



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2022 – 12:08 AM JST

PDB ID : 7DRR  
Title : Structure of SspE-R100A protein  
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Deposited on : 2020-12-29  
Resolution : 3.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

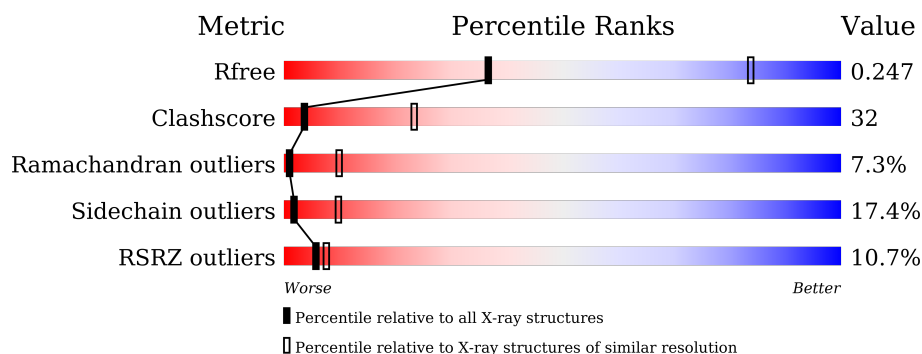
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	771	<div> <div>9%</div> <div>41% 46% 12%</div> </div>
1	B	771	<div> <div>21%</div> <div>44% 43% 11%</div> </div>
1	C	771	<div> <div>5%</div> <div>41% 41% 15%</div> </div>
1	D	771	<div> <div>8%</div> <div>43% 42% 12%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24524 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 SspE protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			
1	A	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			
1	B	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			
1	C	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			

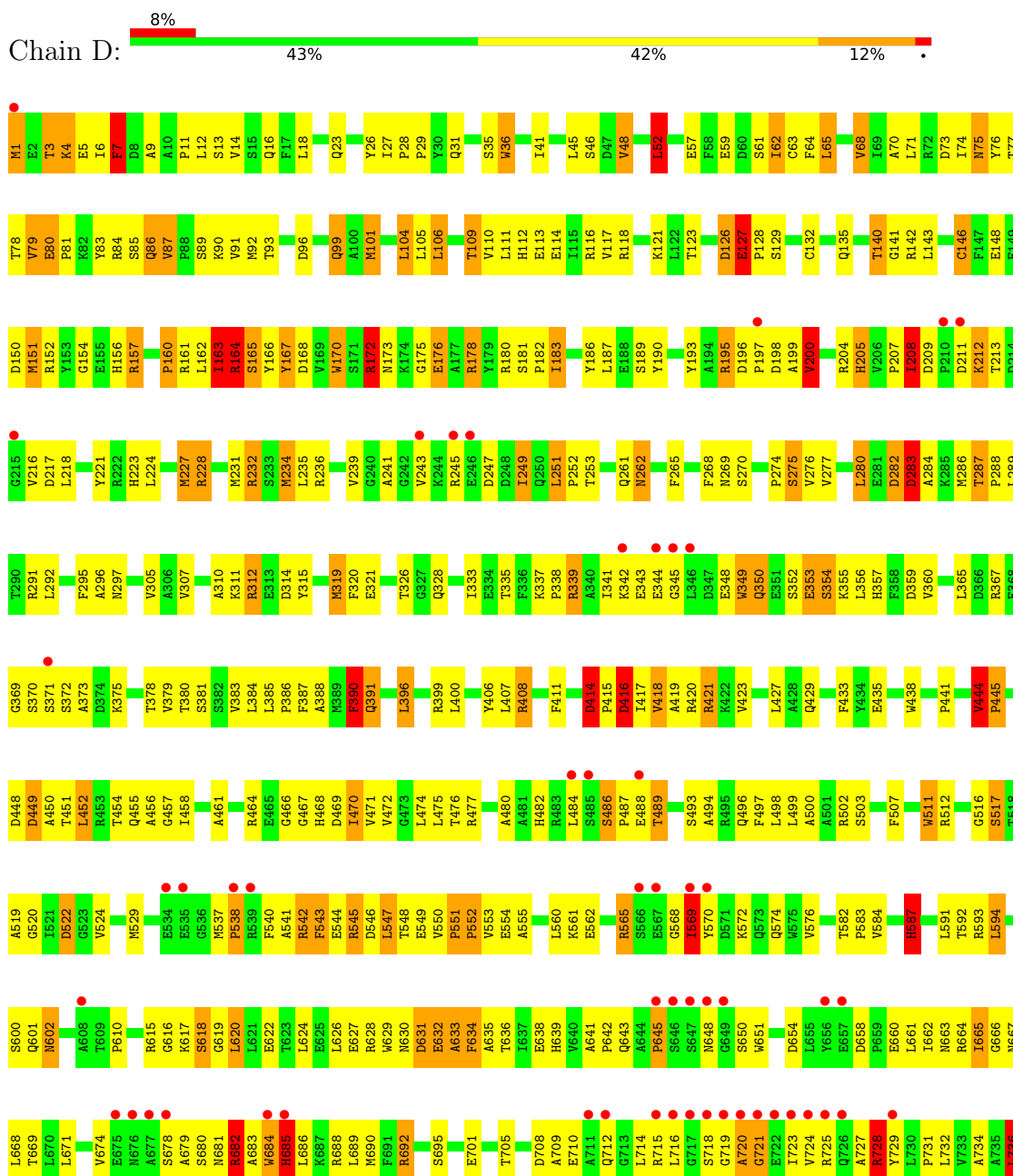
There are 4 discrepancies between the modelled and reference sequences:

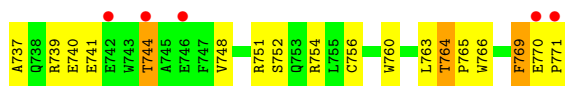
Chain	Residue	Modelled	Actual	Comment	Reference
D	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9
A	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9
B	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9
C	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9

### 3 Residue-property plots

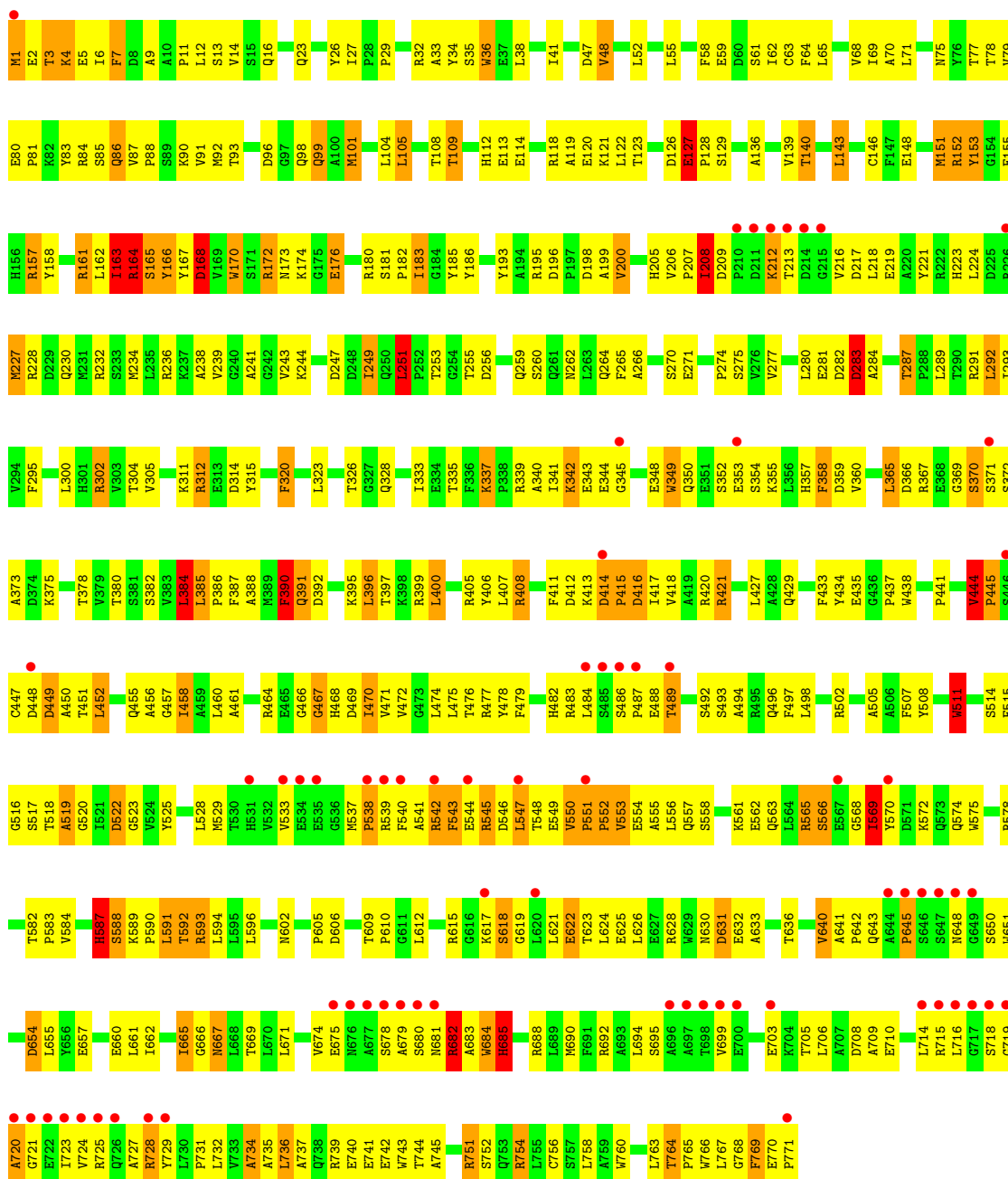
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: SspE protein

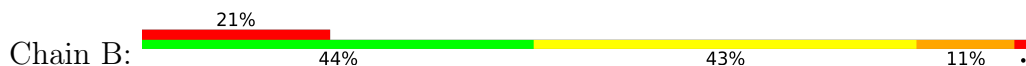


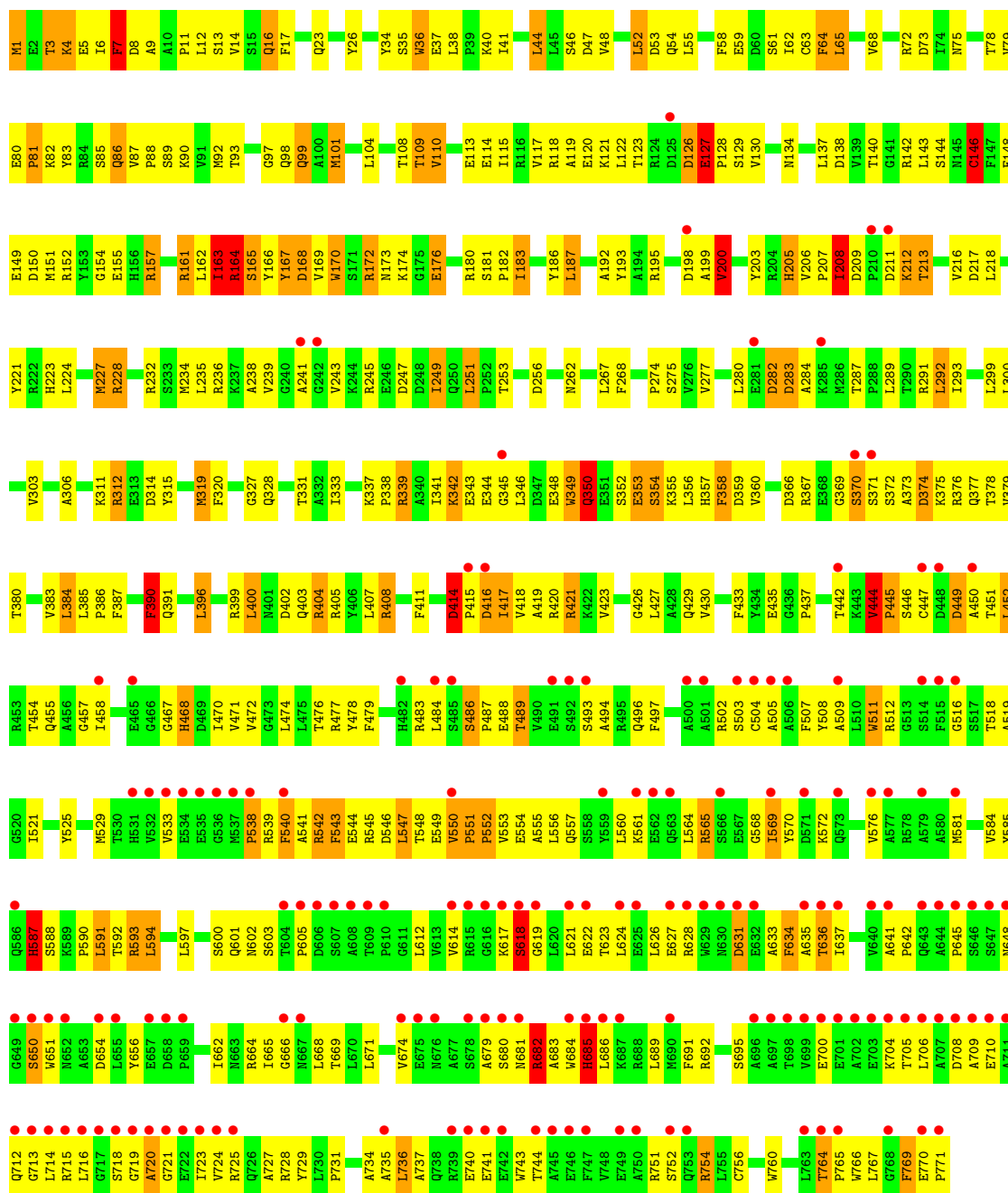


• Molecule 1: SspE protein

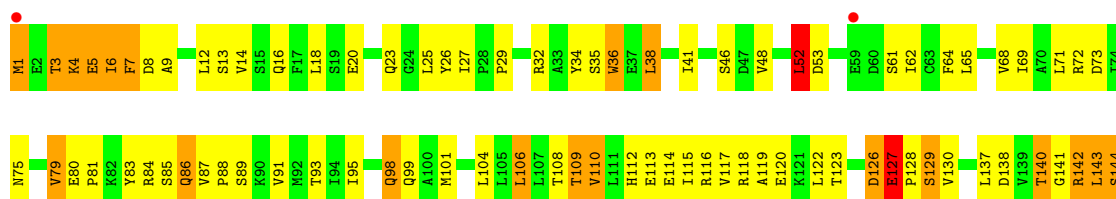


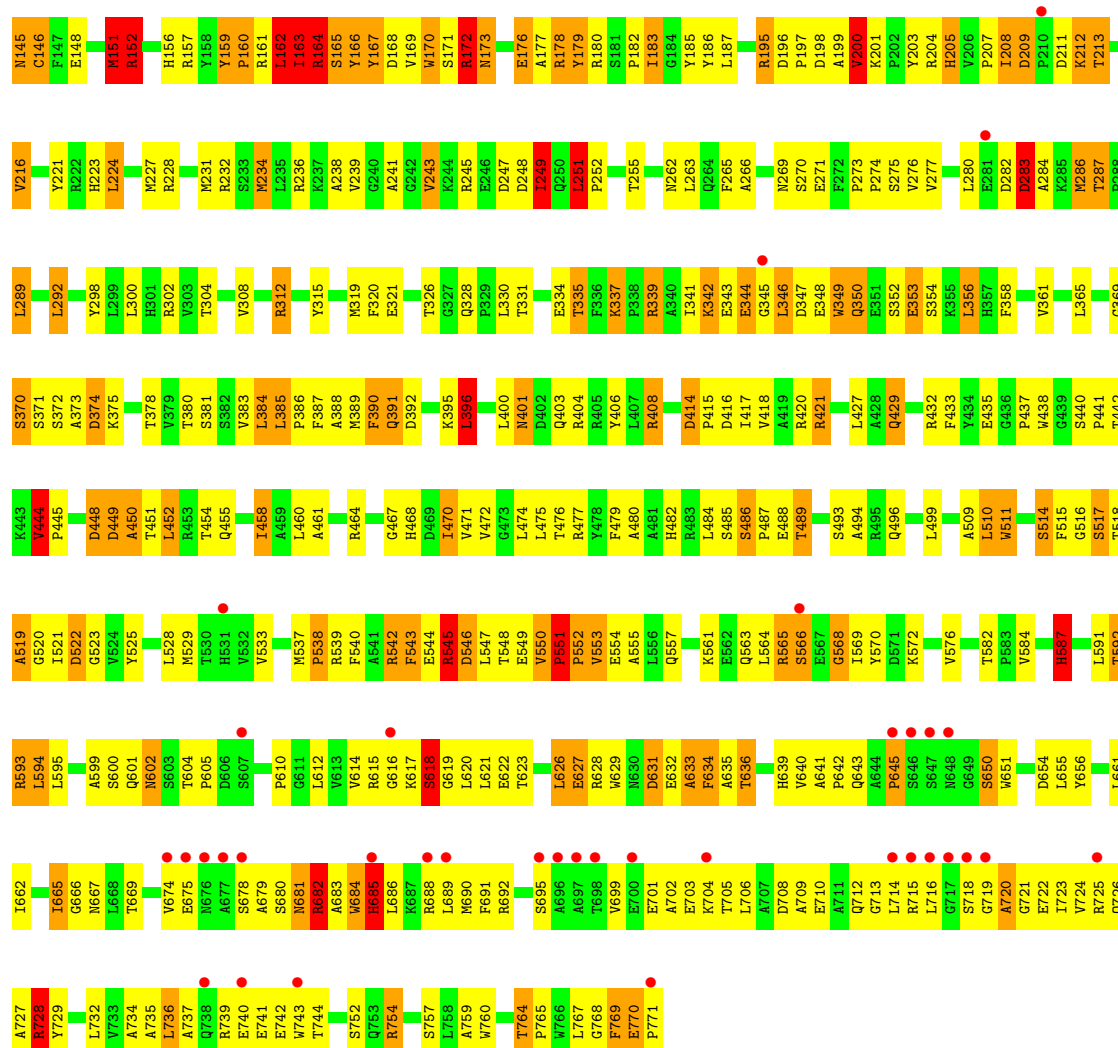
• Molecule 1: SspE protein





• Molecule 1: SspE protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.03Å 137.97Å 292.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.54 – 3.48 36.54 – 3.48	Depositor EDS
% Data completeness (in resolution range)	93.3 (36.54-3.48) 93.4 (36.54-3.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, $R_{free}$	0.224 , 0.294 0.241 , 0.247	Depositor DCC
$R_{free}$ test set	2673 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	24524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.66	3/6266 (0.0%)	0.93	14/8508 (0.2%)
1	B	0.67	2/6266 (0.0%)	0.88	13/8508 (0.2%)
1	C	0.93	12/6266 (0.2%)	1.08	32/8508 (0.4%)
1	D	0.74	8/6266 (0.1%)	0.97	20/8508 (0.2%)
All	All	0.76	25/25064 (0.1%)	0.97	79/34032 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	6
1	D	0	1
All	All	0	9

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	TYR	CD2-CE2	-7.91	1.27	1.39
1	B	146	CYS	CB-SG	-7.87	1.68	1.82
1	D	80	GLU	CB-CG	7.46	1.66	1.52
1	A	756	CYS	CB-SG	-6.60	1.71	1.82
1	C	159	TYR	CE2-CZ	-6.55	1.30	1.38
1	C	146	CYS	CB-SG	-6.45	1.71	1.82
1	C	185	TYR	CD1-CE1	-6.09	1.30	1.39
1	A	511	TRP	CB-CG	6.07	1.61	1.50
1	D	170	TRP	CG-CD2	-5.59	1.34	1.43
1	C	308	VAL	CB-CG2	-5.49	1.41	1.52
1	D	170	TRP	CZ3-CH2	5.40	1.48	1.40
1	D	14	VAL	CB-CG1	-5.36	1.41	1.52
1	C	48	VAL	CB-CG1	-5.34	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLU	CB-CG	5.32	1.62	1.52
1	C	308	VAL	CB-CG1	-5.32	1.41	1.52
1	D	7	PHE	CD1-CE1	-5.27	1.28	1.39
1	C	383	VAL	CB-CG1	-5.25	1.41	1.52
1	C	179	TYR	CE1-CZ	-5.19	1.31	1.38
1	C	321	GLU	CG-CD	5.13	1.59	1.51
1	A	434	TYR	CE2-CZ	-5.11	1.31	1.38
1	D	87	VAL	CB-CG1	-5.09	1.42	1.52
1	C	185	TYR	CB-CG	-5.09	1.44	1.51
1	D	80	GLU	CG-CD	5.06	1.59	1.51
1	C	159	TYR	CD1-CE1	-5.06	1.31	1.39
1	D	127	GLU	C-N	5.02	1.43	1.34

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	LEU	CA-CB-CG	10.39	139.20	115.30
1	B	251	LEU	CA-CB-CG	9.31	136.71	115.30
1	D	152	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	C	142	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	D	319	MET	CB-CG-SD	-8.71	86.26	112.40
1	C	346	LEU	CA-CB-CG	8.57	135.00	115.30
1	A	556	LEU	CA-CB-CG	8.45	134.72	115.30
1	C	345	GLY	N-CA-C	-7.97	93.17	113.10
1	A	337	LYS	CD-CE-NZ	7.57	129.11	111.70
1	C	263	LEU	CB-CG-CD2	-7.19	98.77	111.00
1	C	384	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	D	172	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	251	LEU	CA-CB-CG	6.84	131.03	115.30
1	D	170	TRP	CA-CB-CG	6.82	126.65	113.70
1	D	52	LEU	CA-CB-CG	6.68	130.68	115.30
1	D	251	LEU	CA-CB-CG	6.62	130.53	115.30
1	C	52	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	143	LEU	CB-CG-CD2	-6.42	100.09	111.00
1	C	300	LEU	CB-CG-CD1	-6.40	100.11	111.00
1	D	178	ARG	CB-CG-CD	-6.31	95.19	111.60
1	C	151	MET	C-N-CA	-6.26	106.05	121.70
1	D	151	MET	CG-SD-CE	6.25	110.20	100.20
1	A	105	LEU	CA-CB-CG	6.18	129.52	115.30
1	B	164	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	172	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	249	ILE	CG1-CB-CG2	-6.10	97.98	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	TRP	CA-CB-CG	6.08	125.24	113.70
1	B	152	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	345	GLY	N-CA-C	-5.98	98.14	113.10
1	B	346	LEU	CA-CB-CG	5.96	129.00	115.30
1	D	195	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	C	251	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	170	TRP	CA-CB-CG	5.91	124.94	113.70
1	C	224	LEU	CB-CG-CD2	-5.79	101.17	111.00
1	C	172	ARG	CG-CD-NE	5.78	123.94	111.80
1	C	396	LEU	CA-CB-CG	5.77	128.58	115.30
1	B	7	PHE	CB-CG-CD2	5.74	124.82	120.80
1	D	178	ARG	CG-CD-NE	5.67	123.71	111.80
1	C	661	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	319	MET	CB-CG-SD	-5.67	95.41	112.40
1	D	345	GLY	N-CA-C	-5.66	98.96	113.10
1	C	152	ARG	CB-CG-CD	-5.62	97.00	111.60
1	B	404	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	345	GLY	N-CA-C	-5.60	99.11	113.10
1	C	162	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	A	385	LEU	CB-CG-CD2	5.59	120.50	111.00
1	A	302	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	C	626	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	D	151	MET	C-N-CA	-5.51	107.92	121.70
1	C	187	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	D	121	LYS	O-C-N	-5.49	113.92	122.70
1	A	593	ARG	CG-CD-NE	-5.47	100.32	111.80
1	C	143	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	C	178	ARG	CB-CG-CD	-5.46	97.40	111.60
1	D	104	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	D	48	VAL	CG1-CB-CG2	-5.40	102.27	110.90
1	D	407	LEU	CB-CG-CD2	-5.40	101.83	111.00
1	A	385	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	150	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	289	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	C	170	TRP	CA-CB-CG	5.27	123.71	113.70
1	C	178	ARG	CA-CB-CG	5.26	124.97	113.40
1	C	385	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	D	232	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	12	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	D	101	MET	CB-CG-SD	-5.16	96.92	112.40
1	C	195	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	A	161	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	C	172	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	416	ASP	C-N-CA	5.12	134.51	121.70
1	C	209	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	187	LEU	CA-CB-CG	-5.12	103.53	115.30
1	B	161	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	D	116	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	52	LEU	CA-CB-CG	5.07	126.97	115.30
1	C	178	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	384	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	C	510	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	PRO	Peptide
1	A	553	VAL	Peptide
1	C	173	ASN	Peptide
1	C	344	GLU	Peptide
1	C	551	PRO	Peptide
1	C	553	VAL	Peptide
1	C	681	ASN	Peptide
1	C	79	VAL	Peptide
1	D	175	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6131	0	6038	380	1
1	B	6131	0	6038	374	1
1	C	6131	0	6038	419	2
1	D	6131	0	6038	380	2
All	All	24524	0	24152	1535	3

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 32.

All (1535) 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:126:ASP:HB3	1:D:129:SER:HB3	1.37	1.05
1:A:126:ASP:HB3	1:A:129:SER:HB3	1.36	1.04
1:C:173:ASN:HB2	1:C:176:GLU:OE2	1.57	1.02
1:D:183:ILE:HD12	1:D:183:ILE:H	1.26	0.98
1:C:243:VAL:HG11	1:C:245:ARG:HH21	1.27	0.96
1:A:182:PRO:HB2	1:A:224:LEU:HD13	1.51	0.93
1:A:688:ARG:NH1	1:A:740:GLU:OE2	2.01	0.93
1:A:32:ARG:O	1:A:164:ARG:NH2	2.04	0.91
1:A:612:LEU:HB3	1:A:754:ARG:HD3	1.50	0.90
1:D:692:ARG:HG3	1:D:737:ALA:HB1	1.53	0.89
1:C:688:ARG:NH1	1:C:740:GLU:OE2	2.05	0.89
1:B:126:ASP:HB3	1:B:129:SER:HB3	1.50	0.89
1:A:628:ARG:HA	1:A:631:ASP:HB2	1.55	0.89
1:B:612:LEU:HB3	1:B:754:ARG:HD3	1.55	0.89
1:D:622:GLU:O	1:D:628:ARG:NH1	2.07	0.88
1:D:724:VAL:HG12	1:D:725:ARG:HG3	1.55	0.88
1:C:628:ARG:HA	1:C:631:ASP:HB2	1.53	0.88
1:C:614:VAL:HG12	1:C:754:ARG:HH11	1.38	0.87
1:A:339:ARG:HG2	1:A:408:ARG:HH22	1.39	0.87
1:D:367:ARG:NH1	1:D:435:GLU:OE2	2.09	0.86
1:D:113:GLU:OE2	1:D:232:ARG:NH2	2.07	0.86
1:A:449:ASP:HB3	1:A:452:LEU:HB2	1.57	0.85
1:A:484:LEU:HB3	1:A:548:THR:HG22	1.58	0.85
1:C:1:MET:HA	1:C:4:LYS:HB2	1.56	0.85
1:C:441:PRO:HG2	1:C:461:ALA:HB2	1.59	0.85
1:B:565:ARG:HH21	1:B:771:PRO:HB3	1.41	0.85
1:C:183:ILE:H	1:C:183:ILE:HD12	1.42	0.85
1:D:114:GLU:OE1	1:D:118:ARG:NH1	2.08	0.85
1:A:339:ARG:HG2	1:A:408:ARG:NH2	1.91	0.84
1:A:455:GLN:OE1	1:A:502:ARG:NH2	2.10	0.84
1:A:496:GLN:HA	1:A:553:VAL:HG13	1.59	0.84
1:A:385:LEU:HD22	1:A:396:LEU:HB3	1.60	0.83
1:C:161:ARG:O	1:C:162:LEU:HB2	1.77	0.83
1:B:477:ARG:HD3	1:B:542:ARG:H	1.42	0.83
1:B:628:ARG:HA	1:B:631:ASP:HB2	1.59	0.83
1:D:161:ARG:O	1:D:162:LEU:HB2	1.79	0.82
1:A:449:ASP:O	1:A:452:LEU:N	2.12	0.82
1:A:715:ARG:HB3	1:A:719:GLY:HA2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:GLU:O	1:C:628:ARG:NH1	2.13	0.82
1:C:477:ARG:HD3	1:C:542:ARG:H	1.45	0.82
1:B:614:VAL:HG12	1:B:754:ARG:HH11	1.44	0.81
1:D:617:LYS:O	1:D:619:GLY:N	2.13	0.81
1:A:208:ILE:HG21	1:A:221:TYR:CD2	2.15	0.81
1:A:692:ARG:HG3	1:A:737:ALA:HB1	1.60	0.81
1:B:9:ALA:HB3	1:C:9:ALA:HB3	1.61	0.81
1:C:3:THR:O	1:C:5:GLU:N	2.14	0.81
1:D:209:ASP:OD1	1:D:212:LYS:N	2.13	0.81
1:D:9:ALA:HB3	1:A:9:ALA:HB3	1.61	0.81
1:A:680:SER:O	1:A:682:ARG:NH2	2.13	0.80
1:A:208:ILE:HG21	1:A:221:TYR:HD2	1.47	0.80
1:A:542:ARG:HE	1:A:547:LEU:HD12	1.47	0.80
1:A:1:MET:HA	1:A:4:LYS:HB2	1.64	0.79
1:D:469:ASP:O	1:D:472:VAL:HG23	1.82	0.79
1:D:628:ARG:HA	1:D:631:ASP:HB2	1.64	0.79
1:D:111:LEU:HD22	1:D:296:ALA:HB2	1.65	0.79
1:D:208:ILE:HG21	1:D:221:TYR:CD2	2.18	0.79
1:C:692:ARG:HG3	1:C:737:ALA:HB1	1.63	0.79
1:A:173:ASN:HB2	1:A:176:GLU:OE2	1.83	0.78
1:A:12:LEU:HA	1:A:16:GLN:HE21	1.49	0.78
1:D:760:TRP:O	1:D:764:THR:OG1	2.02	0.78
1:C:485:SER:OG	1:C:489:THR:OG1	2.00	0.78
1:A:337:LYS:HZ1	1:A:358:PHE:HD1	1.29	0.78
1:B:715:ARG:HB3	1:B:719:GLY:HA2	1.64	0.78
1:A:477:ARG:HD3	1:A:542:ARG:H	1.49	0.78
1:D:161:ARG:HA	1:D:170:TRP:HH2	1.48	0.78
1:C:651:TRP:NE1	1:C:683:ALA:HA	1.99	0.78
1:B:692:ARG:HG3	1:B:737:ALA:HB1	1.66	0.77
1:C:344:GLU:OE1	1:C:421:ARG:NH2	2.17	0.77
1:C:511:TRP:HH2	1:C:519:ALA:HB3	1.50	0.77
1:C:617:LYS:O	1:C:619:GLY:N	2.17	0.77
1:D:110:VAL:HA	1:D:228:ARG:HH11	1.49	0.77
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.67	0.77
1:A:542:ARG:HD3	1:A:547:LEU:H	1.50	0.77
1:B:161:ARG:O	1:B:162:LEU:HB2	1.84	0.77
1:D:715:ARG:HB3	1:D:719:GLY:HA2	1.67	0.77
1:C:127:GLU:HB3	1:C:128:PRO:HD2	1.67	0.77
1:D:474:LEU:O	1:D:477:ARG:HB3	1.84	0.77
1:C:612:LEU:HB3	1:C:754:ARG:HD3	1.65	0.77
1:C:665:ILE:HD13	1:C:665:ILE:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASP:OD1	1:B:399:ARG:NH2	2.19	0.76
1:C:208:ILE:HG13	1:C:209:ASP:H	1.47	0.76
1:A:724:VAL:HG12	1:A:725:ARG:HG3	1.67	0.76
1:B:58:PHE:CE2	1:B:405:ARG:HD3	2.20	0.76
1:B:680:SER:O	1:B:682:ARG:NH2	2.19	0.76
1:D:173:ASN:HB2	1:D:176:GLU:OE2	1.85	0.76
1:A:477:ARG:NH2	1:A:547:LEU:O	2.18	0.76
1:B:312:ARG:HD3	1:B:315:TYR:CE2	2.21	0.76
1:A:3:THR:O	1:A:5:GLU:N	2.19	0.76
1:B:3:THR:O	1:B:5:GLU:N	2.19	0.75
1:C:511:TRP:CH2	1:C:519:ALA:HB3	2.21	0.75
1:D:110:VAL:HG12	1:D:228:ARG:HE	1.50	0.75
1:D:543:PHE:O	1:D:545:ARG:NH2	2.16	0.75
1:B:344:GLU:OE1	1:B:421:ARG:NH2	2.19	0.75
1:A:128:PRO:HG3	1:A:275:SER:HB2	1.67	0.75
1:D:3:THR:O	1:D:5:GLU:N	2.20	0.75
1:A:126:ASP:CB	1:A:129:SER:HB3	2.14	0.75
1:A:570:TYR:HB2	1:A:769:PHE:HZ	1.52	0.74
1:B:565:ARG:HG2	1:B:570:TYR:CE2	2.22	0.74
1:C:343:GLU:OE2	1:C:420:ARG:CZ	2.35	0.74
1:D:183:ILE:H	1:D:183:ILE:CD1	1.98	0.74
1:D:680:SER:O	1:D:682:ARG:NH2	2.20	0.74
1:B:26:TYR:HD2	1:B:93:THR:HG22	1.53	0.73
1:C:553:VAL:HB	1:C:554:GLU:HG3	1.68	0.73
1:D:5:GLU:O	1:D:7:PHE:N	2.20	0.73
1:C:167:TYR:CZ	1:C:216:VAL:HG22	2.24	0.73
1:C:390:PHE:HE1	1:C:542:ARG:HG2	1.54	0.73
1:B:36:TRP:CD1	1:B:99:GLN:HG2	2.23	0.73
1:A:183:ILE:H	1:A:183:ILE:HD12	1.53	0.73
1:D:86:GLN:HE22	1:D:172:ARG:H	1.37	0.73
1:C:213:THR:O	1:C:213:THR:OG1	2.05	0.73
1:A:553:VAL:HB	1:A:554:GLU:HG3	1.71	0.73
1:B:5:GLU:O	1:B:7:PHE:N	2.20	0.72
1:C:127:GLU:HB3	1:C:128:PRO:CD	2.18	0.72
1:C:474:LEU:O	1:C:477:ARG:HB3	1.89	0.72
1:B:73:ASP:OD2	1:B:78:THR:OG1	2.05	0.72
1:C:544:GLU:HB2	1:C:545:ARG:NH2	2.05	0.72
1:C:232:ARG:HD3	1:C:236:ARG:CZ	2.20	0.72
1:D:552:PRO:HG2	1:D:555:ALA:H	1.53	0.72
1:B:12:LEU:HB3	1:B:16:GLN:HG3	1.71	0.72
1:B:617:LYS:O	1:B:619:GLY:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ILE:HG21	1:A:522:ASP:HA	1.71	0.72
1:B:312:ARG:HD3	1:B:315:TYR:HE2	1.56	0.71
1:B:710:GLU:HA	1:B:714:LEU:H	1.55	0.71
1:A:544:GLU:HB2	1:A:545:ARG:NH2	2.05	0.71
1:C:715:ARG:HB3	1:C:719:GLY:HA2	1.73	0.71
1:D:529:MET:SD	1:D:541:ALA:HB2	2.31	0.71
1:D:449:ASP:O	1:D:451:THR:N	2.23	0.71
1:C:544:GLU:HB2	1:C:545:ARG:HH22	1.56	0.71
1:B:182:PRO:HD3	1:B:221:TYR:HE1	1.55	0.71
1:D:375:LYS:O	1:D:378:THR:HG22	1.91	0.71
1:C:680:SER:O	1:C:682:ARG:NH2	2.23	0.71
1:A:341:ILE:HG12	1:A:349:TRP:CZ2	2.25	0.71
1:B:333:ILE:HD12	1:B:380:THR:HG23	1.73	0.71
1:D:651:TRP:NE1	1:D:683:ALA:HA	2.05	0.70
1:B:385:LEU:HD22	1:B:396:LEU:HB3	1.73	0.70
1:D:127:GLU:HB3	1:D:128:PRO:HD2	1.73	0.70
1:A:617:LYS:O	1:A:619:GLY:N	2.24	0.70
1:C:172:ARG:HH11	1:C:172:ARG:HG3	1.56	0.70
1:C:517:SER:O	1:C:519:ALA:N	2.24	0.70
1:A:118:ARG:HB2	1:A:289:LEU:HD13	1.71	0.70
1:A:208:ILE:HD13	1:A:209:ASP:H	1.55	0.70
1:B:151:MET:HB3	1:B:172:ARG:HH11	1.57	0.70
1:D:720:ALA:HB1	1:D:723:ILE:HD12	1.73	0.70
1:A:387:PHE:CE2	1:A:427:LEU:HG	2.26	0.70
1:C:113:GLU:O	1:C:117:VAL:HG12	1.91	0.70
1:B:208:ILE:HD13	1:B:209:ASP:H	1.56	0.70
1:C:520:GLY:O	1:C:523:GLY:N	2.25	0.70
1:D:3:THR:HG22	1:A:16:GLN:HE22	1.57	0.70
1:A:12:LEU:HB3	1:A:16:GLN:HG3	1.72	0.70
1:A:47:ASP:OD1	1:A:399:ARG:NH2	2.24	0.70
1:A:391:GLN:OE1	1:A:542:ARG:NH1	2.24	0.70
1:C:3:THR:O	1:C:3:THR:OG1	2.05	0.70
1:A:161:ARG:O	1:A:162:LEU:HB2	1.90	0.70
1:C:496:GLN:HA	1:C:553:VAL:HG13	1.73	0.69
1:B:3:THR:O	1:B:3:THR:OG1	2.11	0.69
1:B:183:ILE:HD12	1:B:183:ILE:H	1.57	0.69
1:D:326:THR:HG21	1:A:323:LEU:O	1.92	0.69
1:D:449:ASP:O	1:D:452:LEU:N	2.26	0.69
1:A:674:VAL:HG11	1:A:679:ALA:H	1.58	0.69
1:A:412:ASP:OD1	1:A:420:ARG:NH2	2.26	0.69
1:B:148:GLU:OE1	1:B:195:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:TRP:CZ3	1:C:684:TRP:HB2	2.28	0.69
1:D:484:LEU:HB3	1:D:548:THR:HG22	1.75	0.69
1:A:36:TRP:CD1	1:A:99:GLN:HG2	2.27	0.69
1:A:618:SER:OG	1:A:619:GLY:N	2.26	0.69
1:C:209:ASP:OD1	1:C:212:LYS:N	2.26	0.69
1:A:572:LYS:HE2	1:A:760:TRP:CZ3	2.27	0.69
1:B:417:ILE:HG23	1:B:418:VAL:HG23	1.75	0.69
1:D:12:LEU:HB3	1:D:16:GLN:HG3	1.75	0.68
1:C:538:PRO:HB3	1:C:550:VAL:HG22	1.75	0.68
1:D:441:PRO:HG2	1:D:461:ALA:HB2	1.75	0.68
1:A:412:ASP:HA	1:A:420:ARG:HH21	1.58	0.68
1:D:641:ALA:HB3	1:D:667:ASN:HD21	1.58	0.68
1:B:418:VAL:HA	1:B:421:ARG:HD2	1.76	0.68
1:B:705:THR:HA	1:B:708:ASP:HB2	1.75	0.68
1:B:127:GLU:OE2	1:B:128:PRO:HD3	1.94	0.68
1:C:183:ILE:H	1:C:183:ILE:CD1	2.07	0.68
1:C:674:VAL:HG11	1:C:679:ALA:H	1.59	0.68
1:A:621:LEU:HD12	1:A:729:TYR:HD2	1.58	0.68
1:B:525:TYR:O	1:B:529:MET:HG2	1.94	0.68
1:C:705:THR:HA	1:C:708:ASP:HB2	1.74	0.68
1:B:208:ILE:HG21	1:B:221:TYR:CD2	2.29	0.68
1:B:651:TRP:CZ3	1:B:684:TRP:HB2	2.29	0.68
1:B:213:THR:O	1:B:213:THR:OG1	2.11	0.67
1:C:470:ILE:HD12	1:C:522:ASP:OD2	1.94	0.67
1:D:208:ILE:HG21	1:D:221:TYR:HD2	1.58	0.67
1:A:114:GLU:OE1	1:A:118:ARG:NH1	2.26	0.67
1:A:239:VAL:HG12	1:A:251:LEU:HD21	1.76	0.67
1:C:666:GLY:H	1:C:752:SER:HB3	1.59	0.67
1:A:666:GLY:H	1:A:752:SER:HB3	1.59	0.67
1:A:414:ASP:O	1:A:416:ASP:N	2.26	0.67
1:A:511:TRP:CZ3	1:A:519:ALA:HB3	2.29	0.67
1:C:168:ASP:OD1	1:C:180:ARG:N	2.24	0.67
1:A:414:ASP:OD2	1:A:416:ASP:OD2	2.12	0.67
1:B:113:GLU:OE2	1:B:232:ARG:NH2	2.28	0.67
1:D:542:ARG:HE	1:D:547:LEU:HD12	1.58	0.67
1:D:728:ARG:HD3	1:D:729:TYR:N	2.09	0.67
1:C:126:ASP:HB3	1:C:129:SER:HB3	1.77	0.67
1:D:418:VAL:H	1:D:421:ARG:HD2	1.60	0.67
1:D:7:PHE:HD1	1:D:319:MET:SD	2.18	0.67
1:C:486:SER:O	1:C:488:GLU:N	2.28	0.67
1:C:599:ALA:HB2	1:C:759:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:O	1:B:477:ARG:HB3	1.93	0.67
1:B:564:LEU:HB3	1:B:570:TYR:HB3	1.77	0.67
1:C:4:LYS:O	1:C:5:GLU:HG3	1.94	0.67
1:A:105:LEU:HD23	1:A:162:LEU:HD12	1.77	0.66
1:C:437:PRO:HD3	1:C:479:PHE:CE2	2.29	0.66
1:D:11:PRO:O	1:D:12:LEU:HD23	1.95	0.66
1:D:438:TRP:CE3	1:D:464:ARG:HG3	2.31	0.66
1:D:445:PRO:HG3	1:D:497:PHE:HD1	1.60	0.66
1:B:128:PRO:HD3	1:B:275:SER:HB2	1.77	0.66
1:B:390:PHE:HE1	1:B:542:ARG:HG2	1.59	0.66
1:B:454:THR:HG21	1:B:627:GLU:OE2	1.95	0.66
1:A:120:GLU:HG2	1:A:200:VAL:HG11	1.76	0.66
1:A:641:ALA:H	1:A:667:ASN:HD21	1.44	0.66
1:B:7:PHE:C	1:B:7:PHE:CD2	2.69	0.66
1:C:449:ASP:O	1:C:451:THR:N	2.28	0.66
1:C:634:PHE:HD1	1:C:634:PHE:H	1.42	0.66
1:A:651:TRP:CZ3	1:A:684:TRP:HB2	2.31	0.66
1:C:114:GLU:OE1	1:C:118:ARG:NH1	2.28	0.66
1:A:83:TYR:CZ	1:A:176:GLU:HB2	2.31	0.66
1:B:208:ILE:HG21	1:B:221:TYR:HD2	1.60	0.65
1:C:387:PHE:CE2	1:C:427:LEU:HG	2.31	0.65
1:C:538:PRO:HB2	1:C:550:VAL:HG13	1.78	0.65
1:C:621:LEU:HD12	1:C:729:TYR:HD2	1.61	0.65
1:D:321:GLU:OE2	1:A:400:LEU:HB2	1.97	0.65
1:A:344:GLU:OE1	1:A:421:ARG:NH2	2.29	0.65
1:C:374:ASP:OD1	1:C:374:ASP:N	2.30	0.65
1:B:173:ASN:HB2	1:B:176:GLU:OE2	1.96	0.65
1:D:477:ARG:HD3	1:D:541:ALA:HA	1.79	0.65
1:A:445:PRO:HD3	1:A:497:PHE:HE1	1.61	0.65
1:B:449:ASP:O	1:B:451:THR:N	2.30	0.65
1:B:486:SER:O	1:B:488:GLU:N	2.30	0.65
1:B:489:THR:O	1:B:489:THR:OG1	2.15	0.65
1:A:168:ASP:OD1	1:A:180:ARG:N	2.28	0.65
1:A:391:GLN:O	1:A:391:GLN:NE2	2.29	0.65
1:D:551:PRO:HB2	1:D:552:PRO:HD3	1.79	0.65
1:C:458:ILE:HD11	1:C:629:TRP:HB2	1.78	0.65
1:D:634:PHE:HD1	1:D:634:PHE:H	1.43	0.65
1:B:4:LYS:O	1:B:5:GLU:HG3	1.97	0.65
1:B:538:PRO:HB2	1:B:550:VAL:HG13	1.78	0.65
1:B:375:LYS:HA	1:B:378:THR:HG22	1.79	0.65
1:B:505:ALA:O	1:B:508:TYR:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:HB3	1:A:128:PRO:HD2	1.78	0.64
1:D:387:PHE:CE2	1:D:427:LEU:HG	2.33	0.64
1:C:265:PHE:CZ	1:C:271:GLU:HG3	2.31	0.64
1:D:496:GLN:HA	1:D:553:VAL:HG13	1.79	0.64
1:A:561:LYS:NZ	1:A:768:GLY:O	2.27	0.64
1:D:27:ILE:HB	1:D:164:ARG:HA	1.80	0.64
1:A:705:THR:HA	1:A:708:ASP:HB2	1.78	0.64
1:B:477:ARG:CZ	1:B:542:ARG:HB3	2.26	0.64
1:C:391:GLN:O	1:C:391:GLN:NE2	2.31	0.64
1:B:37:GLU:H	1:B:40:LYS:HZ1	1.44	0.64
1:B:355:LYS:HD2	1:B:359:ASP:OD2	1.97	0.64
1:C:180:ARG:HH12	1:C:212:LYS:HE2	1.62	0.64
1:A:87:VAL:HG22	1:A:88:PRO:HD2	1.78	0.64
1:C:396:LEU:HD11	1:C:403:GLN:HA	1.77	0.64
1:D:390:PHE:CE1	1:D:542:ARG:HG2	2.32	0.64
1:A:26:TYR:HD2	1:A:93:THR:HG22	1.63	0.64
1:A:168:ASP:OD1	1:A:181:SER:N	2.29	0.64
1:A:474:LEU:O	1:A:477:ARG:HB3	1.98	0.64
1:A:621:LEU:HD12	1:A:729:TYR:CD2	2.33	0.64
1:A:486:SER:O	1:A:488:GLU:N	2.31	0.64
1:B:26:TYR:OH	1:B:165:SER:HB3	1.98	0.64
1:C:474:LEU:HG	1:C:529:MET:HE1	1.80	0.64
1:C:243:VAL:HG11	1:C:245:ARG:NH2	2.09	0.63
1:C:680:SER:HA	1:C:690:MET:HE1	1.79	0.63
1:A:3:THR:O	1:A:3:THR:OG1	2.16	0.63
1:A:13:SER:OG	1:A:16:GLN:HG2	1.99	0.63
1:A:669:THR:HG22	1:A:732:LEU:HD13	1.80	0.63
1:B:86:GLN:HE22	1:B:172:ARG:H	1.46	0.63
1:C:438:TRP:CE3	1:C:464:ARG:HG3	2.33	0.63
1:D:385:LEU:HD22	1:D:396:LEU:HB3	1.79	0.63
1:D:511:TRP:HH2	1:D:519:ALA:HB3	1.64	0.63
1:A:339:ARG:CG	1:A:408:ARG:HH22	2.10	0.63
1:C:514:SER:OG	1:C:515:PHE:N	2.29	0.63
1:D:163:ILE:O	1:D:168:ASP:OD2	2.17	0.63
1:C:282:ASP:O	1:C:284:ALA:N	2.32	0.63
1:C:681:ASN:OD1	1:C:682:ARG:N	2.32	0.63
1:D:23:GLN:HG3	1:D:90:LYS:HD3	1.78	0.63
1:D:86:GLN:NE2	1:D:172:ARG:HD3	2.14	0.63
1:D:284:ALA:O	1:D:286:MET:N	2.32	0.63
1:C:390:PHE:CE1	1:C:542:ARG:HG2	2.34	0.63
1:C:651:TRP:HE1	1:C:683:ALA:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HB2	1:B:289:LEU:HD13	1.79	0.63
1:B:151:MET:HB3	1:B:172:ARG:NH1	2.12	0.63
1:D:396:LEU:HD21	1:D:406:TYR:CG	2.34	0.63
1:A:584:VAL:HG12	1:A:592:THR:HG22	1.81	0.63
1:A:760:TRP:O	1:A:764:THR:OG1	2.15	0.63
1:B:385:LEU:CD2	1:B:396:LEU:HB3	2.28	0.63
1:B:442:THR:HA	1:B:626:LEU:HD21	1.81	0.63
1:B:477:ARG:HD3	1:B:542:ARG:N	2.12	0.63
1:C:584:VAL:HG12	1:C:592:THR:HG22	1.80	0.63
1:D:276:VAL:HG12	1:D:280:LEU:HD22	1.81	0.62
1:D:208:ILE:HG23	1:D:209:ASP:N	2.14	0.62
1:C:13:SER:OG	1:C:16:GLN:HG2	1.98	0.62
1:C:352:SER:O	1:C:354:SER:N	2.31	0.62
1:C:489:THR:OG1	1:C:489:THR:O	2.17	0.62
1:C:433:PHE:CG	1:C:476:THR:HG22	2.33	0.62
1:C:545:ARG:NH2	1:C:545:ARG:H	1.97	0.62
1:D:172:ARG:HG3	1:D:172:ARG:HH11	1.63	0.62
1:B:36:TRP:HE3	1:B:41:ILE:HD13	1.65	0.62
1:C:449:ASP:O	1:C:452:LEU:N	2.32	0.62
1:B:720:ALA:HB1	1:B:723:ILE:HB	1.80	0.62
1:C:546:ASP:HB3	1:C:549:GLU:HG2	1.81	0.62
1:A:355:LYS:HD2	1:A:359:ASP:OD2	2.00	0.62
1:B:449:ASP:O	1:B:452:LEU:N	2.32	0.62
1:D:349:TRP:O	1:D:349:TRP:CD1	2.53	0.62
1:D:600:SER:HB3	1:D:732:LEU:HD21	1.82	0.62
1:C:372:SER:OG	1:C:373:ALA:N	2.31	0.62
1:D:489:THR:O	1:D:489:THR:OG1	2.16	0.62
1:A:605:PRO:HB3	1:A:735:ALA:HB2	1.81	0.62
1:C:688:ARG:HD3	1:C:692:ARG:HH12	1.64	0.61
1:B:411:PHE:HA	1:B:423:VAL:HG11	1.83	0.61
1:D:458:ILE:HG13	1:D:629:TRP:HB2	1.82	0.61
1:D:610:PRO:O	1:D:739:ARG:HB2	2.01	0.61
1:A:34:TYR:HD2	1:A:224:LEU:HD12	1.65	0.61
1:D:127:GLU:HB3	1:D:128:PRO:CD	2.30	0.61
1:D:584:VAL:HG12	1:D:592:THR:HG22	1.83	0.61
1:C:724:VAL:HG12	1:C:725:ARG:HG3	1.80	0.61
1:A:33:ALA:HA	1:A:164:ARG:NH2	2.16	0.61
1:A:441:PRO:HG2	1:A:461:ALA:HB2	1.83	0.61
1:A:333:ILE:HD12	1:A:365:LEU:HD21	1.83	0.61
1:B:26:TYR:O	1:B:93:THR:HA	2.01	0.61
1:B:380:THR:O	1:B:384:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:HD11	1:D:231:MET:HG2	1.83	0.61
1:D:565:ARG:HG2	1:D:570:TYR:CE2	2.35	0.61
1:A:153:TYR:CD1	1:B:134:ASN:HB3	2.35	0.61
1:C:728:ARG:HD3	1:C:729:TYR:N	2.15	0.61
1:A:232:ARG:HD3	1:A:236:ARG:CZ	2.30	0.61
1:D:208:ILE:CD1	1:D:209:ASP:H	2.14	0.61
1:A:208:ILE:HG23	1:A:209:ASP:N	2.15	0.61
1:A:551:PRO:HB2	1:A:552:PRO:HD3	1.83	0.60
1:A:570:TYR:HB2	1:A:769:PHE:CZ	2.36	0.60
1:C:688:ARG:CZ	1:C:740:GLU:OE2	2.49	0.60
1:A:11:PRO:O	1:A:12:LEU:HD23	2.01	0.60
1:A:433:PHE:HE2	1:A:438:TRP:NE1	1.99	0.60
1:C:522:ASP:OD1	1:C:522:ASP:N	2.33	0.60
1:D:631:ASP:O	1:D:633:ALA:N	2.34	0.60
1:A:452:LEU:HB3	1:A:498:LEU:HD13	1.83	0.60
1:B:143:LEU:O	1:B:146:CYS:CB	2.50	0.60
1:B:533:VAL:O	1:B:538:PRO:HD2	2.01	0.60
1:B:516:GLY:O	1:B:587:HIS:NE2	2.33	0.60
1:D:636:THR:HB	1:D:671:LEU:O	2.01	0.60
1:A:489:THR:O	1:A:489:THR:OG1	2.19	0.60
1:A:565:ARG:HG2	1:A:570:TYR:CE2	2.35	0.60
1:C:682:ARG:HE	1:C:716:LEU:HD13	1.65	0.60
1:D:283:ASP:HA	1:D:287:THR:HB	1.83	0.60
1:B:114:GLU:OE1	1:B:118:ARG:NH1	2.33	0.60
1:B:357:HIS:O	1:B:360:VAL:HB	2.01	0.60
1:C:349:TRP:O	1:C:349:TRP:CD1	2.55	0.60
1:D:26:TYR:OH	1:D:165:SER:HB3	2.01	0.60
1:D:583:PRO:HG3	1:D:660:GLU:HG2	1.84	0.60
1:B:377:GLN:HE22	1:B:403:GLN:HE22	1.50	0.60
1:B:729:TYR:CE2	1:B:731:PRO:HG3	2.37	0.60
1:C:471:VAL:HG12	1:C:475:LEU:HG	1.84	0.60
1:C:484:LEU:HB3	1:C:548:THR:HG22	1.84	0.60
1:A:433:PHE:HE2	1:A:438:TRP:CD1	2.19	0.60
1:B:1:MET:HA	1:B:4:LYS:HB2	1.82	0.60
1:C:113:GLU:OE1	1:C:228:ARG:NH1	2.35	0.60
1:D:52:LEU:HD13	1:D:252:PRO:HD2	1.84	0.60
1:D:390:PHE:HE1	1:D:542:ARG:HG2	1.67	0.60
1:A:674:VAL:HG11	1:A:679:ALA:N	2.16	0.60
1:B:542:ARG:HE	1:B:547:LEU:HD12	1.67	0.60
1:C:674:VAL:HG11	1:C:679:ALA:N	2.17	0.60
1:B:7:PHE:C	1:B:7:PHE:HD2	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:LYS:HE3	1:B:769:PHE:HA	1.82	0.59
1:A:163:ILE:HG13	1:A:170:TRP:CH2	2.37	0.59
1:B:26:TYR:CZ	1:B:79:VAL:HA	2.37	0.59
1:C:433:PHE:CD1	1:C:476:THR:HG22	2.37	0.59
1:C:715:ARG:HG2	1:C:720:ALA:HB2	1.84	0.59
1:D:542:ARG:HG3	1:D:542:ARG:O	2.03	0.59
1:A:720:ALA:HB1	1:A:723:ILE:HD12	1.83	0.59
1:B:372:SER:OG	1:B:373:ALA:N	2.33	0.59
1:C:477:ARG:NE	1:C:542:ARG:HB3	2.16	0.59
1:D:674:VAL:HG11	1:D:679:ALA:H	1.67	0.59
1:C:5:GLU:O	1:C:7:PHE:N	2.29	0.59
1:C:764:THR:O	1:C:769:PHE:HB2	2.02	0.59
1:D:414:ASP:HB3	1:D:419:ALA:HB1	1.84	0.59
1:D:651:TRP:CZ3	1:D:684:TRP:HB2	2.37	0.59
1:D:651:TRP:HE1	1:D:683:ALA:HA	1.68	0.59
1:A:682:ARG:HE	1:A:716:LEU:HD13	1.67	0.59
1:B:449:ASP:HB3	1:B:452:LEU:HB2	1.84	0.59
1:B:621:LEU:HD12	1:B:729:TYR:HD2	1.68	0.59
1:D:274:PRO:HA	1:D:277:VAL:HG22	1.83	0.59
1:B:689:LEU:HB3	1:B:709:ALA:HB2	1.83	0.59
1:A:344:GLU:OE2	1:A:352:SER:HB2	2.03	0.59
1:A:544:GLU:HB2	1:A:545:ARG:HH22	1.67	0.59
1:B:299:LEU:HD12	1:B:303:VAL:HG21	1.83	0.59
1:B:474:LEU:HG	1:B:529:MET:SD	2.42	0.59
1:C:167:TYR:OH	1:C:216:VAL:HG13	2.02	0.59
1:D:643:GLN:O	1:D:645:PRO:HD3	2.02	0.59
1:D:343:GLU:OE2	1:D:420:ARG:CZ	2.51	0.58
1:C:234:MET:HG2	1:C:249:ILE:HD11	1.85	0.58
1:A:433:PHE:CG	1:A:476:THR:HG22	2.38	0.58
1:B:642:PRO:O	1:B:656:TYR:OH	2.19	0.58
1:C:551:PRO:HB2	1:C:552:PRO:HD3	1.85	0.58
1:C:631:ASP:C	1:C:633:ALA:H	2.07	0.58
1:D:26:TYR:HD2	1:D:93:THR:HG22	1.67	0.58
1:D:496:GLN:HG2	1:D:553:VAL:HG22	1.85	0.58
1:D:537:MET:HB2	1:D:538:PRO:HD3	1.86	0.58
1:A:569:ILE:HD12	1:A:578:ARG:NH2	2.18	0.58
1:B:182:PRO:HD3	1:B:221:TYR:CE1	2.37	0.58
1:C:418:VAL:HA	1:C:421:ARG:HD2	1.84	0.58
1:D:132:CYS:SG	1:D:289:LEU:HD23	2.43	0.58
1:D:544:GLU:HB2	1:D:545:ARG:NH2	2.19	0.58
1:D:686:LEU:HD21	1:D:712:GLN:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:THR:HG22	1:C:228:ARG:HE	1.68	0.58
1:D:163:ILE:HD12	1:D:170:TRP:CD2	2.39	0.58
1:C:699:VAL:HG12	1:C:703:GLU:HG3	1.84	0.58
1:D:80:GLU:OE1	1:A:342:LYS:HG3	2.04	0.58
1:B:353:GLU:O	1:B:356:LEU:HB2	2.03	0.58
1:C:238:ALA:HB2	1:C:249:ILE:HD13	1.85	0.58
1:D:615:ARG:HG2	1:D:616:GLY:H	1.69	0.58
1:D:163:ILE:HD12	1:D:170:TRP:CE2	2.39	0.57
1:B:86:GLN:NE2	1:B:172:ARG:H	2.01	0.57
1:B:551:PRO:HB2	1:B:552:PRO:HD3	1.85	0.57
1:C:151:MET:HG3	1:C:159:TYR:CZ	2.39	0.57
1:C:552:PRO:HG2	1:C:555:ALA:H	1.69	0.57
1:B:418:VAL:H	1:B:421:ARG:HD2	1.68	0.57
1:A:86:GLN:HE22	1:A:172:ARG:H	1.51	0.57
1:A:151:MET:HB3	1:A:172:ARG:NH1	2.20	0.57
1:B:710:GLU:OE2	1:B:715:ARG:NE	2.37	0.57
1:A:445:PRO:HG3	1:A:497:PHE:CD1	2.39	0.57
1:A:551:PRO:HB2	1:A:552:PRO:CD	2.35	0.57
1:A:643:GLN:O	1:A:645:PRO:HD3	2.05	0.57
1:B:710:GLU:HG2	1:B:715:ARG:HG3	1.85	0.57
1:C:168:ASP:HA	1:C:178:ARG:O	2.04	0.57
1:C:228:ARG:HA	1:C:231:MET:HE2	1.86	0.57
1:A:372:SER:OG	1:A:373:ALA:N	2.34	0.57
1:A:511:TRP:HZ3	1:A:519:ALA:HB3	1.68	0.57
1:C:342:LYS:O	1:C:343:GLU:HG2	2.05	0.57
1:C:642:PRO:HD3	1:C:651:TRP:CZ2	2.39	0.57
1:D:7:PHE:C	1:D:7:PHE:CD2	2.78	0.57
1:D:449:ASP:HB3	1:D:452:LEU:HB2	1.87	0.57
1:D:679:ALA:HA	1:D:716:LEU:O	2.05	0.57
1:D:729:TYR:CE2	1:D:731:PRO:HG3	2.40	0.57
1:A:438:TRP:CE3	1:A:464:ARG:HG3	2.39	0.57
1:A:533:VAL:O	1:A:538:PRO:HD2	2.05	0.57
1:D:186:TYR:OH	1:D:228:ARG:HD2	2.04	0.57
1:D:549:GLU:HB2	1:D:550:VAL:HG23	1.86	0.57
1:D:666:GLY:H	1:D:752:SER:HB3	1.70	0.57
1:D:710:GLU:HG2	1:D:715:ARG:HG3	1.87	0.57
1:A:155:GLU:HG3	1:A:174:LYS:HE2	1.87	0.57
1:C:477:ARG:CZ	1:C:542:ARG:HB3	2.35	0.57
1:C:612:LEU:HD13	1:C:754:ARG:HD2	1.87	0.57
1:A:5:GLU:O	1:A:7:PHE:N	2.32	0.57
1:A:507:PHE:CZ	1:A:511:TRP:HD1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLY:O	1:A:587:HIS:NE2	2.38	0.57
1:B:477:ARG:HD3	1:B:541:ALA:HA	1.87	0.57
1:A:449:ASP:O	1:A:451:THR:N	2.38	0.56
1:B:108:THR:HB	1:B:143:LEU:HD22	1.86	0.56
1:B:312:ARG:NH1	1:B:314:ASP:OD1	2.37	0.56
1:B:418:VAL:CA	1:B:421:ARG:HD2	2.36	0.56
1:C:36:TRP:HE3	1:C:41:ILE:HD13	1.69	0.56
1:C:665:ILE:H	1:C:665:ILE:CD1	2.13	0.56
1:B:349:TRP:O	1:B:349:TRP:CD1	2.58	0.56
1:D:183:ILE:HD12	1:D:183:ILE:N	2.09	0.56
1:D:423:VAL:HA	1:D:542:ARG:HH22	1.70	0.56
1:A:58:PHE:CE2	1:A:405:ARG:HD3	2.40	0.56
1:A:563:GLN:O	1:A:566:SER:OG	2.22	0.56
1:B:455:GLN:HG2	1:B:624:LEU:O	2.05	0.56
1:C:127:GLU:OE2	1:C:127:GLU:C	2.44	0.56
1:C:128:PRO:HD3	1:C:275:SER:HB2	1.88	0.56
1:C:631:ASP:O	1:C:633:ALA:N	2.38	0.56
1:A:445:PRO:HD3	1:A:497:PHE:CE1	2.41	0.56
1:A:507:PHE:CZ	1:A:511:TRP:CD1	2.93	0.56
1:B:26:TYR:CD2	1:B:93:THR:HG22	2.36	0.56
1:B:143:LEU:O	1:B:146:CYS:HB3	2.05	0.56
1:B:457:GLY:HA3	1:B:626:LEU:HD22	1.87	0.56
1:B:715:ARG:HG2	1:B:720:ALA:HB2	1.87	0.56
1:C:270:SER:OG	1:C:271:GLU:N	2.38	0.56
1:C:415:PRO:O	1:C:420:ARG:NH1	2.38	0.56
1:D:36:TRP:HE3	1:D:41:ILE:HD13	1.70	0.56
1:D:355:LYS:HD2	1:D:359:ASP:OD2	2.05	0.56
1:A:238:ALA:HB2	1:A:249:ILE:CD1	2.35	0.56
1:B:173:ASN:ND2	1:B:176:GLU:OE2	2.35	0.56
1:B:180:ARG:HH12	1:B:212:LYS:HE2	1.70	0.56
1:C:542:ARG:O	1:C:542:ARG:HG3	2.05	0.56
1:A:217:ASP:C	1:A:219:GLU:H	2.09	0.56
1:A:239:VAL:HA	1:A:291:ARG:NH1	2.20	0.56
1:B:183:ILE:HG13	1:B:224:LEU:CD1	2.35	0.56
1:B:496:GLN:HA	1:B:553:VAL:HG13	1.88	0.56
1:B:692:ARG:NH2	1:B:740:GLU:OE1	2.39	0.56
1:D:168:ASP:HA	1:D:178:ARG:O	2.04	0.56
1:D:763:LEU:O	1:D:766:TRP:HB2	2.06	0.56
1:A:88:PRO:HG2	1:A:91:VAL:HG12	1.88	0.56
1:B:651:TRP:CH2	1:B:684:TRP:HB2	2.41	0.56
1:B:669:THR:CG2	1:B:751:ARG:HH22	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:ILE:HG12	1:C:349:TRP:CZ2	2.40	0.56
1:C:375:LYS:HA	1:C:378:THR:HG22	1.87	0.56
1:C:684:TRP:HE1	1:C:742:GLU:HA	1.71	0.56
1:D:48:VAL:HG22	1:D:295:PHE:CE1	2.41	0.56
1:D:73:ASP:OD2	1:D:78:THR:OG1	2.10	0.56
1:D:562:GLU:HG2	1:D:565:ARG:NH1	2.21	0.56
1:A:543:PHE:C	1:A:543:PHE:HD2	2.10	0.56
1:B:26:TYR:CE2	1:B:79:VAL:HA	2.41	0.56
1:C:339:ARG:HG2	1:C:408:ARG:CZ	2.35	0.56
1:A:375:LYS:HA	1:A:378:THR:HG22	1.88	0.56
1:A:565:ARG:HH21	1:A:771:PRO:HB3	1.71	0.56
1:D:312:ARG:HD3	1:D:315:TYR:CE2	2.41	0.56
1:A:561:LYS:HE3	1:A:769:PHE:HA	1.87	0.56
1:A:709:ALA:HB3	1:A:714:LEU:HD22	1.87	0.56
1:C:496:GLN:NE2	1:C:553:VAL:HG22	2.20	0.56
1:C:561:LYS:NZ	1:C:768:GLY:O	2.33	0.56
1:D:282:ASP:O	1:D:284:ALA:N	2.38	0.55
1:D:343:GLU:OE2	1:D:420:ARG:NH1	2.39	0.55
1:A:496:GLN:HG2	1:A:553:VAL:HG22	1.88	0.55
1:B:149:GLU:HG2	1:B:150:ASP:N	2.21	0.55
1:B:208:ILE:HG23	1:B:209:ASP:N	2.21	0.55
1:B:239:VAL:HA	1:B:291:ARG:HH12	1.71	0.55
1:B:155:GLU:H	1:B:174:LYS:HE2	1.70	0.55
1:B:110:VAL:CG2	1:B:235:LEU:HD12	2.36	0.55
1:C:26:TYR:CZ	1:C:79:VAL:HA	2.41	0.55
1:A:433:PHE:CE2	1:A:438:TRP:CD1	2.94	0.55
1:B:11:PRO:O	1:B:12:LEU:HD23	2.06	0.55
1:B:496:GLN:HG2	1:B:553:VAL:HG13	1.87	0.55
1:C:87:VAL:HG13	1:C:88:PRO:O	2.06	0.55
1:C:433:PHE:CE2	1:C:438:TRP:CD1	2.94	0.55
1:A:561:LYS:HD2	1:A:767:LEU:HB3	1.89	0.55
1:B:163:ILE:O	1:B:168:ASP:OD2	2.25	0.55
1:C:186:TYR:CE2	1:C:205:HIS:CD2	2.93	0.55
1:D:180:ARG:NH1	1:D:213:THR:HG22	2.22	0.55
1:B:127:GLU:HB3	1:B:128:PRO:HD2	1.89	0.55
1:B:551:PRO:HB2	1:B:552:PRO:CD	2.37	0.55
1:C:602:ASN:OD1	1:C:622:GLU:HG3	2.06	0.55
1:D:388:ALA:HA	1:D:406:TYR:OH	2.07	0.55
1:D:682:ARG:HE	1:D:716:LEU:HD13	1.72	0.55
1:A:180:ARG:NH1	1:A:213:THR:HG22	2.22	0.55
1:A:681:ASN:OD1	1:A:682:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLU:OE2	1:B:420:ARG:CZ	2.55	0.55
1:B:488:GLU:HG2	1:B:489:THR:N	2.22	0.55
1:D:454:THR:HG21	1:D:627:GLU:OE2	2.07	0.55
1:D:511:TRP:CH2	1:D:519:ALA:HB3	2.42	0.55
1:A:260:SER:O	1:A:264:GLN:HG3	2.07	0.55
1:B:78:THR:OG1	1:B:93:THR:HG21	2.06	0.55
1:C:143:LEU:O	1:C:146:CYS:HB3	2.07	0.55
1:C:709:ALA:HB1	1:C:714:LEU:HB2	1.89	0.55
1:A:151:MET:O	1:A:157:ARG:HD3	2.07	0.55
1:A:441:PRO:O	1:A:444:VAL:HG22	2.06	0.55
1:B:486:SER:HB3	1:B:488:GLU:OE2	2.06	0.55
1:C:144:SER:C	1:C:146:CYS:H	2.10	0.55
1:C:496:GLN:HG2	1:C:553:VAL:HG13	1.89	0.55
1:C:684:TRP:HD1	1:C:742:GLU:OE2	1.90	0.55
1:D:565:ARG:HG2	1:D:570:TYR:HE2	1.71	0.55
1:A:119:ALA:O	1:A:122:LEU:HB2	2.07	0.55
1:B:572:LYS:HE2	1:B:760:TRP:CZ3	2.41	0.55
1:B:593:ARG:HH21	1:B:635:ALA:HB1	1.72	0.55
1:C:182:PRO:HG2	1:C:183:ILE:HD12	1.88	0.55
1:B:538:PRO:HB3	1:B:550:VAL:HG22	1.89	0.54
1:D:715:ARG:HG2	1:D:720:ALA:HB2	1.89	0.54
1:A:589:LYS:HA	1:A:592:THR:HG23	1.88	0.54
1:B:642:PRO:HD3	1:B:651:TRP:CZ2	2.41	0.54
1:C:665:ILE:HG12	1:C:752:SER:HB2	1.88	0.54
1:D:208:ILE:HD12	1:D:209:ASP:H	1.72	0.54
1:D:333:ILE:HD12	1:D:380:THR:HG23	1.89	0.54
1:D:561:LYS:HE2	1:D:771:PRO:HD2	1.90	0.54
1:D:674:VAL:HG13	1:D:678:SER:H	1.72	0.54
1:A:114:GLU:OE2	1:A:236:ARG:NE	2.30	0.54
1:A:496:GLN:CA	1:A:553:VAL:HG13	2.34	0.54
1:C:537:MET:HB2	1:C:538:PRO:HD3	1.89	0.54
1:B:7:PHE:HD1	1:B:319:MET:SD	2.31	0.54
1:C:458:ILE:CD1	1:C:629:TRP:HB2	2.37	0.54
1:D:164:ARG:NH1	1:D:183:ILE:HD11	2.22	0.54
1:D:516:GLY:O	1:D:587:HIS:NE2	2.41	0.54
1:A:127:GLU:HB3	1:A:128:PRO:CD	2.37	0.54
1:A:164:ARG:NH1	1:A:183:ILE:HD11	2.22	0.54
1:D:486:SER:O	1:D:488:GLU:N	2.40	0.54
1:D:507:PHE:CD1	1:D:560:LEU:HD22	2.42	0.54
1:A:666:GLY:HA2	1:A:751:ARG:HD3	1.89	0.54
1:A:680:SER:HA	1:A:690:MET:HE1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:NH1	1:A:435:GLU:OE2	2.41	0.54
1:A:455:GLN:HG2	1:A:624:LEU:O	2.08	0.54
1:A:710:GLU:HG2	1:A:715:ARG:HG3	1.88	0.54
1:B:127:GLU:HB3	1:B:128:PRO:CD	2.38	0.54
1:B:565:ARG:NH2	1:B:771:PRO:HB3	2.18	0.54
1:C:86:GLN:HE22	1:C:172:ARG:H	1.54	0.54
1:D:196:ASP:OD1	1:D:197:PRO:HD2	2.08	0.54
1:D:208:ILE:HG23	1:D:209:ASP:HB3	1.90	0.54
1:D:433:PHE:CB	1:D:476:THR:HG22	2.38	0.54
1:C:551:PRO:HB2	1:C:552:PRO:CD	2.38	0.54
1:A:488:GLU:HG2	1:A:489:THR:N	2.22	0.54
1:C:488:GLU:HG2	1:C:489:THR:HG22	1.89	0.54
1:D:180:ARG:HH11	1:D:213:THR:HG22	1.72	0.53
1:B:122:LEU:HD22	1:B:129:SER:OG	2.07	0.53
1:C:312:ARG:HB3	1:C:312:ARG:HH11	1.72	0.53
1:A:181:SER:HB2	1:A:182:PRO:HD2	1.90	0.53
1:B:312:ARG:HB2	1:B:315:TYR:CD2	2.43	0.53
1:C:5:GLU:C	1:C:7:PHE:H	2.12	0.53
1:C:437:PRO:HB2	1:C:460:LEU:CD1	2.37	0.53
1:A:253:THR:N	1:A:256:ASP:OD2	2.19	0.53
1:B:239:VAL:HA	1:B:291:ARG:NH1	2.24	0.53
1:B:387:PHE:CD2	1:B:427:LEU:HG	2.42	0.53
1:B:496:GLN:HG2	1:B:553:VAL:HG22	1.90	0.53
1:B:576:VAL:HG13	1:B:756:CYS:HB2	1.90	0.53
1:D:339:ARG:HG2	1:D:408:ARG:NH1	2.24	0.53
1:C:570:TYR:N	1:C:570:TYR:CD2	2.76	0.53
1:C:667:ASN:ND2	1:C:743:TRP:HE1	2.06	0.53
1:C:710:GLU:HG2	1:C:715:ARG:HG3	1.90	0.53
1:D:544:GLU:HB2	1:D:545:ARG:HH22	1.73	0.53
1:A:27:ILE:HB	1:A:164:ARG:HA	1.89	0.53
1:A:484:LEU:HD23	1:A:548:THR:HG22	1.91	0.53
1:A:688:ARG:HB3	1:A:692:ARG:CZ	2.39	0.53
1:B:414:ASP:HB3	1:B:419:ALA:CB	2.39	0.53
1:C:683:ALA:O	1:C:685:HIS:N	2.42	0.53
1:D:239:VAL:HA	1:D:291:ARG:NH1	2.24	0.53
1:D:262:ASN:H	1:D:262:ASN:ND2	2.06	0.53
1:A:4:LYS:O	1:A:5:GLU:HG3	2.07	0.53
1:A:605:PRO:HG3	1:A:734:ALA:HB3	1.90	0.53
1:A:734:ALA:O	1:A:736:LEU:N	2.36	0.53
1:D:74:ILE:HG23	1:D:75:ASN:OD1	2.09	0.53
1:B:161:ARG:HA	1:B:170:TRP:HH2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:O	1:C:146:CYS:CB	2.57	0.53
1:C:509:ALA:HB2	1:C:594:LEU:HD12	1.90	0.53
1:C:554:GLU:HA	1:C:557:GLN:HG3	1.90	0.53
1:B:119:ALA:O	1:B:122:LEU:HB2	2.09	0.53
1:C:148:GLU:OE1	1:C:195:ARG:NH1	2.36	0.53
1:C:510:LEU:HD12	1:C:564:LEU:HD11	1.89	0.53
1:C:550:VAL:HG13	1:C:551:PRO:HA	1.90	0.53
1:C:692:ARG:HG3	1:C:737:ALA:CB	2.36	0.53
1:D:232:ARG:HD3	1:D:236:ARG:CZ	2.39	0.53
1:A:764:THR:N	1:A:765:PRO:HD2	2.24	0.53
1:B:477:ARG:NE	1:B:542:ARG:HB3	2.24	0.53
1:B:557:GLN:O	1:B:561:LYS:HD3	2.09	0.53
1:B:561:LYS:HD2	1:B:767:LEU:HB3	1.90	0.53
1:C:437:PRO:HD3	1:C:479:PHE:HE2	1.73	0.53
1:A:282:ASP:O	1:A:284:ALA:N	2.42	0.53
1:D:123:THR:O	1:D:129:SER:OG	2.12	0.52
1:D:143:LEU:O	1:D:146:CYS:CB	2.57	0.52
1:D:662:ILE:HD12	1:D:662:ILE:H	1.73	0.52
1:A:543:PHE:C	1:A:543:PHE:CD2	2.83	0.52
1:B:81:PRO:HG2	1:B:169:VAL:HG22	1.91	0.52
1:B:415:PRO:O	1:B:420:ARG:NH1	2.42	0.52
1:B:418:VAL:N	1:B:421:ARG:HD2	2.25	0.52
1:D:385:LEU:CD2	1:D:396:LEU:HB3	2.39	0.52
1:D:630:ASN:O	1:D:632:GLU:N	2.43	0.52
1:A:445:PRO:HG3	1:A:497:PHE:HD1	1.74	0.52
1:B:444:VAL:HG12	1:B:445:PRO:HD3	1.90	0.52
1:B:557:GLN:HB3	1:B:767:LEU:O	2.10	0.52
1:B:706:LEU:HD12	1:B:714:LEU:HD23	1.91	0.52
1:C:682:ARG:HB2	1:C:686:LEU:HB2	1.92	0.52
1:C:701:GLU:HA	1:C:704:LYS:HB2	1.91	0.52
1:A:542:ARG:HD3	1:A:547:LEU:N	2.21	0.52
1:C:343:GLU:OE2	1:C:420:ARG:NH1	2.42	0.52
1:C:401:ASN:H	1:C:401:ASN:ND2	2.06	0.52
1:A:622:GLU:O	1:A:628:ARG:NH1	2.42	0.52
1:B:123:THR:O	1:B:129:SER:OG	2.18	0.52
1:B:671:LEU:HD11	1:B:691:PHE:HE1	1.74	0.52
1:D:418:VAL:HG23	1:D:421:ARG:HH11	1.75	0.52
1:A:113:GLU:OE2	1:A:232:ARG:NH2	2.43	0.52
1:A:562:GLU:HG2	1:A:565:ARG:NH1	2.25	0.52
1:D:268:PHE:O	1:D:270:SER:N	2.42	0.52
1:A:255:THR:O	1:A:259:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:NH1	1:A:314:ASP:OD2	2.42	0.52
1:A:654:ASP:HB2	1:A:745:ALA:HB2	1.91	0.52
1:B:34:TYR:CD2	1:B:224:LEU:HD12	2.44	0.52
1:B:507:PHE:HB2	1:B:560:LEU:HD13	1.92	0.52
1:B:605:PRO:HB3	1:B:735:ALA:HB2	1.92	0.52
1:C:760:TRP:O	1:C:764:THR:OG1	2.27	0.52
1:D:190:TYR:CD1	1:D:190:TYR:C	2.83	0.52
1:D:537:MET:CB	1:D:538:PRO:HD3	2.40	0.52
1:D:705:THR:HA	1:D:708:ASP:HB2	1.92	0.52
1:A:433:PHE:O	1:A:437:PRO:HD2	2.09	0.52
1:A:525:TYR:O	1:A:529:MET:HG2	2.10	0.52
1:B:418:VAL:HA	1:B:421:ARG:CD	2.40	0.52
1:C:326:THR:O	1:C:326:THR:HG23	2.09	0.52
1:B:337:LYS:HE2	1:B:358:PHE:CE1	2.45	0.52
1:C:86:GLN:NE2	1:C:172:ARG:HD3	2.25	0.52
1:C:208:ILE:HG12	1:C:221:TYR:CE2	2.45	0.52
1:D:710:GLU:HA	1:D:714:LEU:H	1.76	0.51
1:A:228:ARG:HD3	1:A:228:ARG:C	2.29	0.51
1:A:396:LEU:HD12	1:A:397:THR:H	1.74	0.51
1:B:584:VAL:HG13	1:B:591:LEU:HD13	1.90	0.51
1:A:537:MET:CB	1:A:538:PRO:HD3	2.41	0.51
1:A:545:ARG:NH2	1:A:545:ARG:H	2.08	0.51
1:B:516:GLY:C	1:B:587:HIS:HE2	2.13	0.51
1:B:681:ASN:OD1	1:B:682:ARG:N	2.44	0.51
1:C:167:TYR:CE1	1:C:216:VAL:HG22	2.45	0.51
1:D:686:LEU:HD21	1:D:712:GLN:CB	2.40	0.51
1:B:455:GLN:NE2	1:B:766:TRP:HZ2	2.08	0.51
1:B:539:ARG:O	1:B:550:VAL:HG11	2.10	0.51
1:C:472:VAL:O	1:C:476:THR:HG23	2.09	0.51
1:D:339:ARG:HG2	1:D:408:ARG:CZ	2.40	0.51
1:D:472:VAL:O	1:D:476:THR:HG23	2.09	0.51
1:A:265:PHE:CZ	1:A:271:GLU:HG3	2.46	0.51
1:B:17:PHE:HE2	1:B:101:MET:SD	2.33	0.51
1:B:183:ILE:HG13	1:B:224:LEU:HD11	1.92	0.51
1:C:106:LEU:HD21	1:C:224:LEU:HG	1.92	0.51
1:C:429:GLN:HG2	1:C:480:ALA:HB2	1.92	0.51
1:C:511:TRP:CE3	1:C:521:ILE:HG12	2.45	0.51
1:C:545:ARG:H	1:C:545:ARG:HH21	1.59	0.51
1:B:104:LEU:HD21	1:B:299:LEU:HD11	1.91	0.51
1:C:538:PRO:HB2	1:C:550:VAL:CG1	2.41	0.51
1:C:722:GLU:O	1:C:726:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:GLU:O	1:D:356:LEU:HB2	2.10	0.51
1:D:445:PRO:HG3	1:D:497:PHE:CD1	2.45	0.51
1:D:511:TRP:HZ3	1:D:517:SER:O	1.92	0.51
1:B:23:GLN:O	1:B:161:ARG:NH1	2.43	0.51
1:B:208:ILE:CD1	1:B:209:ASP:H	2.21	0.51
1:C:73:ASP:HB3	1:C:91:VAL:CG2	2.41	0.51
1:C:120:GLU:HG2	1:C:200:VAL:HG11	1.92	0.51
1:C:600:SER:HB3	1:C:732:LEU:HD21	1.92	0.51
1:D:207:PRO:O	1:D:208:ILE:HG22	2.10	0.51
1:D:626:LEU:HD12	1:D:626:LEU:O	2.11	0.51
1:C:83:TYR:CD1	1:C:169:VAL:HG11	2.46	0.51
1:A:112:HIS:HE2	1:A:140:THR:HG23	1.76	0.51
1:A:720:ALA:HB1	1:A:723:ILE:HB	1.93	0.51
1:C:106:LEU:O	1:C:110:VAL:HG12	2.11	0.51
1:D:415:PRO:O	1:D:420:ARG:NH1	2.44	0.51
1:A:71:LEU:HB3	1:A:93:THR:OG1	2.11	0.51
1:A:312:ARG:HD3	1:A:315:TYR:CE2	2.45	0.51
1:A:413:LYS:O	1:A:415:PRO:HD3	2.11	0.51
1:C:32:ARG:O	1:C:164:ARG:NH2	2.44	0.51
1:C:144:SER:C	1:C:146:CYS:N	2.63	0.51
1:C:418:VAL:HA	1:C:421:ARG:CD	2.40	0.51
1:C:477:ARG:HD3	1:C:542:ARG:N	2.22	0.51
1:A:123:THR:O	1:A:123:THR:OG1	2.24	0.51
1:B:109:THR:HG23	1:B:228:ARG:HH11	1.76	0.51
1:B:584:VAL:HG12	1:B:592:THR:HG22	1.91	0.51
1:C:417:ILE:HD12	1:C:420:ARG:HB2	1.93	0.51
1:C:452:LEU:HD11	1:C:499:LEU:HD23	1.93	0.51
1:C:636:THR:CG2	1:C:675:GLU:HG2	2.41	0.51
1:C:641:ALA:HA	1:C:651:TRP:CH2	2.47	0.50
1:D:62:ILE:HG22	1:A:315:TYR:CE1	2.45	0.50
1:D:73:ASP:HB3	1:D:91:VAL:HG22	1.94	0.50
1:D:199:ALA:O	1:D:200:VAL:HB	2.11	0.50
1:D:641:ALA:N	1:D:667:ASN:OD1	2.44	0.50
1:A:456:ALA:HB3	1:A:498:LEU:HD22	1.93	0.50
1:B:180:ARG:HH22	1:B:212:LYS:NZ	2.09	0.50
1:B:674:VAL:HG11	1:B:679:ALA:N	2.27	0.50
1:C:621:LEU:HD12	1:C:729:TYR:CD2	2.43	0.50
1:D:148:GLU:OE1	1:D:195:ARG:NH1	2.42	0.50
1:D:312:ARG:NH1	1:D:314:ASP:OD1	2.44	0.50
1:D:538:PRO:HB2	1:D:550:VAL:HG13	1.93	0.50
1:D:674:VAL:HG11	1:D:679:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LYS:O	1:D:5:GLU:HG3	2.11	0.50
1:C:385:LEU:CD2	1:C:396:LEU:HB3	2.42	0.50
1:D:630:ASN:O	1:D:632:GLU:HG3	2.12	0.50
1:A:26:TYR:CZ	1:A:79:VAL:HG12	2.45	0.50
1:B:64:PHE:HE1	1:B:306:ALA:HB2	1.75	0.50
1:B:299:LEU:HA	1:B:303:VAL:HG23	1.93	0.50
1:C:163:ILE:O	1:C:168:ASP:OD2	2.29	0.50
1:D:84:ARG:O	1:D:85:SER:C	2.49	0.50
1:D:477:ARG:NH1	1:D:542:ARG:H	2.09	0.50
1:A:484:LEU:HD21	1:A:547:LEU:HD23	1.94	0.50
1:A:542:ARG:NE	1:A:547:LEU:HD12	2.22	0.50
1:B:674:VAL:HG11	1:B:679:ALA:H	1.77	0.50
1:C:561:LYS:HD2	1:C:767:LEU:HB3	1.94	0.50
1:D:135:GLN:HG2	1:D:268:PHE:HE2	1.76	0.50
1:D:470:ILE:HG21	1:D:522:ASP:HA	1.93	0.50
1:A:341:ILE:HG12	1:A:349:TRP:CE2	2.47	0.50
1:C:112:HIS:O	1:C:116:ARG:HB2	2.12	0.50
1:D:326:THR:HG23	1:D:326:THR:O	2.12	0.50
1:D:471:VAL:HG12	1:D:475:LEU:HG	1.92	0.50
1:A:339:ARG:HG2	1:A:408:ARG:CZ	2.41	0.50
1:A:478:TYR:OH	1:A:551:PRO:HG2	2.12	0.50
1:A:683:ALA:O	1:A:685:HIS:N	2.44	0.50
1:B:355:LYS:HD2	1:B:359:ASP:CG	2.32	0.50
1:B:437:PRO:HG3	1:B:479:PHE:HE2	1.77	0.50
1:C:35:SER:O	1:C:223:HIS:NE2	2.44	0.50
1:C:433:PHE:CB	1:C:476:THR:HG22	2.41	0.50
1:C:631:ASP:C	1:C:633:ALA:N	2.65	0.50
1:D:172:ARG:HG3	1:D:172:ARG:NH1	2.27	0.50
1:B:341:ILE:HG12	1:B:349:TRP:CE2	2.46	0.50
1:C:539:ARG:O	1:C:550:VAL:HG11	2.11	0.50
1:D:744:THR:O	1:D:748:VAL:HG23	2.12	0.49
1:A:13:SER:H	1:A:16:GLN:NE2	2.10	0.49
1:A:153:TYR:CE2	1:A:172:ARG:HG3	2.47	0.49
1:A:208:ILE:CD1	1:A:209:ASP:H	2.25	0.49
1:A:542:ARG:HD2	1:A:544:GLU:O	2.12	0.49
1:A:549:GLU:HB2	1:A:550:VAL:HG23	1.93	0.49
1:A:552:PRO:HG2	1:A:555:ALA:H	1.76	0.49
1:B:217:ASP:O	1:B:218:LEU:HB2	2.12	0.49
1:B:581:MET:SD	1:B:664:ARG:NH1	2.84	0.49
1:C:488:GLU:HG2	1:C:489:THR:N	2.27	0.49
1:C:679:ALA:HA	1:C:716:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:GLU:OE2	1:C:725:ARG:NE	2.43	0.49
1:D:204:ARG:O	1:D:205:HIS:CB	2.61	0.49
1:D:344:GLU:OE1	1:D:421:ARG:NH2	2.45	0.49
1:D:477:ARG:HD3	1:D:542:ARG:H	1.76	0.49
1:D:493:SER:OG	1:D:494:ALA:N	2.44	0.49
1:A:337:LYS:NZ	1:A:358:PHE:CD1	2.72	0.49
1:B:163:ILE:HD12	1:B:170:TRP:CD2	2.47	0.49
1:C:433:PHE:C	1:C:433:PHE:CD2	2.86	0.49
1:C:477:ARG:CZ	1:C:542:ARG:CB	2.90	0.49
1:D:204:ARG:O	1:D:205:HIS:HB2	2.12	0.49
1:A:29:PRO:HG3	1:A:80:GLU:HG3	1.94	0.49
1:A:674:VAL:HG13	1:A:678:SER:HB3	1.94	0.49
1:C:52:LEU:HB2	1:C:298:TYR:CG	2.48	0.49
1:C:165:SER:O	1:C:166:TYR:HB2	2.12	0.49
1:C:196:ASP:OD1	1:C:197:PRO:HD2	2.13	0.49
1:C:650:SER:OG	1:C:651:TRP:N	2.45	0.49
1:D:164:ARG:HH12	1:D:183:ILE:HD11	1.76	0.49
1:C:709:ALA:CB	1:C:714:LEU:HB2	2.42	0.49
1:D:62:ILE:HG22	1:A:315:TYR:HE1	1.77	0.49
1:D:602:ASN:HB2	1:D:620:LEU:HB3	1.94	0.49
1:A:180:ARG:HH12	1:A:212:LYS:HE2	1.78	0.49
1:A:615:ARG:NH1	1:A:758:LEU:HG	2.28	0.49
1:B:342:LYS:HG3	1:C:80:GLU:OE1	2.12	0.49
1:B:414:ASP:HB3	1:B:419:ALA:HB1	1.94	0.49
1:B:474:LEU:HG	1:B:529:MET:HE1	1.93	0.49
1:B:713:GLY:O	1:B:716:LEU:HG	2.12	0.49
1:C:119:ALA:O	1:C:122:LEU:HB2	2.13	0.49
1:A:36:TRP:HE3	1:A:41:ILE:HD13	1.77	0.49
1:A:610:PRO:O	1:A:739:ARG:HB2	2.12	0.49
1:A:729:TYR:CE2	1:A:731:PRO:HG3	2.48	0.49
1:B:542:ARG:HG3	1:B:542:ARG:O	2.11	0.49
1:C:86:GLN:NE2	1:C:172:ARG:H	2.10	0.49
1:C:706:LEU:O	1:C:710:GLU:HG3	2.12	0.49
1:D:213:THR:O	1:D:213:THR:OG1	2.31	0.49
1:D:669:THR:HG23	1:D:751:ARG:HH22	1.78	0.49
1:B:341:ILE:HG12	1:B:349:TRP:CZ2	2.48	0.49
1:C:433:PHE:HE2	1:C:438:TRP:CD1	2.31	0.49
1:D:337:LYS:HE3	1:D:337:LYS:HB2	1.47	0.49
1:B:400:LEU:HD13	1:B:400:LEU:HA	1.55	0.49
1:B:400:LEU:HB3	1:B:404:ARG:NH2	2.27	0.49
1:B:512:ARG:HB3	1:B:591:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:PHE:C	1:C:543:PHE:HD2	2.15	0.49
1:D:500:ALA:O	1:D:503:SER:OG	2.26	0.49
1:D:551:PRO:HB2	1:D:552:PRO:CD	2.42	0.49
1:B:109:THR:HG22	1:B:228:ARG:HE	1.77	0.49
1:C:557:GLN:O	1:C:561:LYS:HD3	2.13	0.49
1:C:605:PRO:HB3	1:C:735:ALA:HB2	1.94	0.49
1:D:217:ASP:O	1:D:218:LEU:HB2	2.12	0.49
1:D:764:THR:N	1:D:765:PRO:HD2	2.27	0.49
1:A:667:ASN:O	1:A:667:ASN:ND2	2.45	0.49
1:A:699:VAL:HG12	1:A:703:GLU:HG3	1.95	0.49
1:C:25:LEU:O	1:C:162:LEU:HA	2.12	0.49
1:C:211:ASP:OD1	1:C:211:ASP:O	2.30	0.49
1:C:593:ARG:HH21	1:C:635:ALA:HB1	1.77	0.49
1:C:688:ARG:HB3	1:C:692:ARG:NH1	2.27	0.49
1:C:728:ARG:HD3	1:C:729:TYR:H	1.78	0.49
1:D:253:THR:HA	1:D:291:ARG:NE	2.28	0.48
1:D:418:VAL:N	1:D:421:ARG:HD2	2.27	0.48
1:A:120:GLU:C	1:A:122:LEU:H	2.16	0.48
1:A:153:TYR:CE1	1:B:134:ASN:HB3	2.47	0.48
1:B:35:SER:N	1:B:99:GLN:OE1	2.32	0.48
1:B:120:GLU:C	1:B:122:LEU:H	2.16	0.48
1:B:149:GLU:HB2	1:B:161:ARG:NH2	2.28	0.48
1:B:553:VAL:HB	1:B:554:GLU:HG3	1.94	0.48
1:C:38:LEU:HG	1:C:38:LEU:O	2.13	0.48
1:C:720:ALA:HB1	1:C:723:ILE:HB	1.95	0.48
1:D:126:ASP:OD1	1:D:126:ASP:O	2.31	0.48
1:D:385:LEU:HB2	1:D:386:PRO:HD3	1.95	0.48
1:B:572:LYS:HB3	1:B:760:TRP:CZ3	2.48	0.48
1:C:106:LEU:HB3	1:C:231:MET:HE1	1.95	0.48
1:D:1:MET:HA	1:D:4:LYS:HB2	1.94	0.48
1:D:65:LEU:HD23	1:D:65:LEU:HA	1.62	0.48
1:D:212:LYS:HB3	1:D:213:THR:H	1.42	0.48
1:A:655:LEU:HD23	1:A:745:ALA:HA	1.95	0.48
1:B:203:TYR:CE2	1:B:205:HIS:HB2	2.48	0.48
1:B:417:ILE:HG13	1:B:421:ARG:CZ	2.43	0.48
1:C:116:ARG:HH22	1:C:199:ALA:HB3	1.77	0.48
1:C:209:ASP:O	1:C:209:ASP:CG	2.51	0.48
1:C:337:LYS:HB2	1:C:337:LYS:HZ2	1.78	0.48
1:C:576:VAL:HG11	1:C:757:SER:OG	2.13	0.48
1:D:701:GLU:O	1:D:705:THR:OG1	2.28	0.48
1:A:357:HIS:O	1:A:360:VAL:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ALA:O	1:A:508:TYR:HB3	2.13	0.48
1:A:623:THR:O	1:A:625:GLU:N	2.44	0.48
1:B:186:TYR:OH	1:B:228:ARG:HD2	2.13	0.48
1:C:636:THR:HG23	1:C:675:GLU:HG2	1.95	0.48
1:D:142:ARG:NH2	1:D:297:ASN:OD1	2.47	0.48
1:D:538:PRO:HB3	1:D:550:VAL:HG22	1.95	0.48
1:A:109:THR:CG2	1:A:228:ARG:HE	2.26	0.48
1:A:266:ALA:HB1	1:A:302:ARG:NH1	2.28	0.48
1:B:454:THR:O	1:B:626:LEU:N	2.45	0.48
1:B:689:LEU:HD13	1:B:709:ALA:HA	1.94	0.48
1:D:372:SER:OG	1:D:375:LYS:HB3	2.14	0.48
1:A:390:PHE:CD1	1:A:390:PHE:C	2.86	0.48
1:B:400:LEU:O	1:B:403:GLN:N	2.46	0.48
1:B:621:LEU:HD12	1:B:729:TYR:CD2	2.46	0.48
1:B:634:PHE:HD1	1:B:634:PHE:H	1.60	0.48
1:C:208:ILE:HG21	1:C:221:TYR:CD2	2.48	0.48
1:D:156:HIS:O	1:D:172:ARG:HA	2.14	0.48
1:C:454:THR:HG21	1:C:627:GLU:OE2	2.13	0.48
1:A:575:TRP:CZ3	1:A:760:TRP:HB2	2.49	0.48
1:B:7:PHE:CD2	1:B:8:ASP:N	2.82	0.48
1:C:104:LEU:O	1:C:108:THR:HG23	2.14	0.48
1:C:601:GLN:HA	1:C:623:THR:OG1	2.14	0.48
1:A:514:SER:O	1:A:582:THR:HG21	2.14	0.48
1:B:390:PHE:CD1	1:B:390:PHE:C	2.87	0.48
1:C:26:TYR:CE1	1:C:79:VAL:HG12	2.49	0.48
1:C:312:ARG:HH11	1:C:312:ARG:CB	2.26	0.48
1:C:361:VAL:HG21	1:C:427:LEU:HB3	1.96	0.48
1:D:35:SER:HB2	1:D:99:GLN:OE1	2.14	0.48
1:D:76:TYR:HB3	1:D:79:VAL:HG21	1.96	0.48
1:D:617:LYS:CG	1:D:620:LEU:HB2	2.43	0.48
1:B:163:ILE:HD12	1:B:170:TRP:CE2	2.49	0.48
1:B:228:ARG:HD3	1:B:228:ARG:C	2.34	0.48
1:B:344:GLU:CD	1:B:421:ARG:HH21	2.17	0.48
1:C:122:LEU:HD22	1:C:129:SER:HB2	1.96	0.48
1:C:543:PHE:C	1:C:543:PHE:CD2	2.87	0.48
1:D:496:GLN:HG2	1:D:553:VAL:HG13	1.95	0.47
1:B:7:PHE:O	1:B:8:ASP:HB2	2.14	0.47
1:B:339:ARG:HG2	1:B:408:ARG:CZ	2.43	0.47
1:B:379:VAL:O	1:B:383:VAL:HG12	2.14	0.47
1:D:29:PRO:HG3	1:D:80:GLU:HG3	1.96	0.47
1:D:140:THR:HG22	1:D:141:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:LYS:HG2	1:D:620:LEU:HB2	1.96	0.47
1:D:642:PRO:HD3	1:D:651:TRP:CZ2	2.49	0.47
1:B:447:CYS:HB2	1:B:494:ALA:HB1	1.96	0.47
1:B:518:THR:HG22	1:B:521:ILE:HD12	1.95	0.47
1:C:151:MET:SD	1:C:151:MET:N	2.84	0.47
1:C:171:SER:OG	1:C:176:GLU:HG2	2.14	0.47
1:C:448:ASP:O	1:C:450:ALA:N	2.47	0.47
1:C:496:GLN:CA	1:C:553:VAL:HG13	2.43	0.47
1:C:688:ARG:HD3	1:C:692:ARG:NH1	2.27	0.47
1:D:127:GLU:OE2	1:D:128:PRO:HD3	2.15	0.47
1:D:411:PHE:O	1:D:420:ARG:HG2	2.15	0.47
1:D:553:VAL:HB	1:D:554:GLU:HG3	1.96	0.47
1:B:212:LYS:HB3	1:B:213:THR:H	1.48	0.47
1:B:445:PRO:HG3	1:B:497:PHE:HD1	1.78	0.47
1:C:525:TYR:O	1:C:529:MET:HG2	2.14	0.47
1:A:457:GLY:C	1:A:626:LEU:HB2	2.34	0.47
1:A:709:ALA:HB1	1:A:714:LEU:HD13	1.96	0.47
1:B:35:SER:O	1:B:36:TRP:C	2.52	0.47
1:C:388:ALA:HA	1:C:406:TYR:OH	2.14	0.47
1:D:228:ARG:C	1:D:228:ARG:HD3	2.35	0.47
1:D:232:ARG:HD3	1:D:236:ARG:NH2	2.30	0.47
1:D:683:ALA:O	1:D:685:HIS:N	2.47	0.47
1:A:471:VAL:HG12	1:A:475:LEU:HG	1.97	0.47
1:A:474:LEU:HG	1:A:529:MET:HE2	1.96	0.47
1:A:514:SER:OG	1:A:515:PHE:N	2.47	0.47
1:A:538:PRO:HB3	1:A:550:VAL:HG22	1.97	0.47
1:B:127:GLU:OE2	1:B:275:SER:OG	2.23	0.47
1:B:154:GLY:O	1:B:157:ARG:HB2	2.15	0.47
1:C:203:TYR:CE2	1:C:205:HIS:HB2	2.49	0.47
1:C:565:ARG:O	1:C:568:GLY:N	2.47	0.47
1:D:482:HIS:HA	1:D:493:SER:OG	2.14	0.47
1:A:238:ALA:HB2	1:A:249:ILE:HD13	1.96	0.47
1:A:274:PRO:HA	1:A:277:VAL:HG22	1.95	0.47
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.66	0.47
1:A:417:ILE:HG23	1:A:418:VAL:HG23	1.96	0.47
1:A:447:CYS:HB2	1:A:494:ALA:HB1	1.95	0.47
1:B:126:ASP:CB	1:B:129:SER:HB3	2.35	0.47
1:B:367:ARG:NH1	1:B:435:GLU:OE2	2.47	0.47
1:B:468:HIS:NE2	1:B:521:ILE:HG21	2.29	0.47
1:C:342:LYS:HE3	1:C:342:LYS:HA	1.97	0.47
1:D:689:LEU:HD13	1:D:709:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ALA:N	1:A:667:ASN:HD21	2.10	0.47
1:A:690:MET:O	1:A:694:LEU:HD12	2.15	0.47
1:B:192:ALA:HA	1:B:195:ARG:NH2	2.29	0.47
1:B:601:GLN:HG2	1:B:622:GLU:HG2	1.97	0.47
1:B:662:ILE:HD12	1:B:662:ILE:H	1.80	0.47
1:C:138:ASP:CG	1:C:142:ARG:HH12	2.17	0.47
1:C:516:GLY:HA2	1:C:587:HIS:NE2	2.29	0.47
1:C:610:PRO:O	1:C:739:ARG:HB2	2.15	0.47
1:C:655:LEU:HB2	1:C:656:TYR:CD1	2.49	0.47
1:D:73:ASP:HB3	1:D:91:VAL:CG2	2.45	0.47
1:D:617:LYS:HB3	1:D:620:LEU:HB2	1.97	0.47
1:A:26:TYR:CE2	1:A:79:VAL:HA	2.50	0.47
1:A:642:PRO:HD3	1:A:651:TRP:CZ2	2.49	0.47
1:B:282:ASP:O	1:B:284:ALA:N	2.48	0.47
1:C:341:ILE:HG12	1:C:349:TRP:CE2	2.50	0.47
1:C:390:PHE:HD2	1:C:476:THR:OG1	1.98	0.47
1:C:723:ILE:HG12	1:C:726:GLN:HE22	1.79	0.47
1:D:59:GLU:H	1:D:59:GLU:HG3	1.47	0.47
1:A:136:ALA:HB2	1:A:293:ILE:HD11	1.97	0.47
1:A:340:ALA:HB2	1:A:411:PHE:CZ	2.50	0.47
1:A:386:PRO:HB3	1:A:472:VAL:HB	1.96	0.47
1:A:488:GLU:HG2	1:A:489:THR:HG22	1.97	0.47
1:B:548:THR:OG1	1:B:549:GLU:N	2.47	0.47
1:C:123:THR:O	1:C:123:THR:OG1	2.31	0.47
1:C:160:PRO:N	1:C:170:TRP:HZ3	2.12	0.47
1:C:344:GLU:OE2	1:C:352:SER:HB2	2.15	0.47
1:C:715:ARG:HG2	1:C:720:ALA:CB	2.45	0.47
1:C:764:THR:N	1:C:765:PRO:HD2	2.30	0.47
1:D:457:GLY:C	1:D:626:LEU:HB2	2.36	0.47
1:A:352:SER:O	1:A:354:SER:N	2.48	0.47
1:A:387:PHE:CD2	1:A:427:LEU:HG	2.50	0.47
1:A:437:PRO:HB2	1:A:460:LEU:HD13	1.97	0.47
1:A:529:MET:SD	1:A:541:ALA:HB2	2.55	0.47
1:B:155:GLU:HG3	1:B:174:LYS:HE2	1.97	0.47
1:B:418:VAL:HG22	1:B:421:ARG:HH11	1.80	0.47
1:B:507:PHE:CB	1:B:560:LEU:HD13	2.45	0.47
1:B:666:GLY:H	1:B:752:SER:HB3	1.80	0.47
1:C:84:ARG:O	1:C:85:SER:C	2.52	0.47
1:C:331:THR:HB	1:C:380:THR:HG21	1.97	0.47
1:C:689:LEU:HB3	1:C:709:ALA:HB2	1.97	0.47
1:D:312:ARG:HB2	1:D:315:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:HIS:HA	1:D:667:ASN:O	2.15	0.46
1:A:35:SER:O	1:A:36:TRP:C	2.54	0.46
1:A:539:ARG:O	1:A:550:VAL:HG11	2.15	0.46
1:B:691:PHE:CE2	1:B:736:LEU:HD13	2.51	0.46
1:C:212:LYS:C	1:C:213:THR:HG23	2.35	0.46
1:D:375:LYS:HA	1:D:378:THR:HG22	1.96	0.46
1:D:631:ASP:C	1:D:633:ALA:H	2.18	0.46
1:A:239:VAL:HA	1:A:291:ARG:HH12	1.80	0.46
1:B:484:LEU:CD2	1:B:548:THR:HG22	2.46	0.46
1:B:682:ARG:HA	1:B:682:ARG:HD3	1.40	0.46
1:C:35:SER:O	1:C:36:TRP:C	2.54	0.46
1:C:312:ARG:HD3	1:C:315:TYR:CE2	2.50	0.46
1:D:113:GLU:O	1:D:117:VAL:HG12	2.15	0.46
1:D:542:ARG:HD2	1:D:544:GLU:O	2.14	0.46
1:A:437:PRO:HG3	1:A:479:PHE:HE2	1.80	0.46
1:B:312:ARG:CB	1:B:312:ARG:HH11	2.28	0.46
1:B:570:TYR:HD1	1:B:769:PHE:CZ	2.33	0.46
1:A:13:SER:H	1:A:16:GLN:HE21	1.63	0.46
1:A:312:ARG:HB2	1:A:315:TYR:HD2	1.80	0.46
1:A:433:PHE:CE2	1:A:438:TRP:NE1	2.81	0.46
1:A:588:SER:OG	1:A:591:LEU:HB2	2.15	0.46
1:B:54:GLN:NE2	1:B:402:ASP:OD1	2.48	0.46
1:B:509:ALA:HB2	1:B:594:LEU:HD12	1.97	0.46
1:C:34:TYR:CD2	1:C:224:LEU:HD12	2.49	0.46
1:D:183:ILE:CD1	1:D:183:ILE:N	2.75	0.46
1:D:239:VAL:HA	1:D:291:ARG:HH12	1.79	0.46
1:D:415:PRO:HA	1:D:420:ARG:CZ	2.46	0.46
1:A:270:SER:HB2	1:B:85:SER:HA	1.96	0.46
1:A:326:THR:HG23	1:A:326:THR:O	2.16	0.46
1:B:110:VAL:HG12	1:B:228:ARG:NE	2.30	0.46
1:B:228:ARG:HD3	1:B:228:ARG:O	2.15	0.46
1:B:709:ALA:HB3	1:B:714:LEU:HD22	1.97	0.46
1:C:27:ILE:HB	1:C:164:ARG:HA	1.98	0.46
1:D:161:ARG:HA	1:D:170:TRP:CH2	2.39	0.46
1:A:163:ILE:HD12	1:A:170:TRP:CD2	2.51	0.46
1:B:396:LEU:HD11	1:B:403:GLN:HG2	1.97	0.46
1:C:148:GLU:CD	1:C:195:ARG:NH1	2.69	0.46
1:C:284:ALA:O	1:C:286:MET:N	2.46	0.46
1:C:390:PHE:HD2	1:C:476:THR:HG1	1.62	0.46
1:C:615:ARG:HG2	1:C:616:GLY:H	1.80	0.46
1:A:152:ARG:HD2	1:B:138:ASP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:O	1:A:384:LEU:HB2	2.16	0.46
1:A:520:GLY:O	1:A:522:ASP:N	2.49	0.46
1:A:541:ALA:O	1:A:542:ARG:C	2.54	0.46
1:A:565:ARG:HH21	1:A:771:PRO:CB	2.28	0.46
1:C:20:GLU:HB3	1:C:23:GLN:HB2	1.96	0.46
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.48	0.46
1:C:602:ASN:HB2	1:C:620:LEU:HB3	1.97	0.46
1:D:182:PRO:HB2	1:D:224:LEU:HD13	1.97	0.46
1:D:372:SER:OG	1:D:373:ALA:N	2.48	0.46
1:A:163:ILE:O	1:A:164:ARG:HB2	2.16	0.46
1:A:185:TYR:OH	1:A:206:VAL:O	2.33	0.46
1:A:583:PRO:HD3	1:A:660:GLU:OE1	2.16	0.46
1:B:109:THR:CG2	1:B:228:ARG:HE	2.29	0.46
1:B:337:LYS:HB3	1:B:338:PRO:HD3	1.97	0.46
1:B:503:SER:HB2	1:B:767:LEU:HD23	1.98	0.46
1:B:684:TRP:CE2	1:B:743:TRP:HB2	2.51	0.46
1:B:706:LEU:HD13	1:B:723:ILE:HG22	1.97	0.46
1:C:83:TYR:CE2	1:C:176:GLU:HB2	2.51	0.46
1:C:162:LEU:O	1:C:163:ILE:HG12	2.16	0.46
1:C:684:TRP:CG	1:C:684:TRP:O	2.68	0.46
1:B:167:TYR:CD1	1:B:167:TYR:N	2.84	0.46
1:B:344:GLU:O	1:B:349:TRP:HB3	2.15	0.46
1:B:356:LEU:O	1:B:359:ASP:HB2	2.16	0.46
1:C:563:GLN:O	1:C:566:SER:OG	2.33	0.46
1:D:110:VAL:HA	1:D:228:ARG:NH1	2.24	0.46
1:D:208:ILE:HG23	1:D:209:ASP:CB	2.46	0.46
1:D:664:ARG:O	1:D:668:LEU:HG	2.16	0.46
1:A:477:ARG:NE	1:A:542:ARG:HB3	2.30	0.46
1:A:584:VAL:HG13	1:A:591:LEU:HD13	1.98	0.46
1:B:87:VAL:HG22	1:B:88:PRO:HD2	1.98	0.46
1:B:292:LEU:HD12	1:B:292:LEU:HA	1.58	0.46
1:B:552:PRO:HG2	1:B:555:ALA:H	1.80	0.46
1:B:664:ARG:O	1:B:668:LEU:HG	2.15	0.46
1:D:283:ASP:HA	1:D:287:THR:CB	2.46	0.45
1:A:396:LEU:HD12	1:A:397:THR:N	2.31	0.45
1:B:760:TRP:O	1:B:764:THR:OG1	2.31	0.45
1:C:186:TYR:CZ	1:C:205:HIS:HD2	2.35	0.45
1:C:643:GLN:O	1:C:645:PRO:HD3	2.17	0.45
1:D:681:ASN:OD1	1:D:682:ARG:N	2.49	0.45
1:D:692:ARG:HG3	1:D:737:ALA:CB	2.37	0.45
1:A:388:ALA:HA	1:A:406:TYR:OH	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ASP:N	1:A:469:ASP:OD1	2.48	0.45
1:B:37:GLU:H	1:B:40:LYS:NZ	2.14	0.45
1:B:355:LYS:HD2	1:B:359:ASP:OD1	2.15	0.45
1:D:36:TRP:O	1:D:227:MET:HE2	2.17	0.45
1:A:84:ARG:O	1:A:85:SER:C	2.53	0.45
1:A:414:ASP:C	1:A:416:ASP:H	2.18	0.45
1:D:416:ASP:HB2	1:D:417:ILE:H	1.35	0.45
1:A:369:GLY:O	1:A:371:SER:N	2.46	0.45
1:B:641:ALA:HA	1:B:651:TRP:CH2	2.51	0.45
1:C:120:GLU:CD	1:C:200:VAL:HG21	2.37	0.45
1:C:342:LYS:C	1:C:343:GLU:HG2	2.37	0.45
1:C:686:LEU:HD21	1:C:712:GLN:HB3	1.98	0.45
1:C:710:GLU:OE2	1:C:715:ARG:NE	2.49	0.45
1:D:163:ILE:O	1:D:164:ARG:HB2	2.16	0.45
1:D:234:MET:HG2	1:D:249:ILE:HD11	1.99	0.45
1:D:243:VAL:HG11	1:D:245:ARG:HH21	1.81	0.45
1:D:572:LYS:HB3	1:D:760:TRP:CZ3	2.52	0.45
1:D:594:LEU:HD23	1:D:594:LEU:HA	1.81	0.45
1:A:371:SER:OG	1:A:375:LYS:HG2	2.17	0.45
1:A:538:PRO:HB2	1:A:550:VAL:HG13	1.98	0.45
1:B:433:PHE:O	1:B:437:PRO:HD2	2.17	0.45
1:C:239:VAL:HG11	1:C:292:LEU:HD13	1.98	0.45
1:C:441:PRO:O	1:C:444:VAL:HG22	2.16	0.45
1:C:493:SER:OG	1:C:494:ALA:N	2.50	0.45
1:C:688:ARG:HB3	1:C:692:ARG:CZ	2.47	0.45
1:D:16:GLN:HE22	1:A:3:THR:HG22	1.81	0.45
1:D:352:SER:O	1:D:354:SER:N	2.50	0.45
1:D:414:ASP:HB3	1:D:419:ALA:CB	2.46	0.45
1:D:709:ALA:CB	1:D:714:LEU:HB2	2.47	0.45
1:A:183:ILE:HG13	1:A:224:LEU:CD1	2.47	0.45
1:C:548:THR:OG1	1:C:549:GLU:N	2.49	0.45
1:A:238:ALA:HB2	1:A:249:ILE:HD12	1.97	0.45
1:B:182:PRO:HB2	1:B:224:LEU:HD13	1.99	0.45
1:B:636:THR:HB	1:B:671:LEU:O	2.17	0.45
1:D:3:THR:O	1:D:3:THR:OG1	2.35	0.45
1:D:86:GLN:NE2	1:D:172:ARG:H	2.11	0.45
1:D:455:GLN:HG2	1:D:624:LEU:O	2.17	0.45
1:D:634:PHE:CD1	1:D:634:PHE:N	2.82	0.45
1:A:163:ILE:O	1:A:168:ASP:OD2	2.35	0.45
1:A:209:ASP:OD1	1:A:212:LYS:N	2.50	0.45
1:C:26:TYR:CE2	1:C:79:VAL:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ARG:HB3	1:D:408:ARG:HH22	1.82	0.45
1:D:582:THR:O	1:D:582:THR:OG1	2.33	0.45
1:D:631:ASP:C	1:D:633:ALA:N	2.70	0.45
1:D:632:GLU:HA	1:D:635:ALA:HB3	1.99	0.45
1:A:38:LEU:HD13	1:A:230:GLN:OE1	2.17	0.45
1:A:337:LYS:HB2	1:A:337:LYS:HE3	1.46	0.45
1:A:565:ARG:HH21	1:A:771:PRO:CG	2.30	0.45
1:B:181:SER:HB2	1:B:182:PRO:HD2	1.98	0.45
1:B:588:SER:OG	1:B:591:LEU:HB2	2.16	0.45
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.78	0.45
1:D:499:LEU:HA	1:D:502:ARG:HD3	1.99	0.45
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.63	0.45
1:C:760:TRP:CZ2	1:C:764:THR:HG21	2.52	0.45
1:D:26:TYR:CE2	1:D:79:VAL:HA	2.52	0.44
1:D:469:ASP:OD1	1:D:469:ASP:N	2.49	0.44
1:D:665:ILE:HG13	1:D:756:CYS:SG	2.57	0.44
1:D:764:THR:O	1:D:769:PHE:HB2	2.17	0.44
1:A:606:ASP:OD2	1:A:609:THR:OG1	2.34	0.44
1:A:682:ARG:HD3	1:A:682:ARG:HA	1.57	0.44
1:B:243:VAL:HG11	1:B:245:ARG:HH21	1.81	0.44
1:C:669:THR:HG21	1:C:736:LEU:HD12	1.99	0.44
1:C:682:ARG:HG3	1:C:686:LEU:HD13	1.99	0.44
1:D:641:ALA:HA	1:D:651:TRP:CZ3	2.52	0.44
1:D:669:THR:CG2	1:D:751:ARG:HH22	2.29	0.44
1:C:339:ARG:HB3	1:C:408:ARG:HH22	1.81	0.44
1:D:522:ASP:OD1	1:D:522:ASP:N	2.49	0.44
1:A:433:PHE:CD1	1:A:476:THR:HG22	2.52	0.44
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.77	0.44
1:A:709:ALA:HB1	1:A:714:LEU:HB2	1.99	0.44
1:B:764:THR:N	1:B:765:PRO:HD2	2.32	0.44
1:C:234:MET:CG	1:C:249:ILE:HD11	2.47	0.44
1:D:385:LEU:HD22	1:D:396:LEU:CB	2.47	0.44
1:D:400:LEU:HA	1:D:400:LEU:HD13	1.60	0.44
1:D:429:GLN:HG2	1:D:480:ALA:HB2	1.99	0.44
1:D:441:PRO:O	1:D:444:VAL:HG22	2.17	0.44
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.71	0.44
1:B:720:ALA:HB1	1:B:723:ILE:HD12	2.00	0.44
1:C:87:VAL:HG22	1:C:88:PRO:HD2	1.99	0.44
1:C:199:ALA:C	1:C:201:LYS:H	2.20	0.44
1:C:470:ILE:HG21	1:C:522:ASP:HA	1.98	0.44
1:C:665:ILE:HD13	1:C:665:ILE:N	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:LEU:HD13	1:C:709:ALA:HA	1.99	0.44
1:D:208:ILE:HG21	1:D:221:TYR:CE2	2.53	0.44
1:A:86:GLN:NE2	1:A:172:ARG:H	2.16	0.44
1:A:355:LYS:HD2	1:A:359:ASP:CG	2.38	0.44
1:B:13:SER:OG	1:B:16:GLN:HG2	2.16	0.44
1:B:349:TRP:HA	1:B:352:SER:OG	2.18	0.44
1:C:537:MET:CB	1:C:538:PRO:HD3	2.48	0.44
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.67	0.44
1:D:265:PHE:O	1:D:269:ASN:N	2.51	0.44
1:D:678:SER:OG	1:D:721:GLY:HA3	2.16	0.44
1:A:5:GLU:OE2	1:A:311:LYS:HB2	2.18	0.44
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.44	0.44
1:A:186:TYR:OH	1:A:228:ARG:HD2	2.16	0.44
1:B:369:GLY:O	1:B:371:SER:N	2.51	0.44
1:C:113:GLU:OE2	1:C:232:ARG:NH2	2.50	0.44
1:C:163:ILE:HG13	1:C:170:TRP:CZ2	2.52	0.44
1:C:390:PHE:CD1	1:C:390:PHE:C	2.91	0.44
1:D:5:GLU:C	1:D:7:PHE:N	2.71	0.44
1:D:27:ILE:O	1:D:164:ARG:HA	2.17	0.44
1:A:78:THR:OG1	1:A:93:THR:HG21	2.17	0.44
1:A:742:GLU:HG3	1:A:743:TRP:H	1.83	0.44
1:B:374:ASP:OD1	1:B:374:ASP:N	2.38	0.44
1:C:369:GLY:O	1:C:370:SER:HB3	2.18	0.44
1:C:474:LEU:HA	1:C:474:LEU:HD23	1.62	0.44
1:C:572:LYS:HE2	1:C:760:TRP:CZ3	2.52	0.44
1:D:85:SER:HA	1:C:270:SER:HB2	2.00	0.44
1:D:187:LEU:HA	1:D:187:LEU:HD23	1.77	0.44
1:A:740:GLU:HB3	1:A:741:GLU:H	1.65	0.44
1:B:110:VAL:HG12	1:B:228:ARG:HE	1.81	0.44
1:B:232:ARG:HD3	1:B:236:ARG:CZ	2.48	0.44
1:B:682:ARG:HH21	1:B:716:LEU:HD13	1.82	0.44
1:C:72:ARG:HG3	1:C:72:ARG:O	2.17	0.44
1:C:283:ASP:O	1:C:287:THR:HB	2.17	0.44
1:C:283:ASP:OD2	1:C:283:ASP:N	2.51	0.44
1:D:319:MET:HE2	1:D:319:MET:HB3	1.68	0.44
1:B:543:PHE:C	1:B:543:PHE:CD2	2.92	0.44
1:C:458:ILE:HG12	1:C:626:LEU:HA	1.98	0.44
1:C:640:VAL:HG21	1:C:743:TRP:CH2	2.53	0.44
1:D:143:LEU:O	1:D:146:CYS:HB3	2.18	0.43
1:D:221:TYR:CD1	1:D:221:TYR:N	2.85	0.43
1:D:287:THR:N	1:D:288:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ALA:HB3	1:D:498:LEU:HD22	1.99	0.43
1:D:601:GLN:O	1:D:602:ASN:C	2.56	0.43
1:D:665:ILE:HD13	1:D:665:ILE:H	1.83	0.43
1:A:239:VAL:HG11	1:A:292:LEU:HD13	2.00	0.43
1:B:115:ILE:HD13	1:B:293:ILE:HG12	1.99	0.43
1:B:144:SER:C	1:B:146:CYS:H	2.21	0.43
1:B:173:ASN:HB2	1:B:176:GLU:CD	2.37	0.43
1:B:390:PHE:C	1:B:390:PHE:HD1	2.22	0.43
1:B:618:SER:OG	1:B:619:GLY:N	2.51	0.43
1:C:98:GLN:HE21	1:C:98:GLN:HB2	1.56	0.43
1:C:274:PRO:HA	1:C:277:VAL:HG22	2.00	0.43
1:C:414:ASP:O	1:C:416:ASP:N	2.50	0.43
1:C:593:ARG:NH2	1:C:635:ALA:HB1	2.33	0.43
1:D:661:LEU:O	1:D:663:ASN:N	2.50	0.43
1:D:682:ARG:HB3	1:D:683:ALA:H	1.51	0.43
1:B:349:TRP:O	1:B:350:GLN:HG2	2.18	0.43
1:B:373:ALA:O	1:B:376:ARG:HB3	2.18	0.43
1:B:590:PRO:HA	1:B:593:ARG:HB2	2.00	0.43
1:B:724:VAL:HG12	1:B:725:ARG:HG3	1.99	0.43
1:C:159:TYR:HB3	1:C:170:TRP:CZ3	2.53	0.43
1:C:335:THR:HG21	1:C:404:ARG:HE	1.83	0.43
1:C:339:ARG:HB3	1:C:408:ARG:NH2	2.33	0.43
1:D:13:SER:HB3	1:A:2:GLU:HG2	2.00	0.43
1:D:28:PRO:HD2	1:D:31:GLN:HG2	2.00	0.43
1:D:154:GLY:O	1:D:157:ARG:HB2	2.18	0.43
1:D:520:GLY:O	1:D:524:VAL:HG23	2.17	0.43
1:A:223:HIS:CE1	1:A:227:MET:SD	3.11	0.43
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.69	0.43
1:B:149:GLU:HG2	1:B:150:ASP:H	1.82	0.43
1:C:83:TYR:HD1	1:C:169:VAL:HG11	1.82	0.43
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.67	0.43
1:C:207:PRO:O	1:C:208:ILE:HG22	2.18	0.43
1:C:396:LEU:HD21	1:C:406:TYR:CG	2.53	0.43
1:C:674:VAL:HG13	1:C:678:SER:HB3	2.00	0.43
1:D:618:SER:OG	1:D:619:GLY:N	2.50	0.43
1:D:728:ARG:HD3	1:D:728:ARG:C	2.36	0.43
1:A:706:LEU:O	1:A:710:GLU:HG3	2.18	0.43
1:B:59:GLU:H	1:B:59:GLU:HG3	1.58	0.43
1:B:73:ASP:OD1	1:B:73:ASP:C	2.56	0.43
1:D:420:ARG:O	1:D:423:VAL:HB	2.19	0.43
1:D:682:ARG:HD3	1:D:682:ARG:HA	1.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:THR:OG1	1:A:675:GLU:HG2	2.19	0.43
1:A:662:ILE:HA	1:A:667:ASN:OD1	2.18	0.43
1:B:44:LEU:HD21	1:B:65:LEU:HD21	2.01	0.43
1:C:52:LEU:HB2	1:C:298:TYR:CD2	2.53	0.43
1:C:734:ALA:O	1:C:736:LEU:N	2.43	0.43
1:D:31:GLN:HA	1:D:31:GLN:OE1	2.19	0.43
1:D:261:GLN:CD	1:D:261:GLN:H	2.22	0.43
1:D:337:LYS:HB3	1:D:338:PRO:HD3	1.99	0.43
1:D:502:ARG:NH2	1:D:766:TRP:HE1	2.17	0.43
1:A:493:SER:OG	1:A:494:ALA:N	2.52	0.43
1:B:472:VAL:O	1:B:476:THR:HG23	2.19	0.43
1:B:493:SER:OG	1:B:494:ALA:N	2.51	0.43
1:B:686:LEU:HD21	1:B:712:GLN:CB	2.48	0.43
1:C:437:PRO:HB2	1:C:460:LEU:HD12	1.99	0.43
1:D:128:PRO:HD3	1:D:275:SER:HB2	2.00	0.43
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.87	0.43
1:D:387:PHE:HE2	1:D:427:LEU:N	2.15	0.43
1:A:429:GLN:OE1	1:A:429:GLN:HA	2.18	0.43
1:A:484:LEU:CD2	1:A:547:LEU:HD23	2.48	0.43
1:A:688:ARG:CZ	1:A:740:GLU:OE2	2.64	0.43
1:B:138:ASP:CG	1:B:142:ARG:HH12	2.22	0.43
1:B:385:LEU:HB2	1:B:386:PRO:HD3	2.00	0.43
1:B:650:SER:OG	1:B:683:ALA:HB1	2.19	0.43
1:B:683:ALA:O	1:B:685:HIS:N	2.50	0.43
1:B:706:LEU:HD22	1:B:724:VAL:HA	1.99	0.43
1:C:127:GLU:OE2	1:C:128:PRO:N	2.51	0.43
1:C:353:GLU:O	1:C:356:LEU:HB2	2.18	0.43
1:C:564:LEU:HB3	1:C:570:TYR:HB3	2.00	0.43
1:C:699:VAL:HA	1:C:702:ALA:HB3	2.01	0.43
1:D:68:VAL:HA	1:D:96:ASP:O	2.19	0.43
1:A:34:TYR:CD2	1:A:224:LEU:HD12	2.49	0.43
1:A:55:LEU:HD11	1:A:302:ARG:NH2	2.34	0.43
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.92	0.43
1:B:26:TYR:HB3	1:B:93:THR:HG22	2.01	0.43
1:C:8:ASP:OD1	1:C:8:ASP:C	2.57	0.43
1:C:26:TYR:CD1	1:C:79:VAL:HG12	2.54	0.43
1:C:639:HIS:HA	1:C:667:ASN:O	2.19	0.43
1:D:369:GLY:O	1:D:371:SER:N	2.52	0.43
1:D:680:SER:HA	1:D:690:MET:HE1	2.01	0.43
1:A:165:SER:O	1:A:166:TYR:HB2	2.18	0.43
1:A:417:ILE:O	1:A:418:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:TYR:HD1	1:B:169:VAL:HG11	1.84	0.43
1:B:199:ALA:O	1:B:200:VAL:HB	2.19	0.43
1:C:186:TYR:CZ	1:C:205:HIS:CD2	3.07	0.43
1:C:760:TRP:CE2	1:C:764:THR:HG21	2.54	0.43
1:D:684:TRP:O	1:D:684:TRP:CG	2.72	0.43
1:D:740:GLU:HB3	1:D:741:GLU:H	1.70	0.43
1:B:113:GLU:O	1:B:117:VAL:HG12	2.19	0.43
1:B:238:ALA:HB2	1:B:249:ILE:HD13	2.01	0.43
1:B:375:LYS:O	1:B:378:THR:HG22	2.19	0.43
1:B:623:THR:HG22	1:B:634:PHE:HZ	1.84	0.43
1:B:740:GLU:HB3	1:B:741:GLU:H	1.68	0.43
1:C:675:GLU:O	1:C:680:SER:OG	2.24	0.43
1:D:71:LEU:HD12	1:D:310:ALA:O	2.18	0.42
1:D:561:LYS:CE	1:D:771:PRO:HD2	2.49	0.42
1:A:342:LYS:O	1:A:343:GLU:HG2	2.19	0.42
1:A:395:LYS:HG3	1:A:395:LYS:O	2.19	0.42
1:A:455:GLN:HB3	1:A:502:ARG:HE	1.84	0.42
1:B:113:GLU:OE1	1:B:228:ARG:NH1	2.51	0.42
1:B:344:GLU:HG3	1:B:354:SER:OG	2.19	0.42
1:B:366:ASP:O	1:B:370:SER:HB2	2.18	0.42
1:C:251:LEU:HB2	1:C:252:PRO:HD2	2.00	0.42
1:D:5:GLU:OE2	1:D:311:LYS:HB2	2.19	0.42
1:D:83:TYR:OH	1:D:176:GLU:HB2	2.19	0.42
1:D:181:SER:HB2	1:D:182:PRO:HD2	2.01	0.42
1:D:488:GLU:HG2	1:D:489:THR:N	2.33	0.42
1:A:283:ASP:O	1:A:287:THR:HB	2.19	0.42
1:A:578:ARG:O	1:A:582:THR:HG23	2.19	0.42
1:B:150:ASP:OD1	1:B:151:MET:O	2.37	0.42
1:D:433:PHE:CG	1:D:476:THR:HG22	2.54	0.42
1:D:470:ILE:H	1:D:470:ILE:HG12	1.59	0.42
1:A:96:ASP:HB2	1:A:320:PHE:CE2	2.54	0.42
1:A:520:GLY:O	1:A:523:GLY:N	2.51	0.42
1:B:38:LEU:HB2	1:B:227:MET:HE1	2.01	0.42
1:B:338:PRO:CG	1:C:29:PRO:HG2	2.50	0.42
1:B:414:ASP:HB2	1:B:544:GLU:OE2	2.19	0.42
1:B:486:SER:O	1:B:489:THR:N	2.46	0.42
1:B:624:LEU:HD13	1:B:766:TRP:CH2	2.55	0.42
1:B:666:GLY:O	1:B:751:ARG:HD2	2.20	0.42
1:C:565:ARG:HA	1:C:570:TYR:CE2	2.55	0.42
1:C:617:LYS:CG	1:C:620:LEU:HB2	2.48	0.42
1:C:650:SER:OG	1:C:683:ALA:HB1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:GLU:CD	1:D:311:LYS:HB2	2.40	0.42
1:D:455:GLN:O	1:D:458:ILE:HG22	2.19	0.42
1:D:734:ALA:O	1:D:737:ALA:N	2.52	0.42
1:A:213:THR:O	1:A:213:THR:OG1	2.28	0.42
1:A:390:PHE:C	1:A:390:PHE:HD1	2.22	0.42
1:B:299:LEU:HA	1:B:303:VAL:CG2	2.48	0.42
1:B:331:THR:HB	1:B:380:THR:HG21	2.00	0.42
1:B:356:LEU:HD23	1:B:356:LEU:HA	1.85	0.42
1:B:396:LEU:CD1	1:B:403:GLN:HG2	2.49	0.42
1:B:709:ALA:CB	1:B:714:LEU:HB2	2.49	0.42
1:C:172:ARG:HG3	1:C:172:ARG:NH1	2.30	0.42
1:C:369:GLY:O	1:C:371:SER:N	2.50	0.42
1:C:416:ASP:HB2	1:C:417:ILE:H	1.47	0.42
1:C:433:PHE:CE2	1:C:438:TRP:NE1	2.88	0.42
1:C:533:VAL:O	1:C:538:PRO:HD2	2.19	0.42
1:C:561:LYS:HE2	1:C:771:PRO:HD2	2.02	0.42
1:C:595:LEU:HD23	1:C:595:LEU:HA	1.85	0.42
1:C:713:GLY:O	1:C:716:LEU:HG	2.19	0.42
1:C:740:GLU:HB3	1:C:741:GLU:H	1.68	0.42
1:D:127:GLU:OE2	1:D:127:GLU:C	2.58	0.42
1:D:507:PHE:CG	1:D:560:LEU:HD22	2.53	0.42
1:A:139:VAL:HG12	1:A:143:LEU:HD12	2.00	0.42
1:A:458:ILE:N	1:A:626:LEU:HB2	2.34	0.42
1:A:561:LYS:HD2	1:A:767:LEU:O	2.19	0.42
1:B:274:PRO:HA	1:B:277:VAL:HG22	2.01	0.42
1:B:682:ARG:HE	1:B:716:LEU:HD13	1.84	0.42
1:C:69:ILE:O	1:C:95:ILE:N	2.50	0.42
1:C:152:ARG:HE	1:C:152:ARG:HB2	1.43	0.42
1:C:163:ILE:HG23	1:C:163:ILE:HD13	1.77	0.42
1:C:496:GLN:HG2	1:C:553:VAL:HG22	2.02	0.42
1:D:682:ARG:HE	1:D:716:LEU:CD1	2.32	0.42
1:A:251:LEU:O	1:A:291:ARG:NH2	2.51	0.42
1:A:312:ARG:CB	1:A:312:ARG:HH11	2.31	0.42
1:B:5:GLU:OE2	1:B:311:LYS:HB2	2.19	0.42
1:B:565:ARG:HG2	1:B:570:TYR:CZ	2.53	0.42
1:B:622:GLU:O	1:B:628:ARG:NH1	2.47	0.42
1:C:164:ARG:NH1	1:C:183:ILE:HD11	2.34	0.42
1:C:401:ASN:H	1:C:401:ASN:HD22	1.67	0.42
1:C:604:THR:OG1	1:C:614:VAL:O	2.31	0.42
1:C:617:LYS:HG2	1:C:620:LEU:HB2	2.02	0.42
1:C:769:PHE:O	1:C:770:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:HIS:HD2	1:D:512:ARG:HH21	1.68	0.42
1:D:615:ARG:HG2	1:D:616:GLY:N	2.34	0.42
1:D:734:ALA:O	1:D:736:LEU:N	2.45	0.42
1:A:569:ILE:HG12	1:A:574:GLN:OE1	2.18	0.42
1:B:97:GLY:O	1:B:99:GLN:N	2.53	0.42
1:C:266:ALA:HB1	1:C:302:ARG:NH1	2.34	0.42
1:C:429:GLN:HG2	1:C:480:ALA:CB	2.49	0.42
1:B:223:HIS:CE1	1:B:227:MET:HG2	2.54	0.42
1:B:700:GLU:O	1:B:704:LYS:HD2	2.19	0.42
1:C:71:LEU:HB3	1:C:93:THR:OG1	2.20	0.42
1:C:120:GLU:C	1:C:122:LEU:H	2.23	0.42
1:C:151:MET:HB3	1:C:172:ARG:CZ	2.50	0.42
1:C:204:ARG:O	1:C:205:HIS:CB	2.67	0.42
1:C:542:ARG:NH1	1:C:544:GLU:O	2.53	0.42
1:C:634:PHE:CD1	1:C:634:PHE:N	2.82	0.42
1:D:27:ILE:CG1	1:D:162:LEU:HD22	2.49	0.42
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.78	0.42
1:A:516:GLY:O	1:A:587:HIS:CD2	2.73	0.42
1:A:589:LYS:N	1:A:590:PRO:HD2	2.34	0.42
1:A:630:ASN:O	1:A:632:GLU:N	2.53	0.42
1:B:44:LEU:O	1:B:48:VAL:HG12	2.20	0.42
1:B:282:ASP:OD1	1:B:282:ASP:N	2.53	0.42
1:B:529:MET:HA	1:B:540:PHE:HB3	2.02	0.42
1:B:585:TYR:CD1	1:B:637:ILE:HG21	2.54	0.42
1:C:273:PRO:HG2	1:C:276:VAL:CG2	2.50	0.42
1:C:440:SER:C	1:C:442:THR:H	2.23	0.42
1:C:514:SER:O	1:C:582:THR:HG21	2.20	0.42
1:C:576:VAL:HG21	1:C:757:SER:HA	2.01	0.42
1:D:128:PRO:HG3	1:D:275:SER:HB2	2.02	0.42
1:D:477:ARG:CZ	1:D:542:ARG:H	2.32	0.42
1:D:688:ARG:HD3	1:D:692:ARG:HH12	1.85	0.42
1:A:26:TYR:CE1	1:A:79:VAL:HG12	2.55	0.42
1:A:400:LEU:HD13	1:A:400:LEU:HA	1.53	0.42
1:A:469:ASP:O	1:A:472:VAL:HG23	2.20	0.42
1:A:472:VAL:O	1:A:476:THR:HG23	2.20	0.42
1:B:455:GLN:CD	1:B:766:TRP:HZ2	2.23	0.42
1:B:471:VAL:HG13	1:B:504:CYS:SG	2.60	0.42
1:C:715:ARG:HB3	1:C:719:GLY:CA	2.48	0.42
1:D:29:PRO:HB2	1:D:166:TYR:CE2	2.55	0.41
1:D:162:LEU:O	1:D:163:ILE:HG13	2.20	0.41
1:A:59:GLU:H	1:A:59:GLU:HG3	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HB3	1:A:92:MET:HE3	2.01	0.41
1:A:148:GLU:OE1	1:A:195:ARG:NH1	2.45	0.41
1:A:433:PHE:C	1:A:433:PHE:CD2	2.93	0.41
1:B:207:PRO:O	1:B:208:ILE:HG22	2.19	0.41
1:B:605:PRO:HG3	1:B:734:ALA:HB3	2.02	0.41
1:D:167:TYR:CD1	1:D:167:TYR:N	2.88	0.41
1:D:180:ARG:HD3	1:D:213:THR:CG2	2.49	0.41
1:A:542:ARG:O	1:A:542:ARG:HG3	2.19	0.41
1:A:636:THR:HB	1:A:671:LEU:O	2.20	0.41
1:A:651:TRP:CH2	1:A:684:TRP:HB2	2.55	0.41
1:B:128:PRO:CD	1:B:275:SER:HB2	2.48	0.41
1:B:337:LYS:HE2	1:B:358:PHE:CD1	2.55	0.41
1:C:83:TYR:CZ	1:C:176:GLU:HB2	2.55	0.41
1:D:123:THR:O	1:D:123:THR:OG1	2.29	0.41
1:D:161:ARG:CA	1:D:170:TRP:HH2	2.25	0.41
1:D:390:PHE:HD1	1:D:391:GLN:N	2.19	0.41
1:A:569:ILE:HG12	1:A:574:GLN:CD	2.41	0.41
1:A:763:LEU:O	1:A:766:TRP:HB2	2.21	0.41
1:B:352:SER:O	1:B:354:SER:N	2.53	0.41
1:B:426:GLY:O	1:B:430:VAL:HG23	2.20	0.41
1:C:140:THR:HG22	1:C:141:GLY:N	2.35	0.41
1:C:395:LYS:HG3	1:C:395:LYS:O	2.20	0.41
1:D:70:ALA:HB3	1:D:92:MET:HE3	2.02	0.41
1:D:379:VAL:O	1:D:383:VAL:HG12	2.20	0.41
1:A:482:HIS:HA	1:A:493:SER:CB	2.50	0.41
1:A:557:GLN:O	1:A:561:LYS:HD3	2.21	0.41
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.64	0.41
1:C:339:ARG:HG2	1:C:408:ARG:NH1	2.35	0.41
1:C:617:LYS:HA	1:C:617:LYS:HD2	1.90	0.41
1:C:662:ILE:HD12	1:C:662:ILE:H	1.85	0.41
1:C:723:ILE:HG12	1:C:726:GLN:NE2	2.35	0.41
1:D:337:LYS:O	1:D:341:ILE:HG13	2.21	0.41
1:D:720:ALA:HB1	1:D:723:ILE:HB	2.02	0.41
1:A:366:ASP:O	1:A:370:SER:HB2	2.20	0.41
1:B:377:GLN:HE22	1:B:403:GLN:NE2	2.16	0.41
1:C:330:LEU:HB3	1:C:334:GLU:OE1	2.21	0.41
1:C:666:GLY:N	1:C:752:SER:HB3	2.31	0.41
1:D:576:VAL:HG13	1:D:756:CYS:HB2	2.02	0.41
1:D:658:ASP:OD2	1:D:664:ARG:NH2	2.54	0.41
1:D:665:ILE:HG12	1:D:752:SER:HB2	2.02	0.41
1:D:715:ARG:HG2	1:D:720:ALA:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG22	1:A:295:PHE:CE1	2.56	0.41
1:A:444:VAL:HB	1:A:445:PRO:CD	2.50	0.41
1:A:666:GLY:O	1:A:751:ARG:HD2	2.21	0.41
1:A:709:ALA:CB	1:A:714:LEU:HB2	2.49	0.41
1:B:339:ARG:HG2	1:B:408:ARG:NH1	2.36	0.41
1:A:217:ASP:O	1:A:218:LEU:HB2	2.21	0.41
1:A:312:ARG:HD3	1:A:315:TYR:HE2	1.86	0.41
1:A:466:GLY:O	1:A:467:GLY:O	2.38	0.41
1:B:38:LEU:O	1:B:38:LEU:HG	2.21	0.41
1:B:87:VAL:HG13	1:B:88:PRO:O	2.21	0.41
1:B:455:GLN:OE1	1:B:502:ARG:NH2	2.48	0.41
1:C:391:GLN:O	1:C:391:GLN:CD	2.59	0.41
1:C:482:HIS:HA	1:C:493:SER:HB2	2.02	0.41
1:C:691:PHE:CD2	1:C:736:LEU:HD13	2.54	0.41
1:D:35:SER:O	1:D:223:HIS:NE2	2.48	0.41
1:D:387:PHE:CD2	1:D:427:LEU:HG	2.55	0.41
1:D:445:PRO:CD	1:D:498:LEU:HD21	2.51	0.41
1:A:101:MET:HE1	1:A:104:LEU:HD12	2.02	0.41
1:A:168:ASP:OD1	1:A:168:ASP:N	2.54	0.41
1:A:375:LYS:O	1:A:378:THR:HG22	2.20	0.41
1:A:584:VAL:HG21	1:A:665:ILE:HD13	2.01	0.41
1:B:11:PRO:HB3	1:C:7:PHE:CD2	2.55	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.63	0.41
1:B:391:GLN:HE21	1:B:542:ARG:HH12	1.68	0.41
1:B:417:ILE:HD12	1:B:420:ARG:HB2	2.03	0.41
1:B:511:TRP:HH2	1:B:519:ALA:HB3	1.86	0.41
1:C:391:GLN:OE1	1:C:542:ARG:NH1	2.53	0.41
1:D:9:ALA:HA	1:D:307:VAL:O	2.21	0.41
1:D:83:TYR:CZ	1:D:176:GLU:HB2	2.56	0.41
1:D:112:HIS:NE2	1:D:140:THR:HG23	2.35	0.41
1:D:160:PRO:O	1:D:170:TRP:CZ3	2.74	0.41
1:D:339:ARG:HG2	1:D:408:ARG:NH2	2.36	0.41
1:D:357:HIS:O	1:D:360:VAL:HB	2.20	0.41
1:D:433:PHE:HB3	1:D:476:THR:HG22	2.02	0.41
1:D:449:ASP:C	1:D:451:THR:N	2.74	0.41
1:D:572:LYS:HE2	1:D:760:TRP:CZ3	2.56	0.41
1:D:633:ALA:HB3	1:D:634:PHE:HD1	1.84	0.41
1:A:407:LEU:HA	1:A:407:LEU:HD23	1.78	0.41
1:A:479:PHE:O	1:A:479:PHE:CD1	2.74	0.41
1:A:640:VAL:HG11	1:A:743:TRP:CE2	2.56	0.41
1:B:72:ARG:CZ	1:B:90:LYS:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:MET:HE3	1:B:92:MET:HB3	1.95	0.41
1:C:228:ARG:HD3	1:C:228:ARG:C	2.40	0.41
1:C:432:ARG:O	1:C:435:GLU:N	2.50	0.41
1:C:433:PHE:HE2	1:C:438:TRP:NE1	2.19	0.41
1:C:517:SER:C	1:C:519:ALA:N	2.74	0.41
1:A:108:THR:HB	1:A:143:LEU:HD22	2.03	0.41
1:A:615:ARG:HH22	1:A:758:LEU:C	2.23	0.41
1:C:156:HIS:ND1	1:C:177:ALA:HB3	2.36	0.41
1:C:706:LEU:HD22	1:C:724:VAL:HA	2.03	0.41
1:D:282:ASP:OD1	1:D:282:ASP:N	2.54	0.40
1:D:451:THR:O	1:D:455:GLN:HG3	2.21	0.40
1:D:638:GLU:O	1:D:668:LEU:HA	2.21	0.40
1:A:492:SER:O	1:A:496:GLN:HG3	2.21	0.40
1:A:715:ARG:HG2	1:A:720:ALA:HB2	2.03	0.40
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.82	0.40
1:B:478:TYR:OH	1:B:556:LEU:HG	2.21	0.40
1:C:104:LEU:HA	1:C:104:LEU:HD23	1.78	0.40
1:C:115:ILE:HG23	1:C:289:LEU:HD11	2.03	0.40
1:D:538:PRO:HB2	1:D:550:VAL:CG1	2.51	0.40
1:A:212:LYS:HB3	1:A:213:THR:H	1.57	0.40
1:A:274:PRO:O	1:A:277:VAL:HG22	2.22	0.40
1:A:565:ARG:O	1:A:566:SER:C	2.60	0.40
1:C:148:GLU:OE2	1:C:195:ARG:NH1	2.55	0.40
1:C:182:PRO:HB2	1:C:224:LEU:HD13	2.02	0.40
1:C:211:ASP:O	1:C:212:LYS:HG2	2.20	0.40
1:D:18:LEU:HD23	1:D:18:LEU:HA	1.82	0.40
1:D:106:LEU:O	1:D:109:THR:HG22	2.22	0.40
1:D:617:LYS:HD2	1:D:617:LYS:HA	1.89	0.40
1:A:157:ARG:HD2	1:A:158:TYR:CE2	2.57	0.40
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.65	0.40
1:B:253:THR:O	1:B:256:ASP:HB2	2.20	0.40
1:B:372:SER:OG	1:B:375:LYS:HB3	2.21	0.40
1:B:416:ASP:HB2	1:B:417:ILE:H	1.28	0.40
1:B:474:LEU:HD12	1:B:525:TYR:CD1	2.56	0.40
1:B:597:LEU:HD22	1:B:623:THR:HB	2.03	0.40
1:B:600:SER:HA	1:B:603:SER:OG	2.21	0.40
1:C:5:GLU:CD	1:C:6:ILE:N	2.75	0.40
1:C:284:ALA:C	1:C:286:MET:H	2.25	0.40
1:C:346:LEU:HB3	1:C:347:ASP:H	1.69	0.40
1:C:386:PRO:O	1:C:389:MET:HB2	2.22	0.40
1:C:417:ILE:HD12	1:C:417:ILE:HA	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:HD13	1:A:69:ILE:HG21	1.91	0.40
1:B:65:LEU:HD22	1:B:65:LEU:O	2.21	0.40
1:B:163:ILE:O	1:B:164:ARG:HB2	2.21	0.40
1:C:451:THR:O	1:C:455:GLN:HG3	2.21	0.40
1:C:549:GLU:O	1:C:550:VAL:HB	2.21	0.40
1:C:641:ALA:N	1:C:667:ASN:OD1	2.50	0.40
1:D:417:ILE:HD12	1:D:417:ILE:HA	1.71	0.40
1:D:477:ARG:NE	1:D:542:ARG:HB3	2.36	0.40
1:D:569:ILE:HD13	1:D:574:GLN:HB3	2.02	0.40
1:D:728:ARG:HD3	1:D:729:TYR:H	1.83	0.40
1:A:23:GLN:HG3	1:A:90:LYS:HD3	2.04	0.40
1:A:158:TYR:CD2	1:A:158:TYR:N	2.90	0.40
1:A:484:LEU:CD2	1:A:548:THR:HG22	2.52	0.40
1:B:55:LEU:HG	1:B:55:LEU:O	2.21	0.40
1:B:267:LEU:HB2	1:B:268:PHE:CD1	2.56	0.40
1:C:122:LEU:HD23	1:C:122:LEU:HA	1.78	0.40
1:C:145:ASN:OD1	1:C:145:ASN:N	2.55	0.40
1:C:164:ARG:HH12	1:C:183:ILE:HD11	1.85	0.40
1:C:168:ASP:OD1	1:C:179:TYR:HA	2.21	0.40
1:C:496:GLN:CD	1:C:553:VAL:HG22	2.42	0.40
1:C:618:SER:OG	1:C:619:GLY:N	2.54	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:SER:N	1:C:211:ASP:OD2[4_457]	2.06	0.14
1:D:84:ARG:N	1:C:211:ASP:OD2[4_457]	2.15	0.05
1:A:657:GLU:OE1	1:B:236:ARG:NH1[4_447]	2.15	0.05

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	769/771 (100%)	598 (78%)	112 (15%)	59 (8%)	1	9
1	B	769/771 (100%)	597 (78%)	122 (16%)	50 (6%)	1	12
1	C	769/771 (100%)	601 (78%)	109 (14%)	59 (8%)	1	9
1	D	769/771 (100%)	600 (78%)	113 (15%)	56 (7%)	1	10
All	All	3076/3084 (100%)	2396 (78%)	456 (15%)	224 (7%)	1	10

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	LYS
1	D	36	TRP
1	D	127	GLU
1	D	200	VAL
1	D	205	HIS
1	D	208	ILE
1	D	283	ASP
1	D	353	GLU
1	D	538	PRO
1	D	551	PRO
1	D	552	PRO
1	D	565	ARG
1	D	618	SER
1	D	631	ASP
1	D	633	ALA
1	D	645	PRO
1	D	650	SER
1	D	682	ARG
1	D	727	ALA
1	A	4	LYS
1	A	6	ILE
1	A	127	GLU
1	A	200	VAL
1	A	205	HIS
1	A	208	ILE
1	A	241	ALA
1	A	283	ASP
1	A	353	GLU
1	A	414	ASP
1	A	444	VAL
1	A	445	PRO
1	A	538	PRO
1	A	551	PRO

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Mol	Chain	Res	Type
1	A	552	PRO
1	A	565	ARG
1	A	618	SER
1	A	631	ASP
1	A	633	ALA
1	A	645	PRO
1	A	650	SER
1	A	682	ARG
1	A	727	ALA
1	B	4	LYS
1	B	6	ILE
1	B	127	GLU
1	B	200	VAL
1	B	208	ILE
1	B	241	ALA
1	B	283	ASP
1	B	353	GLU
1	B	444	VAL
1	B	445	PRO
1	B	467	GLY
1	B	538	PRO
1	B	551	PRO
1	B	552	PRO
1	B	565	ARG
1	B	618	SER
1	B	633	ALA
1	B	645	PRO
1	B	650	SER
1	B	682	ARG
1	B	770	GLU
1	C	4	LYS
1	C	127	GLU
1	C	208	ILE
1	C	247	ASP
1	C	283	ASP
1	C	353	GLU
1	C	414	ASP
1	C	444	VAL
1	C	445	PRO
1	C	538	PRO
1	C	551	PRO
1	C	552	PRO

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Mol	Chain	Res	Type
1	C	618	SER
1	C	631	ASP
1	C	633	ALA
1	C	645	PRO
1	C	650	SER
1	C	682	ARG
1	C	727	ALA
1	C	770	GLU
1	D	6	ILE
1	D	81	PRO
1	D	126	ASP
1	D	164	ARG
1	D	241	ALA
1	D	444	VAL
1	D	445	PRO
1	D	450	ALA
1	D	467	GLY
1	D	685	HIS
1	D	695	SER
1	D	720	ALA
1	D	721	GLY
1	A	36	TRP
1	A	450	ALA
1	A	467	GLY
1	A	685	HIS
1	A	695	SER
1	A	721	GLY
1	A	770	GLU
1	B	36	TRP
1	B	81	PRO
1	B	205	HIS
1	B	247	ASP
1	B	450	ALA
1	B	631	ASP
1	B	685	HIS
1	B	695	SER
1	B	721	GLY
1	C	6	ILE
1	C	36	TRP
1	C	200	VAL
1	C	205	HIS
1	C	450	ALA

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Mol	Chain	Res	Type
1	C	467	GLY
1	C	518	THR
1	C	565	ARG
1	C	587	HIS
1	C	685	HIS
1	C	695	SER
1	C	720	ALA
1	C	721	GLY
1	D	569	ILE
1	D	587	HIS
1	D	632	GLU
1	D	684	TRP
1	D	718	SER
1	D	728	ARG
1	D	770	GLU
1	A	164	ARG
1	A	370	SER
1	A	569	ILE
1	A	648	ASN
1	A	718	SER
1	A	720	ALA
1	B	121	LYS
1	B	164	ARG
1	B	370	SER
1	B	587	HIS
1	B	718	SER
1	B	720	ALA
1	B	727	ALA
1	C	81	PRO
1	C	164	ARG
1	C	241	ALA
1	C	350	GLN
1	C	568	GLY
1	C	632	GLU
1	C	684	TRP
1	C	718	SER
1	D	247	ASP
1	D	350	GLN
1	D	370	SER
1	D	390	PHE
1	A	247	ASP
1	A	390	PHE

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Mol	Chain	Res	Type
1	A	448	ASP
1	A	519	ALA
1	A	566	SER
1	A	587	HIS
1	A	684	TRP
1	A	734	ALA
1	B	350	GLN
1	B	568	GLY
1	B	569	ILE
1	C	126	ASP
1	C	269	ASN
1	C	448	ASP
1	C	519	ALA
1	C	569	ILE
1	D	414	ASP
1	D	448	ASP
1	D	620	LEU
1	D	648	ASN
1	D	736	LEU
1	A	81	PRO
1	A	121	LYS
1	A	163	ILE
1	A	281	GLU
1	A	350	GLN
1	A	392	ASP
1	A	487	PRO
1	A	728	ARG
1	B	126	ASP
1	B	163	ILE
1	B	390	PHE
1	B	414	ASP
1	B	487	PRO
1	B	648	ASN
1	C	5	GLU
1	C	160	PRO
1	C	166	TYR
1	C	248	ASP
1	C	392	ASP
1	C	545	ARG
1	C	566	SER
1	C	728	ARG
1	D	57	GLU

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Mol	Chain	Res	Type
1	D	163	ILE
1	D	416	ASP
1	A	166	TYR
1	A	168	ASP
1	A	518	THR
1	B	166	TYR
1	C	162	LEU
1	C	370	SER
1	C	487	PRO
1	D	160	PRO
1	D	568	GLY
1	C	163	ILE
1	C	550	VAL
1	A	640	VAL
1	B	550	VAL
1	D	418	VAL
1	D	487	PRO
1	D	466	GLY
1	A	568	GLY
1	B	327	GLY
1	B	417	ILE
1	A	415	PRO
1	A	550	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/650 (100%)	541 (83%)	109 (17%)	2	11
1	B	650/650 (100%)	537 (83%)	113 (17%)	2	10
1	C	650/650 (100%)	529 (81%)	121 (19%)	1	7
1	D	650/650 (100%)	540 (83%)	110 (17%)	2	11
All	All	2600/2600 (100%)	2147 (83%)	453 (17%)	2	10

All (453) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	MET
1	D	3	THR
1	D	7	PHE
1	D	46	SER
1	D	52	LEU
1	D	61	SER
1	D	62	ILE
1	D	63	CYS
1	D	64	PHE
1	D	65	LEU
1	D	68	VAL
1	D	75	ASN
1	D	77	THR
1	D	79	VAL
1	D	86	GLN
1	D	87	VAL
1	D	89	SER
1	D	99	GLN
1	D	101	MET
1	D	104	LEU
1	D	105	LEU
1	D	106	LEU
1	D	109	THR
1	D	127	GLU
1	D	140	THR
1	D	146	CYS
1	D	151	MET
1	D	157	ARG
1	D	163	ILE
1	D	164	ARG
1	D	165	SER
1	D	167	TYR
1	D	172	ARG
1	D	176	GLU
1	D	183	ILE
1	D	189	SER
1	D	193	TYR
1	D	198	ASP
1	D	200	VAL
1	D	208	ILE
1	D	211	ASP
1	D	212	LYS
1	D	216	VAL

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Mol	Chain	Res	Type
1	D	227	MET
1	D	228	ARG
1	D	234	MET
1	D	249	ILE
1	D	251	LEU
1	D	262	ASN
1	D	275	SER
1	D	280	LEU
1	D	282	ASP
1	D	283	ASP
1	D	287	THR
1	D	292	LEU
1	D	305	VAL
1	D	312	ARG
1	D	320	PHE
1	D	328	GLN
1	D	335	THR
1	D	339	ARG
1	D	342	LYS
1	D	348	GLU
1	D	349	TRP
1	D	350	GLN
1	D	354	SER
1	D	365	LEU
1	D	381	SER
1	D	384	LEU
1	D	390	PHE
1	D	391	GLN
1	D	396	LEU
1	D	399	ARG
1	D	408	ARG
1	D	414	ASP
1	D	416	ASP
1	D	421	ARG
1	D	444	VAL
1	D	449	ASP
1	D	452	LEU
1	D	470	ILE
1	D	486	SER
1	D	489	THR
1	D	511	TRP
1	D	517	SER

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Mol	Chain	Res	Type
1	D	522	ASP
1	D	540	PHE
1	D	542	ARG
1	D	543	PHE
1	D	545	ARG
1	D	546	ASP
1	D	547	LEU
1	D	569	ILE
1	D	587	HIS
1	D	591	LEU
1	D	593	ARG
1	D	594	LEU
1	D	602	ASN
1	D	634	PHE
1	D	654	ASP
1	D	665	ILE
1	D	682	ARG
1	D	685	HIS
1	D	692	ARG
1	D	728	ARG
1	D	736	LEU
1	D	744	THR
1	D	754	ARG
1	D	764	THR
1	D	769	PHE
1	A	1	MET
1	A	3	THR
1	A	7	PHE
1	A	14	VAL
1	A	48	VAL
1	A	52	LEU
1	A	61	SER
1	A	62	ILE
1	A	63	CYS
1	A	64	PHE
1	A	65	LEU
1	A	68	VAL
1	A	75	ASN
1	A	77	THR
1	A	86	GLN
1	A	98	GLN
1	A	99	GLN

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Mol	Chain	Res	Type
1	A	101	MET
1	A	109	THR
1	A	127	GLU
1	A	140	THR
1	A	146	CYS
1	A	151	MET
1	A	152	ARG
1	A	153	TYR
1	A	157	ARG
1	A	163	ILE
1	A	164	ARG
1	A	165	SER
1	A	167	TYR
1	A	168	ASP
1	A	172	ARG
1	A	176	GLU
1	A	183	ILE
1	A	193	TYR
1	A	198	ASP
1	A	208	ILE
1	A	212	LYS
1	A	216	VAL
1	A	227	MET
1	A	234	MET
1	A	243	VAL
1	A	249	ILE
1	A	251	LEU
1	A	262	ASN
1	A	280	LEU
1	A	283	ASP
1	A	287	THR
1	A	292	LEU
1	A	304	THR
1	A	305	VAL
1	A	312	ARG
1	A	320	PHE
1	A	328	GLN
1	A	335	THR
1	A	342	LYS
1	A	348	GLU
1	A	349	TRP
1	A	358	PHE

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Mol	Chain	Res	Type
1	A	365	LEU
1	A	382	SER
1	A	384	LEU
1	A	390	PHE
1	A	391	GLN
1	A	396	LEU
1	A	400	LEU
1	A	408	ARG
1	A	421	ARG
1	A	444	VAL
1	A	449	ASP
1	A	452	LEU
1	A	458	ILE
1	A	468	HIS
1	A	470	ILE
1	A	483	ARG
1	A	489	THR
1	A	511	TRP
1	A	517	SER
1	A	522	ASP
1	A	528	LEU
1	A	540	PHE
1	A	542	ARG
1	A	543	PHE
1	A	545	ARG
1	A	546	ASP
1	A	547	LEU
1	A	558	SER
1	A	569	ILE
1	A	587	HIS
1	A	588	SER
1	A	591	LEU
1	A	592	THR
1	A	593	ARG
1	A	594	LEU
1	A	602	ASN
1	A	622	GLU
1	A	654	ASP
1	A	661	LEU
1	A	665	ILE
1	A	667	ASN
1	A	682	ARG

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Mol	Chain	Res	Type
1	A	685	HIS
1	A	728	ARG
1	A	736	LEU
1	A	744	THR
1	A	751	ARG
1	A	754	ARG
1	A	764	THR
1	A	769	PHE
1	B	1	MET
1	B	3	THR
1	B	7	PHE
1	B	14	VAL
1	B	16	GLN
1	B	46	SER
1	B	52	LEU
1	B	53	ASP
1	B	61	SER
1	B	62	ILE
1	B	63	CYS
1	B	64	PHE
1	B	65	LEU
1	B	68	VAL
1	B	75	ASN
1	B	82	LYS
1	B	86	GLN
1	B	89	SER
1	B	98	GLN
1	B	99	GLN
1	B	101	MET
1	B	109	THR
1	B	110	VAL
1	B	127	GLU
1	B	130	VAL
1	B	137	LEU
1	B	140	THR
1	B	146	CYS
1	B	157	ARG
1	B	163	ILE
1	B	164	ARG
1	B	165	SER
1	B	167	TYR
1	B	168	ASP

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Mol	Chain	Res	Type
1	B	172	ARG
1	B	176	GLU
1	B	183	ILE
1	B	193	TYR
1	B	198	ASP
1	B	200	VAL
1	B	206	VAL
1	B	208	ILE
1	B	211	ASP
1	B	212	LYS
1	B	213	THR
1	B	216	VAL
1	B	227	MET
1	B	228	ARG
1	B	234	MET
1	B	249	ILE
1	B	251	LEU
1	B	262	ASN
1	B	280	LEU
1	B	282	ASP
1	B	283	ASP
1	B	287	THR
1	B	292	LEU
1	B	312	ARG
1	B	320	PHE
1	B	328	GLN
1	B	339	ARG
1	B	342	LYS
1	B	348	GLU
1	B	349	TRP
1	B	350	GLN
1	B	354	SER
1	B	358	PHE
1	B	374	ASP
1	B	384	LEU
1	B	390	PHE
1	B	396	LEU
1	B	400	LEU
1	B	408	ARG
1	B	414	ASP
1	B	416	ASP
1	B	421	ARG

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Mol	Chain	Res	Type
1	B	429	GLN
1	B	444	VAL
1	B	446	SER
1	B	449	ASP
1	B	452	LEU
1	B	458	ILE
1	B	468	HIS
1	B	470	ILE
1	B	483	ARG
1	B	486	SER
1	B	489	THR
1	B	511	TRP
1	B	540	PHE
1	B	542	ARG
1	B	543	PHE
1	B	545	ARG
1	B	546	ASP
1	B	547	LEU
1	B	569	ILE
1	B	587	HIS
1	B	591	LEU
1	B	593	ARG
1	B	594	LEU
1	B	602	ASN
1	B	618	SER
1	B	634	PHE
1	B	636	THR
1	B	654	ASP
1	B	665	ILE
1	B	682	ARG
1	B	685	HIS
1	B	728	ARG
1	B	736	LEU
1	B	744	THR
1	B	754	ARG
1	B	764	THR
1	B	769	PHE
1	C	1	MET
1	C	3	THR
1	C	7	PHE
1	C	14	VAL
1	C	38	LEU

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Mol	Chain	Res	Type
1	C	46	SER
1	C	52	LEU
1	C	53	ASP
1	C	61	SER
1	C	62	ILE
1	C	64	PHE
1	C	65	LEU
1	C	68	VAL
1	C	75	ASN
1	C	86	GLN
1	C	89	SER
1	C	98	GLN
1	C	99	GLN
1	C	101	MET
1	C	106	LEU
1	C	109	THR
1	C	110	VAL
1	C	127	GLU
1	C	129	SER
1	C	130	VAL
1	C	137	LEU
1	C	140	THR
1	C	144	SER
1	C	145	ASN
1	C	151	MET
1	C	152	ARG
1	C	157	ARG
1	C	163	ILE
1	C	164	ARG
1	C	165	SER
1	C	167	TYR
1	C	172	ARG
1	C	176	GLU
1	C	183	ILE
1	C	198	ASP
1	C	200	VAL
1	C	212	LYS
1	C	213	THR
1	C	216	VAL
1	C	227	MET
1	C	234	MET
1	C	243	VAL

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Mol	Chain	Res	Type
1	C	249	ILE
1	C	251	LEU
1	C	255	THR
1	C	262	ASN
1	C	280	LEU
1	C	283	ASP
1	C	286	MET
1	C	287	THR
1	C	292	LEU
1	C	304	THR
1	C	312	ARG
1	C	319	MET
1	C	320	PHE
1	C	328	GLN
1	C	335	THR
1	C	337	LYS
1	C	339	ARG
1	C	342	LYS
1	C	348	GLU
1	C	349	TRP
1	C	350	GLN
1	C	356	LEU
1	C	358	PHE
1	C	365	LEU
1	C	374	ASP
1	C	381	SER
1	C	384	LEU
1	C	390	PHE
1	C	391	GLN
1	C	396	LEU
1	C	400	LEU
1	C	401	ASN
1	C	408	ARG
1	C	421	ARG
1	C	429	GLN
1	C	444	VAL
1	C	449	ASP
1	C	452	LEU
1	C	458	ILE
1	C	468	HIS
1	C	470	ILE
1	C	486	SER

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Mol	Chain	Res	Type
1	C	489	THR
1	C	511	TRP
1	C	514	SER
1	C	517	SER
1	C	522	ASP
1	C	528	LEU
1	C	540	PHE
1	C	542	ARG
1	C	543	PHE
1	C	545	ARG
1	C	546	ASP
1	C	547	LEU
1	C	587	HIS
1	C	591	LEU
1	C	592	THR
1	C	593	ARG
1	C	594	LEU
1	C	602	ASN
1	C	618	SER
1	C	627	GLU
1	C	634	PHE
1	C	636	THR
1	C	654	ASP
1	C	665	ILE
1	C	682	ARG
1	C	685	HIS
1	C	728	ARG
1	C	736	LEU
1	C	744	THR
1	C	754	ARG
1	C	764	THR
1	C	769	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	GLN
1	D	269	ASN
1	D	350	GLN
1	A	16	GLN
1	A	98	GLN
1	A	301	HIS

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Mol	Chain	Res	Type
1	A	667	ASN
1	B	31	GLN
1	B	377	GLN
1	B	663	ASN
1	C	50	HIS
1	C	98	GLN
1	C	350	GLN
1	C	401	ASN
1	C	712	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	771/771 (100%)	0.34	69 (8%) <b>9</b> <b>11</b>	22, 75, 151, 187	0
1	B	771/771 (100%)	0.90	164 (21%) <b>0</b> <b>1</b>	16, 102, 186, 207	0
1	C	771/771 (100%)	-0.07	38 (4%) <b>29</b> <b>28</b>	4, 50, 132, 180	0
1	D	771/771 (100%)	0.18	58 (7%) <b>14</b> <b>16</b>	8, 76, 152, 195	0
All	All	3084/3084 (100%)	0.34	329 (10%) <b>6</b> <b>7</b>	4, 72, 168, 207	0

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	GLY	14.3
1	B	722	GLU	13.0
1	A	719	GLY	10.2
1	D	718	SER	9.5
1	A	211	ASP	9.3
1	B	718	SER	9.1
1	A	718	SER	8.5
1	B	717	GLY	8.5
1	B	723	ILE	8.2
1	D	646	SER	8.1
1	B	702	ALA	7.8
1	A	675	GLU	7.7
1	D	716	LEU	7.7
1	D	717	GLY	7.6
1	A	676	ASN	7.5
1	A	646	SER	7.5
1	B	533	VAL	7.5
1	A	716	LEU	7.4
1	B	535	GLU	7.1
1	B	700	GLU	7.0
1	C	697	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	531	HIS	6.6
1	A	210	PRO	6.6
1	D	676	ASN	6.6
1	A	213	THR	6.3
1	B	532	VAL	6.2
1	B	716	LEU	6.2
1	D	677	ALA	6.1
1	A	647	SER	6.1
1	C	646	SER	6.0
1	C	718	SER	6.0
1	B	699	VAL	5.9
1	B	658	ASP	5.9
1	A	720	ALA	5.8
1	A	531	HIS	5.8
1	C	676	ASN	5.8
1	A	717	GLY	5.8
1	A	677	ALA	5.8
1	B	703	GLU	5.6
1	B	711	ALA	5.6
1	B	747	PHE	5.6
1	B	679	ALA	5.6
1	D	719	GLY	5.6
1	D	345	GLY	5.6
1	B	720	ALA	5.6
1	C	675	GLU	5.6
1	B	696	ALA	5.5
1	B	746	GLU	5.5
1	B	647	SER	5.4
1	B	537	MET	5.4
1	B	646	SER	5.4
1	A	715	ARG	5.3
1	B	630	ASN	5.3
1	B	725	ARG	5.1
1	B	636	THR	5.1
1	B	724	VAL	5.1
1	B	534	GLU	5.0
1	B	618	SER	5.0
1	A	485	SER	5.0
1	C	716	LEU	4.9
1	A	722	GLU	4.9
1	B	569	ILE	4.9
1	C	717	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	606	ASP	4.8
1	A	1	MET	4.8
1	B	621	LEU	4.7
1	A	535	GLU	4.7
1	B	707	ALA	4.7
1	D	675	GLU	4.6
1	D	534	GLU	4.6
1	B	651	TRP	4.5
1	C	647	SER	4.5
1	D	647	SER	4.4
1	C	714	LEU	4.4
1	D	1	MET	4.3
1	B	615	ARG	4.3
1	A	721	GLY	4.3
1	B	719	GLY	4.3
1	B	563	GLN	4.3
1	D	211	ASP	4.2
1	D	771	PRO	4.2
1	B	609	THR	4.2
1	A	729	TYR	4.2
1	B	666	GLY	4.2
1	C	719	GLY	4.2
1	B	516	GLY	4.1
1	B	698	THR	4.1
1	B	608	ALA	4.0
1	B	485	SER	4.0
1	B	617	LYS	4.0
1	B	448	ASP	3.9
1	D	721	GLY	3.9
1	B	211	ASP	3.9
1	B	536	GLY	3.9
1	D	715	ARG	3.9
1	B	680	SER	3.9
1	B	627	GLU	3.8
1	B	712	GLN	3.8
1	A	648	ASN	3.8
1	B	705	THR	3.8
1	B	371	SER	3.8
1	B	616	GLY	3.7
1	A	679	ALA	3.7
1	B	415	PRO	3.7
1	A	448	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	726	GLN	3.7
1	A	649	GLY	3.6
1	D	566	SER	3.6
1	D	723	ILE	3.6
1	B	632	GLU	3.6
1	B	610	PRO	3.6
1	C	616	GLY	3.6
1	B	629	TRP	3.6
1	A	533	VAL	3.6
1	C	715	ARG	3.5
1	B	500	ALA	3.5
1	B	739	ARG	3.5
1	A	540	PHE	3.5
1	B	503	SER	3.5
1	C	1	MET	3.5
1	B	701	GLU	3.5
1	B	607	SER	3.5
1	B	740	GLU	3.5
1	D	210	PRO	3.5
1	B	752	SER	3.5
1	B	708	ASP	3.4
1	A	212	LYS	3.4
1	B	625	GLU	3.4
1	C	740	GLU	3.4
1	B	735	ALA	3.4
1	A	771	PRO	3.4
1	D	729	TYR	3.3
1	B	648	ASN	3.3
1	D	346	LEU	3.3
1	A	215	GLY	3.3
1	B	678	SER	3.3
1	B	697	ALA	3.3
1	C	677	ALA	3.3
1	A	544	GLU	3.3
1	B	750	ALA	3.3
1	A	645	PRO	3.2
1	D	746	GLU	3.2
1	B	345	GLY	3.2
1	D	685	HIS	3.2
1	B	768	GLY	3.2
1	B	685	HIS	3.2
1	B	742	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	241	ALA	3.2
1	A	698	THR	3.2
1	B	491	GLU	3.2
1	B	484	LEU	3.2
1	B	640	VAL	3.2
1	D	722	GLU	3.2
1	D	742	GLU	3.2
1	D	648	ASN	3.2
1	B	450	ALA	3.2
1	B	493	SER	3.2
1	A	680	SER	3.1
1	C	531	HIS	3.1
1	D	538	PRO	3.1
1	A	697	ALA	3.1
1	B	753	GLN	3.1
1	B	764	THR	3.1
1	A	681	ASN	3.1
1	B	492	SER	3.1
1	A	725	ARG	3.1
1	A	534	GLU	3.0
1	B	506	ALA	3.0
1	A	371	SER	3.0
1	B	713	GLY	3.0
1	B	504	CYS	3.0
1	C	685	HIS	3.0
1	B	447	CYS	3.0
1	B	509	ALA	2.9
1	B	675	GLU	2.9
1	D	246	GLU	2.9
1	B	581	MET	2.9
1	C	771	PRO	2.9
1	C	725	ARG	2.9
1	B	710	GLU	2.9
1	A	214	ASP	2.9
1	B	614	VAL	2.9
1	A	486	SER	2.9
1	D	678	SER	2.9
1	D	657	GLU	2.9
1	D	770	GLU	2.9
1	A	547	LEU	2.9
1	A	723	ILE	2.8
1	B	690	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	567	GLU	2.8
1	B	550	VAL	2.8
1	C	738	GLN	2.8
1	D	712	GLN	2.8
1	B	745	ALA	2.8
1	B	654	ASP	2.8
1	B	765	PRO	2.8
1	D	720	ALA	2.8
1	C	59	GLU	2.8
1	B	577	ALA	2.8
1	A	345	GLY	2.8
1	B	514	SER	2.8
1	B	676	ASN	2.8
1	D	656	TYR	2.8
1	C	696	ALA	2.8
1	B	715	ARG	2.7
1	D	344	GLU	2.7
1	D	645	PRO	2.7
1	B	681	ASN	2.7
1	B	741	GLU	2.7
1	B	706	LEU	2.7
1	A	567	GLU	2.7
1	B	659	PRO	2.7
1	B	605	PRO	2.7
1	D	724	VAL	2.7
1	B	624	LEU	2.7
1	D	711	ALA	2.6
1	C	688	ARG	2.6
1	C	678	SER	2.6
1	A	700	GLU	2.6
1	C	345	GLY	2.6
1	B	458	ILE	2.6
1	A	703	GLU	2.6
1	C	698	THR	2.6
1	B	562	GLU	2.6
1	D	342	LYS	2.6
1	A	484	LEU	2.6
1	A	538	PRO	2.6
1	D	539	ARG	2.6
1	B	744	THR	2.6
1	C	704	LYS	2.5
1	B	686	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	704	LYS	2.5
1	B	763	LEU	2.5
1	B	559	TYR	2.5
1	C	743	TRP	2.5
1	B	667	ASN	2.5
1	B	657	GLU	2.5
1	A	644	ALA	2.5
1	B	242	GLY	2.5
1	B	645	PRO	2.5
1	B	465	GLU	2.5
1	D	649	GLY	2.5
1	B	576	VAL	2.5
1	B	573	GLN	2.5
1	D	535	GLU	2.5
1	C	607	SER	2.5
1	D	569	ILE	2.5
1	A	542	ARG	2.5
1	B	749	GLU	2.5
1	B	285	LYS	2.5
1	C	700	GLU	2.4
1	B	714	LEU	2.4
1	D	608	ALA	2.4
1	B	709	ALA	2.4
1	A	724	VAL	2.4
1	C	674	VAL	2.4
1	B	501	ALA	2.4
1	D	484	LEU	2.4
1	A	678	SER	2.4
1	A	699	VAL	2.4
1	B	540	PHE	2.4
1	B	637	ILE	2.4
1	B	684	TRP	2.4
1	B	416	ASP	2.4
1	B	644	ALA	2.4
1	A	446	SER	2.4
1	B	586	GLN	2.4
1	B	655	LEU	2.4
1	D	245	ARG	2.3
1	D	726	GLN	2.3
1	A	617	LYS	2.3
1	B	604	THR	2.3
1	B	652	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	198	ASP	2.3
1	B	538	PRO	2.2
1	B	505	ALA	2.2
1	B	687	LYS	2.2
1	D	371	SER	2.2
1	D	684	TRP	2.2
1	B	566	SER	2.2
1	B	515	PHE	2.2
1	B	125	ASP	2.2
1	B	571	ASP	2.2
1	C	281	GLU	2.2
1	B	210	PRO	2.2
1	D	485	SER	2.2
1	A	714	LEU	2.2
1	D	725	ARG	2.2
1	B	650	SER	2.2
1	B	619	GLY	2.2
1	A	620	LEU	2.2
1	C	689	LEU	2.2
1	A	551	PRO	2.1
1	B	281	GLU	2.1
1	B	622	GLU	2.1
1	C	566	SER	2.1
1	B	631	ASP	2.1
1	B	635	ALA	2.1
1	A	226	ARG	2.1
1	B	482	HIS	2.1
1	B	643	GLN	2.1
1	C	210	PRO	2.1
1	B	579	ALA	2.1
1	D	744	THR	2.1
1	A	489	THR	2.1
1	B	770	GLU	2.1
1	A	487	PRO	2.1
1	A	570	TYR	2.1
1	A	353	GLU	2.1
1	B	442	THR	2.1
1	C	648	ASN	2.1
1	C	645	PRO	2.1
1	B	674	VAL	2.1
1	B	649	GLY	2.1
1	A	728	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	243	VAL	2.1
1	C	695	SER	2.1
1	A	539	ARG	2.1
1	B	370	SER	2.1
1	D	488	GLU	2.0
1	B	641	ALA	2.0
1	B	628	ARG	2.0
1	A	696	ALA	2.0
1	D	215	GLY	2.0
1	B	561	LYS	2.0
1	B	771	PRO	2.0
1	A	414	ASP	2.0
1	D	197	PRO	2.0
1	D	570	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.