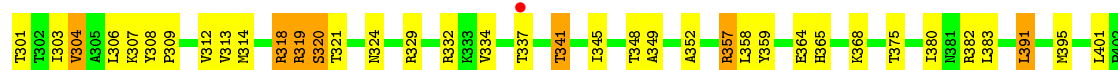




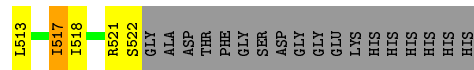
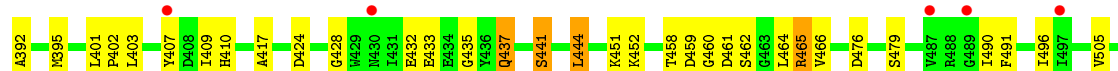
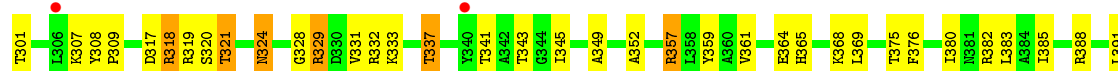
- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit

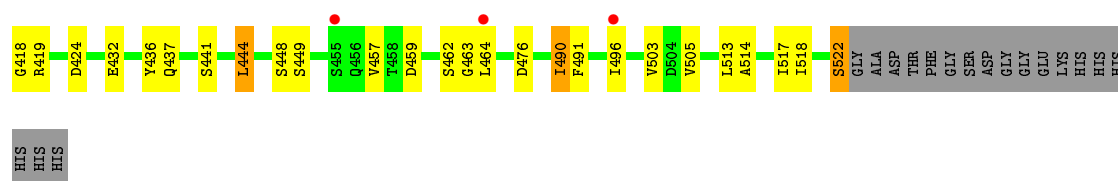


- Molecule 2: proteasome, beta subunit

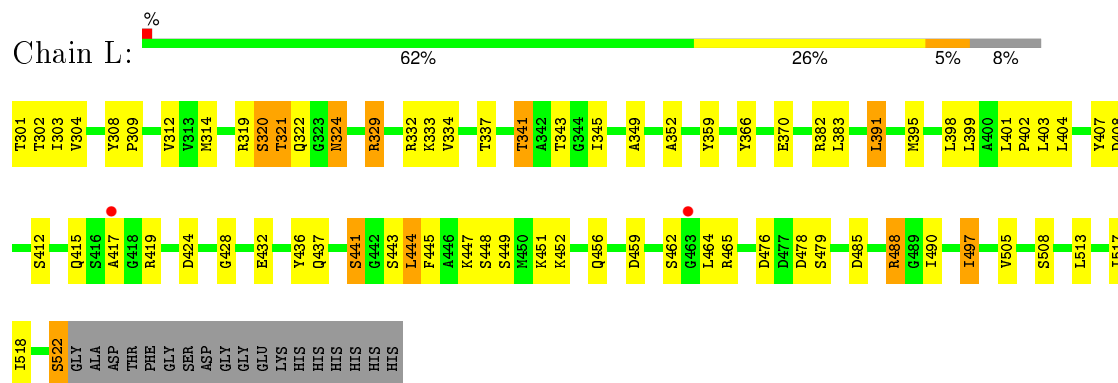


- Molecule 2: proteasome, beta subunit

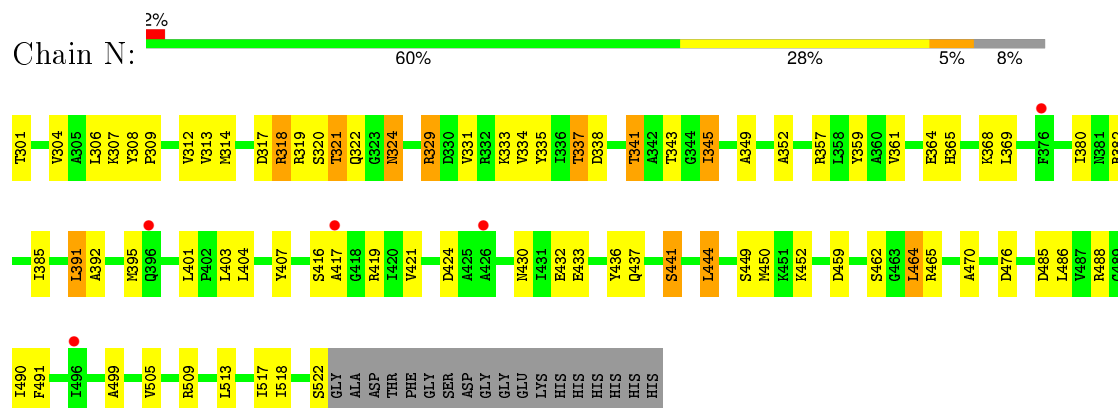




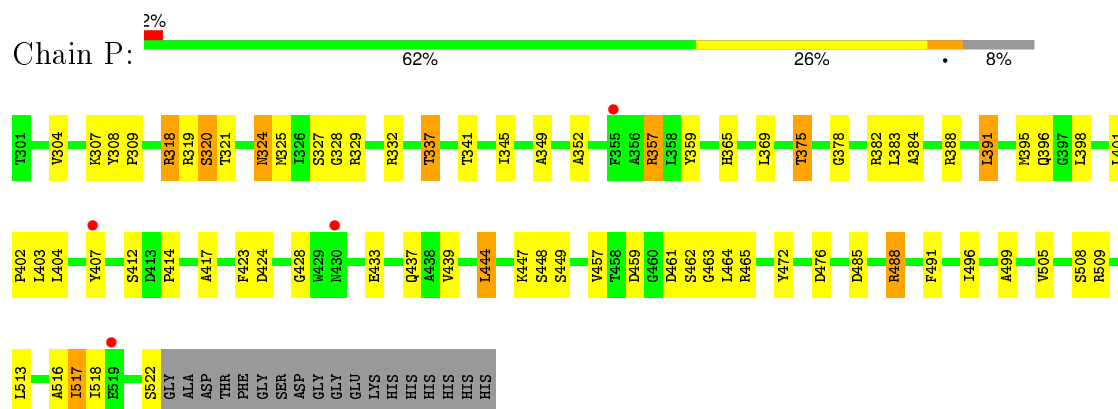
- Molecule 2: proteasome, beta subunit



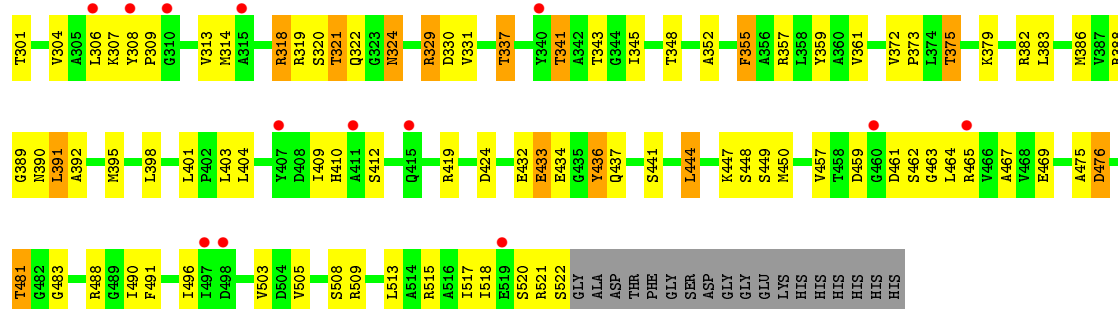
- Molecule 2: proteasome, beta subunit



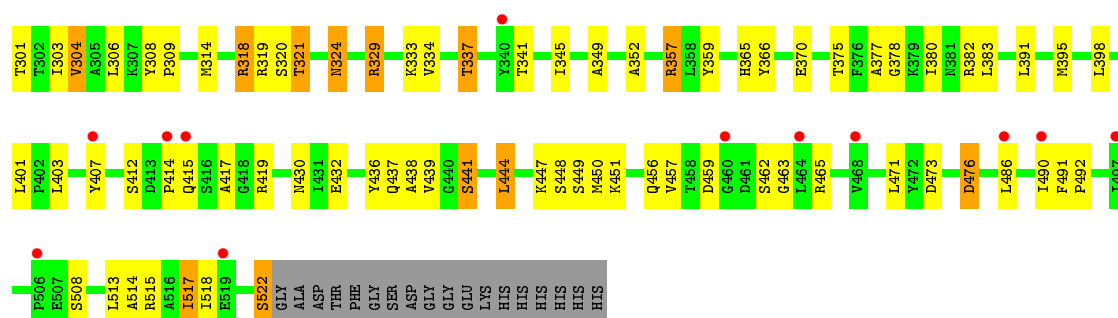
- Molecule 2: proteasome, beta subunit



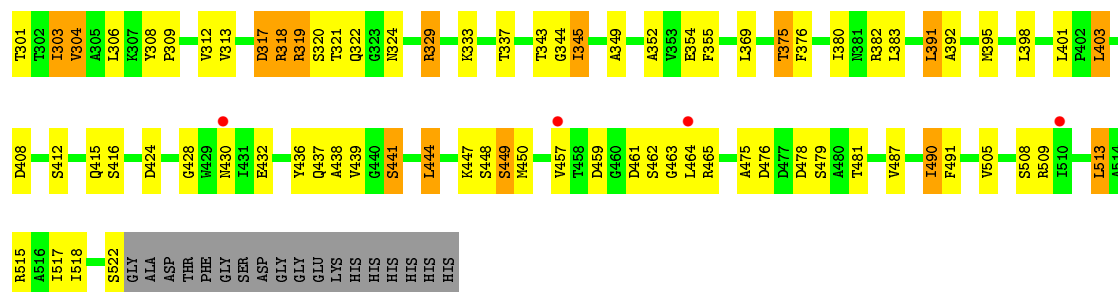
- Molecule 2: proteasome, beta subunit



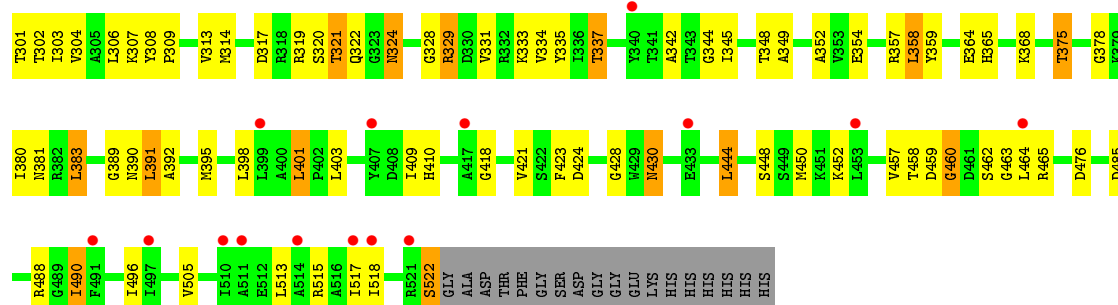
- Molecule 2: proteasome, beta subunit



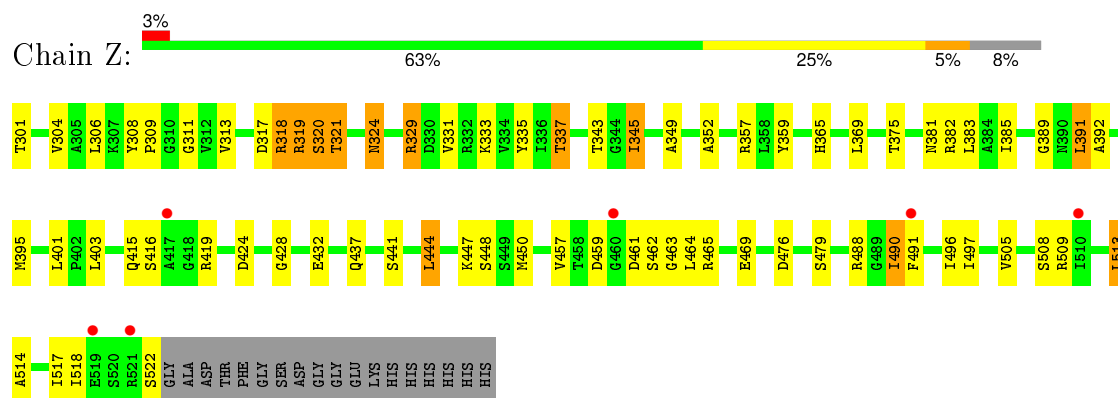
- Molecule 2: proteasome, beta subunit



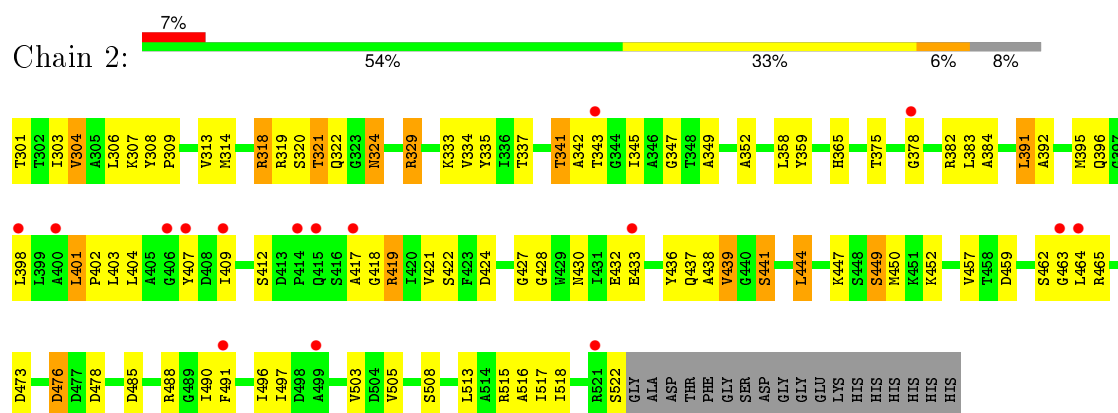
- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.96Å 116.17Å 200.20Å 90.00° 112.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.99 49.77 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.1 (50.00-2.99) 94.1 (49.77-2.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.226 , 0.262 0.227 , 0.229	Depositor DCC
R_{free} test set	4257 reflections (3.14%)	DCC
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 88.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 139841 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47389	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M1N

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	1	0.49	0/1717	0.62	0/2320
1	A	0.45	0/1717	0.61	0/2320
1	B	0.45	0/1717	0.64	0/2320
1	D	0.48	0/1717	0.63	1/2320 (0.0%)
1	F	0.45	0/1717	0.63	0/2320
1	I	0.46	0/1717	0.61	0/2320
1	K	0.46	0/1717	0.63	0/2320
1	M	0.45	0/1717	0.63	0/2320
1	O	0.47	0/1717	0.62	0/2320
1	Q	0.49	0/1717	0.61	0/2320
1	S	0.47	0/1717	0.61	0/2320
1	U	0.47	0/1717	0.63	0/2320
1	W	0.62	2/1717 (0.1%)	0.64	1/2320 (0.0%)
1	Y	0.45	0/1717	0.61	0/2320
2	2	0.55	0/1662	0.71	0/2254
2	C	0.53	0/1662	0.72	0/2254
2	E	0.51	0/1662	0.72	0/2254
2	G	0.51	0/1662	0.69	0/2254
2	H	0.55	0/1662	0.71	0/2254
2	J	0.51	0/1662	0.69	0/2254
2	L	0.53	0/1662	0.70	0/2254
2	N	0.52	0/1662	0.69	0/2254
2	P	0.53	0/1662	0.73	0/2254
2	R	0.60	1/1662 (0.1%)	0.71	0/2254
2	T	0.54	1/1662 (0.1%)	0.68	0/2254
2	V	0.50	0/1662	0.69	0/2254
2	X	0.50	0/1662	0.69	0/2254
2	Z	0.52	0/1662	0.71	0/2254
All	All	0.50	4/47306 (0.0%)	0.66	2/64036 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	173	GLU	CD-OE1	13.22	1.40	1.25
2	R	412	SER	CB-OG	12.49	1.58	1.42
1	W	173	GLU	CD-OE2	11.28	1.38	1.25
2	T	456	GLN	CD-NE2	5.50	1.46	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	LEU	CA-CB-CG	5.71	128.44	115.30
1	W	173	GLU	OE1-CD-OE2	5.57	129.98	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1692	0	1688	68	0
1	A	1692	0	1688	53	1
1	B	1692	0	1688	55	0
1	D	1692	0	1688	54	1
1	F	1692	0	1688	64	0
1	I	1692	0	1688	53	0
1	K	1692	0	1688	64	0
1	M	1692	0	1688	68	0
1	O	1692	0	1688	59	0
1	Q	1692	0	1688	45	0
1	S	1692	0	1688	65	0
1	U	1692	0	1688	53	0
1	W	1692	0	1688	60	0
1	Y	1692	0	1688	54	0
2	2	1638	0	1629	76	0
2	C	1638	0	1629	68	0
2	E	1638	0	1629	55	0
2	G	1638	0	1629	68	0
2	H	1638	0	1629	64	0
2	J	1638	0	1629	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1638	0	1629	67	0
2	N	1638	0	1629	80	0
2	P	1638	0	1629	56	0
2	R	1638	0	1629	55	0
2	T	1638	0	1629	55	0
2	V	1638	0	1629	65	0
2	X	1638	0	1629	73	0
2	Z	1638	0	1629	60	0
3	2	32	0	32	9	0
3	C	32	0	32	12	0
3	E	32	0	32	14	0
3	G	32	0	32	10	0
3	H	32	0	32	12	0
3	J	32	0	32	17	0
3	L	32	0	32	16	0
3	N	32	0	32	16	0
3	P	32	0	32	14	0
3	R	32	0	32	9	0
3	T	32	0	32	11	0
3	V	32	0	32	17	0
3	X	32	0	32	14	0
3	Z	32	0	32	17	0
4	1	6	0	0	4	0
4	2	21	0	0	4	0
4	A	10	0	0	0	0
4	B	10	0	0	2	0
4	C	20	0	0	6	0
4	D	4	0	0	2	0
4	E	10	0	0	1	0
4	F	7	0	0	4	0
4	G	16	0	0	2	0
4	H	16	0	0	4	0
4	I	11	0	0	2	0
4	J	13	0	0	1	0
4	K	9	0	0	0	0
4	L	14	0	0	2	0
4	M	13	0	0	5	0
4	N	12	0	0	3	0
4	O	15	0	0	1	0
4	P	15	0	0	5	0
4	Q	6	0	0	3	0
4	R	12	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	5	0	0	0	0
4	T	8	0	0	2	0
4	U	2	0	0	0	0
4	V	20	0	0	5	0
4	W	7	0	0	2	0
4	X	20	0	0	14	0
4	Y	11	0	0	5	0
4	Z	8	0	0	0	0
All	All	47389	0	46886	1629	1

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 17.

All (1629) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:424:ASP:HA	4:C:542:HOH:O	1.37	1.22
2:X:303:ILE:HG13	4:X:58:HOH:O	1.35	1.22
2:J:444:LEU:HD12	2:Z:444:LEU:HD12	1.31	1.08
2:L:444:LEU:HD12	2:P:444:LEU:HD12	1.35	1.07
3:N:273:M1N:O16	3:N:273:M1N:H221	1.55	1.06
2:N:444:LEU:HD12	2:V:444:LEU:HD12	1.37	1.05
2:H:444:LEU:CD1	2:E:444:LEU:HD12	1.85	1.05
2:H:444:LEU:HD12	2:E:444:LEU:HD12	1.08	1.04
2:H:444:LEU:HD12	2:E:444:LEU:CD1	1.86	1.04
1:D:11:GLN:HG2	1:D:14:ARG:HH12	1.23	1.01
1:K:85:ARG:HG2	1:K:85:ARG:HH11	1.24	0.98
2:E:430:ASN:HB3	4:E:87:HOH:O	1.63	0.98
1:D:59:ARG:HG3	1:D:129:HIS:HD2	1.29	0.96
2:N:304:VAL:HG21	2:N:450:MET:CE	1.96	0.96
1:F:231:GLN:HG3	4:F:252:HOH:O	1.65	0.95
1:U:11:GLN:HG2	1:U:14:ARG:HH12	1.29	0.95
2:C:465:ARG:HG3	2:C:465:ARG:HH11	1.31	0.94
2:V:349:ALA:H	3:V:273:M1N:C35	1.80	0.94
2:N:349:ALA:H	3:N:273:M1N:C35	1.81	0.93
2:N:324:ASN:H	2:N:324:ASN:HD22	1.13	0.92
2:N:337:THR:OG1	2:N:343:THR:HG22	1.70	0.91
1:S:92:ARG:HD2	1:S:129:HIS:CE1	2.05	0.90
1:O:85:ARG:HH11	1:O:85:ARG:CG	1.83	0.90
2:N:349:ALA:H	3:N:273:M1N:H35	1.34	0.90
2:C:301:THR:HG21	3:C:273:M1N:O16	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:321:THR:O	3:R:273:M1N:H51	1.72	0.89
2:V:349:ALA:H	3:V:273:M1N:H35	1.36	0.89
1:M:85:ARG:HH11	1:M:85:ARG:HG2	1.35	0.88
1:O:85:ARG:HH11	1:O:85:ARG:HG2	1.37	0.88
3:Z:273:M1N:O16	3:Z:273:M1N:H221	1.74	0.88
2:L:337:THR:OG1	2:L:343:THR:HG22	1.74	0.88
2:2:403:LEU:HD12	2:2:439:VAL:HG22	1.54	0.87
1:Q:88:ALA:O	2:Z:381:ASN:ND2	2.07	0.87
2:G:444:LEU:HD12	2:2:444:LEU:HD12	1.54	0.87
1:W:83:ASP:OD2	2:X:365:HIS:HD2	1.57	0.87
1:Q:59:ARG:HG3	1:Q:129:HIS:HD2	1.39	0.86
2:N:304:VAL:HG21	2:N:450:MET:HE1	1.55	0.86
2:Z:437:GLN:OE1	2:Z:447:LYS:HD3	1.76	0.85
2:N:349:ALA:N	3:N:273:M1N:H35	1.91	0.85
2:C:444:LEU:HD12	2:R:444:LEU:HD12	1.59	0.85
2:V:349:ALA:N	3:V:273:M1N:H35	1.89	0.85
3:X:273:M1N:H221	3:X:273:M1N:O16	1.76	0.85
3:G:273:M1N:H40	2:N:424:ASP:OD1	1.77	0.85
3:R:273:M1N:HN1	3:R:273:M1N:H252	1.42	0.84
1:S:11:GLN:HG2	1:S:14:ARG:NH1	1.92	0.84
1:M:85:ARG:HH11	1:M:85:ARG:CG	1.90	0.84
2:J:324:ASN:HD22	2:J:324:ASN:H	1.25	0.84
1:1:110:ILE:HG23	1:1:114:GLN:HG3	1.60	0.82
2:X:317:ASP:OD1	2:X:333:LYS:NZ	2.11	0.82
2:X:391:LEU:O	2:X:395:MET:HG2	1.78	0.82
1:D:92:ARG:HD2	1:D:129:HIS:CE1	2.15	0.82
1:Y:37:GLY:HA3	4:Y:256:HOH:O	1.77	0.82
1:A:56:LEU:HD13	1:A:99:LEU:HD23	1.59	0.82
4:Q:254:HOH:O	2:Z:375:THR:HG21	1.78	0.82
2:V:462:SER:O	2:V:465:ARG:HG2	1.78	0.82
2:T:476:ASP:HB2	4:X:20:HOH:O	1.79	0.82
2:2:321:THR:O	3:2:273:M1N:H51	1.80	0.81
2:G:321:THR:O	3:G:273:M1N:H37	1.80	0.81
1:S:83:ASP:OD2	2:T:365:HIS:HD2	1.63	0.81
2:N:321:THR:O	3:N:273:M1N:H37	1.81	0.81
1:K:85:ARG:HH11	1:K:85:ARG:CG	1.94	0.81
2:H:465:ARG:HG3	2:H:465:ARG:HH11	1.46	0.81
3:2:273:M1N:H221	3:2:273:M1N:O16	1.81	0.81
2:2:465:ARG:HD3	4:2:544:HOH:O	1.80	0.81
2:V:319:ARG:HG3	4:V:552:HOH:O	1.81	0.80
2:J:321:THR:O	3:J:273:M1N:H51	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:301:THR:N	2:V:441:SER:HG	1.80	0.80
1:1:92:ARG:HD2	1:1:129:HIS:CE1	2.15	0.80
2:T:301:THR:N	2:T:441:SER:HG	1.80	0.79
2:H:465:ARG:HD3	4:H:547:HOH:O	1.82	0.79
1:S:56:LEU:HD13	1:S:99:LEU:HD22	1.63	0.79
2:C:465:ARG:CG	2:C:465:ARG:HH11	1.95	0.79
1:Y:87:TYR:O	2:Z:357:ARG:NH2	2.16	0.78
2:J:329:ARG:NH2	2:R:476:ASP:O	2.16	0.78
2:G:464:LEU:HD12	2:G:496:ILE:HD11	1.63	0.78
2:H:430:ASN:HB3	4:H:551:HOH:O	1.82	0.78
2:X:345:ILE:N	4:X:58:HOH:O	2.16	0.78
2:X:321:THR:O	3:X:273:M1N:H51	1.82	0.77
2:R:483:GLY:HA2	4:R:46:HOH:O	1.84	0.77
1:K:230:LEU:HD21	1:K:234:LEU:HD13	1.65	0.77
1:F:92:ARG:HG3	1:F:129:HIS:HE1	1.50	0.77
2:X:485:ASP:OD2	2:X:488:ARG:HB2	1.84	0.77
2:X:345:ILE:HD13	2:X:352:ALA:HB1	1.67	0.77
1:I:60:VAL:HG21	1:I:96:GLY:HA3	1.65	0.77
1:B:110:ILE:HG23	1:B:114:GLN:HG3	1.66	0.77
2:G:349:ALA:H	3:G:273:M1N:C35	1.97	0.77
2:Z:465:ARG:HB2	2:Z:513:LEU:HD21	1.66	0.77
2:J:345:ILE:HD13	2:J:352:ALA:HB1	1.65	0.77
2:H:349:ALA:HA	3:H:273:M1N:H243	1.67	0.77
2:L:444:LEU:CD1	2:P:444:LEU:HD12	2.14	0.77
2:T:382:ARG:HD3	1:1:89:TYR:CD1	2.20	0.77
2:Z:349:ALA:HB2	3:Z:273:M1N:H252	1.67	0.76
3:E:273:M1N:C25	3:E:273:M1N:HN1	1.98	0.76
2:X:424:ASP:OD1	3:Z:273:M1N:H40	1.86	0.76
1:Q:110:ILE:HG23	1:Q:114:GLN:HG3	1.66	0.76
2:J:444:LEU:HD12	2:Z:444:LEU:CD1	2.14	0.75
2:T:476:ASP:HA	4:T:88:HOH:O	1.85	0.75
3:C:273:M1N:H221	3:C:273:M1N:O16	1.85	0.75
1:I:83:ASP:OD2	2:J:365:HIS:HD2	1.70	0.75
2:P:321:THR:O	3:P:273:M1N:H37	1.84	0.75
1:1:14:ARG:HH11	1:1:14:ARG:HB3	1.49	0.75
2:H:324:ASN:H	2:H:324:ASN:ND2	1.84	0.75
2:V:321:THR:O	3:V:273:M1N:H37	1.86	0.75
2:L:437:GLN:OE1	2:L:447:LYS:HD3	1.87	0.75
2:Z:321:THR:O	3:Z:273:M1N:H37	1.86	0.74
2:N:337:THR:HG21	2:N:359:TYR:CD2	2.22	0.74
3:H:273:M1N:H221	3:H:273:M1N:O16	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:14:ARG:HB3	1:O:14:ARG:HH11	1.52	0.74
2:X:452:LYS:HA	4:X:4:HOH:O	1.88	0.74
1:D:11:GLN:HG2	1:D:14:ARG:NH1	2.01	0.74
2:H:324:ASN:HD22	2:H:324:ASN:H	1.35	0.74
2:V:301:THR:HG21	3:V:273:M1N:O16	1.88	0.74
2:N:324:ASN:HD22	2:N:324:ASN:N	1.84	0.74
1:D:59:ARG:HG3	1:D:129:HIS:CD2	2.19	0.74
2:E:382:ARG:HD3	1:K:89:TYR:CD1	2.21	0.74
1:O:214:ASP:OD2	1:O:217:ARG:HG2	1.87	0.73
1:A:182:ARG:HG3	1:A:235:VAL:HB	1.69	0.73
2:E:308:TYR:HB2	2:E:309:PRO:HD2	1.70	0.73
1:B:208:LEU:HB3	4:B:251:HOH:O	1.89	0.73
1:B:42:VAL:HG22	1:B:210:VAL:HG22	1.70	0.73
1:I:176:SER:HB3	1:I:179:ASP:OD1	1.88	0.73
2:R:337:THR:HG21	2:R:359:TYR:CD2	2.24	0.73
2:N:304:VAL:HG21	2:N:450:MET:HE3	1.69	0.73
2:N:304:VAL:CG2	2:N:450:MET:HE1	2.19	0.73
2:Z:301:THR:HG21	3:Z:273:M1N:O16	1.87	0.73
1:I:92:ARG:HD2	1:I:129:HIS:CE1	2.24	0.73
1:O:56:LEU:HD13	1:O:99:LEU:HD22	1.71	0.73
1:M:224:ARG:HD2	4:M:255:HOH:O	1.88	0.73
1:O:59:ARG:HG3	1:O:129:HIS:HD2	1.53	0.73
2:J:349:ALA:H	3:J:273:M1N:C35	2.03	0.72
3:E:273:M1N:H252	3:E:273:M1N:HN1	1.53	0.72
2:T:345:ILE:HD13	2:T:352:ALA:HB1	1.70	0.72
2:T:321:THR:O	3:T:273:M1N:C5	2.38	0.72
2:T:321:THR:O	3:T:273:M1N:H51	1.87	0.72
2:Z:459:ASP:H	2:Z:462:SER:HB3	1.53	0.72
2:P:308:TYR:HB2	2:P:309:PRO:HD2	1.71	0.72
1:I:72:ASP:O	1:I:76:ARG:HG3	1.89	0.72
2:R:436:TYR:CD2	2:R:450:MET:HG2	2.24	0.72
1:W:68:PHE:HA	1:W:71:PHE:CE2	2.25	0.72
1:K:59:ARG:HG3	1:K:129:HIS:HD2	1.55	0.72
1:O:94:VAL:HA	1:O:98:GLN:HE22	1.55	0.72
2:N:364:GLU:HG2	2:N:368:LYS:HE2	1.71	0.72
2:R:509:ARG:HG3	4:R:254:HOH:O	1.87	0.72
2:L:444:LEU:HD12	2:P:444:LEU:CD1	2.18	0.72
1:S:85:ARG:HH11	1:S:85:ARG:HG2	1.54	0.72
2:L:464:LEU:HD11	2:L:505:VAL:HG11	1.70	0.71
2:L:456:GLN:HE22	2:L:465:ARG:HH12	1.38	0.71
2:R:462:SER:O	2:R:465:ARG:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:465:ARG:NH1	2:C:465:ARG:HG3	2.00	0.71
1:D:92:ARG:HG3	1:D:129:HIS:HE1	1.54	0.71
1:K:217:ARG:NH2	1:K:223:ARG:HG3	2.06	0.71
2:X:337:THR:HG21	2:X:359:TYR:CD2	2.25	0.71
2:E:462:SER:O	2:E:465:ARG:HG2	1.91	0.71
2:L:345:ILE:HD13	2:L:352:ALA:HB1	1.70	0.71
2:2:464:LEU:HD12	2:2:496:ILE:HD11	1.73	0.71
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.73	0.71
3:V:273:M1N:H221	3:V:273:M1N:O16	1.89	0.71
2:G:321:THR:O	3:G:273:M1N:H51	1.91	0.71
2:T:337:THR:HG21	2:T:359:TYR:CD2	2.24	0.71
2:L:349:ALA:H	3:L:273:M1N:C35	2.03	0.71
2:G:364:GLU:HG2	2:G:368:LYS:HE2	1.73	0.71
2:2:301:THR:N	2:2:441:SER:HG	1.88	0.71
1:1:217:ARG:HH21	1:1:223:ARG:HG3	1.56	0.70
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.72	0.70
2:T:459:ASP:H	2:T:462:SER:HB3	1.56	0.70
2:J:301:THR:HG21	3:J:273:M1N:O16	1.91	0.70
1:S:92:ARG:HD2	1:S:129:HIS:ND1	2.05	0.70
1:D:56:LEU:HD13	1:D:99:LEU:HD23	1.74	0.70
2:V:349:ALA:HA	3:V:273:M1N:H243	1.73	0.70
2:V:391:LEU:O	2:V:395:MET:HG2	1.92	0.70
1:O:59:ARG:HG3	1:O:129:HIS:CD2	2.27	0.70
1:D:55:GLU:OE2	1:D:220:ARG:HD2	1.91	0.70
1:W:85:ARG:HH11	1:W:85:ARG:HG2	1.57	0.70
2:2:485:ASP:OD2	2:2:488:ARG:HB2	1.92	0.69
2:C:318:ARG:HG2	4:C:551:HOH:O	1.90	0.69
2:L:301:THR:N	2:L:441:SER:HG	1.89	0.69
1:Y:72:ASP:OD2	4:Y:258:HOH:O	2.10	0.69
2:T:382:ARG:HD3	1:1:89:TYR:HD1	1.56	0.69
1:W:56:LEU:HD13	1:W:99:LEU:HD22	1.73	0.69
2:C:509:ARG:HG2	4:C:541:HOH:O	1.92	0.69
1:A:217:ARG:HH21	1:A:223:ARG:HG3	1.57	0.69
1:M:56:LEU:HD13	1:M:99:LEU:HD22	1.74	0.69
1:K:56:LEU:HD13	1:K:99:LEU:HD22	1.73	0.69
2:R:437:GLN:OE1	2:R:447:LYS:HD3	1.92	0.69
2:E:485:ASP:OD2	2:E:488:ARG:HB2	1.93	0.69
2:R:308:TYR:HB2	2:R:309:PRO:HD2	1.75	0.69
2:T:321:THR:O	3:T:273:M1N:H37	1.93	0.69
1:B:151:PRO:HD2	4:B:255:HOH:O	1.91	0.69
2:J:337:THR:HG21	2:J:359:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:341:THR:CG2	2:P:404:LEU:HD11	2.23	0.69
2:G:459:ASP:H	2:G:462:SER:HB3	1.57	0.69
2:C:301:THR:N	2:C:441:SER:HG	1.90	0.69
2:T:476:ASP:CB	4:X:20:HOH:O	2.37	0.69
2:Z:465:ARG:HB2	2:Z:513:LEU:CD2	2.22	0.69
1:B:205:VAL:HG12	1:B:206:ALA:H	1.58	0.69
2:C:509:ARG:CG	4:C:541:HOH:O	2.40	0.69
2:T:349:ALA:H	3:T:273:M1N:C35	2.06	0.69
2:Z:345:ILE:HD13	2:Z:352:ALA:HB1	1.75	0.69
1:U:10:GLU:HA	1:I:19:LEU:HD12	1.75	0.68
2:V:321:THR:O	3:V:273:M1N:H52	1.92	0.68
2:G:337:THR:OG1	2:G:343:THR:HG22	1.93	0.68
2:V:459:ASP:H	2:V:462:SER:HB3	1.57	0.68
1:M:92:ARG:HH11	1:M:92:ARG:HB2	1.59	0.68
2:L:518:ILE:O	2:L:522:SER:HB2	1.93	0.68
2:L:314:MET:CE	2:L:334:VAL:HG13	2.24	0.68
1:I:56:LEU:HD13	1:I:99:LEU:HD22	1.74	0.68
2:Z:513:LEU:O	2:Z:517:ILE:HG12	1.94	0.68
1:I:14:ARG:HB3	1:I:14:ARG:NH1	2.07	0.68
2:Z:349:ALA:H	3:Z:273:M1N:C35	2.07	0.68
2:H:321:THR:O	3:H:273:M1N:H37	1.94	0.68
1:B:92:ARG:HD2	1:B:129:HIS:ND1	2.10	0.68
2:C:518:ILE:O	2:C:522:SER:HB2	1.94	0.68
2:G:308:TYR:HB2	2:G:309:PRO:HD2	1.75	0.67
2:N:304:VAL:CG2	2:N:450:MET:CE	2.70	0.67
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.30	0.67
2:X:518:ILE:O	2:X:522:SER:HB2	1.94	0.67
1:B:189:ARG:CZ	1:B:237:GLN:HB3	2.24	0.67
2:G:321:THR:O	3:G:273:M1N:C5	2.43	0.67
2:E:464:LEU:HD11	2:E:505:VAL:HG11	1.76	0.67
1:W:83:ASP:OD2	2:X:365:HIS:CD2	2.45	0.67
2:T:314:MET:CE	2:T:334:VAL:HG13	2.24	0.67
2:J:318:ARG:HD3	2:J:491:PHE:O	1.95	0.67
1:W:49:SER:HB2	1:Y:97:ARG:NH1	2.09	0.67
1:O:9:PRO:HD2	1:U:15:GLU:OE1	1.95	0.67
2:T:318:ARG:HD3	2:T:491:PHE:O	1.93	0.67
2:X:515:ARG:HA	2:X:518:ILE:HD12	1.76	0.67
2:C:308:TYR:HB2	2:C:309:PRO:HD2	1.76	0.67
2:P:464:LEU:HD11	2:P:505:VAL:HG11	1.77	0.67
1:I:23:GLY:HA2	1:I:26:ARG:NH1	2.10	0.66
1:S:217:ARG:NH2	1:S:223:ARG:HG3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:16:ARG:HE	1:1:117:PRO:HD3	1.60	0.66
2:C:329:ARG:NH2	2:E:476:ASP:O	2.28	0.66
2:J:391:LEU:O	2:J:395:MET:HG2	1.95	0.66
2:P:375:THR:HB	2:P:378:GLY:H	1.60	0.66
1:Y:75:ARG:NH2	4:Y:254:HOH:O	2.28	0.66
3:R:273:M1N:N1	3:R:273:M1N:H252	2.09	0.66
2:L:424:ASP:OD1	3:N:273:M1N:H40	1.94	0.66
1:U:11:GLN:HG2	1:U:14:ARG:NH1	2.06	0.66
2:J:324:ASN:ND2	2:J:324:ASN:H	1.93	0.66
2:2:375:THR:HB	2:2:378:GLY:H	1.60	0.66
2:G:437:GLN:HA	2:G:437:GLN:OE1	1.94	0.66
2:C:459:ASP:H	2:C:462:SER:HB3	1.61	0.66
1:U:59:ARG:HG3	1:U:129:HIS:HD2	1.60	0.66
2:P:509:ARG:HG3	4:P:547:HOH:O	1.96	0.66
2:R:301:THR:N	2:R:441:SER:HG	1.94	0.66
1:B:92:ARG:HD2	1:B:129:HIS:CE1	2.31	0.66
2:G:382:ARG:HD3	1:W:89:TYR:HD1	1.62	0.66
2:C:301:THR:CG2	3:C:273:M1N:O16	2.45	0.65
2:P:459:ASP:H	2:P:462:SER:HB3	1.60	0.65
1:I:70:GLU:OE2	1:I:116:LYS:NZ	2.30	0.65
2:L:391:LEU:O	2:L:395:MET:HG2	1.95	0.65
2:2:459:ASP:H	2:2:462:SER:HB3	1.59	0.65
3:P:273:M1N:H253	3:P:273:M1N:HN1	1.61	0.65
2:H:459:ASP:H	2:H:462:SER:HB3	1.62	0.65
2:G:337:THR:HG21	2:G:359:TYR:CD2	2.31	0.65
1:U:59:ARG:HG3	1:U:129:HIS:CD2	2.31	0.65
2:J:349:ALA:HB2	3:J:273:M1N:H252	1.78	0.65
2:E:348:THR:HG23	3:E:273:M1N:H35	1.77	0.65
2:L:456:GLN:HE22	2:L:465:ARG:NH1	1.94	0.65
1:A:161:GLU:O	1:A:165:ASN:HB2	1.95	0.65
1:1:205:VAL:HG12	1:1:206:ALA:H	1.62	0.65
2:J:341:THR:HG22	2:J:404:LEU:HD11	1.76	0.65
2:V:375:THR:HG22	4:V:548:HOH:O	1.97	0.65
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.77	0.65
3:J:273:M1N:O16	3:J:273:M1N:H221	1.97	0.65
2:E:459:ASP:H	2:E:462:SER:HB3	1.61	0.65
2:N:301:THR:N	2:N:441:SER:HG	1.95	0.65
2:L:452:LYS:HD3	4:L:549:HOH:O	1.96	0.65
1:I:121:GLU:OE2	1:I:156:MET:HB3	1.96	0.65
1:O:217:ARG:HH21	1:O:223:ARG:HG3	1.62	0.65
2:L:459:ASP:H	2:L:462:SER:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ARG:HB2	4:F:253:HOH:O	1.96	0.65
2:C:485:ASP:OD2	2:C:488:ARG:HB2	1.98	0.64
2:V:518:ILE:O	2:V:522:SER:HB2	1.96	0.64
1:I:172:ALA:HB3	1:I:175:ALA:HB2	1.80	0.64
1:S:140:ARG:HH11	1:S:140:ARG:HB3	1.61	0.64
2:G:318:ARG:HD3	2:G:491:PHE:O	1.97	0.64
1:D:25:ALA:O	1:D:158:GLY:HA2	1.98	0.64
1:F:165:ASN:HD22	1:F:168:LYS:NZ	1.95	0.64
1:F:56:LEU:HD13	1:F:99:LEU:HD22	1.79	0.64
3:L:273:M1N:HN1	3:L:273:M1N:C25	2.10	0.64
2:C:301:THR:HG21	3:C:273:M1N:H16	1.63	0.64
1:O:14:ARG:HB3	1:O:14:ARG:NH1	2.12	0.64
2:R:357:ARG:O	2:R:361:VAL:HG23	1.98	0.64
1:1:151:PRO:HD2	4:1:253:HOH:O	1.97	0.64
1:1:172:ALA:HB3	1:1:175:ALA:HB2	1.80	0.64
2:E:465:ARG:HH11	2:E:465:ARG:HG3	1.63	0.64
1:Q:92:ARG:HG3	1:Q:129:HIS:CE1	2.32	0.64
1:A:93:ASP:OD1	2:P:375:THR:OG1	2.15	0.64
1:W:20:ALA:O	1:W:24:ILE:HG12	1.98	0.64
2:N:349:ALA:HB2	3:N:273:M1N:H252	1.80	0.63
2:G:382:ARG:HD3	1:W:89:TYR:CD1	2.33	0.63
1:M:55:GLU:OE2	1:M:220:ARG:HD2	1.98	0.63
1:M:226:THR:HA	4:M:252:HOH:O	1.97	0.63
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.80	0.63
2:X:464:LEU:HD12	2:X:496:ILE:HD11	1.80	0.63
1:D:90:ASP:HB3	1:D:93:ASP:OD1	1.98	0.63
2:X:424:ASP:HB3	2:X:428:GLY:H	1.62	0.63
1:M:189:ARG:HH22	1:M:235:VAL:HG13	1.63	0.63
2:C:304:VAL:HG21	2:C:450:MET:CE	2.28	0.63
1:S:48:ARG:HD2	1:1:137:GLU:OE2	1.99	0.63
1:Y:55:GLU:OE2	1:Y:220:ARG:HD2	1.98	0.63
2:N:321:THR:O	3:N:273:M1N:H52	1.99	0.63
1:1:217:ARG:NH2	1:1:223:ARG:HG3	2.14	0.63
2:N:444:LEU:CD1	2:V:444:LEU:HD12	2.22	0.63
2:N:324:ASN:H	2:N:324:ASN:ND2	1.92	0.63
2:C:391:LEU:O	2:C:395:MET:HG2	1.99	0.63
1:U:95:THR:OG1	1:U:98:GLN:HG3	1.98	0.63
1:A:170:SER:HB2	1:A:183:ILE:HD12	1.80	0.63
1:D:48:ARG:HD2	1:K:137:GLU:OE2	1.99	0.63
2:J:459:ASP:H	2:J:462:SER:HB3	1.63	0.63
2:2:518:ILE:O	2:2:522:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:O	2:H:357:ARG:NH2	2.32	0.63
2:X:349:ALA:HA	3:X:273:M1N:H243	1.80	0.63
1:S:14:ARG:HB2	1:S:14:ARG:NH1	2.13	0.63
1:U:60:VAL:HG21	1:U:96:GLY:HA3	1.81	0.63
1:F:11:GLN:HG3	1:F:14:ARG:HH12	1.64	0.63
1:Q:10:GLU:HA	1:Y:19:LEU:HD12	1.79	0.63
1:W:110:ILE:HG23	1:W:114:GLN:HG3	1.80	0.63
1:W:189:ARG:NH2	1:W:237:GLN:HB3	2.14	0.63
1:W:14:ARG:NH1	1:W:14:ARG:HB3	2.14	0.63
2:Z:324:ASN:H	2:Z:324:ASN:HD22	1.47	0.63
1:Y:34:ALA:HB3	4:Y:249:HOH:O	1.99	0.63
1:W:205:VAL:HG12	1:W:206:ALA:H	1.64	0.62
1:M:59:ARG:HG3	1:M:129:HIS:CD2	2.34	0.62
1:O:85:ARG:NH1	1:O:85:ARG:CG	2.52	0.62
2:G:349:ALA:H	3:G:273:M1N:H35	1.64	0.62
2:T:436:TYR:HB2	2:T:450:MET:SD	2.39	0.62
2:Z:392:ALA:O	2:Z:395:MET:HB2	1.99	0.62
2:G:452:LYS:NZ	2:2:449:SER:HB2	2.13	0.62
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.81	0.62
1:A:217:ARG:NH2	1:A:223:ARG:HG3	2.14	0.62
2:P:345:ILE:HD13	2:P:352:ALA:HB1	1.81	0.62
2:L:314:MET:HE3	2:L:334:VAL:HG13	1.79	0.62
2:R:457:VAL:HG22	2:R:463:GLY:HA2	1.80	0.62
3:R:273:M1N:C25	3:R:273:M1N:N1	2.63	0.62
2:E:382:ARG:HD3	1:K:89:TYR:HD1	1.62	0.62
2:R:459:ASP:H	2:R:462:SER:HB3	1.63	0.62
2:Z:318:ARG:HD3	2:Z:491:PHE:O	1.99	0.62
1:U:89:TYR:CD1	2:2:382:ARG:HD3	2.34	0.62
2:H:476:ASP:O	2:L:329:ARG:NH2	2.30	0.62
1:K:85:ARG:HG2	1:K:85:ARG:NH1	2.04	0.62
1:F:92:ARG:HG3	1:F:129:HIS:CE1	2.34	0.62
2:P:462:SER:O	2:P:465:ARG:HG2	2.00	0.62
2:G:345:ILE:HD13	2:G:352:ALA:HB1	1.82	0.62
2:L:349:ALA:N	3:L:273:M1N:H35	2.15	0.62
1:D:176:SER:HB3	1:D:179:ASP:OD1	2.00	0.62
1:1:60:VAL:HG21	1:1:96:GLY:HA3	1.82	0.62
3:R:273:M1N:C25	3:R:273:M1N:HN1	2.13	0.62
2:E:321:THR:O	3:E:273:M1N:H51	2.00	0.62
2:G:518:ILE:O	2:G:522:SER:HB2	1.99	0.61
2:2:308:TYR:HB2	2:2:309:PRO:HD2	1.80	0.61
1:F:73:ASN:HD22	1:W:105:GLN:NE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:444:LEU:HD12	2:V:444:LEU:CD1	2.22	0.61
1:1:56:LEU:HD13	1:1:99:LEU:HD22	1.82	0.61
2:T:444:LEU:HD12	2:X:444:LEU:HD12	1.82	0.61
2:P:513:LEU:O	2:P:517:ILE:HG12	2.00	0.61
1:1:25:ALA:O	1:1:158:GLY:HA2	2.01	0.61
2:2:324:ASN:C	2:2:324:ASN:HD22	2.04	0.61
1:W:14:ARG:HB3	1:W:14:ARG:HH11	1.64	0.61
1:1:230:LEU:HD21	1:1:234:LEU:HD13	1.81	0.61
1:B:172:ALA:HB3	1:B:175:ALA:HB2	1.81	0.61
3:P:273:M1N:H40	2:V:424:ASP:OD1	2.00	0.61
2:C:349:ALA:HB2	3:C:273:M1N:H252	1.81	0.61
1:A:185:VAL:HB	1:A:235:VAL:HG11	1.83	0.61
1:I:20:ALA:O	1:I:24:ILE:HG12	2.01	0.61
2:C:424:ASP:OD1	3:J:273:M1N:H40	2.00	0.61
1:O:205:VAL:C	1:O:207:SER:H	2.03	0.61
1:Q:56:LEU:HD13	1:Q:99:LEU:HD22	1.81	0.61
2:C:321:THR:O	3:C:273:M1N:H51	2.01	0.61
1:F:92:ARG:HD2	1:F:129:HIS:CE1	2.36	0.61
2:H:324:ASN:HD22	2:H:324:ASN:N	1.95	0.61
2:2:441:SER:HB2	2:2:478:ASP:OD2	2.00	0.61
1:D:83:ASP:OD2	2:E:365:HIS:CD2	2.53	0.61
2:X:307:LYS:HD2	2:X:418:GLY:O	2.01	0.61
1:D:92:ARG:HG3	1:D:129:HIS:CE1	2.35	0.61
2:Z:349:ALA:CB	3:Z:273:M1N:H252	2.31	0.61
2:X:462:SER:O	2:X:465:ARG:HG2	2.01	0.61
2:J:306:LEU:HD23	2:J:436:TYR:HB3	1.83	0.61
3:J:273:M1N:C25	3:J:273:M1N:HN1	2.14	0.61
1:Y:25:ALA:O	1:Y:158:GLY:HA2	2.00	0.61
2:H:395:MET:HA	2:H:395:MET:CE	2.31	0.61
1:F:110:ILE:HG12	1:F:114:GLN:HG3	1.83	0.60
1:I:12:ALA:O	1:I:16:ARG:HG2	2.02	0.60
2:2:345:ILE:HD13	2:2:352:ALA:HB1	1.83	0.60
2:L:456:GLN:NE2	2:L:465:ARG:NH1	2.49	0.60
3:L:273:M1N:H252	3:L:273:M1N:HN1	1.66	0.60
2:V:513:LEU:O	2:V:517:ILE:HG12	2.00	0.60
2:N:318:ARG:HD3	2:N:491:PHE:O	2.01	0.60
2:N:459:ASP:H	2:N:462:SER:HB3	1.65	0.60
2:N:380:ILE:HD11	2:N:421:VAL:HG21	1.81	0.60
2:R:518:ILE:O	2:R:522:SER:HB2	2.00	0.60
2:X:329:ARG:NH2	2:2:476:ASP:O	2.34	0.60
2:J:321:THR:O	3:J:273:M1N:C5	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:TYR:O	2:G:357:ARG:NH2	2.34	0.60
1:O:14:ARG:HH11	1:O:14:ARG:CB	2.14	0.60
1:F:20:ALA:O	1:F:24:ILE:HG12	2.01	0.60
1:B:19:LEU:HD12	1:I:10:GLU:HA	1.83	0.60
2:2:419:ARG:HH11	2:2:419:ARG:HG3	1.66	0.60
1:U:11:GLN:CG	1:U:14:ARG:HH12	2.11	0.60
2:E:318:ARG:HD3	2:E:491:PHE:O	2.01	0.60
2:G:444:LEU:HD12	2:2:444:LEU:CD1	2.31	0.60
2:2:515:ARG:HA	2:2:518:ILE:HD12	1.84	0.60
1:K:25:ALA:O	1:K:158:GLY:HA2	2.02	0.60
2:E:391:LEU:O	2:E:395:MET:HG2	2.02	0.60
2:E:314:MET:CE	2:E:334:VAL:HG13	2.31	0.60
1:I:182:ARG:HD3	1:I:235:VAL:HB	1.83	0.60
2:T:473:ASP:HA	4:X:20:HOH:O	2.01	0.60
1:D:110:ILE:HG23	1:D:114:GLN:HG3	1.81	0.60
1:Q:89:TYR:CD1	2:Z:382:ARG:HD3	2.37	0.60
3:H:273:M1N:H40	2:P:424:ASP:OD1	2.02	0.60
1:S:25:ALA:O	1:S:158:GLY:HA2	2.02	0.60
2:J:321:THR:O	3:J:273:M1N:H37	2.02	0.59
1:O:25:ALA:O	1:O:158:GLY:HA2	2.02	0.59
1:Y:205:VAL:C	1:Y:207:SER:H	2.05	0.59
1:O:217:ARG:NH2	1:O:223:ARG:HG3	2.15	0.59
2:R:324:ASN:HD22	2:R:324:ASN:C	2.06	0.59
1:S:85:ARG:NH1	1:S:85:ARG:HG2	2.18	0.59
3:L:273:M1N:C22	3:L:273:M1N:O16	2.50	0.59
1:B:205:VAL:HG12	1:B:206:ALA:N	2.17	0.59
2:G:320:SER:HB2	2:G:331:VAL:HG21	1.84	0.59
1:U:55:GLU:OE2	1:U:220:ARG:HD2	2.02	0.59
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.67	0.59
2:T:518:ILE:O	2:T:522:SER:HB2	2.02	0.59
2:H:345:ILE:HD13	2:H:352:ALA:HB1	1.85	0.59
1:S:217:ARG:HH21	1:S:223:ARG:HG3	1.68	0.59
1:F:25:ALA:O	1:F:158:GLY:HA2	2.03	0.59
2:L:308:TYR:HB2	2:L:309:PRO:HD2	1.84	0.59
1:M:205:VAL:HG12	1:M:206:ALA:N	2.17	0.59
2:C:425:ALA:N	4:C:542:HOH:O	2.34	0.59
1:K:230:LEU:CD2	1:K:234:LEU:HD13	2.33	0.59
2:L:349:ALA:HB2	3:L:273:M1N:H252	1.85	0.59
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.84	0.59
1:Q:217:ARG:HH21	1:Q:223:ARG:HG3	1.68	0.59
1:U:25:ALA:O	1:U:158:GLY:HA2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:437:GLN:OE1	2:V:447:LYS:HD3	2.03	0.59
1:O:205:VAL:HG12	1:O:206:ALA:H	1.66	0.59
1:D:172:ALA:HB3	1:D:175:ALA:HB2	1.85	0.59
1:Y:172:ALA:HB3	1:Y:175:ALA:HB2	1.85	0.59
1:S:20:ALA:O	1:S:24:ILE:HG12	2.02	0.59
2:V:318:ARG:HD3	2:V:491:PHE:O	2.03	0.59
2:L:337:THR:HG1	2:L:343:THR:HG22	1.66	0.59
2:2:349:ALA:HB2	3:2:273:M1N:H252	1.84	0.59
2:G:301:THR:N	2:G:441:SER:OG	2.36	0.59
2:P:349:ALA:HB2	3:P:273:M1N:H252	1.83	0.59
2:X:430:ASN:ND2	4:X:16:HOH:O	2.31	0.58
1:I:205:VAL:C	1:I:207:SER:H	2.05	0.58
1:B:25:ALA:O	1:B:158:GLY:HA2	2.02	0.58
2:C:301:THR:N	2:C:441:SER:OG	2.36	0.58
2:V:424:ASP:HB3	2:V:428:GLY:H	1.67	0.58
2:H:407:TYR:CE1	2:H:417:ALA:HB3	2.38	0.58
1:S:19:LEU:HD12	1:I:10:GLU:HA	1.84	0.58
2:P:349:ALA:HA	3:P:273:M1N:H243	1.85	0.58
1:I:11:GLN:HG2	1:I:14:ARG:HH12	1.68	0.58
2:2:419:ARG:CG	2:2:419:ARG:HH11	2.16	0.58
2:G:513:LEU:O	2:G:517:ILE:HG12	2.03	0.58
2:V:337:THR:OG1	2:V:343:THR:HG22	2.03	0.58
2:T:462:SER:O	2:T:465:ARG:HG2	2.03	0.58
1:M:25:ALA:O	1:M:158:GLY:HA2	2.03	0.58
2:E:518:ILE:O	2:E:522:SER:HB2	2.03	0.58
1:W:98:GLN:O	1:W:102:VAL:HG23	2.03	0.58
2:L:321:THR:O	3:L:273:M1N:H37	2.04	0.58
2:2:419:ARG:NH1	2:2:419:ARG:HG3	2.17	0.58
1:I:14:ARG:CB	1:I:14:ARG:HH11	2.16	0.58
1:M:224:ARG:NH1	4:M:255:HOH:O	2.36	0.58
1:Q:25:ALA:O	1:Q:158:GLY:HA2	2.03	0.58
1:K:205:VAL:C	1:K:207:SER:H	2.07	0.58
2:G:345:ILE:HD12	2:G:345:ILE:O	2.03	0.58
2:T:451:LYS:HB3	4:T:12:HOH:O	2.03	0.58
2:H:349:ALA:H	3:H:273:M1N:C35	2.16	0.58
3:P:273:M1N:C25	3:P:273:M1N:HN1	2.16	0.58
2:L:345:ILE:HD12	2:L:345:ILE:O	2.04	0.58
1:U:96:GLY:HA2	1:U:99:LEU:HD13	1.85	0.58
2:G:464:LEU:HD11	2:G:505:VAL:HG11	1.86	0.58
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.86	0.58
2:C:345:ILE:HD13	2:C:352:ALA:HB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:321:THR:O	3:N:273:M1N:C5	2.52	0.57
2:H:465:ARG:HG3	2:H:465:ARG:NH1	2.18	0.57
2:L:349:ALA:H	3:L:273:M1N:C36	2.17	0.57
2:C:304:VAL:HG21	2:C:450:MET:HE3	1.85	0.57
2:Z:518:ILE:O	2:Z:522:SER:HB2	2.04	0.57
1:I:92:ARG:HD2	1:I:129:HIS:ND1	2.18	0.57
1:M:205:VAL:C	1:M:207:SER:H	2.07	0.57
2:R:409:ILE:HG13	2:R:410:HIS:HD2	1.69	0.57
1:O:60:VAL:HG21	1:O:96:GLY:HA3	1.84	0.57
1:W:25:ALA:O	1:W:158:GLY:HA2	2.03	0.57
2:H:349:ALA:H	3:H:273:M1N:C36	2.17	0.57
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.85	0.57
1:M:87:TYR:O	2:N:357:ARG:NH2	2.37	0.57
1:S:205:VAL:C	1:S:207:SER:H	2.06	0.57
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.86	0.57
1:Q:172:ALA:HB3	1:Q:175:ALA:HB2	1.86	0.57
1:F:19:LEU:HD12	1:W:10:GLU:HA	1.85	0.57
1:O:213:LEU:HA	1:O:221:ALA:O	2.05	0.57
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.87	0.57
2:2:391:LEU:O	2:2:395:MET:HG2	2.04	0.57
2:C:513:LEU:O	2:C:517:ILE:HG12	2.04	0.57
2:V:349:ALA:H	3:V:273:M1N:C36	2.18	0.57
2:C:349:ALA:H	3:C:273:M1N:C35	2.17	0.57
1:A:189:ARG:HH22	1:A:235:VAL:HG13	1.69	0.57
2:G:465:ARG:HB2	2:G:513:LEU:HD21	1.85	0.57
1:U:205:VAL:C	1:U:207:SER:H	2.08	0.57
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.86	0.57
2:T:308:TYR:HB2	2:T:309:PRO:HD2	1.87	0.57
1:Q:205:VAL:C	1:Q:207:SER:H	2.08	0.57
2:G:383:LEU:HD21	2:G:402:PRO:CG	2.35	0.57
1:S:11:GLN:HG2	1:S:14:ARG:HH12	1.66	0.57
2:E:321:THR:O	3:E:273:M1N:C5	2.53	0.57
2:J:382:ARG:HD3	1:S:89:TYR:CD1	2.40	0.57
1:B:135:ARG:HH22	1:B:152:HIS:HD2	1.53	0.57
1:I:25:ALA:O	1:I:158:GLY:HA2	2.05	0.57
1:A:205:VAL:C	1:A:207:SER:H	2.08	0.57
2:C:452:LYS:HE2	2:R:521:ARG:NH2	2.19	0.57
1:I:110:ILE:HG23	1:I:114:GLN:HG3	1.87	0.57
1:A:92:ARG:HD2	1:A:129:HIS:ND1	2.20	0.57
1:Q:151:PRO:HD2	4:Q:249:HOH:O	2.04	0.57
2:E:321:THR:O	3:E:273:M1N:H37	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:318:ARG:HD3	2:P:491:PHE:O	2.05	0.56
1:I:11:GLN:HG3	1:I:14:ARG:HH12	1.69	0.56
1:Y:40:LEU:HD12	1:Y:212:VAL:HG12	1.87	0.56
2:H:318:ARG:HD3	2:H:491:PHE:O	2.05	0.56
2:V:376:PHE:CE2	2:V:380:ILE:HD11	2.39	0.56
2:R:321:THR:O	3:R:273:M1N:C5	2.48	0.56
2:H:391:LEU:O	2:H:395:MET:HG2	2.05	0.56
1:F:110:ILE:HG23	1:F:114:GLN:HG3	1.87	0.56
1:I:73:ASN:HB2	1:S:105:GLN:HE22	1.70	0.56
1:K:19:LEU:HD12	1:M:10:GLU:HA	1.86	0.56
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.87	0.56
1:M:230:LEU:HD21	1:M:234:LEU:HD13	1.85	0.56
2:J:383:LEU:HD21	2:J:402:PRO:HG2	1.86	0.56
2:N:395:MET:HA	2:N:395:MET:CE	2.34	0.56
2:Z:335:TYR:HE1	2:Z:345:ILE:HD11	1.71	0.56
2:P:388:ARG:NH1	4:P:551:HOH:O	2.39	0.56
2:G:444:LEU:CD1	2:2:444:LEU:HD12	2.31	0.56
3:E:273:M1N:O16	3:E:273:M1N:C22	2.53	0.56
2:L:513:LEU:O	2:L:517:ILE:HG12	2.06	0.56
1:W:15:GLU:OE1	1:Y:9:PRO:HD2	2.06	0.56
1:1:182:ARG:HH11	1:1:182:ARG:HB2	1.69	0.56
2:N:349:ALA:H	3:N:273:M1N:C36	2.18	0.56
2:V:321:THR:O	3:V:273:M1N:C5	2.53	0.56
1:1:121:GLU:OE2	1:1:156:MET:HB3	2.06	0.56
2:H:518:ILE:O	2:H:522:SER:HB2	2.06	0.56
1:A:25:ALA:O	1:A:158:GLY:HA2	2.04	0.56
1:F:205:VAL:C	1:F:207:SER:H	2.09	0.56
2:2:329:ARG:O	2:2:490:ILE:HG21	2.06	0.56
1:M:110:ILE:HG23	1:M:114:GLN:HG3	1.87	0.56
2:J:349:ALA:H	3:J:273:M1N:H35	1.70	0.56
2:H:461:ASP:OD1	2:H:509:ARG:HD2	2.06	0.56
2:N:465:ARG:HB2	2:N:513:LEU:CD2	2.35	0.56
1:1:213:LEU:HA	1:1:221:ALA:O	2.06	0.56
1:Y:213:LEU:HA	1:Y:221:ALA:O	2.05	0.56
1:Y:59:ARG:HG3	1:Y:129:HIS:HD2	1.71	0.56
1:Q:127:VAL:HG22	1:Q:215:ALA:HB2	1.87	0.56
2:2:341:THR:HG22	2:2:404:LEU:HD11	1.88	0.56
1:K:205:VAL:HG12	1:K:206:ALA:N	2.21	0.56
2:N:518:ILE:O	2:N:522:SER:HB2	2.06	0.56
2:J:518:ILE:O	2:J:522:SER:HB2	2.06	0.56
1:O:20:ALA:O	1:O:24:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:461:ASP:OD1	2:E:509:ARG:HD2	2.06	0.56
1:B:30:VAL:HG22	1:B:43:ALA:HB1	1.87	0.56
2:Z:317:ASP:OD1	2:Z:333:LYS:NZ	2.37	0.56
1:S:172:ALA:HB3	1:S:175:ALA:HB2	1.86	0.56
1:B:12:ALA:O	1:B:16:ARG:HG2	2.06	0.56
2:C:317:ASP:OD1	2:C:333:LYS:NZ	2.39	0.56
1:B:20:ALA:O	1:B:24:ILE:HG12	2.06	0.56
1:B:182:ARG:HB2	1:B:182:ARG:NH1	2.21	0.56
1:Y:94:VAL:HA	1:Y:98:GLN:HE22	1.71	0.56
2:2:462:SER:O	2:2:465:ARG:HG2	2.06	0.56
2:T:345:ILE:O	2:T:345:ILE:HD12	2.06	0.56
2:T:513:LEU:O	2:T:517:ILE:HG12	2.06	0.56
2:G:452:LYS:HZ3	2:2:449:SER:HB2	1.71	0.56
2:N:318:ARG:O	2:N:331:VAL:HG23	2.06	0.56
2:E:314:MET:HE2	2:E:334:VAL:HG13	1.88	0.56
1:M:83:ASP:OD2	2:N:365:HIS:HD2	1.89	0.56
1:W:155:VAL:HG12	1:W:160:THR:HG22	1.88	0.56
2:J:444:LEU:CD1	2:Z:444:LEU:HD12	2.21	0.55
1:K:56:LEU:HD23	1:K:79:ILE:HG13	1.88	0.55
2:P:341:THR:HG22	2:P:404:LEU:HD11	1.88	0.55
2:T:514:ALA:O	2:T:518:ILE:HG13	2.06	0.55
1:Y:214:ASP:OD2	1:Y:217:ARG:HG2	2.05	0.55
2:L:321:THR:O	3:L:273:M1N:C5	2.54	0.55
1:D:205:VAL:C	1:D:207:SER:H	2.09	0.55
1:M:20:ALA:O	1:M:24:ILE:HG12	2.05	0.55
2:E:513:LEU:O	2:E:517:ILE:HG12	2.06	0.55
1:D:161:GLU:H	1:D:161:GLU:CD	2.10	0.55
2:L:337:THR:OG1	2:L:343:THR:CG2	2.51	0.55
1:B:98:GLN:O	1:B:102:VAL:HG23	2.07	0.55
1:1:205:VAL:C	1:1:207:SER:H	2.10	0.55
1:D:87:TYR:O	2:E:357:ARG:NH2	2.39	0.55
2:T:321:THR:O	3:T:273:M1N:H52	2.05	0.55
1:Q:171:TYR:CE2	1:Q:173:GLU:HA	2.40	0.55
2:G:307:LYS:NZ	2:G:433:GLU:HA	2.21	0.55
2:P:365:HIS:CE1	2:P:369:LEU:HD11	2.41	0.55
2:2:314:MET:CE	2:2:334:VAL:HG13	2.36	0.55
1:U:134:LYS:HA	1:U:134:LYS:HE2	1.89	0.55
1:Q:127:VAL:CG2	1:Q:215:ALA:HB2	2.36	0.55
1:Y:128:ALA:HB2	1:Y:134:LYS:HB3	1.89	0.55
1:A:110:ILE:HG23	1:A:114:GLN:HG3	1.89	0.55
2:L:349:ALA:H	3:L:273:M1N:H35	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:161:GLU:O	1:S:165:ASN:HB2	2.06	0.55
1:F:128:ALA:HB2	1:F:134:LYS:HB3	1.88	0.55
2:J:324:ASN:N	2:J:324:ASN:HD22	1.91	0.55
1:1:110:ILE:HA	1:1:114:GLN:HG2	1.88	0.55
1:W:205:VAL:C	1:W:207:SER:H	2.10	0.55
2:2:341:THR:CG2	2:2:404:LEU:HD11	2.37	0.55
2:N:486:LEU:HD11	2:N:518:ILE:HD13	1.89	0.55
2:P:407:TYR:CE1	2:P:417:ALA:HB3	2.42	0.55
1:K:115:ALA:HB3	1:M:112:THR:HG23	1.88	0.55
1:S:83:ASP:OD2	2:T:365:HIS:CD2	2.53	0.55
2:2:459:ASP:HB2	4:2:552:HOH:O	2.07	0.55
2:T:486:LEU:HD11	2:T:518:ILE:HD13	1.89	0.55
1:B:55:GLU:OE2	1:B:220:ARG:HD2	2.06	0.55
2:G:349:ALA:N	3:G:273:M1N:H35	2.21	0.55
2:L:462:SER:O	2:L:465:ARG:HG2	2.07	0.55
1:1:205:VAL:HG12	1:1:206:ALA:N	2.21	0.55
1:F:23:GLY:HA2	1:F:26:ARG:HE	1.72	0.55
1:K:11:GLN:HG2	1:K:14:ARG:HH12	1.72	0.55
1:U:172:ALA:HB3	1:U:175:ALA:HB2	1.87	0.55
1:O:182:ARG:HD3	1:O:235:VAL:HG23	1.89	0.55
2:Z:349:ALA:H	3:Z:273:M1N:C36	2.20	0.54
2:V:392:ALA:O	2:V:395:MET:HB2	2.07	0.54
1:Y:170:SER:HB2	1:Y:183:ILE:HD12	1.89	0.54
2:2:432:GLU:HG3	2:2:437:GLN:HB2	1.87	0.54
1:O:92:ARG:HH11	1:O:92:ARG:HB2	1.72	0.54
1:W:205:VAL:HG12	1:W:206:ALA:N	2.22	0.54
1:Q:20:ALA:O	1:Q:24:ILE:HG12	2.07	0.54
2:R:355:PHE:CE1	2:R:386:MET:HG2	2.42	0.54
1:U:213:LEU:HA	1:U:221:ALA:O	2.07	0.54
2:G:332:ARG:HD3	4:G:223:HOH:O	2.08	0.54
1:F:10:GLU:HA	1:M:19:LEU:HD12	1.88	0.54
1:Y:139:TYR:CD2	1:Y:149:ASP:HB3	2.42	0.54
1:U:33:LEU:HD11	1:U:180:ALA:HB1	1.88	0.54
2:Z:457:VAL:HG22	2:Z:463:GLY:HA2	1.88	0.54
2:H:308:TYR:HB2	2:H:309:PRO:HD2	1.90	0.54
1:K:16:ARG:HE	1:K:117:PRO:HD3	1.71	0.54
2:R:318:ARG:HB3	2:R:331:VAL:O	2.07	0.54
1:K:110:ILE:HA	1:K:114:GLN:HG2	1.89	0.54
2:J:308:TYR:HB2	2:J:309:PRO:HD2	1.90	0.54
1:F:182:ARG:NH1	1:F:182:ARG:HB2	2.23	0.54
2:R:307:LYS:NZ	2:R:433:GLU:HA	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:59:ARG:HG3	1:Q:129:HIS:CD2	2.30	0.54
3:E:273:M1N:N1	3:E:273:M1N:C25	2.71	0.54
1:O:9:PRO:HD3	4:O:249:HOH:O	2.07	0.54
2:H:307:LYS:HD2	2:H:418:GLY:O	2.06	0.54
1:U:161:GLU:O	1:U:165:ASN:HB2	2.07	0.54
2:X:314:MET:HE3	2:X:334:VAL:HG13	1.89	0.54
2:2:337:THR:HG21	2:2:359:TYR:CD2	2.43	0.54
2:X:459:ASP:H	2:X:462:SER:HB3	1.73	0.54
1:K:115:ALA:HB3	1:M:112:THR:CG2	2.38	0.54
2:V:303:ILE:HG21	4:V:553:HOH:O	2.08	0.54
2:G:329:ARG:O	2:G:490:ILE:HG21	2.07	0.54
2:Z:464:LEU:HD11	2:Z:505:VAL:HG11	1.89	0.54
2:E:437:GLN:OE1	2:E:447:LYS:HD3	2.08	0.54
2:E:319:ARG:HG3	2:E:320:SER:N	2.22	0.54
2:J:514:ALA:O	2:J:518:ILE:HG13	2.07	0.54
1:M:30:VAL:HG22	1:M:43:ALA:HB1	1.89	0.54
1:D:36:ALA:HA	4:D:250:HOH:O	2.07	0.54
2:H:301:THR:N	2:H:441:SER:OG	2.41	0.54
1:Y:209:GLU:OE2	1:Y:224:ARG:NH2	2.41	0.54
1:U:185:VAL:HB	1:U:235:VAL:CG1	2.38	0.54
2:R:306:LEU:HD12	2:R:467:ALA:HB2	1.89	0.54
2:Z:329:ARG:O	2:Z:490:ILE:HG21	2.07	0.54
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.90	0.54
2:P:412:SER:O	2:P:414:PRO:HD3	2.08	0.54
2:L:303:ILE:HD11	2:L:333:LYS:HB3	1.88	0.54
2:T:349:ALA:H	3:T:273:M1N:H35	1.72	0.53
1:F:185:VAL:HB	1:F:235:VAL:HG11	1.90	0.53
1:I:220:ARG:NH2	2:J:367:GLU:OE2	2.36	0.53
2:R:341:THR:HG22	2:R:404:LEU:HD11	1.89	0.53
1:Y:176:SER:H	1:Y:179:ASP:HB2	1.71	0.53
2:N:432:GLU:HG3	2:N:437:GLN:HB2	1.90	0.53
2:T:377:ALA:HA	2:T:380:ILE:HD12	1.90	0.53
2:L:445:PHE:CE1	2:P:444:LEU:HD11	2.43	0.53
1:Q:92:ARG:HG3	1:Q:129:HIS:HE1	1.71	0.53
2:G:349:ALA:HB2	3:G:273:M1N:H252	1.90	0.53
2:G:521:ARG:HH22	2:2:452:LYS:NZ	2.06	0.53
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.44	0.53
2:R:464:LEU:HD11	2:R:505:VAL:HG11	1.89	0.53
1:U:14:ARG:CZ	1:U:14:ARG:HB3	2.38	0.53
1:S:14:ARG:HB2	1:S:14:ARG:HH11	1.71	0.53
2:V:432:GLU:HG3	2:V:437:GLN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:345:ILE:HD13	2:R:352:ALA:HB1	1.89	0.53
2:N:335:TYR:HE1	2:N:345:ILE:HD11	1.72	0.53
2:R:475:ALA:HB2	2:R:481:THR:HG22	1.89	0.53
1:S:213:LEU:HA	1:S:221:ALA:O	2.08	0.53
2:G:424:ASP:OD2	3:X:273:M1N:H34	2.07	0.53
1:W:55:GLU:OE2	1:W:220:ARG:HD2	2.08	0.53
2:C:462:SER:O	2:C:465:ARG:HG2	2.08	0.53
1:I:60:VAL:HG21	1:I:96:GLY:CA	2.37	0.53
1:W:85:ARG:HH11	1:W:85:ARG:CG	2.20	0.53
1:B:205:VAL:C	1:B:207:SER:H	2.11	0.53
1:Y:16:ARG:HE	1:Y:117:PRO:HD3	1.74	0.53
1:Q:63:ALA:O	1:Q:156:MET:HE1	2.09	0.53
1:M:213:LEU:HA	1:M:221:ALA:O	2.09	0.53
2:2:345:ILE:HB	2:2:352:ALA:HB1	1.91	0.53
2:G:465:ARG:HG3	2:G:466:VAL:N	2.24	0.53
1:F:185:VAL:HB	1:F:235:VAL:CG1	2.38	0.53
1:F:226:THR:O	1:F:230:LEU:HB2	2.08	0.53
2:P:457:VAL:HG22	2:P:463:GLY:HA2	1.91	0.53
1:D:135:ARG:HD3	1:D:136:PRO:HD2	1.91	0.53
2:T:457:VAL:HG22	2:T:463:GLY:HA2	1.91	0.53
2:C:437:GLN:OE1	2:C:447:LYS:HD3	2.08	0.53
2:E:380:ILE:HD11	2:E:421:VAL:HG21	1.89	0.53
1:K:182:ARG:HB2	1:K:182:ARG:NH1	2.23	0.53
2:X:464:LEU:HD11	2:X:505:VAL:HG21	1.90	0.53
2:P:391:LEU:O	2:P:395:MET:HG2	2.09	0.53
2:X:457:VAL:HG22	2:X:463:GLY:HA2	1.90	0.53
1:Y:28:LYS:HE3	1:Y:44:GLU:HG3	1.90	0.53
1:A:55:GLU:OE2	1:A:220:ARG:HD2	2.08	0.53
1:O:13:MET:HG3	1:U:19:LEU:HD11	1.90	0.53
1:Y:41:PHE:HE2	1:Y:213:LEU:HD13	1.73	0.53
2:G:451:LYS:NZ	2:2:473:ASP:OD1	2.38	0.53
1:A:176:SER:HB3	1:A:179:ASP:OD1	2.09	0.53
1:D:89:TYR:CE1	2:R:382:ARG:HD3	2.44	0.53
2:P:383:LEU:HD21	2:P:402:PRO:CG	2.38	0.53
2:H:457:VAL:HG22	2:H:463:GLY:HA2	1.91	0.53
2:C:457:VAL:HG22	2:C:463:GLY:HA2	1.90	0.53
1:D:219:ARG:HH11	1:D:219:ARG:HG2	1.73	0.53
2:X:321:THR:O	3:X:273:M1N:C5	2.53	0.53
2:P:349:ALA:H	3:P:273:M1N:C36	2.21	0.53
1:B:54:SER:CB	1:B:75:ARG:HD2	2.39	0.53
1:I:19:LEU:HD12	1:S:10:GLU:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:72:ASP:O	1:1:76:ARG:HG3	2.09	0.53
1:Q:142:THR:OG1	1:Q:146:SER:HB2	2.09	0.53
1:1:140:ARG:NH1	1:1:140:ARG:HB3	2.24	0.53
2:V:349:ALA:N	3:V:273:M1N:C35	2.54	0.53
2:L:382:ARG:HD3	1:M:89:TYR:CD1	2.44	0.53
2:L:312:VAL:HG23	2:L:497:ILE:HD12	1.90	0.53
3:P:273:M1N:H221	3:P:273:M1N:O16	2.10	0.52
2:T:314:MET:HE3	2:T:334:VAL:HG13	1.89	0.52
2:C:450:MET:HE3	2:C:470:ALA:CB	2.38	0.52
2:R:345:ILE:HD12	2:R:345:ILE:O	2.09	0.52
2:X:457:VAL:HB	4:X:115:HOH:O	2.09	0.52
1:W:16:ARG:HE	1:W:117:PRO:HD3	1.73	0.52
1:B:185:VAL:HB	1:B:235:VAL:CG1	2.39	0.52
1:M:12:ALA:O	1:M:16:ARG:HG2	2.09	0.52
2:X:349:ALA:H	3:X:273:M1N:C35	2.23	0.52
2:N:513:LEU:O	2:N:517:ILE:HG12	2.08	0.52
2:P:337:THR:HG21	2:P:359:TYR:CD2	2.44	0.52
2:L:321:THR:O	3:L:273:M1N:H52	2.09	0.52
2:N:317:ASP:OD1	2:N:333:LYS:NZ	2.42	0.52
1:O:203:LEU:HG	1:O:237:GLN:HE22	1.74	0.52
1:U:20:ALA:O	1:U:24:ILE:HG12	2.09	0.52
2:J:301:THR:HG22	2:J:302:THR:N	2.25	0.52
2:Z:321:THR:O	3:Z:273:M1N:H51	2.08	0.52
2:J:338:ASP:OD1	2:J:341:THR:OG1	2.14	0.52
1:D:176:SER:H	1:D:179:ASP:HB2	1.74	0.52
2:V:465:ARG:HB2	2:V:513:LEU:HD21	1.91	0.52
2:P:349:ALA:H	3:P:273:M1N:C35	2.22	0.52
2:T:349:ALA:N	3:T:273:M1N:H35	2.25	0.52
2:L:349:ALA:N	3:L:273:M1N:C35	2.69	0.52
1:F:165:ASN:ND2	1:F:168:LYS:HZ1	2.08	0.52
1:Q:213:LEU:HA	1:Q:221:ALA:O	2.09	0.52
1:Y:185:VAL:HB	1:Y:235:VAL:CG1	2.40	0.52
1:K:176:SER:HB3	1:K:179:ASP:OD1	2.09	0.52
1:A:12:ALA:O	1:A:16:ARG:HG2	2.09	0.52
1:M:33:LEU:HD11	1:M:40:LEU:HD23	1.90	0.52
1:K:92:ARG:HB2	1:K:92:ARG:HH11	1.73	0.52
1:I:178:THR:HB	1:I:233:LEU:HD23	1.91	0.52
2:X:490:ILE:HA	4:X:74:HOH:O	2.10	0.52
1:F:127:VAL:HG11	1:F:213:LEU:HB3	1.92	0.52
2:P:424:ASP:HB3	2:P:428:GLY:N	2.24	0.52
2:X:314:MET:HE2	2:X:342:ALA:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:303:ILE:HD11	2:T:333:LYS:HB3	1.90	0.52
1:A:54:SER:CB	1:A:75:ARG:HD2	2.40	0.52
1:A:64:ALA:CB	1:A:122:LEU:HD12	2.40	0.52
1:U:176:SER:H	1:U:179:ASP:HB2	1.74	0.52
1:M:118:TYR:HB3	1:M:120:VAL:HG22	1.92	0.52
2:P:461:ASP:OD1	2:P:509:ARG:HD2	2.10	0.52
1:F:165:ASN:ND2	1:F:168:LYS:NZ	2.57	0.52
1:F:16:ARG:NH2	1:F:114:GLN:O	2.43	0.52
1:S:185:VAL:HB	1:S:235:VAL:CG1	2.40	0.52
2:X:395:MET:HA	2:X:395:MET:CE	2.39	0.52
3:T:273:M1N:HN1	3:T:273:M1N:C25	2.23	0.52
1:Q:205:VAL:HG12	1:Q:206:ALA:H	1.74	0.52
1:D:185:VAL:HB	1:D:235:VAL:CG1	2.40	0.52
1:W:60:VAL:HG21	1:W:96:GLY:HA3	1.92	0.52
1:F:48:ARG:NH2	1:W:135:ARG:HD2	2.25	0.52
2:P:439:VAL:HG11	4:P:548:HOH:O	2.09	0.52
2:N:321:THR:HG22	4:N:543:HOH:O	2.09	0.51
2:X:320:SER:HB3	2:X:328:GLY:HA3	1.92	0.51
2:P:327:SER:OG	3:P:273:M1N:H38	2.08	0.51
1:F:182:ARG:HH11	1:F:182:ARG:HB2	1.75	0.51
1:I:55:GLU:OE1	1:I:220:ARG:NH1	2.43	0.51
1:I:55:GLU:OE2	1:I:220:ARG:HD2	2.10	0.51
1:A:90:ASP:HB3	1:A:93:ASP:OD1	2.10	0.51
1:F:213:LEU:HA	1:F:221:ALA:O	2.10	0.51
1:W:87:TYR:HA	2:X:357:ARG:HH21	1.75	0.51
1:D:63:ALA:O	1:D:156:MET:HE1	2.10	0.51
1:I:213:LEU:HA	1:I:221:ALA:O	2.10	0.51
1:W:223:ARG:HA	4:W:253:HOH:O	2.10	0.51
1:K:181:LEU:HD23	1:K:233:LEU:HB3	1.92	0.51
1:W:213:LEU:HA	1:W:221:ALA:O	2.10	0.51
2:C:382:ARG:NH1	2:C:385:ILE:HD13	2.26	0.51
2:N:509:ARG:HG3	4:N:541:HOH:O	2.10	0.51
2:X:380:ILE:HD11	2:X:421:VAL:HG21	1.92	0.51
1:O:85:ARG:HG3	1:O:85:ARG:HH11	1.70	0.51
1:A:185:VAL:HB	1:A:235:VAL:CG1	2.40	0.51
1:K:176:SER:H	1:K:179:ASP:HB2	1.75	0.51
1:A:64:ALA:HB2	1:A:122:LEU:HD12	1.92	0.51
1:D:96:GLY:HA2	1:D:99:LEU:HB2	1.92	0.51
2:C:432:GLU:HG3	2:C:437:GLN:HB2	1.92	0.51
1:M:181:LEU:HD23	1:M:233:LEU:HB3	1.90	0.51
1:I:209:GLU:OE2	1:I:224:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:92:ARG:HB2	1:W:92:ARG:HH11	1.75	0.51
2:J:345:ILE:HD12	2:J:345:ILE:O	2.09	0.51
2:T:314:MET:HE2	2:T:334:VAL:HG13	1.93	0.51
1:M:203:LEU:HA	4:M:260:HOH:O	2.09	0.51
1:M:85:ARG:NH1	1:M:85:ARG:CG	2.59	0.51
1:Y:226:THR:HG23	1:Y:227:GLY:N	2.26	0.51
2:2:513:LEU:O	2:2:517:ILE:HG12	2.10	0.51
2:L:329:ARG:O	2:L:490:ILE:HG21	2.11	0.51
2:E:337:THR:HG21	2:E:359:TYR:CE2	2.46	0.51
1:I:132:GLU:HA	4:I:252:HOH:O	2.11	0.51
2:V:345:ILE:HD13	2:V:352:ALA:HB1	1.91	0.51
1:D:59:ARG:CG	1:D:129:HIS:HD2	2.11	0.51
1:K:213:LEU:HA	1:K:221:ALA:O	2.11	0.51
2:G:382:ARG:NH1	2:G:385:ILE:HD13	2.26	0.51
2:C:424:ASP:HB3	2:C:428:GLY:N	2.26	0.51
2:N:345:ILE:HD13	2:N:352:ALA:HB1	1.93	0.51
1:A:213:LEU:HA	1:A:221:ALA:O	2.11	0.51
2:Z:304:VAL:HG21	2:Z:450:MET:HE3	1.92	0.51
2:R:322:GLN:O	2:R:322:GLN:HG2	2.11	0.51
2:E:382:ARG:HD3	1:K:89:TYR:CE1	2.46	0.50
2:R:337:THR:OG1	2:R:343:THR:HG22	2.12	0.50
1:I:59:ARG:HG3	1:I:129:HIS:CD2	2.47	0.50
2:T:306:LEU:HD23	2:T:436:TYR:HB3	1.92	0.50
1:S:182:ARG:HB2	1:S:182:ARG:NH1	2.26	0.50
2:L:407:TYR:CE1	2:L:417:ALA:HB3	2.46	0.50
1:K:59:ARG:CZ	1:K:221:ALA:HB2	2.42	0.50
1:D:20:ALA:O	1:D:24:ILE:HG12	2.11	0.50
1:B:213:LEU:HA	1:B:221:ALA:O	2.11	0.50
1:I:230:LEU:HD21	1:I:234:LEU:HD13	1.92	0.50
2:E:345:ILE:HD13	2:E:352:ALA:HB1	1.93	0.50
1:W:176:SER:H	1:W:179:ASP:HB2	1.76	0.50
1:F:165:ASN:HD22	1:F:168:LYS:HZ3	1.57	0.50
1:O:112:THR:HG22	1:U:115:ALA:HB3	1.92	0.50
1:Q:30:VAL:HG22	1:Q:43:ALA:HB1	1.93	0.50
2:Z:319:ARG:HG3	2:Z:320:SER:N	2.27	0.50
1:D:15:GLU:OE1	1:K:9:PRO:HD2	2.11	0.50
2:R:513:LEU:O	2:R:517:ILE:HG12	2.11	0.50
2:L:456:GLN:NE2	2:L:465:ARG:HH12	2.06	0.50
2:Z:324:ASN:H	2:Z:324:ASN:ND2	2.08	0.50
1:K:205:VAL:CG1	1:K:206:ALA:N	2.75	0.50
1:D:213:LEU:HA	1:D:221:ALA:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:337:THR:OG1	2:C:343:THR:HG22	2.12	0.50
2:N:452:LYS:NZ	2:V:449:SER:HB2	2.25	0.50
2:V:349:ALA:HB2	3:V:273:M1N:H252	1.92	0.50
1:U:185:VAL:HB	1:U:235:VAL:HG11	1.92	0.50
1:M:142:THR:OG1	1:M:146:SER:HB2	2.12	0.50
2:N:341:THR:HG22	2:N:404:LEU:HD11	1.92	0.50
2:X:383:LEU:HD13	2:X:423:PHE:CE1	2.46	0.50
2:X:324:ASN:HD22	2:X:324:ASN:C	2.14	0.50
2:N:349:ALA:HB3	3:N:273:M1N:C34	2.42	0.50
2:X:314:MET:HE2	2:X:342:ALA:HB1	1.93	0.50
1:Y:20:ALA:O	1:Y:24:ILE:HG12	2.11	0.50
3:Z:273:M1N:H221	3:Z:273:M1N:H16	1.73	0.50
1:Y:185:VAL:HB	1:Y:235:VAL:HG11	1.94	0.50
1:D:127:VAL:HG12	1:D:213:LEU:HD23	1.94	0.50
1:F:115:ALA:HB3	1:W:112:THR:HG23	1.94	0.50
2:G:465:ARG:HB2	2:G:513:LEU:CD2	2.42	0.50
1:W:214:ASP:OD2	1:W:217:ARG:HG2	2.11	0.50
1:U:40:LEU:HA	1:U:212:VAL:HG12	1.94	0.50
1:Q:80:GLN:O	1:Q:84:THR:OG1	2.30	0.50
2:N:382:ARG:CZ	2:N:385:ILE:HD12	2.42	0.50
2:L:324:ASN:ND2	2:L:324:ASN:H	2.09	0.50
2:H:513:LEU:O	2:H:517:ILE:HG12	2.11	0.50
2:C:318:ARG:HD3	2:C:491:PHE:O	2.12	0.50
2:P:383:LEU:HD21	2:P:402:PRO:HG3	1.94	0.50
2:C:448:SER:OG	2:R:448:SER:HB3	2.12	0.50
2:J:464:LEU:HD23	2:J:513:LEU:HD12	1.94	0.50
1:O:87:TYR:HA	2:P:357:ARG:HH21	1.77	0.50
2:T:324:ASN:HD22	2:T:324:ASN:C	2.15	0.50
2:N:349:ALA:N	3:N:273:M1N:C35	2.57	0.49
1:D:92:ARG:CD	1:D:129:HIS:CE1	2.92	0.49
2:H:462:SER:O	2:H:465:ARG:HG2	2.12	0.49
1:M:225:ILE:HG22	1:M:230:LEU:HB2	1.93	0.49
1:I:225:ILE:HG22	1:I:230:LEU:HB2	1.93	0.49
4:W:254:HOH:O	2:X:354:GLU:HG3	2.12	0.49
1:K:80:GLN:O	1:K:84:THR:OG1	2.30	0.49
2:J:457:VAL:HG22	2:J:463:GLY:HA2	1.94	0.49
1:O:85:ARG:NH1	1:O:85:ARG:HG2	2.16	0.49
1:S:60:VAL:HG21	1:S:96:GLY:HA3	1.94	0.49
2:C:452:LYS:HE2	2:R:521:ARG:HH22	1.78	0.49
2:N:465:ARG:HB2	2:N:513:LEU:HD22	1.94	0.49
2:2:437:GLN:OE1	2:2:447:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:155:VAL:HG12	1:Y:160:THR:HG22	1.94	0.49
2:T:432:GLU:HG3	2:T:437:GLN:HB2	1.95	0.49
1:U:155:VAL:HG12	1:U:160:THR:HG22	1.94	0.49
2:Z:308:TYR:HB2	2:Z:309:PRO:HD2	1.94	0.49
2:E:395:MET:CE	2:E:395:MET:HA	2.42	0.49
2:E:301:THR:N	2:E:441:SER:OG	2.46	0.49
1:B:63:ALA:O	1:B:156:MET:HE1	2.13	0.49
1:M:83:ASP:OD2	2:N:365:HIS:CD2	2.65	0.49
2:X:381:ASN:ND2	1:Y:88:ALA:O	2.45	0.49
1:B:181:LEU:HD23	1:B:233:LEU:HB3	1.95	0.49
2:V:436:TYR:HB2	2:V:450:MET:SD	2.52	0.49
2:N:322:GLN:O	2:N:322:GLN:HG2	2.13	0.49
2:N:349:ALA:HB3	3:N:273:M1N:C35	2.42	0.49
2:X:322:GLN:HE21	3:X:273:M1N:C38	2.26	0.49
2:X:321:THR:O	3:X:273:M1N:H37	2.12	0.49
1:M:189:ARG:NH2	1:M:235:VAL:HG13	2.26	0.49
2:R:318:ARG:HD3	2:R:491:PHE:O	2.11	0.49
2:X:358:LEU:HD23	4:X:141:HOH:O	2.12	0.49
1:I:30:VAL:HG22	1:I:43:ALA:HB1	1.94	0.49
2:N:464:LEU:HD11	2:N:505:VAL:HG11	1.94	0.49
1:F:55:GLU:OE2	1:F:220:ARG:HD2	2.12	0.49
1:B:14:ARG:HH11	1:B:14:ARG:HB3	1.77	0.49
2:Z:301:THR:N	2:Z:441:SER:OG	2.46	0.49
2:2:392:ALA:O	2:2:395:MET:HB2	2.12	0.49
2:G:409:ILE:HG13	2:G:410:HIS:CD2	2.47	0.49
1:M:217:ARG:HH21	1:M:223:ARG:HG3	1.77	0.49
2:H:382:ARG:HD3	1:B:89:TYR:CD1	2.48	0.49
1:F:176:SER:H	1:F:179:ASP:HB2	1.78	0.49
1:A:172:ALA:HB3	1:A:175:ALA:HB2	1.95	0.49
2:R:391:LEU:O	2:R:395:MET:HG2	2.11	0.49
1:1:56:LEU:HB2	1:1:60:VAL:HG13	1.95	0.49
1:A:11:GLN:HG2	1:A:14:ARG:HH12	1.77	0.49
2:Z:301:THR:N	2:Z:441:SER:HG	2.10	0.49
1:K:226:THR:O	1:K:230:LEU:HB2	2.13	0.49
2:V:424:ASP:HB2	2:V:428:GLY:O	2.13	0.49
1:K:59:ARG:CG	1:K:129:HIS:HD2	2.25	0.49
2:L:465:ARG:HB3	2:L:513:LEU:CD2	2.43	0.49
1:K:42:VAL:HG22	1:K:210:VAL:HG22	1.93	0.49
1:I:161:GLU:O	1:I:165:ASN:HB2	2.13	0.49
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.95	0.49
1:1:182:ARG:NH1	1:1:182:ARG:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:ASP:OD2	2:2:365:HIS:HD2	1.95	0.49
1:U:76:ARG:HG2	2:V:369:LEU:HD22	1.95	0.49
1:Y:83:ASP:OD2	2:Z:365:HIS:HD2	1.96	0.49
2:2:304:VAL:HG23	2:2:438:ALA:HB2	1.95	0.49
1:K:85:ARG:NH1	1:K:85:ARG:CG	2.61	0.49
2:Z:321:THR:O	3:Z:273:M1N:C5	2.61	0.49
1:S:56:LEU:HB2	1:S:60:VAL:HG13	1.93	0.49
1:1:30:VAL:HG22	1:1:43:ALA:HB1	1.94	0.49
1:W:189:ARG:CZ	1:W:237:GLN:HB3	2.43	0.49
2:G:357:ARG:O	2:G:361:VAL:HG23	2.12	0.49
2:N:391:LEU:O	2:N:395:MET:HG2	2.13	0.49
1:U:223:ARG:HH11	1:U:225:ILE:HD11	1.78	0.49
2:L:399:LEU:HD11	2:L:401:LEU:HD13	1.94	0.49
2:G:307:LYS:HE2	2:G:435:GLY:HA2	1.95	0.48
2:R:469:GLU:HG3	2:R:517:ILE:HD12	1.94	0.48
2:L:399:LEU:CD1	2:L:401:LEU:HD13	2.43	0.48
2:J:381:ASN:ND2	1:S:88:ALA:O	2.46	0.48
2:Z:337:THR:HG21	2:Z:359:TYR:CD2	2.47	0.48
1:1:85:ARG:HH11	1:1:85:ARG:HG2	1.76	0.48
1:1:110:ILE:HG21	1:1:118:TYR:CD1	2.47	0.48
2:E:465:ARG:NH1	2:E:465:ARG:HG3	2.25	0.48
1:I:115:ALA:HB3	1:S:112:THR:HG22	1.94	0.48
2:H:364:GLU:HG2	2:H:368:LYS:HE2	1.95	0.48
2:J:349:ALA:N	3:J:273:M1N:H35	2.28	0.48
2:H:331:VAL:HG11	3:H:273:M1N:H251	1.93	0.48
2:P:424:ASP:HB3	2:P:428:GLY:H	1.76	0.48
1:I:92:ARG:HH11	1:I:92:ARG:HB2	1.77	0.48
1:U:85:ARG:NH1	1:U:89:TYR:HE2	2.11	0.48
1:B:185:VAL:HB	1:B:235:VAL:HG11	1.94	0.48
2:V:322:GLN:O	2:V:322:GLN:HG2	2.12	0.48
1:W:56:LEU:HB2	1:W:60:VAL:HG13	1.96	0.48
1:F:48:ARG:HH22	1:W:135:ARG:HD2	1.78	0.48
1:B:209:GLU:OE2	1:B:224:ARG:NH2	2.46	0.48
1:K:172:ALA:HB3	1:K:175:ALA:HB2	1.94	0.48
1:I:48:ARG:HH22	1:S:135:ARG:HB3	1.79	0.48
1:1:177:LEU:CB	4:1:251:HOH:O	2.60	0.48
2:C:324:ASN:HD22	2:C:324:ASN:C	2.15	0.48
2:X:348:THR:HG23	3:X:273:M1N:H35	1.95	0.48
2:2:321:THR:O	3:2:273:M1N:C5	2.56	0.48
1:K:41:PHE:HE2	1:K:213:LEU:HD22	1.79	0.48
2:2:395:MET:HA	2:2:395:MET:CE	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:337:THR:HG21	2:E:359:TYR:CD2	2.49	0.48
1:U:137:GLU:OE2	1:1:48:ARG:HD2	2.14	0.48
2:E:304:VAL:HG23	2:E:438:ALA:HB2	1.95	0.48
2:X:364:GLU:HG2	2:X:368:LYS:HE2	1.94	0.48
1:U:16:ARG:HE	1:U:117:PRO:HD3	1.78	0.48
2:G:321:THR:O	3:G:273:M1N:H52	2.11	0.48
1:S:56:LEU:HD23	1:S:79:ILE:HG13	1.96	0.48
3:P:273:M1N:O16	3:P:273:M1N:C22	2.61	0.48
1:A:182:ARG:HG3	1:A:235:VAL:CB	2.39	0.48
2:C:319:ARG:HG3	2:C:320:SER:N	2.29	0.48
2:E:337:THR:HB	2:E:341:THR:HB	1.95	0.48
1:1:42:VAL:HG22	1:1:210:VAL:HG22	1.95	0.48
1:A:89:TYR:CD1	2:P:382:ARG:HD3	2.48	0.48
2:J:349:ALA:H	3:J:273:M1N:C36	2.27	0.48
1:1:118:TYR:HB3	1:1:120:VAL:HG22	1.94	0.48
1:1:214:ASP:OD2	1:1:217:ARG:HG2	2.13	0.48
1:M:205:VAL:CG1	1:M:206:ALA:N	2.77	0.48
1:Q:127:VAL:HG11	1:Q:213:LEU:HB3	1.96	0.48
2:R:341:THR:CG2	2:R:404:LEU:HD11	2.44	0.48
1:Q:176:SER:H	1:Q:179:ASP:HB2	1.77	0.48
2:C:365:HIS:CE1	2:C:369:LEU:HD11	2.49	0.48
1:K:63:ALA:O	1:K:156:MET:HE1	2.14	0.48
2:L:301:THR:HG22	2:L:302:THR:N	2.29	0.48
2:2:457:VAL:HG22	2:2:463:GLY:HA2	1.94	0.48
1:M:58:ASP:OD1	1:M:219:ARG:NH1	2.47	0.48
2:X:308:TYR:HB2	2:X:309:PRO:HD2	1.96	0.48
2:L:314:MET:HE2	2:L:334:VAL:HG13	1.93	0.47
2:E:496:ILE:HG13	2:E:505:VAL:CG2	2.44	0.47
1:F:110:ILE:HA	1:F:114:GLN:HG2	1.96	0.47
1:1:189:ARG:NH2	1:1:237:GLN:HB3	2.29	0.47
1:Q:112:THR:HG22	1:Y:115:ALA:HB3	1.96	0.47
2:E:349:ALA:H	3:E:273:M1N:C35	2.27	0.47
1:1:205:VAL:CG1	1:1:206:ALA:H	2.25	0.47
2:N:395:MET:HA	2:N:395:MET:HE1	1.96	0.47
1:1:140:ARG:HB3	1:1:140:ARG:HH11	1.79	0.47
1:S:176:SER:H	1:S:179:ASP:HB2	1.79	0.47
1:D:185:VAL:HB	1:D:235:VAL:HG11	1.96	0.47
1:U:80:GLN:O	1:U:84:THR:OG1	2.32	0.47
1:Q:155:VAL:HG12	1:Q:160:THR:HG22	1.95	0.47
1:S:12:ALA:O	1:S:16:ARG:HG2	2.13	0.47
1:O:170:SER:HB2	1:O:183:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:450:MET:HE2	2:N:470:ALA:CB	2.45	0.47
2:2:403:LEU:HB2	2:2:439:VAL:HG21	1.96	0.47
2:2:349:ALA:H	3:2:273:M1N:C36	2.27	0.47
1:Q:68:PHE:HD1	1:Q:71:PHE:CZ	2.32	0.47
2:X:444:LEU:HD22	2:X:444:LEU:HA	1.72	0.47
1:Y:60:VAL:HG21	1:Y:96:GLY:HA3	1.95	0.47
1:O:85:ARG:HG3	1:O:85:ARG:NH1	2.28	0.47
2:G:424:ASP:CG	3:X:273:M1N:H40	2.34	0.47
1:B:135:ARG:HH22	1:B:152:HIS:CD2	2.32	0.47
2:2:314:MET:HE2	2:2:334:VAL:HG13	1.96	0.47
1:O:161:GLU:O	1:O:165:ASN:HB2	2.14	0.47
1:S:226:THR:HG23	1:S:227:GLY:N	2.29	0.47
2:C:424:ASP:HB3	2:C:428:GLY:H	1.80	0.47
2:J:324:ASN:ND2	2:J:324:ASN:N	2.58	0.47
2:X:452:LYS:HD3	4:X:4:HOH:O	2.14	0.47
2:H:514:ALA:O	2:H:518:ILE:HG13	2.14	0.47
2:X:308:TYR:CE2	2:X:460:GLY:HA2	2.48	0.47
1:I:176:SER:H	1:I:179:ASP:HB2	1.80	0.47
1:A:11:GLN:HG2	1:A:14:ARG:NH1	2.28	0.47
2:P:485:ASP:OD2	2:P:488:ARG:HB2	2.14	0.47
2:V:317:ASP:OD1	2:V:333:LYS:NZ	2.47	0.47
2:V:301:THR:CG2	3:V:273:M1N:O16	2.60	0.47
2:H:335:TYR:HE1	2:H:345:ILE:HD11	1.79	0.47
2:E:304:VAL:HG21	2:E:450:MET:HE3	1.97	0.47
1:W:172:ALA:HB3	1:W:175:ALA:HB2	1.96	0.47
2:V:321:THR:HG22	3:V:273:M1N:O3	2.14	0.47
1:W:118:TYR:HB3	1:W:120:VAL:HG22	1.96	0.47
2:2:335:TYR:HE1	2:2:345:ILE:HD11	1.80	0.47
2:G:320:SER:HB3	2:G:328:GLY:HA3	1.97	0.47
1:F:171:TYR:CE2	1:F:173:GLU:HA	2.49	0.47
2:H:337:THR:HG22	2:H:363:LEU:HD12	1.96	0.47
2:R:375:THR:O	2:R:379:LYS:HG3	2.15	0.47
1:I:142:THR:OG1	1:I:146:SER:HB2	2.15	0.47
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.50	0.47
1:Y:110:ILE:HG23	1:Y:114:GLN:HG3	1.97	0.47
1:F:105:GLN:NE2	1:M:73:ASN:HD22	2.13	0.47
1:1:97:ARG:HH11	1:1:97:ARG:HG3	1.80	0.47
2:N:306:LEU:HD23	2:N:436:TYR:HB3	1.95	0.47
2:R:321:THR:O	3:R:273:M1N:H37	2.15	0.47
2:L:432:GLU:HG3	2:L:437:GLN:HB2	1.97	0.47
2:L:349:ALA:HB3	3:L:273:M1N:C35	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:176:SER:HB3	1:S:179:ASP:OD1	2.15	0.47
2:H:382:ARG:NH1	2:H:385:ILE:HD13	2.30	0.47
2:X:344:GLY:C	4:X:58:HOH:O	2.48	0.47
1:S:59:ARG:HG3	1:S:129:HIS:CD2	2.50	0.47
2:L:337:THR:HG21	2:L:359:TYR:CE2	2.50	0.47
2:2:349:ALA:CB	3:2:273:M1N:H252	2.45	0.47
1:M:205:VAL:CG1	1:M:206:ALA:H	2.28	0.47
1:Q:55:GLU:OE2	1:Q:220:ARG:HD2	2.14	0.47
2:2:318:ARG:HD3	2:2:491:PHE:O	2.15	0.47
1:1:185:VAL:HB	1:1:235:VAL:CG1	2.45	0.47
1:D:141:ILE:HG13	1:D:147:ILE:HG12	1.97	0.47
2:R:348:THR:HG23	3:R:273:M1N:H35	1.97	0.46
2:L:321:THR:O	3:L:273:M1N:H51	2.15	0.46
1:D:56:LEU:HD13	1:D:99:LEU:CD2	2.43	0.46
2:C:337:THR:OG1	2:C:343:THR:CG2	2.63	0.46
2:G:407:TYR:CE1	2:G:417:ALA:HB3	2.49	0.46
1:W:19:LEU:HD12	1:Y:10:GLU:HA	1.97	0.46
1:W:72:ASP:O	1:W:76:ARG:HG3	2.15	0.46
1:K:59:ARG:HG3	1:K:129:HIS:CD2	2.43	0.46
2:2:436:TYR:HB2	2:2:450:MET:SD	2.55	0.46
1:S:16:ARG:HE	1:S:117:PRO:HD3	1.80	0.46
2:H:329:ARG:O	2:H:490:ILE:HG21	2.15	0.46
1:Q:154:VAL:HG21	4:Q:253:HOH:O	2.14	0.46
1:1:231:GLN:HA	1:1:231:GLN:HE21	1.80	0.46
1:M:205:VAL:HG12	1:M:206:ALA:H	1.79	0.46
2:2:314:MET:HE1	2:2:342:ALA:HB1	1.96	0.46
2:N:314:MET:CE	2:N:334:VAL:HG13	2.45	0.46
2:L:436:TYR:OH	2:L:451:LYS:HG3	2.15	0.46
2:H:432:GLU:HG3	2:H:437:GLN:HB2	1.96	0.46
1:S:92:ARG:HD2	1:S:129:HIS:HE1	1.70	0.46
2:Z:349:ALA:H	3:Z:273:M1N:H35	1.79	0.46
2:C:318:ARG:HB3	2:C:331:VAL:O	2.15	0.46
2:N:318:ARG:HE	2:N:318:ARG:HB3	1.53	0.46
2:G:301:THR:N	2:G:441:SER:HG	2.13	0.46
2:N:392:ALA:O	2:N:395:MET:HB2	2.14	0.46
2:C:320:SER:HB3	2:C:328:GLY:HA3	1.98	0.46
1:Q:33:LEU:HD11	1:Q:180:ALA:HB1	1.97	0.46
1:M:127:VAL:CG2	1:M:215:ALA:HB2	2.46	0.46
1:F:28:LYS:HE3	1:F:44:GLU:HG3	1.97	0.46
3:P:273:M1N:C25	3:P:273:M1N:N1	2.78	0.46
2:X:464:LEU:HD11	2:X:505:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:321:THR:O	3:2:273:M1N:H37	2.16	0.46
2:L:441:SER:HB2	2:L:478:ASP:OD2	2.15	0.46
1:K:114:GLN:OE1	1:K:114:GLN:HA	2.16	0.46
1:A:137:GLU:HG2	1:A:139:TYR:CE2	2.51	0.46
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.96	0.46
1:O:172:ALA:HB3	1:O:175:ALA:HB2	1.98	0.46
2:R:515:ARG:NH1	4:R:263:HOH:O	2.45	0.46
2:2:303:ILE:HD11	2:2:333:LYS:HB3	1.97	0.46
2:P:324:ASN:C	2:P:324:ASN:HD22	2.18	0.46
2:X:301:THR:HG21	3:X:273:M1N:O16	2.15	0.46
2:Z:395:MET:HA	2:Z:395:MET:CE	2.45	0.46
1:S:73:ASN:HD22	1:1:105:GLN:NE2	2.13	0.46
2:X:375:THR:HB	2:X:378:GLY:H	1.81	0.46
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.97	0.46
1:A:42:VAL:HG22	1:A:210:VAL:HG22	1.98	0.46
2:J:301:THR:CG2	2:J:302:THR:N	2.79	0.46
2:C:349:ALA:H	3:C:273:M1N:C36	2.29	0.46
1:B:110:ILE:HA	1:B:114:GLN:HG2	1.98	0.46
2:H:392:ALA:O	2:H:395:MET:HB2	2.16	0.46
2:C:452:LYS:HA	2:C:452:LYS:HD3	1.76	0.46
1:U:118:TYR:HB3	1:U:120:VAL:HG22	1.97	0.46
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.51	0.46
2:C:307:LYS:HD2	2:C:418:GLY:O	2.15	0.46
1:M:28:LYS:HB2	1:M:52:LYS:NZ	2.30	0.46
1:D:217:ARG:HH21	1:D:223:ARG:HG3	1.80	0.46
1:F:56:LEU:HD23	1:F:79:ILE:HG13	1.98	0.46
1:A:30:VAL:HG22	1:A:43:ALA:HB1	1.97	0.46
1:Y:139:TYR:CE2	1:Y:149:ASP:HB3	2.51	0.46
1:Y:182:ARG:NH1	1:Y:182:ARG:HB2	2.30	0.46
2:C:412:SER:O	2:C:414:PRO:HD3	2.15	0.46
2:X:409:ILE:HG13	2:X:410:HIS:CD2	2.50	0.46
1:B:68:PHE:HA	1:B:71:PHE:CE2	2.51	0.46
2:G:388:ARG:HE	2:G:388:ARG:HB2	1.54	0.46
2:L:319:ARG:HG3	2:L:320:SER:N	2.31	0.46
2:V:349:ALA:HB3	3:V:273:M1N:C34	2.46	0.46
2:G:424:ASP:HB3	2:G:428:GLY:H	1.80	0.46
1:I:96:GLY:HA2	1:I:99:LEU:HB2	1.97	0.46
1:I:55:GLU:OE2	1:I:220:ARG:HD2	2.16	0.46
2:V:345:ILE:HB	2:V:352:ALA:HB1	1.97	0.46
1:F:60:VAL:HG21	1:F:96:GLY:HA3	1.98	0.46
1:I:56:LEU:HB2	1:I:60:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:273:M1N:H36	3:T:273:M1N:H4	1.86	0.45
2:T:349:ALA:HB2	3:T:273:M1N:H252	1.98	0.45
1:S:110:ILE:HA	1:S:114:GLN:HG3	1.97	0.45
2:H:301:THR:N	2:H:441:SER:HG	2.13	0.45
1:W:217:ARG:HH21	1:W:223:ARG:HG3	1.81	0.45
2:Z:365:HIS:CE1	2:Z:369:LEU:HD11	2.50	0.45
1:B:226:THR:OG1	1:B:227:GLY:N	2.49	0.45
2:P:437:GLN:OE1	2:P:447:LYS:HD3	2.17	0.45
2:X:485:ASP:OD2	2:X:488:ARG:CB	2.59	0.45
2:G:437:GLN:CA	2:G:437:GLN:OE1	2.63	0.45
2:P:345:ILE:O	2:P:345:ILE:HD12	2.16	0.45
2:H:307:LYS:NZ	2:H:433:GLU:HA	2.31	0.45
1:F:115:ALA:HB3	1:W:112:THR:CG2	2.46	0.45
1:O:16:ARG:NH2	1:O:114:GLN:O	2.48	0.45
2:J:397:GLY:HA2	4:J:541:HOH:O	2.16	0.45
1:I:85:ARG:HG2	4:I:250:HOH:O	2.15	0.45
2:H:304:VAL:HG21	2:H:450:MET:HE3	1.97	0.45
1:K:24:ILE:HD11	1:K:120:VAL:C	2.37	0.45
1:A:49:SER:HB2	1:B:97:ARG:HH11	1.82	0.45
3:T:273:M1N:O16	3:T:273:M1N:C22	2.64	0.45
1:S:135:ARG:HA	1:S:136:PRO:HD2	1.87	0.45
1:A:226:THR:O	1:A:230:LEU:HB2	2.16	0.45
1:U:214:ASP:OD2	1:U:217:ARG:HG2	2.17	0.45
2:X:304:VAL:HG21	2:X:450:MET:HE3	1.97	0.45
1:O:137:GLU:OE2	1:U:48:ARG:HD2	2.15	0.45
1:S:87:TYR:O	2:T:357:ARG:NH2	2.49	0.45
1:K:55:GLU:OE2	1:K:220:ARG:HD2	2.15	0.45
2:N:349:ALA:CB	3:N:273:M1N:H252	2.45	0.45
1:O:59:ARG:CG	1:O:129:HIS:HD2	2.27	0.45
1:K:11:GLN:CG	1:K:14:ARG:HH12	2.29	0.45
2:G:521:ARG:NH2	2:2:452:LYS:NZ	2.65	0.45
1:D:230:LEU:HD21	1:D:234:LEU:HD13	1.97	0.45
2:L:408:ASP:HA	4:L:548:HOH:O	2.17	0.45
1:U:182:ARG:HB2	1:U:182:ARG:NH1	2.32	0.45
2:L:424:ASP:HB3	2:L:428:GLY:N	2.32	0.45
2:L:465:ARG:HB3	2:L:513:LEU:HD21	1.98	0.45
2:G:309:PRO:HG3	2:G:458:THR:O	2.16	0.45
1:Y:30:VAL:HG22	1:Y:43:ALA:HB1	1.98	0.45
1:A:48:ARG:HH22	1:B:135:ARG:HB3	1.80	0.45
1:I:76:ARG:HA	1:I:79:ILE:HD12	1.98	0.45
1:Y:185:VAL:HG12	1:Y:189:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:437:GLN:OE1	2:T:447:LYS:HD3	2.17	0.45
2:2:424:ASP:HB3	2:2:428:GLY:N	2.31	0.45
2:N:324:ASN:ND2	2:N:324:ASN:N	2.55	0.45
1:I:185:VAL:HB	1:I:235:VAL:CG1	2.46	0.45
1:Y:41:PHE:HZ	1:Y:125:ALA:HB3	1.82	0.45
2:N:338:ASP:C	2:N:338:ASP:OD1	2.55	0.45
2:2:424:ASP:HB2	4:2:545:HOH:O	2.16	0.45
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.98	0.45
2:G:392:ALA:O	2:G:395:MET:HB2	2.17	0.45
1:B:56:LEU:HD13	1:B:99:LEU:HD22	1.98	0.45
1:B:56:LEU:HD23	1:B:79:ILE:HG13	1.98	0.45
1:A:182:ARG:HA	1:A:235:VAL:HB	1.99	0.45
1:D:135:ARG:HH22	1:D:152:HIS:HD2	1.63	0.45
1:I:58:ASP:OD1	1:I:219:ARG:NH1	2.50	0.45
2:E:349:ALA:HA	3:E:273:M1N:H243	1.99	0.45
2:L:301:THR:CG2	2:L:302:THR:N	2.79	0.45
1:O:9:PRO:O	1:O:13:MET:HG2	2.17	0.45
2:T:444:LEU:HD12	2:X:444:LEU:CD1	2.47	0.45
1:B:60:VAL:HG21	1:B:96:GLY:HA3	1.99	0.45
1:S:123:CYS:HB2	1:S:156:MET:CE	2.47	0.45
1:B:170:SER:HB2	1:B:183:ILE:HD12	1.99	0.45
2:T:383:LEU:HD23	2:T:383:LEU:O	2.17	0.45
1:I:83:ASP:OD2	2:J:365:HIS:CD2	2.60	0.45
2:R:436:TYR:N	2:R:436:TYR:CD1	2.85	0.45
2:L:465:ARG:CB	2:L:513:LEU:HD22	2.47	0.45
2:N:465:ARG:HB2	2:N:513:LEU:HD21	1.98	0.45
2:E:432:GLU:HG3	2:E:437:GLN:HB2	1.97	0.45
1:Y:12:ALA:HA	4:Y:251:HOH:O	2.16	0.45
2:H:496:ILE:HG12	2:H:505:VAL:CG2	2.47	0.45
1:D:118:TYR:HB3	1:D:120:VAL:HG22	1.98	0.45
2:J:307:LYS:HD2	2:J:418:GLY:O	2.17	0.45
3:L:273:M1N:H221	3:L:273:M1N:O16	2.16	0.45
1:W:41:PHE:HE2	1:W:213:LEU:HD13	1.81	0.45
2:P:407:TYR:CE2	2:P:499:ALA:HA	2.51	0.45
1:Q:209:GLU:OE2	1:Q:224:ARG:NH2	2.49	0.45
2:2:322:GLN:O	2:2:322:GLN:HG2	2.16	0.45
2:P:321:THR:O	3:P:273:M1N:H51	2.18	0.44
1:B:98:GLN:O	1:B:101:ASN:HB2	2.17	0.44
2:G:376:PHE:CE2	2:G:380:ILE:HD11	2.52	0.44
1:S:115:ALA:HB3	1:1:112:THR:HG23	1.99	0.44
2:Z:459:ASP:O	2:Z:462:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:HA	1:B:136:PRO:HD2	1.90	0.44
2:2:314:MET:HE3	2:2:334:VAL:HG13	1.99	0.44
2:N:308:TYR:HB2	2:N:309:PRO:HD2	1.98	0.44
1:U:230:LEU:HD21	1:U:234:LEU:HD13	1.98	0.44
1:F:137:GLU:HG2	1:F:139:TYR:CE1	2.51	0.44
2:V:461:ASP:OD1	2:V:509:ARG:NH1	2.50	0.44
2:Z:349:ALA:N	3:Z:273:M1N:H35	2.31	0.44
1:I:56:LEU:HD13	1:I:99:LEU:CD2	2.47	0.44
2:L:349:ALA:HB3	3:L:273:M1N:C34	2.47	0.44
1:Y:28:LYS:HE2	1:Y:46:PRO:HD3	1.98	0.44
2:H:436:TYR:HB2	2:H:450:MET:SD	2.57	0.44
1:U:110:ILE:HG23	1:U:114:GLN:HG3	1.98	0.44
1:1:163:ILE:HG23	1:1:188:LEU:HA	1.98	0.44
1:1:70:GLU:OE2	1:1:116:LYS:NZ	2.50	0.44
1:M:176:SER:H	1:M:179:ASP:HB2	1.82	0.44
2:P:384:ALA:HB2	2:P:423:PHE:HE2	1.82	0.44
2:X:306:LEU:HB2	2:X:313:VAL:CG1	2.47	0.44
1:D:16:ARG:HE	1:D:117:PRO:HD3	1.83	0.44
2:H:318:ARG:HB3	2:H:331:VAL:O	2.17	0.44
2:2:464:LEU:HD11	2:2:505:VAL:HG11	1.99	0.44
1:W:70:GLU:OE1	1:W:118:TYR:HA	2.16	0.44
2:Z:391:LEU:O	2:Z:395:MET:HG2	2.18	0.44
1:Y:139:TYR:HD2	1:Y:147:ILE:HD11	1.81	0.44
2:2:319:ARG:O	2:2:333:LYS:NZ	2.45	0.44
2:L:341:THR:HG22	2:L:404:LEU:HD11	1.99	0.44
2:J:301:THR:CG2	3:J:273:M1N:O16	2.62	0.44
1:D:12:ALA:O	1:D:16:ARG:HG2	2.17	0.44
2:P:472:TYR:HE2	4:P:553:HOH:O	2.00	0.44
1:S:189:ARG:CZ	1:S:237:GLN:HB3	2.47	0.44
1:S:209:GLU:OE2	1:S:224:ARG:NH2	2.49	0.44
2:C:321:THR:O	3:C:273:M1N:C5	2.66	0.44
2:2:337:THR:OG1	2:2:343:THR:HG22	2.18	0.44
2:Z:304:VAL:CG2	2:Z:450:MET:SD	3.06	0.44
1:A:133:THR:O	1:A:134:LYS:HE2	2.17	0.44
1:M:54:SER:CB	1:M:75:ARG:HD2	2.47	0.44
2:2:433:GLU:HB3	4:2:554:HOH:O	2.17	0.44
2:N:436:TYR:HB2	2:N:450:MET:SD	2.57	0.44
2:G:518:ILE:HG23	2:V:487:VAL:CG2	2.48	0.44
2:N:365:HIS:CE1	2:N:369:LEU:HD11	2.53	0.44
1:F:172:ALA:HB3	1:F:175:ALA:HB2	1.99	0.44
1:O:226:THR:O	1:O:230:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:366:TYR:CZ	2:T:370:GLU:HG3	2.52	0.44
1:F:70:GLU:OE2	1:F:116:LYS:NZ	2.48	0.44
2:J:364:GLU:HG2	2:J:368:LYS:HE2	2.00	0.44
1:W:127:VAL:HG13	1:W:127:VAL:O	2.16	0.44
2:C:348:THR:HG23	3:C:273:M1N:H35	1.99	0.44
1:I:92:ARG:HD2	1:I:129:HIS:NE2	2.31	0.44
1:W:110:ILE:HA	1:W:114:GLN:HG2	2.00	0.44
1:U:137:GLU:HG2	1:U:139:TYR:CE1	2.53	0.44
1:B:96:GLY:HA2	1:B:99:LEU:HB2	2.00	0.44
2:V:308:TYR:HB2	2:V:309:PRO:HD2	1.99	0.44
1:K:140:ARG:HH11	1:K:154:VAL:HG22	1.83	0.44
1:U:56:LEU:HD13	1:U:99:LEU:HD22	1.99	0.44
2:P:345:ILE:HB	2:P:352:ALA:HB1	2.00	0.44
1:W:30:VAL:HG22	1:W:43:ALA:HB1	1.99	0.44
1:F:179:ASP:O	1:F:183:ILE:HG12	2.18	0.44
2:Z:306:LEU:HB2	2:Z:313:VAL:HG12	2.00	0.44
2:T:412:SER:O	2:T:414:PRO:HD3	2.18	0.44
1:O:127:VAL:CG2	1:O:215:ALA:HB2	2.48	0.44
1:F:45:ASN:HA	1:F:46:PRO:HD2	1.91	0.44
2:J:349:ALA:N	3:J:273:M1N:C35	2.78	0.43
2:J:301:THR:HG21	3:J:273:M1N:H16	1.82	0.43
1:W:205:VAL:CG1	1:W:206:ALA:H	2.29	0.43
2:T:407:TYR:CE1	2:T:417:ALA:HB3	2.53	0.43
1:W:182:ARG:HA	1:W:235:VAL:HB	2.00	0.43
1:A:98:GLN:O	1:A:102:VAL:HG23	2.18	0.43
1:M:70:GLU:OE2	1:M:116:LYS:NZ	2.50	0.43
1:B:141:ILE:N	1:B:141:ILE:HD12	2.33	0.43
1:D:96:GLY:O	1:D:124:VAL:HG11	2.18	0.43
2:H:395:MET:HE1	2:H:395:MET:HA	2.00	0.43
1:F:110:ILE:HG12	1:F:114:GLN:CG	2.46	0.43
1:A:92:ARG:HB2	1:A:92:ARG:HH11	1.83	0.43
2:H:309:PRO:HG2	2:H:458:THR:O	2.17	0.43
2:Z:337:THR:OG1	2:Z:343:THR:HG22	2.17	0.43
1:W:181:LEU:HD23	1:W:233:LEU:HB3	2.00	0.43
1:Y:63:ALA:O	1:Y:156:MET:HE1	2.18	0.43
1:O:54:SER:CB	1:O:75:ARG:HD2	2.48	0.43
2:N:485:ASP:OD2	2:N:488:ARG:HB2	2.17	0.43
2:2:349:ALA:H	3:2:273:M1N:C35	2.31	0.43
3:H:273:M1N:C22	3:H:273:M1N:O16	2.54	0.43
1:Y:59:ARG:HG3	1:Y:129:HIS:CD2	2.52	0.43
2:Z:488:ARG:HB3	2:Z:490:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:189:ARG:CZ	1:1:237:GLN:HB3	2.47	0.43
2:2:424:ASP:HB3	2:2:428:GLY:H	1.83	0.43
1:B:142:THR:OG1	1:B:144:ASP:OD1	2.28	0.43
1:Q:67:LYS:HG2	1:Q:69:ASN:OD1	2.18	0.43
1:Y:205:VAL:HG12	1:Y:206:ALA:H	1.83	0.43
2:T:515:ARG:HA	2:T:518:ILE:HD12	2.01	0.43
1:O:110:ILE:HA	1:O:114:GLN:HG2	2.00	0.43
1:K:24:ILE:HD11	1:K:120:VAL:CA	2.49	0.43
2:E:364:GLU:HG2	2:E:368:LYS:HE2	2.00	0.43
1:W:48:ARG:HH22	1:Y:135:ARG:HD2	1.81	0.43
1:D:97:ARG:HB2	4:D:249:HOH:O	2.17	0.43
1:W:139:TYR:CD2	1:W:149:ASP:HB3	2.53	0.43
2:E:439:VAL:HG23	2:E:439:VAL:O	2.18	0.43
2:C:465:ARG:CB	2:C:465:ARG:HH11	2.31	0.43
2:E:456:GLN:HE22	2:E:465:ARG:NH1	2.16	0.43
1:M:189:ARG:CZ	1:M:237:GLN:HB3	2.48	0.43
1:A:92:ARG:HD2	1:A:129:HIS:CE1	2.53	0.43
2:J:513:LEU:O	2:J:517:ILE:HG12	2.18	0.43
1:Q:182:ARG:HA	1:Q:235:VAL:HB	2.00	0.43
1:M:63:ALA:O	1:M:156:MET:HE1	2.18	0.43
1:A:73:ASN:HD22	1:B:105:GLN:NE2	2.16	0.43
1:K:38:GLY:HA2	1:K:127:VAL:HG21	1.99	0.43
3:J:273:M1N:HN1	3:J:273:M1N:H252	1.83	0.43
2:C:450:MET:CE	2:C:470:ALA:CB	2.97	0.43
1:U:95:THR:C	1:U:97:ARG:H	2.22	0.43
1:M:30:VAL:HG22	1:M:43:ALA:CB	2.49	0.43
1:A:225:ILE:HG22	1:A:230:LEU:HB2	1.99	0.43
2:E:403:LEU:HG	2:E:439:VAL:HG13	2.01	0.43
1:S:70:GLU:OE2	1:S:116:LYS:NZ	2.51	0.43
1:Y:91:ARG:HE	1:Y:91:ARG:HB3	1.68	0.43
3:N:273:M1N:H36	3:N:273:M1N:H4	1.89	0.43
2:Z:432:GLU:HG3	2:Z:437:GLN:HB2	2.00	0.43
2:P:321:THR:O	3:P:273:M1N:C5	2.67	0.43
2:L:464:LEU:HD23	2:L:464:LEU:O	2.19	0.43
2:G:432:GLU:HG3	2:G:437:GLN:HB2	2.00	0.43
2:V:337:THR:OG1	2:V:343:THR:CG2	2.65	0.43
2:R:464:LEU:HD12	2:R:496:ILE:HD11	1.99	0.43
1:Q:30:VAL:HG22	1:Q:43:ALA:CB	2.48	0.43
2:G:365:HIS:CE1	2:G:369:LEU:HD11	2.53	0.43
2:2:401:LEU:HA	2:2:402:PRO:HD3	1.88	0.43
2:E:349:ALA:HB2	3:E:273:M1N:H252	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG22	1:B:43:ALA:CB	2.47	0.43
2:V:395:MET:HA	2:V:395:MET:CE	2.48	0.43
1:U:30:VAL:HG22	1:U:43:ALA:HB1	2.00	0.43
2:N:338:ASP:OD1	2:N:341:THR:OG1	2.28	0.43
1:K:54:SER:OG	1:K:55:GLU:N	2.52	0.43
1:K:94:VAL:HA	1:K:98:GLN:HE22	1.84	0.43
1:M:135:ARG:HA	1:M:136:PRO:HD2	1.91	0.43
2:X:302:THR:O	2:X:303:ILE:HD13	2.18	0.43
2:Z:301:THR:HG21	3:Z:273:M1N:H16	1.83	0.43
1:M:56:LEU:HD23	1:M:79:ILE:HG13	2.01	0.43
1:B:92:ARG:HH11	1:B:92:ARG:HB2	1.84	0.43
2:2:449:SER:OG	2:2:450:MET:N	2.52	0.43
1:O:205:VAL:O	1:O:207:SER:N	2.51	0.43
1:K:12:ALA:O	1:K:16:ARG:HG2	2.18	0.43
1:S:182:ARG:HB2	1:S:182:ARG:HH11	1.84	0.43
1:S:28:LYS:HB2	1:S:52:LYS:NZ	2.33	0.43
2:2:307:LYS:HD2	2:2:418:GLY:O	2.18	0.43
1:B:58:ASP:OD1	1:B:219:ARG:NH1	2.52	0.43
2:P:496:ILE:HG13	2:P:505:VAL:HG22	2.01	0.43
1:U:85:ARG:NH1	1:U:89:TYR:CE2	2.87	0.43
2:H:437:GLN:OE1	2:H:447:LYS:HD3	2.19	0.43
2:H:306:LEU:CD2	2:H:454:TYR:HE1	2.31	0.43
1:M:172:ALA:HB3	1:M:175:ALA:HB2	2.01	0.43
1:A:171:TYR:CE2	1:A:173:GLU:HA	2.54	0.43
1:D:155:VAL:HG12	1:D:160:THR:HG22	2.01	0.43
2:N:349:ALA:CB	3:N:273:M1N:C35	2.97	0.42
2:H:465:ARG:HA	2:H:513:LEU:HD13	2.00	0.42
2:J:337:THR:HG21	2:J:359:TYR:CE2	2.53	0.42
2:J:341:THR:CG2	2:J:404:LEU:HD11	2.45	0.42
1:U:85:ARG:HG2	1:U:85:ARG:HH11	1.84	0.42
1:M:16:ARG:HE	1:M:117:PRO:HD3	1.84	0.42
1:O:147:ILE:HD13	1:O:148:ALA:N	2.33	0.42
2:P:320:SER:HB3	2:P:328:GLY:HA3	2.00	0.42
2:E:306:LEU:HB2	2:E:313:VAL:CG1	2.49	0.42
1:1:176:SER:H	1:1:179:ASP:HB2	1.83	0.42
2:G:317:ASP:OD1	2:G:333:LYS:NZ	2.51	0.42
2:R:337:THR:HG21	2:R:359:TYR:HD2	1.80	0.42
1:K:16:ARG:NH2	1:K:114:GLN:O	2.52	0.42
1:A:176:SER:H	1:A:179:ASP:HB2	1.83	0.42
2:2:513:LEU:O	2:2:516:ALA:HB3	2.19	0.42
2:V:475:ALA:HB2	2:V:481:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:461:ASP:OD1	2:Z:509:ARG:HD2	2.19	0.42
2:X:335:TYR:HE1	2:X:345:ILE:HD11	1.83	0.42
2:X:424:ASP:OD2	3:Z:273:M1N:H34	2.19	0.42
2:Z:349:ALA:N	3:Z:273:M1N:C35	2.79	0.42
2:T:382:ARG:HD3	1:I:89:TYR:CE1	2.53	0.42
2:P:496:ILE:HG13	2:P:505:VAL:CG2	2.49	0.42
1:S:214:ASP:OD2	1:S:217:ARG:HG2	2.20	0.42
1:A:183:ILE:HA	1:A:183:ILE:HD13	1.84	0.42
1:O:89:TYR:CD1	2:V:382:ARG:HD3	2.54	0.42
2:L:383:LEU:HD21	2:L:402:PRO:CG	2.50	0.42
2:G:324:ASN:C	2:G:324:ASN:HD22	2.21	0.42
2:V:301:THR:HG21	3:V:273:M1N:H16	1.80	0.42
2:R:301:THR:N	2:R:441:SER:OG	2.51	0.42
1:Y:139:TYR:CD2	1:Y:147:ILE:HD11	2.53	0.42
1:U:181:LEU:O	1:U:185:VAL:HG23	2.20	0.42
1:D:41:PHE:HE2	1:D:213:LEU:HD13	1.83	0.42
1:K:33:LEU:HD11	1:K:40:LEU:HD23	2.02	0.42
1:B:127:VAL:O	1:B:127:VAL:HG13	2.20	0.42
2:X:401:LEU:HA	2:X:401:LEU:HD12	1.77	0.42
2:X:424:ASP:HB3	2:X:428:GLY:N	2.30	0.42
1:S:179:ASP:O	1:S:182:ARG:HB3	2.19	0.42
1:O:127:VAL:HG22	1:O:215:ALA:HB2	2.01	0.42
2:T:304:VAL:HG23	2:T:438:ALA:HB2	2.01	0.42
1:F:154:VAL:HG13	4:F:254:HOH:O	2.19	0.42
2:X:513:LEU:O	2:X:517:ILE:HG12	2.19	0.42
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.49	0.42
2:N:306:LEU:CD2	2:N:436:TYR:HB3	2.49	0.42
2:C:301:THR:CG2	3:C:273:M1N:H16	2.29	0.42
3:G:273:M1N:C25	3:G:273:M1N:HN1	2.31	0.42
2:X:392:ALA:O	2:X:395:MET:HB2	2.20	0.42
2:H:464:LEU:HD23	2:H:513:LEU:HD12	2.01	0.42
3:E:273:M1N:H221	3:E:273:M1N:O16	2.18	0.42
1:M:56:LEU:HG	1:M:62:PHE:HB2	2.02	0.42
2:G:329:ARG:HB3	2:G:329:ARG:HE	1.64	0.42
1:I:97:ARG:NH1	1:I:97:ARG:HG3	2.34	0.42
1:F:83:ASP:OD2	2:G:365:HIS:HD2	2.02	0.42
2:X:452:LYS:CA	4:X:4:HOH:O	2.59	0.42
1:O:94:VAL:HA	1:O:98:GLN:NE2	2.28	0.42
1:O:205:VAL:C	1:O:207:SER:N	2.73	0.42
2:R:306:LEU:HB2	2:R:313:VAL:HG13	2.02	0.42
1:K:118:TYR:HB3	1:K:120:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:303:ILE:HB	2:E:439:VAL:HG22	2.01	0.42
2:N:407:TYR:CE2	2:N:499:ALA:HA	2.55	0.42
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	2.01	0.42
2:R:372:VAL:HG12	2:R:373:PRO:O	2.19	0.42
1:W:59:ARG:HG3	1:W:129:HIS:CD2	2.54	0.42
1:I:28:LYS:HE2	1:I:46:PRO:HD3	2.02	0.42
2:C:444:LEU:HD22	2:C:444:LEU:HA	1.88	0.42
3:H:273:M1N:HN1	3:H:273:M1N:C25	2.32	0.42
1:Q:217:ARG:HA	1:Q:218:PRO:HD3	1.93	0.42
2:C:513:LEU:O	2:C:516:ALA:HB3	2.20	0.42
2:G:521:ARG:HH22	2:2:452:LYS:HZ1	1.66	0.42
1:O:87:TYR:O	2:P:357:ARG:NH2	2.52	0.42
1:K:54:SER:HB3	1:K:75:ARG:HD2	2.01	0.42
1:K:170:SER:HB2	1:K:183:ILE:HD12	2.01	0.42
2:T:375:THR:HB	2:T:378:GLY:H	1.84	0.42
1:I:171:TYR:CE2	1:I:173:GLU:HA	2.54	0.42
2:E:412:SER:O	2:E:414:PRO:HD3	2.19	0.42
2:X:424:ASP:HB2	2:X:428:GLY:O	2.20	0.42
2:J:318:ARG:HH11	2:J:490:ILE:HG22	1.85	0.42
2:C:436:TYR:OH	2:C:451:LYS:HG3	2.20	0.42
2:C:382:ARG:HA	2:C:382:ARG:HD2	1.78	0.42
1:I:177:LEU:HB2	4:I:251:HOH:O	2.18	0.42
1:M:127:VAL:O	1:M:127:VAL:HG13	2.20	0.42
1:D:95:THR:C	1:D:97:ARG:H	2.23	0.42
1:I:41:PHE:HB3	1:I:53:ILE:HD13	2.01	0.42
2:V:304:VAL:HG23	2:V:438:ALA:HB2	2.02	0.42
1:S:17:SER:O	1:S:21:ARG:HB2	2.19	0.42
1:Y:78:GLY:HA3	1:Y:103:TYR:OH	2.20	0.42
1:F:49:SER:HB2	1:W:97:ARG:HH11	1.85	0.42
2:H:321:THR:O	3:H:273:M1N:H51	2.20	0.42
1:M:217:ARG:NH2	1:M:223:ARG:HG3	2.34	0.42
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.55	0.42
1:F:231:GLN:CG	4:F:252:HOH:O	2.45	0.41
2:V:349:ALA:HB3	3:V:273:M1N:C35	2.49	0.41
1:S:11:GLN:HA	1:S:14:ARG:HH11	1.84	0.41
1:W:110:ILE:HG21	1:W:118:TYR:CD1	2.54	0.41
1:F:182:ARG:HA	1:F:235:VAL:HB	2.01	0.41
1:I:30:VAL:HG13	1:I:43:ALA:HB2	2.01	0.41
2:E:436:TYR:HB2	2:E:450:MET:SD	2.60	0.41
1:B:87:TYR:O	2:C:357:ARG:NH2	2.53	0.41
1:F:181:LEU:HD23	1:F:233:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:306:LEU:HB2	2:V:313:VAL:HG13	2.00	0.41
1:S:41:PHE:HB3	1:S:53:ILE:HD13	2.02	0.41
2:R:329:ARG:HE	2:R:329:ARG:HB3	1.65	0.41
1:1:92:ARG:HB2	1:1:92:ARG:HH11	1.85	0.41
1:F:10:GLU:OE2	1:M:22:LYS:HD2	2.19	0.41
2:V:317:ASP:O	2:V:333:LYS:HD2	2.20	0.41
2:N:314:MET:HE3	2:N:334:VAL:HG13	2.01	0.41
1:K:28:LYS:HE2	1:K:46:PRO:HD3	2.01	0.41
1:F:140:ARG:NH1	1:F:150:GLU:OE2	2.52	0.41
2:V:464:LEU:HD11	2:V:505:VAL:HG21	2.01	0.41
1:U:91:ARG:HE	1:U:91:ARG:HB3	1.66	0.41
2:J:301:THR:N	2:J:441:SER:OG	2.53	0.41
2:X:349:ALA:H	3:X:273:M1N:C36	2.34	0.41
1:S:76:ARG:HA	1:S:79:ILE:HD12	2.02	0.41
2:V:457:VAL:HG22	2:V:463:GLY:HA2	2.03	0.41
1:K:30:VAL:HG13	1:K:43:ALA:HB2	2.02	0.41
3:J:273:M1N:H36	3:J:273:M1N:H4	1.76	0.41
2:Z:424:ASP:HB3	2:Z:428:GLY:N	2.36	0.41
1:M:85:ARG:HG2	1:M:85:ARG:NH1	2.15	0.41
2:C:345:ILE:O	2:C:345:ILE:HD12	2.20	0.41
2:G:383:LEU:HD21	2:G:402:PRO:HG2	2.03	0.41
1:1:127:VAL:HG11	1:1:213:LEU:HB3	2.01	0.41
1:S:182:ARG:HA	1:S:235:VAL:HB	2.02	0.41
1:A:41:PHE:HE2	1:A:213:LEU:HD13	1.85	0.41
2:E:345:ILE:HD12	2:E:345:ILE:O	2.20	0.41
1:Y:110:ILE:HA	1:Y:114:GLN:HG2	2.02	0.41
1:Q:28:LYS:HE2	1:Q:46:PRO:HD3	2.02	0.41
1:F:147:ILE:HD13	1:M:50:LEU:HD11	2.03	0.41
1:F:112:THR:HG22	1:M:115:ALA:HB3	2.01	0.41
2:G:424:ASP:HB3	2:G:428:GLY:N	2.35	0.41
1:F:92:ARG:HH11	1:F:92:ARG:HB2	1.85	0.41
2:Z:469:GLU:HG3	2:Z:517:ILE:HD12	2.02	0.41
2:C:436:TYR:HB2	2:C:450:MET:SD	2.60	0.41
2:H:304:VAL:HG23	2:H:438:ALA:HB2	2.02	0.41
1:Q:234:LEU:HG	1:Q:235:VAL:N	2.35	0.41
2:H:314:MET:CE	2:H:334:VAL:HG13	2.50	0.41
2:N:329:ARG:O	2:N:490:ILE:HG21	2.21	0.41
1:O:55:GLU:OE2	1:O:220:ARG:HD2	2.20	0.41
1:O:95:THR:C	1:O:97:ARG:H	2.24	0.41
2:E:307:LYS:HD2	2:E:418:GLY:O	2.20	0.41
1:D:189:ARG:CZ	1:D:237:GLN:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HG	1:A:237:GLN:OE1	2.19	0.41
1:U:85:ARG:HH11	1:U:89:TYR:HE2	1.69	0.41
2:R:306:LEU:HB2	2:R:313:VAL:CG1	2.50	0.41
1:I:41:PHE:HZ	1:I:125:ALA:HB3	1.85	0.41
1:W:95:THR:C	1:W:97:ARG:H	2.24	0.41
1:O:171:TYR:CE2	1:O:173:GLU:HA	2.55	0.41
2:R:330:ASP:OD1	2:R:330:ASP:N	2.54	0.41
1:Q:21:ARG:HB3	1:Q:21:ARG:NH1	2.35	0.41
1:M:141:ILE:N	1:M:141:ILE:HD12	2.35	0.41
2:J:383:LEU:HD21	2:J:402:PRO:CG	2.50	0.41
2:N:341:THR:CG2	2:N:404:LEU:HD11	2.50	0.41
1:O:30:VAL:HG22	1:O:43:ALA:HB1	2.02	0.41
2:H:311:GLY:HA3	2:H:497:ILE:O	2.21	0.41
1:S:78:GLY:HA3	1:S:103:TYR:OH	2.21	0.41
1:I:27:ALA:HB1	4:I:252:HOH:O	2.21	0.41
2:P:518:ILE:O	2:P:522:SER:HB2	2.20	0.41
2:T:395:MET:CE	2:T:395:MET:HA	2.50	0.41
2:X:345:ILE:HB	2:X:352:ALA:HB1	2.03	0.41
2:C:321:THR:O	3:C:273:M1N:H37	2.21	0.41
3:E:273:M1N:H36	3:E:273:M1N:H4	1.89	0.41
2:R:432:GLU:HG3	2:R:437:GLN:HB2	2.03	0.41
1:O:41:PHE:HE2	1:O:213:LEU:HD13	1.86	0.41
1:D:205:VAL:HG12	1:D:206:ALA:H	1.85	0.41
2:N:345:ILE:HD12	2:N:345:ILE:O	2.19	0.41
1:M:127:VAL:HG22	1:M:215:ALA:HB2	2.02	0.41
2:G:395:MET:CE	2:G:395:MET:HA	2.51	0.41
2:H:306:LEU:CD2	2:H:454:TYR:CE1	3.04	0.41
1:B:128:ALA:HB2	1:B:134:LYS:HB3	2.01	0.41
1:A:31:VAL:HG22	1:A:155:VAL:HG13	2.03	0.41
1:S:22:LYS:HB3	1:S:26:ARG:NH2	2.36	0.41
1:B:163:ILE:HG23	1:B:188:LEU:HA	2.02	0.41
2:T:471:LEU:HD13	2:T:492:PRO:HB3	2.02	0.41
2:L:424:ASP:HB3	2:L:428:GLY:H	1.86	0.41
2:V:441:SER:HB2	2:V:478:ASP:OD2	2.21	0.41
2:H:348:THR:HA	3:H:273:M1N:H36	2.03	0.41
2:E:321:THR:O	3:E:273:M1N:H52	2.21	0.41
2:H:324:ASN:N	2:H:324:ASN:ND2	2.49	0.41
1:B:205:VAL:CG1	1:B:206:ALA:H	2.31	0.41
1:M:226:THR:OG1	1:M:227:GLY:N	2.53	0.41
2:P:513:LEU:O	2:P:516:ALA:HB3	2.21	0.41
1:I:205:VAL:C	1:I:207:SER:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:24:ILE:H	1:O:24:ILE:HG12	1.77	0.41
2:V:344:GLY:C	4:V:553:HOH:O	2.59	0.41
1:D:89:TYR:CD1	2:R:382:ARG:HD3	2.56	0.41
1:Y:182:ARG:HA	1:Y:235:VAL:HB	2.03	0.41
2:Z:320:SER:HB3	2:Z:331:VAL:HG21	2.03	0.41
1:I:30:VAL:HG22	1:I:43:ALA:CB	2.51	0.41
1:F:28:LYS:HB2	1:F:52:LYS:NZ	2.36	0.41
2:N:407:TYR:CE1	2:N:417:ALA:HB3	2.55	0.41
2:T:329:ARG:O	2:T:490:ILE:HG21	2.21	0.41
1:U:87:TYR:OH	2:V:354:GLU:HG2	2.20	0.41
2:2:306:LEU:HB2	2:2:313:VAL:CG1	2.50	0.41
2:2:407:TYR:CE1	2:2:417:ALA:HB3	2.56	0.41
1:S:128:ALA:HB2	1:S:134:LYS:HB3	2.02	0.41
1:I:28:LYS:HE2	1:I:46:PRO:HD3	2.01	0.41
1:M:208:LEU:HB3	4:M:254:HOH:O	2.19	0.41
1:K:91:ARG:HB3	1:K:91:ARG:HE	1.65	0.41
1:M:153:PHE:HZ	1:M:168:LYS:HG2	1.86	0.41
2:V:329:ARG:O	2:V:490:ILE:HG21	2.21	0.41
1:D:171:TYR:CE2	1:D:173:GLU:HA	2.56	0.41
3:R:273:M1N:H40	2:Z:424:ASP:OD1	2.21	0.41
2:G:321:THR:HG22	4:G:153:HOH:O	2.20	0.41
2:2:347:GLY:CA	3:2:273:M1N:H132	2.51	0.41
2:T:465:ARG:HB2	2:T:513:LEU:HD22	2.02	0.41
1:K:96:GLY:HA2	1:K:99:LEU:HB2	2.02	0.41
2:V:515:ARG:HA	2:V:518:ILE:HD12	2.03	0.41
1:M:205:VAL:C	1:M:207:SER:N	2.74	0.41
2:Z:514:ALA:O	2:Z:518:ILE:HG13	2.21	0.41
2:N:345:ILE:HD11	4:N:549:HOH:O	2.21	0.41
1:1:176:SER:HB3	1:1:179:ASP:HB2	2.01	0.41
2:R:392:ALA:HB3	4:R:159:HOH:O	2.21	0.41
1:I:205:VAL:HG12	1:I:206:ALA:H	1.85	0.40
2:Z:311:GLY:HA3	2:Z:497:ILE:O	2.22	0.40
2:H:317:ASP:HB2	4:H:552:HOH:O	2.21	0.40
2:H:413:ASP:HA	2:H:414:PRO:HD3	1.93	0.40
1:1:68:PHE:HA	1:1:71:PHE:CE2	2.56	0.40
1:A:18:GLU:OE1	1:A:21:ARG:NH2	2.54	0.40
1:W:152:HIS:CD2	1:W:171:TYR:CE2	3.09	0.40
2:P:433:GLU:O	2:P:433:GLU:HG3	2.21	0.40
1:D:92:ARG:CG	1:D:129:HIS:CE1	3.03	0.40
2:N:306:LEU:HB2	2:N:313:VAL:HG13	2.04	0.40
3:Z:273:M1N:H4	3:Z:273:M1N:H36	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:382:ARG:NH1	2:Z:385:ILE:HD13	2.37	0.40
1:A:205:VAL:HG12	1:A:206:ALA:H	1.87	0.40
1:D:135:ARG:HA	1:D:136:PRO:HD2	1.88	0.40
1:S:185:VAL:HB	1:S:235:VAL:HG11	2.02	0.40
2:N:452:LYS:HZ3	2:V:449:SER:HB2	1.85	0.40
1:Q:185:VAL:HB	1:Q:235:VAL:CG1	2.51	0.40
1:K:98:GLN:O	1:K:101:ASN:HB2	2.21	0.40
2:L:366:TYR:CZ	2:L:370:GLU:HG3	2.57	0.40
2:C:464:LEU:HD11	2:C:505:VAL:HG11	2.03	0.40
2:V:408:ASP:HA	4:V:551:HOH:O	2.21	0.40
2:N:450:MET:CE	2:N:470:ALA:CB	2.99	0.40
2:X:321:THR:HG23	3:X:273:M1N:O3	2.21	0.40
1:F:92:ARG:HD2	1:F:129:HIS:ND1	2.35	0.40
2:J:306:LEU:CD2	2:J:436:TYR:HB3	2.51	0.40
1:S:205:VAL:O	1:S:207:SER:N	2.54	0.40
1:K:123:CYS:HB3	1:K:156:MET:CE	2.51	0.40
1:B:95:THR:C	1:B:97:ARG:H	2.25	0.40
1:I:54:SER:CB	1:I:75:ARG:HD2	2.51	0.40
2:L:485:ASP:OD2	2:L:488:ARG:HB2	2.22	0.40
2:V:403:LEU:HD12	2:V:439:VAL:HG22	2.03	0.40
2:J:432:GLU:HG3	2:J:437:GLN:HB2	2.04	0.40
2:2:384:ALA:HB1	2:2:427:GLY:O	2.22	0.40
2:X:320:SER:HB2	2:X:331:VAL:HG21	2.03	0.40
1:A:96:GLY:HA2	1:A:99:LEU:HB2	2.02	0.40
2:H:321:THR:HG22	4:H:542:HOH:O	2.20	0.40
2:J:395:MET:HA	2:J:395:MET:CE	2.51	0.40
2:P:388:ARG:HD3	4:P:544:HOH:O	2.21	0.40
2:2:452:LYS:HA	2:2:452:LYS:HD3	1.85	0.40
2:H:313:VAL:HB	2:H:496:ILE:HD13	2.03	0.40
2:J:496:ILE:HG13	2:J:505:VAL:CG2	2.51	0.40
2:R:388:ARG:C	2:R:390:ASN:H	2.24	0.40
2:C:520:SER:HB2	4:C:554:HOH:O	2.21	0.40
2:C:438:ALA:CB	2:C:443:SER:HB2	2.51	0.40
1:U:45:ASN:HA	1:U:46:PRO:HD2	1.97	0.40
2:X:331:VAL:HG11	3:X:273:M1N:H251	2.04	0.40
2:H:347:GLY:H	3:H:273:M1N:H16	1.69	0.40
2:N:357:ARG:O	2:N:361:VAL:HG23	2.22	0.40
1:O:182:ARG:HD3	1:O:235:VAL:CG2	2.52	0.40
2:Z:313:VAL:HG23	2:Z:496:ILE:HG12	2.03	0.40
1:A:95:THR:C	1:A:97:ARG:H	2.25	0.40
1:O:209:GLU:OE2	1:O:224:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:390:ASN:HA	4:X:31:HOH:O	2.22	0.40
1:K:95:THR:C	1:K:97:ARG:H	2.25	0.40
2:L:322:GLN:HG2	2:L:322:GLN:O	2.21	0.40
1:M:161:GLU:H	1:M:161:GLU:CD	2.25	0.40
1:1:165:ASN:HA	1:1:165:ASN:HD22	1.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:O	1:D:133:THR:OG1[2_655]	2.12	0.08

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	1	216/251 (86%)	188 (87%)	23 (11%)	5 (2%)	8	36
1	A	216/251 (86%)	190 (88%)	21 (10%)	5 (2%)	8	36
1	B	216/251 (86%)	189 (88%)	22 (10%)	5 (2%)	8	36
1	D	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	6	30
1	F	216/251 (86%)	192 (89%)	18 (8%)	6 (3%)	6	30
1	I	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	6	30
1	K	216/251 (86%)	190 (88%)	20 (9%)	6 (3%)	6	30
1	M	216/251 (86%)	190 (88%)	21 (10%)	5 (2%)	8	36
1	O	216/251 (86%)	189 (88%)	22 (10%)	5 (2%)	8	36
1	Q	216/251 (86%)	189 (88%)	20 (9%)	7 (3%)	5	27
1	S	216/251 (86%)	188 (87%)	22 (10%)	6 (3%)	6	30
1	U	216/251 (86%)	188 (87%)	23 (11%)	5 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	216/251 (86%)	187 (87%)	23 (11%)	6 (3%)	6	30
1	Y	216/251 (86%)	188 (87%)	24 (11%)	4 (2%)	10	43
2	2	220/240 (92%)	202 (92%)	18 (8%)	0	100	100
2	C	220/240 (92%)	201 (91%)	19 (9%)	0	100	100
2	E	220/240 (92%)	201 (91%)	19 (9%)	0	100	100
2	G	220/240 (92%)	201 (91%)	18 (8%)	1 (0%)	34	76
2	H	220/240 (92%)	201 (91%)	17 (8%)	2 (1%)	21	64
2	J	220/240 (92%)	199 (90%)	21 (10%)	0	100	100
2	L	220/240 (92%)	199 (90%)	21 (10%)	0	100	100
2	N	220/240 (92%)	200 (91%)	19 (9%)	1 (0%)	34	76
2	P	220/240 (92%)	202 (92%)	17 (8%)	1 (0%)	34	76
2	R	220/240 (92%)	204 (93%)	13 (6%)	3 (1%)	14	51
2	T	220/240 (92%)	202 (92%)	18 (8%)	0	100	100
2	V	220/240 (92%)	202 (92%)	16 (7%)	2 (1%)	21	64
2	X	220/240 (92%)	200 (91%)	18 (8%)	2 (1%)	21	64
2	Z	220/240 (92%)	199 (90%)	20 (9%)	1 (0%)	34	76
All	All	6104/6874 (89%)	5457 (89%)	557 (9%)	90 (2%)	13	50

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ALA
1	B	128	ALA
1	D	128	ALA
1	F	128	ALA
1	I	128	ALA
1	K	128	ALA
1	M	128	ALA
1	M	130	TYR
1	O	128	ALA
1	Q	128	ALA
1	S	128	ALA
1	U	128	ALA
1	W	128	ALA
1	Y	128	ALA
1	1	128	ALA

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Mol	Chain	Res	Type
1	A	130	TYR
1	B	130	TYR
1	B	206	ALA
1	B	226	THR
1	D	130	TYR
1	D	206	ALA
1	F	130	TYR
1	I	130	TYR
1	I	206	ALA
1	K	130	TYR
1	K	206	ALA
1	M	206	ALA
1	M	226	THR
1	O	130	TYR
1	O	206	ALA
1	Q	130	TYR
1	S	130	TYR
1	S	206	ALA
1	S	226	THR
1	U	130	TYR
1	U	206	ALA
1	U	226	THR
1	W	130	TYR
1	Y	130	TYR
1	Y	206	ALA
1	1	130	TYR
1	1	206	ALA
1	1	226	THR
1	A	58	ASP
1	A	206	ALA
1	A	226	THR
1	D	226	THR
1	F	206	ALA
1	F	226	THR
1	I	58	ASP
1	I	226	THR
1	K	58	ASP
1	K	226	THR
1	O	226	THR
1	Q	58	ASP
1	Q	206	ALA
1	Q	226	THR

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Mol	Chain	Res	Type
1	U	58	ASP
1	W	206	ALA
1	W	226	THR
1	Y	226	THR
2	P	398	LEU
2	R	398	LEU
2	R	433	GLU
2	H	398	LEU
1	D	58	ASP
1	F	58	ASP
2	N	433	GLU
1	O	132	GLU
2	R	389	GLY
1	S	132	GLU
2	V	317	ASP
2	V	398	LEU
1	W	58	ASP
1	I	58	ASP
1	B	58	ASP
1	Q	132	GLU
2	X	460	GLY
2	Z	389	GLY
2	H	389	GLY
1	F	218	PRO
1	K	218	PRO
2	G	460	GLY
1	I	218	PRO
1	M	218	PRO
1	W	218	PRO
2	X	389	GLY
1	D	218	PRO
1	Q	218	PRO
1	S	218	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	169/195 (87%)	152 (90%)	17 (10%)	9	34
1	A	169/195 (87%)	151 (89%)	18 (11%)	8	31
1	B	169/195 (87%)	149 (88%)	20 (12%)	6	26
1	D	169/195 (87%)	148 (88%)	21 (12%)	6	24
1	F	169/195 (87%)	149 (88%)	20 (12%)	6	26
1	I	169/195 (87%)	147 (87%)	22 (13%)	5	22
1	K	169/195 (87%)	148 (88%)	21 (12%)	6	24
1	M	169/195 (87%)	151 (89%)	18 (11%)	8	31
1	O	169/195 (87%)	148 (88%)	21 (12%)	6	24
1	Q	169/195 (87%)	150 (89%)	19 (11%)	7	29
1	S	169/195 (87%)	147 (87%)	22 (13%)	5	22
1	U	169/195 (87%)	150 (89%)	19 (11%)	7	29
1	W	169/195 (87%)	154 (91%)	15 (9%)	12	42
1	Y	169/195 (87%)	147 (87%)	22 (13%)	5	22
2	2	165/178 (93%)	138 (84%)	27 (16%)	3	14
2	C	165/178 (93%)	140 (85%)	25 (15%)	3	16
2	E	165/178 (93%)	136 (82%)	29 (18%)	2	12
2	G	165/178 (93%)	145 (88%)	20 (12%)	6	25
2	H	165/178 (93%)	140 (85%)	25 (15%)	3	16
2	J	165/178 (93%)	144 (87%)	21 (13%)	5	23
2	L	165/178 (93%)	141 (86%)	24 (14%)	4	18
2	N	165/178 (93%)	143 (87%)	22 (13%)	5	21
2	P	165/178 (93%)	142 (86%)	23 (14%)	4	19
2	R	165/178 (93%)	135 (82%)	30 (18%)	2	11
2	T	165/178 (93%)	139 (84%)	26 (16%)	3	15
2	V	165/178 (93%)	137 (83%)	28 (17%)	2	13
2	X	165/178 (93%)	146 (88%)	19 (12%)	7	28
2	Z	165/178 (93%)	143 (87%)	22 (13%)	5	21
All	All	4676/5222 (90%)	4060 (87%)	616 (13%)	5	22

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	GLU
1	A	60	VAL
1	A	80	GLN
1	A	85	ARG
1	A	91	ARG
1	A	92	ARG
1	A	113	GLU
1	A	116	LYS
1	A	134	LYS
1	A	135	ARG
1	A	147	ILE
1	A	150	GLU
1	A	165	ASN
1	A	182	ARG
1	A	203	LEU
1	A	208	LEU
1	A	237	GLN
2	H	304	VAL
2	H	307	LYS
2	H	318	ARG
2	H	319	ARG
2	H	320	SER
2	H	324	ASN
2	H	329	ARG
2	H	332	ARG
2	H	375	THR
2	H	391	LEU
2	H	401	LEU
2	H	403	LEU
2	H	412	SER
2	H	415	GLN
2	H	422	SER
2	H	424	ASP
2	H	430	ASN
2	H	441	SER
2	H	444	LEU
2	H	449	SER
2	H	476	ASP
2	H	479	SER
2	H	508	SER
2	H	520	SER
2	H	522	SER

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Mol	Chain	Res	Type
1	B	14	ARG
1	B	18	GLU
1	B	28	LYS
1	B	29	SER
1	B	49	SER
1	B	80	GLN
1	B	84	THR
1	B	85	ARG
1	B	92	ARG
1	B	113	GLU
1	B	134	LYS
1	B	135	ARG
1	B	147	ILE
1	B	149	ASP
1	B	150	GLU
1	B	182	ARG
1	B	203	LEU
1	B	208	LEU
1	B	213	LEU
1	B	228	SER
2	C	304	VAL
2	C	318	ARG
2	C	319	ARG
2	C	320	SER
2	C	321	THR
2	C	324	ASN
2	C	329	ARG
2	C	332	ARG
2	C	341	THR
2	C	354	GLU
2	C	355	PHE
2	C	391	LEU
2	C	401	LEU
2	C	403	LEU
2	C	415	GLN
2	C	434	GLU
2	C	439	VAL
2	C	444	LEU
2	C	449	SER
2	C	461	ASP
2	C	465	ARG
2	C	490	ILE

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Mol	Chain	Res	Type
2	C	508	SER
2	C	517	ILE
2	C	522	SER
1	D	11	GLN
1	D	18	GLU
1	D	33	LEU
1	D	84	THR
1	D	85	ARG
1	D	92	ARG
1	D	113	GLU
1	D	133	THR
1	D	134	LYS
1	D	135	ARG
1	D	147	ILE
1	D	150	GLU
1	D	165	ASN
1	D	178	THR
1	D	182	ARG
1	D	188	LEU
1	D	192	SER
1	D	203	LEU
1	D	205	VAL
1	D	208	LEU
1	D	236	ASP
2	E	304	VAL
2	E	312	VAL
2	E	318	ARG
2	E	319	ARG
2	E	320	SER
2	E	324	ASN
2	E	329	ARG
2	E	332	ARG
2	E	341	THR
2	E	357	ARG
2	E	358	LEU
2	E	375	THR
2	E	383	LEU
2	E	391	LEU
2	E	401	LEU
2	E	403	LEU
2	E	415	GLN
2	E	419	ARG

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Mol	Chain	Res	Type
2	E	432	GLU
2	E	444	LEU
2	E	449	SER
2	E	455	SER
2	E	476	ASP
2	E	488	ARG
2	E	490	ILE
2	E	508	SER
2	E	517	ILE
2	E	520	SER
2	E	522	SER
1	F	18	GLU
1	F	26	ARG
1	F	80	GLN
1	F	85	ARG
1	F	92	ARG
1	F	113	GLU
1	F	133	THR
1	F	134	LYS
1	F	135	ARG
1	F	147	ILE
1	F	150	GLU
1	F	159	THR
1	F	173	GLU
1	F	176	SER
1	F	182	ARG
1	F	188	LEU
1	F	203	LEU
1	F	205	VAL
1	F	208	LEU
1	F	213	LEU
2	G	318	ARG
2	G	319	ARG
2	G	321	THR
2	G	324	ASN
2	G	329	ARG
2	G	337	THR
2	G	341	THR
2	G	357	ARG
2	G	375	THR
2	G	391	LEU
2	G	401	LEU

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Mol	Chain	Res	Type
2	G	403	LEU
2	G	437	GLN
2	G	441	SER
2	G	444	LEU
2	G	461	ASP
2	G	465	ARG
2	G	476	ASP
2	G	479	SER
2	G	517	ILE
1	I	18	GLU
1	I	24	ILE
1	I	48	ARG
1	I	60	VAL
1	I	84	THR
1	I	85	ARG
1	I	92	ARG
1	I	113	GLU
1	I	134	LYS
1	I	135	ARG
1	I	137	GLU
1	I	140	ARG
1	I	147	ILE
1	I	150	GLU
1	I	156	MET
1	I	182	ARG
1	I	192	SER
1	I	203	LEU
1	I	208	LEU
1	I	213	LEU
1	I	225	ILE
1	I	237	GLN
2	J	304	VAL
2	J	318	ARG
2	J	319	ARG
2	J	320	SER
2	J	324	ASN
2	J	329	ARG
2	J	337	THR
2	J	341	THR
2	J	375	THR
2	J	391	LEU
2	J	401	LEU

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Mol	Chain	Res	Type
2	J	403	LEU
2	J	419	ARG
2	J	424	ASP
2	J	444	LEU
2	J	448	SER
2	J	449	SER
2	J	476	ASP
2	J	490	ILE
2	J	503	VAL
2	J	522	SER
1	K	18	GLU
1	K	33	LEU
1	K	84	THR
1	K	85	ARG
1	K	91	ARG
1	K	92	ARG
1	K	99	LEU
1	K	113	GLU
1	K	123	CYS
1	K	134	LYS
1	K	135	ARG
1	K	144	ASP
1	K	147	ILE
1	K	150	GLU
1	K	173	GLU
1	K	178	THR
1	K	203	LEU
1	K	208	LEU
1	K	213	LEU
1	K	225	ILE
1	K	237	GLN
2	L	304	VAL
2	L	320	SER
2	L	321	THR
2	L	324	ASN
2	L	329	ARG
2	L	332	ARG
2	L	341	THR
2	L	391	LEU
2	L	398	LEU
2	L	403	LEU
2	L	412	SER

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Mol	Chain	Res	Type
2	L	415	GLN
2	L	419	ARG
2	L	441	SER
2	L	443	SER
2	L	444	LEU
2	L	448	SER
2	L	449	SER
2	L	476	ASP
2	L	479	SER
2	L	488	ARG
2	L	497	ILE
2	L	508	SER
2	L	522	SER
1	M	8	SER
1	M	14	ARG
1	M	18	GLU
1	M	49	SER
1	M	80	GLN
1	M	85	ARG
1	M	92	ARG
1	M	113	GLU
1	M	133	THR
1	M	134	LYS
1	M	135	ARG
1	M	147	ILE
1	M	173	GLU
1	M	176	SER
1	M	188	LEU
1	M	203	LEU
1	M	208	LEU
1	M	213	LEU
2	N	307	LYS
2	N	312	VAL
2	N	318	ARG
2	N	319	ARG
2	N	320	SER
2	N	321	THR
2	N	324	ASN
2	N	329	ARG
2	N	337	THR
2	N	341	THR
2	N	345	ILE

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Mol	Chain	Res	Type
2	N	391	LEU
2	N	401	LEU
2	N	403	LEU
2	N	416	SER
2	N	419	ARG
2	N	430	ASN
2	N	441	SER
2	N	444	LEU
2	N	449	SER
2	N	464	LEU
2	N	476	ASP
1	O	11	GLN
1	O	14	ARG
1	O	18	GLU
1	O	21	ARG
1	O	48	ARG
1	O	84	THR
1	O	85	ARG
1	O	92	ARG
1	O	113	GLU
1	O	134	LYS
1	O	135	ARG
1	O	147	ILE
1	O	150	GLU
1	O	165	ASN
1	O	182	ARG
1	O	188	LEU
1	O	192	SER
1	O	203	LEU
1	O	208	LEU
1	O	225	ILE
1	O	236	ASP
2	P	304	VAL
2	P	307	LYS
2	P	318	ARG
2	P	319	ARG
2	P	320	SER
2	P	324	ASN
2	P	325	MET
2	P	329	ARG
2	P	332	ARG
2	P	337	THR

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Mol	Chain	Res	Type
2	P	357	ARG
2	P	375	THR
2	P	391	LEU
2	P	396	GLN
2	P	401	LEU
2	P	403	LEU
2	P	444	LEU
2	P	448	SER
2	P	449	SER
2	P	476	ASP
2	P	488	ARG
2	P	508	SER
2	P	517	ILE
1	Q	18	GLU
1	Q	21	ARG
1	Q	24	ILE
1	Q	48	ARG
1	Q	84	THR
1	Q	85	ARG
1	Q	92	ARG
1	Q	113	GLU
1	Q	134	LYS
1	Q	135	ARG
1	Q	147	ILE
1	Q	159	THR
1	Q	173	GLU
1	Q	179	ASP
1	Q	203	LEU
1	Q	213	LEU
1	Q	225	ILE
1	Q	236	ASP
1	Q	237	GLN
2	R	304	VAL
2	R	314	MET
2	R	318	ARG
2	R	319	ARG
2	R	320	SER
2	R	321	THR
2	R	324	ASN
2	R	329	ARG
2	R	337	THR
2	R	341	THR

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Mol	Chain	Res	Type
2	R	355	PHE
2	R	375	THR
2	R	383	LEU
2	R	391	LEU
2	R	401	LEU
2	R	403	LEU
2	R	419	ARG
2	R	424	ASP
2	R	434	GLU
2	R	436	TYR
2	R	444	LEU
2	R	449	SER
2	R	461	ASP
2	R	476	ASP
2	R	481	THR
2	R	488	ARG
2	R	490	ILE
2	R	503	VAL
2	R	508	SER
2	R	520	SER
1	S	11	GLN
1	S	17	SER
1	S	18	GLU
1	S	33	LEU
1	S	48	ARG
1	S	49	SER
1	S	84	THR
1	S	85	ARG
1	S	92	ARG
1	S	109	THR
1	S	113	GLU
1	S	133	THR
1	S	134	LYS
1	S	135	ARG
1	S	147	ILE
1	S	150	GLU
1	S	182	ARG
1	S	188	LEU
1	S	192	SER
1	S	203	LEU
1	S	205	VAL
1	S	208	LEU

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Mol	Chain	Res	Type
2	T	304	VAL
2	T	318	ARG
2	T	319	ARG
2	T	320	SER
2	T	321	THR
2	T	324	ASN
2	T	329	ARG
2	T	337	THR
2	T	341	THR
2	T	357	ARG
2	T	391	LEU
2	T	398	LEU
2	T	401	LEU
2	T	403	LEU
2	T	415	GLN
2	T	419	ARG
2	T	430	ASN
2	T	439	VAL
2	T	441	SER
2	T	444	LEU
2	T	448	SER
2	T	449	SER
2	T	476	ASP
2	T	508	SER
2	T	517	ILE
2	T	522	SER
1	U	11	GLN
1	U	18	GLU
1	U	24	ILE
1	U	26	ARG
1	U	84	THR
1	U	85	ARG
1	U	91	ARG
1	U	92	ARG
1	U	113	GLU
1	U	134	LYS
1	U	135	ARG
1	U	147	ILE
1	U	150	GLU
1	U	165	ASN
1	U	188	LEU
1	U	203	LEU

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Mol	Chain	Res	Type
1	U	205	VAL
1	U	208	LEU
1	U	237	GLN
2	V	303	ILE
2	V	304	VAL
2	V	312	VAL
2	V	318	ARG
2	V	319	ARG
2	V	320	SER
2	V	324	ASN
2	V	329	ARG
2	V	345	ILE
2	V	355	PHE
2	V	375	THR
2	V	383	LEU
2	V	391	LEU
2	V	401	LEU
2	V	403	LEU
2	V	412	SER
2	V	415	GLN
2	V	416	SER
2	V	430	ASN
2	V	441	SER
2	V	444	LEU
2	V	448	SER
2	V	449	SER
2	V	476	ASP
2	V	479	SER
2	V	490	ILE
2	V	508	SER
2	V	513	LEU
1	W	11	GLN
1	W	18	GLU
1	W	28	LYS
1	W	85	ARG
1	W	91	ARG
1	W	92	ARG
1	W	113	GLU
1	W	134	LYS
1	W	135	ARG
1	W	137	GLU
1	W	147	ILE

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Mol	Chain	Res	Type
1	W	176	SER
1	W	203	LEU
1	W	225	ILE
1	W	231	GLN
2	X	319	ARG
2	X	321	THR
2	X	324	ASN
2	X	329	ARG
2	X	337	THR
2	X	358	LEU
2	X	375	THR
2	X	383	LEU
2	X	391	LEU
2	X	398	LEU
2	X	401	LEU
2	X	403	LEU
2	X	430	ASN
2	X	444	LEU
2	X	448	SER
2	X	458	THR
2	X	476	ASP
2	X	490	ILE
2	X	522	SER
1	Y	14	ARG
1	Y	18	GLU
1	Y	21	ARG
1	Y	24	ILE
1	Y	33	LEU
1	Y	48	ARG
1	Y	84	THR
1	Y	85	ARG
1	Y	91	ARG
1	Y	92	ARG
1	Y	113	GLU
1	Y	134	LYS
1	Y	135	ARG
1	Y	147	ILE
1	Y	150	GLU
1	Y	161	GLU
1	Y	179	ASP
1	Y	182	ARG
1	Y	188	LEU

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Mol	Chain	Res	Type
1	Y	203	LEU
1	Y	205	VAL
1	Y	237	GLN
2	Z	318	ARG
2	Z	319	ARG
2	Z	320	SER
2	Z	321	THR
2	Z	324	ASN
2	Z	329	ARG
2	Z	337	THR
2	Z	345	ILE
2	Z	383	LEU
2	Z	391	LEU
2	Z	401	LEU
2	Z	403	LEU
2	Z	415	GLN
2	Z	416	SER
2	Z	419	ARG
2	Z	444	LEU
2	Z	448	SER
2	Z	476	ASP
2	Z	479	SER
2	Z	490	ILE
2	Z	508	SER
2	Z	513	LEU
1	1	48	ARG
1	1	49	SER
1	1	85	ARG
1	1	92	ARG
1	1	113	GLU
1	1	134	LYS
1	1	135	ARG
1	1	137	GLU
1	1	147	ILE
1	1	150	GLU
1	1	156	MET
1	1	173	GLU
1	1	179	ASP
1	1	182	ARG
1	1	188	LEU
1	1	203	LEU
1	1	231	GLN

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Mol	Chain	Res	Type
2	2	304	VAL
2	2	318	ARG
2	2	320	SER
2	2	321	THR
2	2	324	ASN
2	2	329	ARG
2	2	341	THR
2	2	358	LEU
2	2	383	LEU
2	2	391	LEU
2	2	396	GLN
2	2	398	LEU
2	2	401	LEU
2	2	409	ILE
2	2	412	SER
2	2	419	ARG
2	2	421	VAL
2	2	422	SER
2	2	430	ASN
2	2	439	VAL
2	2	441	SER
2	2	444	LEU
2	2	449	SER
2	2	476	ASP
2	2	497	ILE
2	2	503	VAL
2	2	508	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	73	ASN
1	A	98	GLN
1	A	105	GLN
1	A	165	ASN
1	A	231	GLN
2	H	324	ASN
2	H	365	HIS
2	H	410	HIS
2	H	415	GLN
2	H	456	GLN

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Mol	Chain	Res	Type
1	B	51	GLN
1	B	73	ASN
1	B	98	GLN
1	B	105	GLN
1	B	152	HIS
1	B	165	ASN
1	B	231	GLN
2	C	324	ASN
2	C	365	HIS
2	C	415	GLN
2	C	456	GLN
1	D	98	GLN
1	D	105	GLN
1	D	129	HIS
1	D	152	HIS
1	D	165	ASN
2	E	324	ASN
2	E	365	HIS
2	E	456	GLN
1	F	51	GLN
1	F	80	GLN
1	F	98	GLN
1	F	105	GLN
1	F	129	HIS
1	F	165	ASN
1	F	231	GLN
2	G	324	ASN
2	G	365	HIS
2	G	410	HIS
2	G	415	GLN
2	G	456	GLN
1	I	51	GLN
1	I	98	GLN
1	I	105	GLN
1	I	129	HIS
1	I	165	ASN
2	J	324	ASN
2	J	365	HIS
2	J	415	GLN
2	J	456	GLN
1	K	51	GLN
1	K	73	ASN

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Mol	Chain	Res	Type
1	K	98	GLN
1	K	105	GLN
1	K	129	HIS
1	K	165	ASN
2	L	324	ASN
2	L	365	HIS
2	L	415	GLN
2	L	456	GLN
1	M	51	GLN
1	M	129	HIS
1	M	231	GLN
2	N	324	ASN
2	N	365	HIS
2	N	410	HIS
2	N	415	GLN
2	N	456	GLN
1	O	51	GLN
1	O	73	ASN
1	O	98	GLN
1	O	129	HIS
1	O	165	ASN
2	P	324	ASN
2	P	365	HIS
2	P	410	HIS
2	P	456	GLN
1	Q	98	GLN
1	Q	129	HIS
1	Q	165	ASN
1	Q	231	GLN
2	R	324	ASN
2	R	365	HIS
2	R	410	HIS
2	R	415	GLN
2	R	456	GLN
1	S	80	GLN
1	S	98	GLN
1	S	105	GLN
1	S	114	GLN
1	S	129	HIS
1	S	165	ASN
2	T	324	ASN
2	T	365	HIS

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Mol	Chain	Res	Type
2	T	390	ASN
2	T	456	GLN
1	U	51	GLN
1	U	98	GLN
1	U	105	GLN
1	U	129	HIS
1	U	165	ASN
1	U	231	GLN
2	V	324	ASN
2	V	410	HIS
2	V	430	ASN
2	V	456	GLN
1	W	51	GLN
1	W	80	GLN
1	W	98	GLN
1	W	105	GLN
1	W	129	HIS
1	W	152	HIS
1	W	165	ASN
1	W	231	GLN
2	X	322	GLN
2	X	324	ASN
2	X	365	HIS
2	X	410	HIS
2	X	456	GLN
1	Y	51	GLN
1	Y	80	GLN
1	Y	98	GLN
1	Y	105	GLN
1	Y	129	HIS
1	Y	165	ASN
1	Y	231	GLN
2	Z	324	ASN
2	Z	365	HIS
1	1	51	GLN
1	1	105	GLN
1	1	129	HIS
1	1	152	HIS
1	1	165	ASN
1	1	231	GLN
2	2	324	ASN
2	2	365	HIS

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Mol	Chain	Res	Type
2	2	456	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	M1N	2	273	2	33,34,34	2.78	14 (42%)	36,46,46	3.51	15 (41%)
3	M1N	C	273	2	33,34,34	2.46	12 (36%)	36,46,46	3.35	15 (41%)
3	M1N	E	273	2	33,34,34	2.57	13 (39%)	36,46,46	3.10	15 (41%)
3	M1N	G	273	2	33,34,34	2.77	15 (45%)	36,46,46	3.05	11 (30%)
3	M1N	H	273	2	33,34,34	2.56	12 (36%)	36,46,46	3.26	12 (33%)
3	M1N	J	273	2	33,34,34	2.63	13 (39%)	36,46,46	2.99	12 (33%)
3	M1N	L	273	2	33,34,34	2.54	13 (39%)	36,46,46	3.36	13 (36%)
3	M1N	N	273	2	33,34,34	2.60	14 (42%)	36,46,46	3.07	14 (38%)
3	M1N	P	273	2	33,34,34	2.66	12 (36%)	36,46,46	3.25	13 (36%)
3	M1N	R	273	2	33,34,34	2.78	14 (42%)	36,46,46	3.14	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	M1N	T	273	2	33,34,34	2.78	15 (45%)	36,46,46	2.94	13 (36%)
3	M1N	V	273	2	33,34,34	2.60	15 (45%)	36,46,46	3.18	13 (36%)
3	M1N	X	273	2	33,34,34	2.78	16 (48%)	36,46,46	3.22	14 (38%)
3	M1N	Z	273	2	33,34,34	2.67	13 (39%)	36,46,46	3.10	13 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M1N	2	273	2	-	2/22/36/36	0/3/3/3
3	M1N	C	273	2	-	2/22/36/36	0/3/3/3
3	M1N	E	273	2	-	2/22/36/36	0/3/3/3
3	M1N	G	273	2	-	2/22/36/36	0/3/3/3
3	M1N	H	273	2	-	2/22/36/36	0/3/3/3
3	M1N	J	273	2	-	3/22/36/36	0/3/3/3
3	M1N	L	273	2	-	2/22/36/36	0/3/3/3
3	M1N	N	273	2	-	2/22/36/36	0/3/3/3
3	M1N	P	273	2	-	2/22/36/36	0/3/3/3
3	M1N	R	273	2	-	3/22/36/36	0/3/3/3
3	M1N	T	273	2	-	2/22/36/36	0/3/3/3
3	M1N	V	273	2	-	3/22/36/36	0/3/3/3
3	M1N	X	273	2	-	2/22/36/36	0/3/3/3
3	M1N	Z	273	2	-	2/22/36/36	0/3/3/3

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	273	M1N	C5-C4	-6.78	1.37	1.54
3	P	273	M1N	C5-C4	-6.77	1.37	1.54
3	G	273	M1N	C5-C4	-6.66	1.37	1.54
3	J	273	M1N	C5-C4	-6.60	1.37	1.54
3	N	273	M1N	C5-C4	-6.53	1.37	1.54
3	H	273	M1N	C5-C4	-6.50	1.37	1.54
3	R	273	M1N	C5-C4	-6.39	1.38	1.54
3	C	273	M1N	C5-C4	-6.36	1.38	1.54
3	Z	273	M1N	C5-C4	-6.30	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	273	M1N	C5-C4	-6.23	1.38	1.54
3	V	273	M1N	C5-C4	-6.14	1.38	1.54
3	L	273	M1N	C5-C4	-6.14	1.38	1.54
3	2	273	M1N	C5-C4	-6.11	1.38	1.54
3	T	273	M1N	C5-C4	-5.97	1.39	1.54
3	R	273	M1N	C4-C2	-3.40	1.43	1.52
3	Z	273	M1N	C4-C2	-3.18	1.44	1.52
3	G	273	M1N	C4-C2	-3.14	1.44	1.52
3	H	273	M1N	C4-C2	-3.13	1.44	1.52
3	C	273	M1N	C4-C2	-3.12	1.44	1.52
3	T	273	M1N	C4-C2	-3.11	1.44	1.52
3	L	273	M1N	C4-C2	-3.08	1.44	1.52
3	E	273	M1N	C4-C2	-2.95	1.44	1.52
3	P	273	M1N	C4-C2	-2.83	1.45	1.52
3	J	273	M1N	C4-C2	-2.82	1.45	1.52
3	N	273	M1N	C4-C2	-2.79	1.45	1.52
3	X	273	M1N	C4-C2	-2.67	1.45	1.52
3	2	273	M1N	C4-C2	-2.37	1.46	1.52
3	V	273	M1N	C4-C2	-2.28	1.46	1.52
3	E	273	M1N	C36-C31	2.01	1.41	1.37
3	L	273	M1N	C36-C31	2.02	1.41	1.37
3	2	273	M1N	C32-C33	2.02	1.46	1.42
3	J	273	M1N	C32-C33	2.06	1.46	1.42
3	X	273	M1N	C4-N6	2.09	1.50	1.45
3	V	273	M1N	C36-C31	2.14	1.41	1.37
3	R	273	M1N	C36-C31	2.14	1.41	1.37
3	Z	273	M1N	C36-C31	2.16	1.41	1.37
3	N	273	M1N	C31-C32	2.18	1.47	1.42
3	L	273	M1N	O12-C11	2.20	1.51	1.42
3	H	273	M1N	O12-C11	2.21	1.51	1.42
3	X	273	M1N	C32-C33	2.23	1.47	1.42
3	N	273	M1N	O12-C11	2.24	1.52	1.42
3	R	273	M1N	C32-C33	2.26	1.47	1.42
3	J	273	M1N	O12-C11	2.28	1.52	1.42
3	X	273	M1N	C31-C32	2.28	1.47	1.42
3	E	273	M1N	O12-C11	2.30	1.52	1.42
3	T	273	M1N	O12-C11	2.30	1.52	1.42
3	C	273	M1N	O12-C11	2.31	1.52	1.42
3	2	273	M1N	C36-C31	2.31	1.41	1.37
3	G	273	M1N	O12-C11	2.32	1.52	1.42
3	G	273	M1N	C32-C33	2.34	1.47	1.42
3	T	273	M1N	C31-C32	2.35	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	273	M1N	O12-C11	2.36	1.52	1.42
3	V	273	M1N	C32-C33	2.38	1.47	1.42
3	V	273	M1N	C31-C32	2.40	1.48	1.42
3	P	273	M1N	O12-C11	2.41	1.52	1.42
3	N	273	M1N	C32-C33	2.42	1.47	1.42
3	R	273	M1N	O12-C11	2.43	1.52	1.42
3	G	273	M1N	C31-C32	2.43	1.48	1.42
3	E	273	M1N	C14-N9	2.48	1.51	1.47
3	T	273	M1N	C36-C31	2.51	1.42	1.37
3	T	273	M1N	C32-C33	2.53	1.47	1.42
3	G	273	M1N	C36-C31	2.56	1.42	1.37
3	V	273	M1N	O12-C11	2.56	1.53	1.42
3	X	273	M1N	C36-C31	2.58	1.42	1.37
3	X	273	M1N	O12-C11	2.58	1.53	1.42
3	Z	273	M1N	O12-C11	2.58	1.53	1.42
3	C	273	M1N	C14-N9	2.59	1.51	1.47
3	H	273	M1N	C14-N9	2.60	1.51	1.47
3	2	273	M1N	C14-N9	2.72	1.51	1.47
3	L	273	M1N	C14-N9	2.82	1.51	1.47
3	V	273	M1N	C35-C34	2.93	1.43	1.36
3	R	273	M1N	C14-N9	2.97	1.52	1.47
3	N	273	M1N	C14-N9	2.99	1.52	1.47
3	2	273	M1N	C35-C34	2.99	1.43	1.36
3	V	273	M1N	C14-N9	3.02	1.52	1.47
3	C	273	M1N	C7-N9	3.06	1.42	1.36
3	H	273	M1N	C10-N9	3.07	1.52	1.47
3	J	273	M1N	C14-N9	3.09	1.52	1.47
3	P	273	M1N	C14-N9	3.10	1.52	1.47
3	N	273	M1N	C35-C34	3.13	1.43	1.36
3	H	273	M1N	C35-C34	3.18	1.43	1.36
3	Z	273	M1N	C14-N9	3.19	1.52	1.47
3	E	273	M1N	C10-N9	3.20	1.52	1.47
3	C	273	M1N	C10-N9	3.22	1.52	1.47
3	Z	273	M1N	C35-C34	3.23	1.44	1.36
3	X	273	M1N	C14-N9	3.23	1.52	1.47
3	R	273	M1N	C10-N9	3.24	1.52	1.47
3	N	273	M1N	C10-N9	3.25	1.52	1.47
3	G	273	M1N	C14-N9	3.26	1.52	1.47
3	L	273	M1N	C35-C34	3.30	1.44	1.36
3	T	273	M1N	C35-C34	3.32	1.44	1.36
3	P	273	M1N	C35-C34	3.36	1.44	1.36
3	X	273	M1N	C35-C34	3.36	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	273	M1N	C10-N9	3.41	1.52	1.47
3	E	273	M1N	C7-N9	3.43	1.43	1.36
3	C	273	M1N	C35-C34	3.44	1.44	1.36
3	L	273	M1N	C10-N9	3.46	1.53	1.47
3	G	273	M1N	C35-C34	3.47	1.44	1.36
3	V	273	M1N	C7-N9	3.47	1.43	1.36
3	G	273	M1N	C10-N9	3.47	1.53	1.47
3	L	273	M1N	C7-N9	3.50	1.43	1.36
3	T	273	M1N	C14-N9	3.50	1.53	1.47
3	N	273	M1N	C7-N9	3.53	1.43	1.36
3	V	273	M1N	C10-N9	3.55	1.53	1.47
3	R	273	M1N	C35-C34	3.57	1.44	1.36
3	J	273	M1N	C10-N9	3.58	1.53	1.47
3	T	273	M1N	C10-N9	3.59	1.53	1.47
3	E	273	M1N	C35-C34	3.64	1.45	1.36
3	E	273	M1N	C7-N6	3.67	1.43	1.35
3	J	273	M1N	C35-C34	3.69	1.45	1.36
3	H	273	M1N	C7-N9	3.73	1.43	1.36
3	N	273	M1N	C35-C36	3.77	1.46	1.38
3	P	273	M1N	C7-N6	3.77	1.43	1.35
3	C	273	M1N	C7-N6	3.78	1.43	1.35
3	X	273	M1N	C7-N9	3.79	1.43	1.36
3	V	273	M1N	C7-N6	3.79	1.43	1.35
3	Z	273	M1N	C10-N9	3.79	1.53	1.47
3	C	273	M1N	C35-C36	3.81	1.46	1.38
3	P	273	M1N	C7-N9	3.84	1.43	1.36
3	X	273	M1N	C10-N9	3.85	1.53	1.47
3	N	273	M1N	C7-N6	3.86	1.44	1.35
3	G	273	M1N	C7-N9	3.87	1.44	1.36
3	J	273	M1N	C7-N9	3.87	1.44	1.36
3	V	273	M1N	C35-C36	3.88	1.46	1.38
3	Z	273	M1N	C35-C36	3.90	1.46	1.38
3	J	273	M1N	C35-C36	3.94	1.47	1.38
3	C	273	M1N	O8-C7	3.94	1.30	1.23
3	E	273	M1N	C35-C36	3.94	1.47	1.38
3	J	273	M1N	C7-N6	3.95	1.44	1.35
3	R	273	M1N	C35-C36	3.98	1.47	1.38
3	T	273	M1N	C35-C36	4.01	1.47	1.38
3	L	273	M1N	C7-N6	4.01	1.44	1.35
3	2	273	M1N	C35-C36	4.02	1.47	1.38
3	L	273	M1N	O8-C7	4.06	1.30	1.23
3	J	273	M1N	C2-N1	4.08	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	273	M1N	C7-N6	4.08	1.44	1.35
3	Z	273	M1N	C7-N6	4.09	1.44	1.35
3	R	273	M1N	C7-N9	4.09	1.44	1.36
3	Z	273	M1N	C2-N1	4.11	1.43	1.34
3	Z	273	M1N	C7-N9	4.12	1.44	1.36
3	P	273	M1N	C35-C36	4.14	1.47	1.38
3	T	273	M1N	C7-N9	4.15	1.44	1.36
3	G	273	M1N	C35-C36	4.16	1.47	1.38
3	C	273	M1N	C2-N1	4.16	1.43	1.34
3	H	273	M1N	C38-C37	4.17	1.46	1.36
3	X	273	M1N	C35-C36	4.24	1.47	1.38
3	H	273	M1N	C35-C36	4.27	1.47	1.38
3	L	273	M1N	C35-C36	4.27	1.47	1.38
3	E	273	M1N	C2-N1	4.27	1.43	1.34
3	C	273	M1N	C38-C37	4.28	1.46	1.36
3	E	273	M1N	O8-C7	4.30	1.31	1.23
3	V	273	M1N	O8-C7	4.32	1.31	1.23
3	2	273	M1N	C10-N9	4.33	1.54	1.47
3	H	273	M1N	O8-C7	4.33	1.31	1.23
3	T	273	M1N	C7-N6	4.34	1.45	1.35
3	E	273	M1N	C38-C37	4.35	1.46	1.36
3	P	273	M1N	O8-C7	4.36	1.31	1.23
3	N	273	M1N	O8-C7	4.43	1.31	1.23
3	H	273	M1N	C2-N1	4.44	1.44	1.34
3	L	273	M1N	C38-C37	4.46	1.46	1.36
3	R	273	M1N	C2-N1	4.47	1.44	1.34
3	G	273	M1N	C7-N6	4.49	1.45	1.35
3	V	273	M1N	C2-N1	4.49	1.44	1.34
3	J	273	M1N	O8-C7	4.50	1.31	1.23
3	2	273	M1N	C7-N6	4.51	1.45	1.35
3	L	273	M1N	C2-N1	4.54	1.44	1.34
3	J	273	M1N	C38-C37	4.56	1.47	1.36
3	X	273	M1N	C38-C37	4.59	1.47	1.36
3	N	273	M1N	C2-N1	4.60	1.44	1.34
3	G	273	M1N	C2-N1	4.61	1.44	1.34
3	V	273	M1N	C38-C37	4.63	1.47	1.36
3	X	273	M1N	C7-N6	4.67	1.46	1.35
3	2	273	M1N	O8-C7	4.68	1.32	1.23
3	Z	273	M1N	C38-C37	4.69	1.47	1.36
3	G	273	M1N	C38-C37	4.70	1.47	1.36
3	P	273	M1N	C2-N1	4.73	1.44	1.34
3	N	273	M1N	C38-C37	4.73	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	273	M1N	C7-N6	4.74	1.46	1.35
3	Z	273	M1N	O8-C7	4.81	1.32	1.23
3	P	273	M1N	C38-C37	4.81	1.47	1.36
3	X	273	M1N	O8-C7	4.84	1.32	1.23
3	T	273	M1N	C2-N1	4.87	1.45	1.34
3	G	273	M1N	O8-C7	4.89	1.32	1.23
3	2	273	M1N	C2-N1	4.89	1.45	1.34
3	T	273	M1N	O8-C7	4.92	1.32	1.23
3	R	273	M1N	O8-C7	4.93	1.32	1.23
3	X	273	M1N	C2-N1	4.96	1.45	1.34
3	2	273	M1N	C7-N9	5.00	1.46	1.36
3	2	273	M1N	C38-C37	5.00	1.48	1.36
3	R	273	M1N	C38-C37	5.09	1.48	1.36
3	T	273	M1N	C38-C37	5.18	1.48	1.36

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	273	M1N	O8-C7-N9	-11.43	104.31	121.77
3	X	273	M1N	O8-C7-N9	-11.00	104.96	121.77
3	C	273	M1N	O8-C7-N9	-10.77	105.31	121.77
3	H	273	M1N	O8-C7-N9	-10.55	105.66	121.77
3	R	273	M1N	O8-C7-N9	-10.45	105.80	121.77
3	E	273	M1N	O8-C7-N9	-10.18	106.23	121.77
3	V	273	M1N	O8-C7-N9	-9.97	106.54	121.77
3	2	273	M1N	O8-C7-N9	-9.89	106.66	121.77
3	Z	273	M1N	O8-C7-N9	-9.67	106.99	121.77
3	G	273	M1N	O8-C7-N9	-9.62	107.07	121.77
3	T	273	M1N	O8-C7-N9	-9.53	107.21	121.77
3	P	273	M1N	O8-C7-N9	-9.37	107.46	121.77
3	N	273	M1N	O8-C7-N9	-9.13	107.82	121.77
3	J	273	M1N	O8-C7-N9	-8.97	108.07	121.77
3	2	273	M1N	O3-C2-N1	-6.53	110.14	122.93
3	V	273	M1N	O3-C2-N1	-6.35	110.49	122.93
3	C	273	M1N	O3-C2-N1	-5.77	111.62	122.93
3	P	273	M1N	O3-C2-N1	-5.74	111.69	122.93
3	N	273	M1N	O3-C2-N1	-5.68	111.81	122.93
3	T	273	M1N	C14-N9-C7	-5.47	102.41	122.03
3	G	273	M1N	O3-C2-N1	-5.43	112.29	122.93
3	J	273	M1N	O3-C2-N1	-5.43	112.29	122.93
3	2	273	M1N	C5-C4-N6	-5.41	99.48	110.80
3	G	273	M1N	C14-N9-C7	-5.33	102.93	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	273	M1N	C14-N9-C7	-5.29	103.05	122.03
3	X	273	M1N	C14-N9-C7	-5.24	103.23	122.03
3	N	273	M1N	C14-N9-C7	-5.12	103.66	122.03
3	H	273	M1N	O3-C2-N1	-5.12	112.90	122.93
3	V	273	M1N	C14-N9-C7	-5.07	103.85	122.03
3	R	273	M1N	C14-N9-C7	-5.07	103.86	122.03
3	E	273	M1N	C14-N9-C7	-5.05	103.92	122.03
3	P	273	M1N	C5-C4-N6	-4.94	100.47	110.80
3	C	273	M1N	C14-N9-C7	-4.93	104.33	122.03
3	E	273	M1N	O3-C2-N1	-4.89	113.36	122.93
3	J	273	M1N	C14-N9-C7	-4.82	104.73	122.03
3	X	273	M1N	O3-C2-N1	-4.80	113.53	122.93
3	H	273	M1N	C14-N9-C7	-4.77	104.91	122.03
3	L	273	M1N	C14-N9-C7	-4.69	105.23	122.03
3	L	273	M1N	O3-C2-N1	-4.66	113.79	122.93
3	2	273	M1N	C14-N9-C7	-4.66	105.31	122.03
3	Z	273	M1N	O3-C2-N1	-4.57	113.98	122.93
3	R	273	M1N	O3-C2-N1	-4.47	114.17	122.93
3	T	273	M1N	O3-C2-N1	-4.39	114.33	122.93
3	Z	273	M1N	C14-N9-C7	-4.26	106.74	122.03
3	R	273	M1N	O3-C2-C4	-4.14	111.22	120.36
3	L	273	M1N	O3-C2-C4	-3.99	111.55	120.36
3	G	273	M1N	O3-C2-C4	-3.73	112.11	120.36
3	H	273	M1N	O3-C2-C4	-3.60	112.40	120.36
3	T	273	M1N	O3-C2-C4	-3.38	112.88	120.36
3	V	273	M1N	C5-C4-N6	-3.29	103.91	110.80
3	C	273	M1N	C5-C4-N6	-3.24	104.02	110.80
3	C	273	M1N	O3-C2-C4	-3.18	113.32	120.36
3	P	273	M1N	O3-C2-C4	-3.16	113.37	120.36
3	Z	273	M1N	O3-C2-C4	-3.09	113.52	120.36
3	E	273	M1N	C5-C4-N6	-3.08	104.36	110.80
3	Z	273	M1N	B-C15-C22	-3.02	104.96	112.79
3	X	273	M1N	O3-C2-C4	-3.01	113.70	120.36
3	2	273	M1N	O8-C7-N6	-2.99	115.19	123.20
3	Z	273	M1N	C11-C10-N9	-2.93	103.62	109.90
3	N	273	M1N	O3-C2-C4	-2.83	114.09	120.36
3	H	273	M1N	C5-C4-N6	-2.75	105.03	110.80
3	V	273	M1N	B-C15-C22	-2.75	105.65	112.79
3	X	273	M1N	B-C15-C22	-2.74	105.67	112.79
3	J	273	M1N	C5-C4-N6	-2.72	105.10	110.80
3	N	273	M1N	C11-C10-N9	-2.68	104.15	109.90
3	L	273	M1N	C40-C33-C34	-2.65	116.95	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	273	M1N	O12-C13-C14	-2.63	105.80	111.84
3	2	273	M1N	O3-C2-C4	-2.62	114.57	120.36
3	R	273	M1N	C10-N9-C7	-2.60	112.71	122.03
3	N	273	M1N	C40-C33-C34	-2.58	117.12	123.22
3	J	273	M1N	O3-C2-C4	-2.58	114.66	120.36
3	E	273	M1N	C10-N9-C7	-2.56	112.86	122.03
3	N	273	M1N	C5-C4-N6	-2.55	105.46	110.80
3	N	273	M1N	B-C15-C22	-2.53	106.23	112.79
3	2	273	M1N	C10-N9-C7	-2.44	113.27	122.03
3	E	273	M1N	O3-C2-C4	-2.43	114.99	120.36
3	H	273	M1N	C10-N9-C7	-2.41	113.39	122.03
3	L	273	M1N	C10-N9-C7	-2.34	113.62	122.03
3	V	273	M1N	C40-C33-C34	-2.33	117.72	123.22
3	P	273	M1N	C40-C33-C34	-2.32	117.73	123.22
3	C	273	M1N	C40-C33-C34	-2.32	117.73	123.22
3	J	273	M1N	C40-C33-C34	-2.27	117.86	123.22
3	T	273	M1N	C40-C33-C34	-2.24	117.92	123.22
3	2	273	M1N	B-C15-C22	-2.23	107.01	112.79
3	H	273	M1N	C40-C33-C34	-2.22	117.98	123.22
3	2	273	M1N	C40-C33-C34	-2.17	118.09	123.22
3	T	273	M1N	C10-N9-C7	-2.17	114.25	122.03
3	X	273	M1N	C10-N9-C7	-2.16	114.27	122.03
3	Z	273	M1N	C5-C4-N6	-2.13	106.33	110.80
3	L	273	M1N	C11-C10-N9	-2.13	105.33	109.90
3	T	273	M1N	C11-C10-N9	-2.12	105.36	109.90
3	T	273	M1N	O12-C13-C14	-2.11	107.00	111.84
3	E	273	M1N	C11-C10-N9	-2.11	105.38	109.90
3	C	273	M1N	C10-N9-C7	-2.11	114.46	122.03
3	E	273	M1N	C40-C33-C34	-2.11	118.24	123.22
3	V	273	M1N	C10-N9-C7	-2.10	114.51	122.03
3	X	273	M1N	C40-C33-C34	-2.08	118.29	123.22
3	G	273	M1N	C11-C10-N9	-2.07	105.46	109.90
3	G	273	M1N	C40-C33-C34	-2.06	118.36	123.22
3	J	273	M1N	C11-C10-N9	-2.06	105.50	109.90
3	N	273	M1N	O12-C13-C14	-2.03	107.18	111.84
3	C	273	M1N	B-C15-C22	-2.03	107.51	112.79
3	P	273	M1N	C11-C10-N9	-2.02	105.58	109.90
3	J	273	M1N	C11-O12-C13	2.02	116.70	109.89
3	2	273	M1N	C40-C33-C32	2.03	121.86	119.10
3	V	273	M1N	C10-N9-C14	2.05	116.37	112.56
3	2	273	M1N	C2-C4-N6	2.11	117.22	111.26
3	E	273	M1N	C10-N9-C14	2.15	116.53	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	273	M1N	C11-O12-C13	2.16	117.17	109.89
3	G	273	M1N	C11-O12-C13	2.25	117.45	109.89
3	Z	273	M1N	C2-C4-N6	2.25	117.60	111.26
3	C	273	M1N	C2-C4-N6	2.25	117.61	111.26
3	L	273	M1N	C11-O12-C13	2.26	117.52	109.89
3	X	273	M1N	C40-C33-C32	2.27	122.18	119.10
3	X	273	M1N	C2-C4-N6	2.27	117.67	111.26
3	E	273	M1N	C40-C33-C32	2.28	122.20	119.10
3	R	273	M1N	C11-O12-C13	2.29	117.59	109.89
3	C	273	M1N	C11-O12-C13	2.30	117.65	109.89
3	P	273	M1N	C10-N9-C14	2.34	116.90	112.56
3	N	273	M1N	C10-N9-C14	2.36	116.94	112.56
3	E	273	M1N	C2-C4-N6	2.39	117.99	111.26
3	V	273	M1N	C40-C33-C32	2.48	122.47	119.10
3	R	273	M1N	C10-N9-C14	2.48	117.17	112.56
3	Z	273	M1N	C10-N9-C14	2.51	117.21	112.56
3	V	273	M1N	C11-O12-C13	2.52	118.38	109.89
3	H	273	M1N	C10-N9-C14	2.52	117.24	112.56
3	C	273	M1N	C10-N9-C14	2.54	117.27	112.56
3	C	273	M1N	C40-C33-C32	2.56	122.58	119.10
3	T	273	M1N	C40-C33-C32	2.57	122.59	119.10
3	J	273	M1N	C40-C33-C32	2.60	122.63	119.10
3	N	273	M1N	C4-N6-C7	2.63	126.54	120.69
3	T	273	M1N	C10-N9-C14	2.66	117.50	112.56
3	E	273	M1N	C11-O12-C13	2.68	118.91	109.89
3	L	273	M1N	C10-N9-C14	2.70	117.56	112.56
3	P	273	M1N	C40-C33-C32	2.72	122.79	119.10
3	X	273	M1N	C11-O12-C13	2.76	119.17	109.89
3	E	273	M1N	C4-N6-C7	2.81	126.95	120.69
3	T	273	M1N	C4-N6-C7	2.89	127.14	120.69
3	Z	273	M1N	C11-O12-C13	2.90	119.64	109.89
3	L	273	M1N	C40-C33-C32	2.92	123.06	119.10
3	G	273	M1N	C10-N9-C14	2.92	117.98	112.56
3	H	273	M1N	C11-O12-C13	2.95	119.81	109.89
3	N	273	M1N	C40-C33-C32	3.10	123.31	119.10
3	G	273	M1N	C4-N6-C7	3.18	127.78	120.69
3	V	273	M1N	C4-N6-C7	3.37	128.20	120.69
3	X	273	M1N	C4-N6-C7	3.43	128.32	120.69
3	R	273	M1N	C4-N6-C7	3.50	128.49	120.69
3	P	273	M1N	C4-N6-C7	3.68	128.90	120.69
3	X	273	M1N	C10-N9-C14	3.85	119.69	112.56
3	L	273	M1N	C4-N6-C7	3.89	129.34	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	273	M1N	C4-N6-C7	4.05	129.71	120.69
3	J	273	M1N	C10-N9-C14	4.16	120.27	112.56
3	Z	273	M1N	C4-N6-C7	4.42	130.53	120.69
3	C	273	M1N	C4-N6-C7	4.44	130.57	120.69
3	2	273	M1N	C4-N6-C7	6.05	134.17	120.69
3	E	273	M1N	C4-C2-N1	6.43	131.60	116.78
3	G	273	M1N	N6-C7-N9	6.44	131.39	117.43
3	N	273	M1N	N6-C7-N9	6.57	131.68	117.43
3	Z	273	M1N	C4-C2-N1	6.77	132.40	116.78
3	X	273	M1N	C4-C2-N1	6.92	132.74	116.78
3	T	273	M1N	C4-C2-N1	6.93	132.76	116.78
3	T	273	M1N	N6-C7-N9	7.02	132.66	117.43
3	J	273	M1N	C4-C2-N1	7.05	133.03	116.78
3	V	273	M1N	C4-C2-N1	7.08	133.10	116.78
3	J	273	M1N	N6-C7-N9	7.15	132.94	117.43
3	N	273	M1N	C4-C2-N1	7.51	134.09	116.78
3	V	273	M1N	N6-C7-N9	7.69	134.10	117.43
3	R	273	M1N	C4-C2-N1	7.73	134.60	116.78
3	L	273	M1N	C4-C2-N1	7.75	134.65	116.78
3	H	273	M1N	C4-C2-N1	7.75	134.65	116.78
3	X	273	M1N	N6-C7-N9	7.83	134.41	117.43
3	P	273	M1N	N6-C7-N9	7.83	134.42	117.43
3	P	273	M1N	C4-C2-N1	7.85	134.88	116.78
3	R	273	M1N	N6-C7-N9	7.85	134.46	117.43
3	C	273	M1N	C4-C2-N1	7.88	134.95	116.78
3	2	273	M1N	C4-C2-N1	8.02	135.27	116.78
3	Z	273	M1N	N6-C7-N9	8.06	134.92	117.43
3	G	273	M1N	C4-C2-N1	8.13	135.53	116.78
3	C	273	M1N	N6-C7-N9	8.27	135.37	117.43
3	E	273	M1N	N6-C7-N9	8.33	135.50	117.43
3	H	273	M1N	N6-C7-N9	8.37	135.59	117.43
3	L	273	M1N	N6-C7-N9	8.59	136.07	117.43
3	2	273	M1N	N6-C7-N9	9.55	138.14	117.43

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	V	273	M1N	O3-C2-N1-C15
3	J	273	M1N	C32-C31-C5-C4
3	R	273	M1N	C32-C31-C5-C4
3	P	273	M1N	O8-C7-N6-C4

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Mol	Chain	Res	Type	Atoms
3	E	273	M1N	O8-C7-N6-C4
3	2	273	M1N	O8-C7-N6-C4
3	Z	273	M1N	O8-C7-N6-C4
3	P	273	M1N	N9-C7-N6-C4
3	X	273	M1N	O8-C7-N6-C4
3	2	273	M1N	N9-C7-N6-C4
3	T	273	M1N	O8-C7-N6-C4
3	V	273	M1N	O8-C7-N6-C4
3	C	273	M1N	O8-C7-N6-C4
3	H	273	M1N	O8-C7-N6-C4
3	E	273	M1N	N9-C7-N6-C4
3	Z	273	M1N	N9-C7-N6-C4
3	J	273	M1N	O8-C7-N6-C4
3	L	273	M1N	O8-C7-N6-C4
3	X	273	M1N	N9-C7-N6-C4
3	V	273	M1N	N9-C7-N6-C4
3	T	273	M1N	N9-C7-N6-C4
3	C	273	M1N	N9-C7-N6-C4
3	H	273	M1N	N9-C7-N6-C4
3	N	273	M1N	O8-C7-N6-C4
3	G	273	M1N	O8-C7-N6-C4
3	L	273	M1N	N9-C7-N6-C4
3	J	273	M1N	N9-C7-N6-C4
3	R	273	M1N	O8-C7-N6-C4
3	N	273	M1N	N9-C7-N6-C4
3	G	273	M1N	N9-C7-N6-C4
3	R	273	M1N	N9-C7-N6-C4

There are no ring outliers.

14 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	273	M1N	9	0
3	C	273	M1N	12	0
3	E	273	M1N	14	0
3	G	273	M1N	10	0
3	H	273	M1N	12	0
3	J	273	M1N	17	0
3	L	273	M1N	16	0
3	N	273	M1N	16	0
3	P	273	M1N	14	0
3	R	273	M1N	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	273	M1N	11	0
3	V	273	M1N	17	0
3	X	273	M1N	14	0
3	Z	273	M1N	17	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	1	220/251 (87%)	1.35	57 (25%) 1 1	75, 100, 100, 100	0
1	A	220/251 (87%)	0.78	15 (6%) 20 7	74, 100, 100, 100	0
1	B	220/251 (87%)	1.00	29 (13%) 4 2	74, 100, 100, 100	0
1	D	220/251 (87%)	1.13	44 (20%) 1 1	74, 100, 100, 100	0
1	F	220/251 (87%)	1.10	37 (16%) 2 1	74, 100, 100, 100	0
1	I	220/251 (87%)	1.03	30 (13%) 4 1	74, 100, 100, 100	0
1	K	220/251 (87%)	1.40	47 (21%) 1 1	74, 100, 100, 100	0
1	M	220/251 (87%)	1.05	35 (15%) 3 1	74, 100, 100, 100	0
1	O	220/251 (87%)	1.36	54 (24%) 1 1	74, 100, 100, 100	0
1	Q	220/251 (87%)	1.46	66 (30%) 1 0	74, 100, 100, 100	0
1	S	220/251 (87%)	1.18	43 (19%) 1 1	74, 100, 100, 100	0
1	U	220/251 (87%)	1.24	49 (22%) 1 1	74, 100, 100, 100	0
1	W	220/251 (87%)	1.20	46 (20%) 1 1	74, 100, 100, 100	0
1	Y	220/251 (87%)	1.71	83 (37%) 0 0	74, 100, 100, 100	0
2	2	222/240 (92%)	0.50	16 (7%) 18 7	52, 72, 91, 100	0
2	C	222/240 (92%)	0.59	2 (0%) 85 64	53, 72, 91, 100	0
2	E	222/240 (92%)	0.47	7 (3%) 51 23	52, 72, 92, 100	0
2	G	222/240 (92%)	0.38	7 (3%) 51 23	52, 72, 91, 100	0
2	H	222/240 (92%)	0.56	3 (1%) 78 51	52, 72, 91, 100	0
2	J	222/240 (92%)	0.44	7 (3%) 51 23	53, 72, 92, 100	0
2	L	222/240 (92%)	0.48	2 (0%) 85 64	53, 72, 92, 100	0
2	N	222/240 (92%)	0.40	5 (2%) 64 33	52, 72, 91, 100	0
2	P	222/240 (92%)	0.42	4 (1%) 71 43	53, 72, 91, 100	0
2	R	222/240 (92%)	0.48	13 (5%) 26 10	53, 72, 92, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	222/240 (92%)	0.52	12 (5%) 29 11	53, 72, 92, 100	0
2	V	222/240 (92%)	0.44	4 (1%) 71 43	53, 72, 92, 100	0
2	X	222/240 (92%)	0.53	15 (6%) 20 7	53, 72, 91, 100	0
2	Z	222/240 (92%)	0.43	6 (2%) 58 28	53, 72, 92, 100	0
All	All	6188/6874 (90%)	0.84	738 (11%) 6 2	52, 88, 100, 100	0

All (738) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	235	VAL	21.4
1	K	236	ASP	19.8
1	S	235	VAL	17.6
1	M	236	ASP	14.9
1	W	235	VAL	14.8
1	1	235	VAL	14.8
1	W	236	ASP	14.8
1	F	236	ASP	12.9
1	U	236	ASP	12.8
1	1	236	ASP	11.9
1	I	235	VAL	11.7
1	M	235	VAL	11.6
1	A	235	VAL	11.3
1	I	237	GLN	11.1
1	M	237	GLN	11.0
1	Q	235	VAL	10.8
1	U	237	GLN	10.7
1	I	236	ASP	10.2
1	S	234	LEU	10.0
1	U	235	VAL	10.0
1	I	203	LEU	9.8
1	Q	236	ASP	9.6
1	O	237	GLN	9.6
1	S	236	ASP	9.5
1	B	235	VAL	9.5
1	U	192	SER	9.2
2	2	414	PRO	9.2
1	D	236	ASP	9.1
1	O	33	LEU	9.1
1	A	237	GLN	8.9
1	O	236	ASP	8.6
1	1	188	LEU	8.5

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Mol	Chain	Res	Type	RSRZ
1	Q	237	GLN	8.5
1	K	237	GLN	8.2
1	F	167	LEU	8.1
1	B	236	ASP	8.0
1	F	177	LEU	7.8
1	S	237	GLN	7.2
1	Y	237	GLN	7.1
1	Q	234	LEU	7.1
1	F	237	GLN	7.0
1	D	188	LEU	7.0
1	Y	188	LEU	6.9
1	K	191	GLY	6.8
1	I	234	LEU	6.8
1	K	13	MET	6.7
1	Q	191	GLY	6.7
1	K	167	LEU	6.6
1	B	237	GLN	6.6
1	1	227	GLY	6.5
1	A	177	LEU	6.5
1	K	234	LEU	6.4
1	I	204	GLY	6.4
1	O	230	LEU	6.3
1	F	235	VAL	6.2
1	1	205	VAL	6.2
1	M	172	ALA	6.2
1	A	236	ASP	6.1
1	O	188	LEU	6.0
1	Q	230	LEU	6.0
1	Q	118	TYR	6.0
1	Q	177	LEU	6.0
1	Y	177	LEU	5.9
1	U	232	ALA	5.9
1	O	172	ALA	5.9
1	K	177	LEU	5.8
1	Y	235	VAL	5.8
1	B	192	SER	5.8
1	Q	33	LEU	5.7
1	Y	171	TYR	5.7
1	M	192	SER	5.7
1	K	111	PHE	5.6
1	Q	192	SER	5.6
1	O	191	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	W	228	SER	5.6
1	Y	230	LEU	5.6
1	1	237	GLN	5.5
1	1	234	LEU	5.5
1	S	19	LEU	5.5
1	D	237	GLN	5.4
1	D	235	VAL	5.4
1	M	182	ARG	5.4
1	Y	10	GLU	5.4
1	D	170	SER	5.4
1	U	234	LEU	5.4
1	D	111	PHE	5.4
1	D	177	LEU	5.3
1	O	232	ALA	5.3
1	U	230	LEU	5.3
1	O	177	LEU	5.3
1	1	115	ALA	5.3
1	Y	156	MET	5.2
1	S	204	GLY	5.2
1	Y	236	ASP	5.2
1	Y	9	PRO	5.2
1	K	172	ALA	5.2
1	K	185	VAL	5.2
1	Q	163	ILE	5.2
1	Y	192	SER	5.1
1	U	111	PHE	5.1
2	2	407	TYR	5.1
1	Y	213	LEU	5.1
1	1	9	PRO	5.0
1	D	171	TYR	5.0
1	B	205	VAL	5.0
1	Y	39	VAL	5.0
2	X	407	TYR	4.9
1	Q	171	TYR	4.9
1	D	191	GLY	4.9
1	Y	167	LEU	4.9
1	Y	31	VAL	4.9
1	Q	9	PRO	4.9
1	K	181	LEU	4.8
1	S	9	PRO	4.8
1	1	177	LEU	4.8
1	Q	232	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	O	235	VAL	4.8
1	M	8	SER	4.8
1	O	234	LEU	4.8
1	W	229	ALA	4.7
2	Z	417	ALA	4.7
1	Y	122	LEU	4.7
1	K	127	VAL	4.7
1	Y	34	ALA	4.7
1	1	225	ILE	4.7
1	U	171	TYR	4.6
1	O	169	GLU	4.6
1	S	192	SER	4.6
1	Q	190	ALA	4.6
1	Y	204	GLY	4.6
1	B	191	GLY	4.6
1	1	172	ALA	4.6
1	B	153	PHE	4.6
1	Y	233	LEU	4.6
1	O	185	VAL	4.5
1	O	138	LEU	4.5
1	U	191	GLY	4.5
1	1	191	GLY	4.5
1	F	171	TYR	4.5
1	O	192	SER	4.5
1	Y	210	VAL	4.5
1	Q	188	LEU	4.5
1	Y	160	THR	4.5
1	Y	38	GLY	4.5
1	W	163	ILE	4.5
1	K	33	LEU	4.5
1	K	34	ALA	4.5
1	D	203	LEU	4.5
1	O	225	ILE	4.4
1	1	40	LEU	4.4
1	K	171	TYR	4.4
1	M	9	PRO	4.4
1	M	177	LEU	4.4
1	K	204	GLY	4.4
1	U	169	GLU	4.4
1	M	189	ARG	4.4
1	B	171	TYR	4.3
1	Y	172	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	T	340	TYR	4.3
1	Y	176	SER	4.3
1	K	143	TYR	4.3
1	M	171	TYR	4.3
1	I	171	TYR	4.3
1	Y	42	VAL	4.3
1	Q	155	VAL	4.3
1	Y	182	ARG	4.2
1	U	177	LEU	4.2
1	S	151	PRO	4.2
2	R	460	GLY	4.2
1	U	181	LEU	4.2
1	I	233	LEU	4.2
1	W	167	LEU	4.2
1	M	204	GLY	4.2
1	S	203	LEU	4.2
1	F	164	ALA	4.1
1	S	13	MET	4.1
1	U	33	LEU	4.1
1	I	135	ARG	4.1
1	S	205	VAL	4.1
1	M	234	LEU	4.1
1	W	237	GLN	4.1
1	U	40	LEU	4.1
1	U	205	VAL	4.0
1	Y	41	PHE	4.0
1	B	167	LEU	4.0
1	Q	220	ARG	4.0
1	K	203	LEU	4.0
1	Y	40	LEU	4.0
1	F	191	GLY	4.0
1	Y	155	VAL	4.0
1	D	36	ALA	4.0
1	Y	208	LEU	4.0
1	M	170	SER	3.9
1	Q	182	ARG	3.9
1	S	135	ARG	3.9
1	Q	225	ILE	3.9
1	O	152	HIS	3.9
1	W	188	LEU	3.9
1	M	178	THR	3.9
1	I	35	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
2	N	417	ALA	3.9
1	U	188	LEU	3.9
1	Y	180	ALA	3.9
1	K	205	VAL	3.9
1	I	230	LEU	3.9
1	D	234	LEU	3.8
1	D	163	ILE	3.8
1	Q	233	LEU	3.8
1	S	175	ALA	3.8
1	F	233	LEU	3.8
1	W	177	LEU	3.8
1	S	114	GLN	3.8
1	O	155	VAL	3.7
1	K	159	THR	3.7
1	D	33	LEU	3.7
1	Y	33	LEU	3.7
1	B	163	ILE	3.7
1	S	172	ALA	3.7
1	I	192	SER	3.7
1	M	13	MET	3.6
2	R	308	TYR	3.6
1	O	181	LEU	3.6
1	D	30	VAL	3.6
1	Y	136	PRO	3.6
1	Y	205	VAL	3.6
1	O	233	LEU	3.6
1	K	114	GLN	3.6
1	I	39	VAL	3.6
1	Y	175	ALA	3.6
1	Y	67	LYS	3.6
1	I	44	GLU	3.6
1	Q	169	GLU	3.6
1	O	160	THR	3.6
1	S	40	LEU	3.6
2	V	510	ILE	3.6
1	F	188	LEU	3.6
1	M	183	ILE	3.6
1	I	9	PRO	3.6
1	Q	186	ALA	3.6
1	O	167	LEU	3.6
1	Y	212	VAL	3.6
1	I	153	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	173	GLU	3.5
1	K	186	ALA	3.5
1	1	117	PRO	3.5
2	C	417	ALA	3.5
1	1	182	ARG	3.5
1	1	33	LEU	3.5
1	D	155	VAL	3.5
1	S	177	LEU	3.5
1	Q	135	ARG	3.5
2	T	486	LEU	3.5
1	W	10	GLU	3.5
1	1	204	GLY	3.5
1	I	172	ALA	3.5
1	Q	187	ALA	3.5
1	Y	13	MET	3.5
1	U	213	LEU	3.5
1	O	179	ASP	3.5
1	S	8	SER	3.4
1	A	169	GLU	3.4
1	U	143	TYR	3.4
1	F	176	SER	3.4
1	I	177	LEU	3.4
1	Y	234	LEU	3.4
1	Y	185	VAL	3.4
1	U	225	ILE	3.4
1	Y	179	ASP	3.4
1	S	224	ARG	3.4
1	O	178	THR	3.4
1	Y	132	GLU	3.4
1	K	115	ALA	3.4
1	W	36	ALA	3.4
1	1	186	ALA	3.4
1	S	138	LEU	3.4
1	Y	225	ILE	3.4
1	K	180	ALA	3.4
1	W	165	ASN	3.4
1	D	31	VAL	3.4
1	O	111	PHE	3.4
1	M	167	LEU	3.4
1	Y	170	SER	3.3
1	Q	167	LEU	3.3
1	B	170	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	172	ALA	3.3
1	U	53	ILE	3.3
1	F	40	LEU	3.3
1	U	138	LEU	3.3
1	1	167	LEU	3.3
1	1	192	SER	3.3
1	Q	189	ARG	3.3
2	L	417	ALA	3.3
1	1	10	GLU	3.3
1	M	185	VAL	3.3
1	S	12	ALA	3.3
1	Q	130	TYR	3.3
1	M	10	GLU	3.3
1	Y	218	PRO	3.3
2	X	491	PHE	3.2
1	S	182	ARG	3.2
1	W	16	ARG	3.2
1	O	205	VAL	3.2
1	D	227	GLY	3.2
1	U	172	ALA	3.2
1	W	191	GLY	3.2
2	2	415	GLN	3.2
1	U	208	LEU	3.2
1	Y	226	THR	3.2
1	B	155	VAL	3.2
1	O	180	ALA	3.2
2	T	464	LEU	3.2
1	Y	178	THR	3.2
1	B	156	MET	3.2
2	2	464	LEU	3.2
1	M	111	PHE	3.2
1	F	13	MET	3.2
1	Y	223	ARG	3.2
1	F	8	SER	3.2
1	Q	205	VAL	3.2
1	Y	211	ALA	3.2
1	O	204	GLY	3.1
1	1	163	ILE	3.1
1	U	203	LEU	3.1
1	Q	36	ALA	3.1
1	K	10	GLU	3.1
1	B	43	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	174	ASN	3.1
2	R	415	GLN	3.1
1	Q	173	GLU	3.1
1	W	169	GLU	3.1
1	I	118	TYR	3.1
1	A	163	ILE	3.0
1	A	188	LEU	3.0
1	S	131	GLY	3.0
1	D	118	TYR	3.0
1	K	214	ASP	3.0
1	M	190	ALA	3.0
1	Q	164	ALA	3.0
1	I	13	MET	3.0
1	Q	181	LEU	3.0
1	F	189	ARG	3.0
1	I	159	THR	3.0
1	Y	174	ASN	3.0
1	I	113	GLU	3.0
1	Y	154	VAL	3.0
1	D	169	GLU	3.0
1	U	186	ALA	3.0
1	F	11	GLN	3.0
1	I	10	GLU	3.0
1	O	208	LEU	3.0
1	W	44	GLU	3.0
1	W	203	LEU	3.0
1	S	191	GLY	3.0
2	2	463	GLY	3.0
1	K	178	THR	3.0
2	T	519	GLU	3.0
1	F	203	LEU	3.0
1	A	111	PHE	3.0
1	Y	159	THR	3.0
2	2	343	THR	3.0
1	Q	218	PRO	3.0
1	I	164	ALA	3.0
1	Q	231	GLN	3.0
1	O	223	ARG	3.0
2	R	306	LEU	3.0
1	K	153	PHE	3.0
1	O	42	VAL	2.9
1	D	135	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	U	233	LEU	2.9
1	Y	68	PHE	2.9
1	Y	153	PHE	2.9
1	I	175	ALA	2.9
1	I	205	VAL	2.9
1	K	138	LEU	2.9
1	Y	140	ARG	2.9
2	V	464	LEU	2.9
1	I	157	GLY	2.9
1	1	179	ASP	2.9
1	F	190	ALA	2.9
1	Y	186	ALA	2.9
1	D	192	SER	2.9
2	T	414	PRO	2.9
2	J	464	LEU	2.9
1	S	111	PHE	2.9
1	U	153	PHE	2.9
1	Y	163	ILE	2.9
1	M	138	LEU	2.9
1	Q	34	ALA	2.9
1	W	9	PRO	2.9
1	Y	181	LEU	2.9
1	Q	160	THR	2.9
1	Y	36	ALA	2.9
1	Q	224	ARG	2.9
1	1	65	ALA	2.9
2	R	340	TYR	2.8
1	Y	135	ARG	2.8
1	W	13	MET	2.8
1	U	189	ARG	2.8
1	D	13	MET	2.8
1	O	16	ARG	2.8
2	T	497	ILE	2.8
2	T	460	GLY	2.8
1	1	180	ALA	2.8
1	F	226	THR	2.8
1	Y	143	TYR	2.8
1	O	125	ALA	2.8
2	N	426	ALA	2.8
1	Q	42	VAL	2.8
1	1	16	ARG	2.8
1	Q	185	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	Q	178	THR	2.8
1	W	187	ALA	2.8
1	I	13	MET	2.8
1	1	169	GLU	2.8
2	2	398	LEU	2.8
1	I	185	VAL	2.8
2	J	455	SER	2.7
2	Z	460	GLY	2.7
1	W	123	CYS	2.7
1	1	187	ALA	2.7
1	D	179	ASP	2.7
1	1	203	LEU	2.7
1	Y	216	ASN	2.7
1	D	190	ALA	2.7
1	O	189	ARG	2.7
1	I	170	SER	2.7
1	M	153	PHE	2.7
1	Q	41	PHE	2.7
1	K	231	GLN	2.7
1	U	36	ALA	2.7
1	1	231	GLN	2.7
1	Y	209	GLU	2.7
1	F	192	SER	2.7
1	Y	54	SER	2.7
1	O	186	ALA	2.7
2	X	511	ALA	2.7
1	U	204	GLY	2.7
1	I	129	HIS	2.7
1	Y	173	GLU	2.7
1	Y	221	ALA	2.7
2	T	415	GLN	2.7
1	K	40	LEU	2.7
1	1	213	LEU	2.7
1	W	132	GLU	2.7
1	F	114	GLN	2.7
1	O	34	ALA	2.7
2	X	514	ALA	2.7
1	B	189	ARG	2.7
2	X	340	TYR	2.7
2	Z	519	GLU	2.7
2	2	409	ILE	2.7
1	D	34	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	39	VAL	2.6
1	O	62	PHE	2.6
1	D	172	ALA	2.6
1	Q	223	ARG	2.6
1	I	41	PHE	2.6
1	S	167	LEU	2.6
1	U	180	ALA	2.6
1	O	31	VAL	2.6
1	M	33	LEU	2.6
1	W	40	LEU	2.6
1	O	171	TYR	2.6
1	A	34	ALA	2.6
2	R	498	ASP	2.6
1	D	153	PHE	2.6
1	K	117	PRO	2.6
1	O	36	ALA	2.6
1	Q	229	ALA	2.6
1	Y	130	TYR	2.6
1	U	185	VAL	2.6
1	O	213	LEU	2.6
1	Y	203	LEU	2.6
1	D	141	ILE	2.6
1	K	65	ALA	2.6
1	Q	10	GLU	2.6
1	D	39	VAL	2.6
1	I	226	THR	2.6
1	Y	131	GLY	2.6
2	X	510	ILE	2.6
2	G	487	VAL	2.6
1	F	138	LEU	2.6
1	S	112	THR	2.6
1	U	170	SER	2.6
1	Q	166	ALA	2.6
1	I	233	LEU	2.5
1	I	189	ARG	2.5
2	2	491	PHE	2.5
1	S	10	GLU	2.5
1	S	123	CYS	2.5
1	W	170	SER	2.5
2	H	407	TYR	2.5
1	Q	153	PHE	2.5
2	2	521	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	36	ALA	2.5
1	F	178	THR	2.5
1	M	175	ALA	2.5
1	Y	164	ALA	2.5
1	W	133	THR	2.5
1	B	234	LEU	2.5
2	R	407	TYR	2.5
1	K	123	CYS	2.5
1	Y	53	ILE	2.5
1	U	13	MET	2.5
1	O	170	SER	2.5
1	W	30	VAL	2.5
1	W	233	LEU	2.5
2	E	407	TYR	2.5
2	G	407	TYR	2.5
1	B	232	ALA	2.5
1	1	34	ALA	2.5
1	U	16	ARG	2.5
1	M	155	VAL	2.5
1	I	40	LEU	2.5
1	1	19	LEU	2.5
1	B	111	PHE	2.5
2	E	522	SER	2.4
1	O	173	GLU	2.4
1	F	232	ALA	2.4
1	Q	53	ILE	2.4
1	I	189	ARG	2.4
1	Y	219	ARG	2.4
1	I	15	GLU	2.4
1	Q	213	LEU	2.4
1	Y	123	CYS	2.4
2	T	407	TYR	2.4
1	K	116	LYS	2.4
1	W	209	GLU	2.4
1	I	180	ALA	2.4
1	Q	151	PRO	2.4
1	S	118	TYR	2.4
1	U	182	ARG	2.4
1	F	162	PRO	2.4
1	W	192	SER	2.4
1	1	36	ALA	2.4
2	T	506	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	X	417	ALA	2.4
2	2	417	ALA	2.4
2	X	521	ARG	2.4
1	D	184	ALA	2.4
1	F	180	ALA	2.4
2	R	411	ALA	2.4
1	A	191	GLY	2.4
1	Q	204	GLY	2.4
1	Y	66	GLY	2.4
1	M	205	VAL	2.4
1	Y	127	VAL	2.4
1	I	230	LEU	2.4
1	K	182	ARG	2.4
1	Y	215	ALA	2.4
1	S	174	ASN	2.4
2	G	489	GLY	2.4
1	D	50	LEU	2.4
2	X	518	ILE	2.4
1	F	111	PHE	2.4
1	F	130	TYR	2.4
1	O	140	ARG	2.4
1	U	42	VAL	2.4
1	M	233	LEU	2.4
2	X	399	LEU	2.4
1	S	187	ALA	2.4
1	W	166	ALA	2.4
1	Q	183	ILE	2.4
1	A	165	ASN	2.4
1	D	212	VAL	2.4
1	K	42	VAL	2.4
1	S	42	VAL	2.4
1	D	40	LEU	2.3
1	W	138	LEU	2.3
1	F	156	MET	2.3
1	B	128	ALA	2.3
1	F	169	GLU	2.3
1	U	132	GLU	2.3
1	K	162	PRO	2.3
1	D	205	VAL	2.3
1	W	226	THR	2.3
1	M	139	TYR	2.3
1	Q	165	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	Y	138	LEU	2.3
1	U	227	GLY	2.3
2	X	464	LEU	2.3
1	D	133	THR	2.3
1	B	177	LEU	2.3
1	S	190	ALA	2.3
2	X	517	ILE	2.3
1	1	111	PHE	2.3
2	N	376	PHE	2.3
1	U	210	VAL	2.3
1	M	203	LEU	2.3
2	N	396	GLN	2.3
2	X	453	LEU	2.3
1	O	176	SER	2.3
2	Z	491	PHE	2.3
1	1	173	GLU	2.3
1	O	114	GLN	2.3
1	W	223	ARG	2.3
1	1	37	GLY	2.3
1	W	172	ALA	2.3
2	R	497	ILE	2.3
1	O	210	VAL	2.3
1	U	122	LEU	2.3
2	2	499	ALA	2.3
1	S	225	ILE	2.3
2	2	433	GLU	2.3
1	B	181	LEU	2.3
1	U	37	GLY	2.3
1	B	34	ALA	2.2
1	D	232	ALA	2.2
1	M	113	GLU	2.2
1	W	219	ARG	2.2
1	I	178	THR	2.2
1	1	11	GLN	2.2
2	2	378	GLY	2.2
1	Q	179	ASP	2.2
1	M	221	ALA	2.2
1	Y	183	ILE	2.2
2	G	340	TYR	2.2
2	G	430	ASN	2.2
2	J	409	ILE	2.2
2	N	496	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	168	LYS	2.2
1	U	127	VAL	2.2
1	O	231	GLN	2.2
2	R	315	ALA	2.2
1	Q	210	VAL	2.2
1	W	131	GLY	2.2
1	K	11	GLN	2.2
2	R	465	ARG	2.2
1	B	143	TYR	2.2
1	W	21	ARG	2.2
2	E	457	VAL	2.2
2	T	468	VAL	2.2
2	V	457	VAL	2.2
1	A	234	LEU	2.2
2	G	306	LEU	2.2
1	Q	111	PHE	2.2
1	O	135	ARG	2.2
2	P	407	TYR	2.2
1	U	19	LEU	2.2
1	U	114	GLN	2.2
1	1	175	ALA	2.2
1	A	48	ARG	2.2
1	I	159	THR	2.2
1	1	223	ARG	2.2
1	S	37	GLY	2.2
2	2	406	GLY	2.2
1	K	192	SER	2.2
1	Q	11	GLN	2.2
2	E	430	ASN	2.2
2	V	430	ASN	2.2
1	Q	184	ALA	2.2
2	J	417	ALA	2.2
1	W	41	PHE	2.2
1	S	216	ASN	2.2
2	C	306	LEU	2.2
1	B	41	PHE	2.2
1	A	40	LEU	2.2
1	B	33	LEU	2.2
1	K	135	ARG	2.2
1	Q	13	MET	2.2
1	S	230	LEU	2.2
1	1	107	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	184	ALA	2.2
1	O	157	GLY	2.1
2	J	306	LEU	2.1
1	W	35	TYR	2.1
2	P	430	ASN	2.1
1	Q	37	GLY	2.1
1	U	224	ARG	2.1
2	T	490	ILE	2.1
1	O	40	LEU	2.1
1	F	166	ALA	2.1
1	D	15	GLU	2.1
1	U	150	GLU	2.1
1	I	62	PHE	2.1
1	M	16	ARG	2.1
2	J	326	ILE	2.1
1	Q	172	ALA	2.1
1	F	170	SER	2.1
1	Y	37	GLY	2.1
2	J	496	ILE	2.1
1	B	190	ALA	2.1
1	Q	16	ARG	2.1
2	P	519	GLU	2.1
1	B	226	THR	2.1
2	E	337	THR	2.1
1	F	165	ASN	2.1
1	S	130	TYR	2.1
1	W	204	GLY	2.1
1	W	227	GLY	2.1
2	R	310	GLY	2.1
2	H	443	SER	2.1
1	Q	219	ARG	2.1
1	B	169	GLU	2.1
1	A	172	ALA	2.1
1	O	190	ALA	2.1
1	F	48	ARG	2.1
1	Y	224	ARG	2.1
1	K	9	PRO	2.1
1	O	127	VAL	2.1
1	D	165	ASN	2.1
2	Z	510	ILE	2.1
1	S	148	ALA	2.1
1	S	180	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	41	PHE	2.1
2	Z	521	ARG	2.1
1	S	132	GLU	2.1
1	D	117	PRO	2.1
1	W	117	PRO	2.1
1	D	189	ARG	2.1
2	2	400	ALA	2.1
1	K	41	PHE	2.0
2	E	415	GLN	2.0
2	E	412	SER	2.0
2	L	463	GLY	2.0
1	D	168	LYS	2.0
1	F	16	ARG	2.0
1	I	118	TYR	2.0
1	W	11	GLN	2.0
1	W	178	THR	2.0
1	Y	231	GLN	2.0
1	D	230	LEU	2.0
1	I	123	CYS	2.0
1	Q	208	LEU	2.0
1	W	212	VAL	2.0
1	B	162	PRO	2.0
1	Q	162	PRO	2.0
1	Y	44	GLU	2.0
2	H	413	ASP	2.0
2	G	497	ILE	2.0
2	X	497	ILE	2.0
1	U	167	LEU	2.0
1	W	130	TYR	2.0
1	K	215	ALA	2.0
1	O	61	GLY	2.0
2	P	355	PHE	2.0
2	R	519	GLU	2.0
2	X	433	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	M1N	2	273	32/32	0.84	0.30	2.63	65,76,78,79	0
3	M1N	T	273	32/32	0.85	0.30	2.08	64,77,78,79	0
3	M1N	V	273	32/32	0.85	0.30	2.02	65,76,78,78	0
3	M1N	J	273	32/32	0.86	0.31	1.77	64,76,77,78	0
3	M1N	X	273	32/32	0.87	0.31	1.64	65,76,78,79	0
3	M1N	R	273	32/32	0.90	0.24	1.22	64,76,78,78	0
3	M1N	E	273	32/32	0.88	0.26	1.16	63,76,78,78	0
3	M1N	Z	273	32/32	0.88	0.24	1.03	66,76,78,78	0
3	M1N	P	273	32/32	0.85	0.25	0.99	65,76,78,79	0
3	M1N	H	273	32/32	0.91	0.25	0.61	64,75,77,78	0
3	M1N	N	273	32/32	0.91	0.24	0.50	65,76,77,78	0
3	M1N	L	273	32/32	0.91	0.24	0.30	65,75,77,78	0
3	M1N	C	273	32/32	0.90	0.24	-0.04	63,75,77,78	0
3	M1N	G	273	32/32	0.89	0.21	-0.25	64,75,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.