W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:32 PM GMT

PDB ID	:	4SBV
Title	:	The REFINEMENT OF SOUTHERN BEAN MOSAIC VIRUS IN RECIP-ROCAL SPACE
Authors	:	Rossmann, M.G.
Deposited on	:	1985-04-01
Resolution	:	2.80 Å(reported)

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

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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		58
Ramachandran outliers		3.9%
Sidechain outliers		29.7%
RSRZ outliers		79.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
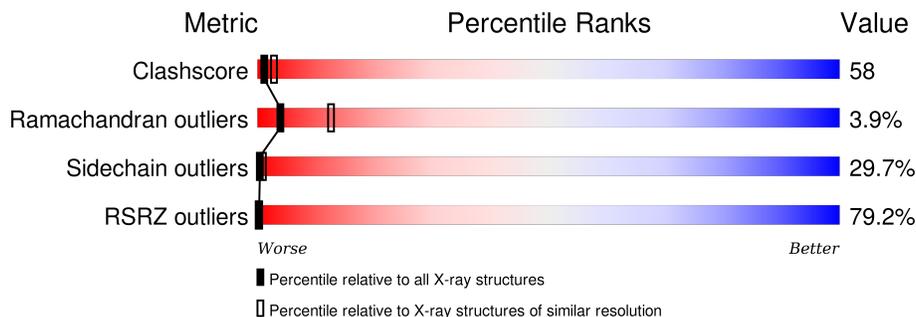
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	260	55% 16% 35% 17% 9% 23%
1	B	260	66% 8% 34% 24% 11% 23%
1	C	260	68% 7% 43% 26% 10% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4723 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 SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total 1506	C 956	N 249	O 292	S 9	0	0	0
1	B	199	Total 1506	C 956	N 249	O 292	S 9	0	0	0
1	C	222	Total 1674	C 1062	N 281	O 319	S 12	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ca 1	0	0
2	A	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total 15	O 15	0	0
3	B	10	Total 10	O 10	0	0
3	C	9	Total 9	O 9	0	0

3   Residue-property plots ⓘ

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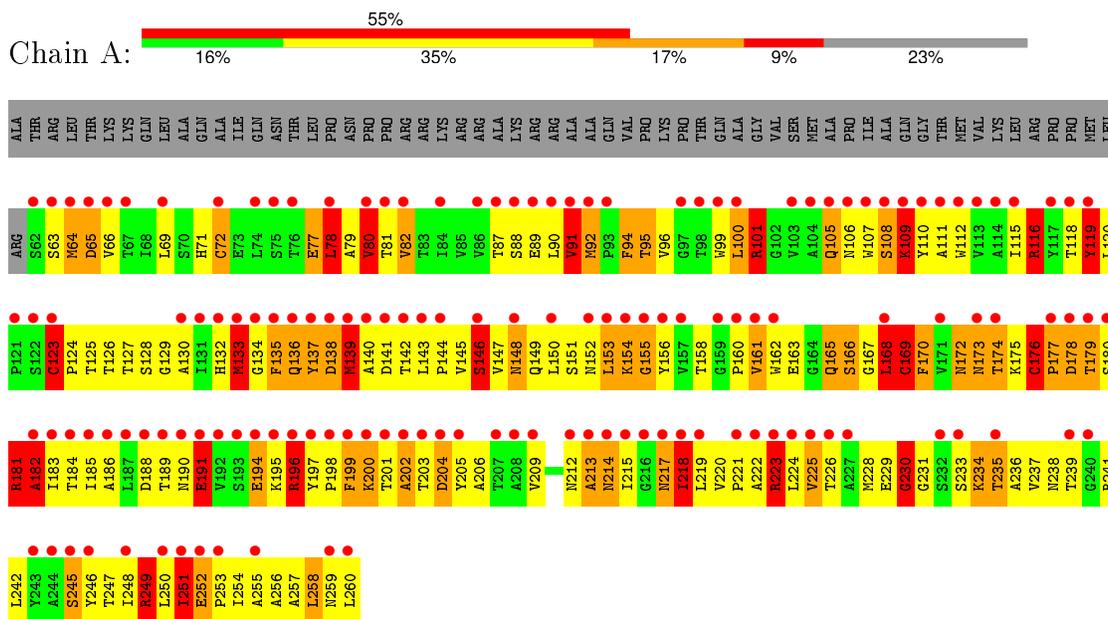
Chain A:

- Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain B:

• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain C:

68%

7%   43%   26%   10%   15%
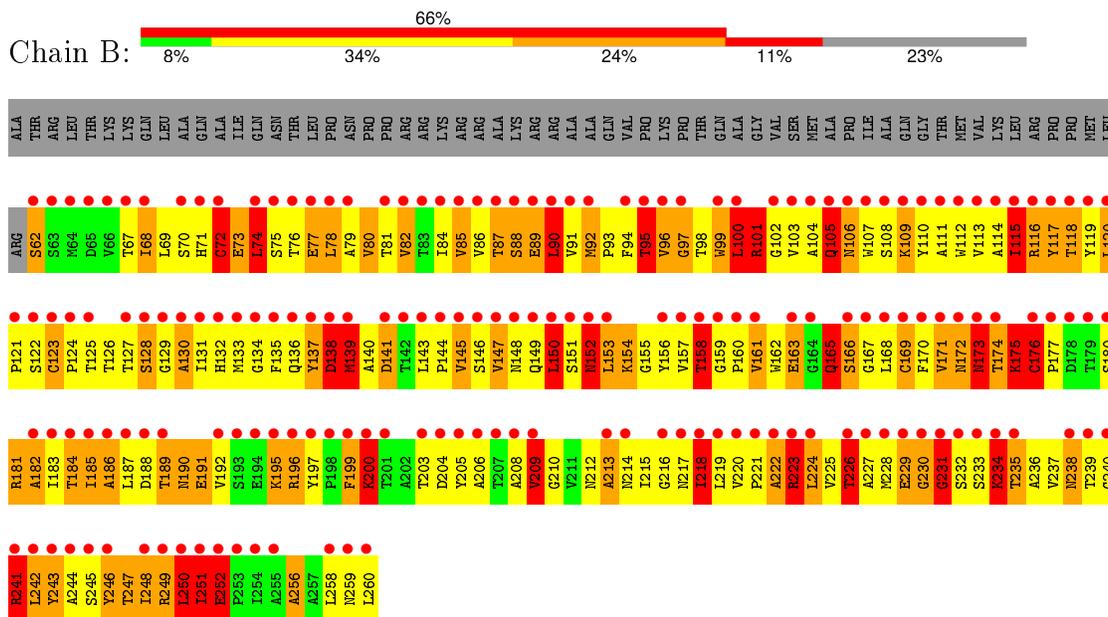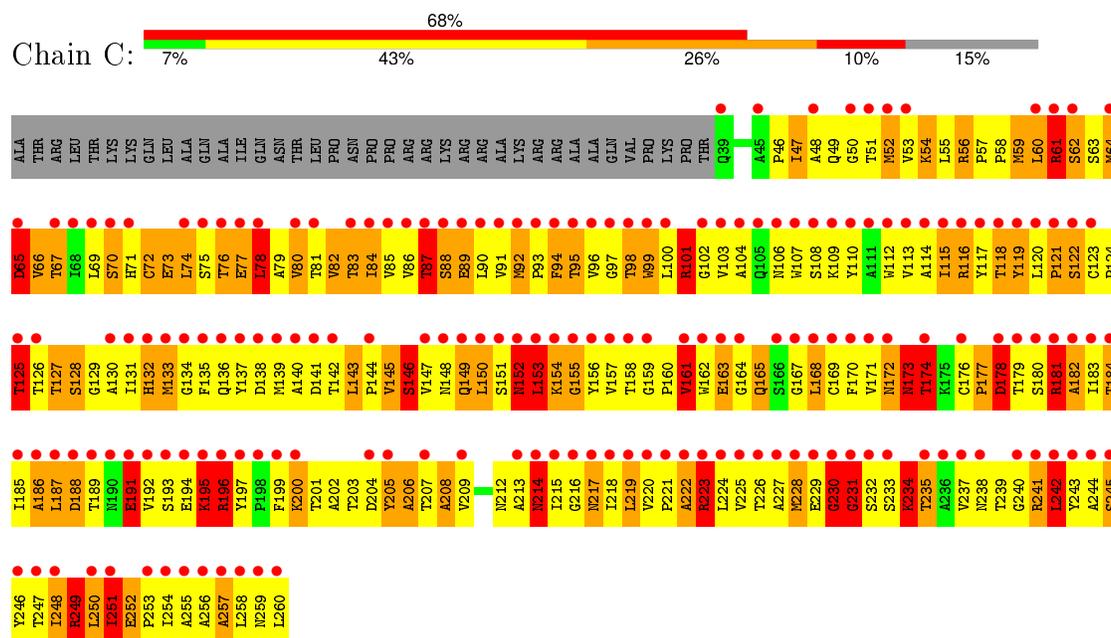
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	334.30Å 334.30Å 757.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) − 2.80 142.18 − 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 75.4 (142.18-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available) 0.515 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 923.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$<|L|> = 0.39, <L^2> = 0.22$	Xtriage
Outliers	10 of 298615 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.22	EDS
Total number of atoms	4723	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.47	8/1537 (0.5%)	2.64	103/2104 (4.9%)
1	B	1.43	7/1537 (0.5%)	2.46	106/2104 (5.0%)
1	C	1.48	11/1708 (0.6%)	2.55	96/2335 (4.1%)
All	All	1.46	26/4782 (0.5%)	2.55	305/6543 (4.7%)

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	3
1	B	0	3
1	C	0	4
All	All	0	10

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	GLU	N-CA	10.24	1.66	1.46
1	C	155	GLY	N-CA	9.10	1.59	1.46
1	B	231	GLY	N-CA	-8.86	1.32	1.46
1	C	231	GLY	N-CA	-8.81	1.32	1.46
1	A	230	GLY	N-CA	8.31	1.58	1.46
1	A	155	GLY	N-CA	7.50	1.57	1.46
1	A	252	GLU	N-CA	6.93	1.60	1.46
1	C	251	ILE	C-O	6.72	1.36	1.23
1	C	231	GLY	CA-C	-6.64	1.41	1.51
1	B	251	ILE	C-O	6.62	1.35	1.23
1	A	194	GLU	CB-CG	6.27	1.64	1.52
1	C	231	GLY	C-O	6.05	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	CD-OE1	-5.74	1.19	1.25
1	A	109	LYS	CA-CB	-5.72	1.41	1.53
1	A	168	LEU	C-O	5.71	1.34	1.23
1	B	252	GLU	CA-CB	-5.67	1.41	1.53
1	B	252	GLU	N-CA	5.65	1.57	1.46
1	B	176	CYS	CB-SG	5.58	1.91	1.82
1	B	137	TYR	C-O	5.52	1.33	1.23
1	C	252	GLU	CA-CB	-5.46	1.42	1.53
1	C	252	GLU	CB-CG	-5.33	1.42	1.52
1	C	64	MET	CA-CB	-5.32	1.42	1.53
1	C	133	MET	CA-CB	-5.32	1.42	1.53
1	B	97	GLY	N-CA	5.14	1.53	1.46
1	C	56	ARG	CZ-NH2	5.06	1.39	1.33
1	A	123	CYS	CB-SG	-5.03	1.73	1.81

All (305) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ARG	NE-CZ-NH1	31.30	135.95	120.30
1	C	101	ARG	NE-CZ-NH1	26.03	133.32	120.30
1	A	109	LYS	CA-CB-CG	25.72	169.98	113.40
1	A	196	ARG	NE-CZ-NH2	-18.85	110.87	120.30
1	A	125	THR	N-CA-CB	17.78	144.08	110.30
1	B	241	ARG	NE-CZ-NH2	-17.49	111.56	120.30
1	C	231	GLY	N-CA-C	16.71	154.87	113.10
1	C	101	ARG	NE-CZ-NH2	-16.52	112.04	120.30
1	C	252	GLU	CA-CB-CG	15.42	147.32	113.40
1	C	196	ARG	NE-CZ-NH2	-15.35	112.62	120.30
1	C	241	ARG	NE-CZ-NH1	-13.64	113.48	120.30
1	C	56	ARG	NE-CZ-NH1	13.19	126.90	120.30
1	B	231	GLY	N-CA-C	12.93	145.43	113.10
1	A	196	ARG	CD-NE-CZ	12.60	141.25	123.60
1	A	223	ARG	CD-NE-CZ	-12.53	106.06	123.60
1	C	173	ASN	C-N-CA	12.13	152.02	121.70
1	B	252	GLU	OE1-CD-OE2	-11.62	109.36	123.30
1	A	181	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	B	251	ILE	CA-C-N	11.34	142.16	117.20
1	A	101	ARG	NE-CZ-NH1	11.21	125.90	120.30
1	C	249	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	C	241	ARG	NE-CZ-NH2	10.99	125.80	120.30
1	C	252	GLU	CB-CA-C	10.79	131.99	110.40
1	C	251	ILE	CA-C-N	10.78	140.91	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	74	LEU	N-CA-CB	10.75	131.90	110.40
1	A	168	LEU	CA-C-N	10.61	140.53	117.20
1	A	176	CYS	CA-CB-SG	10.29	132.53	114.00
1	B	251	ILE	CA-C-O	-10.28	98.52	120.10
1	A	178	ASP	C-N-CA	10.18	147.16	121.70
1	C	153	LEU	CA-CB-CG	10.06	138.45	115.30
1	A	168	LEU	CA-C-O	-10.04	99.02	120.10
1	A	169	CYS	CA-CB-SG	9.90	131.83	114.00
1	A	191	GLU	CA-CB-CG	9.90	135.19	113.40
1	C	214	ASN	CB-CA-C	9.85	130.09	110.40
1	B	90	LEU	CA-CB-CG	9.81	137.88	115.30
1	C	133	MET	CA-CB-CG	9.79	129.94	113.30
1	B	72	CYS	CA-CB-SG	-9.76	96.44	114.00
1	A	241	ARG	NE-CZ-NH1	-9.67	115.46	120.30
1	C	178	ASP	CB-CG-OD1	9.56	126.91	118.30
1	B	223	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	101	ARG	CG-CD-NE	9.32	131.37	111.80
1	B	74	LEU	O-C-N	9.27	137.53	122.70
1	C	73	GLU	CA-CB-CG	9.21	133.65	113.40
1	C	59	MET	CA-CB-CG	-9.08	97.87	113.30
1	B	138	ASP	O-C-N	8.91	136.95	122.70
1	A	181	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	123	CYS	CB-CA-C	-8.63	93.13	110.40
1	C	251	ILE	CA-C-O	-8.62	102.00	120.10
1	C	154	LYS	CA-C-N	8.57	133.35	116.20
1	A	178	ASP	CB-CA-C	8.49	127.37	110.40
1	C	249	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	69	LEU	O-C-N	8.42	136.18	122.70
1	A	138	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	204	ASP	CB-CG-OD1	8.38	125.84	118.30
1	A	249	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	A	146	SER	N-CA-CB	-8.35	97.97	110.50
1	A	218	ILE	CB-CA-C	-8.30	95.00	111.60
1	B	163	GLU	CG-CD-OE2	-8.26	101.78	118.30
1	C	196	ARG	N-CA-CB	8.15	125.27	110.60
1	B	223	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	B	176	CYS	CA-CB-SG	-8.05	99.51	114.00
1	B	230	GLY	C-N-CA	8.04	139.19	122.30
1	A	80	VAL	CB-CA-C	-7.97	96.25	111.40
1	B	223	ARG	NH1-CZ-NH2	7.97	128.16	119.40
1	B	252	GLU	CG-CD-OE1	7.95	134.20	118.30
1	B	246	TYR	CB-CG-CD2	7.91	125.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	165	GLN	CA-CB-CG	-7.82	96.20	113.40
1	A	190	ASN	CB-CA-C	-7.79	94.82	110.40
1	C	110	TYR	CB-CG-CD1	7.75	125.65	121.00
1	B	196	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	251	ILE	N-CA-C	7.75	131.91	111.00
1	A	251	ILE	CA-C-N	7.73	134.21	117.20
1	C	214	ASN	N-CA-CB	-7.73	96.68	110.60
1	C	65	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	B	158	THR	O-C-N	7.46	135.88	123.20
1	C	95	THR	CA-CB-OG1	-7.39	93.48	109.00
1	C	248	ILE	N-CA-CB	-7.34	93.92	110.80
1	A	111	ALA	N-CA-CB	7.33	120.36	110.10
1	B	252	GLU	CA-CB-CG	7.30	129.46	113.40
1	A	175	LYS	N-CA-CB	7.25	123.65	110.60
1	A	101	ARG	CD-NE-CZ	7.20	133.68	123.60
1	C	154	LYS	CA-C-O	-7.20	104.99	120.10
1	A	252	GLU	CB-CA-C	7.12	124.65	110.40
1	C	230	GLY	N-CA-C	7.11	130.88	113.10
1	B	139	MET	CA-CB-CG	-7.06	101.30	113.30
1	B	241	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	B	141	ASP	CB-CA-C	7.02	124.45	110.40
1	C	196	ARG	CA-CB-CG	7.01	128.83	113.40
1	B	241	ARG	CD-NE-CZ	-7.01	113.79	123.60
1	C	64	MET	CA-CB-CG	7.00	125.19	113.30
1	A	179	THR	CA-C-N	-6.99	101.83	117.20
1	B	150	LEU	CA-CB-CG	6.97	131.34	115.30
1	C	133	MET	CB-CA-C	6.97	124.34	110.40
1	C	61	ARG	CA-CB-CG	6.94	128.68	113.40
1	A	170	PHE	CB-CA-C	6.92	124.24	110.40
1	A	251	ILE	CA-C-O	-6.92	105.58	120.10
1	B	246	TYR	CB-CG-CD1	-6.89	116.87	121.00
1	C	62	SER	N-CA-CB	-6.87	100.20	110.50
1	B	92	MET	CA-CB-CG	6.86	124.96	113.30
1	C	56	ARG	CD-NE-CZ	6.86	133.20	123.60
1	C	217	ASN	CA-C-O	-6.84	105.74	120.10
1	A	168	LEU	CA-CB-CG	6.83	131.00	115.30
1	B	191	GLU	CG-CD-OE1	6.83	131.96	118.30
1	B	243	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	B	252	GLU	N-CA-C	-6.82	92.60	111.00
1	B	185	ILE	CB-CG1-CD1	6.79	132.91	113.90
1	C	213	ALA	C-N-CA	-6.78	104.74	121.70
1	C	73	GLU	CG-CD-OE1	6.77	131.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLU	CG-CD-OE1	6.76	131.82	118.30
1	B	115	ILE	CA-CB-CG1	-6.75	98.17	111.00
1	B	130	ALA	CB-CA-C	-6.74	99.99	110.10
1	B	169	CYS	CA-CB-SG	-6.73	101.88	114.00
1	A	153	LEU	CB-CA-C	6.73	122.98	110.20
1	A	178	ASP	CA-C-O	6.70	134.16	120.10
1	A	136	GLN	CB-CA-C	6.69	123.78	110.40
1	A	258	LEU	N-CA-CB	-6.68	97.04	110.40
1	C	146	SER	N-CA-CB	-6.55	100.68	110.50
1	B	105	GLN	CA-CB-CG	6.53	127.77	113.40
1	A	249	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	B	96	VAL	CA-CB-CG1	6.46	120.58	110.90
1	C	73	GLU	CG-CD-OE2	-6.44	105.42	118.30
1	C	242	LEU	CB-CA-C	6.43	122.42	110.20
1	A	116	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	138	ASP	N-CA-C	-6.42	93.65	111.00
1	C	56	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	145	VAL	C-N-CA	6.41	137.71	121.70
1	C	188	ASP	CB-CA-C	6.41	123.21	110.40
1	A	194	GLU	CG-CD-OE2	-6.40	105.50	118.30
1	A	154	LYS	CA-C-N	6.37	128.93	116.20
1	B	168	LEU	CA-CB-CG	6.36	129.94	115.30
1	C	251	ILE	CA-CB-CG1	-6.34	98.96	111.00
1	A	178	ASP	CA-CB-CG	6.33	127.33	113.40
1	B	195	LYS	CD-CE-NZ	6.29	126.16	111.70
1	B	117	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	138	ASP	CA-CB-CG	6.27	127.20	113.40
1	A	78	LEU	O-C-N	6.26	132.72	122.70
1	A	69	LEU	CA-C-N	-6.24	103.47	117.20
1	A	125	THR	CB-CA-C	-6.24	94.75	111.60
1	B	68	ILE	O-C-N	6.23	132.66	122.70
1	C	206	ALA	N-CA-CB	-6.22	101.39	110.10
1	B	166	SER	O-C-N	6.22	133.78	123.20
1	B	251	ILE	CA-CB-CG1	-6.22	99.19	111.00
1	C	77	GLU	N-CA-CB	6.21	121.78	110.60
1	C	204	ASP	N-CA-CB	6.20	121.77	110.60
1	B	89	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	A	133	MET	O-C-N	6.18	133.72	123.20
1	C	188	ASP	N-CA-C	-6.18	94.30	111.00
1	C	196	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	72	CYS	CA-CB-SG	-6.14	102.94	114.00
1	B	96	VAL	CB-CA-C	6.14	123.07	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	ILE	CA-C-O	6.12	132.96	120.10
1	C	94	PHE	CA-C-N	-6.10	103.78	117.20
1	A	169	CYS	O-C-N	6.08	132.44	122.70
1	A	137	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	174	THR	CA-CB-CG2	6.05	120.87	112.40
1	A	182	ALA	O-C-N	6.02	132.33	122.70
1	C	173	ASN	CA-CB-CG	6.02	126.64	113.40
1	A	235	THR	CA-CB-OG1	-6.01	96.37	109.00
1	B	89	GLU	CB-CG-CD	6.00	130.39	114.20
1	B	226	THR	CA-CB-CG2	5.98	120.77	112.40
1	B	174	THR	N-CA-C	-5.95	94.94	111.00
1	A	166	SER	N-CA-CB	-5.95	101.58	110.50
1	B	209	VAL	CB-CA-C	5.95	122.70	111.40
1	A	217	ASN	CB-CG-OD1	5.94	133.49	121.60
1	C	252	GLU	N-CA-C	-5.94	94.96	111.00
1	A	251	ILE	N-CA-C	5.92	126.99	111.00
1	B	181	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	109	LYS	CG-CD-CE	5.92	129.66	111.90
1	C	163	GLU	CG-CD-OE2	-5.92	106.47	118.30
1	B	128	SER	N-CA-CB	-5.91	101.63	110.50
1	B	186	ALA	CB-CA-C	5.87	118.90	110.10
1	B	96	VAL	CA-CB-CG2	-5.83	102.15	110.90
1	B	173	ASN	CA-C-N	-5.83	104.37	117.20
1	B	163	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	A	116	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	224	LEU	CA-C-O	-5.81	107.89	120.10
1	A	179	THR	CA-C-O	5.81	132.29	120.10
1	C	186	ALA	N-CA-CB	-5.80	101.98	110.10
1	C	76	THR	CA-C-O	-5.78	107.96	120.10
1	A	196	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
1	C	146	SER	CA-CB-OG	5.76	126.76	111.20
1	A	91	VAL	CB-CA-C	5.76	122.34	111.40
1	B	95	THR	CA-CB-CG2	5.74	120.43	112.40
1	B	200	LYS	CD-CE-NZ	5.72	124.85	111.70
1	A	241	ARG	NH1-CZ-NH2	5.71	125.67	119.40
1	A	65	ASP	N-CA-CB	5.70	120.86	110.60
1	B	99	TRP	CA-CB-CG	5.68	124.50	113.70
1	B	138	ASP	CA-C-O	-5.67	108.19	120.10
1	C	152	ASN	CA-CB-CG	5.67	125.86	113.40
1	B	158	THR	N-CA-CB	5.65	121.04	110.30
1	C	119	TYR	N-CA-CB	-5.65	100.42	110.60
1	C	234	LYS	C-N-CA	5.65	135.83	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	SER	CB-CA-C	5.65	120.83	110.10
1	C	154	LYS	C-N-CA	-5.62	110.50	122.30
1	B	234	LYS	CA-CB-CG	5.58	125.68	113.40
1	B	73	GLU	CA-CB-CG	5.57	125.66	113.40
1	A	169	CYS	N-CA-C	-5.57	95.96	111.00
1	C	110	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	A	178	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	191	GLU	CG-CD-OE2	-5.54	107.22	118.30
1	C	99	TRP	O-C-N	5.52	131.53	122.70
1	B	80	VAL	O-C-N	5.51	131.52	122.70
1	C	143	LEU	CB-CG-CD2	-5.51	101.64	111.00
1	B	99	TRP	CB-CA-C	5.50	121.40	110.40
1	A	230	GLY	N-CA-C	-5.50	99.36	113.10
1	B	246	TYR	O-C-N	5.50	131.50	122.70
1	C	110	TYR	O-C-N	5.49	131.49	122.70
1	B	77	GLU	CG-CD-OE1	5.49	129.28	118.30
1	A	223	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	174	THR	CA-CB-OG1	-5.46	97.52	109.00
1	A	252	GLU	CG-CD-OE2	-5.46	107.38	118.30
1	B	184	THR	CA-CB-CG2	-5.45	104.77	112.40
1	B	120	LEU	CB-CA-C	5.45	120.55	110.20
1	A	213	ALA	O-C-N	5.44	131.40	122.70
1	C	95	THR	CA-CB-CG2	5.44	120.01	112.40
1	A	105	GLN	O-C-N	5.44	131.40	122.70
1	A	116	ARG	NH1-CZ-NH2	5.43	125.38	119.40
1	C	138	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	243	TYR	CB-CG-CD1	5.41	124.25	121.00
1	B	152	ASN	CA-C-O	-5.40	108.76	120.10
1	C	173	ASN	N-CA-CB	5.39	120.31	110.60
1	C	163	GLU	CG-CD-OE1	5.39	129.08	118.30
1	B	123	CYS	CA-CB-SG	-5.39	104.30	114.00
1	B	174	THR	O-C-N	5.39	131.32	122.70
1	B	182	ALA	O-C-N	5.37	131.29	122.70
1	C	161	VAL	N-CA-CB	-5.37	99.69	111.50
1	C	250	LEU	CB-CA-C	5.37	120.40	110.20
1	A	241	ARG	CD-NE-CZ	-5.37	116.09	123.60
1	A	252	GLU	N-CA-C	-5.37	96.51	111.00
1	A	229	GLU	CA-C-O	-5.36	108.84	120.10
1	C	87	THR	N-CA-CB	-5.36	100.12	110.30
1	A	115	ILE	O-C-N	5.35	131.26	122.70
1	C	101	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
1	C	222	ALA	N-CA-CB	-5.35	102.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	252	GLU	CB-CA-C	5.34	121.09	110.40
1	C	89	GLU	CB-CA-C	-5.34	99.72	110.40
1	C	138	ASP	CB-CA-C	5.34	121.08	110.40
1	B	141	ASP	N-CA-CB	-5.34	101.00	110.60
1	B	100	LEU	O-C-N	5.33	131.23	122.70
1	A	217	ASN	C-N-CA	5.33	135.02	121.70
1	A	247	THR	N-CA-CB	5.33	120.42	110.30
1	A	188	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	191	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	C	230	GLY	O-C-N	-5.31	114.18	123.20
1	B	173	ASN	CA-C-O	5.30	131.24	120.10
1	C	174	THR	CA-CB-CG2	5.30	119.83	112.40
1	A	82	VAL	CA-CB-CG1	5.29	118.84	110.90
1	A	137	TYR	N-CA-CB	-5.28	101.09	110.60
1	B	247	THR	O-C-N	5.28	131.15	122.70
1	C	217	ASN	CB-CG-OD1	-5.28	111.04	121.60
1	C	168	LEU	CA-CB-CG	-5.28	103.16	115.30
1	A	72	CYS	O-C-N	5.28	131.14	122.70
1	A	251	ILE	N-CA-CB	-5.27	98.68	110.80
1	B	256	ALA	CA-C-N	-5.27	105.61	117.20
1	A	111	ALA	O-C-N	5.26	131.11	122.70
1	B	218	ILE	N-CA-CB	5.25	122.88	110.80
1	B	252	GLU	CB-CG-CD	5.25	128.37	114.20
1	A	247	THR	O-C-N	5.24	131.08	122.70
1	A	77	GLU	CG-CD-OE1	5.23	128.77	118.30
1	A	204	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	B	73	GLU	CA-C-O	-5.22	109.15	120.10
1	B	238	ASN	CA-C-O	-5.21	109.15	120.10
1	C	188	ASP	CA-CB-CG	5.21	124.87	113.40
1	A	116	ARG	N-CA-CB	-5.21	101.22	110.60
1	B	222	ALA	N-CA-CB	-5.20	102.82	110.10
1	C	78	LEU	N-CA-CB	-5.20	100.00	110.40
1	A	135	PHE	O-C-N	5.18	131.00	122.70
1	C	116	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	223	ARG	O-C-N	5.17	130.97	122.70
1	B	204	ASP	CA-CB-CG	-5.17	102.04	113.40
1	C	195	LYS	CA-CB-CG	5.16	124.76	113.40
1	C	132	HIS	O-C-N	5.16	130.95	122.70
1	A	128	SER	CA-C-O	-5.16	109.27	120.10
1	B	77	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	95	THR	CB-CA-C	-5.15	97.68	111.60
1	B	250	LEU	O-C-N	5.14	130.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	77	GLU	CA-CB-CG	5.13	124.70	113.40
1	C	208	ALA	CA-C-O	5.13	130.88	120.10
1	B	165	GLN	OE1-CD-NE2	5.12	133.69	121.90
1	B	175	LYS	CB-CA-C	5.12	120.65	110.40
1	A	119	TYR	O-C-N	5.12	130.88	122.70
1	C	216	GLY	O-C-N	5.11	130.88	122.70
1	C	199	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	C	73	GLU	CB-CA-C	5.11	120.61	110.40
1	C	181	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	182	ALA	CB-CA-C	5.10	117.76	110.10
1	A	168	LEU	N-CA-C	-5.10	97.23	111.00
1	C	77	GLU	CG-CD-OE2	-5.10	108.10	118.30
1	B	206	ALA	CB-CA-C	5.09	117.74	110.10
1	B	67	THR	CA-CB-OG1	-5.09	98.31	109.00
1	A	133	MET	N-CA-CB	5.09	119.76	110.60
1	A	194	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	B	206	ALA	N-CA-CB	-5.07	103.00	110.10
1	A	213	ALA	CA-C-O	-5.07	109.46	120.10
1	A	218	ILE	O-C-N	5.07	130.81	122.70
1	B	174	THR	N-CA-CB	5.05	119.89	110.30
1	C	116	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	229	GLU	C-N-CA	-5.03	111.73	122.30
1	B	74	LEU	N-CA-C	-5.03	97.42	111.00
1	C	235	THR	CA-CB-OG1	-5.03	98.44	109.00
1	A	77	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	A	236	ALA	N-CA-CB	-5.02	103.07	110.10
1	A	112	TRP	CA-C-O	-5.01	109.58	120.10
1	A	78	LEU	CA-C-N	-5.01	106.18	117.20
1	B	109	LYS	CB-CA-C	5.01	120.41	110.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	249	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	241	ARG	Sidechain
1	B	249	ARG	Sidechain
1	C	101	ARG	Sidechain
1	C	181	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	196	ARG	Sidechain
1	C	223	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1506	0	1504	207	87
1	B	1506	0	1504	182	1771
1	C	1674	0	1691	187	1943
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	1	1
3	B	10	0	0	0	6
3	C	9	0	0	0	15
All	All	4723	0	4699	540	2046

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 58.

All (540) 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:C:212:ASN:ND2	1:C:214:ASN:H	1.42	1.15
1:C:145:VAL:H	1:C:149:GLN:NE2	1.46	1.11
1:C:161:VAL:HG22	1:C:239:THR:CG2	1.82	1.08
1:C:161:VAL:HG22	1:C:239:THR:HG21	1.09	1.07
1:C:131:ILE:HG13	1:C:228:MET:HE2	1.34	1.06
1:A:168:LEU:O	1:A:169:CYS:HB2	1.57	1.04
1:A:165:GLN:HA	1:A:165:GLN:HE21	1.21	1.03
1:C:187:LEU:HD22	1:C:188:ASP:H	1.19	1.02
1:A:201:THR:HG22	1:A:260:LEU:OXT	1.61	1.01
1:C:54:LYS:H	1:C:172:ASN:HD21	0.99	0.95
1:A:105:GLN:HA	1:A:199:PHE:CE1	2.01	0.95
1:C:119:TYR:OH	1:C:239:THR:HG22	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:VAL:H	1:C:149:GLN:HE22	1.07	0.93
1:C:139:MET:H	1:C:217:ASN:HD21	0.93	0.92
1:C:125:THR:HG22	1:C:162:TRP:CE3	2.04	0.92
1:C:212:ASN:HD22	1:C:214:ASN:N	1.66	0.91
1:A:251:ILE:HG23	1:A:252:GLU:HG2	1.52	0.91
1:B:150:LEU:HA	1:B:153:LEU:HD12	1.53	0.90
1:C:195:LYS:HB3	1:C:195:LYS:HZ3	1.36	0.90
1:A:178:ASP:HB2	1:A:180:SER:OG	1.72	0.90
1:A:168:LEU:O	1:A:169:CYS:CB	2.20	0.89
1:C:187:LEU:CD2	1:C:188:ASP:H	1.86	0.89
1:C:187:LEU:HD22	1:C:188:ASP:N	1.87	0.89
1:B:248:ILE:HD12	1:B:250:LEU:HD13	1.52	0.89
1:C:161:VAL:CG2	1:C:239:THR:HG21	2.01	0.89
1:C:115:ILE:HG23	1:C:187:LEU:HB2	1.54	0.89
1:A:205:TYR:CE2	1:A:209:VAL:HG21	2.08	0.88
1:A:148:ASN:O	1:A:151:SER:HB3	1.75	0.87
1:A:137:TYR:CE1	1:B:252:GLU:HG3	2.10	0.87
1:C:195:LYS:HB3	1:C:195:LYS:NZ	1.90	0.87
1:C:90:LEU:HB2	1:C:95:THR:HG21	1.57	0.87
1:B:82:VAL:HG22	1:B:234:LYS:HA	1.57	0.86
1:C:139:MET:H	1:C:217:ASN:ND2	1.74	0.85
1:A:136:GLN:HE21	1:A:223:ARG:HH11	1.25	0.85
1:C:129:GLY:HA2	1:C:230:GLY:HA3	1.58	0.84
1:B:103:VAL:O	1:B:106:ASN:ND2	2.11	0.84
1:C:129:GLY:O	1:C:161:VAL:HB	1.77	0.83
1:B:78:LEU:HB2	1:B:228:MET:HE2	1.61	0.82
1:B:140:ALA:O	1:C:260:LEU:HD12	1.79	0.82
1:B:131:ILE:O	1:B:158:THR:HG23	1.80	0.80
1:C:145:VAL:N	1:C:149:GLN:NE2	2.29	0.80
1:C:146:SER:H	1:C:149:GLN:HE21	1.28	0.80
1:A:105:GLN:HA	1:A:199:PHE:HE1	1.42	0.80
1:C:139:MET:N	1:C:217:ASN:HD21	1.77	0.80
1:B:120:LEU:HD11	1:B:171:VAL:HG21	1.64	0.80
1:A:90:LEU:HD13	1:A:92:MET:HE1	1.63	0.79
1:A:165:GLN:HA	1:A:165:GLN:NE2	1.97	0.79
1:A:92:MET:O	1:A:96:VAL:HG23	1.83	0.79
1:B:212:ASN:ND2	1:B:214:ASN:HB2	1.98	0.78
1:B:151:SER:HA	1:B:156:TYR:CD2	2.18	0.78
1:C:212:ASN:ND2	1:C:214:ASN:N	2.25	0.78
1:C:212:ASN:HD22	1:C:214:ASN:H	0.81	0.78
1:B:100:LEU:HG	1:B:246:TYR:CE2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LYS:H	1:C:172:ASN:ND2	1.81	0.77
1:C:119:TYR:OH	1:C:239:THR:CG2	2.32	0.77
1:B:124:PRO:HD2	1:B:127:THR:OG1	1.82	0.77
1:B:214:ASN:HD21	1:C:200:LYS:NZ	1.82	0.77
1:A:144:PRO:HA	1:B:258:LEU:HD11	1.66	0.77
1:B:117:TYR:HB3	1:B:242:LEU:HD21	1.65	0.77
1:C:163:GLU:HG3	1:C:164:GLY:N	1.99	0.77
1:A:105:GLN:CA	1:A:199:PHE:HE1	1.97	0.76
1:C:131:ILE:CG1	1:C:228:MET:HE2	2.14	0.76
1:A:181:ARG:O	1:A:181:ARG:HG2	1.84	0.76
1:C:49:GLN:NE2	1:C:165:GLN:HG2	2.00	0.76
1:A:161:VAL:HB	1:A:239:THR:OG1	1.86	0.75
1:A:143:LEU:HD12	1:A:143:LEU:N	2.00	0.75
1:A:123:CYS:HB3	1:A:124:PRO:HD2	1.67	0.75
1:C:169:CYS:O	1:C:173:ASN:N	2.20	0.74
1:A:136:GLN:HE21	1:A:223:ARG:NH1	1.86	0.74
1:A:109:LYS:HE3	1:A:252:GLU:OE1	1.88	0.74
1:C:60:LEU:HD12	1:C:69:LEU:HD13	1.70	0.74
1:A:129:GLY:HA2	1:A:230:GLY:CA	2.18	0.73
1:A:79:ALA:HA	1:A:237:VAL:O	1.89	0.73
1:C:150:LEU:HD13	1:C:150:LEU:O	1.89	0.73
1:C:125:THR:HG22	1:C:162:TRP:CD2	2.24	0.72
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.24	0.72
1:C:66:VAL:HG12	1:C:251:ILE:HD11	1.70	0.72
1:B:146:SER:OG	1:B:148:ASN:HB2	1.89	0.71
1:A:129:GLY:HA2	1:A:230:GLY:HA2	1.72	0.71
1:C:101:ARG:HG2	1:C:102:GLY:N	2.03	0.71
1:A:200:LYS:HE3	1:A:260:LEU:C	2.11	0.70
1:A:105:GLN:HA	1:A:199:PHE:CD1	2.26	0.70
1:B:195:LYS:HE3	1:C:195:LYS:HZ1	1.56	0.70
1:A:258:LEU:HD11	1:C:144:PRO:HA	1.74	0.69
1:C:116:ARG:HH21	1:C:184:THR:HG21	1.57	0.69
1:A:155:GLY:HA3	1:A:185:ILE:HG13	1.74	0.69
1:C:234:LYS:H	1:C:234:LYS:HE3	1.58	0.69
1:C:239:THR:HG22	1:C:240:GLY:N	2.06	0.69
1:B:110:TYR:HB2	1:B:248:ILE:HD11	1.74	0.69
1:B:118:THR:O	1:B:242:LEU:HD23	1.92	0.69
1:C:81:THR:HG23	1:C:83:THR:O	1.92	0.68
1:C:145:VAL:N	1:C:149:GLN:HE22	1.88	0.68
1:B:138:ASP:HA	1:B:217:ASN:HD21	1.58	0.68
1:A:94:PHE:HB2	1:A:199:PHE:HE2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:MET:H	1:B:217:ASN:HD21	1.40	0.68
1:C:205:TYR:O	1:C:209:VAL:HG23	1.93	0.68
1:B:174:THR:HG22	1:B:175:LYS:H	1.58	0.68
1:C:118:THR:HB	1:C:184:THR:OG1	1.94	0.67
1:A:201:THR:HG22	1:A:260:LEU:C	2.14	0.67
1:C:69:LEU:HD12	1:C:70:SER:N	2.10	0.67
1:B:94:PHE:CE1	1:B:101:ARG:HD2	2.29	0.67
1:C:163:GLU:HG3	1:C:164:GLY:H	1.58	0.67
1:A:116:ARG:NE	1:A:170:PHE:HD1	1.92	0.67
1:B:218:ILE:HG12	1:B:219:LEU:CD1	2.25	0.67
1:A:218:ILE:HD11	1:B:218:ILE:HD12	1.77	0.66
1:B:166:SER:O	1:B:176:CYS:SG	2.53	0.66
1:A:148:ASN:HD22	1:A:148:ASN:C	1.98	0.66
1:B:175:LYS:O	1:B:177:PRO:HD3	1.94	0.66
1:B:119:TYR:O	1:B:120:LEU:HD23	1.96	0.66
1:A:108:SER:HB2	1:A:252:GLU:O	1.96	0.66
1:B:71:HIS:HD2	1:B:99:TRP:CZ3	2.13	0.66
1:C:92:MET:O	1:C:96:VAL:HG23	1.94	0.66
1:A:66:VAL:HG21	1:A:249:ARG:HH21	1.61	0.66
1:B:125:THR:HG22	1:B:125:THR:O	1.95	0.66
1:B:137:TYR:CD1	1:C:252:GLU:HG3	2.31	0.66
1:C:78:LEU:HG	1:C:228:MET:HE3	1.77	0.66
1:C:124:PRO:O	1:C:127:THR:OG1	2.14	0.66
1:A:71:HIS:HB3	1:A:246:TYR:CZ	2.31	0.65
1:A:110:TYR:CD1	1:A:248:ILE:HD11	2.32	0.65
1:B:138:ASP:O	1:B:141:ASP:HB2	1.97	0.65
1:A:81:THR:O	1:A:231:GLY:HA2	1.95	0.65
1:C:195:LYS:NZ	1:C:195:LYS:CB	2.57	0.65
1:A:160:PRO:HG2	1:A:163:GLU:HB2	1.78	0.65
1:B:150:LEU:HA	1:B:153:LEU:CD1	2.25	0.65
1:C:115:ILE:CG2	1:C:187:LEU:HB2	2.27	0.64
1:B:73:GLU:OE1	1:B:99:TRP:HB3	1.96	0.64
1:B:189:THR:HA	1:B:192:VAL:HG23	1.79	0.64
1:B:248:ILE:HD13	1:B:249:ARG:H	1.63	0.64
1:B:136:GLN:HE22	1:B:143:LEU:HD23	1.61	0.64
1:A:174:THR:HG22	1:A:176:CYS:SG	2.38	0.64
1:B:106:ASN:H	1:B:106:ASN:ND2	1.94	0.64
1:B:115:ILE:HG13	1:B:246:TYR:HB3	1.79	0.63
1:A:155:GLY:O	1:A:156:TYR:C	2.36	0.63
1:B:135:PHE:HE2	1:B:187:LEU:HA	1.64	0.63
1:A:215:ILE:O	1:A:219:LEU:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:HG	1:C:228:MET:CE	2.28	0.63
1:C:146:SER:H	1:C:149:GLN:NE2	1.97	0.62
1:A:100:LEU:HG	1:A:246:TYR:CE2	2.34	0.62
1:A:144:PRO:CA	1:B:258:LEU:HD11	2.29	0.62
1:A:92:MET:HE2	1:A:220:VAL:CG1	2.29	0.62
1:C:169:CYS:O	1:C:173:ASN:HA	1.99	0.62
1:C:125:THR:CG2	1:C:162:TRP:CE3	2.81	0.62
1:B:81:THR:O	1:B:231:GLY:HA3	2.00	0.62
1:C:144:PRO:CG	1:C:150:LEU:HD23	2.29	0.62
1:B:78:LEU:N	1:B:78:LEU:HD12	2.15	0.62
1:C:169:CYS:O	1:C:173:ASN:CA	2.48	0.62
1:C:155:GLY:HA3	1:C:185:ILE:HG13	1.82	0.61
1:B:79:ALA:HB1	1:B:237:VAL:O	2.00	0.61
1:B:78:LEU:HB2	1:B:228:MET:CE	2.29	0.61
1:A:71:HIS:CG	1:A:72:CYS:H	2.18	0.61
1:A:116:ARG:NE	1:A:170:PHE:CD1	2.68	0.61
1:A:260:LEU:N	1:A:260:LEU:HD23	2.16	0.61
1:A:109:LYS:CE	1:A:252:GLU:OE1	2.49	0.61
1:B:139:MET:CE	1:B:223:ARG:HB3	2.31	0.60
1:A:135:PHE:CE1	1:A:185:ILE:HG12	2.37	0.60
1:A:138:ASP:O	1:A:140:ALA:N	2.35	0.60
1:C:74:LEU:HD12	1:C:75:SER:N	2.16	0.60
1:B:158:THR:HG22	1:B:159:GLY:H	1.66	0.60
1:A:137:TYR:CE2	1:B:252:GLU:OE1	2.55	0.60
1:C:187:LEU:CD2	1:C:188:ASP:N	2.56	0.60
1:B:74:LEU:H	1:B:74:LEU:HD12	1.67	0.60
1:C:192:VAL:HG13	1:C:197:TYR:OH	2.01	0.59
1:A:129:GLY:C	1:A:161:VAL:HG13	2.21	0.59
1:C:133:MET:HA	1:C:225:VAL:O	2.03	0.59
1:C:66:VAL:CG1	1:C:251:ILE:HD11	2.31	0.59
1:A:200:LYS:CE	1:A:260:LEU:OXT	2.51	0.59
1:B:71:HIS:HB3	1:B:246:TYR:CZ	2.38	0.59
1:B:195:LYS:HE3	1:C:195:LYS:CE	2.32	0.59
1:A:123:CYS:CB	1:A:124:PRO:CD	2.79	0.58
1:B:71:HIS:ND1	1:B:72:CYS:N	2.49	0.58
1:C:80:VAL:HG13	1:C:81:THR:N	2.19	0.58
1:B:195:LYS:HE3	1:C:195:LYS:NZ	2.18	0.58
1:A:92:MET:HE2	1:A:220:VAL:HG12	1.84	0.58
1:A:137:TYR:CD1	1:B:252:GLU:HG3	2.39	0.58
1:B:216:GLY:O	1:B:219:LEU:N	2.37	0.58
1:B:218:ILE:HG12	1:B:219:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:N	1:A:196:ARG:HD2	2.18	0.58
1:A:141:ASP:HB3	1:B:258:LEU:O	2.04	0.58
1:A:251:ILE:HG23	1:A:252:GLU:CG	2.31	0.58
1:A:135:PHE:HE1	1:A:185:ILE:HG12	1.67	0.58
1:B:139:MET:H	1:B:217:ASN:ND2	2.01	0.58
1:C:114:ALA:O	1:C:246:TYR:HA	2.04	0.58
1:C:52:MET:SD	1:C:52:MET:N	2.76	0.58
1:A:248:ILE:HG23	1:A:250:LEU:HD13	1.85	0.57
1:B:155:GLY:O	1:B:157:VAL:HG23	2.04	0.57
1:A:212:ASN:OD1	1:A:214:ASN:HB2	2.02	0.57
1:B:82:VAL:HG21	1:B:234:LYS:HG3	1.86	0.57
1:B:212:ASN:HD21	1:B:214:ASN:HB2	1.67	0.57
1:B:246:TYR:N	1:B:246:TYR:CD1	2.72	0.57
1:A:138:ASP:C	1:A:140:ALA:N	2.57	0.57
1:B:139:MET:N	1:B:217:ASN:HD21	2.03	0.57
1:A:129:GLY:HA2	1:A:230:GLY:HA3	1.85	0.57
1:A:71:HIS:HD2	1:A:99:TRP:CE3	2.23	0.57
1:A:200:LYS:HE3	1:A:260:LEU:OXT	2.05	0.57
1:B:131:ILE:O	1:B:158:THR:CG2	2.53	0.57
1:C:135:PHE:O	1:C:153:LEU:HG	2.05	0.57
1:B:94:PHE:O	1:B:101:ARG:NH1	2.35	0.57
1:C:256:ALA:O	1:C:257:ALA:C	2.43	0.57
1:C:144:PRO:HG3	1:C:150:LEU:CD2	2.35	0.56
1:A:91:VAL:HG13	1:A:222:ALA:O	2.05	0.56
1:A:143:LEU:N	1:A:143:LEU:CD1	2.68	0.56
1:A:248:ILE:HG23	1:A:250:LEU:CD1	2.35	0.56
1:B:73:GLU:OE1	1:B:99:TRP:N	2.29	0.56
1:C:234:LYS:H	1:C:234:LYS:CD	2.19	0.56
1:B:135:PHE:CE2	1:B:187:LEU:HA	2.40	0.56
1:A:142:THR:HB	1:B:258:LEU:HD22	1.87	0.56
1:B:158:THR:HG22	1:B:159:GLY:N	2.20	0.56
1:B:189:THR:HA	1:B:192:VAL:CG2	2.35	0.56
1:B:136:GLN:NE2	1:B:143:LEU:HD23	2.19	0.56
1:A:195:LYS:C	1:A:196:ARG:HD2	2.26	0.56
1:A:137:TYR:CZ	1:B:252:GLU:OE1	2.58	0.56
1:B:251:ILE:HG23	1:B:252:GLU:OE2	2.06	0.56
1:B:156:TYR:C	1:B:157:VAL:HG23	2.26	0.56
1:B:70:SER:OG	1:B:247:THR:HG23	2.06	0.56
1:A:116:ARG:HG3	1:A:186:ALA:HB2	1.86	0.56
1:A:179:THR:O	1:A:180:SER:C	2.43	0.56
1:A:71:HIS:CG	1:A:72:CYS:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:HD13	1:B:249:ARG:N	2.20	0.56
1:A:123:CYS:HB3	1:A:124:PRO:CD	2.34	0.56
1:A:199:PHE:O	1:A:200:LYS:HD2	2.05	0.56
1:A:155:GLY:HA3	1:A:185:ILE:CG1	2.36	0.56
1:A:160:PRO:O	1:A:162:TRP:N	2.39	0.55
1:C:60:LEU:CD1	1:C:69:LEU:HD13	2.36	0.55
1:B:195:LYS:HE3	1:C:195:LYS:HE3	1.89	0.55
1:A:138:ASP:C	1:A:140:ALA:H	2.09	0.55
1:B:82:VAL:CG2	1:B:234:LYS:HA	2.33	0.55
1:B:106:ASN:N	1:B:106:ASN:ND2	2.54	0.55
1:A:251:ILE:CG2	1:A:252:GLU:HG2	2.32	0.55
1:C:49:GLN:CD	1:C:165:GLN:HG2	2.26	0.55
1:C:234:LYS:CE	1:C:234:LYS:H	2.19	0.55
1:C:90:LEU:CB	1:C:95:THR:HG21	2.35	0.55
1:C:101:ARG:CG	1:C:102:GLY:N	2.69	0.55
1:C:90:LEU:HD11	1:C:205:TYR:CE1	2.41	0.55
1:B:169:CYS:HA	1:B:172:ASN:HB2	1.89	0.55
1:B:161:VAL:HB	1:B:239:THR:HB	1.89	0.55
1:A:119:TYR:O	1:A:120:LEU:HD23	2.06	0.55
1:B:150:LEU:O	1:B:150:LEU:HD12	2.07	0.54
1:A:200:LYS:HZ2	1:C:140:ALA:HB3	1.72	0.54
1:B:138:ASP:HA	1:B:217:ASN:ND2	2.21	0.54
1:C:144:PRO:HG3	1:C:150:LEU:HD23	1.89	0.54
1:A:259:ASN:C	1:A:260:LEU:HD23	2.27	0.54
1:C:80:VAL:CG1	1:C:81:THR:N	2.70	0.54
1:B:199:PHE:CD2	1:B:199:PHE:C	2.80	0.54
1:C:205:TYR:CE1	1:C:209:VAL:HG21	2.43	0.54
1:A:223:ARG:HG2	1:A:223:ARG:O	2.07	0.54
1:C:101:ARG:HG2	1:C:102:GLY:H	1.73	0.54
1:B:199:PHE:HD2	1:B:199:PHE:C	2.10	0.54
1:B:214:ASN:HD21	1:C:200:LYS:HZ1	1.56	0.54
1:A:123:CYS:HB2	1:A:124:PRO:O	2.07	0.54
1:C:146:SER:N	1:C:149:GLN:NE2	2.56	0.53
1:A:139:MET:HG3	1:A:205:TYR:OH	2.08	0.53
1:B:123:CYS:HB2	1:B:124:PRO:CD	2.38	0.53
1:B:145:VAL:N	1:B:149:GLN:OE1	2.33	0.53
1:B:106:ASN:HD22	1:B:106:ASN:H	1.57	0.53
1:C:218:ILE:O	1:C:220:VAL:N	2.41	0.53
1:B:137:TYR:CE1	1:C:252:GLU:HG3	2.43	0.53
1:A:81:THR:O	1:A:231:GLY:CA	2.56	0.53
1:C:233:SER:HA	1:C:234:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:O	1:C:95:THR:CG2	2.57	0.53
1:A:204:ASP:O	1:A:205:TYR:C	2.46	0.53
1:A:105:GLN:CA	1:A:199:PHE:CE1	2.77	0.53
1:A:147:VAL:HG12	1:A:148:ASN:N	2.24	0.53
1:A:71:HIS:ND1	1:A:72:CYS:N	2.51	0.53
1:C:131:ILE:HG12	1:C:132:HIS:N	2.24	0.53
1:A:139:MET:N	1:A:217:ASN:OD1	2.40	0.53
1:A:218:ILE:CD1	1:B:218:ILE:HD12	2.38	0.52
1:A:124:PRO:HB2	1:A:126:THR:HG22	1.90	0.52
1:B:80:VAL:HG22	1:B:239:THR:CG2	2.39	0.52
1:C:178:ASP:OD1	1:C:180:SER:HB2	2.08	0.52
1:A:78:LEU:HB2	1:A:228:MET:CE	2.38	0.52
1:A:134:GLY:HA3	1:A:153:LEU:HB3	1.91	0.52
1:A:63:SER:HA	1:A:66:VAL:O	2.09	0.52
1:A:165:GLN:O	1:A:167:GLY:N	2.38	0.52
1:A:200:LYS:CG	1:A:219:LEU:HD23	2.39	0.52
1:B:73:GLU:OE1	1:B:99:TRP:CB	2.57	0.52
1:A:218:ILE:O	1:A:218:ILE:HG22	2.09	0.52
1:A:195:LYS:HB3	1:A:196:ARG:HD2	1.92	0.52
1:B:248:ILE:HG23	1:B:250:LEU:HD22	1.91	0.52
1:A:212:ASN:OD1	1:A:213:ALA:N	2.42	0.52
1:A:250:LEU:N	1:A:250:LEU:CD1	2.72	0.52
1:A:201:THR:CG2	1:A:260:LEU:HA	2.41	0.51
1:A:212:ASN:C	1:A:212:ASN:OD1	2.48	0.51
1:A:92:MET:CE	1:A:220:VAL:HG11	2.39	0.51
1:A:123:CYS:CB	1:A:124:PRO:HD2	2.35	0.51
1:C:84:ILE:HG23	1:C:85:VAL:N	2.24	0.51
1:C:107:TRP:CE3	1:C:250:LEU:HD23	2.45	0.51
1:A:194:GLU:HB2	1:A:197:TYR:CZ	2.45	0.51
1:A:132:HIS:CE1	1:A:147:VAL:CG2	2.93	0.51
1:C:116:ARG:NH2	1:C:184:THR:HG21	2.24	0.51
1:B:214:ASN:HD22	1:C:219:LEU:HD11	1.76	0.51
1:B:118:THR:HG23	1:B:184:THR:HB	1.93	0.51
1:C:169:CYS:HB3	1:C:174:THR:HG22	1.93	0.51
1:B:129:GLY:HA2	1:B:230:GLY:CA	2.40	0.51
1:B:62:SER:HA	1:B:68:ILE:CD1	2.41	0.51
1:A:94:PHE:HB2	1:A:199:PHE:CE2	2.43	0.51
1:C:218:ILE:O	1:C:219:LEU:C	2.49	0.51
1:B:131:ILE:O	1:B:158:THR:HA	2.11	0.51
1:B:175:LYS:O	1:B:177:PRO:CD	2.58	0.51
1:B:103:VAL:HG12	1:B:107:TRP:HZ3	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:MET:HG3	1:C:185:ILE:HG21	1.92	0.50
1:C:73:GLU:OE1	1:C:99:TRP:N	2.32	0.50
1:B:138:ASP:CA	1:B:217:ASN:HD21	2.23	0.50
1:A:258:LEU:HD11	1:C:144:PRO:CA	2.40	0.50
1:A:142:THR:HG22	1:A:143:LEU:O	2.11	0.50
1:A:129:GLY:CA	1:A:230:GLY:HA3	2.41	0.50
1:A:228:MET:HE3	1:A:239:THR:HG21	1.94	0.50
1:C:131:ILE:O	1:C:158:THR:HA	2.11	0.50
1:B:139:MET:HE1	1:B:223:ARG:HB3	1.94	0.50
1:A:201:THR:HG22	1:A:260:LEU:CA	2.41	0.50
1:B:205:TYR:O	1:B:208:ALA:HB3	2.11	0.50
1:B:185:ILE:HG23	1:B:185:ILE:O	2.11	0.50
1:C:113:VAL:HB	1:C:247:THR:O	2.12	0.50
1:C:196:ARG:NH1	1:C:249:ARG:HH21	2.10	0.49
1:A:200:LYS:HE3	1:A:260:LEU:O	2.10	0.49
1:B:213:ALA:O	1:B:214:ASN:C	2.50	0.49
1:A:249:ARG:NH2	1:C:191:GLU:OE1	2.45	0.49
1:C:116:ARG:NE	1:C:170:PHE:CE2	2.80	0.49
1:A:107:TRP:CZ3	1:A:250:LEU:HD23	2.47	0.49
1:B:72:CYS:HA	1:B:244:ALA:O	2.12	0.49
1:A:124:PRO:HD2	1:A:127:THR:OG1	2.11	0.49
1:A:139:MET:N	1:A:139:MET:SD	2.80	0.49
1:C:69:LEU:HD12	1:C:70:SER:H	1.77	0.49
1:C:56:ARG:HG2	1:C:57:PRO:HD2	1.95	0.49
1:A:133:MET:HA	1:A:225:VAL:O	2.13	0.49
1:A:215:ILE:HG22	1:A:219:LEU:HD11	1.95	0.49
1:B:138:ASP:OD2	1:B:140:ALA:HB3	2.11	0.49
1:A:124:PRO:HG2	1:A:126:THR:HG22	1.95	0.49
1:C:167:GLY:O	1:C:168:LEU:C	2.51	0.49
1:A:200:LYS:HG3	1:A:219:LEU:HD23	1.95	0.49
1:C:76:THR:CG2	1:C:77:GLU:N	2.75	0.49
1:A:199:PHE:HD2	1:A:200:LYS:N	2.11	0.48
1:B:72:CYS:O	1:B:73:GLU:HB2	2.13	0.48
1:C:201:THR:HG23	1:C:260:LEU:HA	1.94	0.48
1:C:194:GLU:HB2	1:C:197:TYR:CE2	2.48	0.48
1:B:62:SER:HA	1:B:68:ILE:HD12	1.95	0.48
1:B:78:LEU:H	1:B:78:LEU:HD12	1.77	0.48
1:B:105:GLN:HA	1:B:199:PHE:CE1	2.48	0.48
1:B:69:LEU:HB3	1:B:248:ILE:HG22	1.95	0.48
1:C:151:SER:HA	1:C:156:TYR:CD2	2.49	0.48
1:C:99:TRP:O	1:C:100:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:HD22	1:A:238:ASN:N	2.11	0.48
1:A:79:ALA:CA	1:A:237:VAL:O	2.61	0.48
1:B:101:ARG:O	1:B:105:GLN:HB2	2.13	0.48
1:A:89:GLU:OE2	1:A:89:GLU:HA	2.14	0.48
1:A:200:LYS:HE2	1:A:260:LEU:OXT	2.12	0.48
1:A:177:PRO:O	1:A:178:ASP:HB3	2.14	0.48
1:B:69:LEU:HB3	1:B:248:ILE:CG2	2.43	0.48
1:C:150:LEU:HD22	1:C:153:LEU:HD22	1.95	0.48
1:B:213:ALA:O	1:B:216:GLY:N	2.40	0.48
1:B:214:ASN:HD21	1:C:200:LYS:HZ2	1.60	0.48
1:C:116:ARG:CZ	1:C:170:PHE:CE2	2.97	0.47
1:B:188:ASP:OD1	1:B:191:GLU:HB2	2.13	0.47
1:A:155:GLY:HA3	1:A:185:ILE:CD1	2.44	0.47
1:A:169:CYS:N	1:A:172:ASN:HB2	2.30	0.47
1:A:200:LYS:HZ2	1:C:140:ALA:CB	2.27	0.47
1:A:138:ASP:HB3	1:A:141:ASP:OD2	2.15	0.47
1:A:138:ASP:HB3	1:A:141:ASP:CG	2.35	0.47
1:A:92:MET:CE	1:A:220:VAL:CG1	2.93	0.47
1:B:117:TYR:HB3	1:B:242:LEU:CD2	2.41	0.47
1:A:124:PRO:C	1:A:126:THR:H	2.18	0.47
1:C:251:ILE:O	1:C:252:GLU:HB3	2.15	0.47
1:A:94:PHE:O	1:A:101:ARG:NH1	2.41	0.47
1:A:181:ARG:O	1:A:182:ALA:HB2	2.14	0.47
1:B:70:SER:HA	1:B:246:TYR:O	2.14	0.47
1:C:116:ARG:HD3	1:C:170:PHE:CD2	2.50	0.47
1:C:116:ARG:HE	1:C:184:THR:HG21	1.79	0.47
1:B:169:CYS:HB2	1:B:174:THR:HB	1.96	0.47
1:C:197:TYR:CZ	1:C:221:PRO:HB3	2.50	0.47
1:A:64:MET:HA	3:A:262:HOH:O	2.15	0.47
1:A:142:THR:CG2	1:B:258:LEU:HD22	2.45	0.46
1:A:66:VAL:CG2	1:A:249:ARG:HH21	2.27	0.46
1:A:133:MET:CE	1:A:242:LEU:HD11	2.45	0.46
1:B:110:TYR:HB2	1:B:248:ILE:CD1	2.43	0.46
1:B:71:HIS:HD2	1:B:99:TRP:CH2	2.33	0.46
1:A:90:LEU:HD13	1:A:92:MET:CE	2.40	0.46
1:C:119:TYR:C	1:C:119:TYR:CD1	2.89	0.46
1:A:252:GLU:OE2	1:C:137:TYR:CZ	2.67	0.46
1:C:150:LEU:HA	1:C:150:LEU:HD22	1.63	0.46
1:A:203:THR:O	1:A:206:ALA:HB3	2.16	0.46
1:B:93:PRO:CB	1:B:100:LEU:HD13	2.45	0.46
1:C:223:ARG:HG3	1:C:223:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LYS:HA	1:C:200:LYS:HD2	1.62	0.46
1:A:129:GLY:O	1:A:160:PRO:HA	2.15	0.46
1:C:123:CYS:HB2	1:C:127:THR:OG1	2.15	0.46
1:C:145:VAL:CG2	1:C:149:GLN:HE22	2.28	0.46
1:A:71:HIS:HB3	1:A:246:TYR:OH	2.15	0.46
1:A:133:MET:HB2	1:A:224:LEU:HD11	1.98	0.46
1:C:90:LEU:O	1:C:95:THR:HG21	2.16	0.46
1:B:78:LEU:HD22	1:B:228:MET:CE	2.46	0.46
1:B:219:LEU:O	1:B:220:VAL:HG23	2.16	0.46
1:C:84:ILE:O	1:C:85:VAL:HG23	2.14	0.46
1:A:201:THR:HG21	1:A:260:LEU:HA	1.98	0.46
1:C:168:LEU:O	1:C:169:CYS:C	2.54	0.46
1:A:82:VAL:HA	1:A:231:GLY:HA3	1.96	0.46
1:A:78:LEU:HB2	1:A:228:MET:HE1	1.97	0.45
1:A:146:SER:HB3	1:A:149:GLN:HG3	1.97	0.45
1:C:91:VAL:HG12	1:C:91:VAL:O	2.16	0.45
1:B:212:ASN:HD22	1:B:214:ASN:HB2	1.77	0.45
1:B:172:ASN:HD22	1:B:172:ASN:HA	1.20	0.45
1:A:132:HIS:CE1	1:A:147:VAL:HG22	2.51	0.45
1:C:196:ARG:HH11	1:C:249:ARG:HH21	1.63	0.45
1:C:131:ILE:HD12	1:C:228:MET:HE1	1.99	0.45
1:C:59:MET:HG2	1:C:60:LEU:N	2.31	0.45
1:A:150:LEU:HD12	1:A:150:LEU:O	2.17	0.45
1:C:139:MET:HA	1:C:139:MET:CE	2.46	0.45
1:C:205:TYR:O	1:C:208:ALA:N	2.50	0.45
1:C:82:VAL:HB	1:C:234:LYS:HA	1.99	0.45
1:A:233:SER:CB	1:A:235:THR:OG1	2.65	0.45
1:A:138:ASP:O	1:A:139:MET:C	2.56	0.45
1:A:72:CYS:SG	1:A:245:SER:OG	2.75	0.45
1:C:155:GLY:O	1:C:156:TYR:C	2.55	0.45
1:B:139:MET:HE2	1:B:223:ARG:HB3	1.99	0.45
1:C:201:THR:CG2	1:C:260:LEU:HA	2.46	0.45
1:B:170:PHE:HE1	1:B:184:THR:HG21	1.82	0.45
1:B:146:SER:OG	1:B:147:VAL:N	2.49	0.45
1:B:92:MET:HG2	1:B:94:PHE:H	1.82	0.45
1:A:191:GLU:HG3	1:B:251:ILE:CD1	2.48	0.44
1:A:179:THR:C	1:A:181:ARG:N	2.70	0.44
1:B:145:VAL:HG12	1:B:146:SER:N	2.30	0.44
1:A:233:SER:HB3	1:A:235:THR:OG1	2.17	0.44
1:C:176:CYS:HA	1:C:177:PRO:HD3	1.83	0.44
1:B:110:TYR:C	1:B:110:TYR:CD1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:CD	1:C:170:PHE:CD2	3.00	0.44
1:A:170:PHE:CD2	1:A:170:PHE:N	2.85	0.44
1:B:71:HIS:CD2	1:B:99:TRP:CZ3	3.00	0.44
1:B:212:ASN:O	1:B:213:ALA:C	2.55	0.44
1:A:238:ASN:N	1:A:238:ASN:ND2	2.66	0.44
1:A:200:LYS:HD2	1:A:200:LYS:HA	1.73	0.44
1:B:100:LEU:HG	1:B:246:TYR:CZ	2.51	0.44
1:A:130:ALA:N	1:A:161:VAL:HG13	2.33	0.44
1:C:195:LYS:HZ2	1:C:195:LYS:CB	2.30	0.44
1:A:148:ASN:C	1:A:148:ASN:ND2	2.69	0.44
1:C:201:THR:HG23	1:C:260:LEU:CA	2.48	0.44
1:B:151:SER:HA	1:B:156:TYR:CE2	2.51	0.44
1:C:248:ILE:O	1:C:248:ILE:HG23	2.18	0.44
1:C:179:THR:O	1:C:180:SER:C	2.56	0.44
1:A:66:VAL:HG21	1:A:249:ARG:NH2	2.28	0.44
1:C:256:ALA:O	1:C:258:LEU:N	2.50	0.44
1:B:140:ALA:HB2	1:B:214:ASN:OD1	2.18	0.44
1:B:74:LEU:N	1:B:74:LEU:HD12	2.28	0.44
1:C:116:ARG:O	1:C:244:ALA:HA	2.18	0.43
1:C:212:ASN:ND2	1:C:214:ASN:ND2	2.66	0.43
1:B:110:TYR:CD1	1:B:111:ALA:N	2.86	0.43
1:A:107:TRP:CE3	1:A:250:LEU:HD23	2.53	0.43
1:B:69:LEU:HD21	1:B:99:TRP:HZ3	1.83	0.43
1:A:132:HIS:CE1	1:A:147:VAL:HG21	2.54	0.43
1:B:156:TYR:C	1:B:157:VAL:CG2	2.86	0.43
1:C:116:ARG:NE	1:C:170:PHE:CD2	2.86	0.43
1:B:124:PRO:C	1:B:126:THR:H	2.22	0.43
1:C:231:GLY:O	1:C:232:SER:HB3	2.19	0.43
1:C:206:ALA:O	1:C:207:THR:C	2.56	0.43
1:C:227:ALA:C	1:C:228:MET:HG2	2.38	0.43
1:C:78:LEU:HA	1:C:78:LEU:HD12	1.61	0.43
1:B:165:GLN:HB3	1:B:165:GLN:HE21	1.11	0.43
1:A:214:ASN:HD21	1:B:200:LYS:CE	2.31	0.43
1:C:144:PRO:HG2	1:C:150:LEU:HD23	1.99	0.43
1:C:82:VAL:HG12	1:C:83:THR:N	2.34	0.43
1:A:92:MET:HE2	1:A:220:VAL:HG11	2.00	0.43
1:B:72:CYS:SG	1:B:171:VAL:HG13	2.59	0.43
1:B:214:ASN:ND2	1:C:200:LYS:HZ1	2.15	0.43
1:A:80:VAL:HG11	1:A:129:GLY:HA3	2.01	0.43
1:A:82:VAL:HG13	1:A:234:LYS:CA	2.49	0.43
1:C:217:ASN:HD22	1:C:217:ASN:HA	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ALA:O	1:C:205:TYR:HB3	2.19	0.43
1:B:74:LEU:CD1	1:B:74:LEU:H	2.32	0.43
1:A:181:ARG:HD2	1:A:181:ARG:N	2.33	0.43
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.67	0.43
1:A:82:VAL:HG13	1:A:234:LYS:N	2.34	0.43
1:B:79:ALA:HB2	1:B:238:ASN:HA	2.01	0.43
1:A:91:VAL:CG1	1:A:222:ALA:O	2.66	0.43
1:B:200:LYS:HD2	1:B:260:LEU:O	2.19	0.42
1:B:209:VAL:O	1:B:212:ASN:N	2.51	0.42
1:C:80:VAL:CG1	1:C:231:GLY:HA2	2.49	0.42
1:C:55:LEU:HA	1:C:55:LEU:HD23	1.72	0.42
1:B:259:ASN:OD1	1:B:260:LEU:N	2.52	0.42
1:A:135:PHE:O	1:A:153:LEU:HG	2.18	0.42
1:B:167:GLY:C	1:B:169:CYS:N	2.70	0.42
1:C:54:LYS:N	1:C:172:ASN:HD21	1.84	0.42
1:A:116:ARG:HE	1:A:170:PHE:HD1	1.59	0.42
1:B:133:MET:HB2	1:B:133:MET:HE3	1.94	0.42
1:C:205:TYR:O	1:C:208:ALA:HB3	2.19	0.42
1:A:90:LEU:HB3	1:A:92:MET:HE3	2.01	0.42
1:A:78:LEU:HB2	1:A:228:MET:HE2	2.00	0.42
1:B:129:GLY:HA2	1:B:230:GLY:HA3	2.00	0.42
1:A:92:MET:HE1	1:A:220:VAL:HG11	2.00	0.42
1:B:233:SER:HB3	1:B:235:THR:HB	2.01	0.42
1:B:218:ILE:HG12	1:B:219:LEU:HD13	2.00	0.42
1:C:172:ASN:HD22	1:C:172:ASN:HA	1.62	0.42
1:B:113:VAL:HB	1:B:247:THR:O	2.20	0.42
1:A:250:LEU:N	1:A:250:LEU:HD12	2.35	0.42
1:A:92:MET:HE2	1:A:92:MET:HB3	1.60	0.42
1:A:185:ILE:O	1:A:185:ILE:HG23	2.19	0.42
1:A:219:LEU:HD21	1:C:214:ASN:OD1	2.20	0.42
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.50	0.42
1:A:88:SER:HA	1:A:224:LEU:O	2.19	0.41
1:C:71:HIS:CG	1:C:72:CYS:H	2.38	0.41
1:B:115:ILE:HG12	1:B:116:ARG:N	2.34	0.41
1:A:82:VAL:HG13	1:A:233:SER:C	2.41	0.41
1:A:140:ALA:O	1:B:260:LEU:HD12	2.20	0.41
1:C:109:LYS:HB3	1:C:197:TYR:O	2.19	0.41
1:C:82:VAL:CG1	1:C:83:THR:N	2.83	0.41
1:A:170:PHE:HD2	1:A:170:PHE:N	2.18	0.41
1:A:233:SER:C	1:A:235:THR:H	2.22	0.41
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HB2	1:C:243:TYR:CE2	2.56	0.41
1:A:142:THR:HG22	1:B:258:LEU:HD22	2.02	0.41
1:A:160:PRO:HG2	1:A:163:GLU:CB	2.49	0.41
1:A:221:PRO:O	1:A:222:ALA:HB2	2.20	0.41
1:B:133:MET:HA	1:B:225:VAL:O	2.20	0.41
1:A:173:ASN:HA	1:A:173:ASN:HD22	1.27	0.41
1:A:167:GLY:O	1:A:168:LEU:C	2.59	0.41
1:B:248:ILE:HD12	1:B:250:LEU:CD1	2.37	0.41
1:C:116:ARG:CZ	1:C:170:PHE:HE2	2.32	0.41
1:A:71:HIS:HB3	1:A:246:TYR:CE2	2.56	0.41
1:A:202:ALA:O	1:A:203:THR:C	2.58	0.41
1:C:194:GLU:HG3	1:C:218:ILE:HG23	2.01	0.41
1:B:175:LYS:O	1:B:177:PRO:N	2.53	0.41
1:C:79:ALA:CB	1:C:238:ASN:HA	2.50	0.41
1:B:195:LYS:CE	1:C:195:LYS:HE3	2.50	0.41
1:C:194:GLU:OE1	1:C:194:GLU:HA	2.20	0.41
1:B:161:VAL:HG11	1:B:239:THR:HG21	2.03	0.41
1:B:235:THR:HG22	1:B:235:THR:O	2.20	0.41
1:B:123:CYS:HB2	1:B:124:PRO:HD2	2.02	0.41
1:C:69:LEU:O	1:C:248:ILE:HG22	2.20	0.41
1:A:200:LYS:HG3	1:A:219:LEU:CD2	2.51	0.40
1:B:229:GLU:O	1:B:229:GLU:CG	2.65	0.40
1:B:78:LEU:HD22	1:B:228:MET:HE1	2.03	0.40
1:C:219:LEU:HG	1:C:219:LEU:H	1.50	0.40
1:A:71:HIS:CD2	1:A:99:TRP:CE3	3.06	0.40
1:C:79:ALA:HB2	1:C:238:ASN:HA	2.03	0.40
1:B:217:ASN:HD22	1:B:217:ASN:HA	1.47	0.40
1:A:82:VAL:HA	1:A:231:GLY:CA	2.52	0.40
1:B:136:GLN:NE2	1:B:143:LEU:CD2	2.84	0.40
1:C:76:THR:HG22	1:C:77:GLU:N	2.36	0.40
1:B:99:TRP:O	1:B:100:LEU:C	2.59	0.40
1:B:141:ASP:OD1	1:C:259:ASN:HA	2.22	0.40
1:B:213:ALA:O	1:B:215:ILE:N	2.54	0.40
1:B:219:LEU:C	1:B:220:VAL:HG23	2.41	0.40
1:B:197:TYR:CE1	1:B:221:PRO:HB3	2.56	0.40
1:B:132:HIS:HB2	1:B:227:ALA:HB3	2.04	0.40

All (2046) 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:B:185:ILE:CG1	1:C:118:THR:N[3_555]	0.11	2.09
1:B:130:ALA:CB	1:C:136:GLN:N[3_555]	0.18	2.02
1:B:120:LEU:C	1:C:156:TYR:CE1[3_555]	0.23	1.97
1:B:74:LEU:CB	1:C:130:ALA:CB[3_555]	0.25	1.95
1:B:160:PRO:O	1:C:153:LEU:C[3_555]	0.29	1.91
1:C:103:VAL:N	1:C:106:ASN:CG[2_555]	0.31	1.89
1:C:58:PRO:C	1:C:67:THR:N[2_555]	0.33	1.87
1:B:241:ARG:CA	1:C:132:HIS:ND1[3_555]	0.34	1.86
1:A:253:PRO:CG	1:B:162:TRP:CE2[2_555]	0.35	1.85
1:B:73:GLU:CA	1:C:160:PRO:CB[3_555]	0.37	1.83
1:B:236:ALA:CB	1:C:145:VAL:CG1[3_555]	0.38	1.82
1:B:191:GLU:CA	1:C:55:LEU:N[3_555]	0.41	1.79
1:B:154:LYS:C	1:C:244:ALA:C[3_555]	0.42	1.78
1:B:136:GLN:O	1:C:74:LEU:CG[3_555]	0.42	1.78
1:B:89:GLU:C	1:C:78:LEU:N[3_555]	0.44	1.76
1:B:80:VAL:C	1:C:143:LEU:C[3_555]	0.45	1.75
1:B:155:GLY:N	1:C:245:SER:N[3_555]	0.45	1.75
1:B:112:TRP:C	1:C:51:THR:CA[3_555]	0.47	1.73
1:B:243:TYR:CB	1:C:159:GLY:CA[3_555]	0.47	1.73
1:A:106:ASN:ND2	1:B:126:THR:CB[2_555]	0.47	1.73
1:B:73:GLU:C	1:C:160:PRO:CA[3_555]	0.48	1.72
1:B:241:ARG:CB	1:C:132:HIS:CE1[3_555]	0.48	1.72
1:B:158:THR:C	1:C:135:PHE:CD1[3_555]	0.48	1.72
1:B:103:VAL:CG1	1:C:47:ILE:CD1[3_555]	0.49	1.71
1:B:236:ALA:C	1:C:145:VAL:CG2[3_555]	0.49	1.71
1:B:152:ASN:OD1	1:C:93:PRO:C[3_555]	0.51	1.69
1:B:153:LEU:N	1:C:96:VAL:CG1[3_555]	0.51	1.69
1:B:239:THR:CA	1:C:150:LEU:N[3_555]	0.52	1.68
1:B:119:TYR:CA	1:C:157:VAL:C[3_555]	0.53	1.67
1:C:246:TYR:OH	1:C:253:PRO:CB[2_555]	0.54	1.66
1:B:147:VAL:N	1:C:90:LEU:CB[3_555]	0.55	1.65
1:B:228:MET:SD	1:C:225:VAL:CG1[3_555]	0.55	1.65
1:B:117:TYR:CE1	1:C:119:TYR:CE2[3_555]	0.55	1.65
1:B:98:THR:CB	1:C:128:SER:N[3_555]	0.58	1.62
1:B:120:LEU:O	1:C:156:TYR:CZ[3_555]	0.59	1.61
1:B:89:GLU:CA	1:C:78:LEU:CA[3_555]	0.59	1.61
1:B:135:PHE:CD2	1:C:243:TYR:CB[3_555]	0.60	1.60
1:B:131:ILE:CA	1:C:134:GLY:O[3_555]	0.60	1.60
1:B:150:LEU:CD2	1:C:89:GLU:CG[3_555]	0.61	1.59
1:B:147:VAL:CA	1:C:90:LEU:CA[3_555]	0.61	1.59
1:B:95:THR:CB	1:C:239:THR:N[3_555]	0.61	1.59
1:B:155:GLY:O	1:C:116:ARG:C[3_555]	0.62	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:O	1:C:244:ALA:CA[3_555]	0.62	1.58
1:C:99:TRP:CZ3	1:C:107:TRP:CD2[2_555]	0.62	1.58
1:B:132:HIS:C	1:C:224:LEU:CG[3_555]	0.62	1.58
1:B:248:ILE:CA	1:C:50:GLY:N[3_555]	0.63	1.57
1:B:136:GLN:N	1:C:75:SER:N[3_555]	0.63	1.57
1:B:162:TRP:N	1:C:153:LEU:N[3_555]	0.63	1.57
1:B:115:ILE:CD1	1:C:121:PRO:N[3_555]	0.63	1.57
1:B:81:THR:O	1:C:142:THR:C[3_555]	0.64	1.56
1:B:112:TRP:CZ2	1:C:121:PRO:O[3_555]	0.64	1.56
1:A:255:ALA:CA	1:B:127:THR:CA[2_555]	0.65	1.55
1:B:80:VAL:CB	1:C:144:PRO:CD[3_555]	0.65	1.55
1:B:133:MET:SD	1:C:133:MET:SD[3_555]	0.66	1.54
1:A:254:ILE:CG1	1:B:128:SER:C[2_555]	0.66	1.54
1:B:100:LEU:CA	1:C:124:PRO:O[3_555]	0.66	1.54
1:C:99:TRP:N	1:C:254:ILE:CG2[2_555]	0.67	1.53
1:C:99:TRP:CG	1:C:107:TRP:CA[2_555]	0.67	1.53
1:B:99:TRP:C	1:C:126:THR:N[3_555]	0.68	1.52
1:B:100:LEU:CA	1:C:124:PRO:C[3_555]	0.68	1.52
1:B:162:TRP:N	1:C:152:ASN:C[3_555]	0.69	1.51
1:B:135:PHE:CD1	1:C:242:LEU:C[3_555]	0.69	1.51
1:B:190:ASN:O	1:C:54:LYS:CA[3_555]	0.69	1.51
1:B:148:ASN:OD1	1:C:220:VAL:CG1[3_555]	0.70	1.50
1:B:158:THR:N	1:C:135:PHE:CZ[3_555]	0.70	1.50
1:B:153:LEU:CG	1:C:96:VAL:O[3_555]	0.70	1.50
1:B:229:GLU:CA	1:C:223:ARG:NE[3_555]	0.71	1.49
1:B:247:THR:CA	1:C:165:GLN:NE2[3_555]	0.71	1.49
1:B:122:SER:N	1:C:151:SER:CB[3_555]	0.71	1.49
1:B:93:PRO:CA	1:C:122:SER:C[3_555]	0.71	1.49
1:B:76:THR:OG1	1:C:228:MET:CA[3_555]	0.72	1.48
1:B:132:HIS:CD2	1:C:223:ARG:C[3_555]	0.72	1.48
1:B:161:VAL:C	1:C:153:LEU:N[3_555]	0.72	1.48
1:B:89:GLU:CB	1:C:78:LEU:CB[3_555]	0.72	1.48
1:B:95:THR:O	1:C:239:THR:CB[3_555]	0.73	1.47
1:C:57:PRO:CD	1:C:249:ARG:CZ[2_555]	0.74	1.46
1:B:73:GLU:O	1:C:160:PRO:N[3_555]	0.74	1.46
1:B:188:ASP:N	1:C:171:VAL:CG1[3_555]	0.75	1.45
1:C:71:HIS:NE2	1:C:251:ILE:C[2_555]	0.75	1.45
1:B:226:THR:OG1	1:C:226:THR:OG1[3_555]	0.76	1.44
1:B:183:ILE:CD1	1:C:155:GLY:CA[3_555]	0.76	1.44
1:B:69:LEU:CD1	1:C:46:PRO:C[3_555]	0.76	1.44
1:B:155:GLY:C	1:C:116:ARG:O[3_555]	0.76	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:N	1:B:127:THR:C[2_555]	0.76	1.44
1:B:242:LEU:CA	1:C:131:ILE:O[3_555]	0.76	1.44
1:B:191:GLU:N	1:C:54:LYS:C[3_555]	0.76	1.44
1:B:184:THR:N	1:C:184:THR:O[3_555]	0.76	1.44
1:C:58:PRO:CD	1:C:250:LEU:O[2_555]	0.78	1.42
1:B:191:GLU:OE1	1:C:55:LEU:C[3_555]	0.78	1.42
1:B:237:VAL:CG1	1:C:149:GLN:CD[3_555]	0.78	1.42
1:B:71:HIS:ND1	1:C:162:TRP:CH2[3_555]	0.78	1.42
1:B:246:TYR:CA	1:C:49:GLN:NE2[3_555]	0.78	1.42
1:B:93:PRO:CA	1:C:123:CYS:N[3_555]	0.79	1.41
1:B:73:GLU:CD	1:C:162:TRP:CD1[3_555]	0.80	1.40
1:B:135:PHE:CD1	1:C:243:TYR:N[3_555]	0.80	1.40
1:B:98:THR:CA	1:C:127:THR:C[3_555]	0.80	1.40
1:B:100:LEU:CD1	1:C:123:CYS:O[3_555]	0.80	1.40
1:B:190:ASN:O	1:C:54:LYS:CB[3_555]	0.80	1.40
1:B:73:GLU:N	1:C:160:PRO:CG[3_555]	0.81	1.39
1:B:93:PRO:O	1:C:123:CYS:CB[3_555]	0.81	1.39
1:C:59:MET:CE	1:C:63:SER:CA[2_555]	0.81	1.39
1:B:117:TYR:CD2	1:C:119:TYR:CB[3_555]	0.81	1.39
1:B:223:ARG:C	1:C:76:THR:O[3_555]	0.81	1.39
1:B:74:LEU:O	1:C:129:GLY:O[3_555]	0.81	1.39
1:C:98:THR:N	1:C:254:ILE:CG1[2_555]	0.82	1.38
1:B:149:GLN:O	1:C:96:VAL:N[3_555]	0.82	1.38
1:B:152:ASN:CG	1:C:93:PRO:CA[3_555]	0.82	1.38
1:B:117:TYR:O	1:C:183:ILE:C[3_555]	0.82	1.38
1:B:190:ASN:N	1:C:172:ASN:ND2[3_555]	0.82	1.38
1:B:238:ASN:C	1:C:146:SER:O[3_555]	0.82	1.38
1:B:87:THR:OG1	1:C:87:THR:CB[3_555]	0.82	1.38
1:B:237:VAL:CB	1:C:149:GLN:OE1[3_555]	0.83	1.37
1:B:80:VAL:CA	1:C:144:PRO:N[3_555]	0.83	1.37
1:B:115:ILE:CG2	1:C:120:LEU:CB[3_555]	0.83	1.37
1:B:132:HIS:O	1:C:224:LEU:CG[3_555]	0.84	1.36
1:B:244:ALA:O	1:C:163:GLU:CB[3_555]	0.84	1.36
1:B:132:HIS:CA	1:C:224:LEU:CB[3_555]	0.84	1.36
1:C:101:ARG:CG	1:C:255:ALA:C[2_555]	0.84	1.36
1:B:161:VAL:CA	1:C:153:LEU:CB[3_555]	0.84	1.36
1:B:87:THR:N	1:C:87:THR:OG1[3_555]	0.84	1.36
1:C:101:ARG:CG	1:C:256:ALA:N[2_555]	0.85	1.35
1:B:76:THR:N	1:C:130:ALA:O[3_555]	0.85	1.35
1:B:93:PRO:CG	1:C:122:SER:O[3_555]	0.85	1.35
1:C:246:TYR:CZ	1:C:253:PRO:CG[2_555]	0.85	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:MET:CG	1:C:62:SER:C[2_555]	0.85	1.35
1:B:237:VAL:C	1:C:149:GLN:NE2[3_555]	0.85	1.35
1:B:93:PRO:CB	1:C:122:SER:O[3_555]	0.85	1.35
1:B:99:TRP:CD2	1:C:125:THR:O[3_555]	0.86	1.34
1:B:77:GLU:CG	1:C:229:GLU:CB[3_555]	0.86	1.34
1:B:97:GLY:CA	1:C:161:VAL:CG1[3_555]	0.87	1.33
1:A:254:ILE:C	1:B:127:THR:O[2_555]	0.87	1.33
1:C:85:VAL:O	3:B:270:HOH:O[2_555]	0.87	1.33
1:B:87:THR:OG1	1:C:87:THR:CG2[3_555]	0.87	1.33
1:A:258:LEU:O	1:B:231:GLY:C[2_555]	0.87	1.33
1:B:95:THR:O	1:C:239:THR:OG1[3_555]	0.87	1.33
1:B:135:PHE:CG	1:C:243:TYR:CA[3_555]	0.88	1.32
1:B:230:GLY:O	1:C:141:ASP:CB[3_555]	0.88	1.32
1:B:135:PHE:C	1:C:75:SER:N[3_555]	0.88	1.32
1:B:95:THR:N	1:C:238:ASN:O[3_555]	0.88	1.32
1:B:80:VAL:O	1:C:143:LEU:O[3_555]	0.88	1.32
1:B:184:THR:C	1:C:184:THR:CA[3_555]	0.88	1.32
1:C:59:MET:CG	1:C:63:SER:N[2_555]	0.89	1.31
1:B:131:ILE:CG2	1:C:134:GLY:CA[3_555]	0.89	1.31
1:C:57:PRO:O	1:C:66:VAL:CB[2_555]	0.89	1.31
1:B:160:PRO:CD	1:C:154:LYS:CB[3_555]	0.90	1.30
1:B:237:VAL:CG1	1:C:149:GLN:CG[3_555]	0.90	1.30
1:B:156:TYR:CB	1:C:115:ILE:CG1[3_555]	0.90	1.30
1:B:77:GLU:CG	1:C:229:GLU:CG[3_555]	0.90	1.30
1:C:58:PRO:O	1:C:67:THR:N[2_555]	0.90	1.30
1:B:115:ILE:CG1	1:C:121:PRO:CD[3_555]	0.90	1.30
1:B:100:LEU:O	1:C:124:PRO:CB[3_555]	0.91	1.29
1:C:99:TRP:CD2	1:C:107:TRP:CB[2_555]	0.91	1.29
1:B:186:ALA:CA	1:C:118:THR:OG1[3_555]	0.91	1.29
1:C:98:THR:N	1:C:254:ILE:CB[2_555]	0.91	1.29
1:C:99:TRP:CZ3	1:C:107:TRP:CE2[2_555]	0.91	1.29
1:B:183:ILE:CG1	1:C:155:GLY:CA[3_555]	0.92	1.28
1:B:239:THR:CB	1:C:150:LEU:CA[3_555]	0.92	1.28
1:C:55:LEU:CD1	1:C:252:GLU:OE1[2_555]	0.92	1.28
1:B:184:THR:CA	1:C:184:THR:C[3_555]	0.92	1.28
1:B:224:LEU:CD1	1:C:242:LEU:CG[3_555]	0.92	1.28
1:B:73:GLU:OE2	1:C:162:TRP:CG[3_555]	0.92	1.28
1:B:187:LEU:CB	1:C:120:LEU:CD1[3_555]	0.92	1.28
1:B:147:VAL:CG2	1:C:90:LEU:CD2[3_555]	0.92	1.28
1:B:186:ALA:N	1:C:118:THR:OG1[3_555]	0.93	1.27
1:A:254:ILE:CD1	1:B:128:SER:C[2_555]	0.93	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:N	1:C:153:LEU:CB[3_555]	0.93	1.27
1:B:133:MET:O	1:C:117:TYR:CG[3_555]	0.94	1.26
1:A:254:ILE:CA	1:B:127:THR:O[2_555]	0.94	1.26
1:B:98:THR:C	1:C:127:THR:CA[3_555]	0.94	1.26
1:B:161:VAL:CG2	1:C:153:LEU:CD1[3_555]	0.94	1.26
1:B:188:ASP:N	1:C:171:VAL:CB[3_555]	0.94	1.26
1:B:248:ILE:CG2	1:C:48:ALA:C[3_555]	0.94	1.26
1:B:224:LEU:CD1	1:C:242:LEU:CD1[3_555]	0.94	1.26
1:C:101:ARG:CB	1:C:255:ALA:CA[2_555]	0.95	1.25
1:B:229:GLU:CB	1:C:223:ARG:NE[3_555]	0.95	1.25
1:B:184:THR:CA	1:C:184:THR:O[3_555]	0.95	1.25
1:B:73:GLU:OE2	1:C:162:TRP:CD1[3_555]	0.95	1.25
1:B:81:THR:N	1:C:143:LEU:CA[3_555]	0.96	1.24
1:B:147:VAL:N	1:C:90:LEU:CG[3_555]	0.96	1.24
1:B:237:VAL:CB	1:C:149:GLN:CD[3_555]	0.96	1.24
1:B:135:PHE:CG	1:C:243:TYR:N[3_555]	0.97	1.23
1:B:121:PRO:N	1:C:156:TYR:CD1[3_555]	0.97	1.23
1:B:90:LEU:C	1:C:240:GLY:O[3_555]	0.97	1.23
1:B:154:LYS:O	1:C:244:ALA:N[3_555]	0.97	1.23
1:B:95:THR:CB	1:C:238:ASN:C[3_555]	0.97	1.23
1:A:254:ILE:C	1:B:127:THR:C[2_555]	0.97	1.23
1:B:80:VAL:C	1:C:143:LEU:O[3_555]	0.97	1.23
1:B:191:GLU:CD	1:C:56:ARG:N[3_555]	0.97	1.23
1:B:154:LYS:CB	1:C:244:ALA:O[3_555]	0.97	1.23
1:B:148:ASN:CB	1:C:92:MET:SD[3_555]	0.97	1.23
1:B:132:HIS:NE2	1:C:223:ARG:O[3_555]	0.98	1.22
1:B:226:THR:CB	1:C:226:THR:OG1[3_555]	0.98	1.22
1:B:184:THR:C	1:C:184:THR:C[3_555]	0.98	1.22
1:B:227:ALA:CB	1:C:89:GLU:N[3_555]	0.98	1.22
1:B:117:TYR:CE1	1:C:119:TYR:CD2[3_555]	0.98	1.22
1:B:226:THR:OG1	1:C:226:THR:CB[3_555]	0.98	1.22
1:B:157:VAL:C	1:C:135:PHE:CZ[3_555]	0.98	1.22
1:B:247:THR:OG1	1:C:165:GLN:CD[3_555]	0.98	1.22
1:B:162:TRP:CA	1:C:152:ASN:CA[3_555]	0.98	1.22
1:B:247:THR:CB	1:C:165:GLN:NE2[3_555]	0.99	1.21
1:B:236:ALA:O	1:C:145:VAL:CG2[3_555]	0.99	1.21
1:B:162:TRP:CA	1:C:152:ASN:C[3_555]	0.99	1.21
1:B:191:GLU:CB	1:C:55:LEU:CA[3_555]	0.99	1.21
1:B:238:ASN:CA	1:C:146:SER:CA[3_555]	0.99	1.21
1:C:58:PRO:N	1:C:250:LEU:O[2_555]	0.99	1.21
1:C:99:TRP:CE3	1:C:107:TRP:CG[2_555]	0.99	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:THR:O	1:C:185:ILE:N[3_555]	1.00	1.20
1:B:190:ASN:C	1:C:54:LYS:CA[3_555]	1.00	1.20
1:A:255:ALA:N	1:B:127:THR:CA[2_555]	1.00	1.20
1:B:116:ARG:CD	1:C:182:ALA:CB[3_555]	1.01	1.19
1:B:186:ALA:N	1:C:118:THR:CB[3_555]	1.01	1.19
1:B:116:ARG:CD	1:C:182:ALA:CA[3_555]	1.01	1.19
1:B:229:GLU:C	1:C:136:GLN:OE1[3_555]	1.01	1.19
1:B:131:ILE:CB	1:C:134:GLY:O[3_555]	1.02	1.18
1:B:121:PRO:CB	1:C:151:SER:O[3_555]	1.02	1.18
1:A:253:PRO:CB	1:B:162:TRP:NE1[2_555]	1.02	1.18
1:B:89:GLU:OE2	1:C:79:ALA:N[3_555]	1.02	1.18
1:C:99:TRP:CB	1:C:107:TRP:CA[2_555]	1.02	1.18
1:A:259:ASN:N	1:B:232:SER:OG[2_555]	1.02	1.18
1:B:73:GLU:O	1:C:160:PRO:CA[3_555]	1.02	1.18
1:B:238:ASN:CB	1:C:146:SER:CA[3_555]	1.03	1.17
1:B:112:TRP:CA	1:C:51:THR:N[3_555]	1.03	1.17
1:B:152:ASN:OD1	1:C:93:PRO:CA[3_555]	1.03	1.17
1:B:191:GLU:OE1	1:C:55:LEU:O[3_555]	1.03	1.17
1:B:93:PRO:O	1:C:123:CYS:CA[3_555]	1.03	1.17
1:B:225:VAL:CG2	1:C:76:THR:OG1[3_555]	1.03	1.17
1:B:116:ARG:N	1:C:164:GLY:O[3_555]	1.03	1.17
1:C:71:HIS:CE1	1:C:251:ILE:C[2_555]	1.04	1.16
1:B:224:LEU:N	1:C:76:THR:O[3_555]	1.04	1.16
1:C:71:HIS:CE1	1:C:251:ILE:O[2_555]	1.04	1.16
1:C:58:PRO:CD	1:C:250:LEU:C[2_555]	1.05	1.15
1:B:136:GLN:N	1:C:74:LEU:C[3_555]	1.05	1.15
1:B:116:ARG:NE	1:C:182:ALA:CB[3_555]	1.05	1.15
1:B:131:ILE:CG2	1:C:134:GLY:C[3_555]	1.05	1.15
1:B:239:THR:O	1:C:151:SER:N[3_555]	1.06	1.14
1:B:95:THR:C	1:C:239:THR:CA[3_555]	1.06	1.14
1:B:152:ASN:N	1:C:96:VAL:CG2[3_555]	1.06	1.14
1:B:242:LEU:CA	1:C:131:ILE:C[3_555]	1.06	1.14
1:B:69:LEU:CD1	1:C:46:PRO:CA[3_555]	1.06	1.14
1:C:99:TRP:CH2	1:C:107:TRP:CD2[2_555]	1.06	1.14
1:B:191:GLU:CD	1:C:55:LEU:C[3_555]	1.07	1.13
1:B:120:LEU:O	1:C:156:TYR:CE1[3_555]	1.07	1.13
1:B:183:ILE:CD1	1:C:155:GLY:C[3_555]	1.07	1.13
1:C:101:ARG:CB	1:C:255:ALA:C[2_555]	1.07	1.13
1:B:95:THR:CG2	1:C:238:ASN:CA[3_555]	1.08	1.12
1:B:76:THR:CA	1:C:130:ALA:O[3_555]	1.08	1.12
1:C:85:VAL:C	3:B:270:HOH:O[2_555]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:CD1	1:C:133:MET:CA[3_555]	1.08	1.12
1:B:154:LYS:CA	1:C:244:ALA:O[3_555]	1.08	1.12
1:B:185:ILE:N	1:C:184:THR:CA[3_555]	1.08	1.12
1:B:147:VAL:O	1:C:90:LEU:O[3_555]	1.08	1.12
1:B:237:VAL:CG2	1:C:149:GLN:OE1[3_555]	1.09	1.11
1:B:119:TYR:CA	1:C:157:VAL:O[3_555]	1.09	1.11
1:B:148:ASN:O	1:C:92:MET:C[3_555]	1.09	1.11
1:B:133:MET:O	1:C:117:TYR:CD1[3_555]	1.09	1.11
1:B:148:ASN:O	1:C:92:MET:CA[3_555]	1.09	1.11
1:C:56:ARG:C	1:C:251:ILE:CD1[2_555]	1.10	1.10
1:B:248:ILE:CA	1:C:49:GLN:C[3_555]	1.10	1.10
1:B:87:THR:C	3:C:265:HOH:O[3_555]	1.10	1.10
1:B:117:TYR:CD2	1:C:119:TYR:CG[3_555]	1.10	1.10
1:B:227:ALA:O	1:C:224:LEU:O[3_555]	1.10	1.10
1:B:246:TYR:CD1	1:C:162:TRP:O[3_555]	1.10	1.10
1:B:123:CYS:O	1:C:152:ASN:OD1[3_555]	1.10	1.10
1:B:89:GLU:CB	1:C:78:LEU:CA[3_555]	1.10	1.10
1:B:161:VAL:CG1	1:C:153:LEU:CD2[3_555]	1.11	1.09
1:B:114:ALA:O	1:C:165:GLN:CB[3_555]	1.11	1.09
1:B:114:ALA:CB	1:C:165:GLN:O[3_555]	1.11	1.09
1:C:98:THR:C	1:C:254:ILE:CG2[2_555]	1.11	1.09
1:B:239:THR:N	1:C:146:SER:O[3_555]	1.11	1.09
1:B:132:HIS:CG	1:C:224:LEU:N[3_555]	1.11	1.09
1:B:98:THR:C	1:C:127:THR:N[3_555]	1.11	1.09
1:B:158:THR:N	1:C:135:PHE:CE1[3_555]	1.12	1.08
1:B:119:TYR:CE1	1:C:156:TYR:CD2[3_555]	1.12	1.08
1:B:78:LEU:CB	1:C:227:ALA:CB[3_555]	1.12	1.08
1:B:226:THR:CG2	1:C:226:THR:CG2[3_555]	1.12	1.08
1:C:101:ARG:NH1	1:C:258:LEU:CB[2_555]	1.12	1.08
1:B:80:VAL:CG1	1:C:144:PRO:CD[3_555]	1.13	1.07
1:B:157:VAL:CG2	1:C:185:ILE:O[3_555]	1.13	1.07
1:C:56:ARG:O	1:C:251:ILE:CG1[2_555]	1.13	1.07
1:C:101:ARG:CD	1:C:255:ALA:O[2_555]	1.13	1.07
1:B:91:VAL:CG2	1:C:241:ARG:CA[3_555]	1.13	1.07
1:B:92:MET:O	1:C:239:THR:O[3_555]	1.13	1.07
1:C:99:TRP:C	1:C:106:ASN:O[2_555]	1.13	1.07
1:B:89:GLU:CA	1:C:78:LEU:N[3_555]	1.13	1.07
1:B:92:MET:C	1:C:122:SER:CB[3_555]	1.14	1.06
1:B:160:PRO:O	1:C:154:LYS:N[3_555]	1.14	1.06
1:B:192:VAL:CG2	1:C:53:VAL:CB[3_555]	1.15	1.05
1:B:154:LYS:C	1:C:244:ALA:CA[3_555]	1.15	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:TRP:O	1:C:51:THR:C[3_555]	1.15	1.05
1:C:55:LEU:CD1	1:C:252:GLU:CD[2_555]	1.15	1.05
1:B:155:GLY:CA	1:C:116:ARG:O[3_555]	1.15	1.05
1:B:241:ARG:N	1:C:132:HIS:ND1[3_555]	1.15	1.05
1:B:243:TYR:CA	1:C:159:GLY:CA[3_555]	1.16	1.04
1:B:136:GLN:CA	1:C:74:LEU:O[3_555]	1.16	1.04
1:B:100:LEU:N	1:C:124:PRO:O[3_555]	1.16	1.04
1:B:132:HIS:CD2	1:C:223:ARG:O[3_555]	1.16	1.04
1:B:92:MET:CA	1:C:122:SER:CB[3_555]	1.16	1.04
1:B:149:GLN:CB	1:C:95:THR:CA[3_555]	1.16	1.04
1:B:237:VAL:CA	1:C:149:GLN:NE2[3_555]	1.16	1.04
1:B:98:THR:CA	1:C:127:THR:CA[3_555]	1.16	1.04
1:A:254:ILE:CG1	1:B:128:SER:CA[2_555]	1.16	1.04
1:B:155:GLY:O	1:C:116:ARG:O[3_555]	1.17	1.03
1:B:137:TYR:CE1	1:C:73:GLU:C[3_555]	1.17	1.03
1:B:146:SER:OG	1:C:90:LEU:CD1[3_555]	1.17	1.03
1:B:97:GLY:O	1:C:127:THR:CB[3_555]	1.17	1.03
1:C:103:VAL:N	1:C:106:ASN:ND2[2_555]	1.17	1.03
1:B:189:THR:OG1	1:C:168:LEU:CD1[3_555]	1.17	1.03
1:B:76:THR:N	1:C:130:ALA:C[3_555]	1.17	1.03
1:B:170:PHE:CD2	1:C:179:THR:O[3_555]	1.17	1.03
1:C:59:MET:CE	1:C:63:SER:C[2_555]	1.17	1.03
1:B:117:TYR:CG	1:C:119:TYR:CG[3_555]	1.17	1.03
1:B:238:ASN:CA	1:C:146:SER:C[3_555]	1.18	1.02
1:C:73:GLU:OE2	1:C:253:PRO:N[2_555]	1.18	1.02
1:B:100:LEU:O	1:C:124:PRO:CA[3_555]	1.18	1.02
1:B:112:TRP:CE2	1:C:121:PRO:O[3_555]	1.18	1.02
1:B:242:LEU:C	1:C:131:ILE:O[3_555]	1.18	1.02
1:B:103:VAL:CB	1:C:47:ILE:CD1[3_555]	1.18	1.02
1:B:238:ASN:N	1:C:146:SER:N[3_555]	1.18	1.02
1:B:73:GLU:C	1:C:160:PRO:CB[3_555]	1.19	1.01
1:B:112:TRP:CZ2	1:C:121:PRO:C[3_555]	1.19	1.01
1:B:112:TRP:O	1:C:51:THR:CA[3_555]	1.19	1.01
1:B:191:GLU:CG	1:C:55:LEU:CA[3_555]	1.19	1.01
1:B:112:TRP:C	1:C:51:THR:N[3_555]	1.19	1.01
1:A:253:PRO:CA	1:B:162:TRP:NE1[2_555]	1.19	1.01
1:C:71:HIS:CE1	1:C:251:ILE:CA[2_555]	1.19	1.01
1:B:239:THR:OG1	1:C:150:LEU:CB[3_555]	1.20	1.00
1:B:229:GLU:OE1	1:C:139:MET:CE[3_555]	1.20	1.00
1:B:99:TRP:CZ3	1:C:125:THR:CB[3_555]	1.20	1.00
1:B:155:GLY:O	1:C:117:TYR:N[3_555]	1.20	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:O	1:C:124:PRO:CG[3_555]	1.20	1.00
1:B:147:VAL:CA	1:C:90:LEU:CB[3_555]	1.20	1.00
1:B:120:LEU:C	1:C:156:TYR:CD1[3_555]	1.20	1.00
1:B:170:PHE:O	1:C:181:ARG:CB[3_555]	1.20	1.00
1:B:242:LEU:O	1:C:131:ILE:N[3_555]	1.20	1.00
1:B:132:HIS:NE2	1:C:223:ARG:C[3_555]	1.20	1.00
1:B:151:SER:CB	1:C:91:VAL:O[3_555]	1.21	0.99
1:B:227:ALA:O	1:C:224:LEU:C[3_555]	1.21	0.99
1:C:99:TRP:CG	1:C:107:TRP:N[2_555]	1.21	0.99
1:B:241:ARG:CA	1:C:132:HIS:CE1[3_555]	1.21	0.99
1:C:246:TYR:OH	1:C:253:PRO:CG[2_555]	1.21	0.99
1:B:103:VAL:CG1	1:C:47:ILE:CG1[3_555]	1.21	0.99
1:B:93:PRO:N	1:C:122:SER:C[3_555]	1.21	0.99
1:A:253:PRO:CG	1:B:162:TRP:CZ2[2_555]	1.21	0.99
1:B:247:THR:OG1	1:C:165:GLN:OE1[3_555]	1.21	0.99
1:B:236:ALA:CA	1:C:145:VAL:CG1[3_555]	1.22	0.98
1:B:135:PHE:CD2	1:C:243:TYR:CA[3_555]	1.22	0.98
1:B:133:MET:C	1:C:117:TYR:CD2[3_555]	1.22	0.98
1:B:246:TYR:CE1	1:C:162:TRP:O[3_555]	1.22	0.98
1:B:248:ILE:CG2	1:C:48:ALA:O[3_555]	1.22	0.98
1:B:242:LEU:CB	1:C:132:HIS:N[3_555]	1.22	0.98
1:C:73:GLU:OE2	1:C:252:GLU:C[2_555]	1.22	0.98
1:B:229:GLU:O	1:C:136:GLN:OE1[3_555]	1.22	0.98
1:C:73:GLU:CD	1:C:252:GLU:O[2_555]	1.22	0.98
1:B:243:TYR:N	1:C:159:GLY:N[3_555]	1.22	0.98
1:C:97:GLY:O	1:C:255:ALA:N[2_555]	1.22	0.98
1:B:246:TYR:CE1	1:C:162:TRP:C[3_555]	1.22	0.98
1:B:99:TRP:CE3	1:C:125:THR:CB[3_555]	1.23	0.97
1:B:161:VAL:N	1:C:153:LEU:CA[3_555]	1.23	0.97
1:B:157:VAL:CG1	1:C:185:ILE:C[3_555]	1.23	0.97
1:B:185:ILE:CB	1:C:117:TYR:O[3_555]	1.23	0.97
1:C:57:PRO:O	1:C:66:VAL:CA[2_555]	1.23	0.97
1:B:241:ARG:CA	1:C:132:HIS:CG[3_555]	1.23	0.97
1:B:187:LEU:C	1:C:171:VAL:CB[3_555]	1.23	0.97
1:B:188:ASP:OD1	1:C:55:LEU:CD2[3_555]	1.23	0.97
1:B:115:ILE:CD1	1:C:121:PRO:CD[3_555]	1.24	0.96
1:B:133:MET:N	1:C:224:LEU:CD2[3_555]	1.24	0.96
1:B:239:THR:OG1	1:C:150:LEU:CA[3_555]	1.24	0.96
1:A:254:ILE:CB	1:B:128:SER:CA[2_555]	1.24	0.96
1:C:102:GLY:C	1:C:106:ASN:CG[2_555]	1.24	0.96
1:B:246:TYR:CB	1:C:49:GLN:NE2[3_555]	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:TYR:O	1:C:183:ILE:O[3_555]	1.24	0.96
1:B:90:LEU:O	1:C:240:GLY:O[3_555]	1.24	0.96
1:B:221:PRO:CG	1:C:241:ARG:NH2[3_555]	1.24	0.96
1:B:134:GLY:N	1:C:117:TYR:CD2[3_555]	1.25	0.95
1:B:242:LEU:CB	1:C:131:ILE:C[3_555]	1.25	0.95
1:B:132:HIS:CD2	1:C:224:LEU:N[3_555]	1.25	0.95
1:B:137:TYR:CD1	1:C:74:LEU:N[3_555]	1.25	0.95
1:B:132:HIS:CB	1:C:224:LEU:CB[3_555]	1.25	0.95
1:B:237:VAL:N	1:C:145:VAL:CG2[3_555]	1.25	0.95
1:B:99:TRP:O	1:C:126:THR:N[3_555]	1.25	0.95
1:B:170:PHE:CE2	1:C:179:THR:O[3_555]	1.26	0.94
1:B:183:ILE:N	3:C:267:HOH:O[3_555]	1.26	0.94
1:B:156:TYR:O	1:C:115:ILE:C[3_555]	1.26	0.94
1:B:137:TYR:CE1	1:C:74:LEU:N[3_555]	1.26	0.94
1:B:101:ARG:N	1:C:127:THR:OG1[3_555]	1.26	0.94
1:B:117:TYR:CD1	1:C:119:TYR:CD2[3_555]	1.27	0.93
1:B:81:THR:O	1:C:142:THR:CA[3_555]	1.27	0.93
1:C:97:GLY:O	1:C:254:ILE:C[2_555]	1.27	0.93
1:B:242:LEU:N	1:C:131:ILE:O[3_555]	1.27	0.93
1:B:229:GLU:CB	1:C:223:ARG:CD[3_555]	1.27	0.93
1:B:87:THR:CA	1:C:87:THR:OG1[3_555]	1.27	0.93
1:A:253:PRO:CB	1:B:162:TRP:CE2[2_555]	1.27	0.93
1:B:159:GLY:N	1:C:135:PHE:CD1[3_555]	1.27	0.93
1:B:158:THR:CA	1:C:135:PHE:CE1[3_555]	1.27	0.93
1:B:244:ALA:C	1:C:163:GLU:CB[3_555]	1.28	0.92
1:B:238:ASN:CB	1:C:146:SER:C[3_555]	1.28	0.92
1:B:112:TRP:CB	1:C:51:THR:OG1[3_555]	1.28	0.92
1:B:224:LEU:O	1:C:76:THR:CG2[3_555]	1.28	0.92
1:B:90:LEU:CD1	1:C:77:GLU:OE2[3_555]	1.28	0.92
1:B:245:SER:C	1:C:164:GLY:N[3_555]	1.28	0.92
1:B:132:HIS:C	1:C:224:LEU:CD2[3_555]	1.29	0.91
1:B:80:VAL:CB	1:C:144:PRO:N[3_555]	1.29	0.91
1:B:185:ILE:CG1	1:C:117:TYR:C[3_555]	1.29	0.91
1:C:97:GLY:C	1:C:254:ILE:CG1[2_555]	1.29	0.91
1:B:190:ASN:C	1:C:54:LYS:C[3_555]	1.29	0.91
1:B:98:THR:OG1	1:C:128:SER:N[3_555]	1.29	0.91
1:C:56:ARG:O	1:C:251:ILE:CD1[2_555]	1.29	0.91
1:A:254:ILE:CG2	1:B:128:SER:CB[2_555]	1.29	0.91
1:C:100:LEU:N	1:C:106:ASN:O[2_555]	1.29	0.91
1:B:239:THR:CB	1:C:150:LEU:N[3_555]	1.29	0.91
1:B:119:TYR:OH	1:C:150:LEU:O[3_555]	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:TYR:OH	1:C:253:PRO:CA[2_555]	1.29	0.91
1:B:117:TYR:C	1:C:183:ILE:CB[3_555]	1.30	0.90
1:B:81:THR:C	1:C:142:THR:C[3_555]	1.30	0.90
1:B:117:TYR:C	1:C:183:ILE:CG2[3_555]	1.30	0.90
1:B:74:LEU:CA	1:C:130:ALA:CB[3_555]	1.30	0.90
1:B:191:GLU:OE2	1:C:56:ARG:N[3_555]	1.30	0.90
1:C:57:PRO:N	1:C:251:ILE:CD1[2_555]	1.30	0.90
1:B:131:ILE:CD1	1:C:133:MET:C[3_555]	1.30	0.90
1:B:248:ILE:CB	1:C:49:GLN:C[3_555]	1.30	0.90
1:C:71:HIS:ND1	1:C:251:ILE:O[2_555]	1.30	0.90
1:B:115:ILE:C	1:C:164:GLY:O[3_555]	1.30	0.90
1:C:99:TRP:O	1:C:106:ASN:CA[2_555]	1.30	0.90
1:B:117:TYR:CZ	1:C:119:TYR:CD2[3_555]	1.30	0.90
1:B:117:TYR:CG	1:C:119:TYR:CB[3_555]	1.31	0.89
1:B:158:THR:CA	1:C:135:PHE:CD1[3_555]	1.31	0.89
1:B:69:LEU:CD1	1:C:47:ILE:N[3_555]	1.31	0.89
1:B:152:ASN:ND2	1:C:93:PRO:CA[3_555]	1.31	0.89
1:B:147:VAL:O	1:C:90:LEU:C[3_555]	1.31	0.89
1:B:136:GLN:O	1:C:74:LEU:CD1[3_555]	1.31	0.89
1:B:82:VAL:N	1:C:142:THR:CB[3_555]	1.31	0.89
1:B:184:THR:OG1	1:C:184:THR:N[3_555]	1.31	0.89
1:B:123:CYS:N	1:C:151:SER:OG[3_555]	1.32	0.88
1:C:72:CYS:O	1:C:252:GLU:CB[2_555]	1.32	0.88
1:C:58:PRO:C	1:C:66:VAL:C[2_555]	1.32	0.88
1:C:59:MET:CB	1:C:66:VAL:O[2_555]	1.32	0.88
1:B:246:TYR:O	1:C:49:GLN:CD[3_555]	1.32	0.88
1:B:99:TRP:N	1:C:127:THR:N[3_555]	1.32	0.88
1:B:147:VAL:C	1:C:90:LEU:C[3_555]	1.32	0.88
1:B:236:ALA:C	1:C:145:VAL:CB[3_555]	1.32	0.88
1:B:73:GLU:CA	1:C:160:PRO:CG[3_555]	1.32	0.88
1:B:135:PHE:C	1:C:74:LEU:C[3_555]	1.32	0.88
1:B:150:LEU:CD2	1:C:89:GLU:CB[3_555]	1.32	0.88
1:B:95:THR:CA	1:C:238:ASN:C[3_555]	1.33	0.87
1:B:185:ILE:CB	1:C:117:TYR:C[3_555]	1.33	0.87
1:B:119:TYR:N	1:C:157:VAL:CB[3_555]	1.33	0.87
1:B:149:GLN:CB	1:C:95:THR:N[3_555]	1.33	0.87
1:B:160:PRO:C	1:C:153:LEU:CA[3_555]	1.33	0.87
1:B:98:THR:CA	1:C:128:SER:N[3_555]	1.33	0.87
1:C:71:HIS:NE2	1:C:251:ILE:CA[2_555]	1.33	0.87
1:B:154:LYS:CA	1:C:244:ALA:C[3_555]	1.33	0.87
1:B:155:GLY:N	1:C:244:ALA:C[3_555]	1.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ALA:CA	1:C:135:PHE:C[3_555]	1.33	0.87
1:B:243:TYR:CA	1:C:159:GLY:N[3_555]	1.34	0.86
1:B:98:THR:N	1:C:127:THR:C[3_555]	1.34	0.86
1:C:246:TYR:CZ	1:C:253:PRO:CB[2_555]	1.34	0.86
1:B:148:ASN:CA	1:C:92:MET:CB[3_555]	1.34	0.86
1:B:81:THR:N	1:C:143:LEU:C[3_555]	1.34	0.86
1:B:245:SER:O	1:C:165:GLN:N[3_555]	1.35	0.85
1:C:97:GLY:C	1:C:254:ILE:CB[2_555]	1.35	0.85
1:B:98:THR:O	1:C:126:THR:C[3_555]	1.35	0.85
1:B:78:LEU:CG	1:C:227:ALA:CB[3_555]	1.35	0.85
1:B:115:ILE:CD1	1:C:120:LEU:C[3_555]	1.35	0.85
1:B:119:TYR:CA	1:C:157:VAL:CA[3_555]	1.35	0.85
1:B:154:LYS:CG	1:C:72:CYS:CB[3_555]	1.35	0.85
1:B:80:VAL:N	1:C:144:PRO:C[3_555]	1.36	0.84
1:C:102:GLY:C	1:C:106:ASN:OD1[2_555]	1.36	0.84
1:C:59:MET:CE	1:C:63:SER:CB[2_555]	1.36	0.84
1:C:99:TRP:CD2	1:C:107:TRP:CG[2_555]	1.36	0.84
1:B:88:SER:N	3:C:265:HOH:O[3_555]	1.36	0.84
1:B:221:PRO:CG	1:C:241:ARG:CZ[3_555]	1.36	0.84
1:B:183:ILE:CB	1:C:155:GLY:O[3_555]	1.36	0.84
1:B:118:THR:N	1:C:183:ILE:CG2[3_555]	1.36	0.84
1:B:152:ASN:ND2	1:C:93:PRO:N[3_555]	1.36	0.84
1:B:81:THR:O	1:C:143:LEU:N[3_555]	1.36	0.84
1:B:238:ASN:O	1:C:149:GLN:N[3_555]	1.37	0.83
1:B:157:VAL:CG1	1:C:186:ALA:N[3_555]	1.37	0.83
1:C:59:MET:SD	1:C:63:SER:CA[2_555]	1.37	0.83
1:B:146:SER:C	1:C:90:LEU:CB[3_555]	1.37	0.83
1:B:113:VAL:N	1:C:50:GLY:O[3_555]	1.37	0.83
1:A:258:LEU:O	1:B:231:GLY:O[2_555]	1.37	0.83
1:B:76:THR:OG1	1:C:228:MET:CB[3_555]	1.37	0.83
1:B:100:LEU:C	1:C:124:PRO:O[3_555]	1.37	0.83
1:B:81:THR:C	1:C:142:THR:CA[3_555]	1.37	0.83
1:B:119:TYR:C	1:C:157:VAL:C[3_555]	1.37	0.83
1:C:58:PRO:O	1:C:67:THR:CA[2_555]	1.37	0.83
1:C:60:LEU:O	1:C:62:SER:N[2_555]	1.37	0.83
1:B:98:THR:OG1	1:C:128:SER:CA[3_555]	1.37	0.83
1:B:227:ALA:C	1:C:224:LEU:O[3_555]	1.37	0.83
1:B:112:TRP:O	1:C:52:MET:N[3_555]	1.38	0.82
1:B:80:VAL:N	1:C:144:PRO:O[3_555]	1.38	0.82
1:B:123:CYS:C	1:C:152:ASN:OD1[3_555]	1.38	0.82
1:B:160:PRO:O	1:C:153:LEU:O[3_555]	1.38	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:HIS:C	1:C:224:LEU:CB[3_555]	1.39	0.81
1:C:101:ARG:NH2	1:C:258:LEU:N[2_555]	1.39	0.81
1:C:99:TRP:CB	1:C:107:TRP:C[2_555]	1.39	0.81
1:B:132:HIS:N	1:C:224:LEU:CA[3_555]	1.39	0.81
1:B:85:VAL:O	1:C:88:SER:N[3_555]	1.39	0.81
1:B:117:TYR:CA	1:C:183:ILE:CG2[3_555]	1.39	0.81
1:B:245:SER:CA	1:C:163:GLU:CG[3_555]	1.39	0.81
1:B:191:GLU:CB	1:C:55:LEU:CB[3_555]	1.39	0.81
1:B:188:ASP:CB	1:C:171:VAL:O[3_555]	1.39	0.81
1:B:132:HIS:CE1	1:C:223:ARG:N[3_555]	1.39	0.81
1:B:185:ILE:CD1	1:C:118:THR:N[3_555]	1.39	0.81
1:B:160:PRO:C	1:C:153:LEU:C[3_555]	1.39	0.81
1:B:119:TYR:O	1:C:157:VAL:CA[3_555]	1.39	0.81
1:C:99:TRP:CG	1:C:107:TRP:CB[2_555]	1.39	0.81
1:C:101:ARG:NH1	1:C:258:LEU:CG[2_555]	1.39	0.81
1:C:103:VAL:N	1:C:106:ASN:OD1[2_555]	1.39	0.81
1:B:95:THR:CA	1:C:239:THR:N[3_555]	1.39	0.81
1:B:153:LEU:CA	1:C:96:VAL:CG1[3_555]	1.39	0.81
1:B:130:ALA:CB	1:C:136:GLN:CA[3_555]	1.39	0.81
1:C:103:VAL:CG1	1:C:106:ASN:CB[2_555]	1.40	0.80
1:C:97:GLY:C	1:C:254:ILE:CA[2_555]	1.40	0.80
1:B:89:GLU:O	1:C:78:LEU:N[3_555]	1.40	0.80
1:B:87:THR:CB	1:C:87:THR:CG2[3_555]	1.40	0.80
1:B:155:GLY:C	1:C:116:ARG:C[3_555]	1.40	0.80
1:B:86:VAL:CG2	1:C:88:SER:O[3_555]	1.40	0.80
1:B:238:ASN:CA	1:C:146:SER:N[3_555]	1.40	0.80
1:B:154:LYS:C	1:C:245:SER:N[3_555]	1.40	0.80
1:B:95:THR:C	1:C:239:THR:CB[3_555]	1.40	0.80
1:C:73:GLU:OE2	1:C:252:GLU:O[2_555]	1.40	0.80
1:B:117:TYR:CZ	1:C:119:TYR:CE2[3_555]	1.40	0.80
1:B:158:THR:CA	1:C:135:PHE:CZ[3_555]	1.40	0.80
1:B:162:TRP:CB	1:C:152:ASN:CB[3_555]	1.40	0.80
1:B:93:PRO:N	1:C:122:SER:CA[3_555]	1.40	0.80
1:B:149:GLN:CG	1:C:95:THR:OG1[3_555]	1.41	0.79
1:C:71:HIS:NE2	1:C:252:GLU:N[2_555]	1.41	0.79
1:B:96:VAL:CA	1:C:239:THR:CG2[3_555]	1.41	0.79
1:B:191:GLU:N	1:C:55:LEU:N[3_555]	1.41	0.79
1:B:156:TYR:O	1:C:115:ILE:O[3_555]	1.41	0.79
1:A:106:ASN:CG	1:B:126:THR:CG2[2_555]	1.41	0.79
1:B:89:GLU:OE2	1:C:79:ALA:CA[3_555]	1.41	0.79
1:C:59:MET:N	1:C:66:VAL:C[2_555]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASN:C	1:C:54:LYS:N[3_555]	1.41	0.79
1:C:59:MET:CA	1:C:66:VAL:O[2_555]	1.41	0.79
1:C:99:TRP:CE3	1:C:107:TRP:CD2[2_555]	1.41	0.79
1:B:79:ALA:C	1:C:144:PRO:O[3_555]	1.41	0.79
1:B:237:VAL:O	1:C:149:GLN:NE2[3_555]	1.41	0.79
1:B:81:THR:C	1:C:143:LEU:N[3_555]	1.41	0.79
1:B:133:MET:CA	1:C:224:LEU:CD2[3_555]	1.42	0.78
1:B:148:ASN:O	1:C:92:MET:O[3_555]	1.42	0.78
1:B:130:ALA:CB	1:C:135:PHE:C[3_555]	1.42	0.78
1:B:93:PRO:CB	1:C:122:SER:C[3_555]	1.42	0.78
1:C:99:TRP:C	1:C:106:ASN:C[2_555]	1.42	0.78
1:B:99:TRP:CG	1:C:125:THR:O[3_555]	1.42	0.78
1:B:160:PRO:C	1:C:154:LYS:N[3_555]	1.42	0.78
1:A:253:PRO:CG	1:B:162:TRP:NE1[2_555]	1.42	0.78
1:B:152:ASN:OD1	1:C:93:PRO:O[3_555]	1.42	0.78
1:B:243:TYR:CB	1:C:159:GLY:N[3_555]	1.42	0.78
1:B:93:PRO:N	1:C:122:SER:CB[3_555]	1.43	0.77
1:C:205:TYR:CE1	3:B:266:HOH:O[2_555]	1.43	0.77
1:B:223:ARG:CG	1:C:76:THR:C[3_555]	1.43	0.77
1:B:185:ILE:CG1	1:C:118:THR:CA[3_555]	1.43	0.77
1:B:98:THR:O	1:C:127:THR:N[3_555]	1.43	0.77
1:B:133:MET:O	1:C:117:TYR:CD2[3_555]	1.43	0.77
1:B:131:ILE:CB	1:C:134:GLY:C[3_555]	1.43	0.77
1:B:91:VAL:CG2	1:C:241:ARG:CB[3_555]	1.43	0.77
1:B:225:VAL:CB	1:C:76:THR:OG1[3_555]	1.43	0.77
1:C:57:PRO:CD	1:C:249:ARG:NH1[2_555]	1.43	0.77
1:B:162:TRP:CG	1:C:152:ASN:O[3_555]	1.43	0.77
1:C:59:MET:SD	1:C:63:SER:O[2_555]	1.43	0.77
1:B:80:VAL:N	1:C:144:PRO:CA[3_555]	1.43	0.77
1:B:136:GLN:C	1:C:74:LEU:CG[3_555]	1.43	0.77
1:B:99:TRP:CZ3	1:C:125:THR:OG1[3_555]	1.43	0.77
1:A:106:ASN:ND2	1:B:126:THR:CG2[2_555]	1.43	0.77
1:B:93:PRO:C	1:C:123:CYS:CA[3_555]	1.44	0.76
1:B:149:GLN:CB	1:C:95:THR:CB[3_555]	1.44	0.76
1:B:116:ARG:CG	1:C:183:ILE:N[3_555]	1.44	0.76
1:B:191:GLU:CA	1:C:54:LYS:C[3_555]	1.44	0.76
1:A:253:PRO:CD	1:B:162:TRP:CZ2[2_555]	1.44	0.76
1:B:133:MET:C	1:C:117:TYR:CG[3_555]	1.44	0.76
1:B:80:VAL:CA	1:C:143:LEU:C[3_555]	1.44	0.76
1:B:161:VAL:CB	1:C:153:LEU:CD1[3_555]	1.44	0.76
1:C:101:ARG:CZ	1:C:258:LEU:N[2_555]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:O	1:B:126:THR:C[2_555]	1.44	0.76
1:B:183:ILE:C	1:C:184:THR:O[3_555]	1.44	0.76
1:B:237:VAL:CG1	1:C:149:GLN:OE1[3_555]	1.44	0.76
1:A:258:LEU:C	1:B:232:SER:OG[2_555]	1.44	0.76
1:B:72:CYS:O	1:C:162:TRP:CZ2[3_555]	1.44	0.76
1:B:241:ARG:CG	1:C:132:HIS:CE1[3_555]	1.44	0.76
1:B:247:THR:CB	1:C:165:GLN:CD[3_555]	1.44	0.76
1:B:130:ALA:N	1:C:136:GLN:CG[3_555]	1.45	0.75
1:B:242:LEU:N	1:C:131:ILE:C[3_555]	1.45	0.75
1:C:57:PRO:CB	1:C:249:ARG:CG[2_555]	1.45	0.75
1:B:99:TRP:CA	1:C:126:THR:CA[3_555]	1.45	0.75
1:B:136:GLN:CA	1:C:74:LEU:C[3_555]	1.45	0.75
1:B:170:PHE:N	1:C:180:SER:O[3_555]	1.45	0.75
1:B:119:TYR:N	1:C:157:VAL:CA[3_555]	1.45	0.75
1:B:101:ARG:NH1	1:C:237:VAL:CG1[3_555]	1.45	0.75
1:B:81:THR:N	1:C:143:LEU:N[3_555]	1.45	0.75
1:B:99:TRP:CE3	1:C:125:THR:O[3_555]	1.45	0.75
1:B:184:THR:CA	1:C:184:THR:CA[3_555]	1.46	0.74
1:B:95:THR:CA	1:C:238:ASN:O[3_555]	1.46	0.74
1:A:254:ILE:CD1	1:B:129:GLY:N[2_555]	1.46	0.74
1:C:73:GLU:OE2	1:C:253:PRO:CA[2_555]	1.46	0.74
1:B:149:GLN:CB	1:C:95:THR:OG1[3_555]	1.46	0.74
1:B:182:ALA:C	3:C:267:HOH:O[3_555]	1.47	0.73
1:B:114:ALA:N	1:C:51:THR:CG2[3_555]	1.47	0.73
1:B:156:TYR:CE2	1:C:91:VAL:CG2[3_555]	1.47	0.73
1:B:148:ASN:CG	1:C:92:MET:SD[3_555]	1.47	0.73
1:C:99:TRP:CH2	1:C:107:TRP:CE3[2_555]	1.47	0.73
1:B:158:THR:CG2	1:C:135:PHE:CD2[3_555]	1.47	0.73
1:C:102:GLY:C	1:C:106:ASN:ND2[2_555]	1.47	0.73
1:A:254:ILE:CD1	1:B:128:SER:O[2_555]	1.48	0.72
1:B:240:GLY:N	1:C:150:LEU:CB[3_555]	1.48	0.72
1:B:151:SER:CB	1:C:91:VAL:C[3_555]	1.48	0.72
1:B:74:LEU:C	1:C:130:ALA:CA[3_555]	1.48	0.72
1:B:245:SER:O	1:C:164:GLY:C[3_555]	1.48	0.72
1:B:131:ILE:CD1	1:C:134:GLY:N[3_555]	1.48	0.72
1:B:95:THR:C	1:C:239:THR:OG1[3_555]	1.48	0.72
1:A:258:LEU:O	1:B:232:SER:N[2_555]	1.48	0.72
1:C:58:PRO:CG	1:C:250:LEU:C[2_555]	1.48	0.72
1:B:243:TYR:O	1:C:183:ILE:CD1[3_555]	1.48	0.72
1:A:106:ASN:ND2	1:B:126:THR:OG1[2_555]	1.48	0.72
1:B:159:GLY:N	1:C:135:PHE:CG[3_555]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:PHE:CA	1:C:181:ARG:CA[3_555]	1.48	0.72
1:B:158:THR:CA	1:C:135:PHE:CG[3_555]	1.48	0.72
1:C:101:ARG:CB	1:C:255:ALA:CB[2_555]	1.48	0.72
1:B:239:THR:CA	1:C:150:LEU:CA[3_555]	1.48	0.72
1:B:246:TYR:O	1:C:49:GLN:OE1[3_555]	1.48	0.72
1:B:117:TYR:CD2	1:C:119:TYR:CA[3_555]	1.48	0.72
1:B:183:ILE:CG2	1:C:185:ILE:CG1[3_555]	1.48	0.72
1:B:112:TRP:CA	1:C:51:THR:CA[3_555]	1.48	0.72
1:B:99:TRP:CA	1:C:126:THR:N[3_555]	1.48	0.72
1:C:98:THR:CA	1:C:254:ILE:CG1[2_555]	1.49	0.71
1:B:100:LEU:CG	1:C:123:CYS:O[3_555]	1.49	0.71
1:B:80:VAL:C	1:C:144:PRO:N[3_555]	1.49	0.71
1:B:74:LEU:O	1:C:129:GLY:C[3_555]	1.49	0.71
1:B:154:LYS:CG	1:C:72:CYS:CA[3_555]	1.49	0.71
1:B:238:ASN:CA	1:C:146:SER:O[3_555]	1.49	0.71
1:B:191:GLU:OE1	1:C:56:ARG:N[3_555]	1.49	0.71
1:B:78:LEU:CD2	1:C:227:ALA:N[3_555]	1.49	0.71
1:B:189:THR:O	1:C:53:VAL:C[3_555]	1.50	0.70
1:B:80:VAL:O	1:C:143:LEU:C[3_555]	1.50	0.70
1:B:98:THR:C	1:C:127:THR:C[3_555]	1.50	0.70
1:B:227:ALA:O	1:C:225:VAL:N[3_555]	1.50	0.70
1:B:91:VAL:O	1:C:241:ARG:NH1[3_555]	1.50	0.70
1:B:229:GLU:CB	1:C:223:ARG:CZ[3_555]	1.50	0.70
1:C:99:TRP:CZ3	1:C:107:TRP:CG[2_555]	1.50	0.70
3:B:262:HOH:O	3:C:263:HOH:O[3_555]	1.50	0.70
1:B:87:THR:O	3:C:265:HOH:O[3_555]	1.50	0.70
1:B:189:THR:OG1	1:C:168:LEU:CG[3_555]	1.50	0.70
1:B:120:LEU:O	1:C:156:TYR:OH[3_555]	1.50	0.70
1:B:99:TRP:CA	1:C:126:THR:C[3_555]	1.50	0.70
1:B:153:LEU:N	1:C:96:VAL:CB[3_555]	1.50	0.70
1:B:191:GLU:CB	1:C:55:LEU:N[3_555]	1.50	0.70
1:B:118:THR:OG1	1:C:182:ALA:O[3_555]	1.50	0.70
1:B:119:TYR:CB	1:C:157:VAL:N[3_555]	1.51	0.69
1:B:229:GLU:O	1:C:136:GLN:CD[3_555]	1.51	0.69
1:B:238:ASN:CG	1:C:146:SER:CA[3_555]	1.51	0.69
1:A:254:ILE:CG2	1:B:128:SER:CA[2_555]	1.51	0.69
1:B:98:THR:O	1:C:126:THR:O[3_555]	1.51	0.69
1:B:248:ILE:CB	1:C:49:GLN:N[3_555]	1.51	0.69
1:B:241:ARG:CG	1:C:132:HIS:NE2[3_555]	1.51	0.69
1:B:228:MET:N	1:C:88:SER:CB[3_555]	1.51	0.69
1:B:247:THR:O	1:C:50:GLY:O[3_555]	1.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:MET:O	1:C:143:LEU:CD2[3_555]	1.51	0.69
1:B:119:TYR:C	1:C:157:VAL:CA[3_555]	1.51	0.69
1:B:117:TYR:CA	1:C:183:ILE:CB[3_555]	1.51	0.69
1:B:82:VAL:N	1:C:142:THR:CA[3_555]	1.51	0.69
1:B:100:LEU:C	1:C:124:PRO:C[3_555]	1.51	0.69
1:B:80:VAL:CA	1:C:144:PRO:CD[3_555]	1.52	0.68
1:B:191:GLU:N	1:C:54:LYS:O[3_555]	1.52	0.68
1:B:183:ILE:CD1	1:C:155:GLY:N[3_555]	1.52	0.68
1:B:124:PRO:O	1:C:152:ASN:ND2[3_555]	1.52	0.68
1:B:117:TYR:C	1:C:183:ILE:CA[3_555]	1.52	0.68
1:B:238:ASN:N	1:C:146:SER:CB[3_555]	1.52	0.68
1:B:222:ALA:O	1:C:241:ARG:CD[3_555]	1.52	0.68
1:B:184:THR:N	1:C:184:THR:C[3_555]	1.52	0.68
1:B:69:LEU:CG	1:C:46:PRO:CB[3_555]	1.52	0.68
1:B:91:VAL:CG2	1:C:241:ARG:N[3_555]	1.52	0.68
1:B:242:LEU:CD1	1:C:131:ILE:CD1[3_555]	1.52	0.68
1:B:170:PHE:CE2	1:C:179:THR:C[3_555]	1.52	0.68
1:B:228:MET:SD	1:C:225:VAL:CB[3_555]	1.52	0.68
1:B:153:LEU:CD2	1:C:96:VAL:O[3_555]	1.52	0.68
1:B:156:TYR:CZ	1:C:91:VAL:CG1[3_555]	1.52	0.68
1:B:192:VAL:CB	1:C:53:VAL:O[3_555]	1.53	0.67
1:B:81:THR:CA	1:C:143:LEU:N[3_555]	1.53	0.67
1:B:188:ASP:CB	1:C:171:VAL:C[3_555]	1.53	0.67
1:B:248:ILE:CB	1:C:49:GLN:CA[3_555]	1.53	0.67
1:B:149:GLN:CA	1:C:95:THR:N[3_555]	1.53	0.67
1:B:121:PRO:N	1:C:156:TYR:CE1[3_555]	1.53	0.67
1:B:119:TYR:N	1:C:157:VAL:C[3_555]	1.53	0.67
1:B:89:GLU:C	1:C:77:GLU:C[3_555]	1.53	0.67
1:B:161:VAL:CA	1:C:153:LEU:CA[3_555]	1.53	0.67
1:B:158:THR:CB	1:C:135:PHE:CD2[3_555]	1.53	0.67
1:B:87:THR:CB	1:C:87:THR:CB[3_555]	1.53	0.67
1:B:93:PRO:C	1:C:123:CYS:N[3_555]	1.54	0.66
1:C:59:MET:N	1:C:67:THR:N[2_555]	1.54	0.66
1:B:154:LYS:O	1:C:244:ALA:C[3_555]	1.54	0.66
1:B:120:LEU:CA	1:C:156:TYR:CE1[3_555]	1.54	0.66
1:B:154:LYS:C	1:C:244:ALA:O[3_555]	1.54	0.66
1:B:149:GLN:CA	1:C:95:THR:CB[3_555]	1.54	0.66
1:B:230:GLY:N	1:C:136:GLN:OE1[3_555]	1.54	0.66
1:C:99:TRP:O	1:C:106:ASN:C[2_555]	1.54	0.66
1:B:73:GLU:C	1:C:160:PRO:N[3_555]	1.54	0.66
1:B:160:PRO:N	1:C:154:LYS:CB[3_555]	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:OG1	1:C:150:LEU:CG[3_555]	1.54	0.66
1:B:117:TYR:CE2	1:C:119:TYR:CG[3_555]	1.54	0.66
1:B:161:VAL:O	1:C:150:LEU:O[3_555]	1.55	0.65
1:B:117:TYR:CE1	1:C:119:TYR:CZ[3_555]	1.55	0.65
1:B:136:GLN:N	1:C:75:SER:CA[3_555]	1.55	0.65
1:B:74:LEU:CB	1:C:130:ALA:CA[3_555]	1.55	0.65
1:B:96:VAL:O	1:C:161:VAL:CG2[3_555]	1.55	0.65
1:B:246:TYR:N	1:C:49:GLN:NE2[3_555]	1.55	0.65
1:C:101:ARG:CA	1:C:255:ALA:CA[2_555]	1.55	0.65
1:B:147:VAL:C	1:C:90:LEU:O[3_555]	1.55	0.65
1:C:59:MET:SD	1:C:63:SER:N[2_555]	1.55	0.65
1:B:71:HIS:CE1	1:C:162:TRP:CZ2[3_555]	1.55	0.65
1:B:135:PHE:CB	1:C:243:TYR:CA[3_555]	1.55	0.65
1:A:255:ALA:N	1:B:127:THR:O[2_555]	1.55	0.65
1:B:184:THR:O	1:C:184:THR:C[3_555]	1.55	0.65
1:B:93:PRO:CA	1:C:122:SER:O[3_555]	1.55	0.65
1:B:158:THR:C	1:C:135:PHE:CE1[3_555]	1.55	0.65
1:C:58:PRO:CG	1:C:250:LEU:CA[2_555]	1.55	0.65
1:B:96:VAL:O	1:C:161:VAL:CB[3_555]	1.55	0.65
1:B:101:ARG:NH2	1:C:237:VAL:CG2[3_555]	1.56	0.64
1:B:184:THR:CG2	1:C:184:THR:CG2[3_555]	1.56	0.64
1:B:134:GLY:CA	1:C:117:TYR:CD2[3_555]	1.56	0.64
1:C:57:PRO:CD	1:C:249:ARG:NE[2_555]	1.56	0.64
1:B:74:LEU:N	1:C:160:PRO:CA[3_555]	1.56	0.64
1:B:151:SER:OG	1:C:91:VAL:O[3_555]	1.56	0.64
1:C:101:ARG:CG	1:C:255:ALA:O[2_555]	1.56	0.64
1:B:89:GLU:N	1:C:77:GLU:O[3_555]	1.56	0.64
1:B:185:ILE:C	1:C:118:THR:CB[3_555]	1.56	0.64
1:B:159:GLY:O	1:C:135:PHE:N[3_555]	1.56	0.64
1:B:122:SER:N	1:C:151:SER:OG[3_555]	1.56	0.64
1:B:184:THR:C	1:C:185:ILE:N[3_555]	1.56	0.64
1:B:120:LEU:C	1:C:156:TYR:CZ[3_555]	1.56	0.64
1:B:132:HIS:CG	1:C:223:ARG:C[3_555]	1.56	0.64
1:B:228:MET:CG	1:C:225:VAL:CG1[3_555]	1.56	0.64
1:B:117:TYR:O	1:C:183:ILE:CA[3_555]	1.56	0.64
1:B:73:GLU:O	1:C:159:GLY:C[3_555]	1.56	0.64
1:B:112:TRP:CH2	1:C:121:PRO:O[3_555]	1.56	0.64
1:B:112:TRP:CH2	1:C:121:PRO:C[3_555]	1.57	0.63
1:B:158:THR:CA	1:C:135:PHE:CE2[3_555]	1.57	0.63
1:B:98:THR:CB	1:C:128:SER:CA[3_555]	1.57	0.63
1:B:137:TYR:CE2	1:C:243:TYR:CD2[3_555]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:CB	1:C:118:THR:N[3_555]	1.57	0.63
1:C:58:PRO:C	1:C:67:THR:CA[2_555]	1.57	0.63
1:B:245:SER:N	1:C:164:GLY:N[3_555]	1.57	0.63
1:B:146:SER:C	1:C:90:LEU:CG[3_555]	1.57	0.63
1:B:190:ASN:ND2	1:C:172:ASN:CB[3_555]	1.57	0.63
1:B:239:THR:OG1	1:C:150:LEU:CD2[3_555]	1.58	0.62
1:B:248:ILE:CG2	1:C:49:GLN:N[3_555]	1.58	0.62
1:B:131:ILE:CB	1:C:134:GLY:N[3_555]	1.58	0.62
1:B:156:TYR:CB	1:C:115:ILE:CD1[3_555]	1.58	0.62
1:B:93:PRO:CD	1:C:122:SER:O[3_555]	1.58	0.62
1:C:98:THR:CA	1:C:254:ILE:CD1[2_555]	1.58	0.62
1:B:147:VAL:CA	1:C:90:LEU:C[3_555]	1.58	0.62
1:C:98:THR:CB	1:C:254:ILE:CD1[2_555]	1.58	0.62
1:B:241:ARG:CB	1:C:132:HIS:ND1[3_555]	1.58	0.62
1:A:254:ILE:CG1	1:B:129:GLY:N[2_555]	1.58	0.62
1:B:131:ILE:N	1:C:134:GLY:O[3_555]	1.58	0.62
1:B:190:ASN:N	1:C:172:ASN:CG[3_555]	1.58	0.62
1:B:99:TRP:CE3	1:C:125:THR:CA[3_555]	1.58	0.62
1:B:170:PHE:CD2	1:C:180:SER:C[3_555]	1.58	0.62
1:B:242:LEU:CD1	1:C:131:ILE:CG1[3_555]	1.58	0.62
1:B:246:TYR:C	1:C:49:GLN:CD[3_555]	1.59	0.61
1:B:115:ILE:CG2	1:C:120:LEU:CG[3_555]	1.59	0.61
1:B:132:HIS:O	1:C:224:LEU:CD2[3_555]	1.59	0.61
1:B:162:TRP:CB	1:C:152:ASN:CA[3_555]	1.59	0.61
1:B:246:TYR:C	1:C:49:GLN:NE2[3_555]	1.59	0.61
1:B:135:PHE:CZ	1:C:118:THR:O[3_555]	1.59	0.61
1:A:258:LEU:CA	1:B:232:SER:CB[2_555]	1.59	0.61
1:C:101:ARG:NE	1:C:258:LEU:N[2_555]	1.59	0.61
1:B:85:VAL:O	1:C:88:SER:CA[3_555]	1.59	0.61
1:B:73:GLU:O	1:C:160:PRO:C[3_555]	1.59	0.61
1:B:248:ILE:C	1:C:50:GLY:N[3_555]	1.59	0.61
1:B:243:TYR:CA	1:C:159:GLY:C[3_555]	1.59	0.61
1:B:162:TRP:CB	1:C:152:ASN:O[3_555]	1.59	0.61
1:C:101:ARG:N	1:C:254:ILE:O[2_555]	1.60	0.60
1:B:247:THR:OG1	1:C:165:GLN:NE2[3_555]	1.60	0.60
1:B:156:TYR:O	1:C:116:ARG:N[3_555]	1.60	0.60
1:B:148:ASN:C	1:C:92:MET:CB[3_555]	1.60	0.60
1:B:157:VAL:O	1:C:135:PHE:CZ[3_555]	1.60	0.60
1:C:58:PRO:O	1:C:67:THR:C[2_555]	1.60	0.60
1:B:226:THR:CB	1:C:226:THR:CB[3_555]	1.60	0.60
1:B:113:VAL:N	1:C:50:GLY:C[3_555]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:N	1:C:49:GLN:CA[3_555]	1.60	0.60
1:B:130:ALA:CA	1:C:136:GLN:N[3_555]	1.60	0.60
1:B:89:GLU:OE2	1:C:79:ALA:C[3_555]	1.60	0.60
1:B:151:SER:O	1:C:112:TRP:CZ2[3_555]	1.60	0.60
1:B:102:GLY:N	1:C:126:THR:OG1[3_555]	1.61	0.59
1:B:98:THR:CB	1:C:127:THR:C[3_555]	1.61	0.59
1:B:151:SER:O	1:C:112:TRP:CH2[3_555]	1.61	0.59
1:C:103:VAL:CA	1:C:106:ASN:CG[2_555]	1.61	0.59
1:C:64:MET:O	1:C:70:SER:CB[3_555]	1.61	0.59
1:B:158:THR:CA	1:C:135:PHE:CD2[3_555]	1.61	0.59
1:B:99:TRP:N	1:C:127:THR:O[3_555]	1.61	0.59
1:B:245:SER:CA	1:C:164:GLY:N[3_555]	1.61	0.59
1:B:114:ALA:O	1:C:165:GLN:CA[3_555]	1.61	0.59
1:B:96:VAL:CG1	1:C:161:VAL:O[3_555]	1.61	0.59
1:B:130:ALA:CA	1:C:135:PHE:O[3_555]	1.61	0.59
1:B:158:THR:O	1:C:135:PHE:CD1[3_555]	1.61	0.59
1:B:123:CYS:CB	1:C:148:ASN:O[3_555]	1.61	0.59
1:B:245:SER:O	1:C:164:GLY:CA[3_555]	1.61	0.59
1:C:55:LEU:CD1	1:C:252:GLU:OE2[2_555]	1.61	0.59
1:C:59:MET:SD	1:C:63:SER:C[2_555]	1.61	0.59
1:B:131:ILE:CG1	1:C:134:GLY:N[3_555]	1.62	0.58
1:B:95:THR:OG1	1:C:238:ASN:C[3_555]	1.62	0.58
1:B:238:ASN:N	1:C:146:SER:CA[3_555]	1.62	0.58
1:B:118:THR:N	1:C:183:ILE:CB[3_555]	1.62	0.58
1:B:77:GLU:CD	1:C:229:GLU:OE1[3_555]	1.62	0.58
1:B:183:ILE:C	3:C:267:HOH:O[3_555]	1.62	0.58
1:B:160:PRO:O	1:C:153:LEU:CA[3_555]	1.62	0.58
1:A:106:ASN:CG	1:B:126:THR:CB[2_555]	1.62	0.58
1:B:147:VAL:CB	1:C:90:LEU:CA[3_555]	1.62	0.58
1:B:117:TYR:CD1	1:C:119:TYR:CG[3_555]	1.62	0.58
1:B:97:GLY:O	1:C:127:THR:CG2[3_555]	1.62	0.58
1:B:78:LEU:CA	1:C:227:ALA:CB[3_555]	1.62	0.58
1:B:98:THR:OG1	1:C:128:SER:O[3_555]	1.63	0.57
1:B:135:PHE:CE1	1:C:242:LEU:CA[3_555]	1.63	0.57
1:C:99:TRP:CE2	1:C:107:TRP:CB[2_555]	1.63	0.57
1:B:90:LEU:N	1:C:78:LEU:N[3_555]	1.63	0.57
1:B:122:SER:C	1:C:151:SER:OG[3_555]	1.63	0.57
1:B:148:ASN:O	1:C:92:MET:N[3_555]	1.63	0.57
1:B:113:VAL:N	1:C:51:THR:CA[3_555]	1.63	0.57
1:B:186:ALA:C	1:C:118:THR:OG1[3_555]	1.63	0.57
1:C:103:VAL:N	1:C:106:ASN:CB[2_555]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:CA	1:C:157:VAL:CG2[3_555]	1.63	0.57
1:C:102:GLY:O	1:C:106:ASN:OD1[2_555]	1.63	0.57
1:C:99:TRP:CD2	1:C:107:TRP:CA[2_555]	1.63	0.57
1:B:192:VAL:CG2	1:C:53:VAL:CA[3_555]	1.63	0.57
1:C:57:PRO:CD	1:C:249:ARG:NH2[2_555]	1.63	0.57
1:B:183:ILE:CA	3:C:267:HOH:O[3_555]	1.63	0.57
1:B:238:ASN:C	1:C:146:SER:C[3_555]	1.63	0.57
1:B:137:TYR:CE2	1:C:243:TYR:CE2[3_555]	1.64	0.56
1:B:95:THR:CA	1:C:239:THR:CA[3_555]	1.64	0.56
1:B:189:THR:O	1:C:53:VAL:CA[3_555]	1.64	0.56
1:B:238:ASN:CB	1:C:147:VAL:N[3_555]	1.64	0.56
1:B:80:VAL:N	1:C:144:PRO:N[3_555]	1.64	0.56
1:C:246:TYR:CE1	1:C:253:PRO:CG[2_555]	1.64	0.56
1:B:224:LEU:O	1:C:76:THR:CB[3_555]	1.64	0.56
1:B:158:THR:CG2	1:C:135:PHE:CG[3_555]	1.65	0.55
1:B:85:VAL:O	1:C:88:SER:CB[3_555]	1.65	0.55
1:B:81:THR:N	1:C:143:LEU:O[3_555]	1.65	0.55
1:B:113:VAL:N	1:C:51:THR:N[3_555]	1.65	0.55
1:B:158:THR:C	1:C:135:PHE:CG[3_555]	1.65	0.55
1:B:116:ARG:N	1:C:164:GLY:C[3_555]	1.65	0.55
1:C:99:TRP:CH2	1:C:107:TRP:CE2[2_555]	1.65	0.55
1:B:135:PHE:CE1	1:C:243:TYR:N[3_555]	1.65	0.55
1:B:136:GLN:O	1:C:74:LEU:CB[3_555]	1.65	0.55
1:B:190:ASN:CA	1:C:172:ASN:ND2[3_555]	1.65	0.55
1:B:119:TYR:OH	1:C:150:LEU:CD1[3_555]	1.65	0.55
1:A:254:ILE:CG1	1:B:128:SER:O[2_555]	1.65	0.55
1:A:254:ILE:O	1:B:127:THR:N[2_555]	1.65	0.55
1:B:133:MET:SD	1:C:133:MET:CG[3_555]	1.66	0.54
1:B:100:LEU:C	1:C:124:PRO:CA[3_555]	1.66	0.54
1:B:77:GLU:CG	1:C:229:GLU:CD[3_555]	1.66	0.54
1:C:59:MET:CG	1:C:62:SER:CA[2_555]	1.66	0.54
1:B:132:HIS:C	1:C:224:LEU:CD1[3_555]	1.66	0.54
1:B:241:ARG:C	1:C:132:HIS:ND1[3_555]	1.66	0.54
1:B:159:GLY:N	1:C:135:PHE:CB[3_555]	1.66	0.54
1:C:58:PRO:CD	1:C:250:LEU:CA[2_555]	1.66	0.54
1:B:100:LEU:CA	1:C:125:THR:N[3_555]	1.66	0.54
1:B:185:ILE:CB	1:C:118:THR:CA[3_555]	1.66	0.54
1:B:237:VAL:CB	1:C:149:GLN:NE2[3_555]	1.66	0.54
1:B:99:TRP:CE3	1:C:125:THR:C[3_555]	1.66	0.54
1:B:149:GLN:O	1:C:95:THR:C[3_555]	1.66	0.54
1:B:119:TYR:CB	1:C:157:VAL:O[3_555]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:THR:CG2	1:C:238:ASN:C[3_555]	1.66	0.54
1:B:98:THR:C	1:C:126:THR:C[3_555]	1.67	0.53
1:B:81:THR:N	1:C:143:LEU:CB[3_555]	1.67	0.53
1:B:150:LEU:N	1:C:95:THR:CG2[3_555]	1.67	0.53
1:B:132:HIS:CB	1:C:224:LEU:CA[3_555]	1.67	0.53
1:B:119:TYR:N	1:C:157:VAL:CG2[3_555]	1.67	0.53
1:B:156:TYR:CG	1:C:115:ILE:CG1[3_555]	1.67	0.53
1:B:247:THR:N	1:C:165:GLN:CG[3_555]	1.67	0.53
1:B:101:ARG:CZ	1:C:237:VAL:CG1[3_555]	1.67	0.53
1:B:161:VAL:CB	1:C:153:LEU:CG[3_555]	1.67	0.53
1:A:253:PRO:CG	1:B:162:TRP:CD2[2_555]	1.67	0.53
1:C:101:ARG:NH2	1:C:258:LEU:CA[2_555]	1.67	0.53
1:B:160:PRO:CA	1:C:154:LYS:N[3_555]	1.67	0.53
1:B:248:ILE:N	1:C:49:GLN:C[3_555]	1.67	0.53
1:B:160:PRO:CD	1:C:154:LYS:CA[3_555]	1.67	0.53
1:B:132:HIS:CA	1:C:224:LEU:CA[3_555]	1.67	0.53
1:A:255:ALA:CA	1:B:127:THR:CB[2_555]	1.67	0.53
1:B:190:ASN:CB	1:C:54:LYS:CE[3_555]	1.67	0.53
1:B:224:LEU:CD1	1:C:242:LEU:CB[3_555]	1.67	0.53
1:B:102:GLY:CA	1:C:126:THR:OG1[3_555]	1.67	0.53
1:B:245:SER:N	1:C:163:GLU:C[3_555]	1.67	0.53
1:B:135:PHE:CE2	1:C:243:TYR:CB[3_555]	1.67	0.53
1:B:116:ARG:CZ	1:C:182:ALA:CB[3_555]	1.67	0.53
1:B:135:PHE:CD1	1:C:242:LEU:CA[3_555]	1.67	0.53
1:B:97:GLY:N	1:C:161:VAL:CG1[3_555]	1.67	0.53
1:B:185:ILE:C	1:C:118:THR:CA[3_555]	1.67	0.53
1:B:191:GLU:N	1:C:54:LYS:CA[3_555]	1.67	0.53
1:B:243:TYR:CE1	1:C:158:THR:CG2[3_555]	1.67	0.53
1:B:239:THR:C	1:C:147:VAL:O[3_555]	1.68	0.52
1:B:77:GLU:CD	1:C:229:GLU:CD[3_555]	1.68	0.52
1:C:101:ARG:CG	1:C:256:ALA:CA[2_555]	1.68	0.52
1:B:73:GLU:CB	1:C:160:PRO:CB[3_555]	1.68	0.52
1:C:58:PRO:CG	1:C:250:LEU:CB[2_555]	1.68	0.52
1:C:99:TRP:CG	1:C:107:TRP:C[2_555]	1.68	0.52
1:B:226:THR:OG1	1:C:226:THR:CA[3_555]	1.68	0.52
1:B:223:ARG:N	1:C:74:LEU:CD1[3_555]	1.68	0.52
1:C:103:VAL:CA	1:C:106:ASN:OD1[2_555]	1.68	0.52
1:C:99:TRP:NE1	1:C:104:ALA:O[2_555]	1.68	0.52
1:C:73:GLU:CD	1:C:253:PRO:C[2_555]	1.68	0.52
1:B:114:ALA:C	1:C:165:GLN:CA[3_555]	1.69	0.51
1:B:238:ASN:CB	1:C:146:SER:CB[3_555]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:N	1:C:254:ILE:O[2_555]	1.69	0.51
1:B:73:GLU:OE2	1:C:162:TRP:CB[3_555]	1.69	0.51
1:B:123:CYS:N	1:C:148:ASN:O[3_555]	1.69	0.51
1:B:147:VAL:O	1:C:91:VAL:N[3_555]	1.69	0.51
1:B:239:THR:C	1:C:151:SER:N[3_555]	1.69	0.51
1:B:221:PRO:CB	1:C:241:ARG:NH2[3_555]	1.69	0.51
1:B:89:GLU:N	1:C:78:LEU:CD1[3_555]	1.69	0.51
1:B:160:PRO:CD	1:C:154:LYS:CG[3_555]	1.69	0.51
1:B:158:THR:CB	1:C:135:PHE:CG[3_555]	1.69	0.51
1:B:223:ARG:CA	1:C:76:THR:O[3_555]	1.69	0.51
1:B:73:GLU:CA	1:C:160:PRO:CA[3_555]	1.69	0.51
1:C:86:VAL:CG1	3:B:269:HOH:O[2_555]	1.69	0.51
1:B:161:VAL:N	1:C:153:LEU:CG[3_555]	1.69	0.51
1:B:187:LEU:CG	1:C:120:LEU:CD1[3_555]	1.69	0.51
1:B:69:LEU:CD2	1:C:48:ALA:N[3_555]	1.69	0.51
1:B:98:THR:OG1	1:C:128:SER:C[3_555]	1.70	0.50
1:C:99:TRP:CZ2	1:C:107:TRP:CE3[2_555]	1.70	0.50
1:B:77:GLU:OE1	1:C:229:GLU:OE1[3_555]	1.70	0.50
1:B:246:TYR:CD1	1:C:162:TRP:C[3_555]	1.70	0.50
1:B:71:HIS:CG	1:C:162:TRP:CZ3[3_555]	1.70	0.50
1:B:161:VAL:CG1	1:C:153:LEU:CG[3_555]	1.70	0.50
1:B:82:VAL:CA	1:C:142:THR:CG2[3_555]	1.70	0.50
1:C:99:TRP:CZ3	1:C:107:TRP:NE1[2_555]	1.70	0.50
1:B:241:ARG:CB	1:C:132:HIS:NE2[3_555]	1.70	0.50
1:C:101:ARG:CB	1:C:256:ALA:N[2_555]	1.70	0.50
1:B:152:ASN:OD1	1:C:94:PHE:N[3_555]	1.70	0.50
1:B:154:LYS:CD	1:C:72:CYS:CB[3_555]	1.70	0.50
1:B:99:TRP:O	1:C:126:THR:CA[3_555]	1.70	0.50
1:B:99:TRP:C	1:C:126:THR:CA[3_555]	1.70	0.50
1:B:91:VAL:CG1	1:C:120:LEU:O[3_555]	1.70	0.50
1:B:224:LEU:C	1:C:76:THR:CB[3_555]	1.70	0.50
1:C:101:ARG:CD	1:C:255:ALA:C[2_555]	1.70	0.50
1:B:162:TRP:N	1:C:152:ASN:O[3_555]	1.71	0.49
1:B:135:PHE:O	1:C:74:LEU:C[3_555]	1.71	0.49
1:B:88:SER:C	1:C:77:GLU:O[3_555]	1.71	0.49
1:B:248:ILE:N	1:C:50:GLY:N[3_555]	1.71	0.49
1:B:96:VAL:N	1:C:239:THR:CA[3_555]	1.71	0.49
1:B:246:TYR:OH	1:C:162:TRP:CE3[3_555]	1.71	0.49
1:B:152:ASN:CG	1:C:93:PRO:C[3_555]	1.71	0.49
1:C:58:PRO:CA	1:C:67:THR:N[2_555]	1.71	0.49
1:B:71:HIS:ND1	1:C:162:TRP:CZ3[3_555]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:OE1	1:C:162:TRP:CD1[3_555]	1.71	0.49
1:C:97:GLY:O	1:C:254:ILE:CA[2_555]	1.71	0.49
1:B:149:GLN:NE2	1:C:94:PHE:CD2[3_555]	1.71	0.49
1:C:99:TRP:CD1	1:C:107:TRP:O[2_555]	1.71	0.49
1:B:190:ASN:ND2	1:C:172:ASN:CG[3_555]	1.71	0.49
1:B:131:ILE:N	1:C:135:PHE:CA[3_555]	1.71	0.49
1:B:246:TYR:OH	1:C:162:TRP:CD2[3_555]	1.71	0.49
1:B:160:PRO:N	1:C:154:LYS:N[3_555]	1.71	0.49
1:B:237:VAL:C	1:C:146:SER:N[3_555]	1.71	0.49
1:B:111:ALA:O	1:C:50:GLY:CA[3_555]	1.71	0.49
1:B:94:PHE:C	1:C:238:ASN:O[3_555]	1.71	0.49
1:B:230:GLY:CA	1:C:136:GLN:CD[3_555]	1.72	0.48
1:B:74:LEU:CG	1:C:130:ALA:CB[3_555]	1.72	0.48
1:B:183:ILE:CD1	1:C:156:TYR:N[3_555]	1.72	0.48
1:B:227:ALA:CA	1:C:89:GLU:N[3_555]	1.72	0.48
1:B:91:VAL:N	1:C:240:GLY:O[3_555]	1.72	0.48
1:B:148:ASN:C	1:C:92:MET:CG[3_555]	1.72	0.48
1:B:133:MET:O	1:C:117:TYR:CE1[3_555]	1.72	0.48
1:B:153:LEU:CG	1:C:96:VAL:C[3_555]	1.72	0.48
1:C:60:LEU:O	1:C:61:ARG:C[2_555]	1.72	0.48
1:C:73:GLU:OE2	1:C:253:PRO:C[2_555]	1.72	0.48
1:B:237:VAL:O	1:C:145:VAL:N[3_555]	1.72	0.48
1:B:191:GLU:CA	1:C:55:LEU:CA[3_555]	1.72	0.48
1:B:135:PHE:CA	1:C:75:SER:N[3_555]	1.72	0.48
1:B:82:VAL:CA	1:C:142:THR:CB[3_555]	1.72	0.48
1:B:71:HIS:ND1	1:C:162:TRP:CZ2[3_555]	1.72	0.48
1:A:255:ALA:N	1:B:127:THR:CB[2_555]	1.72	0.48
1:B:130:ALA:O	1:C:225:VAL:CG2[3_555]	1.72	0.48
1:B:247:THR:N	1:C:165:GLN:NE2[3_555]	1.72	0.48
1:B:243:TYR:CG	1:C:159:GLY:CA[3_555]	1.72	0.48
1:B:131:ILE:O	1:C:135:PHE:CD2[3_555]	1.72	0.48
1:B:241:ARG:C	1:C:132:HIS:CG[3_555]	1.72	0.48
1:B:132:HIS:CA	1:C:224:LEU:CG[3_555]	1.72	0.48
1:B:190:ASN:C	1:C:54:LYS:O[3_555]	1.72	0.48
1:B:119:TYR:CE1	1:C:156:TYR:CG[3_555]	1.72	0.48
1:B:148:ASN:CB	1:C:92:MET:CG[3_555]	1.73	0.47
1:B:245:SER:O	1:C:164:GLY:N[3_555]	1.73	0.47
1:B:131:ILE:CG2	1:C:134:GLY:N[3_555]	1.73	0.47
1:B:71:HIS:CE1	1:C:162:TRP:CH2[3_555]	1.73	0.47
1:C:99:TRP:CB	1:C:107:TRP:N[2_555]	1.73	0.47
1:A:258:LEU:C	1:B:232:SER:N[2_555]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:CB	1:C:145:VAL:CA[3_555]	1.73	0.47
1:B:123:CYS:CA	1:C:148:ASN:O[3_555]	1.73	0.47
1:B:112:TRP:C	1:C:51:THR:C[3_555]	1.73	0.47
1:B:98:THR:O	1:C:127:THR:CA[3_555]	1.73	0.47
1:B:89:GLU:N	1:C:77:GLU:C[3_555]	1.73	0.47
1:B:121:PRO:C	1:C:151:SER:CB[3_555]	1.73	0.47
1:B:223:ARG:O	1:C:76:THR:N[3_555]	1.73	0.47
1:B:189:THR:O	1:C:54:LYS:N[3_555]	1.73	0.47
1:B:104:ALA:N	1:C:124:PRO:CB[3_555]	1.74	0.46
1:C:59:MET:CB	1:C:63:SER:N[2_555]	1.74	0.46
1:B:230:GLY:O	1:C:141:ASP:CG[3_555]	1.74	0.46
1:B:231:GLY:CA	1:C:142:THR:O[3_555]	1.74	0.46
1:B:81:THR:O	1:C:142:THR:O[3_555]	1.74	0.46
1:B:77:GLU:CD	1:C:229:GLU:CB[3_555]	1.74	0.46
1:B:188:ASP:CA	1:C:171:VAL:C[3_555]	1.74	0.46
1:B:88:SER:C	1:C:78:LEU:CD1[3_555]	1.74	0.46
1:B:148:ASN:ND2	1:C:92:MET:SD[3_555]	1.74	0.46
1:B:154:LYS:CE	1:C:72:CYS:CB[3_555]	1.74	0.46
1:C:59:MET:N	1:C:66:VAL:O[2_555]	1.74	0.46
1:B:132:HIS:CB	1:C:224:LEU:N[3_555]	1.74	0.46
1:B:227:ALA:O	1:C:225:VAL:CA[3_555]	1.74	0.46
1:B:183:ILE:CG1	1:C:155:GLY:C[3_555]	1.74	0.46
1:B:135:PHE:CD2	1:C:243:TYR:CG[3_555]	1.74	0.46
1:B:132:HIS:NE2	1:C:223:ARG:N[3_555]	1.74	0.46
1:B:183:ILE:O	1:C:157:VAL:CG1[3_555]	1.74	0.46
1:B:237:VAL:CA	1:C:149:GLN:CD[3_555]	1.74	0.46
1:C:60:LEU:O	1:C:61:ARG:CA[2_555]	1.74	0.46
1:B:119:TYR:CD1	1:C:156:TYR:CD2[3_555]	1.75	0.45
1:B:187:LEU:CA	1:C:171:VAL:CG2[3_555]	1.75	0.45
1:B:132:HIS:NE2	1:C:223:ARG:CA[3_555]	1.75	0.45
1:B:230:GLY:N	1:C:223:ARG:NH2[3_555]	1.75	0.45
1:C:59:MET:SD	1:C:62:SER:C[2_555]	1.75	0.45
1:B:121:PRO:CD	1:C:156:TYR:CD1[3_555]	1.75	0.45
1:B:115:ILE:O	1:C:120:LEU:CD2[3_555]	1.75	0.45
1:B:222:ALA:O	1:C:241:ARG:CG[3_555]	1.75	0.45
1:B:88:SER:O	3:C:263:HOH:O[3_555]	1.75	0.45
1:B:243:TYR:CG	1:C:159:GLY:N[3_555]	1.75	0.45
1:B:241:ARG:CD	1:C:229:GLU:OE2[3_555]	1.75	0.45
1:B:117:TYR:CG	1:C:119:TYR:CD2[3_555]	1.75	0.45
1:B:131:ILE:N	1:C:134:GLY:C[3_555]	1.75	0.45
1:A:255:ALA:CB	1:B:127:THR:CG2[2_555]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:CB	1:C:229:GLU:CB[3_555]	1.75	0.45
1:B:135:PHE:CG	1:C:242:LEU:C[3_555]	1.75	0.45
1:A:255:ALA:O	1:B:128:SER:N[2_555]	1.75	0.45
1:B:229:GLU:CG	1:C:223:ARG:CG[3_555]	1.75	0.45
1:B:135:PHE:C	1:C:75:SER:CA[3_555]	1.76	0.44
1:B:156:TYR:CE2	1:C:91:VAL:CG1[3_555]	1.76	0.44
1:B:241:ARG:O	1:C:158:THR:CB[3_555]	1.76	0.44
1:B:119:TYR:CG	1:C:133:MET:O[3_555]	1.76	0.44
1:B:144:PRO:CG	1:C:89:GLU:OE1[3_555]	1.76	0.44
1:B:89:GLU:C	1:C:78:LEU:CA[3_555]	1.76	0.44
1:B:133:MET:SD	1:C:133:MET:CE[3_555]	1.76	0.44
1:A:255:ALA:CB	1:B:127:THR:CB[2_555]	1.76	0.44
1:B:229:GLU:O	1:C:136:GLN:CG[3_555]	1.76	0.44
1:B:246:TYR:C	1:C:165:GLN:CG[3_555]	1.76	0.44
1:B:72:CYS:CA	1:C:163:GLU:OE2[3_555]	1.76	0.44
1:B:246:TYR:CG	1:C:162:TRP:O[3_555]	1.76	0.44
1:B:191:GLU:CB	1:C:55:LEU:CG[3_555]	1.76	0.44
1:B:187:LEU:CD1	1:C:243:TYR:CE1[3_555]	1.76	0.44
1:A:258:LEU:N	1:B:232:SER:CB[2_555]	1.76	0.44
1:B:188:ASP:CA	1:C:171:VAL:CG1[3_555]	1.76	0.44
1:B:91:VAL:CG2	1:C:241:ARG:C[3_555]	1.77	0.43
1:B:242:LEU:O	1:C:131:ILE:CA[3_555]	1.77	0.43
1:B:146:SER:CB	1:C:90:LEU:CD1[3_555]	1.77	0.43
1:B:229:GLU:CB	1:C:223:ARG:CG[3_555]	1.77	0.43
1:B:236:ALA:O	1:C:145:VAL:CB[3_555]	1.77	0.43
1:B:72:CYS:N	1:C:162:TRP:CZ3[3_555]	1.77	0.43
1:B:239:THR:O	1:C:147:VAL:O[3_555]	1.77	0.43
1:B:89:GLU:OE2	1:C:79:ALA:O[3_555]	1.77	0.43
1:B:191:GLU:CD	1:C:55:LEU:CA[3_555]	1.77	0.43
1:B:152:ASN:C	1:C:96:VAL:CG1[3_555]	1.77	0.43
1:C:98:THR:N	1:C:254:ILE:CD1[2_555]	1.77	0.43
1:B:119:TYR:CE2	1:C:150:LEU:CD1[3_555]	1.77	0.43
1:B:158:THR:O	1:C:135:PHE:CE1[3_555]	1.77	0.43
1:B:161:VAL:C	1:C:153:LEU:CA[3_555]	1.77	0.43
1:B:119:TYR:CD2	1:C:133:MET:O[3_555]	1.77	0.43
1:B:223:ARG:CG	1:C:77:GLU:N[3_555]	1.77	0.43
1:A:257:ALA:O	1:B:232:SER:CB[2_555]	1.77	0.43
1:B:226:THR:CA	1:C:226:THR:OG1[3_555]	1.77	0.43
1:B:95:THR:O	1:C:239:THR:CA[3_555]	1.77	0.43
1:B:132:HIS:N	1:C:224:LEU:CB[3_555]	1.77	0.43
1:B:89:GLU:CA	1:C:78:LEU:CB[3_555]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASN:ND2	1:C:145:VAL:O[3_555]	1.77	0.43
1:B:156:TYR:CE2	1:C:91:VAL:CB[3_555]	1.77	0.43
1:B:119:TYR:CD1	1:C:156:TYR:CA[3_555]	1.77	0.43
1:B:72:CYS:C	1:C:160:PRO:CG[3_555]	1.77	0.43
1:B:239:THR:CA	1:C:149:GLN:C[3_555]	1.77	0.43
1:B:157:VAL:CB	1:C:185:ILE:O[3_555]	1.77	0.43
1:C:101:ARG:CZ	1:C:258:LEU:CB[2_555]	1.77	0.43
1:B:92:MET:CA	1:C:122:SER:OG[3_555]	1.77	0.43
1:A:258:LEU:CA	1:B:232:SER:OG[2_555]	1.78	0.42
1:B:246:TYR:CG	1:C:49:GLN:NE2[3_555]	1.78	0.42
1:B:84:ILE:CD1	3:C:268:HOH:O[3_555]	1.78	0.42
1:B:152:ASN:C	1:C:96:VAL:CB[3_555]	1.78	0.42
1:B:148:ASN:CG	1:C:220:VAL:CG1[3_555]	1.78	0.42
1:B:133:MET:N	1:C:224:LEU:CG[3_555]	1.78	0.42
1:B:76:THR:OG1	1:C:228:MET:N[3_555]	1.78	0.42
1:A:253:PRO:CB	1:B:162:TRP:CD1[2_555]	1.78	0.42
1:B:80:VAL:C	1:C:143:LEU:CA[3_555]	1.78	0.42
1:B:135:PHE:CD1	1:C:242:LEU:O[3_555]	1.78	0.42
1:B:82:VAL:CA	1:C:142:THR:CA[3_555]	1.78	0.42
1:B:162:TRP:CB	1:C:152:ASN:C[3_555]	1.78	0.42
1:B:162:TRP:CA	1:C:152:ASN:O[3_555]	1.78	0.42
1:C:98:THR:CA	1:C:254:ILE:CG2[2_555]	1.78	0.42
1:B:188:ASP:O	1:C:53:VAL:CG1[3_555]	1.78	0.42
1:B:118:THR:C	1:C:157:VAL:CG2[3_555]	1.78	0.42
1:B:229:GLU:CA	1:C:223:ARG:CZ[3_555]	1.78	0.42
1:B:119:TYR:CZ	1:C:156:TYR:CD2[3_555]	1.78	0.42
1:B:156:TYR:CZ	1:C:91:VAL:CB[3_555]	1.78	0.42
1:B:91:VAL:CG2	1:C:241:ARG:CG[3_555]	1.78	0.42
1:B:243:TYR:O	1:C:183:ILE:CG1[3_555]	1.78	0.42
1:C:101:ARG:CZ	1:C:258:LEU:CG[2_555]	1.78	0.42
1:B:161:VAL:CG1	1:C:153:LEU:CD1[3_555]	1.78	0.42
1:B:189:THR:CB	1:C:168:LEU:CD1[3_555]	1.79	0.41
1:B:78:LEU:N	1:C:227:ALA:CB[3_555]	1.79	0.41
1:B:131:ILE:CA	1:C:134:GLY:C[3_555]	1.79	0.41
1:B:227:ALA:CB	1:C:89:GLU:CA[3_555]	1.79	0.41
1:A:255:ALA:C	1:B:127:THR:CA[2_555]	1.79	0.41
1:A:255:ALA:CA	1:B:127:THR:N[2_555]	1.79	0.41
1:B:161:VAL:CA	1:C:153:LEU:CG[3_555]	1.79	0.41
1:B:227:ALA:CA	1:C:224:LEU:O[3_555]	1.79	0.41
1:B:99:TRP:N	1:C:126:THR:C[3_555]	1.79	0.41
1:B:100:LEU:O	1:C:124:PRO:N[3_555]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:CB	1:C:145:VAL:CB[3_555]	1.79	0.41
1:B:93:PRO:N	1:C:122:SER:O[3_555]	1.79	0.41
1:B:185:ILE:CA	1:C:117:TYR:O[3_555]	1.79	0.41
1:B:98:THR:N	1:C:127:THR:O[3_555]	1.79	0.41
1:C:99:TRP:O	1:C:106:ASN:O[2_555]	1.79	0.41
1:B:71:HIS:CB	1:C:162:TRP:CZ3[3_555]	1.79	0.41
1:B:135:PHE:CD2	1:C:243:TYR:N[3_555]	1.79	0.41
1:B:100:LEU:N	1:C:126:THR:N[3_555]	1.79	0.41
1:B:163:GLU:O	1:C:156:TYR:CB[3_555]	1.79	0.41
1:C:57:PRO:CA	1:C:251:ILE:CD1[2_555]	1.79	0.41
1:B:99:TRP:CA	1:C:127:THR:N[3_555]	1.79	0.41
1:C:100:LEU:N	1:C:254:ILE:N[2_555]	1.80	0.40
1:B:89:GLU:CB	1:C:78:LEU:CG[3_555]	1.80	0.40
1:B:184:THR:CB	1:C:184:THR:N[3_555]	1.80	0.40
1:B:158:THR:CG2	1:C:135:PHE:CB[3_555]	1.80	0.40
1:B:100:LEU:C	1:C:124:PRO:CG[3_555]	1.80	0.40
1:B:192:VAL:N	1:C:53:VAL:O[3_555]	1.80	0.40
1:C:94:PHE:CZ	1:C:257:ALA:CB[2_555]	1.80	0.40
1:B:170:PHE:CA	1:C:180:SER:O[3_555]	1.80	0.40
1:B:80:VAL:CG2	1:C:144:PRO:N[3_555]	1.80	0.40
1:C:57:PRO:CG	1:C:249:ARG:CD[2_555]	1.80	0.40
1:C:60:LEU:N	1:C:62:SER:CA[2_555]	1.80	0.40
1:B:239:THR:N	1:C:150:LEU:N[3_555]	1.80	0.40
1:B:93:PRO:CA	1:C:123:CYS:CA[3_555]	1.80	0.40
1:B:131:ILE:CB	1:C:134:GLY:CA[3_555]	1.80	0.40
1:A:254:ILE:C	1:B:127:THR:CA[2_555]	1.80	0.40
1:B:75:SER:C	1:C:130:ALA:O[3_555]	1.80	0.40
1:B:115:ILE:CG2	1:C:120:LEU:CA[3_555]	1.80	0.40
1:B:148:ASN:C	1:C:92:MET:CA[3_555]	1.80	0.40
1:B:118:THR:OG1	1:C:183:ILE:CA[3_555]	1.80	0.40
1:B:223:ARG:CG	1:C:76:THR:CA[3_555]	1.80	0.40
1:B:101:ARG:NH2	1:C:237:VAL:CB[3_555]	1.80	0.40
1:B:149:GLN:CA	1:C:95:THR:CA[3_555]	1.80	0.40
1:B:132:HIS:O	1:C:224:LEU:CB[3_555]	1.81	0.39
1:B:80:VAL:CG2	1:C:144:PRO:CD[3_555]	1.81	0.39
1:C:99:TRP:CE3	1:C:107:TRP:CD1[2_555]	1.81	0.39
1:C:57:PRO:CG	1:C:249:ARG:NE[2_555]	1.81	0.39
1:B:190:ASN:OD1	1:C:172:ASN:O[3_555]	1.81	0.39
1:B:100:LEU:CB	1:C:124:PRO:O[3_555]	1.81	0.39
1:B:245:SER:N	1:C:163:GLU:CG[3_555]	1.81	0.39
1:B:147:VAL:N	1:C:90:LEU:CA[3_555]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:CB	1:C:87:THR:OG1[3_555]	1.81	0.39
1:B:183:ILE:CG2	1:C:185:ILE:CB[3_555]	1.81	0.39
1:B:225:VAL:N	1:C:242:LEU:CD2[3_555]	1.81	0.39
1:B:99:TRP:O	1:C:126:THR:OG1[3_555]	1.81	0.39
1:B:160:PRO:N	1:C:154:LYS:CA[3_555]	1.81	0.39
1:B:227:ALA:CA	1:C:88:SER:CA[3_555]	1.81	0.39
1:B:73:GLU:CD	1:C:162:TRP:NE1[3_555]	1.81	0.39
1:A:253:PRO:N	1:B:162:TRP:NE1[2_555]	1.81	0.39
1:C:59:MET:SD	1:C:62:SER:O[2_555]	1.81	0.39
1:B:69:LEU:CG	1:C:46:PRO:C[3_555]	1.82	0.38
1:B:69:LEU:CA	1:C:46:PRO:CB[3_555]	1.82	0.38
1:B:87:THR:OG1	1:C:87:THR:CA[3_555]	1.82	0.38
1:C:59:MET:CE	1:C:64:MET:N[2_555]	1.82	0.38
1:B:116:ARG:CD	1:C:182:ALA:C[3_555]	1.82	0.38
1:B:131:ILE:N	1:C:135:PHE:N[3_555]	1.82	0.38
1:B:236:ALA:CA	1:C:145:VAL:CB[3_555]	1.82	0.38
1:C:57:PRO:CG	1:C:249:ARG:NH1[2_555]	1.82	0.38
1:C:58:PRO:CD	1:C:250:LEU:N[2_555]	1.82	0.38
1:B:157:VAL:O	1:C:135:PHE:CE2[3_555]	1.82	0.38
1:B:95:THR:N	1:C:238:ASN:C[3_555]	1.82	0.38
1:B:230:GLY:C	1:C:141:ASP:CB[3_555]	1.82	0.38
1:B:131:ILE:CG1	1:C:225:VAL:O[3_555]	1.82	0.38
1:B:135:PHE:CG	1:C:243:TYR:CB[3_555]	1.82	0.38
1:B:73:GLU:N	1:C:160:PRO:CB[3_555]	1.82	0.38
1:B:225:VAL:CA	1:C:76:THR:OG1[3_555]	1.82	0.38
1:B:117:TYR:CE2	1:C:119:TYR:CD2[3_555]	1.83	0.37
1:B:150:LEU:O	1:C:117:TYR:OH[3_555]	1.83	0.37
1:A:253:PRO:CD	1:B:162:TRP:CE2[2_555]	1.83	0.37
1:B:122:SER:CA	1:C:151:SER:OG[3_555]	1.83	0.37
1:B:230:GLY:CA	1:C:136:GLN:NE2[3_555]	1.83	0.37
1:B:239:THR:C	1:C:150:LEU:CA[3_555]	1.83	0.37
1:B:189:THR:C	1:C:53:VAL:CA[3_555]	1.83	0.37
1:A:254:ILE:O	1:B:126:THR:O[2_555]	1.83	0.37
1:C:58:PRO:O	1:C:67:THR:O[2_555]	1.83	0.37
1:B:162:TRP:N	1:C:153:LEU:CA[3_555]	1.83	0.37
1:B:192:VAL:CA	1:C:53:VAL:O[3_555]	1.83	0.37
1:B:119:TYR:CA	1:C:158:THR:N[3_555]	1.83	0.37
1:B:243:TYR:CA	1:C:159:GLY:O[3_555]	1.83	0.37
1:B:190:ASN:C	1:C:54:LYS:CB[3_555]	1.83	0.37
1:B:120:LEU:O	1:C:156:TYR:CE2[3_555]	1.83	0.37
1:B:96:VAL:O	1:C:161:VAL:CA[3_555]	1.83	0.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:CG2	1:C:86:VAL:O[3_555]	1.83	0.37
1:B:226:THR:CG2	1:C:226:THR:CB[3_555]	1.83	0.37
1:B:170:PHE:CB	1:C:181:ARG:CA[3_555]	1.83	0.37
1:B:229:GLU:N	1:C:223:ARG:NE[3_555]	1.84	0.36
1:B:170:PHE:CD2	1:C:180:SER:O[3_555]	1.84	0.36
1:B:76:THR:O	1:C:132:HIS:CD2[3_555]	1.84	0.36
1:C:58:PRO:O	1:C:66:VAL:C[2_555]	1.84	0.36
1:C:58:PRO:CG	1:C:250:LEU:O[2_555]	1.84	0.36
1:C:246:TYR:OH	1:C:253:PRO:N[2_555]	1.84	0.36
1:B:71:HIS:CG	1:C:162:TRP:CH2[3_555]	1.84	0.36
1:B:89:GLU:CA	1:C:77:GLU:C[3_555]	1.84	0.36
1:C:57:PRO:CG	1:C:249:ARG:CG[2_555]	1.84	0.36
1:C:73:GLU:OE1	1:C:254:ILE:N[2_555]	1.84	0.36
1:B:246:TYR:CE1	1:C:163:GLU:N[3_555]	1.84	0.36
1:B:155:GLY:CA	1:C:245:SER:N[3_555]	1.84	0.36
1:B:136:GLN:C	1:C:74:LEU:CB[3_555]	1.84	0.36
1:B:154:LYS:CG	1:C:244:ALA:O[3_555]	1.84	0.36
1:B:102:GLY:C	1:C:126:THR:OG1[3_555]	1.84	0.36
1:B:131:ILE:C	1:C:134:GLY:O[3_555]	1.84	0.36
1:B:99:TRP:C	1:C:125:THR:C[3_555]	1.85	0.35
1:B:78:LEU:CG	1:C:227:ALA:CA[3_555]	1.85	0.35
1:B:243:TYR:CD1	1:C:158:THR:C[3_555]	1.85	0.35
1:B:85:VAL:C	1:C:88:SER:N[3_555]	1.85	0.35
1:B:74:LEU:CA	1:C:130:ALA:CA[3_555]	1.85	0.35
1:B:103:VAL:N	1:C:126:THR:OG1[3_555]	1.85	0.35
1:B:161:VAL:O	1:C:153:LEU:N[3_555]	1.85	0.35
1:C:101:ARG:C	1:C:256:ALA:N[2_555]	1.85	0.35
1:B:89:GLU:CD	1:C:79:ALA:N[3_555]	1.85	0.35
1:C:98:THR:CG2	1:C:254:ILE:CD1[2_555]	1.85	0.35
1:C:98:THR:CA	1:C:254:ILE:CB[2_555]	1.85	0.35
1:B:85:VAL:CB	3:C:264:HOH:O[3_555]	1.85	0.35
1:C:71:HIS:CD2	1:C:251:ILE:C[2_555]	1.85	0.35
1:B:89:GLU:OE1	1:C:79:ALA:O[3_555]	1.85	0.35
1:B:239:THR:C	1:C:150:LEU:N[3_555]	1.85	0.35
1:B:101:ARG:N	1:C:124:PRO:O[3_555]	1.85	0.35
1:B:245:SER:N	1:C:163:GLU:CB[3_555]	1.86	0.34
1:B:190:ASN:O	1:C:54:LYS:N[3_555]	1.86	0.34
1:B:222:ALA:O	1:C:241:ARG:CB[3_555]	1.86	0.34
1:B:184:THR:CG2	1:C:184:THR:CB[3_555]	1.86	0.34
1:B:136:GLN:N	1:C:74:LEU:O[3_555]	1.86	0.34
1:B:76:THR:N	1:C:131:ILE:N[3_555]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASN:O	1:C:149:GLN:CB[3_555]	1.86	0.34
1:B:184:THR:CA	1:C:184:THR:N[3_555]	1.86	0.34
1:B:98:THR:CG2	1:C:128:SER:OG[3_555]	1.86	0.34
1:B:170:PHE:CA	1:C:181:ARG:N[3_555]	1.86	0.34
1:C:73:GLU:CD	1:C:253:PRO:O[2_555]	1.86	0.34
1:B:132:HIS:CG	1:C:224:LEU:CA[3_555]	1.86	0.34
1:B:114:ALA:CA	1:C:51:THR:CG2[3_555]	1.86	0.34
1:C:246:TYR:OH	1:C:253:PRO:CD[2_555]	1.86	0.34
1:B:95:THR:CG2	1:C:239:THR:N[3_555]	1.86	0.34
1:B:148:ASN:O	1:C:92:MET:CB[3_555]	1.86	0.34
1:B:100:LEU:CB	1:C:124:PRO:C[3_555]	1.87	0.33
1:B:246:TYR:CD2	1:C:49:GLN:CG[3_555]	1.87	0.33
1:B:149:GLN:C	1:C:96:VAL:N[3_555]	1.87	0.33
1:B:70:SER:N	1:C:46:PRO:CG[3_555]	1.87	0.33
1:C:57:PRO:CG	1:C:249:ARG:CZ[2_555]	1.87	0.33
1:B:112:TRP:CG	1:C:51:THR:OG1[3_555]	1.87	0.33
1:B:73:GLU:OE1	1:C:127:THR:O[3_555]	1.87	0.33
1:B:101:ARG:C	1:C:124:PRO:CG[3_555]	1.87	0.33
1:B:117:TYR:CB	1:C:119:TYR:CB[3_555]	1.87	0.33
1:A:255:ALA:N	1:B:128:SER:N[2_555]	1.87	0.33
1:C:101:ARG:CD	1:C:256:ALA:C[2_555]	1.87	0.33
1:B:247:THR:CA	1:C:165:GLN:CD[3_555]	1.87	0.33
1:B:242:LEU:CA	1:C:132:HIS:N[3_555]	1.87	0.33
1:B:101:ARG:O	1:C:124:PRO:CG[3_555]	1.87	0.33
1:B:123:CYS:SG	1:C:149:GLN:O[3_555]	1.87	0.33
1:C:99:TRP:CZ2	1:C:107:TRP:CD2[2_555]	1.87	0.33
1:B:160:PRO:C	1:C:153:LEU:CB[3_555]	1.87	0.33
1:B:170:PHE:CG	1:C:180:SER:O[3_555]	1.87	0.33
1:C:57:PRO:O	1:C:66:VAL:CG1[2_555]	1.87	0.33
1:B:147:VAL:O	1:C:92:MET:N[3_555]	1.88	0.32
1:B:100:LEU:C	1:C:124:PRO:N[3_555]	1.88	0.32
1:A:257:ALA:C	1:B:232:SER:CB[2_555]	1.88	0.32
1:C:97:GLY:CA	1:C:254:ILE:CA[2_555]	1.88	0.32
1:B:223:ARG:O	1:C:76:THR:O[3_555]	1.88	0.32
1:B:189:THR:CA	1:C:53:VAL:CA[3_555]	1.88	0.32
1:B:242:LEU:N	1:C:132:HIS:N[3_555]	1.88	0.32
1:B:149:GLN:C	1:C:95:THR:C[3_555]	1.88	0.32
1:B:90:LEU:O	1:C:240:GLY:C[3_555]	1.88	0.32
1:C:101:ARG:N	1:C:255:ALA:CA[2_555]	1.88	0.32
1:B:161:VAL:CA	1:C:153:LEU:N[3_555]	1.88	0.32
1:B:73:GLU:CG	1:C:162:TRP:CD1[3_555]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:TYR:CE1	1:C:73:GLU:CA[3_555]	1.88	0.32
1:B:117:TYR:CZ	1:C:119:TYR:CG[3_555]	1.88	0.32
1:B:132:HIS:CE1	1:C:223:ARG:CA[3_555]	1.88	0.32
1:B:191:GLU:C	1:C:55:LEU:N[3_555]	1.88	0.32
1:B:70:SER:O	1:C:46:PRO:CD[3_555]	1.88	0.32
1:C:99:TRP:C	1:C:254:ILE:O[2_555]	1.88	0.32
1:B:69:LEU:CB	1:C:46:PRO:CB[3_555]	1.89	0.31
1:B:97:GLY:C	1:C:127:THR:CB[3_555]	1.89	0.31
1:B:184:THR:C	1:C:184:THR:CB[3_555]	1.89	0.31
1:B:162:TRP:CD1	1:C:152:ASN:O[3_555]	1.89	0.31
1:B:185:ILE:CD1	1:C:243:TYR:O[3_555]	1.89	0.31
1:B:80:VAL:CG2	1:C:144:PRO:CB[3_555]	1.89	0.31
1:B:118:THR:CG2	1:C:157:VAL:CG2[3_555]	1.89	0.31
1:B:246:TYR:CA	1:C:49:GLN:CD[3_555]	1.89	0.31
1:B:191:GLU:OE2	1:C:56:ARG:CA[3_555]	1.89	0.31
1:B:75:SER:N	1:C:130:ALA:CA[3_555]	1.89	0.31
1:B:238:ASN:CA	1:C:146:SER:CB[3_555]	1.89	0.31
1:B:78:LEU:CG	1:C:227:ALA:N[3_555]	1.89	0.31
1:B:183:ILE:CG2	1:C:185:ILE:CD1[3_555]	1.89	0.31
1:B:117:TYR:C	1:C:183:ILE:C[3_555]	1.89	0.31
1:B:99:TRP:N	1:C:127:THR:C[3_555]	1.89	0.31
1:C:99:TRP:CZ3	1:C:107:TRP:CE3[2_555]	1.89	0.31
1:B:74:LEU:C	1:C:129:GLY:O[3_555]	1.89	0.31
1:B:241:ARG:CA	1:C:132:HIS:NE2[3_555]	1.89	0.31
1:B:231:GLY:N	1:C:142:THR:O[3_555]	1.89	0.31
1:B:242:LEU:C	1:C:131:ILE:C[3_555]	1.89	0.31
1:B:119:TYR:CD1	1:C:156:TYR:CG[3_555]	1.89	0.31
1:B:188:ASP:CA	1:C:172:ASN:N[3_555]	1.90	0.30
1:B:131:ILE:CG2	1:C:134:GLY:O[3_555]	1.90	0.30
1:C:100:LEU:C	1:C:254:ILE:O[2_555]	1.90	0.30
1:B:120:LEU:CA	1:C:156:TYR:CD1[3_555]	1.90	0.30
1:B:112:TRP:CZ2	1:C:122:SER:N[3_555]	1.90	0.30
1:A:258:LEU:N	1:B:232:SER:OG[2_555]	1.90	0.30
1:B:119:TYR:C	1:C:158:THR:N[3_555]	1.90	0.30
1:B:132:HIS:CE1	1:C:222:ALA:C[3_555]	1.90	0.30
1:C:73:GLU:CG	1:C:252:GLU:O[2_555]	1.90	0.30
1:B:117:TYR:CE2	1:C:120:LEU:N[3_555]	1.90	0.30
1:B:72:CYS:O	1:C:162:TRP:CH2[3_555]	1.90	0.30
1:B:87:THR:OG1	1:C:87:THR:OG1[3_555]	1.90	0.30
1:B:154:LYS:CD	1:C:72:CYS:SG[3_555]	1.90	0.30
1:B:91:VAL:CA	1:C:240:GLY:C[3_555]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:CG	1:C:46:PRO:CA[3_555]	1.90	0.30
1:B:246:TYR:CZ	1:C:162:TRP:O[3_555]	1.90	0.30
1:B:147:VAL:C	1:C:90:LEU:CA[3_555]	1.90	0.30
1:B:155:GLY:N	1:C:245:SER:CA[3_555]	1.90	0.30
1:B:135:PHE:CE1	1:C:242:LEU:C[3_555]	1.90	0.30
1:B:186:ALA:O	1:C:171:VAL:CG2[3_555]	1.90	0.30
1:B:82:VAL:CB	1:C:142:THR:CG2[3_555]	1.90	0.30
1:B:222:ALA:N	1:C:241:ARG:NE[3_555]	1.90	0.30
1:B:185:ILE:CA	1:C:118:THR:CA[3_555]	1.91	0.29
1:B:112:TRP:CB	1:C:51:THR:O[3_555]	1.91	0.29
1:B:224:LEU:CD1	1:C:242:LEU:CD2[3_555]	1.91	0.29
1:A:253:PRO:C	1:B:162:TRP:CD1[2_555]	1.91	0.29
1:B:93:PRO:C	1:C:123:CYS:CB[3_555]	1.91	0.29
1:B:79:ALA:CB	1:C:145:VAL:N[3_555]	1.91	0.29
1:B:161:VAL:C	1:C:152:ASN:C[3_555]	1.91	0.29
1:B:246:TYR:OH	1:C:162:TRP:CG[3_555]	1.91	0.29
1:B:149:GLN:C	1:C:95:THR:CB[3_555]	1.91	0.29
1:B:243:TYR:N	1:C:158:THR:C[3_555]	1.91	0.29
1:A:258:LEU:CA	1:B:232:SER:N[2_555]	1.91	0.29
1:B:243:TYR:CD1	1:C:158:THR:OG1[3_555]	1.91	0.29
1:B:190:ASN:O	1:C:54:LYS:CG[3_555]	1.91	0.29
1:B:80:VAL:CG1	1:C:144:PRO:CG[3_555]	1.91	0.29
1:B:247:THR:CB	1:C:165:GLN:OE1[3_555]	1.91	0.29
1:B:90:LEU:CD1	1:C:77:GLU:CD[3_555]	1.91	0.29
1:B:77:GLU:OE1	1:C:229:GLU:CD[3_555]	1.91	0.29
1:B:119:TYR:CZ	1:C:150:LEU:CD1[3_555]	1.91	0.29
1:A:256:ALA:N	1:B:126:THR:O[2_555]	1.91	0.29
1:B:91:VAL:CB	1:C:241:ARG:CG[3_555]	1.91	0.29
1:C:97:GLY:O	1:C:254:ILE:CG1[2_555]	1.91	0.29
1:B:136:GLN:O	1:C:74:LEU:CD2[3_555]	1.91	0.29
1:B:153:LEU:C	1:C:244:ALA:CB[3_555]	1.91	0.29
1:B:93:PRO:CD	1:C:122:SER:CB[3_555]	1.91	0.29
1:B:156:TYR:OH	1:C:91:VAL:CB[3_555]	1.91	0.29
1:B:163:GLU:N	1:C:153:LEU:O[3_555]	1.92	0.28
1:B:151:SER:C	1:C:96:VAL:CG2[3_555]	1.92	0.28
1:C:99:TRP:CZ3	1:C:107:TRP:CD1[2_555]	1.92	0.28
1:C:99:TRP:CD2	1:C:107:TRP:N[2_555]	1.92	0.28
1:B:122:SER:CA	1:C:151:SER:CB[3_555]	1.92	0.28
1:B:170:PHE:CD2	1:C:179:THR:C[3_555]	1.92	0.28
1:B:238:ASN:ND2	1:C:146:SER:CA[3_555]	1.92	0.28
1:B:244:ALA:CA	1:C:183:ILE:CD1[3_555]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:TYR:CE1	1:C:91:VAL:CG1[3_555]	1.92	0.28
1:B:248:ILE:CG1	1:C:49:GLN:O[3_555]	1.92	0.28
1:B:99:TRP:N	1:C:127:THR:CA[3_555]	1.92	0.28
1:B:247:THR:N	1:C:165:GLN:CB[3_555]	1.92	0.28
1:B:117:TYR:CD1	1:C:119:TYR:CE2[3_555]	1.92	0.28
1:B:245:SER:OG	1:C:163:GLU:CG[3_555]	1.92	0.28
1:C:99:TRP:CE3	1:C:107:TRP:CB[2_555]	1.92	0.28
1:C:71:HIS:NE2	1:C:251:ILE:O[2_555]	1.92	0.28
1:B:158:THR:N	1:C:135:PHE:CE2[3_555]	1.92	0.28
1:B:133:MET:O	1:C:117:TYR:CE2[3_555]	1.92	0.28
1:B:135:PHE:CE1	1:C:118:THR:O[3_555]	1.92	0.28
1:B:93:PRO:CD	1:C:122:SER:C[3_555]	1.92	0.28
1:B:185:ILE:C	1:C:118:THR:OG1[3_555]	1.92	0.28
1:B:77:GLU:CB	1:C:229:GLU:CG[3_555]	1.92	0.28
1:B:118:THR:CB	1:C:157:VAL:CG2[3_555]	1.92	0.28
1:B:149:GLN:C	1:C:95:THR:CA[3_555]	1.92	0.28
1:C:71:HIS:CD2	1:C:252:GLU:N[2_555]	1.93	0.27
1:B:247:THR:N	1:C:165:GLN:CD[3_555]	1.93	0.27
1:B:238:ASN:O	1:C:149:GLN:CA[3_555]	1.93	0.27
1:C:101:ARG:NH2	1:C:258:LEU:CG[2_555]	1.93	0.27
1:B:151:SER:OG	1:C:91:VAL:C[3_555]	1.93	0.27
1:B:170:PHE:CG	1:C:179:THR:O[3_555]	1.93	0.27
1:B:112:TRP:N	1:C:51:THR:O[3_555]	1.93	0.27
1:B:133:MET:N	1:C:224:LEU:CD1[3_555]	1.93	0.27
1:B:241:ARG:CA	1:C:132:HIS:CD2[3_555]	1.93	0.27
1:B:150:LEU:CG	1:C:89:GLU:CG[3_555]	1.93	0.27
1:B:146:SER:CA	1:C:90:LEU:CD1[3_555]	1.93	0.27
1:B:191:GLU:OE2	1:C:56:ARG:CB[3_555]	1.93	0.27
1:B:149:GLN:NE2	1:C:94:PHE:CE2[3_555]	1.93	0.27
1:C:246:TYR:CE2	1:C:253:PRO:CG[2_555]	1.93	0.27
1:B:99:TRP:C	1:C:127:THR:N[3_555]	1.93	0.27
1:B:223:ARG:C	1:C:76:THR:C[3_555]	1.93	0.27
1:C:102:GLY:N	1:C:256:ALA:N[2_555]	1.93	0.27
1:B:90:LEU:O	1:C:240:GLY:N[3_555]	1.93	0.27
1:C:73:GLU:CG	1:C:253:PRO:O[2_555]	1.93	0.27
1:C:98:THR:OG1	1:C:254:ILE:CD1[2_555]	1.94	0.26
1:B:89:GLU:O	1:C:77:GLU:C[3_555]	1.94	0.26
1:B:119:TYR:N	1:C:157:VAL:CG1[3_555]	1.94	0.26
1:B:95:THR:CB	1:C:238:ASN:CA[3_555]	1.94	0.26
1:B:242:LEU:O	1:C:131:ILE:O[3_555]	1.94	0.26
1:B:147:VAL:CB	1:C:90:LEU:CD2[3_555]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PRO:C	1:C:66:VAL:CB[2_555]	1.94	0.26
1:A:253:PRO:C	1:B:162:TRP:NE1[2_555]	1.94	0.26
1:C:55:LEU:O	1:C:196:ARG:NH1[2_555]	1.94	0.26
1:B:93:PRO:CD	1:C:122:SER:CA[3_555]	1.94	0.26
1:B:150:LEU:CD1	1:C:117:TYR:OH[3_555]	1.94	0.26
1:B:71:HIS:O	1:C:163:GLU:CD[3_555]	1.94	0.26
1:B:191:GLU:CG	1:C:55:LEU:C[3_555]	1.94	0.26
1:B:149:GLN:C	1:C:92:MET:O[3_555]	1.94	0.26
1:B:117:TYR:CE1	1:C:119:TYR:CG[3_555]	1.94	0.26
1:B:95:THR:CB	1:C:239:THR:CA[3_555]	1.94	0.26
1:B:150:LEU:N	1:C:95:THR:CB[3_555]	1.94	0.26
1:B:92:MET:C	1:C:122:SER:CA[3_555]	1.94	0.26
1:B:228:MET:CE	1:C:225:VAL:CG1[3_555]	1.94	0.26
1:B:87:THR:CA	1:C:87:THR:CB[3_555]	1.94	0.26
1:B:81:THR:CA	1:C:143:LEU:O[3_555]	1.94	0.26
1:B:150:LEU:CD2	1:C:89:GLU:CD[3_555]	1.94	0.26
1:B:119:TYR:OH	1:C:150:LEU:C[3_555]	1.94	0.26
1:B:112:TRP:CB	1:C:51:THR:CB[3_555]	1.94	0.26
1:B:183:ILE:O	1:C:184:THR:O[3_555]	1.94	0.26
1:B:154:LYS:O	1:C:244:ALA:CB[3_555]	1.94	0.26
1:B:100:LEU:O	1:C:124:PRO:CD[3_555]	1.94	0.26
1:B:189:THR:CG2	1:C:168:LEU:CD1[3_555]	1.94	0.26
1:B:134:GLY:CA	1:C:117:TYR:CE2[3_555]	1.95	0.25
1:B:229:GLU:CA	1:C:223:ARG:CD[3_555]	1.95	0.25
1:B:225:VAL:CG1	1:C:89:GLU:OE2[3_555]	1.95	0.25
1:B:85:VAL:CG2	3:C:264:HOH:O[3_555]	1.95	0.25
1:B:248:ILE:CB	1:C:49:GLN:O[3_555]	1.95	0.25
1:B:190:ASN:O	1:C:54:LYS:C[3_555]	1.95	0.25
1:B:225:VAL:CG2	1:C:76:THR:CB[3_555]	1.95	0.25
1:B:78:LEU:CD2	1:C:226:THR:C[3_555]	1.95	0.25
1:B:119:TYR:CB	1:C:157:VAL:CA[3_555]	1.95	0.25
1:B:89:GLU:CG	1:C:78:LEU:CG[3_555]	1.95	0.25
1:B:98:THR:N	1:C:128:SER:N[3_555]	1.95	0.25
1:B:170:PHE:C	1:C:181:ARG:CA[3_555]	1.95	0.25
1:B:147:VAL:O	1:C:91:VAL:CA[3_555]	1.95	0.25
1:B:191:GLU:N	1:C:54:LYS:N[3_555]	1.95	0.25
1:B:233:SER:O	1:C:142:THR:OG1[3_555]	1.95	0.25
1:B:88:SER:CA	3:C:265:HOH:O[3_555]	1.95	0.25
1:B:154:LYS:CG	1:C:72:CYS:SG[3_555]	1.95	0.25
1:B:82:VAL:CG1	1:C:142:THR:CG2[3_555]	1.95	0.25
1:B:243:TYR:CB	1:C:159:GLY:C[3_555]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ALA:CB	1:C:243:TYR:CZ[3_555]	1.95	0.25
1:B:132:HIS:CD2	1:C:224:LEU:CA[3_555]	1.95	0.25
1:C:99:TRP:CD1	1:C:107:TRP:N[2_555]	1.95	0.25
1:B:154:LYS:CB	1:C:73:GLU:N[3_555]	1.95	0.25
1:B:153:LEU:CB	1:C:96:VAL:O[3_555]	1.95	0.25
1:B:100:LEU:CD1	1:C:123:CYS:C[3_555]	1.95	0.25
1:B:100:LEU:O	1:C:124:PRO:C[3_555]	1.95	0.25
1:B:78:LEU:CB	1:C:227:ALA:CA[3_555]	1.95	0.25
1:B:90:LEU:C	1:C:240:GLY:C[3_555]	1.96	0.24
1:B:95:THR:OG1	1:C:239:THR:N[3_555]	1.96	0.24
1:B:93:PRO:CB	1:C:123:CYS:N[3_555]	1.96	0.24
1:B:156:TYR:CD1	1:C:115:ILE:CG2[3_555]	1.96	0.24
1:B:225:VAL:N	1:C:76:THR:CB[3_555]	1.96	0.24
1:B:99:TRP:CD2	1:C:125:THR:C[3_555]	1.96	0.24
1:A:254:ILE:CD1	1:B:128:SER:CA[2_555]	1.96	0.24
1:B:243:TYR:C	1:C:183:ILE:CD1[3_555]	1.96	0.24
1:B:131:ILE:CD1	1:C:133:MET:CB[3_555]	1.96	0.24
1:B:80:VAL:CA	1:C:144:PRO:CA[3_555]	1.96	0.24
1:C:100:LEU:CA	1:C:254:ILE:O[2_555]	1.96	0.24
1:B:244:ALA:N	1:C:160:PRO:O[3_555]	1.96	0.24
1:B:119:TYR:C	1:C:157:VAL:N[3_555]	1.96	0.24
1:C:73:GLU:CD	1:C:252:GLU:C[2_555]	1.96	0.24
1:B:89:GLU:CG	1:C:78:LEU:CB[3_555]	1.96	0.24
1:B:156:TYR:CZ	1:C:91:VAL:CG2[3_555]	1.96	0.24
1:B:229:GLU:C	1:C:223:ARG:NE[3_555]	1.96	0.24
1:B:190:ASN:CB	1:C:54:LYS:O[3_555]	1.96	0.24
1:B:112:TRP:C	1:C:51:THR:CB[3_555]	1.96	0.24
1:C:59:MET:CE	1:C:63:SER:N[2_555]	1.96	0.24
1:B:95:THR:OG1	1:C:238:ASN:O[3_555]	1.97	0.23
1:C:99:TRP:CA	1:C:107:TRP:N[2_555]	1.97	0.23
1:A:258:LEU:O	1:B:231:GLY:CA[2_555]	1.97	0.23
1:C:56:ARG:CA	1:C:249:ARG:NH2[2_555]	1.97	0.23
1:B:162:TRP:CA	1:C:153:LEU:N[3_555]	1.97	0.23
1:B:170:PHE:CG	1:C:182:ALA:N[3_555]	1.97	0.23
1:B:117:TYR:O	1:C:184:THR:N[3_555]	1.97	0.23
1:C:99:TRP:CA	1:C:106:ASN:C[2_555]	1.97	0.23
1:B:147:VAL:C	1:C:90:LEU:CB[3_555]	1.97	0.23
1:B:73:GLU:N	1:C:160:PRO:CD[3_555]	1.97	0.23
1:C:99:TRP:N	1:C:254:ILE:CB[2_555]	1.97	0.23
1:B:87:THR:N	1:C:87:THR:CB[3_555]	1.97	0.23
1:B:132:HIS:N	1:C:224:LEU:C[3_555]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:CA	1:C:171:VAL:CB[3_555]	1.97	0.23
1:B:187:LEU:C	1:C:171:VAL:CG1[3_555]	1.97	0.23
1:B:100:LEU:CA	1:C:124:PRO:CA[3_555]	1.97	0.23
1:B:73:GLU:C	1:C:160:PRO:C[3_555]	1.97	0.23
1:B:157:VAL:CB	1:C:185:ILE:C[3_555]	1.97	0.23
1:B:147:VAL:CA	1:C:90:LEU:N[3_555]	1.97	0.23
1:B:118:THR:N	1:C:183:ILE:CA[3_555]	1.97	0.23
1:B:115:ILE:CD1	1:C:121:PRO:CA[3_555]	1.97	0.23
1:A:254:ILE:O	1:B:127:THR:O[2_555]	1.97	0.23
1:B:187:LEU:C	1:C:171:VAL:CG2[3_555]	1.98	0.22
1:B:119:TYR:CD2	1:C:133:MET:N[3_555]	1.98	0.22
1:B:73:GLU:O	1:C:160:PRO:CD[3_555]	1.98	0.22
1:A:254:ILE:CA	1:B:127:THR:C[2_555]	1.98	0.22
1:B:69:LEU:CD1	1:C:46:PRO:O[3_555]	1.98	0.22
1:B:89:GLU:CA	1:C:78:LEU:C[3_555]	1.98	0.22
1:B:244:ALA:O	1:C:163:GLU:CG[3_555]	1.98	0.22
1:B:112:TRP:N	1:C:51:THR:N[3_555]	1.98	0.22
1:B:73:GLU:O	1:C:160:PRO:O[3_555]	1.98	0.22
1:B:115:ILE:CG2	1:C:120:LEU:CD2[3_555]	1.98	0.22
1:B:115:ILE:CG1	1:C:121:PRO:N[3_555]	1.98	0.22
1:B:77:GLU:N	1:C:229:GLU:N[3_555]	1.98	0.22
1:B:100:LEU:N	1:C:124:PRO:C[3_555]	1.98	0.22
1:B:117:TYR:CD2	1:C:119:TYR:CD2[3_555]	1.98	0.22
1:B:119:TYR:CA	1:C:157:VAL:N[3_555]	1.98	0.22
1:B:242:LEU:CB	1:C:131:ILE:CA[3_555]	1.98	0.22
1:B:228:MET:CA	1:C:225:VAL:CG2[3_555]	1.98	0.22
1:B:72:CYS:CB	1:C:163:GLU:OE2[3_555]	1.98	0.22
1:B:81:THR:C	1:C:142:THR:CB[3_555]	1.98	0.22
1:B:170:PHE:O	1:C:181:ARG:CA[3_555]	1.98	0.22
1:B:229:GLU:OE2	1:C:223:ARG:N[3_555]	1.98	0.22
1:B:170:PHE:CB	1:C:180:SER:O[3_555]	1.98	0.22
1:B:89:GLU:CB	1:C:78:LEU:C[3_555]	1.99	0.21
1:B:244:ALA:CB	1:C:163:GLU:O[3_555]	1.99	0.21
1:C:85:VAL:CA	3:B:270:HOH:O[2_555]	1.99	0.21
1:B:153:LEU:CB	1:C:96:VAL:CG1[3_555]	1.99	0.21
1:B:100:LEU:CB	1:C:123:CYS:O[3_555]	1.99	0.21
1:C:59:MET:C	1:C:67:THR:OG1[2_555]	1.99	0.21
1:C:73:GLU:OE1	1:C:252:GLU:O[2_555]	1.99	0.21
1:B:73:GLU:CD	1:C:162:TRP:CG[3_555]	1.99	0.21
1:B:116:ARG:CG	1:C:182:ALA:C[3_555]	1.99	0.21
1:B:69:LEU:CD1	1:C:46:PRO:CB[3_555]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:N	1:C:240:GLY:C[3_555]	1.99	0.21
1:B:237:VAL:N	1:C:145:VAL:N[3_555]	1.99	0.21
1:A:254:ILE:O	1:B:127:THR:C[2_555]	1.99	0.21
1:B:99:TRP:O	1:C:126:THR:CB[3_555]	1.99	0.21
1:B:162:TRP:N	1:C:152:ASN:CA[3_555]	1.99	0.21
1:B:117:TYR:CZ	1:C:119:TYR:CZ[3_555]	1.99	0.21
1:C:99:TRP:CD1	1:C:107:TRP:CA[2_555]	1.99	0.21
1:B:170:PHE:CA	1:C:180:SER:C[3_555]	1.99	0.21
1:B:248:ILE:CA	1:C:49:GLN:CA[3_555]	1.99	0.21
1:B:80:VAL:CG2	1:C:144:PRO:CA[3_555]	1.99	0.21
1:B:246:TYR:O	1:C:49:GLN:CG[3_555]	1.99	0.21
1:B:183:ILE:O	1:C:157:VAL:CB[3_555]	1.99	0.21
1:B:71:HIS:C	1:C:162:TRP:CZ3[3_555]	1.99	0.21
1:B:95:THR:C	1:C:239:THR:N[3_555]	1.99	0.21
1:B:98:THR:C	1:C:126:THR:O[3_555]	1.99	0.21
1:A:255:ALA:CB	1:B:127:THR:CA[2_555]	1.99	0.21
1:B:148:ASN:CB	1:C:92:MET:CB[3_555]	1.99	0.21
1:B:89:GLU:N	1:C:78:LEU:N[3_555]	1.99	0.21
1:B:149:GLN:O	1:C:96:VAL:CA[3_555]	1.99	0.21
1:B:243:TYR:CE1	1:C:158:THR:OG1[3_555]	1.99	0.21
1:B:237:VAL:CG1	1:C:149:GLN:NE2[3_555]	1.99	0.21
1:C:58:PRO:CA	1:C:250:LEU:O[2_555]	2.00	0.20
1:B:85:VAL:CG1	1:C:143:LEU:CD1[3_555]	2.00	0.20
1:B:149:GLN:CD	1:C:95:THR:OG1[3_555]	2.00	0.20
1:B:222:ALA:CA	1:C:74:LEU:CD2[3_555]	2.00	0.20
1:B:153:LEU:CD1	1:C:96:VAL:O[3_555]	2.00	0.20
1:B:239:THR:C	1:C:150:LEU:CB[3_555]	2.00	0.20
1:B:135:PHE:N	1:C:75:SER:CB[3_555]	2.00	0.20
1:B:116:ARG:NH1	1:C:182:ALA:CB[3_555]	2.00	0.20
1:C:100:LEU:CA	1:C:106:ASN:O[2_555]	2.00	0.20
1:B:152:ASN:CG	1:C:93:PRO:N[3_555]	2.00	0.20
1:B:228:MET:O	1:C:143:LEU:CD1[3_555]	2.00	0.20
1:B:75:SER:C	1:C:130:ALA:C[3_555]	2.00	0.20
1:B:149:GLN:N	1:C:95:THR:CB[3_555]	2.00	0.20
1:B:132:HIS:CE1	1:C:223:ARG:C[3_555]	2.00	0.20
1:B:246:TYR:CD2	1:C:49:GLN:CB[3_555]	2.00	0.20
1:B:80:VAL:N	1:C:144:PRO:CG[3_555]	2.00	0.20
1:B:91:VAL:CB	1:C:241:ARG:N[3_555]	2.00	0.20
1:A:255:ALA:CA	1:B:127:THR:C[2_555]	2.00	0.20
1:B:187:LEU:CD2	1:C:120:LEU:CD1[3_555]	2.00	0.20
1:C:72:CYS:C	1:C:252:GLU:CB[2_555]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:CB	1:C:226:THR:CG2[3_555]	2.01	0.19
1:B:147:VAL:N	1:C:90:LEU:CD2[3_555]	2.01	0.19
1:B:118:THR:OG1	1:C:182:ALA:C[3_555]	2.01	0.19
1:B:93:PRO:O	1:C:123:CYS:N[3_555]	2.01	0.19
1:A:254:ILE:CB	1:B:128:SER:C[2_555]	2.01	0.19
1:B:227:ALA:CB	1:C:224:LEU:O[3_555]	2.01	0.19
1:B:86:VAL:CB	1:C:88:SER:O[3_555]	2.01	0.19
1:B:155:GLY:O	1:C:117:TYR:CA[3_555]	2.01	0.19
1:B:187:LEU:CD1	1:C:243:TYR:CD1[3_555]	2.01	0.19
1:B:121:PRO:N	1:C:156:TYR:CG[3_555]	2.01	0.19
1:A:258:LEU:C	1:B:232:SER:CA[2_555]	2.01	0.19
1:B:131:ILE:CG2	1:C:135:PHE:N[3_555]	2.01	0.19
1:C:101:ARG:CZ	1:C:258:LEU:CA[2_555]	2.01	0.19
1:C:101:ARG:NH2	1:C:258:LEU:CB[2_555]	2.01	0.19
1:C:60:LEU:C	1:C:62:SER:N[2_555]	2.01	0.19
1:B:243:TYR:CD1	1:C:158:THR:CG2[3_555]	2.01	0.19
1:B:137:TYR:CG	1:C:74:LEU:CB[3_555]	2.01	0.19
1:B:190:ASN:N	1:C:172:ASN:OD1[3_555]	2.01	0.19
1:B:227:ALA:CA	1:C:88:SER:C[3_555]	2.01	0.19
1:B:184:THR:N	3:C:267:HOH:O[3_555]	2.02	0.18
1:B:170:PHE:CZ	1:C:179:THR:O[3_555]	2.02	0.18
1:B:89:GLU:N	1:C:78:LEU:CA[3_555]	2.02	0.18
1:B:112:TRP:CA	1:C:51:THR:C[3_555]	2.02	0.18
1:B:146:SER:O	1:C:90:LEU:CB[3_555]	2.02	0.18
1:B:230:GLY:CA	1:C:136:GLN:OE1[3_555]	2.02	0.18
1:B:135:PHE:O	1:C:75:SER:N[3_555]	2.02	0.18
1:B:76:THR:C	1:C:130:ALA:O[3_555]	2.02	0.18
1:A:253:PRO:O	1:B:162:TRP:CD1[2_555]	2.02	0.18
1:B:99:TRP:CH2	1:C:46:PRO:O[3_555]	2.02	0.18
1:B:221:PRO:CG	1:C:241:ARG:NE[3_555]	2.02	0.18
1:B:238:ASN:N	1:C:149:GLN:NE2[3_555]	2.02	0.18
1:B:152:ASN:CG	1:C:93:PRO:CB[3_555]	2.02	0.18
1:A:258:LEU:C	1:B:231:GLY:C[2_555]	2.02	0.18
1:B:239:THR:C	1:C:150:LEU:C[3_555]	2.02	0.18
1:A:258:LEU:C	1:B:232:SER:CB[2_555]	2.02	0.18
1:C:57:PRO:C	1:C:250:LEU:O[2_555]	2.02	0.18
1:B:161:VAL:O	1:C:152:ASN:N[3_555]	2.02	0.18
1:B:101:ARG:CA	1:C:124:PRO:CG[3_555]	2.02	0.18
1:B:225:VAL:CG1	1:C:89:GLU:OE1[3_555]	2.02	0.18
1:B:229:GLU:C	1:C:136:GLN:CD[3_555]	2.02	0.18
1:B:152:ASN:N	1:C:96:VAL:CB[3_555]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:THR:C	1:C:54:LYS:N[3_555]	2.02	0.18
1:B:236:ALA:CA	1:C:145:VAL:CG2[3_555]	2.02	0.18
1:B:80:VAL:CB	1:C:144:PRO:CG[3_555]	2.02	0.18
1:B:159:GLY:O	1:C:135:PHE:O[3_555]	2.02	0.18
1:B:72:CYS:O	1:C:162:TRP:CE2[3_555]	2.03	0.17
1:B:72:CYS:N	1:C:162:TRP:CH2[3_555]	2.03	0.17
1:B:150:LEU:C	1:C:96:VAL:CG2[3_555]	2.03	0.17
1:B:119:TYR:CG	1:C:157:VAL:N[3_555]	2.03	0.17
1:B:185:ILE:N	1:C:184:THR:CB[3_555]	2.03	0.17
1:B:115:ILE:CD1	1:C:120:LEU:CA[3_555]	2.03	0.17
1:B:159:GLY:O	1:C:135:PHE:CA[3_555]	2.03	0.17
1:B:96:VAL:C	1:C:161:VAL:O[3_555]	2.03	0.17
1:C:73:GLU:OE1	1:C:253:PRO:C[2_555]	2.03	0.17
1:B:98:THR:N	1:C:127:THR:CA[3_555]	2.03	0.17
1:C:99:TRP:CE2	1:C:107:TRP:CG[2_555]	2.03	0.17
1:B:136:GLN:CG	1:C:75:SER:O[3_555]	2.03	0.17
1:B:157:VAL:C	1:C:135:PHE:CE2[3_555]	2.03	0.17
1:B:135:PHE:O	1:C:74:LEU:O[3_555]	2.03	0.17
1:B:124:PRO:O	1:C:152:ASN:CG[3_555]	2.03	0.17
1:B:103:VAL:CG1	1:C:47:ILE:CB[3_555]	2.03	0.17
1:B:156:TYR:OH	1:C:91:VAL:CG2[3_555]	2.03	0.17
1:C:99:TRP:CD1	1:C:104:ALA:O[2_555]	2.03	0.17
1:A:106:ASN:ND2	1:B:126:THR:CA[2_555]	2.03	0.17
1:C:102:GLY:CA	1:C:256:ALA:CB[2_555]	2.03	0.17
1:C:60:LEU:CD1	1:C:67:THR:OG1[2_555]	2.03	0.17
1:B:190:ASN:CG	1:C:172:ASN:ND2[3_555]	2.03	0.17
1:B:154:LYS:NZ	1:C:245:SER:CB[3_555]	2.03	0.17
1:B:148:ASN:CA	1:C:92:MET:CG[3_555]	2.04	0.16
1:C:71:HIS:ND1	1:C:251:ILE:C[2_555]	2.04	0.16
1:A:106:ASN:CB	1:B:126:THR:CG2[2_555]	2.04	0.16
1:B:157:VAL:CG1	1:C:185:ILE:O[3_555]	2.04	0.16
1:B:95:THR:CB	1:C:238:ASN:O[3_555]	2.04	0.16
1:B:133:MET:CG	1:C:133:MET:SD[3_555]	2.04	0.16
1:B:76:THR:OG1	1:C:228:MET:CG[3_555]	2.04	0.16
1:B:245:SER:CB	1:C:163:GLU:CG[3_555]	2.04	0.16
1:B:249:ARG:N	1:C:50:GLY:CA[3_555]	2.04	0.16
1:B:225:VAL:CG2	1:C:75:SER:O[3_555]	2.04	0.16
1:B:238:ASN:O	1:C:146:SER:O[3_555]	2.04	0.16
1:B:190:ASN:CA	1:C:54:LYS:CG[3_555]	2.04	0.16
1:B:239:THR:O	1:C:151:SER:CA[3_555]	2.04	0.16
1:B:119:TYR:CB	1:C:157:VAL:C[3_555]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:TYR:CE1	1:C:73:GLU:O[3_555]	2.04	0.16
1:B:161:VAL:CB	1:C:153:LEU:CB[3_555]	2.04	0.16
1:B:103:VAL:CA	1:C:47:ILE:CD1[3_555]	2.04	0.16
1:B:237:VAL:N	1:C:145:VAL:CB[3_555]	2.04	0.16
1:B:154:LYS:O	1:C:243:TYR:C[3_555]	2.04	0.16
1:B:241:ARG:CG	1:C:229:GLU:OE2[3_555]	2.04	0.16
1:B:241:ARG:N	1:C:132:HIS:CG[3_555]	2.04	0.16
1:B:222:ALA:CB	1:C:243:TYR:OH[3_555]	2.04	0.16
1:C:59:MET:N	1:C:67:THR:CA[2_555]	2.04	0.16
1:B:170:PHE:C	1:C:181:ARG:CB[3_555]	2.04	0.16
1:B:148:ASN:C	1:C:92:MET:N[3_555]	2.04	0.16
1:C:59:MET:CG	1:C:62:SER:O[2_555]	2.04	0.16
1:B:85:VAL:O	1:C:87:THR:C[3_555]	2.04	0.16
1:B:121:PRO:CA	1:C:151:SER:O[3_555]	2.04	0.16
1:A:254:ILE:C	1:B:127:THR:N[2_555]	2.04	0.16
1:B:98:THR:CA	1:C:127:THR:O[3_555]	2.04	0.16
1:B:152:ASN:OD1	1:C:93:PRO:CB[3_555]	2.04	0.16
1:B:71:HIS:O	1:C:163:GLU:OE1[3_555]	2.05	0.15
1:B:186:ALA:CB	1:C:167:GLY:CA[3_555]	2.05	0.15
1:C:59:MET:CA	1:C:66:VAL:C[2_555]	2.05	0.15
1:B:133:MET:O	1:C:117:TYR:CZ[3_555]	2.05	0.15
1:B:80:VAL:O	1:C:144:PRO:N[3_555]	2.05	0.15
1:B:134:GLY:C	1:C:75:SER:CB[3_555]	2.05	0.15
1:B:155:GLY:N	1:C:244:ALA:CA[3_555]	2.05	0.15
1:B:242:LEU:CG	1:C:131:ILE:CG1[3_555]	2.05	0.15
1:B:117:TYR:CB	1:C:183:ILE:CG2[3_555]	2.05	0.15
1:B:156:TYR:N	1:C:116:ARG:O[3_555]	2.05	0.15
1:B:246:TYR:OH	1:C:162:TRP:CB[3_555]	2.05	0.15
1:B:242:LEU:N	1:C:132:HIS:CG[3_555]	2.05	0.15
1:B:100:LEU:CD2	1:C:124:PRO:CA[3_555]	2.05	0.15
1:C:99:TRP:CD1	1:C:107:TRP:CB[2_555]	2.05	0.15
1:C:99:TRP:CD2	1:C:107:TRP:CD2[2_555]	2.05	0.15
1:C:101:ARG:NH2	1:C:257:ALA:C[2_555]	2.05	0.15
1:B:114:ALA:C	1:C:165:GLN:CB[3_555]	2.05	0.15
1:B:170:PHE:CB	1:C:182:ALA:N[3_555]	2.05	0.15
1:B:226:THR:OG1	1:C:226:THR:N[3_555]	2.05	0.15
1:B:77:GLU:O	1:C:228:MET:N[3_555]	2.05	0.15
1:B:244:ALA:C	1:C:163:GLU:CG[3_555]	2.05	0.15
1:B:191:GLU:CG	1:C:56:ARG:N[3_555]	2.05	0.15
1:B:112:TRP:CA	1:C:51:THR:O[3_555]	2.05	0.15
1:B:248:ILE:CA	1:C:50:GLY:CA[3_555]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:CB	1:B:127:THR:OG1[2_555]	2.06	0.14
1:B:183:ILE:CB	1:C:155:GLY:C[3_555]	2.06	0.14
1:B:134:GLY:N	1:C:117:TYR:CE2[3_555]	2.06	0.14
1:B:189:THR:C	1:C:172:ASN:ND2[3_555]	2.06	0.14
1:B:155:GLY:O	1:C:116:ARG:CA[3_555]	2.06	0.14
1:B:80:VAL:N	1:C:144:PRO:CB[3_555]	2.06	0.14
1:B:69:LEU:CG	1:C:47:ILE:N[3_555]	2.06	0.14
1:B:133:MET:C	1:C:117:TYR:CE2[3_555]	2.06	0.14
1:B:96:VAL:C	1:C:239:THR:CG2[3_555]	2.06	0.14
1:A:254:ILE:C	1:B:128:SER:N[2_555]	2.06	0.14
1:B:242:LEU:CB	1:C:131:ILE:CG1[3_555]	2.06	0.14
1:B:91:VAL:CG2	1:C:241:ARG:O[3_555]	2.06	0.14
1:B:237:VAL:C	1:C:149:GLN:CD[3_555]	2.06	0.14
1:B:192:VAL:CG2	1:C:53:VAL:N[3_555]	2.06	0.14
1:A:254:ILE:CG1	1:B:128:SER:N[2_555]	2.06	0.14
1:B:190:ASN:CA	1:C:54:LYS:N[3_555]	2.06	0.14
1:B:159:GLY:CA	1:C:154:LYS:CB[3_555]	2.06	0.14
1:B:93:PRO:CG	1:C:122:SER:C[3_555]	2.06	0.14
1:C:60:LEU:N	1:C:62:SER:CB[2_555]	2.07	0.13
1:B:98:THR:CG2	1:C:128:SER:N[3_555]	2.07	0.13
1:B:243:TYR:CD1	1:C:158:THR:CB[3_555]	2.07	0.13
1:B:130:ALA:N	1:C:136:GLN:CB[3_555]	2.07	0.13
1:C:98:THR:N	1:C:254:ILE:CG2[2_555]	2.07	0.13
1:B:170:PHE:CB	1:C:181:ARG:C[3_555]	2.07	0.13
1:C:101:ARG:CA	1:C:256:ALA:N[2_555]	2.07	0.13
1:B:96:VAL:CG2	1:C:119:TYR:OH[3_555]	2.07	0.13
1:B:244:ALA:C	1:C:163:GLU:CA[3_555]	2.07	0.13
1:B:246:TYR:CG	1:C:49:GLN:CD[3_555]	2.07	0.13
1:B:189:THR:O	1:C:52:MET:O[3_555]	2.07	0.13
1:C:60:LEU:CA	1:C:62:SER:CB[2_555]	2.07	0.13
1:B:86:VAL:CA	1:C:88:SER:N[3_555]	2.07	0.13
1:B:117:TYR:CE2	1:C:119:TYR:CA[3_555]	2.07	0.13
1:B:116:ARG:CA	1:C:164:GLY:O[3_555]	2.07	0.13
1:A:253:PRO:CB	1:B:162:TRP:CD2[2_555]	2.07	0.13
1:B:99:TRP:C	1:C:124:PRO:O[3_555]	2.07	0.13
1:B:192:VAL:N	1:C:53:VAL:C[3_555]	2.07	0.13
1:B:116:ARG:N	1:C:164:GLY:CA[3_555]	2.07	0.13
1:B:86:VAL:C	1:C:87:THR:OG1[3_555]	2.07	0.13
1:B:79:ALA:CB	1:C:144:PRO:C[3_555]	2.07	0.13
1:B:187:LEU:CB	1:C:120:LEU:CG[3_555]	2.07	0.13
1:B:224:LEU:N	1:C:76:THR:C[3_555]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:CD2	1:C:132:HIS:O[3_555]	2.07	0.13
1:B:136:GLN:CA	1:C:75:SER:N[3_555]	2.07	0.13
1:B:182:ALA:O	3:C:267:HOH:O[3_555]	2.08	0.12
1:B:157:VAL:C	1:C:135:PHE:CE1[3_555]	2.08	0.12
1:C:102:GLY:N	1:C:106:ASN:ND2[2_555]	2.08	0.12
1:B:99:TRP:CE2	1:C:125:THR:O[3_555]	2.08	0.12
1:B:248:ILE:CB	1:C:50:GLY:N[3_555]	2.08	0.12
1:B:184:THR:O	1:C:184:THR:CA[3_555]	2.08	0.12
1:B:187:LEU:O	1:C:168:LEU:O[3_555]	2.08	0.12
1:C:73:GLU:CB	1:C:252:GLU:O[2_555]	2.08	0.12
1:B:151:SER:C	1:C:112:TRP:CZ2[3_555]	2.08	0.12
1:B:225:VAL:CG1	1:C:89:GLU:CD[3_555]	2.08	0.12
1:C:60:LEU:N	1:C:67:THR:OG1[2_555]	2.08	0.12
1:B:229:GLU:OE2	1:C:136:GLN:O[3_555]	2.08	0.12
1:B:243:TYR:CD1	1:C:159:GLY:N[3_555]	2.08	0.12
1:C:97:GLY:C	1:C:254:ILE:C[2_555]	2.08	0.12
1:B:161:VAL:CB	1:C:153:LEU:CD2[3_555]	2.08	0.12
1:B:78:LEU:CD1	1:C:132:HIS:CB[3_555]	2.08	0.12
1:B:224:LEU:C	1:C:242:LEU:CD2[3_555]	2.08	0.12
1:B:159:GLY:C	1:C:154:LYS:CB[3_555]	2.08	0.12
1:B:229:GLU:O	1:C:136:GLN:CB[3_555]	2.08	0.12
1:B:98:THR:OG1	1:C:128:SER:CB[3_555]	2.08	0.12
1:B:117:TYR:CE2	1:C:119:TYR:C[3_555]	2.08	0.12
1:B:223:ARG:CB	1:C:76:THR:C[3_555]	2.08	0.12
1:C:101:ARG:N	1:C:254:ILE:C[2_555]	2.08	0.12
1:B:239:THR:CB	1:C:149:GLN:C[3_555]	2.08	0.12
1:C:246:TYR:CE2	1:C:253:PRO:CB[2_555]	2.08	0.12
1:C:65:ASP:O	1:C:70:SER:O[3_555]	2.08	0.12
1:B:228:MET:O	1:C:143:LEU:CG[3_555]	2.09	0.11
1:A:253:PRO:CD	1:B:162:TRP:NE1[2_555]	2.09	0.11
1:B:93:PRO:N	1:C:123:CYS:N[3_555]	2.09	0.11
1:B:95:THR:O	1:C:239:THR:CG2[3_555]	2.09	0.11
1:B:135:PHE:CA	1:C:75:SER:CB[3_555]	2.09	0.11
1:C:99:TRP:CB	1:C:108:SER:N[2_555]	2.09	0.11
1:B:183:ILE:CG1	1:C:155:GLY:O[3_555]	2.09	0.11
1:B:184:THR:N	1:C:185:ILE:N[3_555]	2.09	0.11
1:B:79:ALA:C	1:C:144:PRO:C[3_555]	2.09	0.11
1:B:149:GLN:OE1	1:C:95:THR:OG1[3_555]	2.09	0.11
1:B:87:THR:OG1	1:C:87:THR:N[3_555]	2.09	0.11
1:B:117:TYR:OH	1:C:119:TYR:CE2[3_555]	2.09	0.11
1:B:158:THR:CB	1:C:135:PHE:CE2[3_555]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PRO:N	1:C:152:ASN:OD1[3_555]	2.09	0.11
1:B:242:LEU:N	1:C:132:HIS:CA[3_555]	2.09	0.11
1:B:246:TYR:CD1	1:C:163:GLU:N[3_555]	2.09	0.11
1:B:150:LEU:N	1:C:90:LEU:O[3_555]	2.09	0.11
1:B:96:VAL:O	1:C:161:VAL:O[3_555]	2.10	0.10
1:B:79:ALA:CB	1:C:144:PRO:O[3_555]	2.10	0.10
1:B:189:THR:OG1	1:C:168:LEU:CD2[3_555]	2.10	0.10
1:B:147:VAL:N	1:C:90:LEU:CD1[3_555]	2.10	0.10
1:B:241:ARG:N	1:C:156:TYR:OH[3_555]	2.10	0.10
1:C:101:ARG:CA	1:C:255:ALA:C[2_555]	2.10	0.10
1:B:132:HIS:N	1:C:225:VAL:N[3_555]	2.10	0.10
1:A:258:LEU:CA	1:B:232:SER:CA[2_555]	2.10	0.10
1:B:190:ASN:OD1	1:C:172:ASN:C[3_555]	2.10	0.10
1:B:224:LEU:CA	1:C:242:LEU:CD2[3_555]	2.10	0.10
1:B:229:GLU:CD	1:C:139:MET:CE[3_555]	2.10	0.10
1:B:92:MET:N	1:C:122:SER:CB[3_555]	2.10	0.10
1:B:90:LEU:CD1	1:C:77:GLU:CB[3_555]	2.10	0.10
1:B:93:PRO:CA	1:C:122:SER:CA[3_555]	2.10	0.10
1:B:133:MET:CG	1:C:224:LEU:CD1[3_555]	2.10	0.10
1:B:147:VAL:C	1:C:91:VAL:N[3_555]	2.10	0.10
1:B:184:THR:CB	1:C:184:THR:O[3_555]	2.10	0.10
1:B:237:VAL:CA	1:C:149:GLN:OE1[3_555]	2.10	0.10
1:B:152:ASN:ND2	1:C:93:PRO:CB[3_555]	2.10	0.10
1:B:188:ASP:OD2	1:C:171:VAL:CG1[3_555]	2.10	0.10
1:B:185:ILE:CA	1:C:118:THR:CB[3_555]	2.10	0.10
1:B:154:LYS:N	1:C:244:ALA:CB[3_555]	2.10	0.10
1:B:123:CYS:SG	1:C:152:ASN:N[3_555]	2.11	0.09
1:B:96:VAL:C	1:C:161:VAL:CG1[3_555]	2.11	0.09
1:B:134:GLY:O	1:C:75:SER:CB[3_555]	2.11	0.09
1:B:157:VAL:CG1	1:C:185:ILE:CA[3_555]	2.11	0.09
1:B:135:PHE:CD1	1:C:243:TYR:CA[3_555]	2.11	0.09
1:B:153:LEU:O	1:C:244:ALA:CB[3_555]	2.11	0.09
1:B:246:TYR:CD1	1:C:163:GLU:CA[3_555]	2.11	0.09
1:B:114:ALA:C	1:C:51:THR:CG2[3_555]	2.11	0.09
1:B:242:LEU:O	1:C:131:ILE:C[3_555]	2.11	0.09
1:B:95:THR:CG2	1:C:238:ASN:CB[3_555]	2.11	0.09
1:B:237:VAL:C	1:C:145:VAL:N[3_555]	2.11	0.09
1:B:133:MET:CE	1:C:133:MET:CE[3_555]	2.11	0.09
1:B:149:GLN:N	1:C:92:MET:CG[3_555]	2.11	0.09
1:B:90:LEU:CA	1:C:240:GLY:O[3_555]	2.11	0.09
1:B:119:TYR:CD1	1:C:157:VAL:N[3_555]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:THR:OG1	1:C:152:ASN:ND2[3_555]	2.11	0.09
1:A:253:PRO:CA	1:B:162:TRP:CD1[2_555]	2.11	0.09
1:B:151:SER:OG	1:C:92:MET:N[3_555]	2.11	0.09
1:B:87:THR:CG2	1:C:87:THR:CG2[3_555]	2.11	0.09
1:C:101:ARG:CB	1:C:255:ALA:O[2_555]	2.11	0.09
1:C:99:TRP:CG	1:C:107:TRP:O[2_555]	2.11	0.09
1:B:188:ASP:CA	1:C:171:VAL:CA[3_555]	2.11	0.09
1:C:101:ARG:CD	1:C:256:ALA:O[2_555]	2.11	0.09
1:C:60:LEU:C	1:C:62:SER:CB[2_555]	2.11	0.09
1:B:150:LEU:O	1:C:96:VAL:CG2[3_555]	2.11	0.09
1:B:239:THR:CA	1:C:150:LEU:CB[3_555]	2.11	0.09
1:B:184:THR:CB	1:C:184:THR:CA[3_555]	2.11	0.09
1:B:76:THR:CB	1:C:228:MET:CA[3_555]	2.11	0.09
1:B:190:ASN:N	1:C:54:LYS:N[3_555]	2.12	0.08
1:B:146:SER:CA	1:C:90:LEU:CG[3_555]	2.12	0.08
1:B:69:LEU:CG	1:C:46:PRO:CG[3_555]	2.12	0.08
1:C:71:HIS:NE2	1:C:251:ILE:N[2_555]	2.12	0.08
1:B:156:TYR:CA	1:C:115:ILE:CG1[3_555]	2.12	0.08
1:B:185:ILE:O	1:C:183:ILE:O[3_555]	2.12	0.08
1:B:91:VAL:CA	1:C:241:ARG:N[3_555]	2.12	0.08
1:B:147:VAL:CG1	1:C:223:ARG:CA[3_555]	2.12	0.08
1:B:246:TYR:CZ	1:C:162:TRP:CE3[3_555]	2.12	0.08
1:B:242:LEU:O	1:C:159:GLY:O[3_555]	2.12	0.08
1:B:132:HIS:ND1	1:C:223:ARG:C[3_555]	2.12	0.08
1:B:112:TRP:C	1:C:50:GLY:C[3_555]	2.12	0.08
1:C:102:GLY:CA	1:C:106:ASN:ND2[2_555]	2.12	0.08
1:B:121:PRO:CB	1:C:151:SER:C[3_555]	2.12	0.08
1:A:255:ALA:C	1:B:126:THR:O[2_555]	2.12	0.08
1:B:189:THR:C	1:C:172:ASN:OD1[3_555]	2.12	0.08
1:B:119:TYR:O	1:C:157:VAL:N[3_555]	2.12	0.08
1:C:99:TRP:CH2	1:C:107:TRP:CG[2_555]	2.12	0.08
1:B:156:TYR:CD1	1:C:115:ILE:CG1[3_555]	2.12	0.08
1:B:154:LYS:C	1:C:244:ALA:CB[3_555]	2.12	0.08
1:B:228:MET:CB	1:C:225:VAL:CG1[3_555]	2.12	0.08
1:C:99:TRP:CH2	1:C:107:TRP:CZ3[2_555]	2.12	0.08
1:B:188:ASP:N	1:C:171:VAL:CA[3_555]	2.12	0.08
1:B:117:TYR:C	1:C:183:ILE:O[3_555]	2.12	0.08
1:B:116:ARG:NH2	1:C:170:PHE:CE1[3_555]	2.12	0.08
1:B:155:GLY:CA	1:C:245:SER:OG[3_555]	2.12	0.08
1:B:135:PHE:CA	1:C:242:LEU:O[3_555]	2.12	0.08
1:B:119:TYR:CE1	1:C:156:TYR:CB[3_555]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:OG	1:C:77:GLU:O[3_555]	2.12	0.08
1:C:57:PRO:N	1:C:249:ARG:CZ[2_555]	2.12	0.08
1:B:113:VAL:C	1:C:51:THR:CG2[3_555]	2.12	0.08
1:B:77:GLU:OE2	1:C:229:GLU:CB[3_555]	2.12	0.08
1:B:156:TYR:O	1:C:116:ARG:CA[3_555]	2.12	0.08
1:B:89:GLU:CD	1:C:79:ALA:O[3_555]	2.12	0.08
1:B:228:MET:CG	1:C:226:THR:N[3_555]	2.12	0.08
1:B:73:GLU:CG	1:C:162:TRP:NE1[3_555]	2.12	0.08
1:B:101:ARG:NH2	1:C:237:VAL:CG1[3_555]	2.12	0.08
1:B:158:THR:OG1	1:C:135:PHE:CE2[3_555]	2.13	0.07
1:B:170:PHE:CE2	1:C:180:SER:N[3_555]	2.13	0.07
1:B:243:TYR:CB	1:C:158:THR:C[3_555]	2.13	0.07
1:C:71:HIS:CB	1:C:253:PRO:CD[2_555]	2.13	0.07
1:B:151:SER:N	1:C:96:VAL:CG2[3_555]	2.13	0.07
1:B:187:LEU:O	1:C:171:VAL:CB[3_555]	2.13	0.07
1:C:101:ARG:CG	1:C:256:ALA:C[2_555]	2.13	0.07
1:B:86:VAL:N	1:C:88:SER:N[3_555]	2.13	0.07
1:B:246:TYR:N	1:C:49:GLN:CD[3_555]	2.13	0.07
1:B:160:PRO:CG	1:C:154:LYS:CA[3_555]	2.13	0.07
1:B:86:VAL:CA	1:C:88:SER:O[3_555]	2.13	0.07
1:C:99:TRP:CA	1:C:254:ILE:CG2[2_555]	2.13	0.07
1:B:100:LEU:C	1:C:124:PRO:CB[3_555]	2.13	0.07
1:C:71:HIS:CE1	1:C:251:ILE:CB[2_555]	2.13	0.07
1:B:74:LEU:O	1:C:130:ALA:N[3_555]	2.13	0.07
1:B:156:TYR:CD2	1:C:117:TYR:OH[3_555]	2.13	0.07
1:B:224:LEU:CB	1:C:242:LEU:N[3_555]	2.13	0.07
1:A:254:ILE:N	1:B:127:THR:O[2_555]	2.13	0.07
1:B:77:GLU:CD	1:C:229:GLU:CG[3_555]	2.13	0.07
1:B:137:TYR:CD1	1:C:73:GLU:C[3_555]	2.13	0.07
1:B:225:VAL:CA	1:C:76:THR:CB[3_555]	2.13	0.07
1:B:115:ILE:CA	1:C:164:GLY:O[3_555]	2.13	0.07
1:C:99:TRP:CZ2	1:C:250:LEU:CD2[2_555]	2.13	0.07
1:B:80:VAL:CB	1:C:143:LEU:C[3_555]	2.13	0.07
1:B:151:SER:OG	1:C:92:MET:CA[3_555]	2.13	0.07
1:B:248:ILE:CB	1:C:48:ALA:C[3_555]	2.13	0.07
1:C:94:PHE:CA	1:C:255:ALA:CB[2_555]	2.14	0.06
1:B:92:MET:O	1:C:239:THR:C[3_555]	2.14	0.06
1:B:70:SER:O	1:C:46:PRO:CG[3_555]	2.14	0.06
1:B:134:GLY:O	1:C:242:LEU:CD2[3_555]	2.14	0.06
1:B:152:ASN:ND2	1:C:93:PRO:CD[3_555]	2.14	0.06
1:B:191:GLU:CD	1:C:55:LEU:O[3_555]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:C	1:C:127:THR:O[3_555]	2.14	0.06
1:B:74:LEU:O	1:C:130:ALA:CA[3_555]	2.14	0.06
1:B:154:LYS:CB	1:C:244:ALA:C[3_555]	2.14	0.06
1:B:73:GLU:O	1:C:160:PRO:CB[3_555]	2.14	0.06
1:B:244:ALA:N	1:C:183:ILE:CD1[3_555]	2.14	0.06
1:B:185:ILE:CA	1:C:184:THR:OG1[3_555]	2.14	0.06
1:B:224:LEU:CB	1:C:242:LEU:CB[3_555]	2.14	0.06
1:C:56:ARG:C	1:C:251:ILE:CG1[2_555]	2.14	0.06
1:C:73:GLU:OE2	1:C:253:PRO:O[2_555]	2.14	0.06
1:B:230:GLY:O	1:C:141:ASP:OD1[3_555]	2.14	0.06
1:B:224:LEU:CA	1:C:242:LEU:N[3_555]	2.14	0.06
1:B:239:THR:CB	1:C:150:LEU:CB[3_555]	2.14	0.06
1:C:59:MET:O	1:C:62:SER:OG[2_555]	2.15	0.05
1:B:229:GLU:N	1:C:223:ARG:CD[3_555]	2.15	0.05
1:B:170:PHE:N	1:C:180:SER:C[3_555]	2.15	0.05
1:C:73:GLU:OE1	1:C:254:ILE:CB[2_555]	2.15	0.05
1:B:192:VAL:CG2	1:C:53:VAL:C[3_555]	2.15	0.05
1:B:236:ALA:C	1:C:145:VAL:CG1[3_555]	2.15	0.05
1:B:242:LEU:CB	1:C:131:ILE:O[3_555]	2.15	0.05
1:B:72:CYS:N	1:C:163:GLU:OE2[3_555]	2.15	0.05
1:B:115:ILE:N	1:C:165:GLN:CA[3_555]	2.15	0.05
1:B:119:TYR:N	1:C:158:THR:N[3_555]	2.15	0.05
1:B:246:TYR:OH	1:C:125:THR:CG2[3_555]	2.15	0.05
1:C:99:TRP:CZ3	1:C:107:TRP:CZ2[2_555]	2.15	0.05
1:B:112:TRP:CB	1:C:51:THR:CA[3_555]	2.15	0.05
1:B:157:VAL:CG2	1:C:117:TYR:N[3_555]	2.15	0.05
1:B:157:VAL:CG2	1:C:185:ILE:C[3_555]	2.15	0.05
1:B:96:VAL:O	1:C:161:VAL:C[3_555]	2.15	0.05
1:B:137:TYR:CD2	1:C:243:TYR:CE2[3_555]	2.15	0.05
1:B:149:GLN:O	1:C:92:MET:O[3_555]	2.15	0.05
1:B:247:THR:C	1:C:165:GLN:NE2[3_555]	2.15	0.05
1:B:181:ARG:NH1	3:A:272:HOH:O[3_555]	2.15	0.05
1:B:96:VAL:CG2	1:C:240:GLY:CA[3_555]	2.15	0.05
1:B:185:ILE:N	1:C:184:THR:N[3_555]	2.15	0.05
1:B:240:GLY:C	1:C:132:HIS:ND1[3_555]	2.15	0.05
1:B:237:VAL:CA	1:C:145:VAL:CG2[3_555]	2.15	0.05
1:B:75:SER:N	1:C:130:ALA:C[3_555]	2.15	0.05
1:B:191:GLU:OE1	1:C:55:LEU:CA[3_555]	2.15	0.05
1:B:79:ALA:CB	1:C:145:VAL:C[3_555]	2.15	0.05
1:C:59:MET:C	1:C:62:SER:CA[2_555]	2.15	0.05
1:B:162:TRP:CA	1:C:152:ASN:N[3_555]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:TYR:CD2	1:C:119:TYR:C[3_555]	2.15	0.05
1:B:112:TRP:CD2	1:C:121:PRO:O[3_555]	2.15	0.05
1:B:112:TRP:CA	1:C:51:THR:OG1[3_555]	2.15	0.05
1:B:152:ASN:CA	1:C:96:VAL:CB[3_555]	2.15	0.05
1:B:90:LEU:CD1	1:C:77:GLU:CG[3_555]	2.16	0.04
1:B:136:GLN:C	1:C:74:LEU:C[3_555]	2.16	0.04
1:B:240:GLY:N	1:C:147:VAL:O[3_555]	2.16	0.04
1:B:80:VAL:CG2	1:C:144:PRO:CG[3_555]	2.16	0.04
1:C:72:CYS:O	1:C:252:GLU:CA[2_555]	2.16	0.04
1:C:97:GLY:O	1:C:254:ILE:CB[2_555]	2.16	0.04
1:B:154:LYS:O	1:C:244:ALA:O[3_555]	2.16	0.04
1:A:255:ALA:N	1:B:127:THR:N[2_555]	2.16	0.04
1:B:224:LEU:N	1:C:242:LEU:N[3_555]	2.16	0.04
1:B:152:ASN:ND2	1:C:92:MET:C[3_555]	2.16	0.04
1:B:192:VAL:CG2	1:C:53:VAL:O[3_555]	2.16	0.04
1:B:157:VAL:N	1:C:117:TYR:CD1[3_555]	2.16	0.04
1:B:96:VAL:O	1:C:239:THR:CG2[3_555]	2.16	0.04
1:B:75:SER:CA	1:C:161:VAL:CG2[3_555]	2.16	0.04
1:C:72:CYS:O	1:C:252:GLU:CG[2_555]	2.16	0.04
1:C:94:PHE:CE1	1:C:257:ALA:CB[2_555]	2.16	0.04
1:C:101:ARG:NH2	1:C:258:LEU:CD2[2_555]	2.16	0.04
1:B:227:ALA:CB	1:C:88:SER:C[3_555]	2.16	0.04
1:B:224:LEU:CG	1:C:242:LEU:CG[3_555]	2.16	0.04
1:B:74:LEU:CD2	1:C:130:ALA:N[3_555]	2.16	0.04
1:B:81:THR:CA	1:C:142:THR:C[3_555]	2.16	0.04
1:B:223:ARG:O	1:C:74:LEU:CD1[3_555]	2.16	0.04
1:B:243:TYR:C	1:C:159:GLY:CA[3_555]	2.16	0.04
1:B:103:VAL:CG2	1:C:47:ILE:CD1[3_555]	2.17	0.03
1:C:99:TRP:CD1	1:C:107:TRP:C[2_555]	2.17	0.03
1:B:111:ALA:O	1:C:50:GLY:C[3_555]	2.17	0.03
1:B:229:GLU:CB	1:C:223:ARG:NH1[3_555]	2.17	0.03
1:B:250:LEU:CD2	1:C:48:ALA:CB[3_555]	2.17	0.03
1:B:191:GLU:CB	1:C:55:LEU:CD2[3_555]	2.17	0.03
1:B:244:ALA:C	1:C:163:GLU:C[3_555]	2.17	0.03
1:C:57:PRO:C	1:C:66:VAL:CA[2_555]	2.17	0.03
1:B:69:LEU:CB	1:C:48:ALA:O[3_555]	2.17	0.03
1:B:228:MET:N	1:C:88:SER:CA[3_555]	2.17	0.03
1:B:148:ASN:C	1:C:92:MET:C[3_555]	2.17	0.03
1:B:96:VAL:N	1:C:239:THR:CB[3_555]	2.17	0.03
1:B:74:LEU:N	1:C:160:PRO:CB[3_555]	2.17	0.03
1:B:99:TRP:C	1:C:126:THR:C[3_555]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASN:ND2	1:C:145:VAL:C[3_555]	2.17	0.03
1:C:55:LEU:CD2	1:C:252:GLU:OE2[2_555]	2.17	0.03
1:B:76:THR:OG1	1:C:228:MET:C[3_555]	2.17	0.03
1:B:73:GLU:C	1:C:160:PRO:CG[3_555]	2.17	0.03
1:B:114:ALA:CA	1:C:165:GLN:O[3_555]	2.17	0.03
1:B:96:VAL:O	1:C:161:VAL:CG1[3_555]	2.17	0.03
1:B:130:ALA:C	1:C:135:PHE:C[3_555]	2.17	0.03
1:B:115:ILE:C	1:C:164:GLY:C[3_555]	2.17	0.03
1:B:185:ILE:N	1:C:184:THR:C[3_555]	2.17	0.03
1:B:239:THR:CG2	1:C:144:PRO:CB[3_555]	2.17	0.03
1:B:92:MET:C	1:C:239:THR:O[3_555]	2.17	0.03
1:B:186:ALA:N	1:C:118:THR:CA[3_555]	2.17	0.03
1:B:77:GLU:C	1:C:227:ALA:CB[3_555]	2.17	0.03
1:C:99:TRP:NE1	1:C:107:TRP:CB[2_555]	2.18	0.02
1:B:130:ALA:CA	1:C:136:GLN:CA[3_555]	2.18	0.02
1:B:117:TYR:N	1:C:183:ILE:CB[3_555]	2.18	0.02
1:B:245:SER:N	1:C:163:GLU:CA[3_555]	2.18	0.02
1:B:90:LEU:O	1:C:240:GLY:CA[3_555]	2.18	0.02
1:B:116:ARG:NE	1:C:182:ALA:CA[3_555]	2.18	0.02
1:B:189:THR:C	1:C:53:VAL:C[3_555]	2.18	0.02
1:B:79:ALA:CA	1:C:144:PRO:O[3_555]	2.18	0.02
1:B:185:ILE:N	1:C:184:THR:OG1[3_555]	2.18	0.02
1:B:154:LYS:CG	1:C:72:CYS:C[3_555]	2.18	0.02
1:B:184:THR:C	1:C:184:THR:O[3_555]	2.18	0.02
1:B:239:THR:O	1:C:150:LEU:C[3_555]	2.18	0.02
1:B:237:VAL:CG1	1:C:149:GLN:CB[3_555]	2.18	0.02
1:B:96:VAL:CG2	1:C:240:GLY:N[3_555]	2.18	0.02
1:B:80:VAL:N	1:C:144:PRO:CD[3_555]	2.18	0.02
1:B:228:MET:CG	1:C:225:VAL:CA[3_555]	2.18	0.02
1:B:153:LEU:CD1	1:C:96:VAL:CA[3_555]	2.18	0.02
1:B:152:ASN:CG	1:C:93:PRO:O[3_555]	2.18	0.02
1:B:137:TYR:CZ	1:C:73:GLU:C[3_555]	2.18	0.02
1:B:135:PHE:C	1:C:74:LEU:O[3_555]	2.18	0.02
1:B:184:THR:CA	1:C:185:ILE:N[3_555]	2.18	0.02
1:B:93:PRO:CD	1:C:122:SER:OG[3_555]	2.18	0.02
1:B:96:VAL:N	1:C:123:CYS:SG[3_555]	2.18	0.02
1:B:89:GLU:O	1:C:77:GLU:CA[3_555]	2.18	0.02
1:B:154:LYS:C	1:C:244:ALA:N[3_555]	2.18	0.02
1:B:71:HIS:N	1:C:49:GLN:OE1[3_555]	2.18	0.02
1:B:161:VAL:CG2	1:C:153:LEU:CG[3_555]	2.18	0.02
1:B:147:VAL:O	1:C:91:VAL:C[3_555]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:CD1	1:C:117:TYR:C[3_555]	2.18	0.02
1:B:224:LEU:CG	1:C:242:LEU:CB[3_555]	2.18	0.02
1:B:146:SER:O	1:C:95:THR:CG2[3_555]	2.18	0.02
1:B:247:THR:CG2	1:C:165:GLN:NE2[3_555]	2.18	0.02
1:B:79:ALA:O	1:C:144:PRO:O[3_555]	2.19	0.01
1:B:246:TYR:N	1:C:49:GLN:OE1[3_555]	2.19	0.01
1:B:136:GLN:C	1:C:74:LEU:O[3_555]	2.19	0.01
1:B:137:TYR:CZ	1:C:243:TYR:CD2[3_555]	2.19	0.01
1:B:115:ILE:CB	1:C:121:PRO:CD[3_555]	2.19	0.01
1:B:188:ASP:OD1	1:C:55:LEU:CG[3_555]	2.19	0.01
1:B:190:ASN:CB	1:C:172:ASN:ND2[3_555]	2.19	0.01
1:B:246:TYR:N	1:C:164:GLY:N[3_555]	2.19	0.01
1:C:103:VAL:CB	1:C:106:ASN:CB[2_555]	2.19	0.01
1:B:118:THR:OG1	1:C:183:ILE:N[3_555]	2.19	0.01
1:B:80:VAL:O	1:C:144:PRO:CA[3_555]	2.19	0.01
1:B:237:VAL:N	1:C:149:GLN:NE2[3_555]	2.19	0.01
1:B:135:PHE:CB	1:C:242:LEU:O[3_555]	2.19	0.01
1:B:132:HIS:N	1:C:224:LEU:CG[3_555]	2.19	0.01
1:B:170:PHE:CD2	1:C:180:SER:CA[3_555]	2.19	0.01
1:B:71:HIS:O	1:C:163:GLU:OE2[3_555]	2.19	0.01
1:B:116:ARG:CG	1:C:182:ALA:CA[3_555]	2.19	0.01
1:A:254:ILE:CB	1:B:127:THR:O[2_555]	2.19	0.01
1:C:98:THR:N	1:C:254:ILE:CA[2_555]	2.19	0.01
1:B:161:VAL:C	1:C:153:LEU:CB[3_555]	2.19	0.01
1:B:248:ILE:CG1	1:C:49:GLN:C[3_555]	2.19	0.01
1:B:191:GLU:OE1	1:C:56:ARG:CA[3_555]	2.19	0.01
1:B:243:TYR:CG	1:C:158:THR:C[3_555]	2.19	0.01
1:B:162:TRP:CA	1:C:152:ASN:CB[3_555]	2.19	0.01
1:B:121:PRO:CA	1:C:156:TYR:CD1[3_555]	2.19	0.01
1:C:58:PRO:N	1:C:250:LEU:C[2_555]	2.19	0.01
1:B:224:LEU:CG	1:C:242:LEU:CD1[3_555]	2.19	0.01
1:B:248:ILE:CG2	1:C:48:ALA:CA[3_555]	2.19	0.01
1:B:93:PRO:C	1:C:122:SER:C[3_555]	2.19	0.01
1:C:101:ARG:NE	1:C:255:ALA:O[2_555]	2.19	0.01
1:B:117:TYR:CE2	1:C:119:TYR:CB[3_555]	2.19	0.01
1:B:151:SER:CB	1:C:91:VAL:CG1[3_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/260 (76%)	160 (81%)	27 (14%)	10 (5%)	2	8
1	B	197/260 (76%)	163 (83%)	29 (15%)	5 (2%)	7	24
1	C	220/260 (85%)	182 (83%)	29 (13%)	9 (4%)	3	11
All	All	614/780 (79%)	505 (82%)	85 (14%)	24 (4%)	4	12

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	B	231	GLY
1	C	219	LEU
1	C	230	GLY
1	C	231	GLY
1	A	161	VAL
1	A	166	SER
1	A	169	CYS
1	B	210	GLY
1	C	177	PRO
1	A	139	MET
1	A	202	ALA
1	B	173	ASN
1	A	94	PHE
1	A	182	ALA
1	B	213	ALA
1	B	256	ALA
1	C	125	THR
1	C	205	TYR
1	C	257	ALA
1	C	173	ASN
1	C	251	ILE
1	A	177	PRO
1	A	230	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/217 (77%)	121 (72%)	46 (28%)	0	1
1	B	167/217 (77%)	116 (70%)	51 (30%)	0	1
1	C	185/217 (85%)	128 (69%)	57 (31%)	0	1
All	All	519/651 (80%)	365 (70%)	154 (30%)	0	1

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	MET
1	A	65	ASP
1	A	77	GLU
1	A	78	LEU
1	A	80	VAL
1	A	87	THR
1	A	91	VAL
1	A	92	MET
1	A	95	THR
1	A	100	LEU
1	A	101	ARG
1	A	108	SER
1	A	109	LYS
1	A	116	ARG
1	A	118	THR
1	A	119	TYR
1	A	123	CYS
1	A	133	MET
1	A	139	MET
1	A	145	VAL
1	A	146	SER
1	A	148	ASN
1	A	152	ASN
1	A	154	LYS
1	A	158	THR
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	172	ASN
1	A	173	ASN
1	A	176	CYS
1	A	181	ARG
1	A	183	ILE
1	A	184	THR
1	A	191	GLU
1	A	196	ARG
1	A	198	PRO
1	A	199	PHE
1	A	200	LYS
1	A	214	ASN
1	A	218	ILE
1	A	223	ARG
1	A	225	VAL
1	A	226	THR
1	A	234	LYS
1	A	245	SER
1	A	251	ILE
1	B	62	SER
1	B	72	CYS
1	B	74	LEU
1	B	78	LEU
1	B	82	VAL
1	B	85	VAL
1	B	87	THR
1	B	88	SER
1	B	90	LEU
1	B	95	THR
1	B	100	LEU
1	B	105	GLN
1	B	106	ASN
1	B	108	SER
1	B	109	LYS
1	B	115	ILE
1	B	116	ARG
1	B	118	THR
1	B	138	ASP
1	B	139	MET
1	B	147	VAL
1	B	150	LEU

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Mol	Chain	Res	Type
1	B	152	ASN
1	B	153	LEU
1	B	154	LYS
1	B	158	THR
1	B	161	VAL
1	B	165	GLN
1	B	171	VAL
1	B	172	ASN
1	B	173	ASN
1	B	175	LYS
1	B	176	CYS
1	B	180	SER
1	B	189	THR
1	B	190	ASN
1	B	196	ARG
1	B	199	PHE
1	B	200	LYS
1	B	203	THR
1	B	209	VAL
1	B	218	ILE
1	B	223	ARG
1	B	226	THR
1	B	234	LYS
1	B	235	THR
1	B	242	LEU
1	B	248	ILE
1	B	250	LEU
1	B	251	ILE
1	B	252	GLU
1	C	47	ILE
1	C	52	MET
1	C	54	LYS
1	C	60	LEU
1	C	61	ARG
1	C	65	ASP
1	C	66	VAL
1	C	67	THR
1	C	70	SER
1	C	72	CYS
1	C	74	LEU
1	C	78	LEU
1	C	80	VAL

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Mol	Chain	Res	Type
1	C	82	VAL
1	C	83	THR
1	C	84	ILE
1	C	87	THR
1	C	88	SER
1	C	92	MET
1	C	98	THR
1	C	115	ILE
1	C	118	THR
1	C	121	PRO
1	C	122	SER
1	C	125	THR
1	C	127	THR
1	C	128	SER
1	C	145	VAL
1	C	146	SER
1	C	149	GLN
1	C	150	LEU
1	C	152	ASN
1	C	153	LEU
1	C	161	VAL
1	C	165	GLN
1	C	172	ASN
1	C	173	ASN
1	C	174	THR
1	C	178	ASP
1	C	181	ARG
1	C	184	THR
1	C	187	LEU
1	C	189	THR
1	C	191	GLU
1	C	193	SER
1	C	195	LYS
1	C	196	ARG
1	C	200	LYS
1	C	203	THR
1	C	214	ASN
1	C	228	MET
1	C	234	LYS
1	C	235	THR
1	C	242	LEU
1	C	245	SER

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Mol	Chain	Res	Type
1	C	249	ARG
1	C	251	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	136	GLN
1	A	148	ASN
1	A	165	GLN
1	A	172	ASN
1	A	173	ASN
1	A	190	ASN
1	A	214	ASN
1	A	238	ASN
1	B	106	ASN
1	B	136	GLN
1	B	152	ASN
1	B	165	GLN
1	B	172	ASN
1	B	173	ASN
1	B	190	ASN
1	B	212	ASN
1	B	214	ASN
1	B	217	ASN
1	B	238	ASN
1	C	49	GLN
1	C	149	GLN
1	C	172	ASN
1	C	173	ASN
1	C	212	ASN
1	C	217	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	199/260 (76%)	2.57	142 (71%)	0	0	12, 22, 60, 83	0
1	B	199/260 (76%)	3.14	172 (86%)	0	0	10, 21, 50, 65	0
1	C	222/260 (85%)	2.93	177 (79%)	0	0	8, 21, 37, 60	0
All	All	620/780 (79%)	2.88	491 (79%)	0	0	8, 21, 46, 83	0

All (491) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ALA	7.5
1	B	240	GLY	7.3
1	C	70	SER	6.7
1	A	193	SER	6.7
1	C	65	ASP	6.6
1	B	193	SER	6.6
1	B	217	ASN	6.3
1	B	176	CYS	6.2
1	C	105	GLN	6.2
1	B	244	ALA	6.0
1	C	104	ALA	5.9
1	B	216	GLY	5.9
1	B	104	ALA	5.6
1	C	158	THR	5.5
1	C	100	LEU	5.5
1	B	221	PRO	5.4
1	B	111	ALA	5.4
1	C	222	ALA	5.4
1	A	91	VAL	5.4
1	B	230	GLY	5.3
1	B	150	LEU	5.3
1	C	81	THR	5.2
1	C	194	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	80	VAL	5.2
1	C	218	ILE	5.1
1	B	151	SER	5.0
1	B	110	TYR	5.0
1	B	107	TRP	4.9
1	C	94	PHE	4.9
1	C	125	THR	4.9
1	B	124	PRO	4.9
1	C	108	SER	4.9
1	B	90	LEU	4.8
1	C	69	LEU	4.8
1	B	197	TYR	4.8
1	C	187	LEU	4.8
1	B	119	TYR	4.7
1	C	137	TYR	4.7
1	A	136	GLN	4.7
1	B	83	THR	4.6
1	B	206	ALA	4.6
1	C	112	TRP	4.6
1	A	107	TRP	4.6
1	C	89	GLU	4.5
1	A	217	ASN	4.5
1	B	259	ASN	4.5
1	C	240	GLY	4.5
1	A	90	LEU	4.5
1	C	169	CYS	4.5
1	C	170	PHE	4.5
1	C	150	LEU	4.5
1	A	65	ASP	4.4
1	A	92	MET	4.4
1	A	100	LEU	4.4
1	B	213	ALA	4.4
1	A	191	GLU	4.4
1	B	239	THR	4.4
1	C	68	ILE	4.4
1	A	64	MET	4.3
1	C	233	SER	4.3
1	C	197	TYR	4.3
1	C	215	ILE	4.3
1	A	198	PRO	4.3
1	A	222	ALA	4.3
1	B	134	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	220	VAL	4.3
1	C	168	LEU	4.3
1	C	243	TYR	4.3
1	B	226	THR	4.3
1	B	67	THR	4.3
1	C	220	VAL	4.2
1	C	185	ILE	4.2
1	C	226	THR	4.2
1	B	78	LEU	4.2
1	B	243	TYR	4.2
1	C	189	THR	4.2
1	C	139	MET	4.2
1	C	86	VAL	4.1
1	B	97	GLY	4.1
1	B	146	SER	4.1
1	B	92	MET	4.1
1	B	122	SER	4.1
1	C	117	TYR	4.1
1	A	62	SER	4.1
1	B	96	VAL	4.0
1	B	125	THR	4.0
1	B	91	VAL	4.0
1	C	246	TYR	4.0
1	B	209	VAL	4.0
1	C	60	LEU	4.0
1	C	109	LYS	4.0
1	A	260	LEU	4.0
1	B	171	VAL	4.0
1	B	152	ASN	4.0
1	B	139	MET	4.0
1	C	141	ASP	4.0
1	A	224	LEU	3.9
1	B	233	SER	3.9
1	B	183	ILE	3.9
1	B	180	SER	3.9
1	B	85	VAL	3.9
1	C	91	VAL	3.9
1	C	241	ARG	3.9
1	C	183	ILE	3.9
1	A	137	TYR	3.9
1	B	218	ILE	3.8
1	B	142	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	194	GLU	3.8
1	C	84	ILE	3.8
1	A	253	PRO	3.8
1	B	86	VAL	3.8
1	C	221	PRO	3.8
1	C	253	PRO	3.8
1	C	119	TYR	3.8
1	A	197	TYR	3.8
1	A	187	LEU	3.8
1	B	235	THR	3.8
1	C	88	SER	3.8
1	C	216	GLY	3.8
1	C	93	PRO	3.7
1	B	205	TYR	3.7
1	B	88	SER	3.7
1	A	104	ALA	3.7
1	C	132	HIS	3.7
1	C	219	LEU	3.7
1	B	167	GLY	3.7
1	A	245	SER	3.7
1	C	151	SER	3.7
1	C	166	SER	3.7
1	C	133	MET	3.7
1	C	228	MET	3.7
1	B	161	VAL	3.7
1	B	75	SER	3.7
1	B	187	LEU	3.7
1	C	260	LEU	3.6
1	A	103	VAL	3.6
1	B	157	VAL	3.6
1	B	153	LEU	3.6
1	A	179	THR	3.6
1	C	205	TYR	3.6
1	B	172	ASN	3.6
1	C	161	VAL	3.6
1	B	156	TYR	3.6
1	C	92	MET	3.6
1	A	153	LEU	3.6
1	C	156	TYR	3.6
1	A	192	VAL	3.6
1	A	80	VAL	3.6
1	A	108	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	120	LEU	3.6
1	B	250	LEU	3.6
1	B	132	HIS	3.6
1	B	82	VAL	3.5
1	B	137	TYR	3.5
1	B	148	ASN	3.5
1	C	71	HIS	3.5
1	A	213	ALA	3.5
1	C	148	ASN	3.5
1	B	70	SER	3.5
1	B	145	VAL	3.5
1	C	198	PRO	3.5
1	C	242	LEU	3.5
1	A	199	PHE	3.5
1	A	218	ILE	3.5
1	C	131	ILE	3.5
1	C	236	ALA	3.5
1	A	183	ILE	3.5
1	C	193	SER	3.5
1	A	208	ALA	3.5
1	A	239	THR	3.5
1	B	242	LEU	3.5
1	B	112	TRP	3.5
1	B	121	PRO	3.4
1	A	251	ILE	3.4
1	A	195	LYS	3.4
1	C	195	LYS	3.4
1	B	246	TYR	3.4
1	A	76	THR	3.4
1	C	51	THR	3.4
1	C	171	VAL	3.4
1	B	84	ILE	3.4
1	B	168	LEU	3.4
1	B	118	THR	3.4
1	C	140	ALA	3.4
1	B	223	ARG	3.4
1	C	217	ASN	3.4
1	C	98	THR	3.4
1	B	245	SER	3.3
1	B	79	ALA	3.3
1	B	174	THR	3.3
1	B	74	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	256	ALA	3.3
1	A	252	GLU	3.3
1	C	192	VAL	3.3
1	B	144	PRO	3.3
1	A	214	ASN	3.3
1	B	147	VAL	3.3
1	A	81	THR	3.3
1	A	201	THR	3.3
1	B	138	ASP	3.3
1	C	77	GLU	3.3
1	C	115	ILE	3.3
1	B	160	PRO	3.3
1	C	136	GLN	3.3
1	A	112	TRP	3.3
1	C	172	ASN	3.3
1	C	196	ARG	3.3
1	B	179	THR	3.3
1	A	150	LEU	3.3
1	B	143	LEU	3.3
1	C	114	ALA	3.2
1	C	74	LEU	3.2
1	C	152	ASN	3.2
1	B	120	LEU	3.2
1	B	192	VAL	3.2
1	A	118	THR	3.2
1	B	72	CYS	3.2
1	B	113	VAL	3.2
1	C	53	VAL	3.2
1	B	182	ALA	3.2
1	A	141	ASP	3.2
1	A	88	SER	3.2
1	C	110	TYR	3.2
1	C	199	PHE	3.2
1	A	148	ASN	3.2
1	B	129	GLY	3.2
1	B	123	CYS	3.2
1	C	123	CYS	3.2
1	A	174	THR	3.2
1	C	116	ARG	3.1
1	A	115	ILE	3.1
1	A	159	GLY	3.1
1	A	130	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	ALA	3.1
1	A	110	TYR	3.1
1	B	184	THR	3.1
1	C	67	THR	3.1
1	A	216	GLY	3.1
1	C	155	GLY	3.1
1	C	190	ASN	3.1
1	C	90	LEU	3.1
1	A	188	ASP	3.1
1	C	50	GLY	3.1
1	A	87	THR	3.1
1	C	247	THR	3.1
1	A	186	ALA	3.1
1	B	255	ALA	3.1
1	C	259	ASN	3.1
1	B	141	ASP	3.1
1	B	208	ALA	3.0
1	C	232	SER	3.0
1	A	259	ASN	3.0
1	C	61	ARG	3.0
1	C	237	VAL	3.0
1	A	133	MET	3.0
1	A	63	SER	3.0
1	A	111	ALA	3.0
1	B	186	ALA	3.0
1	B	254	ILE	3.0
1	A	143	LEU	3.0
1	B	189	THR	3.0
1	C	138	ASP	3.0
1	B	241	ARG	3.0
1	A	240	GLY	3.0
1	B	224	LEU	3.0
1	B	253	PRO	3.0
1	A	212	ASN	3.0
1	A	244	ALA	3.0
1	C	188	ASP	3.0
1	A	168	LEU	3.0
1	A	93	PRO	3.0
1	A	248	ILE	3.0
1	A	98	THR	3.0
1	C	107	TRP	3.0
1	A	117	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	66	VAL	2.9
1	B	199	PHE	2.9
1	A	205	TYR	2.9
1	B	94	PHE	2.9
1	C	179	THR	2.9
1	B	251	ILE	2.9
1	B	117	TYR	2.9
1	B	87	THR	2.9
1	A	132	HIS	2.9
1	C	245	SER	2.9
1	A	135	PHE	2.9
1	B	66	VAL	2.9
1	A	196	ARG	2.9
1	C	248	ILE	2.9
1	A	219	LEU	2.9
1	B	133	MET	2.9
1	A	226	THR	2.9
1	A	225	VAL	2.9
1	B	71	HIS	2.9
1	C	85	VAL	2.8
1	A	160	PRO	2.8
1	B	99	TRP	2.8
1	C	97	GLY	2.8
1	A	173	ASN	2.8
1	B	115	ILE	2.8
1	A	146	SER	2.8
1	B	108	SER	2.8
1	C	176	CYS	2.8
1	A	221	PRO	2.8
1	A	223	ARG	2.8
1	A	235	THR	2.8
1	B	166	SER	2.8
1	C	214	ASN	2.8
1	B	204	ASP	2.8
1	C	106	ASN	2.8
1	C	178	ASP	2.8
1	A	140	ALA	2.8
1	A	182	ALA	2.8
1	A	171	VAL	2.8
1	C	111	ALA	2.8
1	B	219	LEU	2.7
1	C	78	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	149	GLN	2.7
1	B	231	GLY	2.7
1	A	200	LYS	2.7
1	C	87	THR	2.7
1	C	103	VAL	2.7
1	A	122	SER	2.7
1	B	109	LYS	2.7
1	B	106	ASN	2.7
1	A	246	TYR	2.7
1	A	203	THR	2.7
1	B	169	CYS	2.7
1	C	83	THR	2.7
1	C	235	THR	2.7
1	B	89	GLU	2.7
1	B	159	GLY	2.7
1	B	201	THR	2.7
1	C	174	THR	2.7
1	A	89	GLU	2.7
1	C	181	ARG	2.7
1	C	227	ALA	2.7
1	A	243	TYR	2.7
1	A	185	ILE	2.7
1	B	178	ASP	2.7
1	C	147	VAL	2.7
1	A	69	LEU	2.7
1	A	75	SER	2.7
1	A	233	SER	2.7
1	A	194	GLU	2.7
1	C	102	GLY	2.7
1	C	157	VAL	2.6
1	A	152	ASN	2.6
1	C	64	MET	2.6
1	B	130	ALA	2.6
1	B	227	ALA	2.6
1	C	204	ASP	2.6
1	C	75	SER	2.6
1	C	209	VAL	2.6
1	B	100	LEU	2.6
1	B	249	ARG	2.6
1	A	97	GLY	2.6
1	A	156	TYR	2.6
1	C	213	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	118	THR	2.6
1	C	142	THR	2.6
1	C	223	ARG	2.6
1	A	142	THR	2.6
1	C	224	LEU	2.6
1	B	164	GLY	2.6
1	B	105	GLN	2.6
1	C	164	GLY	2.6
1	B	214	ASN	2.6
1	C	186	ALA	2.6
1	A	119	TYR	2.6
1	A	161	VAL	2.6
1	A	138	ASP	2.5
1	A	139	MET	2.5
1	C	200	LYS	2.5
1	B	136	GLN	2.5
1	A	131	ILE	2.5
1	C	122	SER	2.5
1	A	123	CYS	2.5
1	B	170	PHE	2.5
1	C	159	GLY	2.5
1	A	178	ASP	2.5
1	A	184	THR	2.5
1	C	52	MET	2.5
1	B	128	SER	2.5
1	B	102	GLY	2.5
1	B	64	MET	2.5
1	C	238	ASN	2.5
1	C	257	ALA	2.5
1	A	109	LYS	2.5
1	C	95	THR	2.5
1	B	63	SER	2.4
1	A	121	PRO	2.4
1	A	189	THR	2.4
1	C	62	SER	2.4
1	B	198	PRO	2.4
1	A	154	LYS	2.4
1	B	185	ILE	2.4
1	C	48	ALA	2.4
1	C	76	THR	2.4
1	C	191	GLU	2.4
1	B	260	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	154	LYS	2.4
1	C	258	LEU	2.4
1	C	244	ALA	2.4
1	C	134	GLY	2.4
1	B	65	ASP	2.4
1	A	106	ASN	2.4
1	B	173	ASN	2.4
1	B	188	ASP	2.4
1	C	96	VAL	2.4
1	A	67	THR	2.4
1	B	228	MET	2.4
1	B	234	LYS	2.4
1	C	121	PRO	2.4
1	A	113	VAL	2.4
1	B	252	GLU	2.4
1	A	180	SER	2.4
1	B	81	THR	2.4
1	C	207	THR	2.4
1	A	250	LEU	2.3
1	C	153	LEU	2.3
1	A	105	GLN	2.3
1	B	149	GLN	2.3
1	C	130	ALA	2.3
1	A	99	TRP	2.3
1	C	250	LEU	2.3
1	B	163	GLU	2.3
1	A	232	SER	2.3
1	B	195	LYS	2.3
1	B	127	THR	2.3
1	C	45	ALA	2.3
1	B	131	ILE	2.3
1	A	144	PRO	2.3
1	A	78	LEU	2.3
1	B	238	ASN	2.3
1	C	167	GLY	2.3
1	A	207	THR	2.3
1	A	215	ILE	2.3
1	B	135	PHE	2.3
1	A	157	VAL	2.3
1	C	230	GLY	2.3
1	B	95	THR	2.3
1	B	158	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	144	PRO	2.3
1	A	190	ASN	2.3
1	A	227	ALA	2.2
1	B	114	ALA	2.2
1	B	232	SER	2.2
1	B	248	ILE	2.2
1	A	162	TRP	2.2
1	A	134	GLY	2.2
1	A	72	CYS	2.2
1	C	229	GLU	2.2
1	B	68	ILE	2.2
1	C	251	ILE	2.2
1	B	62	SER	2.2
1	C	113	VAL	2.2
1	C	231	GLY	2.2
1	B	196	ARG	2.2
1	A	155	GLY	2.2
1	A	74	LEU	2.2
1	B	207	THR	2.2
1	B	177	PRO	2.1
1	C	254	ILE	2.1
1	C	225	VAL	2.1
1	B	77	GLU	2.1
1	B	229	GLU	2.1
1	A	209	VAL	2.1
1	B	76	THR	2.1
1	C	255	ALA	2.1
1	A	84	ILE	2.1
1	C	180	SER	2.1
1	A	82	VAL	2.1
1	C	162	TRP	2.1
1	A	86	VAL	2.1
1	A	114	ALA	2.1
1	C	126	THR	2.1
1	C	39	GLN	2.1
1	B	200	LYS	2.1
1	B	103	VAL	2.0
1	A	255	ALA	2.0
1	C	182	ALA	2.0
1	C	99	TRP	2.0
1	A	177	PRO	2.0
1	C	163	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	116	ARG	2.0
1	B	258	LEU	2.0
1	C	135	PHE	2.0
1	A	204	ASP	2.0
1	B	203	THR	2.0
1	C	184	THR	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	C	261	1/1	0.82	0.22	-3.49	20,20,20,20	0
2	CA	B	261	1/1	0.93	0.32	-3.77	16,16,16,16	0
2	CA	A	261	1/1	0.82	0.21	-4.75	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.