



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 08:43 AM EDT

PDB ID : 4DW2  
Title : The crystal structure of uPA in complex with the Fab fragment of mAb-112  
Authors : Jiang, L.; Botkjaer, K.A.; Andersen, L.M.; Yuan, C.; Andreasen, P.A.; Huang, M.  
Deposited on : 2012-02-24  
Resolution : 2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

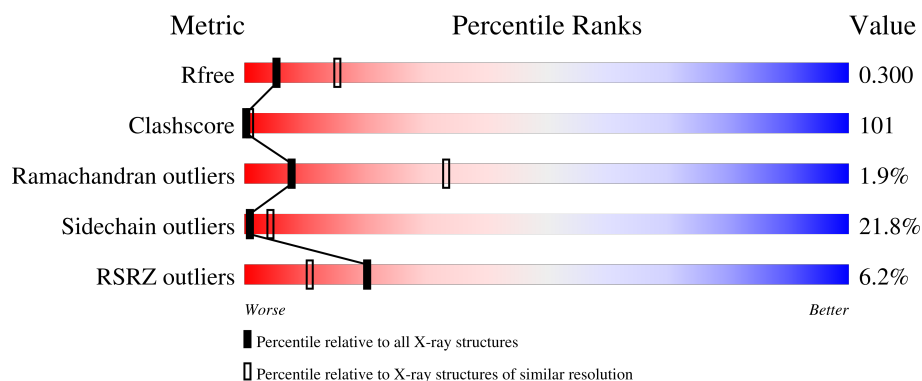
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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

Mol	Chain	Length	Quality of chain
1	U	246	
2	H	212	
3	L	215	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5022 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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	221	Total	C	N	O	S	0	0	0
			1763	1121	304	325	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	122	ALA	CYS	ENGINEERED MUTATION	UNP P00749
U	145	GLN	ASN	ENGINEERED MUTATION	UNP P00749

- Molecule 2 is a protein called Fab fragment of pro-uPA antibody mAb-112.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1596	1007	265	315	9			

- Molecule 3 is a protein called Fab fragment of pro-uPA antibody mAb-112.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1648	1026	275	339	8			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	S	0	0
			5	4	1		

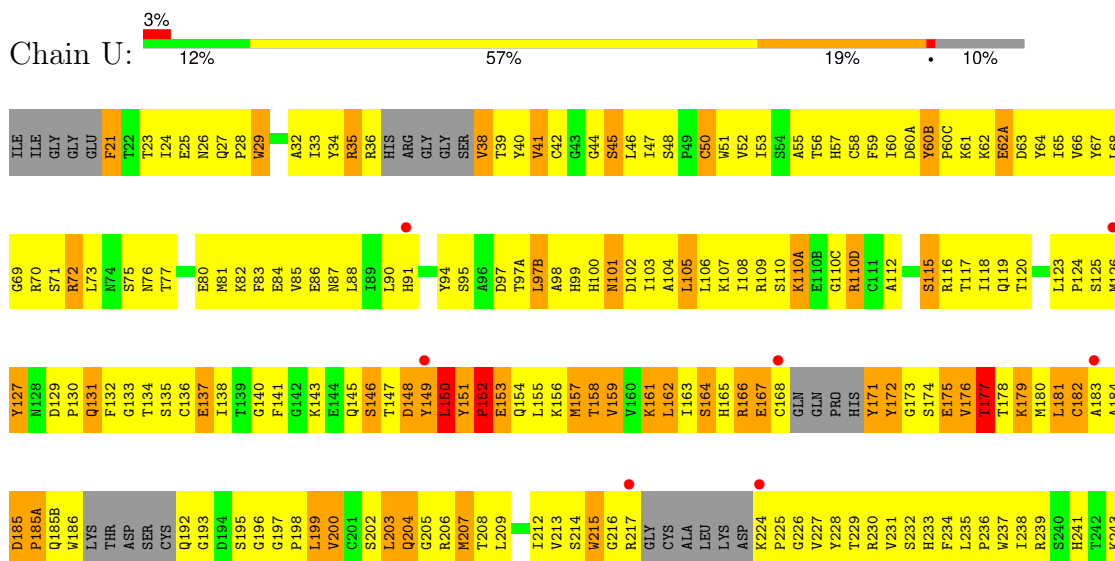
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	U	2	Total	O	0	0
			2	2		
5	H	4	Total	O	0	0
			4	4		
5	L	4	Total	O	0	0
			4	4		

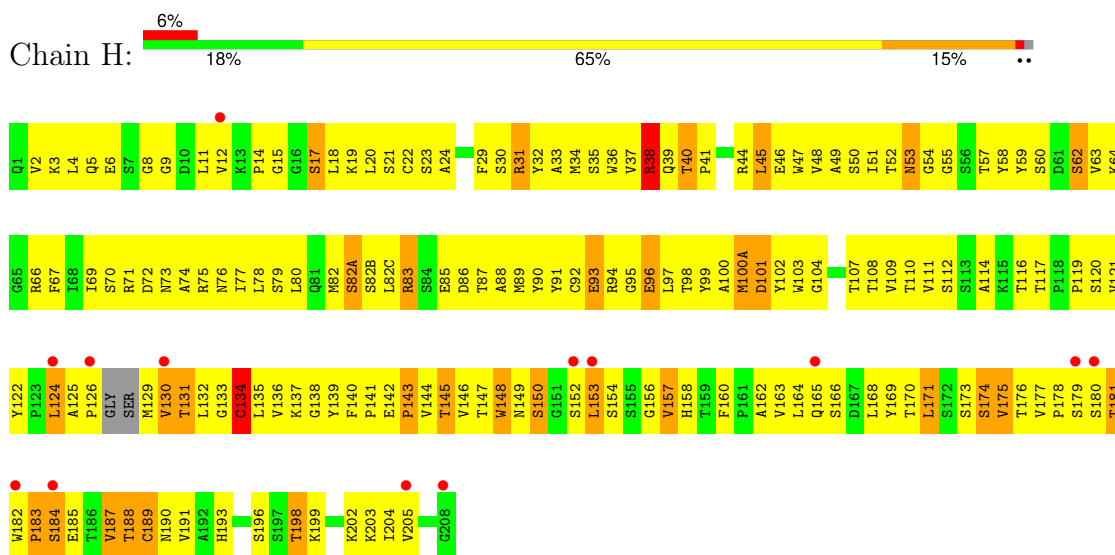
### 3 Residue-property plots

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

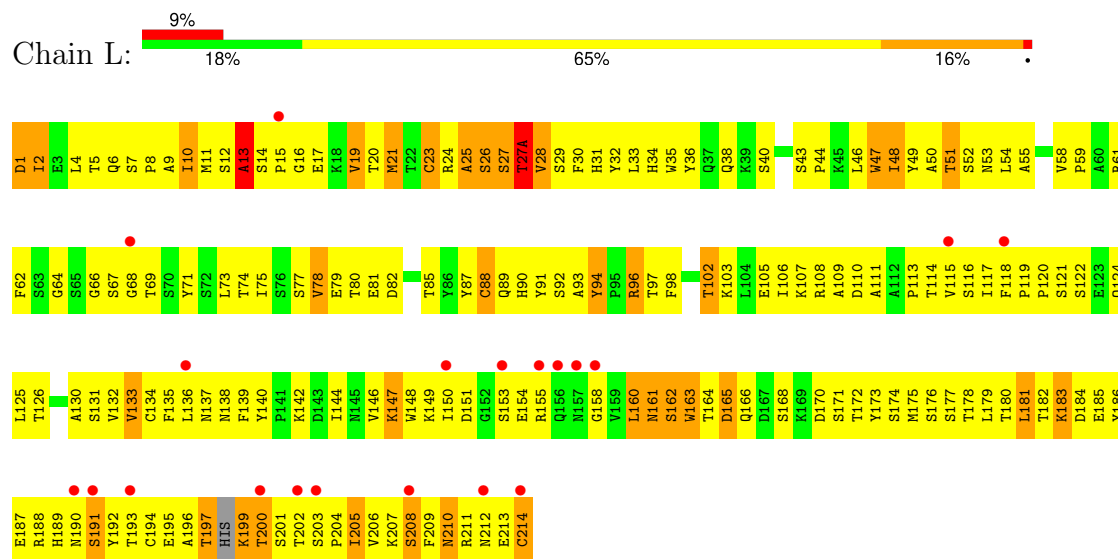
- Molecule 1: Urokinase-type plasminogen activator



- Molecule 2: Fab fragment of pro-uPA antibody mAb-112



- Molecule 3: Fab fragment of pro-uPA antibody mAb-112



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.96Å 94.95Å 154.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.93 – 2.97 45.33 – 2.97	Depositor EDS
% Data completeness (in resolution range)	90.8 (80.93-2.97) 90.9 (45.33-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.240 , 0.300 0.242 , 0.300	Depositor DCC
$R_{free}$ test set	557 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	U	0.87	0/1805	0.95	3/2442 (0.1%)
2	H	0.76	3/1633 (0.2%)	0.84	2/2222 (0.1%)
3	L	0.77	1/1687 (0.1%)	0.85	1/2290 (0.0%)
All	All	0.80	4/5125 (0.1%)	0.89	6/6954 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1
3	L	0	3
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	82(A)	SER	C-N	6.37	1.48	1.34
3	L	88	CYS	CB-SG	-5.89	1.72	1.81
2	H	148	TRP	CD2-CE2	5.17	1.47	1.41
2	H	38	ARG	C-N	-5.09	1.22	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	23	CYS	CA-CB-SG	-6.08	103.06	114.00
1	U	150	LEU	CA-CB-CG	5.54	128.04	115.30
2	H	134	CYS	CA-CB-SG	-5.50	104.10	114.00
2	H	130	VAL	CB-CA-C	-5.49	100.96	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	50	CYS	CA-CB-SG	-5.05	104.91	114.00
1	U	185	ASP	C-N-CD	-5.02	109.55	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	13	ALA	Peptide
3	L	25	ALA	Peptide
3	L	26	SER	Peptide
1	U	150	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1763	0	1721	386	1
2	H	1596	0	1576	315	0
3	L	1648	0	1565	360	1
4	L	5	0	0	0	0
5	H	4	0	0	1	0
5	L	4	0	0	0	0
5	U	2	0	0	0	0
All	All	5022	0	4862	1001	2

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 101.

All (1001) 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:H:94:ARG:NE	2:H:101:ASP:OD2	1.69	1.25
2:H:39:GLN:OE1	3:L:38:GLN:NE2	1.67	1.25
1:U:150:LEU:C	1:U:152:PRO:HA	1.61	1.19
1:U:150:LEU:O	1:U:152:PRO:HA	1.44	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:177:THR:O	1:U:178:THR:HG22	1.46	1.15
3:L:2:ILE:HD13	3:L:27:SER:HB2	1.15	1.14
2:H:94:ARG:CZ	2:H:101:ASP:OD2	1.98	1.12
3:L:190:ASN:O	3:L:210:ASN:HA	1.50	1.11
2:H:38:ARG:HD3	2:H:48:VAL:HG22	1.26	1.10
3:L:52:SER:HA	3:L:64:GLY:HA3	1.29	1.09
1:U:36:ARG:HB3	1:U:65:ILE:HD11	1.27	1.08
3:L:185:GLU:HA	3:L:188:ARG:HD3	1.35	1.07
3:L:51:THR:HG22	3:L:52:SER:N	1.63	1.06
1:U:110(A):LYS:HD2	1:U:110(A):LYS:N	1.69	1.06
1:U:109:ARG:HE	1:U:110(C):GLY:HA2	1.11	1.05
1:U:98:ALA:HB2	1:U:215:TRP:CZ2	1.91	1.05
2:H:94:ARG:NH2	2:H:101:ASP:OD2	1.89	1.05
1:U:204:GLN:OE1	1:U:204:GLN:HA	1.56	1.04
1:U:35:ARG:NH2	1:U:60(B):TYR:CG	2.25	1.03
3:L:181:LEU:HD13	3:L:185:GLU:HG2	1.34	1.02
1:U:192:GLN:HG2	1:U:217:ARG:HB3	1.41	1.02
1:U:84:GLU:HG3	1:U:110(A):LYS:NZ	1.74	1.02
3:L:27(A):THR:H	3:L:69:THR:HG22	1.22	1.01
3:L:59:PRO:HG2	3:L:62:PHE:HE1	1.24	1.01
3:L:14:SER:O	3:L:17:GLU:HB2	1.58	1.01
2:H:11:LEU:HB2	2:H:141:PRO:HG3	1.40	1.01
1:U:84:GLU:HG3	1:U:110(A):LYS:HZ2	1.25	1.01
1:U:172:TYR:CE1	1:U:215:TRP:CZ3	2.48	1.00
3:L:13:ALA:HA	3:L:107:LYS:HB2	1.41	1.00
3:L:2:ILE:HD12	3:L:26:SER:O	1.60	1.00
1:U:192:GLN:OE1	1:U:217:ARG:HD2	1.61	0.99
1:U:171:TYR:O	1:U:172:TYR:O	1.79	0.99
3:L:13:ALA:HA	3:L:107:LYS:CB	1.94	0.98
1:U:35:ARG:NH2	1:U:60(B):TYR:CD2	2.32	0.97
3:L:52:SER:HB2	3:L:64:GLY:O	1.64	0.97
1:U:200:VAL:HG12	1:U:200:VAL:O	1.61	0.97
1:U:109:ARG:NE	1:U:110(C):GLY:HA2	1.79	0.97
2:H:178:PRO:O	2:H:181:THR:OG1	1.82	0.97
3:L:2:ILE:CD1	3:L:26:SER:O	2.12	0.96
3:L:49:TYR:O	3:L:53:ASN:HB2	1.65	0.96
1:U:127:TYR:CE1	1:U:230:ARG:NH1	2.31	0.96
1:U:172:TYR:CD1	1:U:215:TRP:CZ3	2.53	0.96
1:U:138:ILE:HD11	1:U:192:GLN:HG3	1.47	0.96
2:H:132:LEU:HD13	2:H:204:ILE:HG21	1.46	0.95
1:U:159:VAL:O	1:U:185:ASP:OD2	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:50:ALA:O	3:L:51:THR:HB	1.66	0.94
1:U:172:TYR:HB3	1:U:175:GLU:HG2	1.51	0.93
2:H:87:THR:HG23	2:H:110:THR:HA	1.47	0.93
3:L:2:ILE:HD13	3:L:27:SER:CB	1.99	0.93
1:U:230:ARG:NH2	1:U:233:HIS:HB2	1.83	0.93
1:U:98:ALA:CB	1:U:215:TRP:CZ2	2.51	0.93
2:H:144:VAL:HG12	2:H:193:HIS:HD2	1.32	0.92
2:H:59:TYR:HE2	2:H:69:ILE:H	1.12	0.92
1:U:151:TYR:N	1:U:152:PRO:HA	1.77	0.92
1:U:177:THR:OG1	1:U:180:MET:SD	2.28	0.92
3:L:2:ILE:HG23	3:L:2:ILE:O	1.69	0.91
3:L:151:ASP:OD2	3:L:189:HIS:ND1	2.03	0.91
1:U:110(A):LYS:N	1:U:110(A):LYS:CD	2.32	0.91
3:L:59:PRO:HG2	3:L:62:PHE:CE1	2.06	0.90
3:L:213:GLU:O	3:L:214:CYS:HB2	1.68	0.90
3:L:211:ARG:HB3	3:L:211:ARG:NH1	1.87	0.90
3:L:2:ILE:HG23	3:L:93:ALA:HA	1.51	0.90
1:U:150:LEU:O	1:U:152:PRO:CA	2.19	0.89
2:H:51:ILE:HG13	2:H:57:THR:HG22	1.54	0.89
2:H:39:GLN:CD	3:L:38:GLN:HE22	1.74	0.89
1:U:36:ARG:HB3	1:U:65:ILE:CD1	2.03	0.89
2:H:160:PHE:HB3	3:L:162:SER:HB3	1.56	0.88
3:L:96:ARG:HH11	3:L:96:ARG:HG2	1.36	0.88
1:U:152:PRO:HG2	1:U:152:PRO:O	1.71	0.88
2:H:142:GLU:HG3	2:H:143:PRO:HB3	1.54	0.88
2:H:182:TRP:CZ2	2:H:204:ILE:HG22	2.09	0.88
3:L:48:ILE:HG21	3:L:51:THR:O	1.73	0.87
3:L:51:THR:CG2	3:L:52:SER:N	2.33	0.87
1:U:123:LEU:HB3	1:U:124:PRO:HD2	1.55	0.87
2:H:99:TYR:O	2:H:100:ALA:HB3	1.74	0.87
3:L:52:SER:HA	3:L:64:GLY:CA	2.05	0.86
3:L:68:GLY:O	3:L:71:TYR:HE1	1.58	0.86
2:H:182:TRP:CD1	2:H:183:PRO:HA	2.10	0.86
3:L:15:PRO:HA	3:L:78:VAL:O	1.75	0.86
2:H:93:GLU:HB3	2:H:100(A):MET:HG2	1.57	0.86
2:H:130:VAL:O	2:H:130:VAL:HG13	1.76	0.85
2:H:47:TRP:CD2	2:H:97:LEU:HD11	2.11	0.85
2:H:144:VAL:HG12	2:H:193:HIS:CD2	2.11	0.85
3:L:211:ARG:NH1	3:L:211:ARG:CB	2.39	0.85
1:U:23:THR:HB	3:L:30:PHE:HE2	1.41	0.85
1:U:172:TYR:CD1	1:U:215:TRP:HZ3	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.56	0.85
3:L:4:LEU:HD13	3:L:88:CYS:HB3	1.58	0.85
3:L:190:ASN:O	3:L:210:ASN:CA	2.24	0.85
3:L:211:ARG:HB3	3:L:211:ARG:CZ	2.07	0.84
1:U:109:ARG:HE	1:U:110(C):GLY:CA	1.89	0.84
1:U:127:TYR:HE1	1:U:230:ARG:HH12	1.22	0.84
1:U:151:TYR:CZ	1:U:153:GLU:OE1	2.31	0.84
1:U:185(B):GLN:HG2	1:U:186:TRP:N	1.90	0.84
3:L:15:PRO:HA	3:L:78:VAL:HG22	1.60	0.84
2:H:38:ARG:NH1	2:H:90:TYR:OH	2.09	0.84
3:L:187:GLU:OE2	3:L:211:ARG:HD3	1.78	0.84
1:U:72:ARG:HE	1:U:153:GLU:HB3	1.41	0.83
1:U:177:THR:C	1:U:179:LYS:H	1.79	0.83
1:U:192:GLN:CG	1:U:217:ARG:HB3	2.07	0.83
3:L:186:TYR:O	3:L:192:TYR:OH	1.95	0.83
1:U:155:LEU:O	3:L:31:HIS:NE2	2.12	0.83
1:U:164:SER:N	1:U:167:GLU:OE1	2.11	0.83
3:L:68:GLY:O	3:L:71:TYR:CE1	2.31	0.82
1:U:172:TYR:HB3	1:U:175:GLU:CG	2.09	0.82
1:U:109:ARG:HG2	1:U:110:SER:O	1.80	0.81
2:H:2:VAL:HG22	2:H:2:VAL:O	1.80	0.81
2:H:3:LYS:HG2	2:H:5:GLN:NE2	1.95	0.81
2:H:178:PRO:N	2:H:181:THR:OG1	2.14	0.81
2:H:60:SER:HB3	2:H:62:SER:OG	1.80	0.81
2:H:119:PRO:CA	2:H:139:TYR:HB3	2.11	0.81
2:H:40:THR:HG22	2:H:41:PRO:HD2	1.61	0.80
2:H:93:GLU:CB	2:H:100(A):MET:HG2	2.11	0.80
2:H:182:TRP:CG	2:H:183:PRO:HA	2.17	0.80
1:U:67:TYR:O	1:U:68:LEU:HD23	1.82	0.80
1:U:177:THR:OG1	1:U:180:MET:CE	2.30	0.80
1:U:145:GLN:N	1:U:145:GLN:OE1	2.14	0.80
1:U:177:THR:O	1:U:178:THR:CG2	2.29	0.80
1:U:72:ARG:NH1	1:U:75:SER:OG	2.15	0.80
1:U:172:TYR:CB	1:U:175:GLU:OE1	2.29	0.80
2:H:136:VAL:HG23	2:H:139:TYR:HD2	1.47	0.79
3:L:146:VAL:HA	3:L:195:GLU:O	1.81	0.79
2:H:154:SER:O	2:H:157:VAL:HG12	1.83	0.79
1:U:157:MET:H	3:L:31:HIS:CE1	2.01	0.79
1:U:38:VAL:CG1	1:U:38:VAL:O	2.31	0.78
1:U:83:PHE:CZ	1:U:112:ALA:HB2	2.18	0.78
3:L:52:SER:CB	3:L:64:GLY:O	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:78:VAL:HG23	3:L:106:ILE:HD12	1.64	0.78
2:H:89:MET:SD	2:H:108:THR:OG1	2.41	0.78
3:L:2:ILE:CD1	3:L:27:SER:HB2	2.08	0.78
1:U:203:LEU:HB2	1:U:208:THR:OG1	1.84	0.77
1:U:60(C):PRO:O	1:U:88:LEU:HD23	1.85	0.77
3:L:2:ILE:HG21	3:L:92:SER:O	1.84	0.77
1:U:28:PRO:HG2	1:U:119:GLN:HB2	1.65	0.77
2:H:177:VAL:HB	2:H:181:THR:CB	2.15	0.77
2:H:53:ASN:HD22	2:H:53:ASN:N	1.80	0.77
2:H:130:VAL:O	2:H:130:VAL:CG1	2.33	0.77
3:L:62:PHE:CD2	3:L:75:ILE:HG12	2.20	0.77
3:L:199:LYS:O	3:L:199:LYS:CD	2.33	0.76
1:U:181:LEU:O	1:U:228:TYR:N	2.14	0.76
3:L:28:VAL:O	3:L:71:TYR:OH	2.02	0.76
1:U:23:THR:HB	3:L:30:PHE:CE2	2.20	0.76
1:U:171:TYR:C	1:U:172:TYR:O	2.22	0.76
1:U:192:GLN:CD	1:U:217:ARG:HD2	2.05	0.76
2:H:133:GLY:HA2	2:H:173:SER:O	1.86	0.76
1:U:46:LEU:HD13	1:U:68:LEU:HD11	1.67	0.76
1:U:127:TYR:HE1	1:U:230:ARG:NH1	1.77	0.76
1:U:98:ALA:HA	1:U:215:TRP:CE2	2.21	0.76
2:H:142:GLU:HG3	2:H:143:PRO:CB	2.16	0.76
1:U:45:SER:OG	1:U:198:PRO:HB3	1.86	0.75
2:H:46:GLU:OE2	3:L:96:ARG:NH2	2.19	0.75
2:H:47:TRP:CE3	2:H:97:LEU:HD11	2.22	0.75
2:H:39:GLN:NE2	3:L:38:GLN:OE1	2.18	0.75
3:L:14:SER:O	3:L:17:GLU:CB	2.35	0.75
1:U:86:GLU:HB3	1:U:107:LYS:HG2	1.69	0.75
2:H:150:SER:HA	2:H:190:ASN:HD22	1.51	0.75
1:U:172:TYR:CE1	1:U:215:TRP:HZ3	2.03	0.75
3:L:49:TYR:O	3:L:50:ALA:HB3	1.87	0.75
3:L:122:SER:HA	3:L:125:LEU:HD12	1.67	0.75
3:L:184:ASP:O	3:L:187:GLU:N	2.19	0.75
1:U:21:PHE:HB3	3:L:53:ASN:OD1	1.87	0.75
3:L:29:SER:O	3:L:90:HIS:HE1	1.69	0.74
1:U:124:PRO:HA	1:U:208:THR:HG21	1.69	0.74
2:H:100:ALA:HA	3:L:36:TYR:OH	1.87	0.74
2:H:119:PRO:HB3	2:H:139:TYR:HB3	1.67	0.74
2:H:139:TYR:OH	2:H:162:ALA:HB2	1.86	0.74
3:L:78:VAL:CG2	3:L:106:ILE:HD12	2.17	0.74
1:U:60(B):TYR:CD1	1:U:60(B):TYR:N	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:177:VAL:HB	2:H:181:THR:HB	1.68	0.74
3:L:2:ILE:CG2	3:L:93:ALA:HA	2.17	0.74
3:L:134:CYS:N	3:L:177:SER:O	2.20	0.74
1:U:94:TYR:HA	1:U:100:HIS:O	1.87	0.74
1:U:164:SER:O	1:U:167:GLU:HB2	1.87	0.74
2:H:117:THR:HG22	2:H:138:GLY:O	1.86	0.74
2:H:117:THR:CG2	2:H:138:GLY:O	2.35	0.74
3:L:50:ALA:O	3:L:51:THR:CB	2.33	0.74
3:L:2:ILE:O	3:L:2:ILE:CG2	2.36	0.74
2:H:114:ALA:HB3	2:H:140:PHE:CE2	2.24	0.73
2:H:82(C):LEU:HB3	2:H:111:VAL:HG11	1.70	0.73
3:L:51:THR:HG22	3:L:52:SER:H	1.51	0.73
3:L:48:ILE:HA	3:L:53:ASN:O	1.88	0.73
1:U:65:ILE:HG21	1:U:82:LYS:HE3	1.70	0.73
1:U:149:TYR:HA	1:U:151:TYR:HB3	1.71	0.73
1:U:175:GLU:N	1:U:175:GLU:CD	2.42	0.73
2:H:132:LEU:N	2:H:175:VAL:O	2.17	0.73
2:H:53:ASN:HA	2:H:71:ARG:NH2	2.04	0.72
3:L:90:HIS:HD2	3:L:92:SER:H	1.35	0.72
3:L:210:ASN:N	3:L:210:ASN:ND2	2.32	0.72
3:L:29:SER:O	3:L:90:HIS:CE1	2.42	0.72
2:H:196:SER:OG	2:H:198:THR:OG1	2.08	0.72
1:U:115:SER:OG	1:U:117:THR:N	2.22	0.72
1:U:33:ILE:HG22	1:U:41:VAL:HG13	1.72	0.72
2:H:99:TYR:O	2:H:100:ALA:CB	2.38	0.72
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.20	0.72
2:H:35:SER:OG	2:H:96:GLU:HA	1.90	0.72
3:L:90:HIS:CD2	3:L:92:SER:HB2	2.24	0.72
3:L:211:ARG:CB	3:L:211:ARG:HH11	2.02	0.72
2:H:119:PRO:CB	2:H:139:TYR:HB3	2.20	0.72
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.72	0.71
1:U:151:TYR:N	1:U:152:PRO:CA	2.52	0.71
3:L:103:LYS:HE3	3:L:165:ASP:OD1	1.90	0.71
3:L:106:ILE:HB	3:L:166:GLN:HE22	1.55	0.71
1:U:172:TYR:HB3	1:U:175:GLU:CD	2.10	0.71
2:H:15:GLY:N	2:H:82(C):LEU:O	2.19	0.71
3:L:48:ILE:CG2	3:L:51:THR:O	2.39	0.71
2:H:2:VAL:O	2:H:2:VAL:CG2	2.38	0.71
3:L:166:GLN:HB2	3:L:173:TYR:CZ	2.25	0.71
1:U:57:HIS:CE1	1:U:195:SER:HB3	2.26	0.71
3:L:13:ALA:CB	3:L:17:GLU:OE2	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:173:GLY:C	1:U:175:GLU:OE2	2.29	0.70
2:H:19:LYS:HE2	2:H:79:SER:HB3	1.73	0.70
2:H:185:GLU:H	2:H:185:GLU:CD	1.94	0.70
3:L:160:LEU:HD12	3:L:178:THR:HB	1.71	0.70
2:H:183:PRO:O	2:H:184:SER:C	2.29	0.70
1:U:124:PRO:HA	1:U:208:THR:CG2	2.22	0.70
1:U:133:GLY:N	1:U:162:LEU:O	2.23	0.70
3:L:199:LYS:CD	3:L:199:LYS:C	2.59	0.70
1:U:123:LEU:HB3	1:U:124:PRO:CD	2.21	0.70
1:U:110:SER:OG	1:U:110(D):ARG:N	2.24	0.70
2:H:120:SER:HB3	2:H:122:TYR:CZ	2.26	0.70
3:L:116:SER:HB2	3:L:135:PHE:HB2	1.74	0.70
1:U:50:CYS:O	1:U:108:ILE:N	2.20	0.69
2:H:14:PRO:HD3	2:H:112:SER:C	2.12	0.69
1:U:172:TYR:HB2	1:U:175:GLU:OE1	1.92	0.69
1:U:184:ALA:HB2	1:U:225:PRO:HB3	1.73	0.69
2:H:29:PHE:CD2	2:H:76:ASN:HA	2.26	0.69
2:H:174:SER:OG	3:L:137:ASN:ND2	2.24	0.69
2:H:6:GLU:OE2	2:H:92:CYS:N	2.22	0.69
3:L:12:SER:HA	3:L:105:GLU:O	1.93	0.69
1:U:163:ILE:HD11	1:U:182:CYS:HB2	1.72	0.69
1:U:172:TYR:C	1:U:175:GLU:OE1	2.30	0.69
2:H:94:ARG:HH21	2:H:101:ASP:CG	1.95	0.69
3:L:62:PHE:HZ	3:L:82:ASP:OD1	1.76	0.69
1:U:138:ILE:CD1	1:U:192:GLN:HG3	2.22	0.69
1:U:148:ASP:HB3	2:H:99:TYR:CG	2.28	0.69
1:U:38:VAL:O	1:U:38:VAL:HG12	1.92	0.68
1:U:177:THR:C	1:U:179:LYS:N	2.46	0.68
1:U:151:TYR:CE1	1:U:153:GLU:OE1	2.46	0.68
1:U:131:GLN:O	1:U:134:THR:OG1	2.07	0.68
1:U:150:LEU:HD12	1:U:150:LEU:H	1.58	0.68
2:H:119:PRO:HA	2:H:139:TYR:HB3	1.74	0.68
3:L:108:ARG:HG2	3:L:140:TYR:CD2	2.29	0.68
2:H:136:VAL:HG23	2:H:139:TYR:CD2	2.29	0.68
2:H:136:VAL:CG2	2:H:139:TYR:CD2	2.77	0.68
2:H:66:ARG:NH2	2:H:86:ASP:OD1	2.22	0.68
3:L:107:LYS:HD2	3:L:140:TYR:OH	1.94	0.68
1:U:127:TYR:OH	1:U:233:HIS:ND1	2.26	0.68
2:H:48:VAL:HG12	2:H:63:VAL:HG21	1.76	0.68
3:L:13:ALA:HA	3:L:107:LYS:HB3	1.76	0.67
3:L:30:PHE:HB3	3:L:71:TYR:HE2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:LEU:O	3:L:51:THR:N	2.28	0.67
3:L:183:LYS:HG3	3:L:184:ASP:H	1.58	0.67
1:U:23:THR:HG21	3:L:31:HIS:NE2	2.10	0.67
3:L:211:ARG:HH11	3:L:211:ARG:HB2	1.59	0.67
2:H:53:ASN:ND2	2:H:54:GLY:H	1.93	0.67
3:L:161:ASN:HB3	3:L:175:MET:HE3	1.77	0.67
3:L:14:SER:N	3:L:17:GLU:OE2	2.27	0.67
1:U:46:LEU:HD13	1:U:68:LEU:CD1	2.24	0.66
3:L:27(A):THR:N	3:L:69:THR:HG22	2.04	0.66
3:L:163:TRP:CD1	3:L:175:MET:HG3	2.30	0.66
1:U:146:SER:OG	2:H:52:THR:HB	1.95	0.66
2:H:108:THR:HB	2:H:143:PRO:HD3	1.78	0.66
3:L:187:GLU:OE2	3:L:187:GLU:HA	1.96	0.66
1:U:36:ARG:HG2	1:U:63:ASP:O	1.95	0.66
3:L:117:ILE:HG13	3:L:209:PHE:HD2	1.60	0.66
1:U:99:HIS:O	1:U:180:MET:HE2	1.96	0.66
3:L:23:CYS:N	3:L:71:TYR:O	2.28	0.66
1:U:48:SER:OG	1:U:51:TRP:HB2	1.96	0.66
1:U:60(A):ASP:C	1:U:60(B):TYR:CD1	2.69	0.66
2:H:39:GLN:HB2	2:H:45:LEU:CD1	2.26	0.66
2:H:132:LEU:HD13	2:H:204:ILE:CG2	2.22	0.66
3:L:210:ASN:H	3:L:210:ASN:HD22	1.43	0.66
1:U:27:GLN:HA	1:U:29:TRP:CZ2	2.31	0.65
1:U:72:ARG:CZ	1:U:75:SER:OG	2.44	0.65
1:U:110(A):LYS:CD	1:U:110(A):LYS:H	2.08	0.65
1:U:152:PRO:O	1:U:153:GLU:C	2.33	0.65
1:U:173:GLY:N	1:U:175:GLU:OE1	2.29	0.65
1:U:174:SER:N	1:U:175:GLU:OE2	2.30	0.65
2:H:38:ARG:HD3	2:H:48:VAL:CG2	2.16	0.65
2:H:11:LEU:HD13	2:H:141:PRO:HB3	1.77	0.65
3:L:185:GLU:HA	3:L:188:ARG:CD	2.21	0.65
3:L:196:ALA:O	3:L:204:PRO:CB	2.44	0.65
3:L:199:LYS:O	3:L:199:LYS:HD3	1.97	0.65
2:H:131:THR:O	2:H:132:LEU:HD23	1.97	0.64
1:U:177:THR:O	1:U:179:LYS:N	2.30	0.64
2:H:30:SER:O	2:H:53:ASN:HB2	1.97	0.64
1:U:34:TYR:HB3	1:U:38:VAL:HG22	1.79	0.64
1:U:175:GLU:N	1:U:175:GLU:OE2	2.29	0.64
3:L:136:LEU:HD13	3:L:175:MET:HE2	1.79	0.64
2:H:94:ARG:HH21	2:H:101:ASP:CB	2.11	0.64
2:H:148:TRP:HB2	2:H:153:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:197:GLY:O	1:U:213:VAL:HG23	1.97	0.64
1:U:164:SER:OG	1:U:167:GLU:OE1	2.13	0.64
1:U:177:THR:OG1	1:U:180:MET:HE3	1.97	0.64
2:H:39:GLN:HB2	2:H:45:LEU:HD11	1.80	0.64
1:U:97(B):LEU:HG	1:U:215:TRP:CZ3	2.33	0.63
1:U:203:LEU:C	1:U:205:GLY:N	2.50	0.63
3:L:2:ILE:HD13	3:L:26:SER:O	1.98	0.63
2:H:158:HIS:CE1	3:L:174:SER:HG	2.16	0.63
3:L:90:HIS:CD2	3:L:92:SER:H	2.15	0.63
1:U:164:SER:O	1:U:167:GLU:CB	2.45	0.63
2:H:122:TYR:HB3	3:L:121:SER:OG	1.98	0.63
2:H:47:TRP:O	2:H:60:SER:HB2	1.99	0.63
2:H:83:ARG:HD2	2:H:85:GLU:OE1	1.98	0.63
2:H:51:ILE:HB	2:H:69:ILE:HD13	1.80	0.63
1:U:98:ALA:HB2	1:U:215:TRP:CH2	2.32	0.63
3:L:147:LYS:HG3	3:L:154:GLU:HG3	1.81	0.63
2:H:140:PHE:CD1	2:H:141:PRO:HA	2.34	0.63
3:L:1:ASP:OD1	3:L:1:ASP:N	2.32	0.63
1:U:53:ILE:HD11	1:U:103:ILE:HD11	1.80	0.62
3:L:13:ALA:HB1	3:L:17:GLU:OE2	1.98	0.62
1:U:72:ARG:NH2	1:U:153:GLU:OE1	2.32	0.62
1:U:141:PHE:CD1	1:U:153:GLU:O	2.52	0.62
2:H:139:TYR:CD1	2:H:139:TYR:O	2.52	0.62
1:U:60(C):PRO:O	1:U:88:LEU:CD2	2.47	0.62
1:U:146:SER:HB3	2:H:33:ALA:HB2	1.81	0.62
3:L:210:ASN:ND2	3:L:210:ASN:H	1.98	0.62
1:U:186:TRP:CH2	2:H:98:THR:HG21	2.35	0.62
1:U:60(A):ASP:HB3	1:U:60(B):TYR:CE1	2.34	0.62
2:H:60:SER:CB	2:H:62:SER:OG	2.48	0.62
1:U:175:GLU:CD	1:U:175:GLU:H	2.02	0.62
3:L:199:LYS:O	3:L:199:LYS:HD2	1.98	0.62
2:H:11:LEU:CD1	2:H:141:PRO:HB3	2.29	0.62
2:H:138:GLY:HA2	2:H:168:LEU:HB3	1.80	0.62
2:H:141:PRO:O	2:H:193:HIS:NE2	2.33	0.62
3:L:163:TRP:CE3	3:L:163:TRP:N	2.68	0.62
3:L:186:TYR:HA	3:L:192:TYR:OH	1.99	0.62
3:L:209:PHE:CD1	3:L:209:PHE:C	2.73	0.62
1:U:110:SER:HG	1:U:110(D):ARG:H	1.46	0.62
2:H:130:VAL:CG2	2:H:132:LEU:HD21	2.29	0.62
3:L:166:GLN:HE21	3:L:171:SER:HA	1.64	0.62
3:L:190:ASN:C	3:L:210:ASN:HB3	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:165:HIS:O	1:U:166:ARG:C	2.37	0.61
1:U:178:THR:HG23	1:U:178:THR:O	1.98	0.61
2:H:93:GLU:N	2:H:93:GLU:CD	2.53	0.61
3:L:24:ARG:NH2	3:L:26:SER:OG	2.34	0.61
2:H:93:GLU:HB3	2:H:100(A):MET:CG	2.30	0.61
3:L:197:THR:HG23	3:L:204:PRO:HB3	1.81	0.61
2:H:146:VAL:HG11	2:H:173:SER:CB	2.30	0.61
3:L:132:VAL:HG12	3:L:148:TRP:CH2	2.35	0.61
1:U:47:ILE:HG13	1:U:51:TRP:O	2.01	0.61
1:U:72:ARG:NE	1:U:153:GLU:CB	2.64	0.61
2:H:51:ILE:HG23	2:H:51:ILE:O	1.99	0.61
3:L:1:ASP:O	3:L:94:TYR:O	2.18	0.61
3:L:28:VAL:HG12	3:L:92:SER:HB2	1.81	0.61
3:L:187:GLU:OE2	3:L:211:ARG:CD	2.48	0.61
3:L:107:LYS:HA	3:L:140:TYR:OH	2.01	0.61
2:H:139:TYR:CE1	2:H:169:TYR:HB2	2.36	0.61
1:U:51:TRP:CH2	1:U:107:LYS:HB2	2.34	0.60
2:H:144:VAL:CG1	2:H:193:HIS:HD2	2.10	0.60
1:U:152:PRO:O	1:U:152:PRO:CG	2.36	0.60
2:H:34:MET:CB	2:H:78:LEU:HD22	2.30	0.60
1:U:27:GLN:HE22	3:L:30:PHE:HZ	1.47	0.60
2:H:53:ASN:HD22	2:H:54:GLY:H	1.48	0.60
2:H:119:PRO:HB3	2:H:139:TYR:CB	2.32	0.60
1:U:77:THR:O	1:U:80:GLU:HB3	2.01	0.60
1:U:115:SER:OG	1:U:116:ARG:N	2.35	0.60
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.82	0.60
2:H:142:GLU:HG3	2:H:143:PRO:CA	2.31	0.60
3:L:134:CYS:O	3:L:177:SER:N	2.31	0.60
1:U:150:LEU:H	1:U:150:LEU:CD1	2.13	0.60
2:H:87:THR:HA	2:H:109:VAL:O	2.01	0.60
2:H:146:VAL:HG11	2:H:173:SER:HB2	1.83	0.60
3:L:15:PRO:CA	3:L:78:VAL:O	2.49	0.60
1:U:51:TRP:CE3	1:U:105:LEU:HD22	2.37	0.60
2:H:60:SER:C	2:H:62:SER:N	2.54	0.60
3:L:124:GLN:HE22	3:L:131:SER:N	1.99	0.60
1:U:29:TRP:HA	1:U:119:GLN:O	2.02	0.60
1:U:72:ARG:HE	1:U:153:GLU:CB	2.11	0.60
2:H:30:SER:HA	2:H:73:ASN:ND2	2.17	0.60
1:U:72:ARG:HD2	1:U:75:SER:CB	2.32	0.59
1:U:124:PRO:HD2	1:U:235:LEU:HD21	1.84	0.59
2:H:101:ASP:HB2	2:H:102:TYR:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:55:ALA:HA	1:U:102:ASP:O	2.03	0.59
1:U:203:LEU:C	1:U:205:GLY:H	2.04	0.59
2:H:93:GLU:HG3	2:H:103:TRP:CE2	2.38	0.59
2:H:182:TRP:HA	2:H:183:PRO:C	2.22	0.59
1:U:41:VAL:HG22	1:U:42:CYS:HB2	1.84	0.59
1:U:84:GLU:N	1:U:109:ARG:O	2.36	0.59
3:L:16:GLY:HA2	3:L:77:SER:OG	2.02	0.59
1:U:86:GLU:OE2	1:U:107:LYS:HE2	2.03	0.59
1:U:172:TYR:HB3	1:U:175:GLU:OE1	2.01	0.59
2:H:31:ARG:HG3	2:H:31:ARG:NH1	2.17	0.59
2:H:47:TRP:CG	2:H:97:LEU:HD21	2.38	0.59
2:H:116:THR:CG2	2:H:196:SER:HB3	2.33	0.59
2:H:37:VAL:CG1	2:H:46:GLU:O	2.51	0.59
1:U:25:GLU:OE1	1:U:116:ARG:HD2	2.03	0.58
1:U:186:TRP:CZ2	2:H:98:THR:HG21	2.38	0.58
3:L:166:GLN:HE21	3:L:171:SER:CA	2.16	0.58
2:H:53:ASN:N	2:H:53:ASN:ND2	2.51	0.58
3:L:193:THR:OG1	3:L:208:SER:HB3	2.03	0.58
1:U:181:LEU:N	1:U:228:TYR:O	2.29	0.58
1:U:59:PHE:O	1:U:60(B):TYR:N	2.36	0.58
1:U:125:SER:O	1:U:126:MET:C	2.39	0.58
1:U:56:THR:HG23	1:U:90:LEU:HD13	1.86	0.58
2:H:116:THR:HG22	2:H:196:SER:HB3	1.85	0.58
1:U:72:ARG:HD3	1:U:73:LEU:N	2.19	0.58
1:U:172:TYR:CB	1:U:175:GLU:HG2	2.30	0.58
2:H:36:TRP:HE1	2:H:78:LEU:HG	1.68	0.58
1:U:67:TYR:CE2	1:U:70:ARG:NH1	2.72	0.57
1:U:70:ARG:HB2	1:U:80:GLU:HG3	1.86	0.57
1:U:233:HIS:O	1:U:236:PRO:HD2	2.04	0.57
2:H:114:ALA:HB3	2:H:140:PHE:HE2	1.69	0.57
2:H:35:SER:HA	2:H:50:SER:HA	1.87	0.57
3:L:155:ARG:NH1	3:L:185:GLU:OE1	2.37	0.57
2:H:164:LEU:HD21	2:H:169:TYR:CE1	2.39	0.57
3:L:9:ALA:O	3:L:102:THR:HA	2.04	0.57
1:U:44:GLY:O	1:U:198:PRO:HD3	2.04	0.57
1:U:50:CYS:O	1:U:108:ILE:HG12	2.05	0.57
1:U:72:ARG:NE	1:U:153:GLU:HB3	2.14	0.57
1:U:185(B):GLN:O	1:U:186:TRP:CG	2.57	0.57
3:L:90:HIS:HD2	3:L:92:SER:HB2	1.67	0.57
3:L:120:PRO:HD2	3:L:186:TYR:CZ	2.39	0.57
3:L:17:GLU:HB2	3:L:78:VAL:CG1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.39	0.57
1:U:185(B):GLN:CG	1:U:186:TRP:N	2.66	0.57
2:H:98:THR:HA	3:L:91:TYR:HB3	1.86	0.57
3:L:175:MET:CE	3:L:177:SER:HB2	2.35	0.57
1:U:137:GLU:OE1	1:U:200:VAL:HG11	2.05	0.57
1:U:185(B):GLN:O	1:U:186:TRP:CB	2.52	0.57
3:L:181:LEU:CD1	3:L:185:GLU:HG2	2.23	0.57
1:U:23:THR:O	1:U:26:ASN:O	2.23	0.56
1:U:172:TYR:HE1	1:U:215:TRP:CZ3	2.18	0.56
3:L:161:ASN:ND2	3:L:177:SER:OG	2.38	0.56
1:U:84:GLU:HG3	1:U:110(A):LYS:HZ1	1.63	0.56
1:U:150:LEU:HD12	1:U:150:LEU:N	2.20	0.56
2:H:82(C):LEU:HB3	2:H:111:VAL:CG1	2.34	0.56
3:L:142:LYS:HD2	3:L:173:TYR:CE1	2.40	0.56
1:U:47:ILE:HD11	1:U:51:TRP:CB	2.35	0.56
2:H:59:TYR:HE2	2:H:69:ILE:N	1.94	0.56
3:L:30:PHE:CB	3:L:71:TYR:HE2	2.17	0.56
1:U:47:ILE:HD11	1:U:51:TRP:HB2	1.87	0.56
1:U:179:LYS:HG2	1:U:233:HIS:CD2	2.40	0.56
1:U:181:LEU:HD22	1:U:230:ARG:HA	1.86	0.56
1:U:192:GLN:CD	1:U:217:ARG:HB3	2.26	0.56
2:H:93:GLU:HB3	2:H:100(A):MET:HB3	1.86	0.56
3:L:190:ASN:O	3:L:210:ASN:CB	2.52	0.56
1:U:175:GLU:CG	1:U:215:TRP:HH2	2.19	0.56
1:U:157:MET:N	3:L:31:HIS:ND1	2.52	0.56
1:U:184:ALA:HB2	1:U:225:PRO:CB	2.35	0.56
2:H:163:VAL:O	2:H:169:TYR:HA	2.06	0.56
3:L:62:PHE:HA	3:L:74:THR:O	2.06	0.56
3:L:117:ILE:HG13	3:L:209:PHE:CD2	2.40	0.56
1:U:35:ARG:O	1:U:38:VAL:HA	2.06	0.56
1:U:162:LEU:HD12	1:U:183:ALA:HB2	1.88	0.55
1:U:182:CYS:HA	1:U:226:GLY:O	2.06	0.55
2:H:149:ASN:HB2	2:H:152:SER:HB2	1.88	0.55
3:L:47:TRP:CD2	3:L:58:VAL:HG22	2.41	0.55
3:L:80:THR:HB	3:L:171:SER:OG	2.05	0.55
1:U:192:GLN:NE2	1:U:217:ARG:HG3	2.21	0.55
1:U:203:LEU:O	1:U:206:ARG:N	2.31	0.55
3:L:28:VAL:HG12	3:L:92:SER:CB	2.37	0.55
1:U:132:PHE:HB2	1:U:163:ILE:C	2.26	0.55
2:H:130:VAL:HG22	2:H:132:LEU:CD2	2.36	0.55
3:L:4:LEU:HD13	3:L:88:CYS:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:57:HIS:C	1:U:57:HIS:CD2	2.79	0.55
2:H:130:VAL:HG22	2:H:132:LEU:HD21	1.88	0.55
1:U:91:HIS:HD2	1:U:103:ILE:CG2	2.19	0.55
1:U:148:ASP:OD1	1:U:148:ASP:N	2.35	0.55
2:H:163:VAL:HG22	2:H:170:THR:O	2.07	0.55
2:H:178:PRO:HD2	2:H:181:THR:HG21	1.89	0.55
1:U:76:ASN:HA	1:U:80:GLU:OE1	2.07	0.55
1:U:183:ALA:HB3	1:U:228:TYR:CE1	2.41	0.55
2:H:31:ARG:HG3	2:H:31:ARG:HH11	1.71	0.55
3:L:51:THR:O	3:L:64:GLY:HA3	2.07	0.55
1:U:47:ILE:HG21	1:U:123:LEU:HD21	1.88	0.55
1:U:185(B):GLN:O	1:U:186:TRP:HB2	2.07	0.55
1:U:234:PHE:C	1:U:238:ILE:HD12	2.27	0.55
1:U:56:THR:CG2	1:U:90:LEU:HB3	2.37	0.55
3:L:51:THR:HG22	3:L:52:SER:HB3	1.88	0.55
3:L:149:LYS:O	3:L:193:THR:N	2.39	0.55
3:L:199:LYS:C	3:L:199:LYS:HD2	2.27	0.55
1:U:181:LEU:HB2	1:U:228:TYR:HB2	1.88	0.54
2:H:86:ASP:HB2	2:H:111:VAL:HG21	1.89	0.54
1:U:59:PHE:O	1:U:60:ILE:C	2.44	0.54
1:U:124:PRO:CA	1:U:208:THR:CG2	2.84	0.54
1:U:52:VAL:HG21	1:U:66:VAL:HG11	1.90	0.54
1:U:56:THR:HA	1:U:104:ALA:HB2	1.89	0.54
2:H:182:TRP:CD1	2:H:187:VAL:HG13	2.42	0.54
3:L:36:TYR:HE1	3:L:89:GLN:HB3	1.72	0.54
3:L:113:PRO:HB2	3:L:115:VAL:HG22	1.90	0.54
1:U:148:ASP:HB3	2:H:99:TYR:CB	2.38	0.54
3:L:27(A):THR:H	3:L:69:THR:CG2	2.09	0.54
3:L:85:THR:OG1	3:L:103:LYS:HG2	2.06	0.54
1:U:130:PRO:HB2	1:U:162:LEU:CD2	2.37	0.54
2:H:117:THR:O	2:H:139:TYR:HA	2.07	0.54
3:L:96:ARG:HG2	3:L:96:ARG:NH1	2.11	0.54
1:U:204:GLN:OE1	1:U:204:GLN:CA	2.41	0.54
2:H:93:GLU:HG3	2:H:103:TRP:CD2	2.43	0.54
3:L:47:TRP:CE3	3:L:58:VAL:HG22	2.43	0.54
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.34	0.54
2:H:53:ASN:ND2	2:H:54:GLY:N	2.55	0.54
3:L:132:VAL:HG12	3:L:148:TRP:HH2	1.73	0.54
3:L:136:LEU:O	3:L:175:MET:N	2.32	0.54
1:U:82:LYS:HG2	1:U:110(A):LYS:HE2	1.89	0.53
2:H:124:LEU:HB2	2:H:133:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:THR:C	2:H:132:LEU:HD23	2.27	0.53
3:L:132:VAL:HG13	3:L:209:PHE:HE2	1.73	0.53
3:L:62:PHE:CE2	3:L:75:ILE:HG12	2.44	0.53
3:L:96:ARG:HH11	3:L:96:ARG:CG	2.12	0.53
3:L:30:PHE:HB3	3:L:71:TYR:CE2	2.41	0.53
1:U:23:THR:OG1	3:L:31:HIS:CE1	2.61	0.53
2:H:139:TYR:CD1	2:H:139:TYR:C	2.82	0.53
2:H:184:SER:HB3	2:H:185:GLU:CD	2.29	0.53
3:L:8:PRO:HB2	3:L:10:ILE:O	2.09	0.53
3:L:201:SER:O	3:L:203:SER:O	2.27	0.53
3:L:149:LYS:N	3:L:193:THR:O	2.29	0.53
1:U:57:HIS:HE1	1:U:195:SER:HB3	1.72	0.53
1:U:83:PHE:CZ	1:U:112:ALA:CB	2.91	0.53
2:H:131:THR:HA	2:H:176:THR:HA	1.91	0.53
3:L:210:ASN:N	3:L:210:ASN:HD22	1.99	0.53
2:H:146:VAL:HG22	2:H:191:VAL:HG22	1.91	0.53
1:U:47:ILE:HG23	1:U:53:ILE:HG22	1.91	0.53
1:U:175:GLU:HG2	1:U:215:TRP:HH2	1.74	0.53
1:U:130:PRO:HB2	1:U:162:LEU:HD23	1.91	0.53
1:U:230:ARG:CZ	1:U:233:HIS:HB2	2.36	0.53
2:H:57:THR:HB	2:H:69:ILE:HG22	1.90	0.53
2:H:108:THR:CB	2:H:143:PRO:HD3	2.38	0.53
2:H:160:PHE:CG	3:L:176:SER:HB2	2.44	0.53
2:H:196:SER:C	2:H:198:THR:H	2.10	0.53
3:L:14:SER:CB	3:L:15:PRO:HD2	2.38	0.53
3:L:136:LEU:O	3:L:174:SER:HA	2.09	0.53
3:L:182:THR:OG1	3:L:185:GLU:N	2.37	0.53
3:L:190:ASN:O	3:L:210:ASN:HB3	2.07	0.53
2:H:37:VAL:HG13	2:H:46:GLU:O	2.09	0.53
1:U:59:PHE:O	1:U:60(B):TYR:C	2.47	0.52
2:H:139:TYR:CE1	2:H:169:TYR:CB	2.91	0.52
3:L:28:VAL:CG1	3:L:92:SER:HB2	2.39	0.52
1:U:100:HIS:C	1:U:101:ASN:OD1	2.47	0.52
1:U:141:PHE:HB3	1:U:152:PRO:HG2	1.90	0.52
2:H:135:LEU:CD2	3:L:131:SER:HB2	2.39	0.52
1:U:200:VAL:CG1	1:U:207:MET:CE	2.87	0.52
3:L:124:GLN:NE2	3:L:131:SER:N	2.58	0.52
3:L:147:LYS:HD3	3:L:154:GLU:OE2	2.09	0.52
2:H:156:GLY:O	2:H:175:VAL:HA	2.08	0.52
3:L:25:ALA:N	3:L:69:THR:O	2.40	0.52
3:L:170:ASP:C	3:L:170:ASP:OD1	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:192:TYR:N	3:L:209:PHE:O	2.31	0.52
2:H:145:THR:O	2:H:191:VAL:HA	2.10	0.52
3:L:35:TRP:HA	3:L:87:TYR:O	2.10	0.52
1:U:53:ILE:HG21	1:U:209:LEU:HD22	1.91	0.52
1:U:145:GLN:O	1:U:146:SER:HB2	2.10	0.52
1:U:159:VAL:O	1:U:159:VAL:CG1	2.58	0.52
3:L:136:LEU:HD13	3:L:175:MET:HB3	1.90	0.52
1:U:60(B):TYR:O	1:U:64:TYR:HE2	1.92	0.52
2:H:126:PRO:HG3	2:H:130:VAL:HG23	1.91	0.52
2:H:160:PHE:CE2	3:L:175:MET:C	2.84	0.52
2:H:162:ALA:HB2	2:H:171:LEU:HB2	1.92	0.52
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.91	0.52
2:H:142:GLU:CG	2:H:143:PRO:HB3	2.34	0.52
1:U:71:SER:HB3	1:U:77:THR:HG21	1.93	0.51
1:U:172:TYR:HD1	1:U:215:TRP:HZ3	1.51	0.51
1:U:234:PHE:O	1:U:238:ILE:HD12	2.10	0.51
2:H:39:GLN:HB3	2:H:91:TYR:HE2	1.73	0.51
2:H:94:ARG:HH21	2:H:101:ASP:HB2	1.75	0.51
3:L:2:ILE:HD13	3:L:27:SER:O	2.10	0.51
1:U:55:ALA:O	1:U:59:PHE:CE2	2.64	0.51
2:H:94:ARG:O	2:H:100(A):MET:HA	2.10	0.51
3:L:147:LYS:HD3	3:L:154:GLU:CD	2.31	0.51
1:U:148:ASP:OD2	1:U:156:LYS:NZ	2.44	0.51
2:H:139:TYR:OH	2:H:162:ALA:CB	2.57	0.51
3:L:132:VAL:HG13	3:L:209:PHE:CE2	2.45	0.51
1:U:32:ALA:HB1	1:U:34:TYR:HE1	1.75	0.51
2:H:50:SER:N	2:H:58:TYR:O	2.36	0.51
2:H:60:SER:C	2:H:62:SER:H	2.14	0.51
3:L:78:VAL:CG2	3:L:106:ILE:CD1	2.87	0.51
1:U:35:ARG:NH2	1:U:60(B):TYR:CD1	2.77	0.51
1:U:132:PHE:HA	1:U:162:LEU:HB3	1.92	0.51
1:U:138:ILE:O	1:U:158:THR:HG23	2.10	0.51
5:H:304:HOH:O	3:L:96:ARG:HD3	2.10	0.51
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.92	0.51
2:H:17:SER:HB2	2:H:82(A):SER:HA	1.91	0.51
2:H:140:PHE:HE1	2:H:169:TYR:HE1	1.59	0.51
3:L:5:THR:HG21	3:L:24:ARG:NH1	2.26	0.51
1:U:184:ALA:HB2	1:U:225:PRO:HA	1.92	0.51
2:H:22:CYS:O	2:H:77:ILE:HA	2.11	0.51
2:H:47:TRP:HE1	2:H:50:SER:HG	1.59	0.51
2:H:183:PRO:O	2:H:185:GLU:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:166:GLN:HE21	3:L:171:SER:CB	2.24	0.51
2:H:32:TYR:CG	2:H:94:ARG:HD2	2.45	0.51
3:L:150:ILE:N	3:L:153:SER:O	2.43	0.51
3:L:186:TYR:CD1	3:L:192:TYR:CZ	2.99	0.50
1:U:34:TYR:HD2	1:U:38:VAL:HG13	1.77	0.50
1:U:61:LYS:O	1:U:63:ASP:HB2	2.12	0.50
1:U:172:TYR:CE1	1:U:215:TRP:CE3	2.97	0.50
2:H:3:LYS:HG2	2:H:5:GLN:HE22	1.75	0.50
2:H:130:VAL:HG21	2:H:132:LEU:HD21	1.93	0.50
2:H:177:VAL:CB	2:H:181:THR:HB	2.41	0.50
2:H:70:SER:O	2:H:78:LEU:HD12	2.12	0.50
3:L:162:SER:O	3:L:175:MET:HA	2.12	0.50
1:U:57:HIS:HA	1:U:60:ILE:HG12	1.93	0.50
2:H:160:PHE:CD1	3:L:176:SER:HB2	2.46	0.50
1:U:29:TRP:O	1:U:46:LEU:N	2.43	0.50
1:U:33:ILE:HG13	1:U:66:VAL:HG22	1.93	0.50
2:H:140:PHE:O	2:H:193:HIS:CE1	2.65	0.50
2:H:178:PRO:C	2:H:181:THR:OG1	2.50	0.50
3:L:147:LYS:O	3:L:195:GLU:N	2.44	0.50
3:L:155:ARG:CZ	3:L:185:GLU:OE1	2.59	0.50
1:U:109:ARG:CG	1:U:110:SER:O	2.58	0.50
1:U:178:THR:CG2	1:U:179:LYS:N	2.68	0.50
2:H:6:GLU:HB3	2:H:107:THR:CG2	2.41	0.50
2:H:36:TRP:NE1	2:H:78:LEU:HG	2.26	0.50
2:H:138:GLY:HA2	2:H:168:LEU:HD13	1.92	0.50
3:L:5:THR:HG21	3:L:24:ARG:HH11	1.76	0.50
1:U:124:PRO:CA	1:U:208:THR:HG21	2.38	0.50
1:U:152:PRO:C	1:U:154:GLN:N	2.59	0.50
2:H:91:TYR:O	2:H:93:GLU:OE1	2.29	0.50
2:H:100:ALA:HB2	3:L:34:HIS:ND1	2.26	0.50
3:L:89:GLN:HA	3:L:97:THR:O	2.12	0.50
1:U:70:ARG:NH2	1:U:73:LEU:O	2.45	0.50
1:U:173:GLY:O	1:U:175:GLU:OE1	2.29	0.50
1:U:84:GLU:CG	1:U:110(A):LYS:NZ	2.62	0.50
2:H:190:ASN:OD1	2:H:199:LYS:HE2	2.12	0.50
3:L:108:ARG:NE	3:L:170:ASP:O	2.43	0.50
3:L:113:PRO:CA	3:L:139:PHE:HB3	2.42	0.50
1:U:152:PRO:HB3	1:U:156:LYS:NZ	2.27	0.49
1:U:200:VAL:HG22	1:U:208:THR:O	2.12	0.49
3:L:8:PRO:O	3:L:102:THR:OG1	2.21	0.49
1:U:25:GLU:OE1	1:U:116:ARG:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:123:LEU:CB	1:U:124:PRO:CD	2.87	0.49
1:U:150:LEU:O	1:U:152:PRO:CB	2.60	0.49
1:U:157:MET:SD	1:U:158:THR:N	2.85	0.49
2:H:37:VAL:HA	2:H:48:VAL:HG23	1.94	0.49
2:H:126:PRO:HD3	3:L:118:PHE:HE1	1.77	0.49
3:L:6:GLN:HG3	3:L:88:CYS:SG	2.52	0.49
1:U:109:ARG:HG3	1:U:110(C):GLY:HA2	1.95	0.49
2:H:72:ASP:OD1	2:H:74:ALA:HB3	2.12	0.49
3:L:117:ILE:CG1	3:L:209:PHE:HD2	2.24	0.49
3:L:120:PRO:HG2	3:L:130:ALA:HB1	1.94	0.49
1:U:163:ILE:CD1	1:U:182:CYS:HB2	2.40	0.49
2:H:149:ASN:OD1	2:H:187:VAL:HA	2.12	0.49
2:H:157:VAL:O	2:H:157:VAL:HG13	2.12	0.49
3:L:147:LYS:HE3	3:L:147:LYS:HA	1.94	0.49
1:U:46:LEU:HD23	1:U:119:GLN:C	2.32	0.49
2:H:51:ILE:O	2:H:51:ILE:CG2	2.60	0.49
2:H:178:PRO:CD	2:H:181:THR:OG1	2.61	0.49
2:H:181:THR:O	2:H:185:GLU:OE1	2.30	0.49
3:L:31:HIS:O	3:L:50:ALA:HA	2.12	0.49
3:L:103:LYS:HB3	3:L:103:LYS:NZ	2.28	0.49
1:U:127:TYR:HE1	1:U:230:ARG:CZ	2.26	0.49
2:H:8:GLY:O	2:H:18:LEU:HD21	2.13	0.49
3:L:27:SER:O	3:L:27(A):THR:O	2.31	0.49
3:L:49:TYR:O	3:L:50:ALA:CB	2.54	0.49
3:L:212:ASN:OD1	3:L:213:GLU:OE1	2.30	0.49
1:U:135:SER:C	1:U:136:CYS:SG	2.91	0.49
1:U:145:GLN:O	1:U:146:SER:CB	2.61	0.49
2:H:14:PRO:HD3	2:H:112:SER:O	2.12	0.49
2:H:117:THR:HG21	2:H:138:GLY:O	2.11	0.49
3:L:51:THR:OG1	3:L:71:TYR:CD2	2.66	0.49
3:L:149:LYS:HA	3:L:153:SER:O	2.12	0.49
3:L:182:THR:HG1	3:L:185:GLU:H	1.59	0.49
1:U:47:ILE:CG2	1:U:123:LEU:HD21	2.43	0.49
1:U:51:TRP:CZ3	1:U:107:LYS:HB2	2.48	0.49
3:L:47:TRP:O	3:L:58:VAL:HG21	2.13	0.49
3:L:139:PHE:CE2	3:L:144:ILE:HD12	2.48	0.49
1:U:165:HIS:O	1:U:168:CYS:N	2.43	0.48
2:H:19:LYS:HA	2:H:80:LEU:O	2.12	0.48
2:H:20:LEU:HD21	2:H:109:VAL:HG21	1.95	0.48
2:H:137:LYS:HG2	2:H:138:GLY:N	2.28	0.48
2:H:188:THR:HA	2:H:202:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:36:ARG:CZ	1:U:62(A):GLU:O	2.61	0.48
1:U:166:ARG:O	1:U:167:GLU:C	2.50	0.48
2:H:63:VAL:HG12	2:H:66:ARG:NH2	2.28	0.48
2:H:157:VAL:O	2:H:157:VAL:CG1	2.60	0.48
3:L:2:ILE:HD13	3:L:27:SER:C	2.34	0.48
3:L:90:HIS:HD2	3:L:92:SER:CB	2.26	0.48
3:L:108:ARG:HG2	3:L:140:TYR:CG	2.48	0.48
1:U:24:ILE:HG13	1:U:28:PRO:HA	1.95	0.48
1:U:140:GLY:HA2	1:U:155:LEU:CD1	2.42	0.48
2:H:147:THR:OG1	2:H:190:ASN:HB3	2.12	0.48
2:H:184:SER:CB	2:H:185:GLU:OE2	2.61	0.48
3:L:115:VAL:HA	3:L:135:PHE:O	2.13	0.48
1:U:68:LEU:O	1:U:80:GLU:HA	2.14	0.48
3:L:164:THR:CG2	3:L:174:SER:HB2	2.43	0.48
1:U:214:SER:HB2	1:U:227:VAL:O	2.13	0.48
3:L:46:LEU:HG	3:L:55:ALA:HB2	1.95	0.48
1:U:61:LYS:HB3	1:U:62(A):GLU:HG2	1.94	0.48
2:H:29:PHE:CE1	2:H:34:MET:HG3	2.49	0.48
3:L:108:ARG:NH1	3:L:109:ALA:O	2.46	0.48
1:U:103:ILE:HG23	1:U:237:TRP:CZ3	2.48	0.48
1:U:109:ARG:NE	1:U:110(C):GLY:CA	2.63	0.48
1:U:115:SER:OG	1:U:117:THR:HG22	2.13	0.48
2:H:147:THR:O	2:H:190:ASN:N	2.31	0.48
1:U:21:PHE:CB	3:L:53:ASN:OD1	2.61	0.48
2:H:40:THR:CG2	2:H:41:PRO:HD2	2.38	0.48
3:L:38:GLN:HG3	3:L:44:PRO:N	2.29	0.48
3:L:66:GLY:HA3	3:L:71:TYR:HA	1.96	0.48
3:L:96:ARG:NH1	3:L:96:ARG:CG	2.71	0.48
2:H:51:ILE:HD13	2:H:71:ARG:HG2	1.96	0.48
3:L:17:GLU:O	3:L:77:SER:HA	2.14	0.48
3:L:108:ARG:HD2	3:L:171:SER:O	2.13	0.48
1:U:209:LEU:HD21	1:U:212:ILE:HD11	1.96	0.47
2:H:59:TYR:HB2	2:H:64:LYS:HB2	1.96	0.47
1:U:137:GLU:OE2	1:U:157:MET:HE2	2.14	0.47
2:H:126:PRO:CD	3:L:118:PHE:HE1	2.26	0.47
2:H:126:PRO:N	3:L:118:PHE:HE1	2.13	0.47
1:U:156:LYS:HA	3:L:31:HIS:CE1	2.49	0.47
3:L:12:SER:OG	3:L:13:ALA:N	2.47	0.47
2:H:136:VAL:HG21	2:H:144:VAL:HG21	1.95	0.47
3:L:30:PHE:CE2	3:L:31:HIS:CE1	3.03	0.47
3:L:148:TRP:CZ2	3:L:194:CYS:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:PHE:HB3	3:L:162:SER:CB	2.37	0.47
1:U:27:GLN:HA	1:U:29:TRP:CE2	2.50	0.47
1:U:91:HIS:HD2	1:U:103:ILE:HG22	1.80	0.47
1:U:156:LYS:HA	3:L:31:HIS:CG	2.49	0.47
1:U:178:THR:HG22	1:U:179:LYS:N	2.30	0.47
1:U:184:ALA:HB2	1:U:225:PRO:CA	2.45	0.47
1:U:215:TRP:CD1	1:U:215:TRP:N	2.82	0.47
2:H:37:VAL:CA	2:H:48:VAL:HG23	2.44	0.47
2:H:40:THR:OG1	2:H:44:ARG:O	2.32	0.47
2:H:119:PRO:CD	2:H:193:HIS:HB2	2.45	0.47
2:H:174:SER:CB	3:L:137:ASN:HD21	2.25	0.47
2:H:178:PRO:HD2	2:H:181:THR:CG2	2.45	0.47
2:H:178:PRO:CA	2:H:181:THR:OG1	2.62	0.47
3:L:23:CYS:HB3	3:L:71:TYR:HB2	1.97	0.47
3:L:48:ILE:HG13	3:L:54:LEU:HD23	1.97	0.47
3:L:139:PHE:CE2	3:L:144:ILE:HB	2.49	0.47
3:L:211:ARG:NH1	3:L:211:ARG:HB2	2.18	0.47
2:H:6:GLU:HA	2:H:21:SER:O	2.15	0.47
2:H:184:SER:HB3	2:H:185:GLU:OE2	2.15	0.47
2:H:184:SER:OG	2:H:185:GLU:OE2	2.22	0.47
2:H:189:CYS:HB2	2:H:191:VAL:HG23	1.97	0.47
3:L:2:ILE:CD1	3:L:27:SER:O	2.63	0.47
3:L:115:VAL:HG13	3:L:136:LEU:HG	1.97	0.47
1:U:34:TYR:CE1	1:U:40:TYR:HD1	2.33	0.47
1:U:212:ILE:HB	1:U:229:THR:HB	1.96	0.47
3:L:62:PHE:CZ	3:L:82:ASP:OD1	2.64	0.47
3:L:90:HIS:CD2	3:L:92:SER:CB	2.96	0.47
3:L:111:ALA:HB3	3:L:139:PHE:HA	1.96	0.47
1:U:117:THR:HG23	1:U:118:ILE:HG13	1.95	0.46
2:H:5:GLN:O	2:H:22:CYS:HA	2.15	0.46
2:H:160:PHE:HE2	3:L:174:SER:C	2.19	0.46
3:L:78:VAL:HG23	3:L:106:ILE:CD1	2.39	0.46
3:L:115:VAL:HG23	3:L:205:ILE:HD12	1.97	0.46
3:L:118:PHE:O	3:L:132:VAL:HA	2.15	0.46
2:H:67:PHE:CE2	2:H:82:MET:HG2	2.50	0.46
2:H:93:GLU:HB3	2:H:100(A):MET:CB	2.45	0.46
3:L:4:LEU:HA	3:L:25:ALA:HA	1.97	0.46
1:U:172:TYR:CD1	1:U:215:TRP:CH2	3.03	0.46
1:U:173:GLY:N	1:U:175:GLU:CD	2.68	0.46
2:H:38:ARG:HG2	2:H:46:GLU:HB2	1.97	0.46
2:H:117:THR:O	2:H:140:PHE:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:15:PRO:O	3:L:15:PRO:HG2	2.15	0.46
2:H:6:GLU:OE2	2:H:91:TYR:HA	2.16	0.46
3:L:2:ILE:CG2	3:L:94:TYR:H	2.27	0.46
3:L:196:ALA:O	3:L:204:PRO:HB2	2.14	0.46
1:U:149:TYR:OH	3:L:46:LEU:HD23	2.16	0.46
1:U:155:LEU:O	3:L:31:HIS:CE1	2.68	0.46
1:U:185(B):GLN:O	1:U:186:TRP:CD2	2.68	0.46
2:H:51:ILE:HB	2:H:69:ILE:CG2	2.46	0.46
3:L:90:HIS:HD2	3:L:92:SER:N	2.09	0.46
1:U:161:LYS:HE3	1:U:163:ILE:HG22	1.98	0.46
2:H:129:MET:SD	2:H:179:SER:HB2	2.56	0.46
2:H:140:PHE:CG	2:H:141:PRO:HA	2.49	0.46
3:L:10:ILE:HD12	3:L:11:MET:N	2.30	0.46
3:L:59:PRO:CG	3:L:62:PHE:HE1	2.11	0.46
1:U:97(A):THR:OG1	1:U:97(B):LEU:N	2.48	0.46
1:U:98:ALA:HA	1:U:215:TRP:CD2	2.50	0.46
2:H:4:LEU:C	2:H:5:GLN:NE2	2.69	0.46
3:L:97:THR:HG23	3:L:98:PHE:CD2	2.50	0.46
3:L:122:SER:O	3:L:126:THR:HG23	2.15	0.46
3:L:147:LYS:HE3	3:L:147:LYS:CA	2.45	0.46
1:U:53:ILE:HG21	1:U:209:LEU:CD2	2.46	0.46
2:H:39:GLN:HE22	3:L:38:GLN:CD	2.15	0.46
3:L:81:GLU:HA	3:L:168:SER:O	2.16	0.46
3:L:124:GLN:CD	3:L:131:SER:H	2.19	0.46
1:U:23:THR:HG21	3:L:31:HIS:HE2	1.79	0.46
1:U:124:PRO:O	1:U:235:LEU:HD11	2.15	0.46
2:H:20:LEU:HD22	2:H:107:THR:CG2	2.46	0.46
1:U:55:ALA:HB3	1:U:58:CYS:SG	2.56	0.45
1:U:98:ALA:CB	1:U:215:TRP:CE2	2.99	0.45
1:U:99:HIS:O	1:U:180:MET:CE	2.63	0.45
3:L:61:ARG:NH1	3:L:79:GLU:OE1	2.49	0.45
1:U:72:ARG:NE	1:U:153:GLU:HB2	2.29	0.45
1:U:183:ALA:HB3	1:U:228:TYR:HE1	1.80	0.45
3:L:148:TRP:CE2	3:L:194:CYS:HB3	2.51	0.45
1:U:177:THR:O	1:U:178:THR:CB	2.63	0.45
3:L:11:MET:O	3:L:105:GLU:N	2.26	0.45
3:L:26:SER:O	3:L:27:SER:CB	2.64	0.45
3:L:62:PHE:CD1	3:L:62:PHE:N	2.83	0.45
3:L:113:PRO:HA	3:L:139:PHE:HB3	1.97	0.45
1:U:56:THR:OG1	1:U:90:LEU:HA	2.16	0.45
1:U:56:THR:HG21	1:U:90:LEU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:68:LEU:HB3	1:U:118:ILE:HG12	1.98	0.45
1:U:59:PHE:C	1:U:60(A):ASP:N	2.68	0.45
1:U:91:HIS:CD2	1:U:103:ILE:HG22	2.52	0.45
1:U:115:SER:HG	1:U:117:THR:H	1.63	0.45
1:U:138:ILE:HG23	1:U:199:LEU:HD12	1.98	0.45
1:U:152:PRO:HB3	1:U:156:LYS:HZ3	1.80	0.45
2:H:46:GLU:HG2	3:L:96:ARG:CZ	2.46	0.45
3:L:117:ILE:HB	3:L:207:LYS:HB3	1.97	0.45
1:U:57:HIS:CD2	1:U:58:CYS:N	2.85	0.45
1:U:72:ARG:HD2	1:U:75:SER:HB2	1.97	0.45
1:U:110:SER:HG	1:U:110(D):ARG:N	2.08	0.45
1:U:127:TYR:CE1	1:U:230:ARG:CZ	2.99	0.45
1:U:150:LEU:CD1	1:U:150:LEU:N	2.80	0.45
1:U:163:ILE:HG12	1:U:182:CYS:O	2.17	0.45
1:U:200:VAL:CG1	1:U:207:MET:HE1	2.46	0.45
2:H:182:TRP:HZ2	2:H:204:ILE:HG22	1.71	0.45
3:L:2:ILE:HD12	3:L:2:ILE:HA	1.84	0.45
3:L:124:GLN:NE2	3:L:131:SER:H	2.15	0.45
3:L:164:THR:HG23	3:L:174:SER:HB2	1.98	0.45
1:U:33:ILE:O	1:U:41:VAL:HG13	2.15	0.45
1:U:149:TYR:O	1:U:151:TYR:CD2	2.70	0.45
2:H:24:ALA:O	2:H:76:ASN:HB3	2.16	0.45
2:H:37:VAL:HG23	2:H:93:GLU:OE1	2.17	0.45
2:H:136:VAL:CG2	2:H:139:TYR:CE2	3.00	0.45
3:L:102:THR:O	3:L:102:THR:HG22	2.17	0.45
1:U:53:ILE:HD13	1:U:212:ILE:HD11	1.98	0.45
2:H:203:LYS:O	2:H:203:LYS:HG2	2.17	0.45
3:L:51:THR:OG1	3:L:71:TYR:HD2	1.99	0.45
3:L:136:LEU:HD23	3:L:196:ALA:HB2	1.99	0.45
1:U:98:ALA:CA	1:U:215:TRP:CE2	2.95	0.44
1:U:239:ARG:CZ	1:U:243:LYS:HE3	2.47	0.44
2:H:136:VAL:O	2:H:136:VAL:HG22	2.17	0.44
2:H:142:GLU:HA	2:H:143:PRO:HA	1.78	0.44
3:L:36:TYR:HE1	3:L:89:GLN:CB	2.30	0.44
3:L:124:GLN:HE22	3:L:131:SER:CB	2.31	0.44
2:H:36:TRP:CD1	2:H:80:LEU:HB2	2.52	0.44
1:U:21:PHE:CD1	1:U:21:PHE:N	2.85	0.44
1:U:51:TRP:HA	1:U:106:LEU:O	2.17	0.44
1:U:168:CYS:O	1:U:171:TYR:O	2.35	0.44
1:U:237:TRP:CD1	1:U:241:HIS:CE1	3.05	0.44
2:H:48:VAL:CG1	2:H:63:VAL:HG21	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:61:ARG:HD2	3:L:77:SER:O	2.18	0.44
3:L:119:PRO:HA	3:L:209:PHE:CZ	2.53	0.44
1:U:145:GLN:N	1:U:145:GLN:CD	2.71	0.44
2:H:154:SER:O	2:H:157:VAL:CG1	2.60	0.44
2:H:6:GLU:OE1	2:H:104:GLY:HA3	2.17	0.44
2:H:101:ASP:HB2	2:H:102:TYR:CD1	2.49	0.44
2:H:125:ALA:O	2:H:126:PRO:C	2.55	0.44
2:H:174:SER:HB2	3:L:135:PHE:CD2	2.52	0.44
3:L:26:SER:HA	3:L:69:THR:HG22	2.00	0.44
1:U:46:LEU:HB3	1:U:120:THR:HA	2.00	0.44
1:U:69:GLY:HA3	1:U:118:ILE:HG13	1.99	0.44
1:U:216:GLY:HA3	1:U:226:GLY:HA2	2.00	0.44
2:H:37:VAL:HG12	2:H:46:GLU:O	2.17	0.44
1:U:97:ASP:C	1:U:97(B):LEU:N	2.69	0.44
1:U:140:GLY:HA2	1:U:155:LEU:HD12	1.99	0.44
2:H:51:ILE:N	2:H:69:ILE:HD13	2.33	0.44
2:H:121:VAL:HG13	2:H:134:CYS:SG	2.58	0.44
2:H:140:PHE:CE1	2:H:169:TYR:HE1	2.36	0.44
3:L:19:VAL:CG2	3:L:21:MET:HE2	2.47	0.44
3:L:48:ILE:CA	3:L:53:ASN:O	2.62	0.44
1:U:38:VAL:O	1:U:38:VAL:HG13	2.11	0.44
2:H:36:TRP:NE1	2:H:80:LEU:HB2	2.33	0.44
3:L:186:TYR:CA	3:L:192:TYR:OH	2.65	0.44
1:U:137:GLU:OE1	1:U:200:VAL:CG1	2.66	0.44
1:U:152:PRO:HB2	1:U:156:LYS:CD	2.48	0.44
3:L:17:GLU:HB2	3:L:78:VAL:HG13	1.99	0.44
2:H:9:GLY:HA3	2:H:107:THR:OG1	2.17	0.43
2:H:82:MET:HE3	2:H:82(C):LEU:HD11	2.00	0.43
2:H:160:PHE:CD1	2:H:160:PHE:N	2.85	0.43
1:U:56:THR:CA	1:U:104:ALA:HB2	2.48	0.43
2:H:87:THR:O	2:H:88:ALA:HB2	2.18	0.43
2:H:150:SER:HA	2:H:190:ASN:ND2	2.27	0.43
3:L:170:ASP:OD1	3:L:172:THR:HG23	2.18	0.43
3:L:186:TYR:CE1	3:L:192:TYR:CE1	3.06	0.43
1:U:56:THR:HG22	1:U:60:ILE:CG2	2.48	0.43
1:U:101:ASN:HA	1:U:234:PHE:CZ	2.52	0.43
1:U:192:GLN:NE2	1:U:217:ARG:CG	2.81	0.43
2:H:66:ARG:HB2	2:H:82(B):SER:HB2	2.00	0.43
3:L:21:MET:CE	3:L:73:LEU:HD22	2.48	0.43
3:L:32:TYR:CG	3:L:91:TYR:HE2	2.36	0.43
1:U:60(B):TYR:O	1:U:64:TYR:CE2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:72:ARG:HD3	1:U:73:LEU:H	1.82	0.43
2:H:165:GLN:NE2	2:H:170:THR:OG1	2.52	0.43
3:L:14:SER:O	3:L:78:VAL:HG13	2.18	0.43
3:L:163:TRP:HA	3:L:174:SER:O	2.18	0.43
1:U:60(B):TYR:N	1:U:60(B):TYR:HD1	2.13	0.43
1:U:149:TYR:CE1	3:L:49:TYR:CD2	3.07	0.43
1:U:158:THR:HB	3:L:32:TYR:CE2	2.54	0.43
2:H:20:LEU:HD21	2:H:109:VAL:CG2	2.48	0.43
3:L:34:HIS:HB2	3:L:89:GLN:OE1	2.19	0.43
3:L:197:THR:HA	3:L:204:PRO:HB3	1.99	0.43
2:H:177:VAL:C	2:H:181:THR:OG1	2.56	0.43
2:H:182:TRP:CG	2:H:183:PRO:CA	2.96	0.43
2:H:158:HIS:HE1	3:L:138:ASN:ND2	2.17	0.43
3:L:113:PRO:O	3:L:115:VAL:HG23	2.19	0.43
2:H:153:LEU:HD11	2:H:177:VAL:CG1	2.49	0.43
3:L:136:LEU:N	3:L:175:MET:O	2.46	0.43
1:U:56:THR:HG23	1:U:90:LEU:HB3	1.99	0.43
1:U:156:LYS:HA	3:L:31:HIS:CD2	2.54	0.43
1:U:176:VAL:HG12	1:U:176:VAL:O	2.19	0.43
3:L:108:ARG:HD2	3:L:171:SER:C	2.39	0.43
3:L:148:TRP:O	3:L:155:ARG:N	2.46	0.43
1:U:33:ILE:HG21	1:U:59:PHE:HE1	1.84	0.42
2:H:6:GLU:CB	2:H:107:THR:HB	2.49	0.42
3:L:49:TYR:N	3:L:53:ASN:O	2.46	0.42
1:U:56:THR:HG22	1:U:60:ILE:HG23	2.02	0.42
2:H:100:ALA:HB2	3:L:34:HIS:CE1	2.54	0.42
3:L:13:ALA:HB3	3:L:17:GLU:OE2	2.15	0.42
3:L:139:PHE:CZ	3:L:144:ILE:HD12	2.54	0.42
3:L:166:GLN:NE2	3:L:171:SER:HB3	2.34	0.42
3:L:191:SER:HA	3:L:209:PHE:O	2.18	0.42
1:U:103:ILE:HG21	1:U:234:PHE:CD2	2.54	0.42
3:L:163:TRP:HE3	3:L:163:TRP:H	1.67	0.42
1:U:192:GLN:CG	1:U:193:GLY:H	2.33	0.42
1:U:33:ILE:HG22	1:U:33:ILE:O	2.18	0.42
1:U:173:GLY:C	1:U:175:GLU:CD	2.78	0.42
1:U:185(A):PRO:O	1:U:185(A):PRO:HG2	2.19	0.42
2:H:70:SER:OG	2:H:79:SER:HB2	2.20	0.42
2:H:119:PRO:HD3	2:H:193:HIS:HB2	2.00	0.42
2:H:182:TRP:CD1	2:H:187:VAL:CG1	3.02	0.42
3:L:132:VAL:CG1	3:L:209:PHE:HE2	2.33	0.42
1:U:72:ARG:HD2	1:U:75:SER:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:ASP:CG	2:H:75:ARG:HG3	2.39	0.42
3:L:132:VAL:CG1	3:L:148:TRP:CZ3	3.03	0.42
3:L:150:ILE:CD1	3:L:181:LEU:HD11	2.49	0.42
3:L:163:TRP:N	3:L:163:TRP:CD2	2.87	0.42
3:L:183:LYS:HG3	3:L:184:ASP:N	2.29	0.42
1:U:60:ILE:HG13	1:U:60(A):ASP:N	2.35	0.42
1:U:101:ASN:OD1	1:U:101:ASN:N	2.52	0.42
2:H:178:PRO:O	2:H:181:THR:N	2.40	0.42
1:U:85:VAL:CG2	1:U:106:LEU:HD23	2.50	0.42
2:H:49:ALA:HA	2:H:59:TYR:HA	2.01	0.42
3:L:33:LEU:HG	3:L:71:TYR:CG	2.55	0.42
1:U:28:PRO:HD2	1:U:29:TRP:CE3	2.54	0.42
1:U:60:ILE:HG21	1:U:94:TYR:CE2	2.54	0.42
1:U:129:ASP:HA	1:U:130:PRO:HD3	1.90	0.42
1:U:137:GLU:HB3	1:U:157:MET:CE	2.50	0.42
3:L:106:ILE:HD12	3:L:106:ILE:HG23	1.75	0.42
3:L:148:TRP:HA	3:L:193:THR:O	2.19	0.42
1:U:158:THR:HG22	3:L:32:TYR:OH	2.20	0.42
1:U:171:TYR:O	1:U:172:TYR:C	2.47	0.42
1:U:192:GLN:CD	1:U:217:ARG:CD	2.83	0.42
1:U:214:SER:HB3	1:U:215:TRP:HD1	1.85	0.42
2:H:67:PHE:CE1	2:H:82:MET:HB3	2.55	0.42
2:H:135:LEU:CD2	3:L:131:SER:CB	2.98	0.42
3:L:14:SER:HB3	3:L:15:PRO:HD2	2.02	0.42
3:L:27(A):THR:HA	3:L:69:THR:HA	2.01	0.42
1:U:148:ASP:HB3	2:H:99:TYR:HB3	2.02	0.41
2:H:18:LEU:HB3	2:H:82:MET:HE2	2.02	0.41
2:H:66:ARG:HH12	2:H:86:ASP:CG	2.19	0.41
3:L:2:ILE:HD13	3:L:27:SER:CA	2.50	0.41
3:L:79:GLU:O	3:L:82:ASP:HB2	2.19	0.41
3:L:213:GLU:O	3:L:214:CYS:CB	2.51	0.41
2:H:30:SER:HA	2:H:73:ASN:HD22	1.83	0.41
1:U:46:LEU:O	1:U:120:THR:HA	2.20	0.41
2:H:37:VAL:HG21	2:H:103:TRP:CH2	2.56	0.41
1:U:47:ILE:HD11	1:U:51:TRP:HB3	2.01	0.41
1:U:212:ILE:O	1:U:228:TYR:HA	2.20	0.41
2:H:18:LEU:HB3	2:H:82:MET:CE	2.50	0.41
2:H:38:ARG:HA	2:H:89:MET:O	2.20	0.41
2:H:60:SER:O	2:H:62:SER:N	2.54	0.41
3:L:47:TRP:HA	3:L:58:VAL:HG21	2.00	0.41
3:L:78:VAL:HG21	3:L:106:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:78:VAL:HG21	3:L:106:ILE:HD12	2.00	0.41
1:U:35:ARG:HH21	1:U:60(B):TYR:CB	2.33	0.41
1:U:124:PRO:HG2	1:U:235:LEU:HD11	2.03	0.41
1:U:202:SER:HB2	1:U:207:MET:HE3	2.02	0.41
1:U:231:VAL:O	1:U:234:PHE:N	2.53	0.41
1:U:159:VAL:H	3:L:29:SER:HB2	1.85	0.41
2:H:132:LEU:HB2	2:H:175:VAL:HG12	2.02	0.41
2:H:178:PRO:C	2:H:181:THR:HG1	2.05	0.41
2:H:202:LYS:HD3	2:H:202:LYS:HA	1.79	0.41
3:L:146:VAL:HG21	3:L:175:MET:CE	2.50	0.41
1:U:81:MET:HB3	1:U:83:PHE:CE2	2.55	0.41
1:U:123:LEU:HD23	1:U:123:LEU:HA	1.97	0.41
2:H:137:LYS:HG3	2:H:170:THR:OG1	2.21	0.41
2:H:177:VAL:CG2	2:H:181:THR:HB	2.50	0.41
3:L:47:TRP:CE2	3:L:58:VAL:HG13	2.56	0.41
3:L:166:GLN:NE2	3:L:171:SER:CB	2.83	0.41
1:U:55:ALA:H	1:U:196:GLY:HA2	1.85	0.41
1:U:87:ASN:H	1:U:107:LYS:HB3	1.85	0.41
1:U:172:TYR:HE1	1:U:215:TRP:CE3	2.38	0.41
2:H:45:LEU:HD12	2:H:45:LEU:HA	1.67	0.41
1:U:72:ARG:HG3	1:U:72:ARG:HH11	1.86	0.41
1:U:163:ILE:HD11	1:U:168:CYS:SG	2.61	0.41
2:H:19:LYS:HE2	2:H:79:SER:CB	2.46	0.41
2:H:57:THR:HB	2:H:69:ILE:CG2	2.50	0.41
2:H:94:ARG:HG2	2:H:95:GLY:N	2.35	0.41
2:H:124:LEU:HD21	3:L:133:VAL:HG11	2.03	0.41
2:H:126:PRO:HD3	3:L:118:PHE:CE1	2.56	0.41
2:H:158:HIS:CE1	3:L:138:ASN:ND2	2.89	0.41
3:L:30:PHE:HA	3:L:71:TYR:CE2	2.56	0.41
3:L:47:TRP:CE3	3:L:47:TRP:HA	2.53	0.41
3:L:121:SER:O	3:L:125:LEU:HG	2.21	0.41
3:L:185:GLU:CA	3:L:188:ARG:HD3	2.26	0.41
1:U:166:ARG:O	1:U:168:CYS:N	2.54	0.41
2:H:132:LEU:HD12	2:H:187:VAL:HG21	2.02	0.41
3:L:136:LEU:HD22	3:L:144:ILE:HD13	2.01	0.41
2:H:148:TRP:CD1	2:H:157:VAL:HG23	2.55	0.40
3:L:51:THR:HG22	3:L:52:SER:CB	2.50	0.40
3:L:158:GLY:O	3:L:179:LEU:HD12	2.21	0.40
1:U:98:ALA:HB1	1:U:215:TRP:CZ2	2.51	0.40
1:U:146:SER:HG	2:H:52:THR:HB	1.83	0.40
2:H:135:LEU:HD11	2:H:170:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:56:THR:N	1:U:102:ASP:O	2.46	0.40
1:U:98:ALA:CA	1:U:215:TRP:CZ2	3.03	0.40
1:U:127:TYR:CE1	1:U:230:ARG:NH2	2.89	0.40
3:L:32:TYR:CD2	3:L:91:TYR:HE2	2.39	0.40
3:L:161:ASN:HB3	3:L:175:MET:CE	2.48	0.40
1:U:100:HIS:HB3	1:U:101:ASN:OD1	2.21	0.40
1:U:151:TYR:CD1	1:U:153:GLU:HG2	2.57	0.40
2:H:55:GLY:O	2:H:57:THR:HG23	2.21	0.40
2:H:82(C):LEU:HD23	2:H:82(C):LEU:HA	1.81	0.40
2:H:92:CYS:C	2:H:93:GLU:OE2	2.60	0.40
2:H:122:TYR:CD2	3:L:124:GLN:HG3	2.56	0.40
2:H:122:TYR:CG	3:L:124:GLN:HG3	2.57	0.40
3:L:33:LEU:HD22	3:L:34:HIS:N	2.36	0.40

All (2) 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:U:151:TYR:OH	1:U:164:SER:OG[1_655]	1.37	0.83
3:L:67:SER:OG	3:L:200:THR:O[4_445]	2.08	0.12

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	211/246 (86%)	186 (88%)	18 (8%)	7 (3%)	4	19
2	H	206/212 (97%)	186 (90%)	18 (9%)	2 (1%)	15	50
3	L	210/215 (98%)	189 (90%)	18 (9%)	3 (1%)	11	41
All	All	627/673 (93%)	561 (90%)	54 (9%)	12 (2%)	8	33

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	146	SER
1	U	172	TYR
1	U	176	VAL
1	U	177	THR
1	U	185(A)	PRO
3	L	27(A)	THR
3	L	13	ALA
1	U	151	TYR
3	L	2	ILE
1	U	152	PRO
2	H	143	PRO
2	H	183	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	U	195/214 (91%)	145 (74%)	50 (26%)	0	2
2	H	183/184 (100%)	150 (82%)	33 (18%)	1	8
3	L	186/187 (100%)	146 (78%)	40 (22%)	1	4
All	All	564/585 (96%)	441 (78%)	123 (22%)	1	4

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	21	PHE
1	U	29	TRP
1	U	35	ARG
1	U	38	VAL
1	U	39	THR
1	U	41	VAL
1	U	45	SER
1	U	60(B)	TYR
1	U	62	LYS
1	U	62(A)	GLU
1	U	72	ARG

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Mol	Chain	Res	Type
1	U	95	SER
1	U	97(B)	LEU
1	U	101	ASN
1	U	105	LEU
1	U	110(A)	LYS
1	U	110(D)	ARG
1	U	115	SER
1	U	127	TYR
1	U	131	GLN
1	U	137	GLU
1	U	143	LYS
1	U	147	THR
1	U	148	ASP
1	U	149	TYR
1	U	150	LEU
1	U	152	PRO
1	U	153	GLU
1	U	157	MET
1	U	158	THR
1	U	159	VAL
1	U	161	LYS
1	U	162	LEU
1	U	164	SER
1	U	166	ARG
1	U	167	GLU
1	U	171	TYR
1	U	175	GLU
1	U	177	THR
1	U	179	LYS
1	U	181	LEU
1	U	182	CYS
1	U	199	LEU
1	U	200	VAL
1	U	203	LEU
1	U	204	GLN
1	U	207	MET
1	U	215	TRP
1	U	224	LYS
1	U	232	SER
2	H	12	VAL
2	H	17	SER
2	H	23	SER

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Mol	Chain	Res	Type
2	H	31	ARG
2	H	38	ARG
2	H	40	THR
2	H	45	LEU
2	H	53	ASN
2	H	62	SER
2	H	83	ARG
2	H	93	GLU
2	H	96	GLU
2	H	100(A)	MET
2	H	101	ASP
2	H	124	LEU
2	H	131	THR
2	H	134	CYS
2	H	145	THR
2	H	150	SER
2	H	153	LEU
2	H	157	VAL
2	H	166	SER
2	H	171	LEU
2	H	174	SER
2	H	175	VAL
2	H	180	SER
2	H	181	THR
2	H	184	SER
2	H	187	VAL
2	H	188	THR
2	H	189	CYS
2	H	198	THR
2	H	205	VAL
3	L	1	ASP
3	L	7	SER
3	L	10	ILE
3	L	19	VAL
3	L	20	THR
3	L	21	MET
3	L	27	SER
3	L	27(A)	THR
3	L	28	VAL
3	L	40	SER
3	L	43	SER
3	L	47	TRP

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Mol	Chain	Res	Type
3	L	48	ILE
3	L	51	THR
3	L	78	VAL
3	L	94	TYR
3	L	96	ARG
3	L	102	THR
3	L	110	ASP
3	L	114	THR
3	L	133	VAL
3	L	147	LYS
3	L	160	LEU
3	L	161	ASN
3	L	162	SER
3	L	163	TRP
3	L	165	ASP
3	L	180	THR
3	L	181	LEU
3	L	183	LYS
3	L	191	SER
3	L	197	THR
3	L	199	LYS
3	L	200	THR
3	L	202	THR
3	L	205	ILE
3	L	206	VAL
3	L	208	SER
3	L	210	ASN
3	L	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	27	GLN
1	U	91	HIS
1	U	99	HIS
1	U	119	GLN
2	H	5	GLN
2	H	39	GLN
2	H	53	ASN
2	H	165	GLN
2	H	190	ASN
3	L	38	GLN

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Mol	Chain	Res	Type
3	L	90	HIS
3	L	124	GLN
3	L	137	ASN
3	L	138	ASN
3	L	161	ASN
3	L	166	GLN
3	L	210	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z  > 2$
4	SO4	L	301	-	4,4,4	0.51	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	U	221/246 (89%)	0.41	7 (3%) 47 29	23, 44, 70, 88	0
2	H	210/212 (99%)	0.52	13 (6%) 20 11	25, 41, 64, 79	0
3	L	214/215 (99%)	0.55	20 (9%) 8 5	27, 43, 63, 83	0
All	All	645/673 (95%)	0.49	40 (6%) 20 11	23, 43, 66, 88	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	179	SER	5.6
3	L	200	THR	4.0
2	H	180	SER	3.8
3	L	156	GLN	3.7
2	H	124	LEU	3.6
3	L	118	PHE	3.3
3	L	136	LEU	3.2
2	H	184	SER	3.2
2	H	205	VAL	3.0
3	L	68	GLY	2.9
2	H	182	TRP	2.9
3	L	158	GLY	2.9
3	L	202	THR	2.8
2	H	126	PRO	2.7
1	U	126	MET	2.6
2	H	153	LEU	2.6
3	L	208	SER	2.6
1	U	217	ARG	2.6
1	U	224	LYS	2.5
2	H	152	SER	2.5
3	L	150	ILE	2.5
3	L	214	CYS	2.3
3	L	190	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	203	SER	2.2
3	L	153	SER	2.2
1	U	149	TYR	2.2
2	H	12	VAL	2.2
2	H	130	VAL	2.2
2	H	165	GLN	2.1
3	L	157	ASN	2.1
1	U	91	HIS	2.1
1	U	183	ALA	2.1
3	L	15	PRO	2.1
3	L	115	VAL	2.1
2	H	208	GLY	2.1
3	L	193	THR	2.0
1	U	168	CYS	2.0
3	L	155	ARG	2.0
3	L	191	SER	2.0
3	L	212	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	L	301	5/5	0.95	0.14	50,50,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.