



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:18 PM UTC

PDB ID : 3KRD / pdb_00003krd
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome in complex with
Fellutamide B
Authors : Li, D.; Li, H.
Deposited on : 2009-11-18
Resolution : 2.50 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

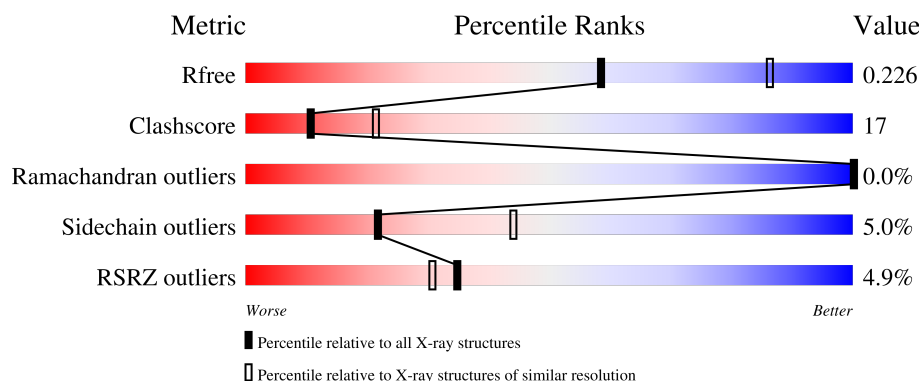
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	1	248	3% 50% 30% 6% 13%
1	A	248	5% 52% 30% • 14%
1	B	248	9% 55% 29% • 14%
1	D	248	19% 42% 35% 8% • 14%
1	F	248	5% 52% 30% 5% 13%

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Mol	Chain	Length	Quality of chain
1	I	248	
1	K	248	
1	M	248	
1	O	248	
1	Q	248	
1	S	248	
1	U	248	
1	W	248	
1	Y	248	
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	
3	a	3	
3	b	3	

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Mol	Chain	Length	Quality of chain
3	c	3	 67%33%
3	d	3	 67%33%
3	e	3	 67%33%
3	f	3	 67%33%
3	g	3	 67%33%
3	h	3	 67%33%
3	i	3	 67%33%
3	j	3	 67%33%
3	k	3	 67%33%
3	l	3	 67%33%
3	m	3	 67%33%
3	n	3	 67%33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48828 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	B	213	Total	C	N	O	S	0	0	0
			1642	1027	301	311	3			
1	D	213	Total	C	N	O	S	0	0	0
			1646	1031	301	311	3			
1	F	216	Total	C	N	O	S	0	0	0
			1661	1040	304	314	3			
1	I	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	K	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	M	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	O	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	Q	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	S	215	Total	C	N	O	S	0	0	0
			1657	1038	303	313	3			
1	U	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	W	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	Y	216	Total	C	N	O	S	0	0	0
			1661	1040	304	314	3			
1	1	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	E	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	G	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	H	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	J	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	L	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	N	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	P	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	R	229	Total 1683	C 1054	N 289	O 335	S 5	0	0	0
2	T	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	V	229	Total 1683	C 1054	N 289	O 335	S 5	0	0	0
2	X	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	Z	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	2	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	535	HIS	-	expression tag	UNP A5U4D6
C	536	HIS	-	expression tag	UNP A5U4D6
C	537	HIS	-	expression tag	UNP A5U4D6
C	538	HIS	-	expression tag	UNP A5U4D6
C	539	HIS	-	expression tag	UNP A5U4D6
C	540	HIS	-	expression tag	UNP A5U4D6
E	535	HIS	-	expression tag	UNP A5U4D6
E	536	HIS	-	expression tag	UNP A5U4D6
E	537	HIS	-	expression tag	UNP A5U4D6
E	538	HIS	-	expression tag	UNP A5U4D6
E	539	HIS	-	expression tag	UNP A5U4D6
E	540	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	535	HIS	-	expression tag	UNP A5U4D6
G	536	HIS	-	expression tag	UNP A5U4D6
G	537	HIS	-	expression tag	UNP A5U4D6
G	538	HIS	-	expression tag	UNP A5U4D6
G	539	HIS	-	expression tag	UNP A5U4D6
G	540	HIS	-	expression tag	UNP A5U4D6
H	535	HIS	-	expression tag	UNP A5U4D6
H	536	HIS	-	expression tag	UNP A5U4D6
H	537	HIS	-	expression tag	UNP A5U4D6
H	538	HIS	-	expression tag	UNP A5U4D6
H	539	HIS	-	expression tag	UNP A5U4D6
H	540	HIS	-	expression tag	UNP A5U4D6
J	535	HIS	-	expression tag	UNP A5U4D6
J	536	HIS	-	expression tag	UNP A5U4D6
J	537	HIS	-	expression tag	UNP A5U4D6
J	538	HIS	-	expression tag	UNP A5U4D6
J	539	HIS	-	expression tag	UNP A5U4D6
J	540	HIS	-	expression tag	UNP A5U4D6
L	535	HIS	-	expression tag	UNP A5U4D6
L	536	HIS	-	expression tag	UNP A5U4D6
L	537	HIS	-	expression tag	UNP A5U4D6
L	538	HIS	-	expression tag	UNP A5U4D6
L	539	HIS	-	expression tag	UNP A5U4D6
L	540	HIS	-	expression tag	UNP A5U4D6
N	535	HIS	-	expression tag	UNP A5U4D6
N	536	HIS	-	expression tag	UNP A5U4D6
N	537	HIS	-	expression tag	UNP A5U4D6
N	538	HIS	-	expression tag	UNP A5U4D6
N	539	HIS	-	expression tag	UNP A5U4D6
N	540	HIS	-	expression tag	UNP A5U4D6
P	535	HIS	-	expression tag	UNP A5U4D6
P	536	HIS	-	expression tag	UNP A5U4D6
P	537	HIS	-	expression tag	UNP A5U4D6
P	538	HIS	-	expression tag	UNP A5U4D6
P	539	HIS	-	expression tag	UNP A5U4D6
P	540	HIS	-	expression tag	UNP A5U4D6
R	535	HIS	-	expression tag	UNP A5U4D6
R	536	HIS	-	expression tag	UNP A5U4D6
R	537	HIS	-	expression tag	UNP A5U4D6
R	538	HIS	-	expression tag	UNP A5U4D6
R	539	HIS	-	expression tag	UNP A5U4D6
R	540	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
T	535	HIS	-	expression tag	UNP A5U4D6
T	536	HIS	-	expression tag	UNP A5U4D6
T	537	HIS	-	expression tag	UNP A5U4D6
T	538	HIS	-	expression tag	UNP A5U4D6
T	539	HIS	-	expression tag	UNP A5U4D6
T	540	HIS	-	expression tag	UNP A5U4D6
V	535	HIS	-	expression tag	UNP A5U4D6
V	536	HIS	-	expression tag	UNP A5U4D6
V	537	HIS	-	expression tag	UNP A5U4D6
V	538	HIS	-	expression tag	UNP A5U4D6
V	539	HIS	-	expression tag	UNP A5U4D6
V	540	HIS	-	expression tag	UNP A5U4D6
X	535	HIS	-	expression tag	UNP A5U4D6
X	536	HIS	-	expression tag	UNP A5U4D6
X	537	HIS	-	expression tag	UNP A5U4D6
X	538	HIS	-	expression tag	UNP A5U4D6
X	539	HIS	-	expression tag	UNP A5U4D6
X	540	HIS	-	expression tag	UNP A5U4D6
Z	535	HIS	-	expression tag	UNP A5U4D6
Z	536	HIS	-	expression tag	UNP A5U4D6
Z	537	HIS	-	expression tag	UNP A5U4D6
Z	538	HIS	-	expression tag	UNP A5U4D6
Z	539	HIS	-	expression tag	UNP A5U4D6
Z	540	HIS	-	expression tag	UNP A5U4D6
2	535	HIS	-	expression tag	UNP A5U4D6
2	536	HIS	-	expression tag	UNP A5U4D6
2	537	HIS	-	expression tag	UNP A5U4D6
2	538	HIS	-	expression tag	UNP A5U4D6
2	539	HIS	-	expression tag	UNP A5U4D6
2	540	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is a protein called Fellutamide B.

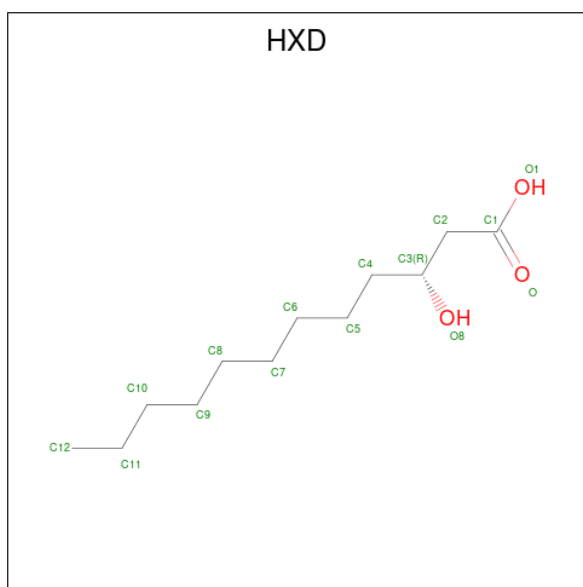
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	b	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	c	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	d	3	Total	C	N	O	0	0	0
			25	15	5	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	e	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	f	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	g	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	h	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	i	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	j	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	k	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	l	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	m	3	Total	C	N	O	0	0	0
			25	15	5	5			
3	n	3	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 4 is (3R)-3-HYDROXYDODECANOIC ACID (CCD ID: HXD) (formula: $C_{12}H_{24}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	C	O	0	0
			7	5	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	b	1	Total C O 7 5 2	0	0
4	c	1	Total C O 7 5 2	0	0
4	d	1	Total C O 7 5 2	0	0
4	e	1	Total C O 7 5 2	0	0
4	f	1	Total C O 7 5 2	0	0
4	g	1	Total C O 7 5 2	0	0
4	h	1	Total C O 7 5 2	0	0
4	i	1	Total C O 7 5 2	0	0
4	j	1	Total C O 7 5 2	0	0
4	k	1	Total C O 7 5 2	0	0
4	l	1	Total C O 7 5 2	0	0
4	m	1	Total C O 7 5 2	0	0
4	n	1	Total C O 7 5 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	42	Total O 42 42	0	0
5	C	131	Total O 131 131	0	0
5	D	25	Total O 25 25	0	0
5	E	130	Total O 130 130	0	0
5	F	41	Total O 41 41	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	113	Total O 113 113	0	0
5	H	126	Total O 126 126	0	0
5	I	38	Total O 38 38	0	0
5	J	122	Total O 122 122	0	0
5	K	33	Total O 33 33	0	0
5	L	132	Total O 132 132	0	0
5	M	42	Total O 42 42	0	0
5	N	121	Total O 121 121	0	0
5	O	39	Total O 39 39	0	0
5	P	111	Total O 111 111	0	0
5	Q	34	Total O 34 34	0	0
5	R	143	Total O 143 143	0	0
5	S	43	Total O 43 43	0	0
5	T	103	Total O 103 103	0	0
5	U	33	Total O 33 33	0	0
5	V	149	Total O 149 149	0	0
5	W	26	Total O 26 26	0	0
5	X	115	Total O 115 115	0	0
5	Y	22	Total O 22 22	0	0
5	Z	106	Total O 106 106	0	0
5	1	55	Total O 55 55	0	0

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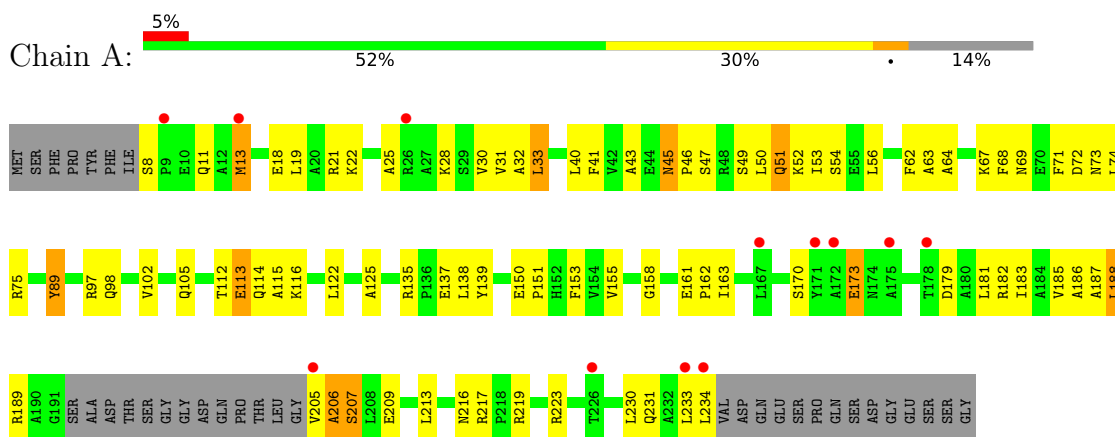
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2	118	Total 118	O 118	0	0

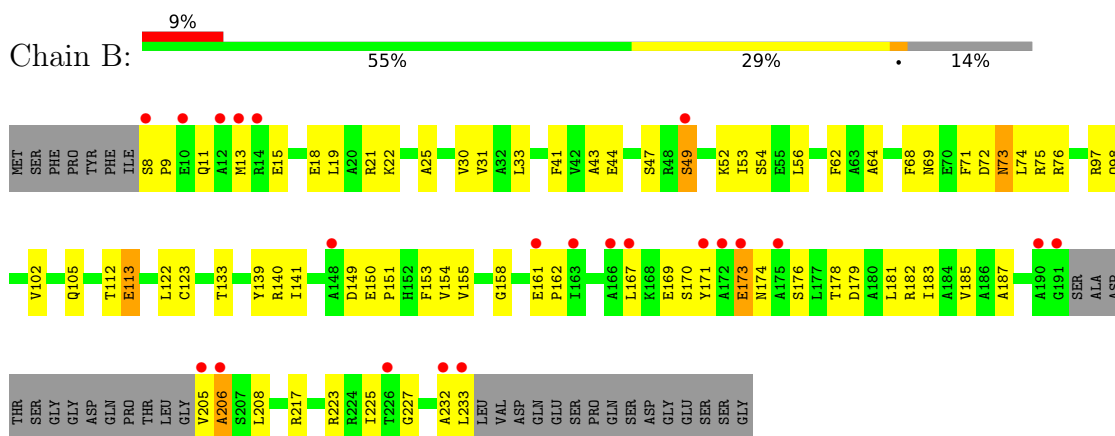
3 Residue-property plots [i](#)

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

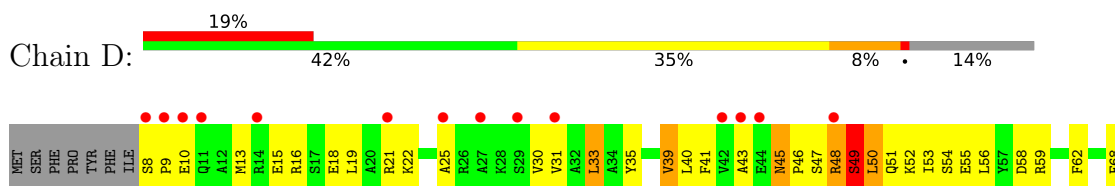
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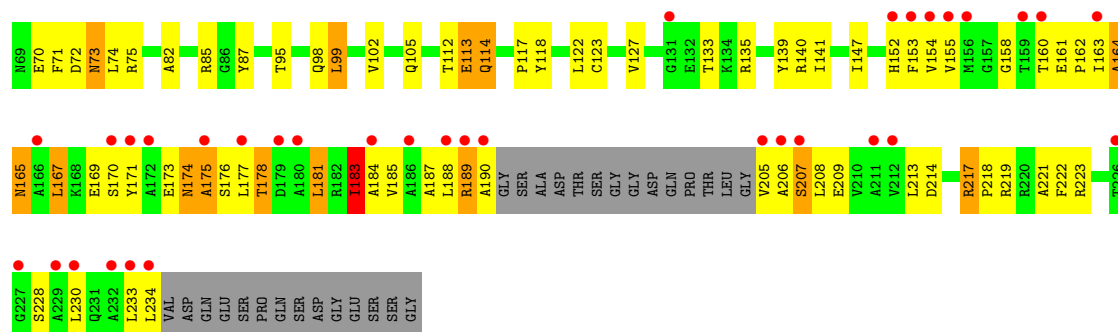


• Molecule 1: Proteasome subunit alpha

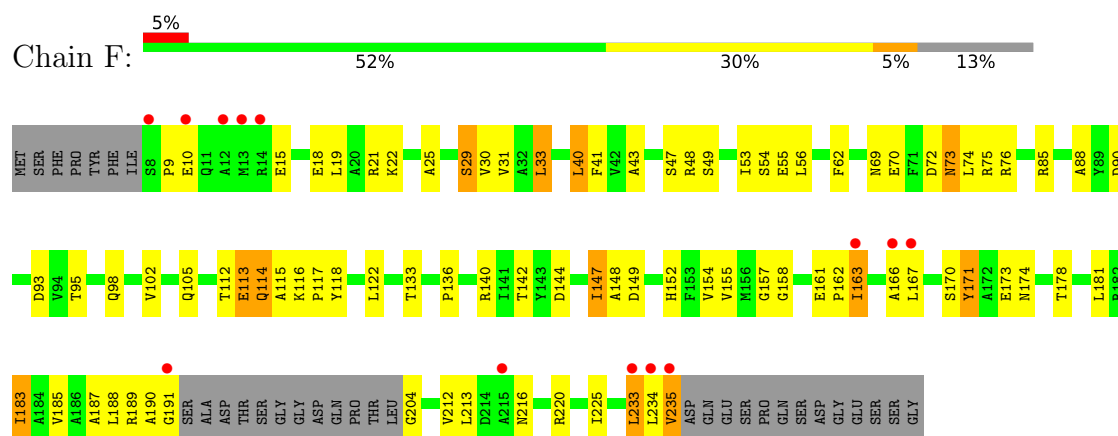


• Molecule 1: Proteasome subunit alpha

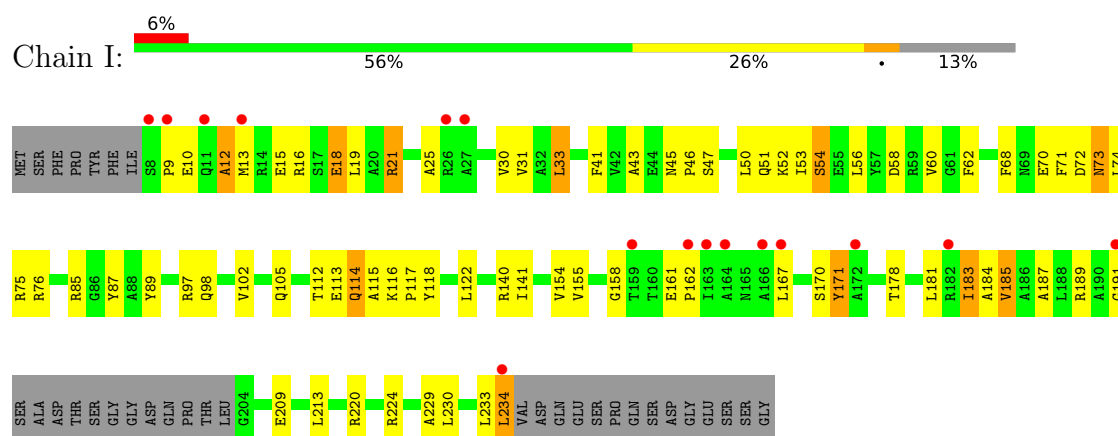




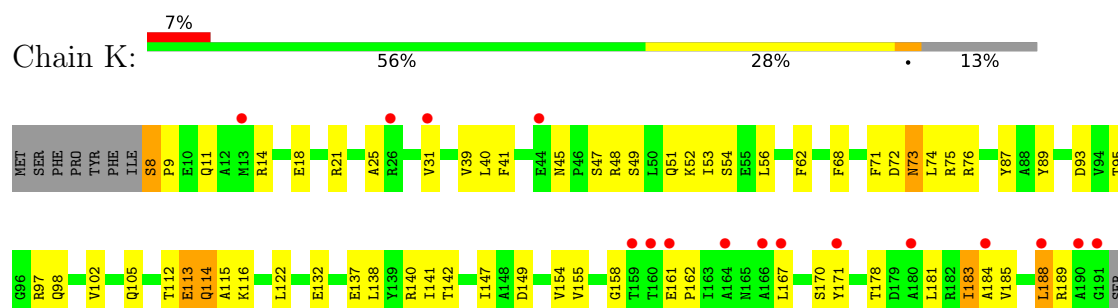
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

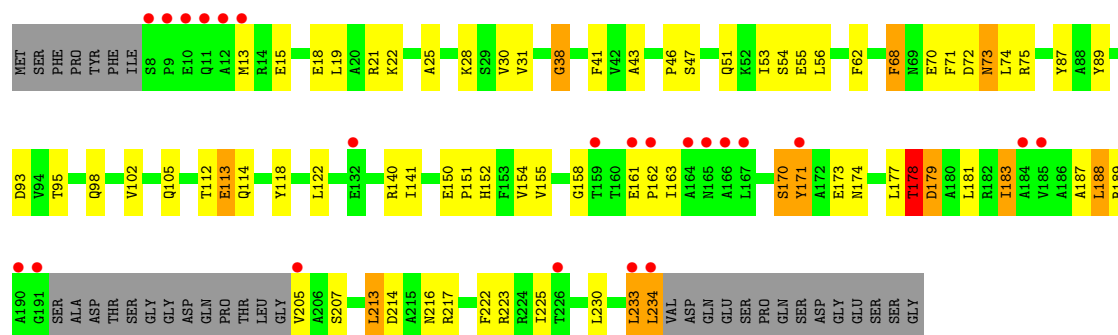


- Molecule 1: Proteasome subunit alpha

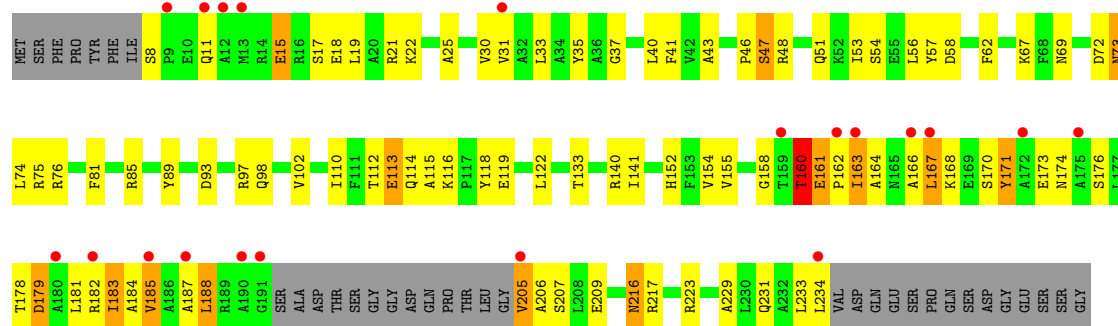




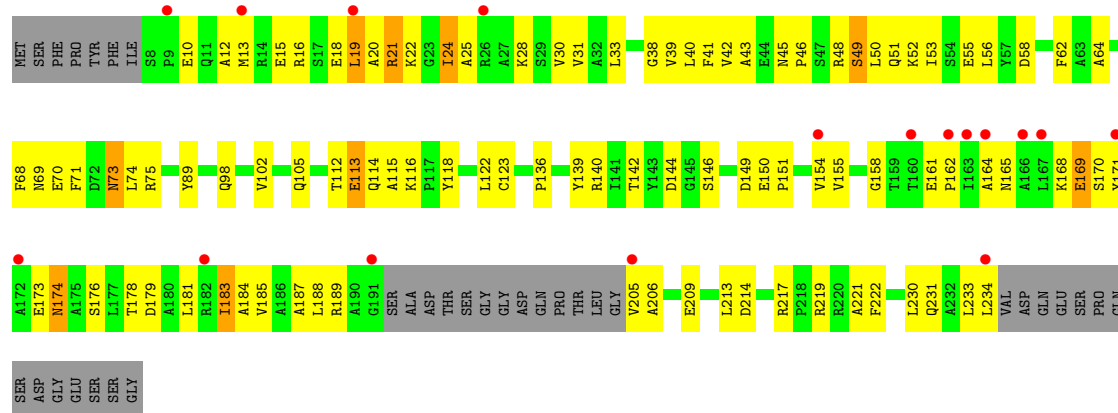
● Molecule 1: Proteasome subunit alpha



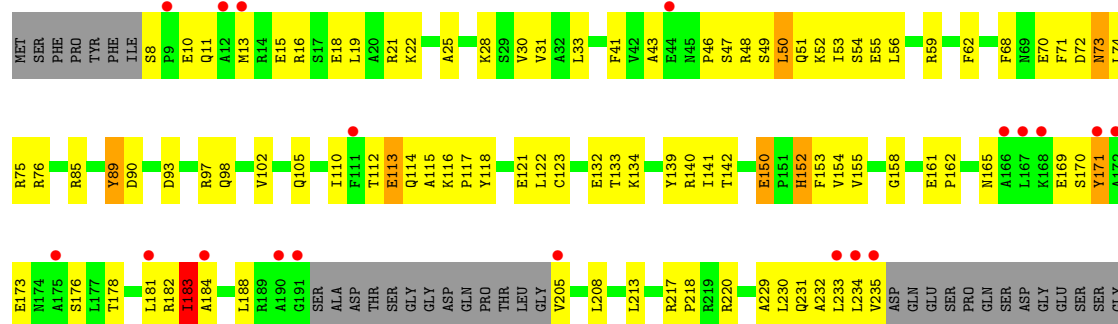
● Molecule 1: Proteasome subunit alpha



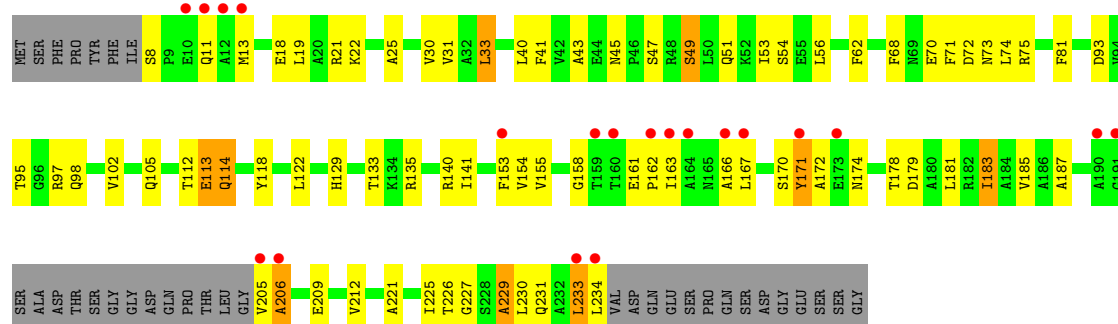
● Molecule 1: Proteasome subunit alpha



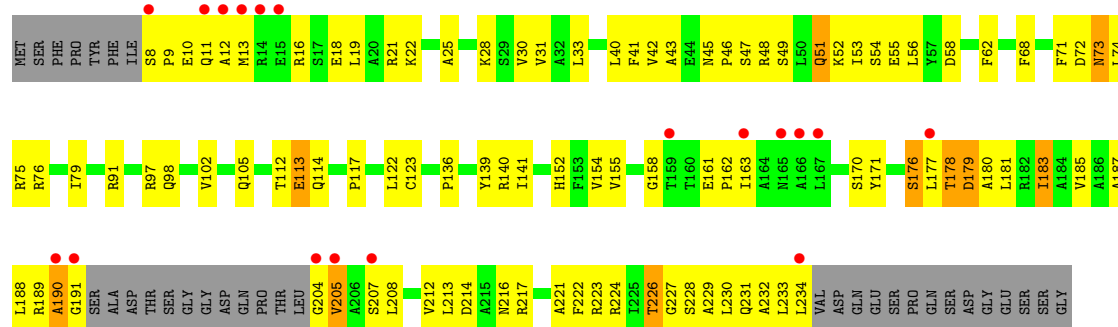
● Molecule 1: Proteasome subunit alpha



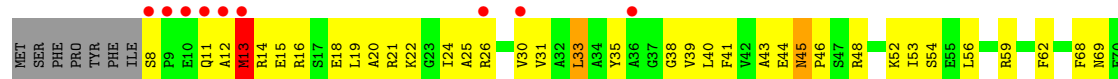
• Molecule 1: Proteasome subunit alpha

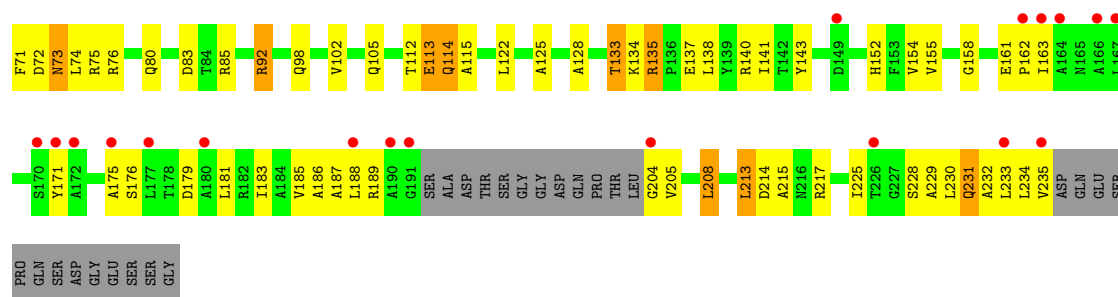


• Molecule 1: Proteasome subunit alpha

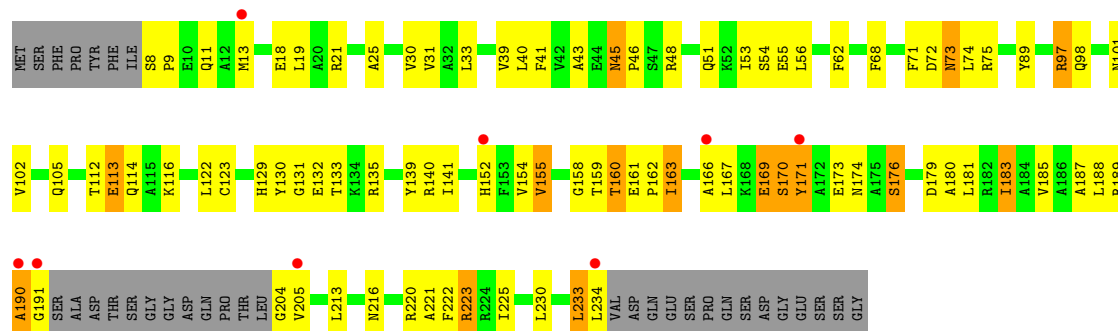


• Molecule 1: Proteasome subunit alpha

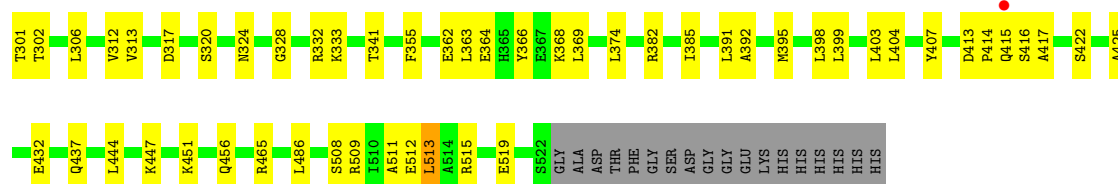




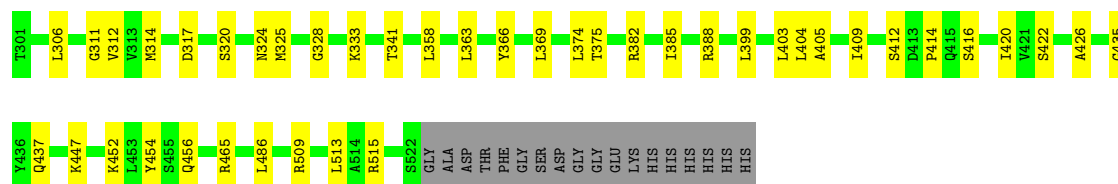
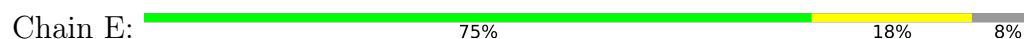
- Molecule 1: Proteasome subunit alpha



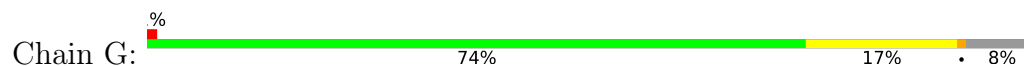
- Molecule 2: Proteasome subunit beta

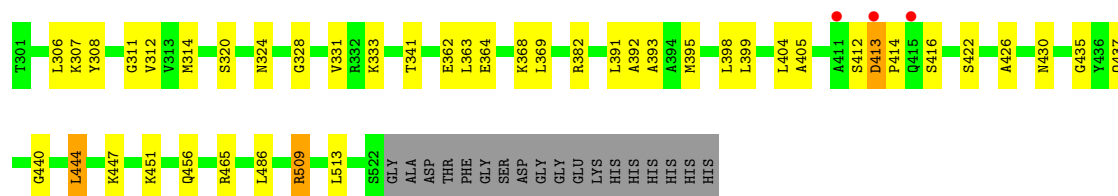


- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

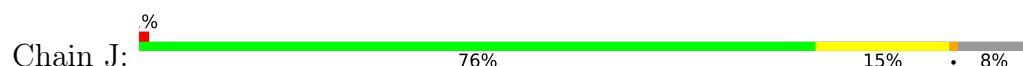




• Molecule 2: Proteasome subunit beta



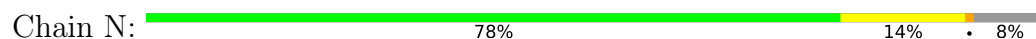
• Molecule 2: Proteasome subunit beta



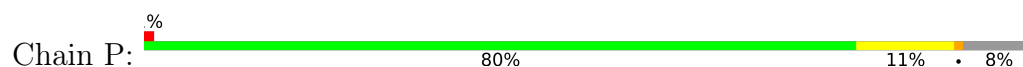
• Molecule 2: Proteasome subunit beta

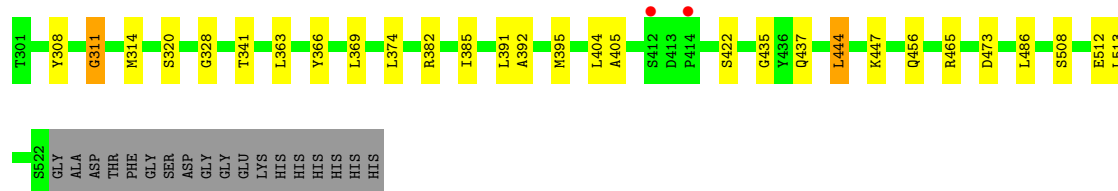


• Molecule 2: Proteasome subunit beta

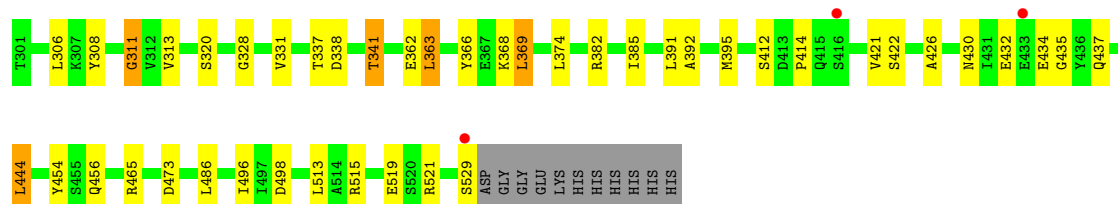
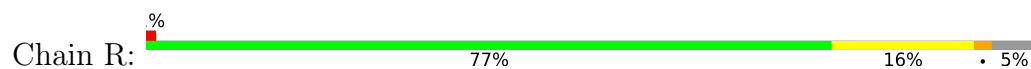


• Molecule 2: Proteasome subunit beta

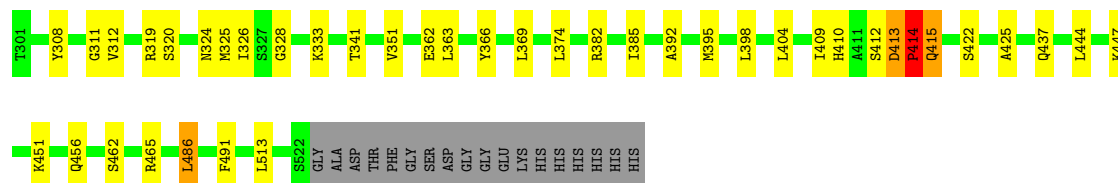




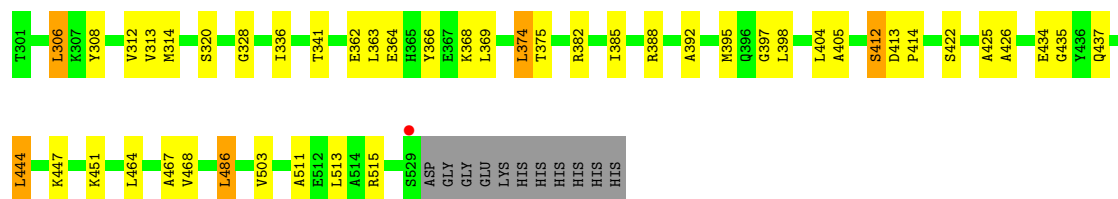
- Molecule 2: Proteasome subunit beta



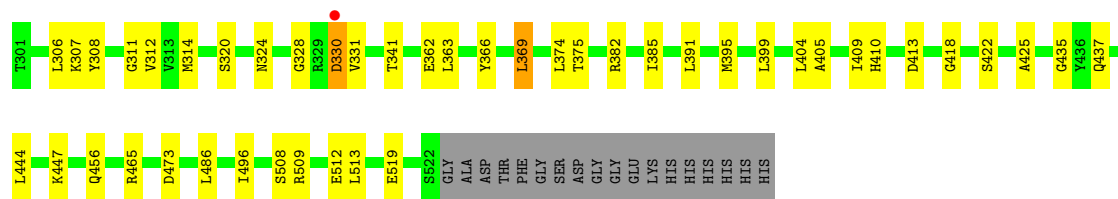
- Molecule 2: Proteasome subunit beta



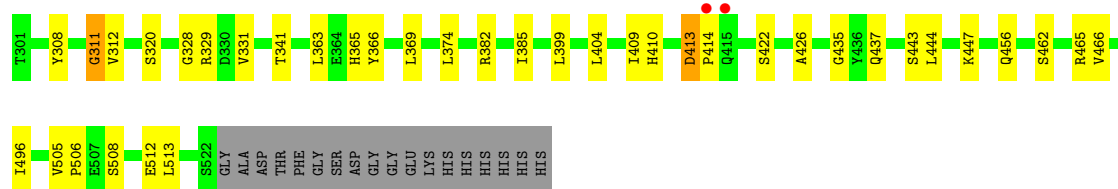
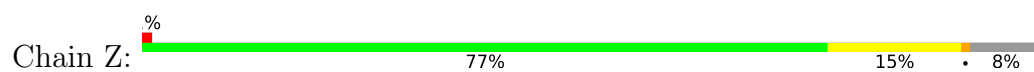
- Molecule 2: Proteasome subunit beta



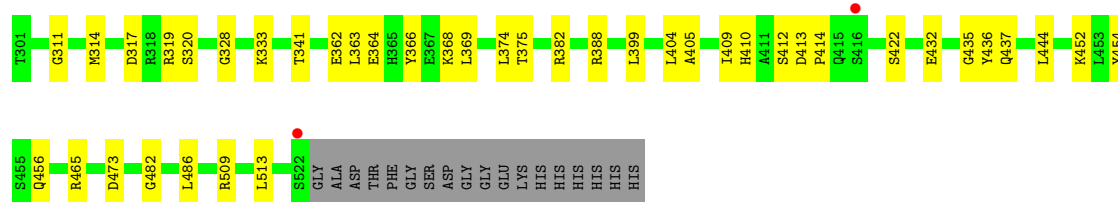
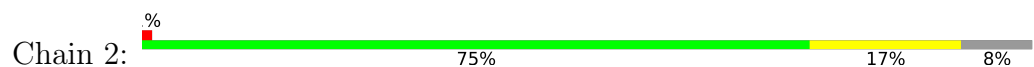
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 3: Fellutamide B



- Molecule 3: Fellutamide B



- Molecule 3: Fellutamide B



- Molecule 3: Fellutamide B



- Molecule 3: Fellutamide B



- Molecule 3: Fellutamide B

Chain f:  67% 33%



● Molecule 3: Fellutamide B

Chain g:  67% 33%



● Molecule 3: Fellutamide B

Chain h:  67% 33%



● Molecule 3: Fellutamide B

Chain i:  67% 33%



● Molecule 3: Fellutamide B

Chain j:  67% 33%



● Molecule 3: Fellutamide B

Chain k:  67% 33%



● Molecule 3: Fellutamide B

Chain l:  67% 33%



● Molecule 3: Fellutamide B

Chain m:  67% 33%



● Molecule 3: Fellutamide B

Chain n:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	170.19Å 118.10Å 194.35Å 90.00° 112.62° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-2.50) 96.5 (25.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.229 0.207 , 0.226	Depositor DCC
R_{free} test set	12081 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	48828	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.333 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: HXD

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	1.06	0/1679	1.11	11/2268 (0.5%)
1	A	0.88	2/1675 (0.1%)	1.03	8/2263 (0.4%)
1	B	0.78	0/1667	1.00	9/2252 (0.4%)
1	D	0.83	0/1671	1.17	16/2258 (0.7%)
1	F	0.95	0/1686	1.06	8/2278 (0.4%)
1	I	0.90	1/1679 (0.1%)	1.07	10/2268 (0.4%)
1	K	0.96	0/1679	1.08	8/2268 (0.4%)
1	M	0.84	1/1675 (0.1%)	1.05	9/2263 (0.4%)
1	O	0.94	0/1675	1.07	7/2263 (0.3%)
1	Q	0.89	0/1675	1.04	7/2263 (0.3%)
1	S	0.85	1/1682 (0.1%)	1.08	8/2273 (0.4%)
1	U	0.85	0/1675	1.05	12/2263 (0.5%)
1	W	0.77	0/1679	1.06	12/2268 (0.5%)
1	Y	0.92	0/1686	1.11	12/2278 (0.5%)
2	2	0.94	1/1662 (0.1%)	1.00	6/2254 (0.3%)
2	C	0.88	0/1662	1.03	5/2254 (0.2%)
2	E	0.98	0/1662	1.04	4/2254 (0.2%)
2	G	0.88	2/1662 (0.1%)	0.99	5/2254 (0.2%)
2	H	0.94	0/1662	1.01	5/2254 (0.2%)
2	J	0.96	0/1662	1.03	5/2254 (0.2%)
2	L	0.97	1/1662 (0.1%)	1.01	4/2254 (0.2%)
2	N	0.85	1/1662 (0.1%)	0.97	2/2254 (0.1%)
2	P	0.94	1/1662 (0.1%)	0.99	3/2254 (0.1%)
2	R	1.01	0/1708	1.06	4/2316 (0.2%)
2	T	1.02	1/1662 (0.1%)	1.08	7/2254 (0.3%)
2	V	1.03	4/1708 (0.2%)	1.02	4/2316 (0.2%)
2	X	0.90	1/1662 (0.1%)	1.03	6/2254 (0.3%)
2	Z	0.82	0/1662	1.02	6/2254 (0.3%)
3	a	2.63	1/24 (4.2%)	1.76	0/30
3	b	2.58	1/24 (4.2%)	1.74	0/30
3	c	2.56	1/24 (4.2%)	1.85	0/30
3	d	2.66	1/24 (4.2%)	1.77	0/30

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	2.59	1/24 (4.2%)	1.93	0/30
3	f	2.70	1/24 (4.2%)	1.76	0/30
3	g	2.68	1/24 (4.2%)	1.66	0/30
3	h	2.64	1/24 (4.2%)	1.93	0/30
3	i	2.42	1/24 (4.2%)	1.74	0/30
3	j	2.59	1/24 (4.2%)	2.04	0/30
3	k	2.61	1/24 (4.2%)	1.62	0/30
3	l	2.56	1/24 (4.2%)	1.69	0/30
3	m	2.56	1/24 (4.2%)	1.72	0/30
3	n	2.58	1/24 (4.2%)	1.75	0/30
All	All	0.94	31/47179 (0.1%)	1.05	203/63826 (0.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	3	LEU	C-OXT	11.04	1.45	1.23
3	b	3	LEU	C-OXT	10.74	1.45	1.23
3	d	3	LEU	C-OXT	10.66	1.44	1.23
3	m	3	LEU	C-OXT	10.61	1.44	1.23
3	f	3	LEU	C-OXT	10.61	1.44	1.23
3	n	3	LEU	C-OXT	10.51	1.44	1.23
3	g	3	LEU	C-OXT	10.50	1.44	1.23
3	l	3	LEU	C-OXT	10.44	1.44	1.23
3	h	3	LEU	C-OXT	10.24	1.44	1.23
3	j	3	LEU	C-OXT	10.19	1.44	1.23
3	c	3	LEU	C-OXT	10.10	1.43	1.23
3	k	3	LEU	C-OXT	9.91	1.43	1.23
3	e	3	LEU	C-OXT	9.87	1.43	1.23
3	i	3	LEU	C-OXT	9.57	1.42	1.23
1	S	89	TYR	CA-C	-6.20	1.49	1.52
2	X	308	TYR	C-O	-6.12	1.17	1.24
2	V	467	ALA	CA-CB	-6.01	1.43	1.53
2	V	312	VAL	C-O	-5.69	1.18	1.23
1	M	38	GLY	C-O	-5.59	1.19	1.23
2	V	503	VAL	C-O	-5.51	1.18	1.23
1	I	185	VAL	CA-CB	-5.49	1.47	1.54
2	V	308	TYR	C-O	-5.46	1.19	1.24
1	A	89	TYR	CA-C	-5.32	1.49	1.52
2	G	308	TYR	C-O	-5.30	1.19	1.24
2	G	440	GLY	C-O	-5.18	1.18	1.23
2	2	482	GLY	C-O	-5.16	1.18	1.23
2	T	326	ILE	C-O	-5.16	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	306	LEU	C-O	-5.15	1.17	1.23
1	A	206	ALA	CA-CB	-5.12	1.47	1.54
2	P	311	GLY	C-O	-5.08	1.18	1.23
2	L	326	ILE	C-O	-5.02	1.18	1.24

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	190	ALA	N-CA-C	-9.38	100.15	112.34
1	S	183	ILE	CB-CA-C	-9.23	99.67	112.14
1	D	49	SER	N-CA-C	8.99	124.48	112.88
1	Q	183	ILE	CB-CA-C	-8.85	100.20	112.14
1	1	221	ALA	N-CA-C	8.54	120.67	111.36
1	1	190	ALA	N-CA-C	-8.14	102.41	111.28
1	O	160	THR	N-CA-C	8.04	120.12	111.36
1	M	171	TYR	N-CA-C	7.94	120.56	110.24
2	E	311	GLY	N-CA-C	7.88	121.17	110.69
2	V	413	ASP	CA-C-N	7.74	128.44	119.47
2	V	413	ASP	C-N-CA	7.74	128.44	119.47
1	D	47	SER	N-CA-C	7.73	121.62	110.10
1	W	229	ALA	N-CA-C	-7.59	102.95	111.07
2	2	311	GLY	N-CA-C	7.58	121.49	110.80
1	D	206	ALA	N-CA-C	-7.48	101.37	113.19
1	D	183	ILE	CB-CA-C	-7.42	102.12	112.14
1	F	188	LEU	N-CA-C	-7.31	103.31	111.28
1	D	165	ASN	N-CA-C	-7.29	103.34	111.28
1	I	72	ASP	N-CA-C	-7.14	103.54	111.82
1	1	171	TYR	N-CA-C	7.07	121.19	109.46
1	U	233	LEU	N-CA-C	-7.03	104.58	113.01
2	X	413	ASP	CA-C-N	7.02	127.00	119.28
2	X	413	ASP	C-N-CA	7.02	127.00	119.28
1	Y	230	LEU	N-CA-C	-6.99	103.67	111.28
1	W	49	SER	N-CA-C	6.94	124.02	113.61
1	K	72	ASP	N-CA-C	-6.91	103.81	111.82
1	B	47	SER	N-CA-C	6.90	120.23	110.23
2	Z	413	ASP	CA-C-N	6.88	126.85	119.28
2	Z	413	ASP	C-N-CA	6.88	126.85	119.28
1	O	72	ASP	N-CA-C	-6.85	103.89	111.36
1	K	171	TYR	N-CA-C	6.81	120.17	109.96
2	L	311	GLY	N-CA-C	6.79	120.37	110.80
1	D	175	ALA	N-CA-C	-6.79	100.39	110.23
1	A	51	GLN	N-CA-C	6.73	121.01	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	47	SER	N-CA-C	6.68	119.98	109.96
1	K	49	SER	N-CA-C	6.63	121.59	112.90
1	S	72	ASP	N-CA-C	-6.59	103.92	112.23
2	G	311	GLY	N-CA-C	6.57	121.32	110.55
1	F	171	TYR	N-CA-C	6.55	119.79	109.96
1	B	72	ASP	N-CA-C	-6.54	104.23	111.36
1	B	171	TYR	N-CA-C	6.53	119.95	110.28
2	2	413	ASP	CA-C-N	6.53	128.00	119.84
2	2	413	ASP	C-N-CA	6.53	128.00	119.84
1	S	213	LEU	N-CA-C	-6.50	97.09	108.20
1	A	72	ASP	N-CA-C	-6.48	104.07	112.23
1	1	72	ASP	N-CA-C	-6.48	104.30	111.36
1	M	179	ASP	N-CA-C	-6.47	104.23	111.28
1	W	213	LEU	N-CA-C	-6.44	97.19	108.20
1	D	213	LEU	N-CA-C	-6.42	97.22	108.20
1	Y	133	THR	N-CA-C	-6.41	98.07	108.52
1	Q	206	ALA	N-CA-C	-6.39	105.48	113.28
1	U	72	ASP	N-CA-C	-6.34	104.45	111.36
2	C	415	GLN	N-CA-C	-6.31	105.44	113.01
1	M	72	ASP	N-CA-C	-6.30	104.49	111.36
1	W	51	GLN	N-CA-C	6.30	119.80	110.48
1	1	170	SER	N-CA-C	6.30	121.11	113.17
2	C	413	ASP	CA-C-N	6.29	125.70	118.85
2	C	413	ASP	C-N-CA	6.29	125.70	118.85
1	I	213	LEU	N-CA-C	-6.28	97.46	108.20
2	H	311	GLY	N-CA-C	6.28	120.85	110.55
1	U	171	TYR	N-CA-C	6.24	119.31	109.96
2	G	413	ASP	CA-C-N	6.23	125.97	119.05
2	G	413	ASP	C-N-CA	6.23	125.97	119.05
1	S	208	LEU	N-CA-C	6.20	118.60	109.24
1	K	47	SER	N-CA-C	6.20	119.45	110.28
1	D	183	ILE	N-CA-C	-6.18	104.31	110.62
1	F	33	LEU	N-CA-C	6.18	118.81	109.23
2	X	435	GLY	N-CA-C	6.16	122.26	114.25
1	D	45	ASN	CA-C-N	6.15	125.77	119.56
1	D	45	ASN	C-N-CA	6.15	125.77	119.56
1	U	51	GLN	N-CA-C	6.15	119.51	109.24
1	Q	49	SER	N-CA-C	6.12	120.81	113.23
2	P	391	LEU	N-CA-C	6.11	117.94	111.28
1	Q	187	ALA	N-CA-C	-6.11	104.62	111.28
2	J	454	TYR	N-CA-C	6.10	118.73	111.71
1	U	206	ALA	N-CA-C	-6.10	105.69	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	227	GLY	N-CA-C	6.08	122.33	111.02
1	W	72	ASP	N-CA-C	-6.08	104.77	111.82
1	F	216	ASN	N-CA-C	6.07	117.89	111.28
1	Y	205	VAL	N-CA-C	6.05	116.79	110.62
1	Y	45	ASN	CA-C-N	6.03	125.58	119.19
1	Y	45	ASN	C-N-CA	6.03	125.58	119.19
1	D	113	GLU	N-CA-C	6.01	120.75	113.17
1	1	45	ASN	CA-C-N	5.96	125.35	118.85
1	1	45	ASN	C-N-CA	5.96	125.35	118.85
2	G	435	GLY	N-CA-C	5.96	121.99	114.25
1	U	229	ALA	N-CA-C	-5.95	104.79	111.28
1	W	183	ILE	CB-CA-C	-5.95	104.11	112.14
1	F	72	ASP	N-CA-C	-5.94	104.75	112.23
1	I	54	SER	N-CA-C	5.92	118.18	109.24
1	O	171	TYR	N-CA-C	5.92	118.92	110.10
1	1	113	GLU	N-CA-C	5.92	120.63	113.17
1	Y	72	ASP	N-CA-C	-5.92	104.95	111.82
1	D	72	ASP	N-CA-C	-5.91	104.96	111.82
1	I	171	TYR	N-CA-C	5.90	119.02	110.28
1	A	113	GLU	N-CA-C	5.90	120.63	113.38
2	E	435	GLY	N-CA-C	5.88	121.90	114.25
1	U	113	GLU	N-CA-C	5.88	120.61	113.38
1	1	213	LEU	N-CA-C	-5.86	98.18	108.20
1	M	113	GLU	N-CA-C	5.86	120.55	113.17
1	I	33	LEU	N-CA-C	5.83	118.26	109.23
1	S	47	SER	N-CA-C	5.82	118.89	110.28
1	A	207	SER	N-CA-C	-5.81	104.89	113.61
1	I	184	ALA	N-CA-C	5.78	117.25	111.07
2	R	311	GLY	N-CA-C	5.77	120.02	110.55
1	Y	213	LEU	N-CA-C	-5.75	98.36	108.20
1	K	213	LEU	N-CA-C	-5.75	98.37	108.20
1	D	160	THR	N-CA-C	5.75	118.76	111.69
2	H	399	LEU	N-CA-C	5.75	118.58	109.96
1	O	113	GLU	N-CA-C	5.72	120.38	113.17
2	T	414	PRO	N-CA-C	5.72	121.48	113.53
1	Y	13	MET	N-CA-C	-5.71	106.40	113.19
1	A	213	LEU	N-CA-C	-5.70	98.45	108.20
1	M	170	SER	N-CA-C	5.70	117.29	111.14
2	E	399	LEU	N-CA-C	5.69	118.81	109.76
2	Z	311	GLY	N-CA-C	5.65	119.82	110.55
2	T	413	ASP	CA-C-N	5.64	125.31	119.05
2	T	413	ASP	C-N-CA	5.64	125.31	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	399	LEU	N-CA-C	5.63	118.41	109.96
2	2	454	TYR	N-CA-C	5.63	118.14	111.33
1	W	113	GLU	N-CA-C	5.62	120.29	113.38
1	Y	208	LEU	N-CA-C	5.60	118.35	109.50
1	M	178	THR	N-CA-C	5.59	117.46	111.36
2	C	399	LEU	N-CA-C	5.59	118.34	109.96
1	F	113	GLU	N-CA-C	5.57	120.23	113.38
1	S	113	GLU	N-CA-C	5.57	120.19	113.17
2	V	435	GLY	N-CA-C	5.56	121.31	114.69
1	W	205	VAL	N-CA-C	5.55	116.94	110.62
1	Y	33	LEU	N-CA-C	5.54	117.82	109.23
2	R	454	TYR	N-CA-C	5.53	118.07	111.71
1	1	51	GLN	N-CA-C	5.53	119.08	110.17
1	M	213	LEU	N-CA-C	-5.52	98.76	108.20
1	U	174	ASN	N-CA-C	5.51	119.18	111.74
2	J	435	GLY	N-CA-C	5.51	121.25	114.69
2	E	454	TYR	N-CA-C	5.50	118.03	111.71
1	A	45	ASN	CA-C-N	5.49	124.84	118.85
1	A	45	ASN	C-N-CA	5.49	124.84	118.85
1	O	47	SER	N-CA-C	5.49	118.28	110.10
1	A	49	SER	N-CA-C	5.48	121.84	113.61
1	Q	113	GLU	N-CA-C	5.47	120.11	113.38
2	R	435	GLY	N-CA-C	5.46	121.58	115.08
2	2	435	GLY	N-CA-C	5.46	121.58	115.08
1	B	227	GLY	N-CA-C	5.45	121.15	111.02
2	H	391	LEU	N-CA-C	5.45	117.22	111.28
2	T	311	GLY	N-CA-C	5.44	117.93	110.69
2	H	435	GLY	N-CA-C	5.44	121.32	114.25
1	U	47	SER	N-CA-C	5.44	118.20	110.10
1	S	152	HIS	N-CA-C	5.43	119.67	112.72
1	O	216	ASN	N-CA-C	5.42	119.51	113.01
2	L	319	ARG	N-CA-C	5.42	118.50	110.48
1	W	176	SER	N-CA-C	-5.40	103.40	110.53
1	I	58	ASP	N-CA-C	5.40	117.86	111.33
2	2	399	LEU	N-CA-C	5.40	118.06	109.96
2	N	519	GLU	N-CA-C	-5.39	105.48	111.36
2	R	391	LEU	N-CA-C	5.35	117.12	111.28
1	K	51	GLN	N-CA-C	5.35	118.53	109.76
1	D	52	LYS	N-CA-C	-5.35	106.14	113.30
1	O	185	VAL	CB-CA-C	-5.34	104.93	112.14
1	B	113	GLU	N-CA-C	5.34	119.90	113.17
1	Q	169	GLU	N-CA-C	5.33	117.17	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	399	LEU	N-CA-C	5.33	118.03	110.10
2	L	454	TYR	N-CA-C	5.32	117.77	111.33
1	B	49	SER	N-CA-C	5.32	121.59	113.61
1	S	171	TYR	N-CA-C	5.32	117.94	110.23
1	B	44	GLU	N-CA-C	-5.27	101.18	109.25
1	F	213	LEU	N-CA-C	-5.24	99.24	108.20
2	G	399	LEU	N-CA-C	5.23	118.08	109.76
2	H	454	TYR	N-CA-C	5.22	117.65	111.33
2	T	415	GLN	N-CA-C	-5.20	106.19	112.54
1	K	113	GLU	N-CA-C	5.20	119.72	113.17
1	I	176	SER	N-CA-C	-5.18	104.03	110.41
2	P	311	GLY	N-CA-C	5.18	120.50	110.66
1	Y	176	SER	N-CA-C	5.17	116.77	110.41
1	B	208	LEU	N-CA-C	5.17	118.15	110.14
1	M	68	PHE	N-CA-C	5.17	117.31	111.11
1	W	221	ALA	N-CA-C	5.17	116.99	111.36
2	T	462	SER	N-CA-C	-5.16	105.83	111.82
1	U	49	SER	N-CA-C	5.16	119.70	113.41
1	Q	221	ALA	N-CA-C	5.15	116.97	111.36
1	F	29	SER	N-CA-C	5.14	118.13	110.52
2	J	501	GLY	N-CA-C	5.12	118.53	112.33
2	J	319	ARG	N-CA-C	5.12	118.06	110.48
2	P	435	GLY	N-CA-C	5.11	120.90	114.25
2	V	336	ILE	N-CA-C	-5.11	100.97	108.54
1	Y	113	GLU	N-CA-C	5.11	119.61	113.17
1	K	183	ILE	CB-CA-C	-5.10	105.26	112.14
2	X	330	ASP	CB-CA-C	-5.10	101.88	110.64
2	J	413	ASP	CB-CA-C	-5.09	105.86	110.44
2	Z	435	GLY	N-CA-C	5.08	120.86	114.25
1	U	221	ALA	N-CA-C	5.08	116.89	111.36
2	C	403	LEU	N-CA-C	-5.08	100.18	108.76
1	D	207	SER	N-CA-C	-5.07	105.82	112.41
1	I	12	ALA	N-CA-C	-5.06	105.77	111.28
2	T	319	ARG	N-CA-C	5.05	117.96	110.48
1	W	178	THR	N-CA-C	5.04	116.47	111.07
2	X	311	GLY	N-CA-C	5.04	118.82	110.55
1	D	164	ALA	N-CA-C	5.04	116.58	111.14
2	L	435	GLY	N-CA-C	5.04	120.80	114.25
1	I	47	SER	N-CA-C	5.03	117.52	110.23
2	N	311	GLY	N-CA-C	5.03	117.89	110.80
2	Z	443	SER	N-CA-C	5.03	116.76	111.28
1	I	183	ILE	CB-CA-C	-5.02	105.36	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ALA	N-CA-C	-5.01	107.00	113.01

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	1654	0	1651	95	0
1	A	1650	0	1648	74	0
1	B	1642	0	1637	63	0
1	D	1646	0	1645	148	0
1	F	1661	0	1660	70	0
1	I	1654	0	1651	62	0
1	K	1654	0	1651	86	0
1	M	1650	0	1648	72	0
1	O	1650	0	1648	97	0
1	Q	1650	0	1648	90	0
1	S	1657	0	1657	100	0
1	U	1650	0	1648	64	0
1	W	1654	0	1651	90	0
1	Y	1661	0	1660	123	0
2	2	1638	0	1629	28	0
2	C	1638	0	1629	41	0
2	E	1638	0	1629	32	0
2	G	1638	0	1629	35	0
2	H	1638	0	1629	25	0
2	J	1638	0	1629	33	0
2	L	1638	0	1629	54	0
2	N	1638	0	1629	23	0
2	P	1638	0	1629	20	0
2	R	1683	0	1665	39	0
2	T	1638	0	1629	37	0
2	V	1683	0	1665	31	0
2	X	1638	0	1629	30	0
2	Z	1638	0	1629	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	a	25	0	24	0	0
3	b	25	0	24	1	0
3	c	25	0	24	3	0
3	d	25	0	24	0	0
3	e	25	0	24	0	0
3	f	25	0	24	1	0
3	g	25	0	24	1	0
3	h	25	0	24	0	0
3	i	25	0	24	1	0
3	j	25	0	24	1	0
3	k	25	0	24	0	0
3	l	25	0	24	1	0
3	m	25	0	24	1	0
3	n	25	0	24	1	0
4	a	7	0	6	2	0
4	b	7	0	6	1	0
4	c	7	0	6	0	0
4	d	7	0	6	0	0
4	e	7	0	6	1	0
4	f	7	0	6	0	0
4	g	7	0	6	1	0
4	h	7	0	6	2	0
4	i	7	0	6	2	0
4	j	7	0	6	1	0
4	k	7	0	6	0	0
4	l	7	0	6	1	0
4	m	7	0	6	1	0
4	n	7	0	6	1	0
5	1	55	0	0	2	0
5	2	118	0	0	6	0
5	A	32	0	0	3	0
5	B	42	0	0	3	0
5	C	131	0	0	10	0
5	D	25	0	0	3	0
5	E	130	0	0	7	0
5	F	41	0	0	6	0
5	G	113	0	0	8	0
5	H	126	0	0	6	0
5	I	38	0	0	6	0
5	J	122	0	0	3	0
5	K	33	0	0	6	0
5	L	132	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	42	0	0	0	0
5	N	121	0	0	3	0
5	O	39	0	0	6	0
5	P	111	0	0	2	0
5	Q	34	0	0	0	0
5	R	143	0	0	9	0
5	S	43	0	0	19	0
5	T	103	0	0	5	0
5	U	33	0	0	2	0
5	V	149	0	0	5	0
5	W	26	0	0	3	0
5	X	115	0	0	4	0
5	Y	22	0	0	3	0
5	Z	106	0	0	1	0
All	All	48828	0	46401	1557	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HB2	1:D:217:ARG:NH1	1.41	1.30
1:A:13:MET:CE	1:O:116:LYS:HD3	1.62	1.27
1:M:217:ARG:HD3	1:M:223:ARG:NH2	1.53	1.24
1:B:170:SER:OG	1:B:183:ILE:HG23	1.39	1.23
1:Y:229:ALA:O	1:Y:233:LEU:HD13	1.41	1.20
1:D:49:SER:C	1:D:50:LEU:HD23	1.65	1.19
1:W:176:SER:HB3	1:W:179:ASP:OD2	1.42	1.19
1:Q:10:GLU:HG3	1:Y:15:GLU:OE1	1.41	1.18
1:I:155:VAL:CG1	1:I:160:THR:HG23	1.71	1.18
1:F:166:ALA:O	1:F:170:SER:HB2	1.43	1.17
1:A:13:MET:HE2	1:O:116:LYS:CD	1.75	1.16
1:I:179:ASP:O	1:I:183:ILE:HG22	1.42	1.16
1:D:152:HIS:HB3	1:D:171:TYR:CZ	1.82	1.13
1:M:205:VAL:HG12	1:M:234:LEU:HD23	1.29	1.13
2:L:451:LYS:HE3	5:L:3067:HOH:O	1.44	1.13
2:L:456:GLN:NE2	2:L:465:ARG:HH22	1.45	1.13
1:O:178:THR:CG2	1:O:182:ARG:HH12	1.63	1.12
1:B:232:ALA:O	1:B:233:LEU:HB2	1.41	1.11
1:S:170:SER:OG	1:S:183:ILE:HG12	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:92:ARG:HH11	1:Y:92:ARG:CG	1.60	1.10
1:1:152:HIS:HB3	1:1:171:TYR:CE2	1.86	1.10
1:D:214:ASP:HB3	1:D:217:ARG:NH1	1.66	1.10
1:O:152:HIS:HB3	1:O:171:TYR:CE2	1.87	1.09
1:M:205:VAL:HG12	1:M:234:LEU:CD2	1.83	1.08
2:R:529:SER:HB3	5:R:1999:HOH:O	1.53	1.08
2:Z:456:GLN:NE2	2:Z:465:ARG:HH12	1.51	1.07
1:D:217:ARG:HH11	1:D:217:ARG:CB	1.67	1.07
1:1:155:VAL:HG12	1:1:160:THR:HG23	1.17	1.07
2:T:409:ILE:HD11	2:T:410:HIS:HE1	1.20	1.06
1:U:231:GLN:HA	1:U:234:LEU:HD12	1.11	1.06
1:A:51:GLN:HG2	1:A:209:GLU:OE2	1.56	1.05
1:A:13:MET:HE2	1:O:116:LYS:HD3	1.06	1.05
1:D:214:ASP:HB3	1:D:217:ARG:HH12	0.94	1.05
2:G:465:ARG:HD2	5:G:2889:HOH:O	1.52	1.05
1:Y:92:ARG:HH11	1:Y:92:ARG:HG2	1.13	1.05
2:T:491:PHE:HB2	5:T:3058:HOH:O	1.55	1.04
1:D:13:MET:HE2	1:Q:19:LEU:HD21	1.40	1.04
1:Y:22:LYS:HG2	1:Y:26:ARG:HH21	1.23	1.03
1:D:173:GLU:HB3	1:D:174:ASN:OD1	1.59	1.02
1:Q:171:TYR:HE2	1:Q:173:GLU:HG3	1.25	1.02
1:S:150:GLU:HA	1:S:150:GLU:OE1	1.58	1.01
1:Y:8:SER:CB	1:Y:11:GLN:HB3	1.89	1.01
1:W:181:LEU:O	1:W:185:VAL:HG23	1.58	1.01
1:D:177:LEU:HD23	1:D:233:LEU:HD21	1.43	1.00
1:K:217:ARG:HH11	1:K:217:ARG:CG	1.72	1.00
2:E:465:ARG:HD2	5:E:2886:HOH:O	1.62	1.00
1:K:217:ARG:HH11	1:K:217:ARG:HG3	0.85	0.99
1:M:170:SER:OG	1:M:183:ILE:HG12	1.62	0.99
1:O:178:THR:CG2	1:O:182:ARG:NH1	2.26	0.99
2:2:388:ARG:HD2	5:2:3066:HOH:O	1.60	0.98
1:D:13:MET:CE	1:Q:19:LEU:HD21	1.93	0.98
1:F:18:GLU:CD	1:F:21:ARG:HH12	1.70	0.98
1:M:217:ARG:CD	1:M:223:ARG:NH2	2.27	0.98
2:T:409:ILE:HG13	2:T:410:HIS:ND1	1.77	0.98
2:L:456:GLN:HE22	2:L:465:ARG:NH2	1.62	0.98
1:U:166:ALA:O	1:U:170:SER:HB2	1.63	0.98
1:K:116:LYS:HD2	1:M:13:MET:HE1	1.45	0.97
1:Y:152:HIS:CD2	1:Y:171:TYR:HE2	1.82	0.97
1:Y:8:SER:OG	1:Y:11:GLN:HB3	1.65	0.96
1:D:49:SER:O	1:D:50:LEU:HD23	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:409:ILE:HD11	2:T:410:HIS:CE1	2.01	0.96
1:Y:152:HIS:HB3	1:Y:171:TYR:CZ	2.01	0.95
1:K:217:ARG:HG3	1:K:217:ARG:NH1	1.57	0.95
1:A:170:SER:OG	1:A:183:ILE:HG23	1.65	0.95
1:1:169:GLU:HA	1:1:169:GLU:OE1	1.63	0.95
1:D:234:LEU:HD23	1:D:234:LEU:O	1.67	0.94
1:F:167:LEU:HA	1:F:170:SER:HB3	1.49	0.94
1:1:152:HIS:CD2	1:1:171:TYR:HE2	1.87	0.94
1:Y:152:HIS:CD2	1:Y:171:TYR:CE2	2.56	0.93
2:Z:456:GLN:HE22	2:Z:465:ARG:HH12	1.05	0.93
1:M:205:VAL:CG1	1:M:234:LEU:HD23	1.97	0.93
2:R:456:GLN:NE2	2:R:465:ARG:HH21	1.66	0.93
2:X:444:LEU:HB2	5:X:2899:HOH:O	1.67	0.93
2:R:456:GLN:HE21	2:R:465:ARG:HH21	1.05	0.93
1:1:155:VAL:HG12	1:1:160:THR:CG2	1.99	0.93
1:M:217:ARG:HD3	1:M:223:ARG:CZ	1.98	0.92
1:Q:20:ALA:O	1:Q:24:ILE:HG13	1.69	0.92
2:T:409:ILE:HG13	2:T:410:HIS:CE1	2.04	0.92
1:1:31:VAL:HG22	1:1:155:VAL:HG22	1.51	0.92
2:H:456:GLN:NE2	2:H:465:ARG:HH21	1.68	0.91
1:S:152:HIS:CD2	1:S:171:TYR:HE2	1.87	0.91
1:Y:8:SER:HB2	1:Y:11:GLN:HB3	1.50	0.91
1:A:219:ARG:HB3	5:A:1319:HOH:O	1.68	0.91
1:D:48:ARG:HH12	1:K:137:GLU:HB3	1.34	0.91
1:Q:164:ALA:O	1:Q:168:LYS:HG3	1.70	0.91
1:U:231:GLN:CA	1:U:234:LEU:HD12	2.00	0.91
2:R:456:GLN:HE21	2:R:465:ARG:NH2	1.69	0.90
1:M:41:PHE:HB3	1:M:53:ILE:HD13	1.51	0.90
1:K:142:THR:HA	5:K:2919:HOH:O	1.70	0.90
1:S:182:ARG:NH2	1:S:235:VAL:HB	1.85	0.90
2:P:456:GLN:HE21	2:P:465:ARG:NH2	1.68	0.90
1:O:76:ARG:HD3	5:O:1070:HOH:O	1.70	0.90
1:D:48:ARG:CG	1:K:149:ASP:OD1	2.20	0.89
1:D:181:LEU:HD12	1:D:181:LEU:O	1.72	0.89
1:D:10:GLU:HG3	1:Q:15:GLU:HG3	1.54	0.89
2:J:456:GLN:NE2	2:J:465:ARG:HH21	1.70	0.89
1:O:18:GLU:O	1:O:22:LYS:HG3	1.71	0.89
1:Q:18:GLU:HG3	1:Q:22:LYS:HE3	1.52	0.89
2:J:456:GLN:NE2	2:J:465:ARG:NH2	2.20	0.89
1:M:170:SER:HG	1:M:183:ILE:HG12	1.38	0.88
2:H:456:GLN:HE21	2:H:465:ARG:NH2	1.69	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:231:GLN:HA	1:U:234:LEU:CD1	2.03	0.88
2:C:355:PHE:HE1	5:C:2910:HOH:O	1.57	0.88
2:H:456:GLN:HE21	2:H:465:ARG:HH21	1.17	0.87
5:S:2958:HOH:O	1:1:112:THR:CG2	2.22	0.87
1:U:231:GLN:O	1:U:234:LEU:HB2	1.74	0.87
2:T:409:ILE:CD1	2:T:410:HIS:CE1	2.58	0.87
1:S:152:HIS:CD2	1:S:171:TYR:CE2	2.63	0.87
2:T:409:ILE:CG1	2:T:410:HIS:ND1	2.37	0.87
1:1:155:VAL:CG1	1:1:160:THR:CG2	2.50	0.86
1:Y:92:ARG:HG2	1:Y:92:ARG:NH1	1.86	0.86
1:1:152:HIS:CG	1:1:171:TYR:HE2	1.93	0.86
2:T:409:ILE:CG1	2:T:410:HIS:CE1	2.58	0.86
2:L:372:VAL:CG2	2:L:373:PRO:HD2	2.05	0.86
2:L:372:VAL:CG2	2:L:373:PRO:CD	2.53	0.85
1:B:8:SER:N	1:B:11:GLN:H	1.73	0.85
2:G:392:ALA:HA	2:G:395:MET:HE3	1.58	0.85
1:I:170:SER:OG	1:I:183:ILE:HG23	1.76	0.85
5:C:3006:HOH:O	4:a:4:HXD:H22	1.75	0.85
2:V:388:ARG:HD2	5:V:2903:HOH:O	1.76	0.85
1:O:178:THR:HG23	1:O:182:ARG:HH12	1.39	0.85
1:Q:174:ASN:N	1:Q:174:ASN:HD22	1.74	0.85
1:M:163:ILE:HG23	1:M:187:ALA:O	1.76	0.85
2:P:456:GLN:HE21	2:P:465:ARG:HH21	1.25	0.85
1:F:18:GLU:HG3	1:F:22:LYS:HE2	1.59	0.84
1:U:13:MET:HE1	1:1:116:LYS:HD2	1.57	0.84
2:J:392:ALA:HA	2:J:395:MET:HE2	1.59	0.84
1:Y:92:ARG:CG	1:Y:92:ARG:NH1	2.31	0.84
2:G:509:ARG:HD3	5:G:3043:HOH:O	1.75	0.84
1:D:217:ARG:NH1	1:D:217:ARG:CB	2.30	0.84
1:1:163:ILE:HG23	1:1:187:ALA:O	1.77	0.83
2:P:456:GLN:NE2	2:P:465:ARG:HH21	1.75	0.83
1:K:18:GLU:CD	1:K:21:ARG:HH12	1.86	0.83
1:K:140:ARG:HG2	1:K:140:ARG:HH11	1.42	0.83
1:Y:152:HIS:CG	1:Y:171:TYR:CE2	2.67	0.83
1:Y:25:ALA:O	1:Y:158:GLY:HA2	1.79	0.83
1:Y:19:LEU:C	1:Y:19:LEU:HD23	2.04	0.82
1:Q:31:VAL:HG22	1:Q:155:VAL:HG22	1.58	0.82
1:B:31:VAL:HG22	1:B:155:VAL:HG22	1.61	0.82
1:1:152:HIS:CB	1:1:171:TYR:CE2	2.62	0.82
1:K:31:VAL:HG22	1:K:155:VAL:HG22	1.61	0.82
1:W:31:VAL:HG22	1:W:155:VAL:HG22	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:VAL:HG22	1:M:155:VAL:HG22	1.61	0.82
1:O:178:THR:HG22	1:O:182:ARG:NH1	1.92	0.82
1:D:217:ARG:HH21	1:D:223:ARG:HB3	1.45	0.82
1:W:8:SER:N	1:W:12:ALA:H	1.78	0.82
1:A:230:LEU:O	1:A:234:LEU:HD13	1.80	0.82
1:O:182:ARG:HD3	1:O:234:LEU:HA	1.62	0.81
1:F:116:LYS:HD2	1:W:13:MET:HE1	1.60	0.81
1:M:163:ILE:HG23	1:M:187:ALA:C	2.04	0.81
1:B:170:SER:HG	1:B:183:ILE:HG23	1.41	0.81
2:L:372:VAL:HG22	2:L:373:PRO:HD2	1.62	0.81
2:N:456:GLN:NE2	2:N:465:ARG:HH21	1.78	0.81
1:D:31:VAL:HG22	1:D:155:VAL:HG22	1.61	0.81
1:S:28:LYS:HE3	1:S:46:PRO:HG2	1.61	0.81
1:S:170:SER:O	1:S:183:ILE:HD11	1.80	0.81
1:B:205:VAL:HG23	1:B:206:ALA:H	1.46	0.80
2:C:355:PHE:CE1	5:C:2910:HOH:O	2.31	0.80
1:S:31:VAL:HG22	1:S:155:VAL:HG22	1.63	0.80
1:U:31:VAL:HG22	1:U:155:VAL:HG22	1.63	0.80
1:I:31:VAL:HG22	1:I:155:VAL:HG22	1.60	0.80
2:N:456:GLN:HE21	2:N:465:ARG:HH21	1.25	0.80
1:Q:171:TYR:CE2	1:Q:173:GLU:HG3	2.14	0.80
1:Y:8:SER:OG	1:Y:11:GLN:CG	2.30	0.80
2:J:382:ARG:NH2	2:J:385:ILE:HD13	1.97	0.80
1:S:150:GLU:OE1	1:S:150:GLU:CA	2.30	0.80
1:Y:8:SER:OG	1:Y:11:GLN:CB	2.30	0.80
2:L:509:ARG:HD3	5:L:2882:HOH:O	1.81	0.80
1:D:152:HIS:HB3	1:D:171:TYR:CE1	2.17	0.79
1:S:170:SER:OG	1:S:183:ILE:CG1	2.29	0.79
1:Y:31:VAL:HG22	1:Y:155:VAL:HG22	1.64	0.79
1:O:179:ASP:O	1:O:183:ILE:CG2	2.30	0.79
1:W:179:ASP:O	1:W:183:ILE:HG13	1.82	0.79
1:Q:112:THR:CG2	1:Y:115:ALA:HB3	2.12	0.79
1:I:185:VAL:O	1:I:189:ARG:HG3	1.82	0.79
1:A:31:VAL:HG22	1:A:155:VAL:HG22	1.63	0.79
1:D:234:LEU:O	1:D:234:LEU:CD2	2.30	0.79
1:U:135:ARG:HD3	1:I:48:ARG:HH12	1.48	0.79
1:M:152:HIS:HB3	1:M:171:TYR:CE2	2.17	0.79
2:J:392:ALA:HA	2:J:395:MET:CE	2.11	0.78
2:V:306:LEU:HD12	2:V:313:VAL:HG12	1.65	0.78
1:Y:20:ALA:O	1:Y:24:ILE:HG13	1.83	0.78
2:2:409:ILE:HG23	5:2:2949:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:25:ALA:O	1:W:158:GLY:HA2	1.83	0.78
1:1:155:VAL:HG11	1:1:160:THR:HG23	1.65	0.78
1:Q:10:GLU:HG3	1:Y:15:GLU:CD	2.08	0.78
1:S:121:GLU:HG3	5:S:3022:HOH:O	1.81	0.78
2:L:372:VAL:HG22	2:L:373:PRO:CD	2.12	0.78
1:Q:25:ALA:O	1:Q:158:GLY:HA2	1.83	0.78
1:K:45:ASN:HD22	1:K:52:LYS:HG3	1.47	0.78
1:A:25:ALA:O	1:A:158:GLY:HA2	1.84	0.78
1:D:50:LEU:CD2	5:D:2921:HOH:O	2.31	0.78
2:L:306:LEU:HD12	2:L:313:VAL:CG1	2.14	0.78
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.65	0.78
2:L:456:GLN:HE22	2:L:465:ARG:HH22	0.82	0.78
1:O:31:VAL:HG22	1:O:155:VAL:HG22	1.64	0.77
1:O:166:ALA:O	1:O:170:SER:CB	2.32	0.77
1:D:39:VAL:HG23	1:D:127:VAL:CG1	2.15	0.77
1:W:189:ARG:C	1:W:191:GLY:N	2.39	0.77
1:S:25:ALA:O	1:S:158:GLY:HA2	1.84	0.77
1:S:49:SER:C	1:S:50:LEU:HD23	2.10	0.77
1:D:25:ALA:O	1:D:158:GLY:HA2	1.84	0.77
1:O:173:GLU:CG	1:O:174:ASN:OD1	2.32	0.76
1:U:25:ALA:O	1:U:158:GLY:HA2	1.85	0.76
1:M:25:ALA:O	1:M:158:GLY:HA2	1.85	0.76
1:W:180:ALA:HA	1:W:183:ILE:HD12	1.65	0.76
1:1:205:VAL:HG12	1:1:230:LEU:HG	1.66	0.76
1:D:177:LEU:CD2	1:D:233:LEU:HD21	2.15	0.76
1:F:31:VAL:HG22	1:F:155:VAL:HG22	1.66	0.76
1:D:152:HIS:CD2	1:D:171:TYR:CE2	2.73	0.76
1:Q:105:GLN:HG3	1:Y:73:ASN:HD21	1.49	0.76
1:O:173:GLU:HG2	1:O:174:ASN:OD1	1.84	0.76
1:A:116:LYS:HD2	1:B:13:MET:HE1	1.66	0.76
1:U:163:ILE:HG23	1:U:187:ALA:O	1.86	0.76
1:W:48:ARG:NH2	1:Y:137:GLU:HG2	2.01	0.76
1:Q:112:THR:HG23	1:Y:115:ALA:HB3	1.67	0.76
1:S:182:ARG:HH21	1:S:235:VAL:HB	1.51	0.75
1:Y:229:ALA:O	1:Y:233:LEU:CD1	2.29	0.75
1:D:217:ARG:HB2	1:D:217:ARG:HH11	0.72	0.75
2:2:319:ARG:HD3	5:2:877:HOH:O	1.86	0.75
1:S:176:SER:HB3	5:S:2939:HOH:O	1.85	0.75
1:1:179:ASP:O	1:1:183:ILE:CG2	2.30	0.75
1:D:48:ARG:HG3	1:K:149:ASP:OD1	1.85	0.75
2:C:515:ARG:HD2	5:C:1980:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:306:LEU:CD1	2:L:313:VAL:CG1	2.64	0.75
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.69	0.75
1:D:173:GLU:C	1:D:174:ASN:OD1	2.29	0.74
2:X:456:GLN:HE21	2:X:465:ARG:HH21	1.33	0.74
1:1:152:HIS:CG	1:1:171:TYR:CE2	2.75	0.74
1:Y:92:ARG:HH11	1:Y:92:ARG:HG3	1.52	0.74
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.68	0.74
2:E:456:GLN:HE21	2:E:465:ARG:NH2	1.85	0.74
1:O:152:HIS:CB	1:O:171:TYR:CE2	2.68	0.74
1:U:230:LEU:O	1:U:234:LEU:HG	1.86	0.74
1:B:25:ALA:O	1:B:158:GLY:HA2	1.86	0.74
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.67	0.74
1:Y:41:PHE:HB3	1:Y:53:ILE:HD13	1.70	0.74
1:B:15:GLU:OE1	1:I:9:PRO:HD2	1.88	0.73
1:D:184:ALA:O	1:D:188:LEU:HD13	1.87	0.73
1:Y:18:GLU:CD	1:Y:21:ARG:HH12	1.96	0.73
2:L:372:VAL:HG23	2:L:373:PRO:CD	2.19	0.73
2:C:456:GLN:HE21	2:C:465:ARG:HH21	1.36	0.73
1:O:178:THR:HG22	1:O:182:ARG:CZ	2.18	0.73
1:D:152:HIS:CB	1:D:171:TYR:CZ	2.70	0.73
1:D:48:ARG:HH12	1:K:137:GLU:CB	2.02	0.73
1:F:85:ARG:HB3	5:F:3030:HOH:O	1.89	0.73
2:T:392:ALA:HA	2:T:395:MET:HE2	1.69	0.73
2:2:456:GLN:NE2	2:2:465:ARG:HH21	1.87	0.73
1:1:161:GLU:HB2	1:1:162:PRO:CD	2.19	0.73
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.71	0.72
2:2:412:SER:O	2:2:414:PRO:HD3	1.89	0.72
2:V:451:LYS:HE3	5:V:1254:HOH:O	1.87	0.72
1:D:48:ARG:CD	1:K:149:ASP:OD1	2.37	0.72
2:H:409:ILE:HG12	5:H:2877:HOH:O	1.88	0.72
1:D:178:THR:CG2	1:D:233:LEU:O	2.38	0.72
1:1:97:ARG:NH2	1:1:101:ASN:HD22	1.87	0.72
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.71	0.72
2:J:362:GLU:OE2	2:J:382:ARG:HD3	1.89	0.72
1:S:152:HIS:HB3	1:S:171:TYR:CE2	2.25	0.72
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.72	0.71
1:F:15:GLU:HB3	1:W:10:GLU:HG3	1.72	0.71
2:H:329:ARG:HD3	5:H:3008:HOH:O	1.89	0.71
1:I:19:LEU:HD23	1:I:19:LEU:C	2.15	0.71
1:Q:205:VAL:HG11	1:Q:231:GLN:HE22	1.55	0.71
1:Y:85:ARG:HD2	5:Y:1301:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:233:LEU:N	1:Y:233:LEU:HD12	2.04	0.71
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.72	0.71
1:F:167:LEU:HA	1:F:170:SER:CB	2.20	0.71
1:O:163:ILE:HD13	1:O:188:LEU:HA	1.72	0.71
1:M:170:SER:OG	1:M:183:ILE:CG1	2.36	0.71
2:T:413:ASP:OD2	2:T:413:ASP:C	2.30	0.71
1:B:18:GLU:CD	1:B:21:ARG:HH12	1.98	0.71
2:G:456:GLN:HE21	2:G:465:ARG:HH21	1.38	0.71
1:D:217:ARG:HG3	1:D:218:PRO:HD2	1.72	0.71
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.73	0.71
2:T:456:GLN:NE2	2:T:465:ARG:HH21	1.88	0.71
1:1:135:ARG:NH2	1:1:173:GLU:OE2	2.24	0.71
1:1:180:ALA:HA	1:1:183:ILE:CG2	2.21	0.70
2:J:456:GLN:HE22	2:J:465:ARG:HH21	1.36	0.70
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.73	0.70
1:D:177:LEU:HD23	1:D:233:LEU:CD2	2.20	0.70
1:I:16:ARG:HB3	1:I:117:PRO:HG2	1.72	0.70
1:Y:152:HIS:HB3	1:Y:171:TYR:CE2	2.25	0.70
1:1:190:ALA:O	1:1:191:GLY:C	2.34	0.70
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.74	0.70
1:D:51:GLN:HG2	1:D:209:GLU:OE2	1.91	0.70
1:F:170:SER:OG	1:F:183:ILE:HD12	1.92	0.70
1:M:18:GLU:CD	1:M:21:ARG:HH12	2.00	0.70
5:S:2958:HOH:O	1:1:112:THR:HG21	1.90	0.70
1:D:177:LEU:CD2	1:D:233:LEU:CD2	2.69	0.70
1:M:18:GLU:HG3	1:M:22:LYS:HE3	1.74	0.70
1:O:166:ALA:O	1:O:170:SER:HB2	1.92	0.70
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.73	0.70
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.74	0.70
2:L:456:GLN:NE2	2:L:465:ARG:NH2	2.30	0.70
1:W:45:ASN:OD1	1:W:46:PRO:HD2	1.90	0.70
1:D:8:SER:HA	1:Q:15:GLU:OE2	1.92	0.69
1:S:18:GLU:CD	1:S:21:ARG:HH12	1.99	0.69
1:S:28:LYS:HE3	1:S:46:PRO:CG	2.22	0.69
1:S:230:LEU:HG	1:S:234:LEU:HD11	1.74	0.69
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.75	0.69
1:S:231:GLN:HA	1:S:234:LEU:HD12	1.73	0.69
1:I:25:ALA:O	1:I:158:GLY:HA2	1.92	0.69
1:M:177:LEU:HD21	1:M:233:LEU:HD21	1.74	0.69
2:N:465:ARG:HD2	5:N:2586:HOH:O	1.93	0.69
1:O:19:LEU:C	1:O:19:LEU:HD23	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2958:HOH:O	1:I:112:THR:HG22	1.89	0.69
2:V:306:LEU:CD1	2:V:313:VAL:HG12	2.23	0.69
1:Y:45:ASN:ND2	1:Y:52:LYS:HG3	2.08	0.69
1:Y:231:GLN:O	1:Y:235:VAL:HG23	1.92	0.69
2:Z:456:GLN:HE22	2:Z:465:ARG:NH1	1.85	0.69
2:Z:508:SER:O	2:Z:512:GLU:HG3	1.93	0.69
1:F:18:GLU:O	1:F:22:LYS:HG3	1.93	0.69
2:G:324:ASN:HB2	5:G:2032:HOH:O	1.93	0.69
1:A:41:PHE:HB3	1:A:53:ILE:HD13	1.75	0.69
1:M:161:GLU:HB2	1:M:162:PRO:CD	2.23	0.69
1:F:234:LEU:O	1:F:235:VAL:C	2.35	0.68
1:U:41:PHE:HB3	1:U:53:ILE:HD13	1.73	0.68
1:D:177:LEU:O	1:D:181:LEU:CB	2.40	0.68
1:U:205:VAL:HG12	1:U:234:LEU:HD13	1.75	0.68
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.75	0.68
1:K:230:LEU:O	1:K:234:LEU:HD13	1.94	0.68
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.76	0.68
1:F:140:ARG:HD3	1:F:154:VAL:HG13	1.76	0.68
2:X:375:THR:HG21	1:Y:92:ARG:HB3	1.74	0.68
1:D:177:LEU:HG	1:D:233:LEU:HD23	1.73	0.68
1:M:140:ARG:HD3	1:M:154:VAL:HG13	1.76	0.68
1:O:152:HIS:CG	1:O:171:TYR:HE2	2.11	0.68
1:Q:140:ARG:HD3	1:Q:154:VAL:HG13	1.75	0.68
1:S:121:GLU:HA	5:S:3022:HOH:O	1.92	0.68
1:S:132:GLU:HG3	1:S:133:THR:H	1.59	0.68
1:D:177:LEU:O	1:D:181:LEU:HB3	1.94	0.68
1:F:21:ARG:HG2	5:F:1785:HOH:O	1.92	0.68
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.75	0.68
1:K:142:THR:CA	5:K:2919:HOH:O	2.32	0.68
1:Q:181:LEU:HD23	1:Q:233:LEU:HB3	1.76	0.68
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.75	0.68
1:W:189:ARG:C	1:W:191:GLY:H	1.98	0.68
1:Q:181:LEU:O	1:Q:185:VAL:HG23	1.93	0.68
1:S:140:ARG:HD3	1:S:154:VAL:HG13	1.76	0.68
2:J:382:ARG:NH2	2:J:385:ILE:CD1	2.57	0.67
1:Y:140:ARG:HD3	1:Y:154:VAL:HG13	1.76	0.67
1:D:234:LEU:HD23	1:D:234:LEU:C	2.19	0.67
1:O:140:ARG:HD3	1:O:154:VAL:HG13	1.77	0.67
1:A:18:GLU:CD	1:A:21:ARG:HH12	2.01	0.67
1:A:13:MET:CE	1:O:116:LYS:CD	2.47	0.67
1:F:136:PRO:HG3	5:F:2981:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:382:ARG:HH21	2:J:385:ILE:CD1	2.08	0.67
1:S:76:ARG:HD3	5:S:1506:HOH:O	1.95	0.67
1:D:18:GLU:CD	1:D:21:ARG:HH12	2.03	0.67
1:D:181:LEU:O	1:D:185:VAL:HG23	1.95	0.67
1:I:140:ARG:HD3	1:I:154:VAL:HG13	1.76	0.67
1:W:18:GLU:CD	1:W:21:ARG:HH12	2.03	0.67
2:2:409:ILE:HG12	5:2:2949:HOH:O	1.95	0.67
1:U:140:ARG:HD3	1:U:154:VAL:HG13	1.75	0.67
1:W:8:SER:N	1:W:11:GLN:N	2.43	0.67
1:Y:12:ALA:O	1:Y:16:ARG:HG3	1.95	0.66
1:W:228:SER:O	1:W:232:ALA:CB	2.43	0.66
1:1:152:HIS:CD2	1:1:171:TYR:CE2	2.78	0.66
1:B:18:GLU:HG3	1:B:22:LYS:HE3	1.77	0.66
1:U:18:GLU:CD	1:U:21:ARG:HH12	2.02	0.66
1:D:170:SER:O	1:D:183:ILE:HD11	1.96	0.66
1:D:161:GLU:C	1:D:165:ASN:HD22	2.03	0.66
1:F:73:ASN:HD21	1:W:105:GLN:HG3	1.60	0.66
1:F:170:SER:OG	1:F:183:ILE:CD1	2.43	0.66
1:I:12:ALA:O	1:I:16:ARG:HG3	1.95	0.66
1:K:25:ALA:O	1:K:158:GLY:HA2	1.96	0.66
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.75	0.66
1:S:50:LEU:HD23	1:S:50:LEU:N	2.09	0.66
1:S:132:GLU:CG	1:S:133:THR:N	2.59	0.66
1:W:48:ARG:HH22	1:Y:137:GLU:HG2	1.60	0.66
2:P:456:GLN:NE2	2:P:465:ARG:NH2	2.37	0.66
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.76	0.66
1:O:152:HIS:CD2	1:O:171:TYR:HE2	2.13	0.66
2:Z:366:TYR:CD2	2:Z:374:LEU:HD13	2.31	0.66
1:1:31:VAL:CG2	1:1:155:VAL:HG22	2.24	0.66
1:M:28:LYS:HE3	1:M:46:PRO:CG	2.26	0.65
1:Q:161:GLU:HB2	1:Q:162:PRO:HD3	1.78	0.65
2:X:456:GLN:NE2	2:X:465:ARG:HH21	1.94	0.65
2:G:456:GLN:NE2	2:G:465:ARG:HH21	1.94	0.65
1:B:140:ARG:HD3	1:B:154:VAL:HG13	1.77	0.65
1:D:163:ILE:HG23	1:D:187:ALA:C	2.21	0.65
1:O:179:ASP:O	1:O:183:ILE:HG22	1.96	0.65
2:T:456:GLN:HE21	2:T:465:ARG:HH21	1.41	0.65
1:U:18:GLU:HG3	1:U:22:LYS:HE3	1.78	0.65
1:1:167:LEU:O	1:1:171:TYR:N	2.30	0.65
1:A:73:ASN:ND2	1:B:105:GLN:OE1	2.30	0.65
1:D:50:LEU:HD23	1:D:50:LEU:N	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ARG:HD3	1:D:154:VAL:HG13	1.77	0.65
1:I:220:ARG:HH22	2:J:367:GLU:CD	2.05	0.65
1:K:18:GLU:OE2	1:K:21:ARG:NH1	2.30	0.65
1:Y:18:GLU:CD	1:Y:21:ARG:NH1	2.54	0.65
1:A:13:MET:HE1	1:O:116:LYS:HD3	1.72	0.65
1:D:181:LEU:HD12	1:D:181:LEU:C	2.18	0.65
1:F:235:VAL:HA	5:F:778:HOH:O	1.96	0.65
1:O:178:THR:HG23	1:O:182:ARG:NH1	2.03	0.65
1:W:8:SER:N	1:W:11:GLN:H	1.95	0.65
2:J:413:ASP:C	2:J:413:ASP:OD1	2.40	0.65
2:R:430:ASN:ND2	5:R:2917:HOH:O	2.30	0.64
1:U:229:ALA:O	1:U:233:LEU:HD13	1.97	0.64
1:Y:45:ASN:HD22	1:Y:52:LYS:HG3	1.62	0.64
1:W:140:ARG:HD3	1:W:154:VAL:HG13	1.78	0.64
1:Y:18:GLU:OE1	1:Y:21:ARG:NH1	2.30	0.64
1:I:18:GLU:OE2	1:I:21:ARG:NH1	2.30	0.64
1:F:173:GLU:O	1:F:174:ASN:HB2	1.97	0.64
1:K:18:GLU:OE1	1:K:21:ARG:NH1	2.30	0.64
1:A:13:MET:HE2	1:O:116:LYS:HD2	1.78	0.64
1:F:40:LEU:HD12	1:F:212:VAL:HG12	1.77	0.64
1:S:73:ASN:HD21	1:I:105:GLN:HG3	1.63	0.64
1:W:18:GLU:HG3	1:W:22:LYS:HE3	1.79	0.64
1:Y:18:GLU:OE2	1:Y:21:ARG:NH1	2.30	0.64
1:Y:161:GLU:HB2	1:Y:162:PRO:HD3	1.80	0.64
1:W:176:SER:CB	1:W:179:ASP:OD2	2.34	0.64
1:W:181:LEU:CD2	1:W:234:LEU:HD21	2.28	0.64
1:Y:33:LEU:HD11	1:Y:40:LEU:HD23	1.80	0.64
1:I:31:VAL:HG22	1:I:155:VAL:CG2	2.24	0.64
1:I:140:ARG:HD3	1:I:154:VAL:HG13	1.79	0.64
2:E:456:GLN:HE21	2:E:465:ARG:HH21	1.44	0.64
1:F:161:GLU:HB2	1:F:162:PRO:HD3	1.80	0.64
1:K:18:GLU:OE2	1:K:21:ARG:NH2	2.30	0.64
1:O:173:GLU:HG3	1:O:174:ASN:OD1	1.98	0.64
1:Q:181:LEU:HD23	1:Q:233:LEU:CB	2.28	0.64
2:R:432:GLU:OE2	2:R:434:GLU:N	2.29	0.64
1:O:155:VAL:HG12	1:O:160:THR:HG22	1.80	0.64
1:S:18:GLU:HG3	1:S:22:LYS:HE3	1.78	0.64
1:S:152:HIS:NE2	1:S:173:GLU:OE2	2.23	0.64
1:K:76:ARG:HD3	5:K:2440:HOH:O	1.96	0.64
1:O:33:LEU:HD21	1:O:184:ALA:HB2	1.80	0.64
2:C:456:GLN:NE2	2:C:465:ARG:HH21	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:CG1	1:A:206:ALA:N	2.61	0.63
1:D:152:HIS:CG	1:D:171:TYR:CE2	2.87	0.63
1:M:177:LEU:CD2	1:M:233:LEU:HD21	2.28	0.63
1:O:18:GLU:OE2	1:O:21:ARG:NH1	2.30	0.63
1:S:161:GLU:HB2	1:S:162:PRO:HD3	1.78	0.63
1:D:161:GLU:HB2	1:D:162:PRO:HD3	1.81	0.63
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.78	0.63
1:Q:230:LEU:O	1:Q:234:LEU:HD13	1.98	0.63
1:S:116:LYS:HD2	1:I:13:MET:HE1	1.80	0.63
1:O:167:LEU:HD13	1:O:187:ALA:CB	2.27	0.63
1:U:161:GLU:HB2	1:U:162:PRO:HD3	1.79	0.63
1:F:40:LEU:HD12	1:F:212:VAL:CG1	2.28	0.63
1:Q:10:GLU:CG	1:Y:15:GLU:OE1	2.33	0.63
1:Y:22:LYS:HG2	1:Y:26:ARG:NH2	2.07	0.63
2:C:511:ALA:O	2:C:515:ARG:HG3	1.99	0.63
1:D:18:GLU:HG3	1:D:22:LYS:HE3	1.81	0.63
2:H:301:THR:N	5:H:3024:HOH:O	2.31	0.63
1:K:11:GLN:OE1	1:K:14:ARG:NH1	2.31	0.63
1:W:161:GLU:HB2	1:W:162:PRO:HD3	1.81	0.63
1:Y:233:LEU:CD1	1:Y:233:LEU:N	2.60	0.63
2:Z:456:GLN:NE2	2:Z:465:ARG:NH1	2.36	0.63
1:A:186:ALA:O	1:A:189:ARG:HB2	1.98	0.63
1:D:10:GLU:HG3	1:Q:15:GLU:CG	2.27	0.63
1:I:97:ARG:NH2	5:I:1244:HOH:O	2.32	0.63
1:I:155:VAL:HG11	1:I:160:THR:CG2	2.21	0.63
1:D:167:LEU:HA	1:D:170:SER:OG	1.99	0.63
1:D:174:ASN:OD1	1:D:174:ASN:N	2.31	0.63
1:I:76:ARG:HD3	5:I:252:HOH:O	1.98	0.63
2:L:372:VAL:HG23	2:L:373:PRO:HD2	1.75	0.63
1:O:115:ALA:HB3	5:O:2956:HOH:O	1.99	0.63
2:E:456:GLN:NE2	2:E:465:ARG:NH2	2.47	0.62
1:D:13:MET:HE1	1:Q:116:LYS:HD2	1.81	0.62
2:T:366:TYR:CD2	2:T:374:LEU:HD13	2.34	0.62
1:D:189:ARG:O	1:D:190:ALA:C	2.42	0.62
1:K:45:ASN:ND2	1:K:52:LYS:HG3	2.11	0.62
2:L:383:LEU:HD23	2:L:423:PHE:CZ	2.34	0.62
1:O:97:ARG:HD2	1:U:49:SER:HB2	1.82	0.62
2:X:366:TYR:CD2	2:X:374:LEU:HD13	2.33	0.62
1:I:130:TYR:C	1:I:132:GLU:H	2.08	0.62
1:A:47:SER:OG	1:A:50:LEU:N	2.30	0.62
1:A:161:GLU:HB2	1:A:162:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:306:LEU:HD12	2:L:313:VAL:HG12	1.82	0.62
1:O:205:VAL:C	1:O:207:SER:H	2.08	0.62
1:A:18:GLU:HG3	1:A:22:LYS:HE3	1.80	0.62
1:1:180:ALA:O	1:1:183:ILE:HG23	1.99	0.62
1:U:205:VAL:HG12	1:U:234:LEU:CD1	2.29	0.62
1:I:52:LYS:NZ	5:I:1197:HOH:O	2.32	0.62
2:J:413:ASP:OD1	2:J:414:PRO:HD2	1.99	0.62
2:V:366:TYR:CD2	2:V:374:LEU:HD13	2.34	0.62
1:B:161:GLU:HB2	1:B:162:PRO:HD3	1.82	0.62
1:B:178:THR:HG22	1:B:182:ARG:NE	2.15	0.62
1:M:217:ARG:CD	1:M:223:ARG:HH22	2.11	0.62
1:O:166:ALA:O	1:O:170:SER:HB3	1.98	0.62
1:1:204:GLY:N	5:1:2895:HOH:O	2.31	0.62
1:B:178:THR:HG23	1:B:233:LEU:HA	1.81	0.61
1:K:18:GLU:CD	1:K:21:ARG:NH1	2.58	0.61
1:O:115:ALA:CB	5:O:2956:HOH:O	2.47	0.61
1:A:205:VAL:HG12	1:A:206:ALA:N	2.13	0.61
1:I:16:ARG:HB3	1:I:117:PRO:CG	2.30	0.61
1:I:73:ASN:ND2	1:S:105:GLN:HE21	1.98	0.61
1:M:214:ASP:OD2	1:M:223:ARG:NH2	2.30	0.61
1:M:95:THR:OG1	1:M:98:GLN:HG3	2.01	0.61
2:H:456:GLN:NE2	2:H:465:ARG:NH2	2.35	0.61
1:I:51:GLN:HA	1:I:209:GLU:OE1	2.01	0.61
1:I:161:GLU:HB2	1:I:162:PRO:HD3	1.82	0.61
1:Y:33:LEU:HD12	1:Y:40:LEU:HB3	1.81	0.61
1:K:8:SER:OG	1:K:11:GLN:HB3	1.99	0.61
1:U:205:VAL:CG1	1:U:234:LEU:HD13	2.30	0.61
1:B:33:LEU:HB3	1:B:153:PHE:HB3	1.82	0.61
1:D:147:ILE:HD13	1:Q:50:LEU:HD21	1.82	0.61
1:U:97:ARG:NH2	5:U:1015:HOH:O	2.33	0.61
1:U:135:ARG:HD3	1:1:48:ARG:NH1	2.14	0.61
1:1:170:SER:O	1:1:183:ILE:HD12	2.00	0.61
1:D:205:VAL:N	1:D:208:LEU:HD13	2.16	0.61
1:F:18:GLU:OE2	1:F:21:ARG:NH1	2.30	0.61
1:K:161:GLU:HB2	1:K:162:PRO:HD3	1.83	0.60
1:S:181:LEU:HD23	1:S:233:LEU:HB3	1.82	0.60
1:S:183:ILE:HG22	1:S:184:ALA:N	2.07	0.60
1:U:13:MET:CE	1:1:116:LYS:HD2	2.30	0.60
1:U:181:LEU:O	1:U:185:VAL:HG23	2.01	0.60
2:J:366:TYR:CD2	2:J:374:LEU:HD13	2.37	0.60
2:L:412:SER:O	2:L:414:PRO:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:451:LYS:NZ	2:2:473:ASP:OD1	2.34	0.60
1:Y:19:LEU:C	1:Y:19:LEU:CD2	2.75	0.60
2:T:486:LEU:HB2	5:T:1332:HOH:O	2.01	0.60
1:W:163:ILE:HG23	1:W:187:ALA:O	2.02	0.60
1:D:163:ILE:HG23	1:D:187:ALA:O	2.01	0.60
1:Q:58:ASP:OD1	1:Q:219:ARG:NH1	2.35	0.60
1:K:73:ASN:HD21	1:M:105:GLN:HG3	1.66	0.60
1:Q:165:ASN:HA	1:Q:168:LYS:HD2	1.82	0.60
1:K:167:LEU:CD1	1:K:183:ILE:HG22	2.32	0.60
2:N:456:GLN:HE21	2:N:465:ARG:NH2	1.96	0.60
2:2:319:ARG:HG3	2:2:320:SER:N	2.15	0.59
1:A:32:ALA:HA	1:A:40:LEU:O	2.01	0.59
1:K:140:ARG:HG2	1:K:140:ARG:NH1	2.08	0.59
2:2:366:TYR:CD2	2:2:374:LEU:HD13	2.37	0.59
2:L:451:LYS:NZ	2:P:473:ASP:OD1	2.30	0.59
1:S:152:HIS:CG	1:S:171:TYR:CE2	2.91	0.59
1:D:184:ALA:O	1:D:188:LEU:CD1	2.50	0.59
1:Y:152:HIS:CB	1:Y:171:TYR:CE2	2.85	0.59
1:1:97:ARG:NH2	1:1:101:ASN:ND2	2.50	0.59
1:D:48:ARG:NH1	1:K:137:GLU:HG2	2.18	0.59
1:D:152:HIS:HB3	1:D:171:TYR:CE2	2.36	0.59
2:T:392:ALA:HA	2:T:395:MET:CE	2.32	0.59
1:O:33:LEU:HD11	1:O:40:LEU:HD23	1.83	0.59
2:T:444:LEU:HB3	2:X:444:LEU:HD21	1.84	0.59
2:V:306:LEU:CD1	2:V:313:VAL:CG1	2.80	0.59
1:Y:214:ASP:HB3	1:Y:217:ARG:HG2	1.84	0.59
1:Y:234:LEU:O	1:Y:235:VAL:C	2.46	0.59
1:A:67:LYS:HG2	1:A:69:ASN:ND2	2.18	0.59
1:B:217:ARG:HH12	1:B:223:ARG:HB3	1.67	0.59
1:F:170:SER:OG	1:F:183:ILE:HG23	2.03	0.59
1:B:181:LEU:O	1:B:185:VAL:HG23	2.03	0.59
1:Y:225:ILE:HG21	1:Y:233:LEU:HD22	1.84	0.59
1:D:164:ALA:O	1:D:167:LEU:N	2.35	0.59
2:T:451:LYS:NZ	2:X:473:ASP:OD1	2.30	0.59
1:D:161:GLU:O	1:D:162:PRO:C	2.42	0.58
1:M:98:GLN:O	1:M:102:VAL:HG23	2.03	0.58
2:X:456:GLN:HE21	2:X:465:ARG:NH2	2.00	0.58
1:Y:12:ALA:C	1:Y:14:ARG:H	2.12	0.58
2:G:391:LEU:HG	2:G:395:MET:HE2	1.85	0.58
2:H:417:ALA:HA	5:H:3049:HOH:O	2.02	0.58
1:K:181:LEU:HD21	1:K:234:LEU:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:232:ALA:HA	1:Y:235:VAL:CG2	2.33	0.58
2:2:456:GLN:HE21	2:2:465:ARG:NH2	2.00	0.58
1:D:39:VAL:HG23	1:D:127:VAL:HG12	1.85	0.58
1:O:178:THR:HG22	1:O:182:ARG:NH2	2.17	0.58
1:Q:12:ALA:O	1:Q:16:ARG:HG3	2.02	0.58
2:X:391:LEU:HG	2:X:395:MET:HE2	1.86	0.58
1:Y:19:LEU:HD23	1:Y:19:LEU:O	2.03	0.58
1:I:220:ARG:NH2	2:J:367:GLU:OE2	2.36	0.58
2:L:382:ARG:NH2	2:L:385:ILE:HD13	2.19	0.58
1:S:152:HIS:HD2	1:S:171:TYR:CE2	2.20	0.58
1:B:178:THR:O	1:B:182:ARG:HD2	2.04	0.58
1:F:115:ALA:HB3	1:W:112:THR:CG2	2.33	0.58
1:K:87:TYR:O	2:L:357:ARG:NH2	2.35	0.58
1:K:115:ALA:HB3	1:M:112:THR:HG23	1.86	0.58
2:R:430:ASN:ND2	5:R:548:HOH:O	2.30	0.58
1:S:170:SER:OG	1:S:183:ILE:CD1	2.52	0.58
1:D:105:GLN:HE21	1:Q:73:ASN:ND2	2.01	0.58
1:I:73:ASN:HD21	1:S:105:GLN:HG3	1.67	0.58
2:E:320:SER:HB3	2:E:328:GLY:HA3	1.86	0.58
1:1:161:GLU:HB2	1:1:162:PRO:HD3	1.86	0.58
1:F:25:ALA:O	1:F:158:GLY:HA2	2.04	0.57
1:F:166:ALA:O	1:F:170:SER:CB	2.36	0.57
2:L:306:LEU:CD1	2:L:313:VAL:HG13	2.33	0.57
1:Q:105:GLN:HG3	1:Y:73:ASN:ND2	2.19	0.57
1:U:167:LEU:HA	1:U:170:SER:HB3	1.85	0.57
1:Y:76:ARG:NH2	5:Y:2938:HOH:O	2.37	0.57
1:Y:128:ALA:HB2	1:Y:134:LYS:HB3	1.85	0.57
1:A:33:LEU:HB3	1:A:153:PHE:HB3	1.85	0.57
1:A:170:SER:OG	1:A:183:ILE:CG2	2.49	0.57
2:C:324:ASN:HB2	5:C:2066:HOH:O	2.03	0.57
1:U:171:TYR:C	1:U:171:TYR:CD2	2.81	0.57
2:R:426:ALA:HB2	4:b:4:HXD:H41	1.86	0.57
2:V:306:LEU:HD11	2:V:313:VAL:CG1	2.34	0.57
2:L:511:ALA:O	2:L:515:ARG:HG3	2.04	0.57
1:O:11:GLN:O	1:O:15:GLU:CG	2.52	0.57
1:U:105:GLN:HG3	1:1:73:ASN:HD21	1.68	0.57
1:K:167:LEU:HD12	1:K:183:ILE:HG22	1.84	0.57
2:V:362:GLU:OE2	2:V:382:ARG:HD3	2.05	0.57
1:Y:135:ARG:NH1	1:Y:135:ARG:HG3	2.18	0.57
1:Y:141:ILE:N	1:Y:141:ILE:HD12	2.19	0.57
1:K:140:ARG:HD3	1:K:154:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:164:ALA:O	1:O:168:LYS:N	2.30	0.57
2:T:413:ASP:OD2	2:T:414:PRO:N	2.37	0.57
1:B:217:ARG:NH1	1:B:217:ARG:HG3	2.19	0.57
2:C:515:ARG:NH2	5:C:1432:HOH:O	2.37	0.57
1:D:49:SER:O	1:D:50:LEU:CD2	2.48	0.57
2:L:372:VAL:HG22	2:L:373:PRO:N	2.16	0.57
1:W:228:SER:O	1:W:232:ALA:N	2.33	0.57
1:Y:232:ALA:HA	1:Y:235:VAL:HG23	1.86	0.57
1:A:105:GLN:HG3	1:O:73:ASN:HD21	1.70	0.57
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.69	0.57
1:F:55:GLU:CD	1:F:220:ARG:HH21	2.13	0.57
1:M:161:GLU:HB2	1:M:162:PRO:HD2	1.86	0.57
1:O:110:ILE:HA	1:O:114:GLN:HG3	1.87	0.57
1:B:182:ARG:NE	1:B:233:LEU:O	2.33	0.57
2:V:392:ALA:HA	2:V:395:MET:HE3	1.87	0.57
1:D:152:HIS:CD2	1:D:171:TYR:HE2	2.19	0.57
2:C:508:SER:O	2:C:512:GLU:HG3	2.05	0.56
2:N:366:TYR:CD2	2:N:374:LEU:HD13	2.40	0.56
2:R:366:TYR:CD2	2:R:374:LEU:HD13	2.40	0.56
2:V:362:GLU:OE2	2:V:382:ARG:CD	2.53	0.56
1:W:181:LEU:HD21	1:W:234:LEU:HD21	1.86	0.56
1:I:129:HIS:O	1:I:132:GLU:HB3	2.05	0.56
2:L:306:LEU:HD11	2:L:313:VAL:CG1	2.35	0.56
1:Y:135:ARG:HG3	1:Y:135:ARG:HH11	1.69	0.56
1:D:48:ARG:HG3	1:D:49:SER:H	1.70	0.56
1:D:161:GLU:C	1:D:165:ASN:ND2	2.63	0.56
1:I:185:VAL:O	1:I:189:ARG:N	2.30	0.56
1:O:179:ASP:O	1:O:183:ILE:HG23	2.03	0.56
1:A:205:VAL:O	1:A:206:ALA:HB3	2.05	0.56
1:D:161:GLU:O	1:D:165:ASN:ND2	2.27	0.56
1:D:178:THR:HG23	1:D:233:LEU:O	2.04	0.56
1:F:115:ALA:HB3	1:W:112:THR:HG23	1.88	0.56
1:I:230:LEU:O	1:I:234:LEU:HD22	2.05	0.56
1:I:114:GLN:NE2	5:I:1024:HOH:O	2.39	0.56
2:P:366:TYR:CD2	2:P:374:LEU:HD13	2.40	0.56
1:Q:179:ASP:O	1:Q:183:ILE:HG13	2.06	0.56
1:B:179:ASP:O	1:B:183:ILE:HG13	2.05	0.56
2:G:307:LYS:HG3	2:G:312:VAL:HG12	1.88	0.56
1:Q:233:LEU:C	1:Q:234:LEU:HD12	2.30	0.56
1:D:170:SER:O	1:D:183:ILE:CD1	2.53	0.56
1:Q:233:LEU:HD12	1:Q:233:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:509:ARG:O	2:C:513:LEU:HD22	2.06	0.56
2:L:306:LEU:HD12	2:L:313:VAL:HG13	1.86	0.56
1:D:13:MET:HE2	1:Q:19:LEU:CD2	2.25	0.56
2:J:511:ALA:O	2:J:515:ARG:HG3	2.06	0.56
1:W:163:ILE:HG23	1:W:187:ALA:C	2.31	0.56
1:B:19:LEU:C	1:B:19:LEU:HD23	2.32	0.55
1:B:141:ILE:N	1:B:141:ILE:HD12	2.20	0.55
1:D:73:ASN:HD21	1:K:105:GLN:HG3	1.71	0.55
1:F:19:LEU:C	1:F:19:LEU:HD23	2.31	0.55
1:I:115:ALA:HB3	1:S:112:THR:CG2	2.37	0.55
1:S:132:GLU:HG3	1:S:133:THR:N	2.18	0.55
1:M:141:ILE:N	1:M:141:ILE:HD12	2.21	0.55
1:A:179:ASP:O	1:A:183:ILE:HG13	2.06	0.55
2:G:509:ARG:NH1	2:G:509:ARG:HG3	2.22	0.55
1:I:25:ALA:O	1:I:158:GLY:HA2	2.05	0.55
1:I:180:ALA:HA	1:I:183:ILE:HG23	1.88	0.55
1:O:51:GLN:HG2	1:O:209:GLU:OE2	2.07	0.55
1:F:185:VAL:O	1:F:189:ARG:N	2.28	0.55
1:Q:136:PRO:O	1:Y:48:ARG:NH2	2.32	0.55
2:V:515:ARG:HD3	5:V:2326:HOH:O	2.06	0.55
1:B:49:SER:HB2	1:I:97:ARG:HD2	1.89	0.55
1:O:19:LEU:HD23	1:O:19:LEU:O	2.07	0.55
2:C:432:GLU:HB2	5:C:135:HOH:O	2.06	0.55
1:Y:22:LYS:CG	1:Y:26:ARG:HH21	2.08	0.55
1:D:163:ILE:O	1:D:187:ALA:HB1	2.07	0.55
1:D:217:ARG:NH2	1:D:223:ARG:HB3	2.19	0.55
1:B:8:SER:HB3	1:B:11:GLN:HB3	1.89	0.55
2:C:366:TYR:CD2	2:C:374:LEU:HD13	2.42	0.55
1:K:116:LYS:HD2	1:M:13:MET:CE	2.30	0.55
2:V:392:ALA:HA	2:V:395:MET:CE	2.36	0.55
2:Z:437:GLN:OE1	2:Z:447:LYS:HD3	2.07	0.55
1:I:141:ILE:N	1:I:141:ILE:HD12	2.22	0.55
2:C:451:LYS:NZ	2:R:473:ASP:OD1	2.39	0.55
1:I:45:ASN:ND2	1:I:50:LEU:O	2.38	0.55
2:P:508:SER:O	2:P:512:GLU:HG3	2.07	0.55
1:U:129:HIS:HE1	5:U:2960:HOH:O	1.89	0.55
1:D:58:ASP:OD2	1:D:219:ARG:HD2	2.08	0.54
1:O:97:ARG:NH2	5:O:1513:HOH:O	2.40	0.54
2:P:341:THR:CG2	2:P:404:LEU:HD11	2.37	0.54
1:I:8:SER:OG	1:I:11:GLN:HB3	2.07	0.54
1:B:76:ARG:HD3	5:B:341:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:GLU:HG2	1:S:10:GLU:HG3	1.89	0.54
1:U:141:ILE:HD12	1:U:141:ILE:N	2.21	0.54
2:V:444:LEU:HB2	5:V:855:HOH:O	2.06	0.54
2:H:422:SER:HB3	2:H:437:GLN:HG2	1.90	0.54
1:O:183:ILE:HG12	1:O:184:ALA:N	2.21	0.54
2:T:382:ARG:NH2	2:T:385:ILE:HD13	2.22	0.54
1:U:205:VAL:CG1	1:U:234:LEU:CD1	2.86	0.54
1:D:178:THR:HG22	1:D:233:LEU:O	2.05	0.54
1:I:130:TYR:O	1:I:132:GLU:N	2.40	0.54
2:2:456:GLN:NE2	2:2:465:ARG:NH2	2.56	0.54
1:B:173:GLU:O	1:B:174:ASN:HB2	2.06	0.54
2:R:308:TYR:CZ	2:R:311:GLY:HA3	2.42	0.54
1:Y:8:SER:HB2	1:Y:11:GLN:CB	2.32	0.54
1:I:166:ALA:O	1:I:170:SER:N	2.38	0.54
1:K:98:GLN:O	1:K:102:VAL:HG23	2.07	0.54
2:C:407:TYR:CE1	2:C:417:ALA:HB3	2.43	0.54
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.90	0.54
1:I:170:SER:OG	1:I:183:ILE:CG2	2.53	0.54
1:O:205:VAL:HG21	1:O:231:GLN:HE22	1.71	0.54
1:W:189:ARG:O	1:W:191:GLY:N	2.40	0.54
1:O:11:GLN:O	1:O:15:GLU:HG3	2.08	0.54
1:Y:13:MET:O	1:Y:13:MET:HG3	2.07	0.54
2:J:456:GLN:HE21	2:J:465:ARG:NH2	2.00	0.54
1:K:181:LEU:CD2	1:K:234:LEU:HD12	2.38	0.54
2:V:382:ARG:NH2	2:V:385:ILE:HD13	2.22	0.54
1:Y:80:GLN:HG2	5:Y:1507:HOH:O	2.06	0.54
1:I:205:VAL:HG13	1:I:234:LEU:HD12	1.90	0.54
1:D:74:LEU:HD13	1:D:122:LEU:HD11	1.90	0.53
2:X:341:THR:CG2	2:X:404:LEU:HD11	2.39	0.53
1:D:173:GLU:CB	1:D:174:ASN:OD1	2.46	0.53
1:O:152:HIS:HB3	1:O:171:TYR:CZ	2.42	0.53
1:S:205:VAL:CG2	5:S:2979:HOH:O	2.56	0.53
1:W:226:THR:OG1	1:W:227:GLY:N	2.40	0.53
1:F:90:ASP:HB3	1:F:93:ASP:OD2	2.08	0.53
1:W:228:SER:O	1:W:232:ALA:HB2	2.08	0.53
2:Z:366:TYR:CE2	2:Z:374:LEU:HD13	2.42	0.53
2:E:366:TYR:CD2	2:E:374:LEU:HD13	2.43	0.53
1:F:142:THR:OG1	1:F:144:ASP:OD1	2.26	0.53
1:Q:164:ALA:HB1	1:Q:168:LYS:HE3	1.89	0.53
1:S:231:GLN:CA	1:S:234:LEU:HD12	2.37	0.53
2:X:366:TYR:CG	2:X:374:LEU:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:173:GLU:C	1:Q:174:ASN:HD22	2.17	0.53
2:E:452:LYS:NZ	5:E:814:HOH:O	2.33	0.53
1:M:181:LEU:CD2	1:M:233:LEU:HB3	2.39	0.53
1:O:74:LEU:HD13	1:O:122:LEU:HD11	1.90	0.53
1:W:141:ILE:HD12	1:W:141:ILE:N	2.24	0.53
1:M:152:HIS:CD2	1:M:171:TYR:HE2	2.27	0.53
2:2:320:SER:HB3	2:2:328:GLY:HA3	1.90	0.53
1:S:8:SER:OG	1:S:11:GLN:HB3	2.09	0.53
1:S:74:LEU:HD13	1:S:122:LEU:HD11	1.91	0.53
1:W:28:LYS:HB2	1:W:52:LYS:NZ	2.24	0.53
1:W:189:ARG:O	1:W:190:ALA:C	2.51	0.53
1:B:19:LEU:HD23	1:B:19:LEU:O	2.08	0.53
1:O:152:HIS:CG	1:O:171:TYR:CE2	2.93	0.53
1:U:166:ALA:O	1:U:170:SER:CB	2.49	0.53
1:Y:125:ALA:HB2	1:Y:138:LEU:HD23	1.91	0.53
1:A:19:LEU:C	1:A:19:LEU:HD23	2.34	0.52
1:I:19:LEU:HD23	1:I:19:LEU:O	2.07	0.52
1:K:181:LEU:HD21	1:K:234:LEU:HD11	1.90	0.52
1:S:19:LEU:C	1:S:19:LEU:HD23	2.34	0.52
1:Y:152:HIS:CB	1:Y:171:TYR:CZ	2.86	0.52
2:C:416:SER:HA	5:C:2935:HOH:O	2.08	0.52
1:Q:205:VAL:HG21	1:Q:231:GLN:HE21	1.75	0.52
2:R:529:SER:C	5:R:3074:HOH:O	2.51	0.52
2:2:456:GLN:HE21	2:2:465:ARG:HH21	1.53	0.52
2:C:425:ALA:HB3	4:e:4:HXD:H42	1.91	0.52
2:G:456:GLN:HE21	2:G:465:ARG:NH2	2.04	0.52
1:I:74:LEU:HD13	1:I:122:LEU:HD11	1.92	0.52
2:V:366:TYR:CG	2:V:374:LEU:HD13	2.44	0.52
1:B:22:LYS:HD2	1:I:10:GLU:OE1	2.09	0.52
2:E:515:ARG:NE	5:E:1107:HOH:O	2.38	0.52
1:S:115:ALA:HB3	5:S:2958:HOH:O	2.09	0.52
1:U:19:LEU:HD23	1:U:19:LEU:C	2.34	0.52
1:W:8:SER:N	1:W:9:PRO:C	2.68	0.52
1:B:74:LEU:HD13	1:B:122:LEU:HD11	1.92	0.52
1:D:50:LEU:HD22	5:D:2921:HOH:O	2.01	0.52
2:L:374:LEU:HD11	1:M:89:TYR:CD1	2.45	0.52
2:T:456:GLN:HE21	2:T:465:ARG:NH2	2.06	0.52
1:W:170:SER:OG	1:W:183:ILE:HG23	2.09	0.52
1:A:8:SER:OG	1:A:11:GLN:CB	2.58	0.52
1:O:53:ILE:HD12	1:O:209:GLU:HG2	1.92	0.52
1:Q:205:VAL:HG21	1:Q:231:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:214:ASP:HB3	1:Q:217:ARG:HG2	1.92	0.52
1:S:141:ILE:HD12	1:S:141:ILE:N	2.24	0.52
2:V:341:THR:CG2	2:V:404:LEU:HD11	2.39	0.52
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.90	0.52
1:M:161:GLU:CB	1:M:162:PRO:CD	2.87	0.52
1:S:121:GLU:CB	5:S:3022:HOH:O	2.57	0.52
2:T:320:SER:HB3	2:T:328:GLY:HA3	1.92	0.52
1:Y:163:ILE:HG23	1:Y:187:ALA:O	2.09	0.52
2:G:341:THR:CG2	2:G:404:LEU:HD11	2.40	0.52
2:N:392:ALA:HA	2:N:395:MET:CE	2.39	0.52
1:U:205:VAL:HG23	1:U:206:ALA:N	2.24	0.52
1:Y:56:LEU:HG	1:Y:62:PHE:HB2	1.92	0.52
1:A:182:ARG:NH2	5:A:2141:HOH:O	2.41	0.52
2:Z:366:TYR:CG	2:Z:374:LEU:HD13	2.45	0.52
2:C:422:SER:HB3	2:C:437:GLN:HG2	1.92	0.52
1:D:40:LEU:HD13	1:D:177:LEU:HD11	1.92	0.52
2:J:320:SER:HB3	2:J:328:GLY:HA3	1.92	0.52
1:M:163:ILE:HG23	1:M:188:LEU:HA	1.93	0.52
1:1:173:GLU:O	1:1:174:ASN:HB2	2.09	0.52
2:N:437:GLN:OE1	2:N:447:LYS:HD3	2.10	0.51
2:T:409:ILE:HG12	2:T:410:HIS:ND1	2.24	0.51
1:Y:233:LEU:CD1	1:Y:233:LEU:H	2.21	0.51
1:D:13:MET:HE1	1:Q:19:LEU:HD21	1.88	0.51
2:T:422:SER:HB3	2:T:437:GLN:HG2	1.91	0.51
2:X:362:GLU:HG3	5:X:2197:HOH:O	2.10	0.51
1:A:98:GLN:O	1:A:102:VAL:HG23	2.10	0.51
2:R:456:GLN:NE2	2:R:465:ARG:NH2	2.39	0.51
1:A:8:SER:OG	1:A:11:GLN:HB2	2.09	0.51
1:K:170:SER:OG	1:K:183:ILE:HG23	2.10	0.51
1:W:74:LEU:HD13	1:W:122:LEU:HD11	1.93	0.51
1:A:233:LEU:C	1:A:234:LEU:HD12	2.35	0.51
1:D:48:ARG:NH1	1:K:137:GLU:CG	2.74	0.51
1:D:177:LEU:O	1:D:181:LEU:HB2	2.09	0.51
1:D:217:ARG:NH2	1:D:221:ALA:O	2.44	0.51
1:F:18:GLU:OE1	1:F:21:ARG:NH1	2.43	0.51
2:G:320:SER:HB3	2:G:328:GLY:HA3	1.92	0.51
1:I:98:GLN:O	1:I:102:VAL:HG23	2.11	0.51
1:O:183:ILE:CG1	1:O:184:ALA:N	2.73	0.51
2:T:325:MET:HE2	5:T:1035:HOH:O	2.10	0.51
1:D:45:ASN:OD1	1:D:46:PRO:HD2	2.10	0.51
2:P:392:ALA:HA	2:P:395:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:40:LEU:HD12	1:W:212:VAL:HG12	1.93	0.51
1:Y:11:GLN:O	1:Y:14:ARG:CB	2.59	0.51
1:D:82:ALA:HB2	1:D:99:LEU:HD11	1.92	0.51
2:L:509:ARG:HH11	2:L:509:ARG:HA	1.74	0.51
1:A:181:LEU:HD21	1:A:234:LEU:HD11	1.92	0.51
2:C:320:SER:HB3	2:C:328:GLY:HA3	1.93	0.51
2:H:366:TYR:CD2	2:H:374:LEU:HD13	2.46	0.51
1:Q:52:LYS:HE3	1:Q:64:ALA:O	2.11	0.51
1:Y:8:SER:CB	1:Y:11:GLN:CB	2.76	0.51
1:B:178:THR:HG23	1:B:233:LEU:CA	2.40	0.50
1:D:48:ARG:NE	1:K:149:ASP:OD1	2.44	0.50
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.92	0.50
2:L:324:ASN:ND2	5:L:654:HOH:O	2.44	0.50
2:R:320:SER:HB3	2:R:328:GLY:HA3	1.93	0.50
1:U:95:THR:OG1	1:U:98:GLN:HG3	2.10	0.50
1:A:51:GLN:CG	1:A:209:GLU:OE2	2.45	0.50
1:B:205:VAL:HG23	1:B:206:ALA:N	2.22	0.50
1:I:181:LEU:HD23	1:I:233:LEU:HB3	1.93	0.50
1:K:18:GLU:OE2	1:K:21:ARG:CZ	2.59	0.50
2:L:341:THR:CG2	2:L:404:LEU:HD11	2.41	0.50
2:L:357:ARG:NH1	5:L:1225:HOH:O	2.30	0.50
1:O:217:ARG:NH2	1:O:223:ARG:HH11	2.08	0.50
2:V:412:SER:O	2:V:414:PRO:HD3	2.11	0.50
2:C:444:LEU:HB2	5:C:1970:HOH:O	2.10	0.50
1:D:48:ARG:HG3	1:D:49:SER:N	2.27	0.50
1:D:95:THR:O	1:D:98:GLN:HB2	2.11	0.50
2:E:324:ASN:HB2	5:E:543:HOH:O	2.11	0.50
1:I:141:ILE:HD12	1:I:141:ILE:N	2.26	0.50
1:S:28:LYS:HE3	1:S:46:PRO:CD	2.42	0.50
1:U:33:LEU:HB3	1:U:153:PHE:HB3	1.93	0.50
2:2:333:LYS:HE2	3:n:3:LEU:HD22	1.92	0.50
1:D:19:LEU:HD23	1:D:19:LEU:C	2.36	0.50
1:F:152:HIS:HB3	1:F:171:TYR:CE2	2.46	0.50
1:D:181:LEU:HD23	1:D:233:LEU:HB3	1.92	0.50
1:Q:18:GLU:O	1:Q:22:LYS:HG3	2.12	0.50
1:Q:142:THR:OG1	1:Q:144:ASP:OD1	2.30	0.50
1:B:33:LEU:HB3	1:B:153:PHE:CB	2.41	0.50
2:C:392:ALA:HA	2:C:395:MET:HE3	1.92	0.50
1:M:38:GLY:HA3	1:M:213:LEU:O	2.11	0.50
1:1:167:LEU:HA	1:1:170:SER:OG	2.11	0.50
1:A:234:LEU:HD12	1:A:234:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:515:ARG:O	2:C:519:GLU:HG3	2.12	0.50
1:Q:42:VAL:HG12	1:Q:188:LEU:CD2	2.41	0.50
1:U:81:PHE:CZ	1:U:102:VAL:HG21	2.47	0.50
1:Y:135:ARG:HH11	1:Y:135:ARG:CG	2.24	0.50
2:G:331:VAL:HG11	3:c:3:LEU:CD2	2.41	0.50
2:T:362:GLU:OE2	2:T:382:ARG:HD3	2.11	0.50
1:W:19:LEU:C	1:W:19:LEU:HD23	2.37	0.50
1:Y:12:ALA:C	1:Y:14:ARG:N	2.67	0.50
2:J:392:ALA:HA	2:J:395:MET:HE3	1.93	0.50
1:Y:179:ASP:O	1:Y:183:ILE:HG13	2.12	0.50
2:2:452:LYS:HD3	5:2:2578:HOH:O	2.10	0.50
1:A:135:ARG:NH2	1:A:173:GLU:OE2	2.37	0.49
1:D:233:LEU:O	1:D:234:LEU:C	2.53	0.49
2:E:409:ILE:HG23	5:E:2808:HOH:O	2.11	0.49
2:P:382:ARG:NH2	2:P:385:ILE:HD13	2.27	0.49
1:Q:144:ASP:OD1	1:Q:146:SER:OG	2.30	0.49
1:D:112:THR:CG2	1:Q:115:ALA:HB3	2.43	0.49
1:Q:21:ARG:CZ	1:Q:21:ARG:HB3	2.38	0.49
2:Z:382:ARG:NH2	2:Z:385:ILE:HD13	2.27	0.49
2:L:437:GLN:OE1	2:L:447:LYS:HD3	2.12	0.49
1:O:116:LYS:NZ	1:O:119:GLU:OE2	2.40	0.49
1:O:205:VAL:HG23	1:O:206:ALA:H	1.77	0.49
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.93	0.49
1:A:181:LEU:HD23	1:A:233:LEU:HB3	1.95	0.49
2:H:366:TYR:CG	2:H:374:LEU:HD13	2.47	0.49
2:L:314:MET:HE3	2:L:405:ALA:HB2	1.95	0.49
5:R:2894:HOH:O	4:i:4:HXD:H22	2.11	0.49
1:1:39:VAL:CG1	1:1:40:LEU:N	2.76	0.49
1:B:21:ARG:HB3	1:B:21:ARG:CZ	2.42	0.49
2:E:374:LEU:HD11	1:K:89:TYR:CD1	2.47	0.49
1:M:19:LEU:C	1:M:19:LEU:HD23	2.37	0.49
2:N:341:THR:CG2	2:N:404:LEU:HD11	2.43	0.49
2:N:444:LEU:HB2	5:N:793:HOH:O	2.12	0.49
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.93	0.49
1:O:8:SER:OG	1:O:11:GLN:HB3	2.13	0.49
1:Q:140:ARG:HD3	1:Q:154:VAL:CG1	2.42	0.49
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.93	0.49
1:S:181:LEU:CD2	1:S:233:LEU:HB3	2.43	0.49
2:T:366:TYR:CG	2:T:374:LEU:HD13	2.47	0.49
1:W:152:HIS:HB3	1:W:171:TYR:CZ	2.48	0.49
1:1:169:GLU:OE1	1:1:169:GLU:CA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:ASN:ND2	1:W:105:GLN:HE21	2.11	0.49
2:G:509:ARG:CD	5:G:3043:HOH:O	2.46	0.49
1:K:181:LEU:HD23	1:K:234:LEU:HD12	1.95	0.49
2:Z:320:SER:HB3	2:Z:328:GLY:HA3	1.95	0.49
1:D:48:ARG:HH22	1:K:138:LEU:H	1.59	0.49
1:F:105:GLN:HG3	1:M:73:ASN:HD21	1.78	0.49
1:I:18:GLU:OE2	1:I:21:ARG:NH1	2.45	0.49
1:I:116:LYS:HD2	1:S:13:MET:HE1	1.94	0.49
1:K:142:THR:CB	5:K:2919:HOH:O	2.58	0.49
1:O:11:GLN:O	1:O:15:GLU:HG2	2.12	0.49
2:R:422:SER:HB3	2:R:437:GLN:HG2	1.93	0.49
1:S:142:THR:HA	5:S:3022:HOH:O	2.13	0.49
1:U:171:TYR:CD2	1:U:172:ALA:N	2.81	0.49
1:Y:8:SER:HG	1:Y:11:GLN:HB3	1.71	0.49
1:D:87:TYR:CZ	2:E:358:LEU:HD13	2.48	0.49
1:D:207:SER:C	1:D:208:LEU:HD12	2.38	0.49
1:K:97:ARG:NH2	5:K:1202:HOH:O	2.45	0.49
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.94	0.49
2:P:314:MET:HE3	2:P:405:ALA:HB2	1.94	0.49
1:U:167:LEU:O	1:U:171:TYR:N	2.34	0.49
1:Y:13:MET:O	1:Y:13:MET:CG	2.61	0.49
1:Y:83:ASP:OD2	2:Z:365:HIS:ND1	2.37	0.49
1:I:39:VAL:HG12	1:I:40:LEU:N	2.27	0.49
1:D:85:ARG:HB3	5:D:797:HOH:O	2.13	0.49
1:D:141:ILE:HD12	1:D:141:ILE:N	2.28	0.49
1:Q:39:VAL:CG1	1:Q:40:LEU:N	2.76	0.49
1:W:73:ASN:HD21	1:Y:105:GLN:HG3	1.78	0.49
1:W:98:GLN:O	1:W:102:VAL:HG23	2.12	0.49
2:L:393:ALA:HB1	2:L:398:LEU:HD12	1.93	0.48
1:I:171:TYR:C	1:I:171:TYR:CD2	2.91	0.48
1:K:87:TYR:CZ	2:L:358:LEU:HD13	2.49	0.48
2:V:397:GLY:O	2:V:398:LEU:HD23	2.13	0.48
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.95	0.48
2:H:413:ASP:HA	2:H:414:PRO:HD2	1.65	0.48
1:K:39:VAL:CG1	1:K:40:LEU:N	2.77	0.48
1:K:132:GLU:HB2	5:K:2964:HOH:O	2.14	0.48
2:L:426:ALA:HB2	4:g:4:HxD:H41	1.95	0.48
1:O:140:ARG:HD3	1:O:154:VAL:CG1	2.42	0.48
1:S:121:GLU:CA	5:S:3022:HOH:O	2.59	0.48
2:T:308:TYR:CD1	2:T:308:TYR:C	2.91	0.48
1:W:58:ASP:OD1	1:W:91:ARG:NH2	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:205:VAL:HG12	1:W:230:LEU:HG	1.95	0.48
2:C:414:PRO:C	2:C:416:SER:N	2.69	0.48
1:F:140:ARG:HD3	1:F:154:VAL:CG1	2.43	0.48
2:H:320:SER:HB3	2:H:328:GLY:HA3	1.94	0.48
1:K:39:VAL:HG12	1:K:40:LEU:N	2.28	0.48
2:L:324:ASN:HB2	5:L:1305:HOH:O	2.13	0.48
1:M:56:LEU:HG	1:M:62:PHE:HB2	1.95	0.48
1:Q:98:GLN:O	1:Q:102:VAL:HG23	2.12	0.48
2:R:382:ARG:NH2	2:R:385:ILE:HD13	2.28	0.48
1:S:8:SER:O	1:S:11:GLN:N	2.46	0.48
1:S:205:VAL:CG1	5:S:2979:HOH:O	2.62	0.48
1:U:225:ILE:HG21	1:U:233:LEU:HD22	1.94	0.48
1:1:74:LEU:HD13	1:1:122:LEU:HD11	1.94	0.48
2:J:366:TYR:CG	2:J:374:LEU:HD13	2.49	0.48
1:M:140:ARG:HD3	1:M:154:VAL:CG1	2.42	0.48
1:O:181:LEU:HD23	1:O:233:LEU:HB3	1.95	0.48
1:S:140:ARG:HD3	1:S:154:VAL:CG1	2.41	0.48
1:U:140:ARG:HD3	1:U:154:VAL:CG1	2.41	0.48
1:Y:140:ARG:HD3	1:Y:154:VAL:CG1	2.42	0.48
1:1:112:THR:HG22	1:1:113:GLU:HG3	1.96	0.48
1:K:8:SER:CB	1:K:11:GLN:HB3	2.43	0.48
1:K:74:LEU:HD13	1:K:122:LEU:HD11	1.94	0.48
1:M:74:LEU:HD13	1:M:122:LEU:HD11	1.94	0.48
1:Y:38:GLY:HA3	1:Y:213:LEU:O	2.14	0.48
1:I:140:ARG:HD3	1:I:154:VAL:CG1	2.42	0.48
2:L:366:TYR:CD2	2:L:374:LEU:HD13	2.49	0.48
2:P:374:LEU:HB2	5:P:208:HOH:O	2.13	0.48
1:U:19:LEU:HD23	1:U:19:LEU:O	2.13	0.48
1:W:56:LEU:HG	1:W:62:PHE:HB2	1.95	0.48
1:D:147:ILE:CD1	1:Q:50:LEU:HD21	2.44	0.48
1:K:53:ILE:HB	1:K:209:GLU:OE2	2.14	0.48
1:O:229:ALA:O	1:O:233:LEU:HD13	2.14	0.48
1:Y:59:ARG:NH2	1:Y:215:ALA:O	2.47	0.48
1:A:74:LEU:HD13	1:A:122:LEU:HD11	1.96	0.48
1:Y:11:GLN:NE2	1:Y:15:GLU:HG3	2.29	0.48
2:Z:422:SER:HB3	2:Z:437:GLN:HG2	1.94	0.48
2:L:372:VAL:HG23	2:L:373:PRO:HD3	1.96	0.48
2:V:511:ALA:O	2:V:515:ARG:HG3	2.14	0.48
1:K:115:ALA:HB3	1:M:112:THR:CG2	2.44	0.47
2:R:366:TYR:CG	2:R:374:LEU:HD13	2.49	0.47
2:C:416:SER:O	2:C:416:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:231:GLN:HA	1:S:231:GLN:OE1	2.14	0.47
2:V:320:SER:HB3	2:V:328:GLY:HA3	1.95	0.47
1:M:205:VAL:C	1:M:207:SER:H	2.21	0.47
1:D:73:ASN:ND2	1:K:105:GLN:HG3	2.30	0.47
2:E:456:GLN:NE2	2:E:465:ARG:HH21	2.11	0.47
2:N:415:GLN:OE1	2:N:415:GLN:HA	2.15	0.47
2:P:437:GLN:OE1	2:P:447:LYS:HD3	2.14	0.47
1:Y:228:SER:O	1:Y:231:GLN:HB3	2.14	0.47
2:2:366:TYR:CG	2:2:374:LEU:HD13	2.50	0.47
1:F:74:LEU:HD13	1:F:122:LEU:HD11	1.96	0.47
1:I:73:ASN:ND2	1:S:105:GLN:HG3	2.29	0.47
2:J:444:LEU:HB2	5:J:543:HOH:O	2.14	0.47
2:N:320:SER:HB3	2:N:328:GLY:HA3	1.95	0.47
1:W:223:ARG:NH1	5:W:1623:HOH:O	2.45	0.47
2:X:437:GLN:OE1	2:X:447:LYS:HD3	2.15	0.47
1:Y:152:HIS:CD2	1:Y:171:TYR:CZ	3.01	0.47
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.97	0.47
1:A:205:VAL:C	1:A:207:SER:H	2.21	0.47
1:B:140:ARG:HD3	1:B:154:VAL:CG1	2.44	0.47
2:C:414:PRO:C	2:C:416:SER:H	2.23	0.47
1:I:56:LEU:HB2	1:I:60:VAL:HG12	1.96	0.47
1:I:85:ARG:HB3	5:I:791:HOH:O	2.13	0.47
2:L:422:SER:HB3	2:L:437:GLN:HG2	1.96	0.47
1:Q:105:GLN:HE21	1:Y:73:ASN:ND2	2.12	0.47
2:C:366:TYR:CG	2:C:374:LEU:HD13	2.49	0.47
1:F:204:GLY:N	5:F:2909:HOH:O	2.47	0.47
2:H:362:GLU:OE2	2:H:382:ARG:CD	2.63	0.47
2:L:375:THR:HG23	1:M:93:ASP:OD1	2.14	0.47
2:N:333:LYS:HE2	3:g:3:LEU:HD22	1.97	0.47
1:Q:74:LEU:HD13	1:Q:122:LEU:HD11	1.97	0.47
1:Q:112:THR:HG22	1:Y:115:ALA:HB3	1.94	0.47
1:Q:112:THR:HG22	1:Q:113:GLU:HG3	1.97	0.47
1:Q:174:ASN:N	1:Q:174:ASN:ND2	2.46	0.47
1:S:19:LEU:HD23	1:S:19:LEU:O	2.14	0.47
1:S:115:ALA:HB3	1:I:112:THR:CG2	2.44	0.47
1:Y:11:GLN:O	1:Y:14:ARG:HB3	2.14	0.47
1:Y:163:ILE:HD13	1:Y:188:LEU:HD12	1.97	0.47
1:Y:232:ALA:O	1:Y:235:VAL:HB	2.15	0.47
2:G:306:LEU:C	2:G:306:LEU:HD12	2.40	0.47
1:K:56:LEU:HG	1:K:62:PHE:HB2	1.96	0.47
1:W:46:PRO:CD	1:W:47:SER:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:140:ARG:HD3	1:1:154:VAL:CG1	2.45	0.47
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.96	0.47
1:F:73:ASN:ND2	1:W:105:GLN:HG3	2.29	0.47
1:M:28:LYS:HE3	1:M:46:PRO:HG3	1.97	0.47
2:N:329:ARG:HD3	5:N:930:HOH:O	2.14	0.47
1:S:152:HIS:HB3	1:S:171:TYR:CZ	2.50	0.47
1:W:40:LEU:HG	1:W:41:PHE:N	2.30	0.47
1:W:181:LEU:CD2	1:W:234:LEU:CD2	2.93	0.47
1:Y:92:ARG:NH1	1:Y:92:ARG:HG3	2.18	0.47
1:Y:231:GLN:O	1:Y:231:GLN:OE1	2.32	0.47
1:1:55:GLU:CD	1:1:220:ARG:HH21	2.22	0.47
1:D:48:ARG:HH12	1:K:137:GLU:CG	2.27	0.47
1:F:9:PRO:HD2	1:M:15:GLU:CD	2.40	0.47
1:K:140:ARG:NH1	1:K:140:ARG:CG	2.76	0.47
2:N:392:ALA:HA	2:N:395:MET:HE3	1.95	0.47
2:R:306:LEU:HD12	2:R:313:VAL:HG12	1.97	0.47
1:S:98:GLN:O	1:S:102:VAL:HG23	2.15	0.47
1:U:74:LEU:HD13	1:U:122:LEU:HD11	1.97	0.47
2:V:314:MET:HE3	2:V:405:ALA:HB2	1.96	0.47
1:Y:137:GLU:C	1:Y:138:LEU:HG	2.38	0.47
1:D:140:ARG:HD3	1:D:154:VAL:CG1	2.42	0.46
1:F:55:GLU:OE1	1:F:220:ARG:NH2	2.39	0.46
2:L:382:ARG:NH2	2:L:385:ILE:CD1	2.78	0.46
2:N:366:TYR:CG	2:N:374:LEU:HD13	2.50	0.46
1:O:98:GLN:O	1:O:102:VAL:HG23	2.15	0.46
1:S:170:SER:C	1:S:183:ILE:HD11	2.37	0.46
1:1:130:TYR:C	1:1:132:GLU:N	2.69	0.46
1:F:170:SER:OG	1:F:183:ILE:HD13	2.15	0.46
1:O:11:GLN:HG3	1:O:15:GLU:OE1	2.15	0.46
1:S:97:ARG:NH2	5:S:683:HOH:O	2.47	0.46
1:W:40:LEU:HD21	1:W:42:VAL:CG2	2.46	0.46
1:W:112:THR:HG22	1:W:113:GLU:HG3	1.98	0.46
1:W:230:LEU:HD12	1:W:230:LEU:O	2.15	0.46
2:Z:409:ILE:HG13	2:Z:410:HIS:ND1	2.31	0.46
2:2:364:GLU:HG2	2:2:368:LYS:HD3	1.98	0.46
1:I:114:GLN:HE21	1:I:114:GLN:HB3	1.52	0.46
5:I:1024:HOH:O	1:S:112:THR:HG21	2.14	0.46
2:J:324:ASN:ND2	5:J:541:HOH:O	2.48	0.46
1:K:181:LEU:O	1:K:185:VAL:HG23	2.14	0.46
1:S:55:GLU:OE1	1:S:220:ARG:NH2	2.39	0.46
2:V:362:GLU:OE2	2:V:382:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:SER:OG	1:F:157:GLY:O	2.29	0.46
2:G:509:ARG:HH11	2:G:509:ARG:CG	2.28	0.46
1:B:97:ARG:NH2	5:B:1763:HOH:O	2.47	0.46
1:M:54:SER:CB	1:M:75:ARG:HD2	2.46	0.46
1:M:161:GLU:HB2	1:M:162:PRO:HD3	1.98	0.46
1:M:163:ILE:O	1:M:187:ALA:HB1	2.14	0.46
1:Q:52:LYS:HG2	1:Q:71:PHE:CZ	2.51	0.46
1:S:152:HIS:CB	1:S:171:TYR:CE2	2.96	0.46
1:W:79:ILE:HG21	2:X:369:LEU:HD13	1.97	0.46
1:W:152:HIS:HB3	1:W:171:TYR:CE2	2.51	0.46
1:1:97:ARG:HH22	1:1:101:ASN:ND2	2.11	0.46
1:B:8:SER:HA	1:B:9:PRO:C	2.40	0.46
2:C:362:GLU:OE2	2:C:382:ARG:CD	2.64	0.46
2:C:437:GLN:OE1	2:C:447:LYS:HD3	2.15	0.46
2:E:388:ARG:HD3	2:E:426:ALA:O	2.14	0.46
1:F:18:GLU:CD	1:F:21:ARG:NH1	2.55	0.46
1:I:54:SER:CB	1:I:75:ARG:HD2	2.45	0.46
1:K:112:THR:HG22	1:K:113:GLU:HG3	1.98	0.46
1:O:33:LEU:O	1:O:33:LEU:HD12	2.16	0.46
1:O:205:VAL:HG21	1:O:231:GLN:NE2	2.30	0.46
1:A:45:ASN:OD1	1:A:47:SER:N	2.48	0.46
1:D:68:PHE:HA	1:D:71:PHE:CE2	2.51	0.46
1:D:161:GLU:CA	1:D:165:ASN:ND2	2.79	0.46
1:F:114:GLN:HE21	1:F:114:GLN:HB3	1.54	0.46
1:1:54:SER:CB	1:1:75:ARG:HD2	2.45	0.46
1:1:163:ILE:CG2	1:1:187:ALA:O	2.55	0.46
1:K:184:ALA:O	1:K:188:LEU:HB2	2.15	0.46
2:P:320:SER:HB3	2:P:328:GLY:HA3	1.97	0.46
1:A:112:THR:HG22	1:A:113:GLU:HG3	1.98	0.46
1:A:125:ALA:HB2	1:A:138:LEU:HD23	1.98	0.46
1:D:217:ARG:NH2	1:D:223:ARG:HD3	2.30	0.46
1:I:181:LEU:HD23	1:I:233:LEU:CB	2.46	0.46
1:O:17:SER:O	1:O:21:ARG:HB2	2.16	0.46
1:O:112:THR:HG22	1:O:113:GLU:HG3	1.98	0.46
1:W:51:GLN:HG2	1:W:224:ARG:NH2	2.31	0.46
1:Y:74:LEU:HD13	1:Y:122:LEU:HD11	1.98	0.46
1:Y:98:GLN:O	1:Y:102:VAL:HG23	2.15	0.46
1:A:188:LEU:HD12	1:A:188:LEU:HA	1.79	0.46
1:M:173:GLU:O	1:M:174:ASN:HB2	2.15	0.46
1:1:56:LEU:HG	1:1:62:PHE:HB2	1.97	0.46
1:A:234:LEU:N	1:A:234:LEU:CD1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:116:LYS:CD	1:M:13:MET:HE1	2.32	0.45
1:O:54:SER:CB	1:O:75:ARG:HD2	2.46	0.45
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.51	0.45
1:B:68:PHE:HA	1:B:71:PHE:CE2	2.51	0.45
1:F:98:GLN:O	1:F:102:VAL:HG23	2.16	0.45
2:J:425:ALA:HB3	4:j:4:HXD:H42	1.97	0.45
1:M:112:THR:HG22	1:M:113:GLU:HG3	1.98	0.45
1:S:205:VAL:HG21	5:S:2979:HOH:O	2.14	0.45
1:1:205:VAL:CG1	1:1:234:LEU:HD12	2.45	0.45
2:H:425:ALA:HB3	4:a:4:HXD:H42	1.98	0.45
2:J:317:ASP:OD2	2:J:333:LYS:NZ	2.47	0.45
2:N:364:GLU:HG2	2:N:368:LYS:HD3	1.98	0.45
1:S:112:THR:HG22	1:S:113:GLU:HG3	1.98	0.45
1:S:114:GLN:HE21	1:S:114:GLN:HB3	1.53	0.45
1:U:8:SER:HB2	1:U:11:GLN:HB2	1.98	0.45
1:D:167:LEU:CD1	1:D:183:ILE:CG2	2.95	0.45
2:L:392:ALA:HA	2:L:395:MET:HE3	1.98	0.45
2:V:426:ALA:HB2	4:h:4:HXD:H41	1.97	0.45
1:W:140:ARG:HD3	1:W:154:VAL:CG1	2.44	0.45
2:E:382:ARG:NH2	2:E:385:ILE:HD13	2.32	0.45
1:F:70:GLU:HB3	1:F:118:TYR:CD2	2.52	0.45
1:F:112:THR:HG22	1:F:113:GLU:HG3	1.98	0.45
2:H:362:GLU:OE2	2:H:382:ARG:HD3	2.17	0.45
1:I:56:LEU:CG	1:I:62:PHE:HB2	2.44	0.45
2:R:529:SER:CB	5:R:1999:HOH:O	2.34	0.45
2:2:422:SER:HB3	2:2:437:GLN:HG2	1.98	0.45
1:A:52:LYS:HE2	1:A:64:ALA:O	2.16	0.45
1:A:163:ILE:HG23	1:A:187:ALA:C	2.41	0.45
1:D:135:ARG:HH22	1:D:173:GLU:CD	2.24	0.45
1:Q:185:VAL:O	1:Q:189:ARG:N	2.42	0.45
1:S:165:ASN:O	1:S:169:GLU:OE2	2.34	0.45
1:Y:8:SER:OG	1:Y:11:GLN:HG2	2.14	0.45
1:Y:128:ALA:HB2	1:Y:134:LYS:CB	2.45	0.45
1:1:33:LEU:HD12	1:1:33:LEU:O	2.17	0.45
1:1:97:ARG:HH22	1:1:101:ASN:HD22	1.60	0.45
1:A:45:ASN:OD1	1:A:45:ASN:C	2.59	0.45
1:A:97:ARG:NH2	5:A:1568:HOH:O	2.42	0.45
1:B:112:THR:HG22	1:B:113:GLU:HG3	1.99	0.45
2:E:422:SER:HB3	2:E:437:GLN:HG2	1.98	0.45
2:H:308:TYR:CZ	2:H:311:GLY:HA3	2.52	0.45
1:K:54:SER:CB	1:K:75:ARG:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:41:PHE:CB	1:M:53:ILE:HD13	2.36	0.45
1:O:182:ARG:NH1	1:O:233:LEU:O	2.36	0.45
2:P:366:TYR:CG	2:P:374:LEU:HD13	2.51	0.45
2:R:392:ALA:HA	2:R:395:MET:CE	2.46	0.45
1:S:152:HIS:HD2	1:S:171:TYR:OH	1.99	0.45
2:E:375:THR:HG23	1:K:93:ASP:OD1	2.17	0.45
1:I:45:ASN:OD1	1:I:46:PRO:HD2	2.17	0.45
1:I:73:ASN:HD21	1:S:105:GLN:HE21	1.65	0.45
1:U:112:THR:HG22	1:U:113:GLU:HG3	1.99	0.45
1:W:114:GLN:HE21	1:W:114:GLN:HB3	1.52	0.45
1:W:152:HIS:CD2	1:W:171:TYR:CE2	3.05	0.45
1:W:207:SER:O	1:W:208:LEU:HD23	2.17	0.45
1:B:54:SER:CB	1:B:75:ARG:HD2	2.46	0.45
2:C:391:LEU:HG	2:C:395:MET:HE2	1.99	0.45
1:S:85:ARG:HB3	5:S:786:HOH:O	2.16	0.45
2:T:444:LEU:HD23	2:X:444:LEU:HD22	1.97	0.45
1:Q:144:ASP:CG	1:Q:146:SER:HG	2.24	0.45
1:Q:188:LEU:HA	1:Q:188:LEU:HD12	1.80	0.45
1:W:54:SER:CB	1:W:75:ARG:HD2	2.47	0.45
2:C:456:GLN:HE21	2:C:465:ARG:NH2	2.09	0.44
2:C:509:ARG:HA	2:C:509:ARG:HD2	1.79	0.44
2:G:422:SER:HB3	2:G:437:GLN:HG2	1.97	0.44
2:L:391:LEU:HG	2:L:395:MET:HE2	1.99	0.44
1:Q:33:LEU:HD12	1:Q:33:LEU:O	2.16	0.44
2:R:331:VAL:HG11	3:i:3:LEU:HD22	1.98	0.44
2:R:465:ARG:HD3	5:R:712:HOH:O	2.17	0.44
1:S:153:PHE:CD1	1:S:153:PHE:C	2.95	0.44
1:U:45:ASN:ND2	1:U:209:GLU:OE1	2.48	0.44
1:W:33:LEU:HD12	1:W:33:LEU:O	2.17	0.44
1:A:114:GLN:HE21	1:A:114:GLN:HB3	1.51	0.44
2:R:392:ALA:HA	2:R:395:MET:HE3	2.00	0.44
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.99	0.44
1:Y:232:ALA:CA	1:Y:235:VAL:HG23	2.48	0.44
2:G:324:ASN:ND2	5:G:1829:HOH:O	2.50	0.44
1:I:229:ALA:O	1:I:233:LEU:HD13	2.17	0.44
1:K:114:GLN:HE21	1:K:114:GLN:HB3	1.52	0.44
2:L:320:SER:HB3	2:L:328:GLY:HA3	1.99	0.44
2:N:422:SER:HB3	2:N:437:GLN:HG2	1.99	0.44
2:R:515:ARG:O	2:R:519:GLU:HG3	2.17	0.44
1:Y:45:ASN:HA	1:Y:46:PRO:HD2	1.68	0.44
1:I:223:ARG:O	1:I:223:ARG:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:225:ILE:HG21	1:1:233:LEU:CD2	2.46	0.44
2:2:432:GLU:HG2	2:2:436:TYR:O	2.18	0.44
2:2:509:ARG:HG2	5:2:2188:HOH:O	2.16	0.44
1:D:105:GLN:HG3	1:Q:73:ASN:HD21	1.82	0.44
2:J:437:GLN:OE1	2:J:447:LYS:HD3	2.16	0.44
1:O:167:LEU:HA	1:O:167:LEU:HD12	1.67	0.44
2:T:341:THR:CG2	2:T:404:LEU:HD11	2.48	0.44
1:W:76:ARG:HD3	5:W:2805:HOH:O	2.18	0.44
1:A:54:SER:CB	1:A:75:ARG:HD2	2.47	0.44
1:A:233:LEU:N	1:A:233:LEU:HD12	2.32	0.44
1:B:133:THR:HG23	1:B:133:THR:O	2.17	0.44
1:M:230:LEU:HD12	1:M:230:LEU:O	2.16	0.44
2:P:422:SER:HB3	2:P:437:GLN:HG2	1.99	0.44
1:W:73:ASN:ND2	1:Y:105:GLN:HE21	2.15	0.44
1:Y:181:LEU:O	1:Y:185:VAL:HG23	2.18	0.44
1:Y:186:ALA:O	1:Y:189:ARG:N	2.51	0.44
1:A:67:LYS:HG2	1:A:69:ASN:HD21	1.82	0.44
1:A:217:ARG:NH1	1:A:223:ARG:HB3	2.33	0.44
2:C:301:THR:CG2	2:C:302:THR:N	2.80	0.44
1:D:45:ASN:HA	1:D:46:PRO:HD3	1.85	0.44
2:E:314:MET:HE3	2:E:405:ALA:HB2	1.99	0.44
2:E:325:MET:SD	2:R:444:LEU:HD21	2.58	0.44
1:I:62:PHE:CZ	1:I:122:LEU:HD22	2.53	0.44
1:I:112:THR:HG22	1:I:113:GLU:HG3	2.00	0.44
1:K:205:VAL:C	1:K:207:SER:H	2.26	0.44
1:M:71:PHE:CD1	1:M:71:PHE:C	2.95	0.44
1:O:141:ILE:N	1:O:141:ILE:HD12	2.32	0.44
1:S:54:SER:CB	1:S:75:ARG:HD2	2.48	0.44
1:S:59:ARG:NH1	1:S:217:ARG:O	2.47	0.44
1:S:73:ASN:ND2	1:1:105:GLN:HG3	2.30	0.44
1:U:93:ASP:OD1	2:2:375:THR:HG23	2.17	0.44
2:Z:308:TYR:CZ	2:Z:311:GLY:HA3	2.52	0.44
1:D:152:HIS:CB	1:D:171:TYR:CE2	3.00	0.44
2:J:416:SER:C	2:J:418:GLY:H	2.26	0.44
1:O:85:ARG:NH2	5:O:2922:HOH:O	2.39	0.44
1:Q:45:ASN:ND2	1:Q:209:GLU:OE1	2.51	0.44
1:Y:112:THR:HG22	1:Y:113:GLU:HG3	1.98	0.44
1:A:89:TYR:CD1	2:P:374:LEU:HD11	2.53	0.44
1:D:33:LEU:HB3	1:D:153:PHE:HB3	1.99	0.44
1:D:184:ALA:C	1:D:188:LEU:HD13	2.42	0.44
1:K:183:ILE:HD13	1:K:183:ILE:HG21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:48:ARG:H	1:Q:48:ARG:HG2	1.39	0.44
1:U:179:ASP:O	1:U:183:ILE:HG13	2.18	0.44
1:Y:15:GLU:O	1:Y:16:ARG:C	2.57	0.44
1:D:152:HIS:CD2	1:D:171:TYR:CZ	3.05	0.44
1:I:189:ARG:O	1:I:191:GLY:N	2.49	0.44
1:K:167:LEU:HD12	1:K:183:ILE:CG2	2.48	0.44
2:T:444:LEU:HB2	5:T:2189:HOH:O	2.18	0.44
1:1:181:LEU:HD23	1:1:233:LEU:HB3	1.98	0.44
1:Q:181:LEU:HD23	1:Q:233:LEU:HB2	1.99	0.43
1:Q:184:ALA:O	1:Q:188:LEU:HB2	2.18	0.43
1:S:121:GLU:CG	5:S:3022:HOH:O	2.50	0.43
1:U:114:GLN:HE21	1:U:114:GLN:HB3	1.53	0.43
1:1:55:GLU:OE1	1:1:220:ARG:NH2	2.43	0.43
1:F:163:ILE:HG23	1:F:187:ALA:O	2.18	0.43
2:G:331:VAL:HG11	3:c:3:LEU:HD22	2.00	0.43
2:G:364:GLU:HG2	2:G:368:LYS:HD3	1.99	0.43
2:G:509:ARG:HG3	2:G:509:ARG:HH11	1.80	0.43
1:I:70:GLU:HB3	1:I:118:TYR:CD2	2.54	0.43
1:Q:38:GLY:HA3	1:Q:213:LEU:O	2.17	0.43
2:R:515:ARG:NE	5:R:1326:HOH:O	2.42	0.43
1:1:19:LEU:C	1:1:19:LEU:HD23	2.43	0.43
1:A:21:ARG:CZ	1:A:21:ARG:HB3	2.49	0.43
1:A:45:ASN:HA	1:A:46:PRO:HD2	1.82	0.43
1:B:149:ASP:OD2	1:B:149:ASP:N	2.49	0.43
1:D:54:SER:CB	1:D:75:ARG:HD2	2.48	0.43
1:I:51:GLN:OE1	1:I:224:ARG:NH2	2.51	0.43
2:J:374:LEU:HB2	5:J:182:HOH:O	2.18	0.43
2:J:422:SER:HB3	2:J:437:GLN:HG2	2.00	0.43
1:M:55:GLU:HB2	1:M:222:PHE:CG	2.53	0.43
2:P:444:LEU:HB2	5:P:88:HOH:O	2.18	0.43
1:S:48:ARG:H	1:S:48:ARG:HG2	1.57	0.43
2:X:307:LYS:HE3	2:X:418:GLY:O	2.18	0.43
1:Y:228:SER:O	1:Y:232:ALA:N	2.41	0.43
2:Z:331:VAL:HG11	3:m:3:LEU:HD22	2.01	0.43
2:C:332:ARG:NH2	5:C:550:HOH:O	2.40	0.43
2:E:437:GLN:OE1	2:E:447:LYS:HD3	2.18	0.43
1:K:141:ILE:HD12	1:K:141:ILE:N	2.33	0.43
2:L:317:ASP:OD2	2:L:333:LYS:NZ	2.47	0.43
2:L:366:TYR:CG	2:L:374:LEU:HD13	2.53	0.43
1:M:18:GLU:CG	1:M:22:LYS:HE3	2.45	0.43
1:S:123:CYS:HA	1:S:139:TYR:O	2.19	0.43

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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	0.43
2:V:422:SER:HB3	2:V:437:GLN:HG2	1.99	0.43
1:W:21:ARG:CZ	1:W:21:ARG:HB3	2.49	0.43
1:W:46:PRO:HD2	1:W:47:SER:H	1.83	0.43
1:Y:54:SER:CB	1:Y:75:ARG:HD2	2.48	0.43
2:Z:341:THR:CG2	2:Z:404:LEU:HD11	2.49	0.43
1:1:133:THR:HG23	1:1:133:THR:O	2.18	0.43
1:D:21:ARG:CZ	1:D:21:ARG:HB3	2.48	0.43
1:F:54:SER:CB	1:F:75:ARG:HD2	2.49	0.43
1:F:167:LEU:CA	1:F:170:SER:HB3	2.35	0.43
2:J:314:MET:HE3	2:J:405:ALA:HB2	1.99	0.43
2:J:320:SER:HB3	2:J:328:GLY:CA	2.48	0.43
2:L:362:GLU:OE2	2:L:382:ARG:HD2	2.19	0.43
1:M:87:TYR:CZ	2:N:358:LEU:HD13	2.54	0.43
1:O:161:GLU:HB3	1:O:162:PRO:CD	2.48	0.43
1:Q:149:ASP:OD2	1:Q:149:ASP:N	2.51	0.43
1:W:227:GLY:O	1:W:231:GLN:N	2.29	0.43
1:Y:13:MET:HA	1:Y:16:ARG:HD3	2.00	0.43
1:Y:135:ARG:NH1	1:Y:135:ARG:CG	2.82	0.43
1:1:129:HIS:O	1:1:132:GLU:CB	2.65	0.43
1:D:16:ARG:HB3	1:D:117:PRO:HG2	1.99	0.43
2:E:320:SER:HB3	2:E:328:GLY:CA	2.48	0.43
2:H:306:LEU:HD12	2:H:306:LEU:C	2.44	0.43
2:N:412:SER:O	2:N:414:PRO:HD3	2.18	0.43
1:Q:150:GLU:HA	1:Q:151:PRO:HD3	1.89	0.43
2:R:412:SER:O	2:R:414:PRO:HD3	2.18	0.43
1:W:68:PHE:HA	1:W:71:PHE:CE2	2.53	0.43
1:A:28:LYS:HE3	1:A:46:PRO:HG2	2.00	0.43
1:B:73:ASN:HD21	1:I:105:GLN:HG3	1.83	0.43
1:D:35:TYR:HB2	1:D:175:ALA:O	2.19	0.43
1:M:68:PHE:HA	1:M:71:PHE:CE2	2.54	0.43
2:X:324:ASN:HD22	2:X:324:ASN:HA	1.61	0.43
1:A:115:ALA:HB3	1:B:112:THR:CG2	2.48	0.43
1:A:137:GLU:OE1	1:A:139:TYR:OH	2.30	0.43
1:D:8:SER:CA	1:Q:15:GLU:OE2	2.64	0.43
2:E:341:THR:CG2	2:E:404:LEU:HD11	2.49	0.43
2:G:306:LEU:HD12	2:G:306:LEU:O	2.18	0.43
1:O:57:TYR:O	1:O:58:ASP:C	2.62	0.43
1:1:98:GLN:O	1:1:102:VAL:HG23	2.19	0.43
2:C:306:LEU:HD12	2:C:313:VAL:HG12	2.00	0.43
2:E:317:ASP:OD2	2:E:333:LYS:NZ	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:LEU:C	1:I:19:LEU:CD2	2.86	0.43
1:K:140:ARG:HD3	1:K:154:VAL:CG1	2.48	0.43
1:K:229:ALA:O	1:K:233:LEU:HD13	2.19	0.43
1:Q:170:SER:O	1:Q:170:SER:OG	2.37	0.43
2:R:362:GLU:OE2	2:R:382:ARG:HD3	2.19	0.43
1:W:19:LEU:HD23	1:W:19:LEU:O	2.19	0.43
1:A:150:GLU:HA	1:A:151:PRO:HD3	1.87	0.43
2:G:314:MET:HE3	2:G:405:ALA:HB2	2.01	0.43
2:H:430:ASN:ND2	5:H:2966:HOH:O	2.52	0.43
1:Q:123:CYS:HA	1:Q:139:TYR:O	2.19	0.43
1:U:21:ARG:CZ	1:U:21:ARG:HB3	2.49	0.43
1:U:133:THR:HG23	1:U:133:THR:O	2.18	0.43
1:Y:204:GLY:O	1:Y:208:LEU:HG	2.18	0.43
1:B:150:GLU:HA	1:B:151:PRO:HD3	1.89	0.42
1:D:123:CYS:HA	1:D:139:TYR:O	2.19	0.42
2:G:393:ALA:HB1	2:G:398:LEU:HD12	2.01	0.42
2:G:426:ALA:HB2	4:I:4:H XD:H41	2.01	0.42
2:H:341:THR:CG2	2:H:404:LEU:HD11	2.49	0.42
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.54	0.42
1:M:28:LYS:HE3	1:M:46:PRO:HG2	2.01	0.42
1:M:163:ILE:HG23	1:M:188:LEU:CA	2.48	0.42
2:N:382:ARG:NH2	2:N:385:ILE:HD13	2.34	0.42
2:R:521:ARG:HD3	2:R:521:ARG:HA	1.87	0.42
1:S:170:SER:C	1:S:183:ILE:CD1	2.92	0.42
1:Y:181:LEU:HD21	1:Y:234:LEU:CD1	2.49	0.42
1:A:163:ILE:HG23	1:A:187:ALA:O	2.19	0.42
1:D:70:GLU:HB3	1:D:118:TYR:CD2	2.54	0.42
1:D:112:THR:HG22	1:D:113:GLU:HG3	2.00	0.42
1:D:133:THR:HG23	1:D:133:THR:O	2.20	0.42
1:F:88:ALA:O	2:N:381:ASN:ND2	2.51	0.42
2:G:393:ALA:O	2:G:398:LEU:HB2	2.18	0.42
1:O:35:TYR:CZ	1:O:37:GLY:HA3	2.53	0.42
1:Q:56:LEU:O	2:R:368:LYS:HE3	2.19	0.42
1:W:179:ASP:O	1:W:183:ILE:CG1	2.61	0.42
1:W:204:GLY:O	1:W:208:LEU:HG	2.19	0.42
1:I:8:SER:N	5:I:1515:HOH:O	2.52	0.42
1:A:19:LEU:HD23	1:A:19:LEU:O	2.19	0.42
2:C:362:GLU:OE2	2:C:382:ARG:HD3	2.18	0.42
2:E:324:ASN:HD22	2:E:324:ASN:HA	1.62	0.42
1:F:116:LYS:HG2	1:F:117:PRO:O	2.19	0.42
1:F:170:SER:C	1:F:183:ILE:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:362:GLU:OE2	2:L:382:ARG:CD	2.66	0.42
2:L:509:ARG:CD	5:L:2882:HOH:O	2.53	0.42
2:T:351:VAL:HG21	2:T:398:LEU:HB3	2.00	0.42
2:X:331:VAL:HG11	3:l:3:LEU:HD22	2.00	0.42
2:X:508:SER:O	2:X:512:GLU:HG3	2.20	0.42
1:D:105:GLN:HE21	1:Q:73:ASN:HD21	1.65	0.42
2:E:306:LEU:C	2:E:420:ILE:HD11	2.45	0.42
2:E:366:TYR:CG	2:E:374:LEU:HD13	2.54	0.42
2:E:412:SER:O	2:E:414:PRO:HD3	2.19	0.42
1:K:230:LEU:O	1:K:231:GLN:C	2.62	0.42
1:K:231:GLN:O	1:K:232:ALA:C	2.62	0.42
2:L:333:LYS:HE2	3:f:3:LEU:HD22	2.01	0.42
1:O:19:LEU:C	1:O:19:LEU:CD2	2.87	0.42
1:O:25:ALA:O	1:O:158:GLY:HA2	2.20	0.42
1:U:54:SER:CB	1:U:75:ARG:HD2	2.49	0.42
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.54	0.42
1:Y:152:HIS:HD2	1:Y:171:TYR:OH	2.02	0.42
2:C:398:LEU:HD23	2:C:398:LEU:HA	1.75	0.42
1:D:40:LEU:HD13	1:D:177:LEU:CD1	2.49	0.42
1:F:19:LEU:HD23	1:F:19:LEU:O	2.20	0.42
2:G:509:ARG:NE	5:G:3043:HOH:O	2.52	0.42
1:K:149:ASP:OD2	1:K:149:ASP:N	2.53	0.42
1:Q:28:LYS:HE3	1:Q:46:PRO:HG3	2.01	0.42
2:R:430:ASN:OD1	2:R:430:ASN:C	2.63	0.42
1:S:21:ARG:HB3	1:S:21:ARG:CZ	2.49	0.42
2:T:374:LEU:HD11	1:l:89:TYR:CD1	2.55	0.42
1:W:181:LEU:HD23	1:W:234:LEU:CD2	2.48	0.42
1:W:205:VAL:HG11	1:W:231:GLN:HB2	2.00	0.42
1:l:45:ASN:HA	1:l:46:PRO:HD2	1.87	0.42
2:2:317:ASP:OD2	2:2:333:LYS:NZ	2.50	0.42
2:2:362:GLU:OE2	2:2:382:ARG:CD	2.67	0.42
2:C:317:ASP:OD2	2:C:333:LYS:NZ	2.52	0.42
1:D:19:LEU:HD23	1:D:19:LEU:O	2.20	0.42
1:D:73:ASN:ND2	1:K:105:GLN:HE21	2.17	0.42
2:E:324:ASN:ND2	5:E:893:HOH:O	2.51	0.42
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.54	0.42
1:O:89:TYR:CD1	2:V:374:LEU:HD11	2.55	0.42
1:Q:75:ARG:NH2	2:R:369:LEU:O	2.36	0.42
1:Q:214:ASP:HB3	1:Q:217:ARG:CG	2.49	0.42
2:R:320:SER:HB2	2:R:331:VAL:HG21	2.01	0.42
2:T:324:ASN:HD22	2:T:324:ASN:HA	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:8:SER:OG	1:Y:11:GLN:HG3	2.18	0.42
2:2:409:ILE:HG13	2:2:410:HIS:ND1	2.33	0.42
2:C:364:GLU:HG2	2:C:368:LYS:HD3	2.02	0.42
2:E:366:TYR:CE2	2:E:374:LEU:HD13	2.54	0.42
2:G:444:LEU:HB2	5:G:869:HOH:O	2.18	0.42
2:H:392:ALA:HA	2:H:395:MET:HE2	2.01	0.42
2:J:341:THR:CG2	2:J:404:LEU:HD11	2.49	0.42
1:Q:171:TYR:HE2	1:Q:173:GLU:CG	2.13	0.42
2:V:437:GLN:OE1	2:V:447:LYS:HD3	2.19	0.42
1:W:207:SER:C	1:W:208:LEU:HD23	2.45	0.42
1:W:214:ASP:HB3	1:W:217:ARG:HG2	2.02	0.42
2:X:382:ARG:NH2	2:X:385:ILE:HD13	2.35	0.42
2:X:409:ILE:HG13	2:X:410:HIS:ND1	2.34	0.42
2:2:366:TYR:CE2	2:2:374:LEU:HD13	2.55	0.42
1:F:147:ILE:CG1	1:F:148:ALA:N	2.83	0.42
2:G:333:LYS:HE2	3:c:3:LEU:HD22	2.01	0.42
2:G:437:GLN:OE1	2:G:447:LYS:HD3	2.20	0.42
1:I:9:PRO:O	1:I:13:MET:HB2	2.20	0.42
2:J:374:LEU:HD11	1:S:89:TYR:CD1	2.55	0.42
1:K:181:LEU:CD2	1:K:234:LEU:CD1	2.97	0.42
1:O:67:LYS:HD3	1:O:69:ASN:HD21	1.84	0.42
1:O:110:ILE:HG21	1:O:118:TYR:CD1	2.55	0.42
2:T:425:ALA:HB3	4:n:4:HXD:H42	2.02	0.42
1:W:28:LYS:HB2	1:W:52:LYS:HZ1	1.82	0.42
2:X:425:ALA:HB3	4:m:4:HXD:H42	2.00	0.42
1:l:129:HIS:O	1:l:130:TYR:C	2.59	0.42
1:A:231:GLN:HA	1:A:231:GLN:NE2	2.35	0.42
1:B:123:CYS:HA	1:B:139:TYR:O	2.20	0.42
2:G:413:ASP:OD2	2:G:416:SER:HB2	2.19	0.42
2:H:508:SER:O	2:H:512:GLU:HG3	2.20	0.42
1:M:178:THR:O	1:M:179:ASP:C	2.60	0.42
1:M:205:VAL:C	1:M:207:SER:N	2.78	0.42
1:Q:55:GLU:HB2	1:Q:222:PHE:CG	2.55	0.42
1:S:52:LYS:NZ	5:S:2897:HOH:O	2.30	0.42
1:U:8:SER:OG	1:U:11:GLN:HB3	2.20	0.42
1:U:33:LEU:HB3	1:U:153:PHE:CB	2.49	0.42
1:U:163:ILE:HG23	1:U:187:ALA:C	2.44	0.42
2:X:320:SER:HB3	2:X:328:GLY:HA3	2.02	0.42
1:Y:114:GLN:HE21	1:Y:114:GLN:HB3	1.54	0.42
2:Z:426:ALA:HB2	4:i:4:HXD:H41	2.01	0.42
1:F:149:ASP:OD2	1:F:149:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:390:ASN:CG	2:H:390:ASN:O	2.63	0.42
1:O:8:SER:N	5:O:986:HOH:O	2.53	0.42
2:T:491:PHE:C	5:T:3058:HOH:O	2.62	0.42
1:W:136:PRO:HG3	5:W:2971:HOH:O	2.19	0.42
2:X:306:LEU:C	2:X:306:LEU:HD12	2.45	0.42
1:I:180:ALA:C	1:I:183:ILE:HG23	2.45	0.42
1:A:18:GLU:CG	1:A:22:LYS:HE3	2.49	0.41
1:D:55:GLU:HB2	1:D:222:PHE:CG	2.55	0.41
1:F:76:ARG:HD3	5:F:990:HOH:O	2.19	0.41
1:F:133:THR:HG23	1:F:133:THR:O	2.20	0.41
1:M:21:ARG:CZ	1:M:21:ARG:HB3	2.49	0.41
1:M:163:ILE:CG2	1:M:188:LEU:HA	2.50	0.41
2:X:444:LEU:CB	5:X:2899:HOH:O	2.46	0.41
2:C:306:LEU:HD12	2:C:306:LEU:C	2.45	0.41
1:I:167:LEU:HD13	1:I:187:ALA:CB	2.50	0.41
1:O:81:PHE:CZ	1:O:102:VAL:HG21	2.55	0.41
1:S:15:GLU:CD	1:I:9:PRO:HD2	2.45	0.41
1:S:233:LEU:HD12	1:S:233:LEU:N	2.35	0.41
1:I:123:CYS:HA	1:I:139:TYR:O	2.20	0.41
1:I:180:ALA:O	1:I:181:LEU:C	2.60	0.41
1:A:68:PHE:HA	1:A:71:PHE:CE2	2.55	0.41
1:B:232:ALA:O	1:B:233:LEU:CB	2.30	0.41
1:D:164:ALA:O	1:D:167:LEU:CB	2.67	0.41
1:I:87:TYR:CZ	2:J:358:LEU:HD13	2.55	0.41
1:O:133:THR:O	1:O:133:THR:HG23	2.20	0.41
2:Z:413:ASP:HA	2:Z:414:PRO:HD3	1.89	0.41
1:I:55:GLU:HB2	1:I:222:PHE:CG	2.55	0.41
1:B:21:ARG:HB3	1:B:21:ARG:NH1	2.35	0.41
1:D:48:ARG:HG2	1:K:149:ASP:OD1	2.17	0.41
1:D:98:GLN:O	1:D:102:VAL:HG23	2.20	0.41
1:D:152:HIS:CG	1:D:171:TYR:CZ	3.07	0.41
2:G:430:ASN:ND2	5:G:1095:HOH:O	2.53	0.41
2:J:324:ASN:HD22	2:J:324:ASN:HA	1.63	0.41
2:L:390:ASN:HA	5:L:963:HOH:O	2.20	0.41
1:O:182:ARG:HG2	1:O:234:LEU:HD23	2.02	0.41
1:S:110:ILE:HG21	1:S:118:TYR:CD1	2.55	0.41
1:S:229:ALA:O	1:S:232:ALA:HB3	2.20	0.41
1:W:16:ARG:HB3	1:W:117:PRO:HG2	2.02	0.41
1:W:55:GLU:HB2	1:W:222:PHE:CG	2.56	0.41
1:Y:68:PHE:HA	1:Y:71:PHE:CE2	2.54	0.41
2:2:314:MET:HE3	2:2:405:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:HD13	1:A:188:LEU:HD12	2.03	0.41
1:F:49:SER:HB3	1:W:97:ARG:HD2	2.03	0.41
2:H:393:ALA:HB1	2:H:398:LEU:HD12	2.03	0.41
1:M:150:GLU:HA	1:M:151:PRO:HD3	1.86	0.41
1:O:56:LEU:HD23	1:O:56:LEU:HA	1.86	0.41
1:S:70:GLU:HB3	1:S:118:TYR:CD2	2.55	0.41
1:S:90:ASP:HB3	1:S:93:ASP:OD2	2.19	0.41
2:Z:329:ARG:HD3	5:Z:924:HOH:O	2.20	0.41
1:D:114:GLN:HE21	1:D:114:GLN:HB3	1.52	0.41
1:F:93:ASP:OD1	2:N:375:THR:HG23	2.20	0.41
1:M:70:GLU:HB3	1:M:118:TYR:CD2	2.55	0.41
1:Q:89:TYR:CD1	2:Z:374:LEU:HD11	2.56	0.41
2:V:486:LEU:HB2	5:V:1158:HOH:O	2.21	0.41
1:W:18:GLU:CG	1:W:22:LYS:HE3	2.48	0.41
1:W:228:SER:O	1:W:232:ALA:HB3	2.21	0.41
2:X:422:SER:HB3	2:X:437:GLN:HG2	2.02	0.41
2:2:341:THR:CG2	2:2:404:LEU:HD11	2.51	0.41
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.90	0.41
1:B:18:GLU:CG	1:B:22:LYS:HE3	2.49	0.41
1:D:176:SER:O	1:D:177:LEU:C	2.62	0.41
2:E:509:ARG:NE	5:E:1528:HOH:O	2.43	0.41
1:O:233:LEU:N	1:O:233:LEU:HD12	2.36	0.41
2:T:333:LYS:HE2	3:j:3:LEU:HD22	2.03	0.41
1:W:123:CYS:HA	1:W:139:TYR:O	2.20	0.41
2:Z:462:SER:O	2:Z:466:VAL:HG23	2.20	0.41
2:C:374:LEU:HD11	1:I:89:TYR:CD1	2.56	0.41
2:G:362:GLU:OE2	2:G:382:ARG:CD	2.69	0.41
2:P:308:TYR:CZ	2:P:311:GLY:HA3	2.54	0.41
1:U:230:LEU:O	1:U:234:LEU:CG	2.62	0.41
2:V:364:GLU:HG2	2:V:368:LYS:HD3	2.03	0.41
1:W:170:SER:OG	1:W:170:SER:O	2.34	0.41
1:W:177:LEU:HG	1:W:233:LEU:HD21	2.03	0.41
1:A:116:LYS:HD2	1:B:13:MET:CE	2.43	0.41
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.80	0.41
1:D:58:ASP:OD2	1:D:219:ARG:CG	2.69	0.41
1:K:95:THR:OG1	1:K:98:GLN:HG3	2.21	0.41
1:K:147:ILE:HG21	1:K:147:ILE:HD13	1.84	0.41
2:L:444:LEU:HB2	5:L:2568:HOH:O	2.20	0.41
2:N:517:ILE:O	2:N:520:SER:HB3	2.21	0.41
2:R:306:LEU:CD1	2:R:313:VAL:CG1	2.99	0.41
2:R:363:LEU:HD12	2:R:363:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:16:ARG:HB3	1:S:117:PRO:HG2	2.03	0.41
2:X:314:MET:HE3	2:X:405:ALA:HB2	2.03	0.41
2:X:366:TYR:CE2	2:X:374:LEU:HD13	2.56	0.41
1:B:21:ARG:HG2	5:B:1479:HOH:O	2.19	0.41
1:D:15:GLU:CD	1:K:9:PRO:HD2	2.46	0.41
1:F:181:LEU:O	1:F:185:VAL:HG23	2.21	0.41
1:F:190:ALA:O	1:F:191:GLY:C	2.61	0.41
2:L:392:ALA:HB3	5:L:813:HOH:O	2.21	0.41
1:M:68:PHE:CD2	1:M:68:PHE:C	2.99	0.41
1:O:46:PRO:HG2	1:O:47:SER:N	2.36	0.41
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.55	0.41
1:U:40:LEU:HD12	1:U:212:VAL:HG12	2.03	0.41
1:B:167:LEU:HD13	1:B:187:ALA:CB	2.51	0.40
1:B:176:SER:HB3	1:B:179:ASP:OD2	2.21	0.40
2:C:341:THR:CG2	2:C:404:LEU:HD11	2.51	0.40
1:O:40:LEU:HD21	1:O:181:LEU:HA	2.03	0.40
1:O:93:ASP:OD1	2:V:375:THR:HG23	2.20	0.40
2:R:320:SER:HB3	2:R:328:GLY:CA	2.51	0.40
2:R:338:ASP:CG	2:R:341:THR:HG1	2.22	0.40
2:R:498:ASP:HB2	5:R:144:HOH:O	2.20	0.40
1:U:231:GLN:O	1:U:234:LEU:CB	2.56	0.40
1:Y:152:HIS:CD2	1:Y:171:TYR:OH	2.75	0.40
1:B:33:LEU:HD23	1:B:167:LEU:HD21	2.03	0.40
1:B:52:LYS:HE2	1:B:64:ALA:O	2.21	0.40
1:B:98:GLN:O	1:B:102:VAL:HG23	2.21	0.40
1:D:9:PRO:HD2	1:Q:15:GLU:HG2	2.02	0.40
2:E:333:LYS:HE2	3:b:3:LEU:HD22	2.02	0.40
2:H:416:SER:C	5:H:3049:HOH:O	2.64	0.40
1:I:115:ALA:HB3	1:S:112:THR:HG22	2.03	0.40
1:M:163:ILE:HG23	1:M:188:LEU:N	2.36	0.40
1:S:205:VAL:HG11	5:S:2979:HOH:O	2.20	0.40
1:Y:35:TYR:HB2	1:Y:175:ALA:O	2.21	0.40
2:Z:505:VAL:HA	2:Z:506:PRO:HD3	1.97	0.40
1:A:41:PHE:CD1	1:A:63:ALA:HB2	2.56	0.40
2:C:382:ARG:NH2	2:C:385:ILE:HD13	2.37	0.40
1:D:33:LEU:HD12	1:D:40:LEU:HB3	2.03	0.40
1:K:231:GLN:O	1:K:234:LEU:HB2	2.21	0.40
2:L:452:LYS:NZ	2:P:473:ASP:OD2	2.47	0.40
1:O:217:ARG:NH2	1:O:223:ARG:HD3	2.36	0.40
2:V:464:LEU:O	2:V:468:VAL:HG23	2.21	0.40
2:X:509:ARG:HA	2:X:509:ARG:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:PHE:HA	1:1:71:PHE:CE2	2.56	0.40
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.85	0.40
2:G:412:SER:O	2:G:414:PRO:HD3	2.22	0.40
1:Q:70:GLU:HB3	1:Q:118:TYR:CD2	2.57	0.40
1:U:8:SER:O	1:U:11:GLN:N	2.55	0.40
1:U:105:GLN:HG3	1:1:73:ASN:ND2	2.36	0.40
2:V:425:ALA:HB3	4:h:4:HXD:H42	2.04	0.40
2:X:444:LEU:HD12	5:X:2899:HOH:O	2.21	0.40
1:Y:39:VAL:HG12	1:Y:40:LEU:N	2.36	0.40
1:Y:163:ILE:HG23	1:Y:187:ALA:C	2.47	0.40
1:D:58:ASP:O	1:D:59:ARG:HD2	2.21	0.40
2:E:403:LEU:HD12	2:E:403:LEU:HA	1.90	0.40
1:F:95:THR:OG1	1:F:98:GLN:HG3	2.21	0.40
1:F:225:ILE:HG21	1:F:233:LEU:HD23	2.03	0.40
2:R:362:GLU:OE2	2:R:382:ARG:CD	2.69	0.40
1:S:217:ARG:HA	1:S:218:PRO:HD3	1.98	0.40
1:U:70:GLU:HB3	1:U:118:TYR:CD2	2.57	0.40
1:Y:143:TYR:CD1	1:Y:143:TYR:C	3.00	0.40
1:1:114:GLN:HE21	1:1:114:GLN:HB3	1.52	0.40
1:1:225:ILE:HG21	1:1:233:LEU:HD22	2.03	0.40
2:2:320:SER:HB3	2:2:328:GLY:CA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	211/248 (85%)	199 (94%)	11 (5%)	1 (0%)	24	43
1	A	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
1	B	209/248 (84%)	203 (97%)	6 (3%)	0	100	100
1	D	209/248 (84%)	203 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	212/248 (86%)	208 (98%)	4 (2%)	0	100	100
1	I	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	K	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	M	210/248 (85%)	204 (97%)	6 (3%)	0	100	100
1	O	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
1	Q	210/248 (85%)	202 (96%)	8 (4%)	0	100	100
1	S	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	U	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	W	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	Y	212/248 (86%)	206 (97%)	6 (3%)	0	100	100
2	2	220/240 (92%)	220 (100%)	0	0	100	100
2	C	220/240 (92%)	220 (100%)	0	0	100	100
2	E	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	H	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	J	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	L	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	N	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	R	227/240 (95%)	224 (99%)	3 (1%)	0	100	100
2	T	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	V	227/240 (95%)	226 (100%)	1 (0%)	0	100	100
2	X	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
3	a	1/3 (33%)	1 (100%)	0	0	100	100
3	b	1/3 (33%)	1 (100%)	0	0	100	100
3	c	1/3 (33%)	1 (100%)	0	0	100	100
3	d	1/3 (33%)	1 (100%)	0	0	100	100
3	e	1/3 (33%)	1 (100%)	0	0	100	100
3	f	1/3 (33%)	1 (100%)	0	0	100	100
3	g	1/3 (33%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	h	1/3 (33%)	1 (100%)	0	0	100	100
3	i	1/3 (33%)	1 (100%)	0	0	100	100
3	j	1/3 (33%)	1 (100%)	0	0	100	100
3	k	1/3 (33%)	1 (100%)	0	0	100	100
3	l	1/3 (33%)	1 (100%)	0	0	100	100
3	m	1/3 (33%)	1 (100%)	0	0	100	100
3	n	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6055/6874 (88%)	5942 (98%)	112 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	131	GLY

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	164/192 (85%)	151 (92%)	13 (8%)	11	24
1	A	164/192 (85%)	158 (96%)	6 (4%)	30	57
1	B	163/192 (85%)	158 (97%)	5 (3%)	35	62
1	D	164/192 (85%)	146 (89%)	18 (11%)	6	13
1	F	165/192 (86%)	151 (92%)	14 (8%)	10	22
1	I	164/192 (85%)	157 (96%)	7 (4%)	26	51
1	K	164/192 (85%)	155 (94%)	9 (6%)	19	40
1	M	164/192 (85%)	153 (93%)	11 (7%)	15	31
1	O	164/192 (85%)	150 (92%)	14 (8%)	10	22
1	Q	164/192 (85%)	151 (92%)	13 (8%)	11	24
1	S	165/192 (86%)	156 (94%)	9 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	164/192 (85%)	158 (96%)	6 (4%)	30	57
1	W	164/192 (85%)	158 (96%)	6 (4%)	30	57
1	Y	165/192 (86%)	156 (94%)	9 (6%)	19	40
2	2	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	C	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	E	165/178 (93%)	159 (96%)	6 (4%)	31	58
2	G	165/178 (93%)	159 (96%)	6 (4%)	31	58
2	H	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	J	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	L	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	N	165/178 (93%)	158 (96%)	7 (4%)	26	52
2	P	165/178 (93%)	160 (97%)	5 (3%)	36	64
2	R	169/178 (95%)	160 (95%)	9 (5%)	20	42
2	T	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	V	169/178 (95%)	160 (95%)	9 (5%)	20	42
2	X	165/178 (93%)	157 (95%)	8 (5%)	23	46
2	Z	165/178 (93%)	159 (96%)	6 (4%)	31	58
3	a	3/3 (100%)	3 (100%)	0	100	100
3	b	3/3 (100%)	3 (100%)	0	100	100
3	c	3/3 (100%)	3 (100%)	0	100	100
3	d	3/3 (100%)	3 (100%)	0	100	100
3	e	3/3 (100%)	3 (100%)	0	100	100
3	f	3/3 (100%)	3 (100%)	0	100	100
3	g	3/3 (100%)	3 (100%)	0	100	100
3	h	3/3 (100%)	3 (100%)	0	100	100
3	i	3/3 (100%)	3 (100%)	0	100	100
3	j	3/3 (100%)	3 (100%)	0	100	100
3	k	3/3 (100%)	3 (100%)	0	100	100
3	l	3/3 (100%)	3 (100%)	0	100	100
3	m	3/3 (100%)	3 (100%)	0	100	100
3	n	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4658/5222 (89%)	4423 (95%)	235 (5%)	22	44

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	33	LEU
1	A	173	GLU
1	A	185	VAL
1	A	188	LEU
1	A	216	ASN
1	B	69	ASN
1	B	73	ASN
1	B	169	GLU
1	B	173	GLU
1	B	225	ILE
2	C	312	VAL
2	C	363	LEU
2	C	369	LEU
2	C	486	LEU
2	C	513	LEU
1	D	33	LEU
1	D	39	VAL
1	D	48	ARG
1	D	49	SER
1	D	50	LEU
1	D	73	ASN
1	D	99	LEU
1	D	114	GLN
1	D	167	LEU
1	D	169	GLU
1	D	174	ASN
1	D	178	THR
1	D	181	LEU
1	D	183	ILE
1	D	189	ARG
1	D	217	ARG
1	D	228	SER
1	D	230	LEU
2	E	312	VAL
2	E	363	LEU
2	E	369	LEU

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Mol	Chain	Res	Type
2	E	416	SER
2	E	486	LEU
2	E	513	LEU
1	F	10	GLU
1	F	33	LEU
1	F	40	LEU
1	F	47	SER
1	F	48	ARG
1	F	69	ASN
1	F	73	ASN
1	F	114	GLN
1	F	147	ILE
1	F	163	ILE
1	F	178	THR
1	F	183	ILE
1	F	233	LEU
1	F	235	VAL
2	G	363	LEU
2	G	369	LEU
2	G	444	LEU
2	G	486	LEU
2	G	509	ARG
2	G	513	LEU
2	H	312	VAL
2	H	363	LEU
2	H	369	LEU
2	H	412	SER
2	H	416	SER
2	H	444	LEU
2	H	486	LEU
2	H	513	LEU
1	I	18	GLU
1	I	21	ARG
1	I	33	LEU
1	I	73	ASN
1	I	114	GLN
1	I	178	THR
1	I	234	LEU
2	J	324	ASN
2	J	363	LEU
2	J	369	LEU
2	J	486	LEU

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Mol	Chain	Res	Type
2	J	513	LEU
1	K	8	SER
1	K	48	ARG
1	K	73	ASN
1	K	114	GLN
1	K	178	THR
1	K	188	LEU
1	K	189	ARG
1	K	216	ASN
1	K	217	ARG
2	L	306	LEU
2	L	363	LEU
2	L	369	LEU
2	L	374	LEU
2	L	412	SER
2	L	444	LEU
2	L	486	LEU
2	L	513	LEU
1	M	51	GLN
1	M	73	ASN
1	M	114	GLN
1	M	178	THR
1	M	183	ILE
1	M	188	LEU
1	M	189	ARG
1	M	216	ASN
1	M	225	ILE
1	M	233	LEU
1	M	234	LEU
2	N	363	LEU
2	N	369	LEU
2	N	412	SER
2	N	444	LEU
2	N	486	LEU
2	N	513	LEU
2	N	522	SER
1	O	15	GLU
1	O	48	ARG
1	O	73	ASN
1	O	160	THR
1	O	161	GLU
1	O	163	ILE

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Mol	Chain	Res	Type
1	O	167	LEU
1	O	176	SER
1	O	179	ASP
1	O	183	ILE
1	O	185	VAL
1	O	188	LEU
1	O	205	VAL
1	O	216	ASN
2	P	363	LEU
2	P	369	LEU
2	P	444	LEU
2	P	486	LEU
2	P	513	LEU
1	Q	13	MET
1	Q	19	LEU
1	Q	21	ARG
1	Q	24	ILE
1	Q	49	SER
1	Q	51	GLN
1	Q	69	ASN
1	Q	73	ASN
1	Q	114	GLN
1	Q	169	GLU
1	Q	174	ASN
1	Q	176	SER
1	Q	178	THR
2	R	337	THR
2	R	341	THR
2	R	363	LEU
2	R	369	LEU
2	R	421	VAL
2	R	444	LEU
2	R	486	LEU
2	R	496	ILE
2	R	513	LEU
1	S	33	LEU
1	S	50	LEU
1	S	51	GLN
1	S	73	ASN
1	S	134	LYS
1	S	150	GLU
1	S	178	THR

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Mol	Chain	Res	Type
1	S	183	ILE
1	S	188	LEU
2	T	312	VAL
2	T	363	LEU
2	T	369	LEU
2	T	412	SER
2	T	414	PRO
2	T	415	GLN
2	T	486	LEU
2	T	513	LEU
1	U	33	LEU
1	U	73	ASN
1	U	114	GLN
1	U	178	THR
1	U	183	ILE
1	U	226	THR
2	V	306	LEU
2	V	363	LEU
2	V	369	LEU
2	V	374	LEU
2	V	412	SER
2	V	434	GLU
2	V	444	LEU
2	V	486	LEU
2	V	513	LEU
1	W	73	ASN
1	W	178	THR
1	W	179	ASP
1	W	188	LEU
1	W	216	ASN
1	W	226	THR
2	X	312	VAL
2	X	330	ASP
2	X	363	LEU
2	X	369	LEU
2	X	486	LEU
2	X	496	ILE
2	X	513	LEU
2	X	519	GLU
1	Y	13	MET
1	Y	44	GLU
1	Y	69	ASN

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Mol	Chain	Res	Type
1	Y	73	ASN
1	Y	92	ARG
1	Y	114	GLN
1	Y	133	THR
1	Y	135	ARG
1	Y	231	GLN
2	Z	312	VAL
2	Z	363	LEU
2	Z	369	LEU
2	Z	444	LEU
2	Z	496	ILE
2	Z	513	LEU
1	1	73	ASN
1	1	97	ARG
1	1	155	VAL
1	1	159	THR
1	1	160	THR
1	1	163	ILE
1	1	169	GLU
1	1	176	SER
1	1	183	ILE
1	1	188	LEU
1	1	216	ASN
1	1	223	ARG
1	1	233	LEU
2	2	363	LEU
2	2	369	LEU
2	2	444	LEU
2	2	486	LEU
2	2	513	LEU

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	69	ASN
1	A	114	GLN
1	A	165	ASN
1	A	231	GLN
1	B	11	GLN
1	B	51	GLN
1	B	69	ASN

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Mol	Chain	Res	Type
1	B	73	ASN
1	B	114	GLN
1	B	165	ASN
2	C	322	GLN
2	C	324	ASN
2	C	456	GLN
1	D	11	GLN
1	D	69	ASN
1	D	73	ASN
1	D	105	GLN
1	D	114	GLN
1	D	129	HIS
1	D	152	HIS
1	D	165	ASN
2	E	322	GLN
2	E	324	ASN
2	E	410	HIS
2	E	456	GLN
1	F	11	GLN
1	F	69	ASN
1	F	73	ASN
1	F	101	ASN
1	F	114	GLN
1	F	165	ASN
2	G	324	ASN
2	G	430	ASN
2	G	456	GLN
2	H	322	GLN
2	H	324	ASN
2	H	415	GLN
2	H	456	GLN
1	I	69	ASN
1	I	73	ASN
1	I	114	GLN
1	I	129	HIS
1	I	165	ASN
2	J	322	GLN
2	J	324	ASN
2	J	456	GLN
1	K	69	ASN
1	K	73	ASN
1	K	114	GLN

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Mol	Chain	Res	Type
1	K	165	ASN
1	K	231	GLN
2	L	322	GLN
2	L	324	ASN
2	L	396	GLN
2	L	456	GLN
1	M	11	GLN
1	M	69	ASN
1	M	73	ASN
1	M	114	GLN
1	M	165	ASN
2	N	322	GLN
2	N	324	ASN
2	N	456	GLN
1	O	69	ASN
1	O	73	ASN
1	O	101	ASN
1	O	114	GLN
1	O	152	HIS
1	O	231	GLN
2	P	322	GLN
2	P	324	ASN
2	P	456	GLN
1	Q	69	ASN
1	Q	73	ASN
1	Q	105	GLN
1	Q	114	GLN
1	Q	152	HIS
1	Q	165	ASN
1	Q	174	ASN
1	Q	231	GLN
2	R	322	GLN
2	R	324	ASN
2	R	396	GLN
2	R	456	GLN
1	S	11	GLN
1	S	51	GLN
1	S	69	ASN
1	S	73	ASN
1	S	105	GLN
1	S	114	GLN
1	S	165	ASN

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Mol	Chain	Res	Type
2	T	322	GLN
2	T	324	ASN
2	T	456	GLN
1	U	11	GLN
1	U	69	ASN
1	U	73	ASN
1	U	114	GLN
1	U	165	ASN
2	V	322	GLN
2	V	324	ASN
2	V	456	GLN
1	W	11	GLN
1	W	69	ASN
1	W	73	ASN
1	W	105	GLN
1	W	114	GLN
1	W	152	HIS
1	W	165	ASN
1	W	231	GLN
2	X	322	GLN
2	X	324	ASN
2	X	456	GLN
1	Y	11	GLN
1	Y	69	ASN
1	Y	73	ASN
1	Y	114	GLN
1	Y	152	HIS
1	Y	165	ASN
2	Z	324	ASN
2	Z	396	GLN
2	Z	456	GLN
1	1	11	GLN
1	1	69	ASN
1	1	73	ASN
1	1	101	ASN
1	1	105	GLN
1	1	114	GLN
1	1	129	HIS
1	1	152	HIS
1	1	174	ASN
2	2	322	GLN
2	2	324	ASN

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Mol	Chain	Res	Type
2	2	396	GLN
2	2	456	GLN
3	c	1	ASN
3	g	1	ASN
3	n	2	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	HXD	c	4	3	5,6,14	1.21	1 (20%)	5,6,15	1.29	0
4	HXD	b	4	3	5,6,14	1.18	0	5,6,15	1.15	0
4	HXD	m	4	3	5,6,14	1.14	0	5,6,15	1.17	1 (20%)
4	HXD	n	4	3	5,6,14	1.13	0	5,6,15	1.34	1 (20%)
4	HXD	j	4	3	5,6,14	1.16	1 (20%)	5,6,15	1.29	0
4	HXD	e	4	3	5,6,14	1.10	0	5,6,15	1.29	1 (20%)
4	HXD	f	4	3	5,6,14	1.05	0	5,6,15	1.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HXD	k	4	3	5,6,14	1.04	0	5,6,15	1.21	1 (20%)
4	HXD	a	4	3	5,6,14	1.01	0	5,6,15	1.32	1 (20%)
4	HXD	g	4	3	5,6,14	1.11	0	5,6,15	1.43	1 (20%)
4	HXD	l	4	3	5,6,14	1.33	1 (20%)	5,6,15	1.42	1 (20%)
4	HXD	h	4	3	5,6,14	1.41	1 (20%)	5,6,15	1.46	1 (20%)
4	HXD	i	4	3	5,6,14	1.28	1 (20%)	5,6,15	1.05	0
4	HXD	d	4	3	5,6,14	1.51	1 (20%)	5,6,15	1.39	1 (20%)

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
4	HXD	c	4	3	-	0/5/5/13	-
4	HXD	b	4	3	-	0/5/5/13	-
4	HXD	m	4	3	-	0/5/5/13	-
4	HXD	n	4	3	-	0/5/5/13	-
4	HXD	j	4	3	-	0/5/5/13	-
4	HXD	e	4	3	-	0/5/5/13	-
4	HXD	f	4	3	-	0/5/5/13	-
4	HXD	k	4	3	-	0/5/5/13	-
4	HXD	a	4	3	-	0/5/5/13	-
4	HXD	g	4	3	-	0/5/5/13	-
4	HXD	l	4	3	-	0/5/5/13	-
4	HXD	h	4	3	-	0/5/5/13	-
4	HXD	i	4	3	-	0/5/5/13	-
4	HXD	d	4	3	-	0/5/5/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	4	HXD	C2-C1	2.85	1.57	1.50
4	h	4	HXD	C2-C1	2.42	1.56	1.50
4	l	4	HXD	C2-C1	2.17	1.55	1.50
4	c	4	HXD	C2-C1	2.08	1.55	1.50
4	i	4	HXD	C2-C1	2.07	1.55	1.50
4	j	4	HXD	C2-C1	2.02	1.55	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	g	4	HXD	O8-C3-C2	-2.49	102.81	109.45
4	a	4	HXD	C3-C2-C1	2.46	116.90	112.70
4	d	4	HXD	C3-C2-C1	2.40	116.79	112.70
4	h	4	HXD	C3-C2-C1	2.40	116.79	112.70
4	l	4	HXD	C3-C2-C1	2.38	116.75	112.70
4	e	4	HXD	C3-C2-C1	2.21	116.46	112.70
4	m	4	HXD	O8-C3-C2	-2.19	103.63	109.45
4	n	4	HXD	C3-C2-C1	2.04	116.18	112.70
4	k	4	HXD	O8-C3-C2	-2.02	104.06	109.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	b	4	HXD	1	0
4	m	4	HXD	1	0
4	n	4	HXD	1	0
4	j	4	HXD	1	0
4	e	4	HXD	1	0
4	a	4	HXD	2	0
4	g	4	HXD	1	0
4	l	4	HXD	1	0
4	h	4	HXD	2	0
4	i	4	HXD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	215/248 (86%)	0.55	8 (3%) 45 40	23, 51, 86, 94	0
1	A	214/248 (86%)	0.69	12 (5%) 30 26	24, 53, 88, 100	0
1	B	213/248 (85%)	0.76	22 (10%) 12 10	24, 52, 87, 94	0
1	D	213/248 (85%)	1.13	48 (22%) 2 2	25, 55, 93, 112	0
1	F	216/248 (87%)	0.71	13 (6%) 27 24	23, 53, 86, 93	0
1	I	215/248 (86%)	0.77	16 (7%) 20 18	24, 52, 87, 95	0
1	K	215/248 (86%)	0.71	18 (8%) 17 15	24, 53, 87, 95	0
1	M	214/248 (86%)	0.78	23 (10%) 11 9	23, 54, 88, 96	0
1	O	214/248 (86%)	0.70	20 (9%) 14 12	22, 53, 88, 95	0
1	Q	214/248 (86%)	0.75	17 (7%) 18 16	26, 52, 87, 95	0
1	S	215/248 (86%)	0.75	19 (8%) 15 14	24, 53, 89, 99	0
1	U	214/248 (86%)	0.76	20 (9%) 14 12	23, 53, 87, 95	0
1	W	215/248 (86%)	0.86	18 (8%) 17 15	24, 54, 93, 98	0
1	Y	216/248 (87%)	0.89	28 (12%) 7 6	26, 55, 90, 98	0
2	2	222/240 (92%)	-0.41	2 (0%) 81 78	12, 23, 41, 66	0
2	C	222/240 (92%)	-0.45	1 (0%) 87 85	12, 24, 41, 68	0
2	E	222/240 (92%)	-0.43	0 100 100	13, 24, 41, 65	0
2	G	222/240 (92%)	-0.39	3 (1%) 73 70	14, 24, 43, 68	0
2	H	222/240 (92%)	-0.43	0 100 100	11, 24, 42, 66	0
2	J	222/240 (92%)	-0.41	2 (0%) 81 78	12, 24, 43, 65	0
2	L	222/240 (92%)	-0.38	0 100 100	13, 24, 42, 65	0
2	N	222/240 (92%)	-0.45	1 (0%) 87 85	13, 24, 43, 67	0
2	P	222/240 (92%)	-0.41	2 (0%) 81 78	14, 24, 42, 67	0
2	R	229/240 (95%)	-0.45	3 (1%) 75 71	13, 24, 46, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	222/240 (92%)	-0.36	0 100 100	15, 25, 43, 67	0
2	V	229/240 (95%)	-0.44	1 (0%) 88 86	12, 23, 44, 67	0
2	X	222/240 (92%)	-0.40	1 (0%) 87 85	13, 25, 43, 67	0
2	Z	222/240 (92%)	-0.34	2 (0%) 81 78	13, 25, 43, 67	0
3	a	3/3 (100%)	-0.52	0 100 100	24, 24, 24, 26	0
3	b	3/3 (100%)	-0.41	0 100 100	20, 20, 22, 23	0
3	c	3/3 (100%)	-0.31	0 100 100	23, 23, 24, 28	0
3	d	3/3 (100%)	-0.67	0 100 100	22, 22, 25, 27	0
3	e	3/3 (100%)	-0.50	0 100 100	21, 21, 23, 24	0
3	f	3/3 (100%)	-0.13	0 100 100	21, 21, 24, 28	0
3	g	3/3 (100%)	-0.37	0 100 100	21, 21, 22, 28	0
3	h	3/3 (100%)	-0.47	0 100 100	23, 23, 28, 28	0
3	i	3/3 (100%)	-0.35	0 100 100	25, 25, 26, 27	0
3	j	3/3 (100%)	-0.41	0 100 100	26, 26, 27, 30	0
3	k	3/3 (100%)	-0.62	0 100 100	22, 22, 25, 28	0
3	l	3/3 (100%)	-0.20	0 100 100	23, 23, 27, 27	0
3	m	3/3 (100%)	-0.36	0 100 100	30, 30, 30, 31	0
3	n	3/3 (100%)	-0.45	0 100 100	25, 25, 27, 28	0
All	All	6167/6874 (89%)	0.16	300 (4%) 35 31	11, 35, 84, 112	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	172	ALA	4.9
1	D	233	LEU	4.6
1	B	205	VAL	4.6
1	Y	9	PRO	4.1
1	Y	235	VAL	4.1
1	Y	12	ALA	4.0
1	D	184	ALA	3.8
1	K	191	GLY	3.8
1	D	190	ALA	3.8
1	B	191	GLY	3.8
1	A	172	ALA	3.7
1	F	10	GLU	3.6
1	D	205	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	235	VAL	3.6
1	D	188	LEU	3.5
1	K	234	LEU	3.5
1	S	235	VAL	3.5
1	U	166	ALA	3.5
1	U	13	MET	3.4
1	S	175	ALA	3.4
1	O	13	MET	3.4
1	D	166	ALA	3.4
1	S	191	GLY	3.4
1	U	191	GLY	3.4
1	W	234	LEU	3.4
1	M	191	GLY	3.4
1	Q	166	ALA	3.4
1	A	13	MET	3.3
1	B	233	LEU	3.3
1	B	13	MET	3.3
1	A	205	VAL	3.3
1	A	171	TYR	3.3
1	W	191	GLY	3.3
1	Y	10	GLU	3.2
1	D	180	ALA	3.2
1	W	8	SER	3.2
1	B	166	ALA	3.2
1	F	191	GLY	3.2
1	I	191	GLY	3.2
1	F	12	ALA	3.2
1	M	233	LEU	3.2
1	M	234	LEU	3.2
1	Y	191	GLY	3.2
1	Y	175	ALA	3.1
1	F	13	MET	3.1
1	D	159	THR	3.1
1	A	234	LEU	3.1
1	D	42	VAL	3.1
1	I	26	ARG	3.1
1	O	172	ALA	3.1
1	A	9	PRO	3.1
1	D	31	VAL	3.1
1	M	190	ALA	3.0
1	S	166	ALA	3.0
1	Y	166	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	W	205	VAL	3.0
1	Q	234	LEU	3.0
2	R	529	SER	3.0
1	O	191	GLY	3.0
1	D	11	GLN	3.0
1	S	205	VAL	3.0
1	S	13	MET	3.0
1	I	167	LEU	3.0
1	W	11	GLN	3.0
1	D	8	SER	2.9
2	C	415	GLN	2.9
1	U	205	VAL	2.9
1	D	206	ALA	2.9
1	O	190	ALA	2.9
1	S	172	ALA	2.9
1	D	44	GLU	2.9
1	B	172	ALA	2.9
1	D	234	LEU	2.9
1	W	13	MET	2.9
1	K	204	GLY	2.9
1	I	182	ARG	2.9
1	O	9	PRO	2.9
1	Q	160	THR	2.9
1	D	232	ALA	2.9
1	U	12	ALA	2.9
1	Y	172	ALA	2.9
1	W	167	LEU	2.9
1	O	185	VAL	2.8
1	I	13	MET	2.8
1	K	13	MET	2.8
1	I	163	ILE	2.8
1	U	206	ALA	2.8
1	W	159	THR	2.8
1	Q	191	GLY	2.8
1	D	230	LEU	2.8
1	Y	204	GLY	2.7
1	Q	205	VAL	2.7
1	F	14	ARG	2.7
1	W	204	GLY	2.7
1	O	167	LEU	2.7
1	U	190	ALA	2.7
1	M	205	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	1	205	VAL	2.7
2	P	412	SER	2.7
1	O	234	LEU	2.7
1	I	172	ALA	2.7
1	Y	180	ALA	2.7
1	D	163	ILE	2.7
1	I	234	LEU	2.7
1	M	167	LEU	2.7
1	U	234	LEU	2.7
1	B	175	ALA	2.7
1	W	14	ARG	2.6
1	A	167	LEU	2.6
1	D	171	TYR	2.6
1	D	229	ALA	2.6
1	K	166	ALA	2.6
1	Q	162	PRO	2.6
1	Y	13	MET	2.6
1	U	233	LEU	2.6
1	M	8	SER	2.6
1	S	181	LEU	2.6
1	U	10	GLU	2.6
1	D	160	THR	2.6
1	O	166	ALA	2.6
1	Y	164	ALA	2.6
1	B	171	TYR	2.6
1	D	189	ARG	2.5
1	D	43	ALA	2.5
1	D	179	ASP	2.5
1	1	191	GLY	2.5
1	Y	177	LEU	2.5
1	B	12	ALA	2.5
1	M	12	ALA	2.5
1	M	166	ALA	2.5
1	1	190	ALA	2.5
1	D	226	THR	2.5
1	U	159	THR	2.5
1	S	171	TYR	2.5
1	F	234	LEU	2.5
2	G	415	GLN	2.5
1	D	175	ALA	2.5
1	K	180	ALA	2.5
1	M	184	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	180	ALA	2.5
1	Y	8	SER	2.5
1	O	163	ILE	2.5
1	O	182	ARG	2.5
1	W	190	ALA	2.5
1	O	159	THR	2.5
1	M	9	PRO	2.4
1	K	167	LEU	2.4
1	M	165	ASN	2.4
1	B	206	ALA	2.4
1	A	226	THR	2.4
1	I	159	THR	2.4
1	B	163	ILE	2.4
1	Q	163	ILE	2.4
1	Q	171	TYR	2.4
1	W	177	LEU	2.4
1	A	26	ARG	2.4
1	B	14	ARG	2.4
1	M	185	VAL	2.4
1	M	13	MET	2.4
1	F	166	ALA	2.4
1	I	27	ALA	2.4
1	D	9	PRO	2.4
1	I	9	PRO	2.4
1	F	163	ILE	2.4
1	W	163	ILE	2.4
1	Y	233	LEU	2.4
1	1	152	HIS	2.4
1	D	153	PHE	2.4
1	O	205	VAL	2.4
1	Q	154	VAL	2.4
1	B	232	ALA	2.4
1	D	186	ALA	2.4
1	D	10	GLU	2.4
1	O	162	PRO	2.4
1	S	44	GLU	2.4
2	Z	414	PRO	2.4
2	R	416	SER	2.4
2	V	529	SER	2.4
1	B	167	LEU	2.4
1	Q	167	LEU	2.4
2	N	415	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	Z	415	GLN	2.4
1	K	171	TYR	2.4
1	K	190	ALA	2.4
1	K	44	GLU	2.4
1	F	233	LEU	2.3
1	U	163	ILE	2.3
1	U	171	TYR	2.3
1	B	10	GLU	2.3
1	D	211	ALA	2.3
1	I	164	ALA	2.3
1	S	184	ALA	2.3
1	S	190	ALA	2.3
1	D	14	ARG	2.3
1	O	11	GLN	2.3
1	Y	11	GLN	2.3
1	S	234	LEU	2.3
1	M	171	TYR	2.3
1	O	31	VAL	2.3
1	W	12	ALA	2.3
1	M	159	THR	2.3
1	I	11	GLN	2.3
1	S	233	LEU	2.3
1	D	212	VAL	2.3
2	R	433	GLU	2.3
1	1	171	TYR	2.3
1	O	12	ALA	2.3
1	S	9	PRO	2.3
1	K	161	GLU	2.3
1	K	31	VAL	2.3
1	I	162	PRO	2.3
2	P	414	PRO	2.3
1	Y	190	ALA	2.2
1	1	166	ALA	2.2
1	D	152	HIS	2.2
1	D	207	SER	2.2
2	G	413	ASP	2.2
1	M	10	GLU	2.2
1	U	162	PRO	2.2
1	B	190	ALA	2.2
1	D	27	ALA	2.2
1	D	227	GLY	2.2
1	M	132	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	2.2
1	W	166	ALA	2.2
1	M	226	THR	2.2
1	S	167	LEU	2.2
1	B	173	GLU	2.2
1	U	173	GLU	2.2
1	W	15	GLU	2.2
1	K	184	ALA	2.2
1	Q	164	ALA	2.2
1	W	165	ASN	2.2
1	U	167	LEU	2.2
1	I	8	SER	2.2
1	W	207	SER	2.2
1	B	161	GLU	2.2
1	M	162	PRO	2.2
1	Q	9	PRO	2.2
1	D	155	VAL	2.1
1	D	25	ALA	2.1
1	D	156	MET	2.1
1	K	164	ALA	2.1
1	M	11	GLN	2.1
1	M	164	ALA	2.1
1	F	167	LEU	2.1
1	D	48	ARG	2.1
1	Y	170	SER	2.1
1	B	148	ALA	2.1
1	Y	36	ALA	2.1
1	A	178	THR	2.1
1	A	233	LEU	2.1
1	K	188	LEU	2.1
1	Y	167	LEU	2.1
1	Y	188	LEU	2.1
1	Y	226	THR	2.1
1	M	161	GLU	2.1
1	Y	149	ASP	2.1
1	U	11	GLN	2.1
1	O	175	ALA	2.1
2	G	411	ALA	2.1
1	D	131	GLY	2.1
1	K	159	THR	2.1
1	Q	26	ARG	2.1
1	Y	26	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	Y	163	ILE	2.1
1	Y	171	TYR	2.1
1	B	8	SER	2.1
1	D	170	SER	2.1
2	2	416	SER	2.1
1	1	13	MET	2.1
1	D	154	VAL	2.1
1	Y	30	VAL	2.1
1	I	166	ALA	2.1
1	Q	172	ALA	2.1
1	D	177	LEU	2.1
1	F	8	SER	2.1
1	D	21	ARG	2.0
1	F	215	ALA	2.0
1	O	187	ALA	2.0
1	S	12	ALA	2.0
1	B	226	THR	2.0
1	K	160	THR	2.0
1	U	160	THR	2.0
1	B	49	SER	2.0
1	Y	162	PRO	2.0
2	J	522	SER	2.0
2	2	522	SER	2.0
1	K	26	ARG	2.0
1	Q	182	ARG	2.0
1	S	111	PHE	2.0
1	U	153	PHE	2.0
1	Q	19	LEU	2.0
1	U	164	ALA	2.0
1	1	234	LEU	2.0
1	S	168	LYS	2.0
1	Q	13	MET	2.0
2	X	330	ASP	2.0
1	D	29	SER	2.0
2	J	412	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
4	HXD	d	4	7/15	0.80	0.14	23,30,34,38	0
4	HXD	m	4	7/15	0.80	0.15	28,33,37,37	0
4	HXD	j	4	7/15	0.82	0.14	25,30,33,37	0
4	HXD	e	4	7/15	0.84	0.14	18,28,37,38	0
4	HXD	i	4	7/15	0.84	0.14	25,31,38,40	0
4	HXD	k	4	7/15	0.85	0.12	30,33,36,37	0
4	HXD	g	4	7/15	0.85	0.12	28,29,32,33	0
4	HXD	c	4	7/15	0.86	0.13	29,29,33,34	0
4	HXD	h	4	7/15	0.86	0.13	32,34,37,37	0
4	HXD	l	4	7/15	0.86	0.14	26,28,30,32	0
4	HXD	f	4	7/15	0.86	0.12	23,29,32,35	0
4	HXD	n	4	7/15	0.86	0.12	24,28,29,30	0
4	HXD	b	4	7/15	0.88	0.14	22,28,36,37	0
4	HXD	a	4	7/15	0.91	0.10	23,26,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.