



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:43 am BST

PDB ID : 2XQA
Title : Pentameric ligand gated ion channel GLIC in complex with tetrabutylammonium (TBSb)
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on : 2010-09-01
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

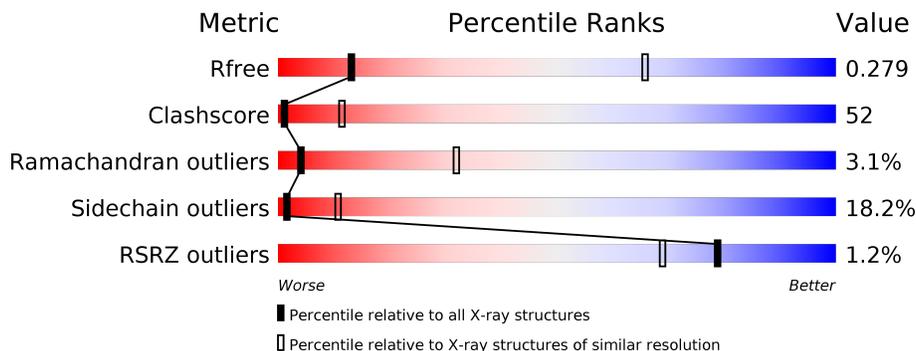
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	317	 2% 32% 53% 12%
1	B	317	 31% 55% 12%
1	C	317	 2% 33% 52% 12%
1	D	317	 % 32% 53% 12%
1	E	317	 2% 33% 53% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12606 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 GLR4197 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2521	1662	403	452	4	0	0	0
1	B	310	2521	1662	403	452	4	0	0	0
1	C	310	2521	1662	403	452	4	0	0	0
1	D	310	2521	1662	403	452	4	0	0	0
1	E	310	2521	1662	403	452	4	0	0	0

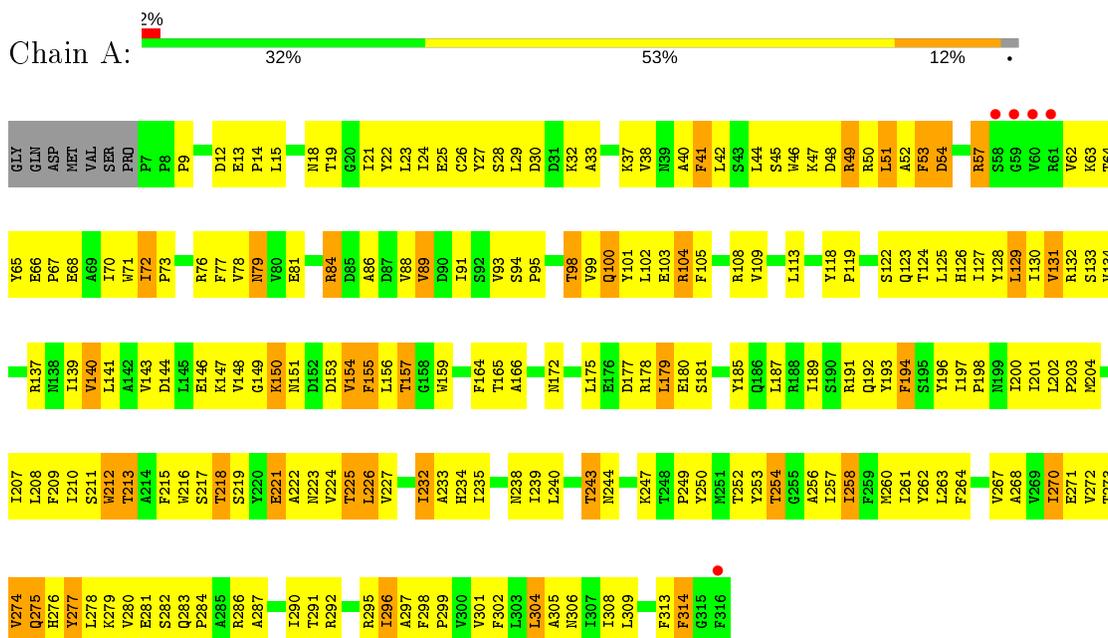
- Molecule 2 is ANTIMONY (III) ION (three-letter code: SB) (formula: Sb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Sb	0	0
			1	1		

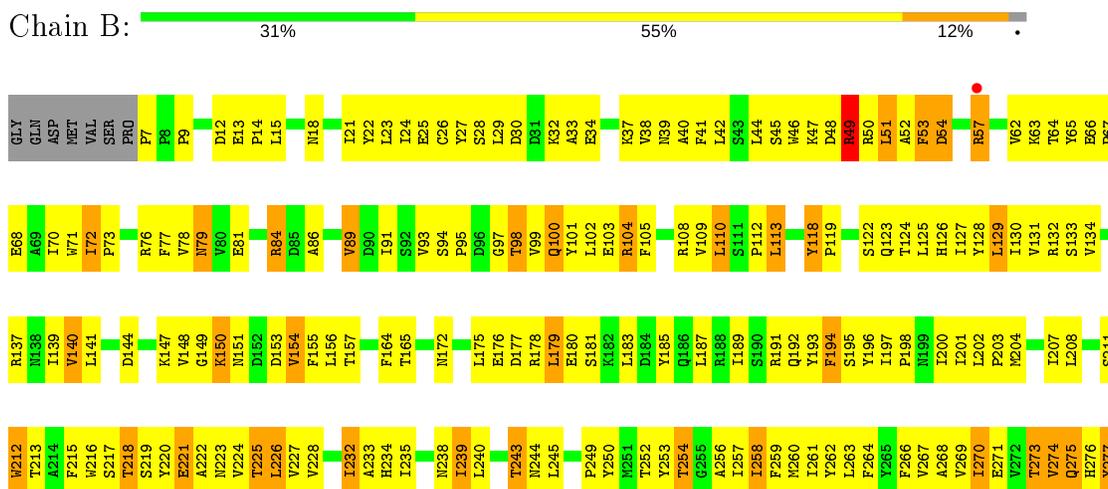
3 Residue-property plots

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

- Molecule 1: GLR4197 PROTEIN

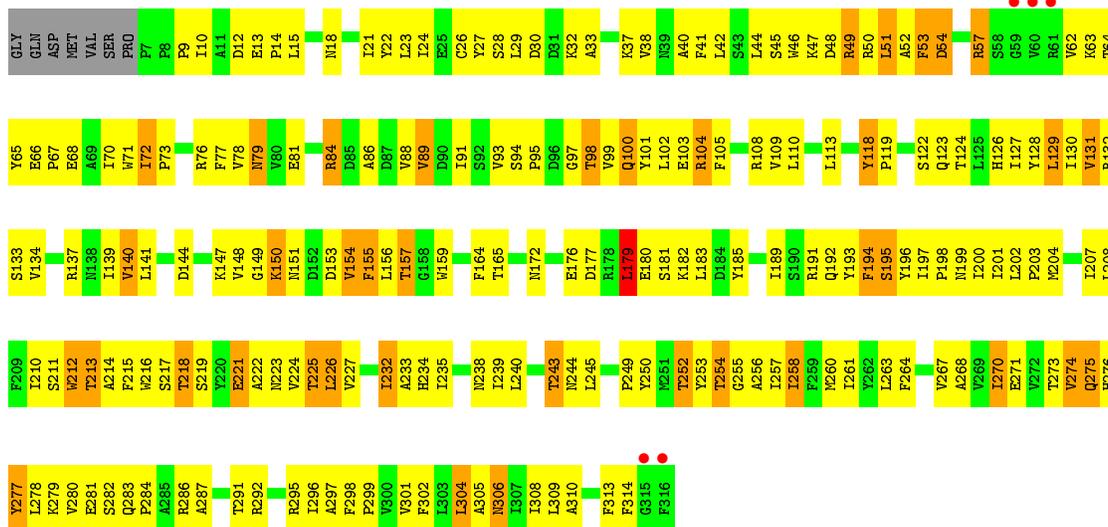


- Molecule 1: GLR4197 PROTEIN

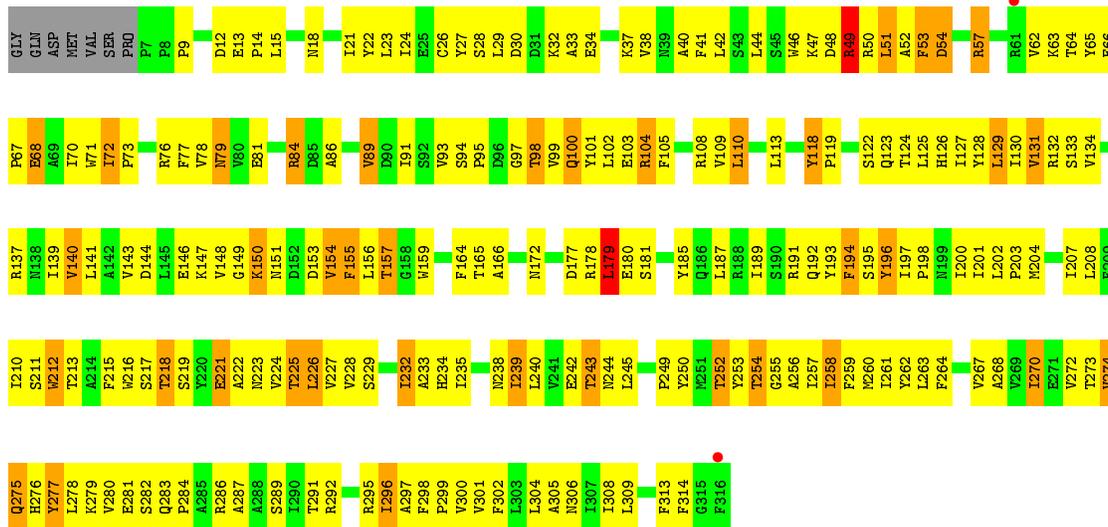




• Molecule 1: GLR4197 PROTEIN



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• Molecule 1: GLR4197 PROTEIN



Y65	S133	W212	L278
E66	V134	T213	K279
P67	R137	A214	V280
E68	M138	F215	E281
I70	I139	W216	S282
W71	V140	S217	Q283
I72	L141	T218	P284
P73	A142	S219	A285
	V143	Y220	R286
R76	D144	E221	A287
F77	K147	N223	T291
V78	V146	A222	R292
M79	G149	V224	R295
V80	K150	T225	I296
E81	M151	L226	A297
	D152	V227	F298
R84	D153	V228	P299
D85	V154	I232	V300
A86	F155	A233	V301
	L156	E234	F302
V89	T157		L303
D90	F164	N238	I304
I91	T165	I239	A305
S92	M172	L240	B306
V93		T243	I307
S94	L175	N244	I308
P95	D96	L245	L309
G97	E176	P246	F313
T98	D177	K247	F314
V99	R178	T248	G315
Q100	L179	P249	F316
Y101	E180	Y250	
L102	S181	T252	
E103	Y185	Y253	
R104	I189	T254	
F105	S190	G255	
	L110	A256	
R108	R191	I257	
V109	Q192	I258	
L110	Y193	F259	
S111	F194	M260	
P112	S195	L261	
L113	I197	Y262	
	P198	L263	
Y118	W199	F264	
P119	I200	V267	
	L201	A268	
S122	L202	V269	
Q123	P203	I270	
T124	M204	E271	
L125	I207	V272	
H126	L208	T273	
H127	S211	V274	
I128		Q275	
L129		H276	
I130		Y277	
V131			
R132			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.31Å 128.31Å 164.37Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	40.20 – 3.70 40.20 – 3.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.20-3.70) 92.4 (40.20-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.57Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.256 , 0.274 0.259 , 0.279	Depositor DCC
R_{free} test set	2172 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtrriage
Anisotropy	0.399	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 100.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/2589	0.73	2/3535 (0.1%)
1	B	0.53	0/2589	0.73	2/3535 (0.1%)
1	C	0.52	0/2589	0.74	3/3535 (0.1%)
1	D	0.53	0/2589	0.73	3/3535 (0.1%)
1	E	0.53	0/2589	0.73	2/3535 (0.1%)
All	All	0.53	0/12945	0.73	12/17675 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	129	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	129	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	129	LEU	CA-CB-CG	5.53	128.01	115.30
1	D	129	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	129	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	134	VAL	CB-CA-C	5.02	120.94	111.40
1	D	134	VAL	CB-CA-C	5.02	120.93	111.40
1	E	134	VAL	CB-CA-C	5.01	120.92	111.40
1	A	134	VAL	CB-CA-C	5.01	120.92	111.40
1	C	179	LEU	CA-CB-CG	5.01	126.82	115.30
1	C	134	VAL	CB-CA-C	5.01	120.91	111.40
1	D	179	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2521	0	2537	314	0
1	B	2521	0	2537	316	0
1	C	2521	0	2537	270	0
1	D	2521	0	2537	287	0
1	E	2521	0	2537	264	0
2	E	1	0	0	0	0
All	All	12606	0	12685	1319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (1319) 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:A:155:PHE:CE1	1:B:112:PRO:HB3	1.83	1.12
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.68	1.08
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.70	1.06
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.73	1.03
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.20	1.03
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.38	1.02
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.76	1.01
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.76	1.01
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.42	0.99
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.46	0.98
1:B:257:ILE:O	1:B:261:ILE:HG12	1.63	0.97
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.46	0.97
1:D:257:ILE:O	1:D:261:ILE:HG12	1.65	0.97
1:A:257:ILE:O	1:A:261:ILE:HG12	1.63	0.96
1:D:155:PHE:CE1	1:E:112:PRO:HB3	1.99	0.96
1:E:257:ILE:O	1:E:261:ILE:HG12	1.65	0.96
1:A:104:ARG:NH2	1:B:78:VAL:HA	1.80	0.95
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.47	0.95
1:C:257:ILE:O	1:C:261:ILE:HG12	1.66	0.94
1:D:104:ARG:HH22	1:E:78:VAL:HA	1.29	0.94
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:CG2	1:E:224:VAL:HG23	1.98	0.93
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.49	0.93
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.51	0.93
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.03	0.93
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.04	0.91
1:A:226:LEU:CD2	1:B:224:VAL:HB	2.00	0.91
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.36	0.91
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.06	0.90
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.07	0.90
1:A:297:ALA:O	1:A:301:VAL:HG23	1.71	0.90
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.29	0.90
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.54	0.89
1:C:22:TYR:HA	1:C:149:GLY:CA	2.02	0.89
1:C:297:ALA:O	1:C:301:VAL:HG23	1.72	0.88
1:A:253:TYR:HD1	1:A:313:PHE:HD2	1.20	0.88
1:D:253:TYR:HA	1:D:313:PHE:HE2	1.36	0.88
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.08	0.88
1:D:253:TYR:HD1	1:D:313:PHE:HD2	1.17	0.88
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.55	0.87
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.56	0.87
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.37	0.87
1:D:304:LEU:O	1:D:308:ILE:HG12	1.74	0.87
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.36	0.87
1:C:253:TYR:HA	1:C:313:PHE:HE2	1.37	0.87
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.38	0.86
1:B:22:TYR:HA	1:B:149:GLY:CA	2.06	0.86
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.58	0.86
1:D:22:TYR:HA	1:D:149:GLY:CA	2.06	0.85
1:E:253:TYR:HA	1:E:313:PHE:HE2	1.40	0.85
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.41	0.85
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.41	0.85
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.40	0.85
1:D:139:ILE:HG12	1:D:172:ASN:HD21	1.41	0.85
1:B:79:ASN:H	1:B:79:ASN:HD22	1.24	0.84
1:A:22:TYR:HA	1:A:149:GLY:CA	2.07	0.84
1:A:221:GLU:HB3	1:B:221:GLU:HG2	1.59	0.84
1:E:253:TYR:HD1	1:E:313:PHE:HD2	1.25	0.84
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.60	0.83
1:B:253:TYR:HD1	1:B:313:PHE:HD2	1.27	0.83
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.42	0.83
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ALA:O	1:E:301:VAL:HG23	1.78	0.83
1:A:155:PHE:CZ	1:B:112:PRO:HB3	2.13	0.82
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.39	0.82
1:C:253:TYR:HD1	1:C:313:PHE:HD2	1.26	0.82
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.59	0.82
1:A:27:TYR:CB	1:B:110:LEU:HD11	2.10	0.81
1:B:297:ALA:O	1:B:301:VAL:HG23	1.81	0.81
1:E:22:TYR:HA	1:E:149:GLY:CA	2.09	0.81
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.62	0.80
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.64	0.80
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.64	0.80
1:A:260:MET:HE2	1:A:309:LEU:HD22	1.63	0.80
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.45	0.80
1:E:304:LEU:O	1:E:308:ILE:HG12	1.83	0.79
1:B:304:LEU:O	1:B:308:ILE:HG12	1.82	0.79
1:D:297:ALA:O	1:D:301:VAL:HG23	1.83	0.79
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.64	0.79
1:A:283:GLN:N	1:A:284:PRO:HD3	1.98	0.79
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.03	0.79
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.64	0.79
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.64	0.79
1:B:260:MET:HE2	1:B:309:LEU:HD22	1.64	0.79
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.64	0.79
1:E:147:LYS:O	1:E:147:LYS:HG2	1.83	0.79
1:E:79:ASN:HD22	1:E:79:ASN:H	1.31	0.79
1:A:226:LEU:HD23	1:B:224:VAL:HB	1.64	0.78
1:C:147:LYS:O	1:C:147:LYS:HG2	1.83	0.78
1:C:149:GLY:O	1:C:164:PHE:HD1	1.67	0.78
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.19	0.78
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.19	0.77
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.67	0.77
1:A:147:LYS:O	1:A:147:LYS:HG2	1.83	0.77
1:D:283:GLN:N	1:D:284:PRO:HD3	2.00	0.77
1:E:149:GLY:O	1:E:164:PHE:HD1	1.68	0.77
1:B:254:THR:O	1:B:258:ILE:HB	1.84	0.77
1:B:197:ILE:HA	1:B:201:ILE:HB	1.67	0.77
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.66	0.77
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.66	0.77
1:B:283:GLN:N	1:B:284:PRO:HD3	2.00	0.77
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.67	0.76
1:A:217:SER:OG	1:B:220:TYR:HE2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLN:N	1:C:284:PRO:HD3	1.99	0.76
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.20	0.76
1:A:254:THR:O	1:A:258:ILE:HB	1.86	0.76
1:D:147:LYS:O	1:D:147:LYS:HG2	1.83	0.76
1:D:225:THR:HG22	1:E:224:VAL:HG23	1.66	0.76
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.20	0.76
1:A:79:ASN:HD22	1:A:79:ASN:H	1.34	0.76
1:B:147:LYS:HG2	1:B:147:LYS:O	1.83	0.76
1:E:283:GLN:N	1:E:284:PRO:HD3	2.00	0.76
1:A:226:LEU:HD21	1:B:224:VAL:HB	1.66	0.76
1:C:260:MET:HE2	1:C:309:LEU:HD22	1.66	0.76
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.22	0.75
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.66	0.75
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.68	0.75
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.21	0.75
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.69	0.75
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.67	0.75
1:D:197:ILE:HA	1:D:201:ILE:HB	1.69	0.75
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.69	0.75
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.22	0.75
1:E:260:MET:HE2	1:E:309:LEU:HD22	1.68	0.74
1:D:254:THR:O	1:D:258:ILE:HB	1.87	0.74
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.69	0.74
1:E:254:THR:O	1:E:258:ILE:HB	1.87	0.74
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.01	0.74
1:D:253:TYR:HD1	1:D:313:PHE:CD2	2.04	0.74
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.68	0.74
1:E:147:LYS:CG	1:E:147:LYS:O	2.35	0.74
1:A:217:SER:OG	1:B:220:TYR:CE2	2.39	0.74
1:B:149:GLY:O	1:B:164:PHE:HD1	1.70	0.74
1:C:226:LEU:HD21	1:D:224:VAL:HB	1.69	0.74
1:D:147:LYS:CG	1:D:147:LYS:O	2.35	0.74
1:B:147:LYS:O	1:B:147:LYS:CG	2.35	0.73
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.23	0.73
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.22	0.73
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.70	0.73
1:D:253:TYR:CD1	1:D:313:PHE:HD2	2.04	0.73
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.69	0.73
1:B:100:GLN:HA	1:B:100:GLN:HE21	1.54	0.73
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.71	0.73
1:C:147:LYS:CG	1:C:147:LYS:O	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.54	0.72
1:A:146:GLU:HG3	1:B:176:GLU:HG2	1.71	0.72
1:C:254:THR:O	1:C:258:ILE:HB	1.89	0.72
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.70	0.72
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.54	0.72
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.71	0.72
1:A:149:GLY:O	1:A:164:PHE:HD1	1.73	0.72
1:A:253:TYR:CD1	1:A:313:PHE:HD2	2.06	0.72
1:C:304:LEU:O	1:C:308:ILE:HG12	1.89	0.72
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.20	0.71
1:A:147:LYS:O	1:A:147:LYS:CG	2.35	0.71
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.72	0.71
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.01	0.71
1:A:304:LEU:O	1:A:308:ILE:HG12	1.90	0.71
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.71	0.71
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.71	0.71
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.72	0.71
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.20	0.71
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.73	0.71
1:D:79:ASN:HD22	1:D:79:ASN:H	1.36	0.71
1:D:149:GLY:O	1:D:164:PHE:HD1	1.73	0.71
1:D:146:GLU:HG3	1:E:176:GLU:HG2	1.73	0.71
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.73	0.70
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.73	0.70
1:D:260:MET:HE2	1:D:309:LEU:HD22	1.73	0.70
1:C:157:THR:HG21	1:D:34:GLU:HG3	1.73	0.70
1:E:100:GLN:HE21	1:E:100:GLN:HA	1.55	0.70
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.26	0.70
1:A:253:TYR:HD1	1:A:313:PHE:CD2	2.06	0.70
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.74	0.70
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.75	0.70
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.22	0.70
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.22	0.70
1:C:79:ASN:HD22	1:C:79:ASN:H	1.39	0.70
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.74	0.69
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.74	0.69
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.74	0.69
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.22	0.69
1:E:84:ARG:HB2	1:E:84:ARG:NH1	2.07	0.69
1:C:193:TYR:O	1:C:194:PHE:HB2	1.92	0.69
1:B:253:TYR:HD1	1:B:313:PHE:CD2	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ILE:HA	1:E:201:ILE:HB	1.75	0.69
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.74	0.69
1:E:267:VAL:HA	1:E:270:ILE:HB	1.74	0.69
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.23	0.69
1:B:253:TYR:CD1	1:B:313:PHE:HD2	2.11	0.68
1:C:223:ASN:O	1:C:227:VAL:HG23	1.93	0.68
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.75	0.68
1:B:223:ASN:O	1:B:227:VAL:HG23	1.92	0.68
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.74	0.68
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.23	0.68
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.23	0.68
1:A:197:ILE:HA	1:A:201:ILE:HB	1.76	0.68
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.75	0.68
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.29	0.68
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.76	0.68
1:E:84:ARG:HB2	1:E:84:ARG:HH11	1.58	0.68
1:B:216:TRP:HA	1:B:295:ARG:HH21	1.59	0.68
1:C:118:TYR:CE1	1:C:245:LEU:HD11	2.29	0.68
1:C:216:TRP:HA	1:C:295:ARG:HH21	1.57	0.68
1:D:216:TRP:HA	1:D:295:ARG:HH21	1.57	0.68
1:D:218:THR:HG22	1:D:279:LYS:HE2	1.76	0.68
1:D:94:SER:OG	1:D:95:PRO:HD2	1.94	0.68
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.75	0.67
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.42	0.67
1:A:194:PHE:HE2	1:B:250:TYR:O	1.77	0.67
1:C:197:ILE:HA	1:C:201:ILE:HB	1.75	0.67
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.74	0.67
1:A:27:TYR:CG	1:B:110:LEU:HD11	2.29	0.67
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.29	0.67
1:B:218:THR:HG22	1:B:279:LYS:HE2	1.77	0.67
1:C:94:SER:OG	1:C:95:PRO:HD2	1.95	0.67
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.30	0.67
1:A:41:PHE:HE2	1:B:175:LEU:HD23	1.58	0.67
1:D:225:THR:CG2	1:E:224:VAL:CG2	2.71	0.67
1:D:155:PHE:HE1	1:E:112:PRO:HB3	1.52	0.67
1:A:94:SER:OG	1:A:95:PRO:HD2	1.95	0.67
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.25	0.67
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.77	0.67
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.30	0.67
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.77	0.67
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.76	0.67
1:C:216:TRP:HA	1:C:295:ARG:NH2	2.09	0.67
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.75	0.67
1:E:193:TYR:O	1:E:194:PHE:HB2	1.94	0.67
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.76	0.67
1:C:267:VAL:HA	1:C:270:ILE:HB	1.77	0.66
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.10	0.66
1:A:223:ASN:O	1:A:227:VAL:HG23	1.94	0.66
1:A:216:TRP:HA	1:A:295:ARG:HH21	1.60	0.66
1:B:267:VAL:HA	1:B:270:ILE:HB	1.77	0.66
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.76	0.66
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.77	0.66
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.60	0.66
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.76	0.66
1:C:118:TYR:CE1	1:C:245:LEU:CD1	2.78	0.66
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.31	0.66
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.78	0.66
1:A:225:THR:HG21	1:B:225:THR:OG1	1.96	0.66
1:E:223:ASN:O	1:E:227:VAL:HG23	1.95	0.66
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.61	0.66
1:B:118:TYR:CE1	1:B:245:LEU:CD1	2.79	0.66
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.78	0.66
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.30	0.66
1:B:21:ILE:O	1:B:149:GLY:HA3	1.96	0.66
1:C:147:LYS:C	1:C:149:GLY:H	1.99	0.66
1:E:118:TYR:CE1	1:E:245:LEU:CD1	2.79	0.66
1:E:253:TYR:CD1	1:E:313:PHE:HD2	2.10	0.66
1:C:199:ASN:HB3	1:D:242:GLU:OE1	1.96	0.66
1:C:202:LEU:HD12	1:D:259:PHE:HE1	1.60	0.66
1:D:118:TYR:CE1	1:D:245:LEU:CD1	2.79	0.66
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.31	0.66
1:B:84:ARG:NH1	1:B:84:ARG:HB2	2.11	0.66
1:E:47:LYS:HD3	1:E:49:ARG:NH2	2.10	0.66
1:E:84:ARG:CB	1:E:84:ARG:HH11	2.08	0.66
1:C:253:TYR:HD1	1:C:313:PHE:CD2	2.10	0.65
1:C:48:ASP:O	1:C:51:LEU:HD23	1.96	0.65
1:A:77:PHE:H	1:A:84:ARG:HD3	1.60	0.65
1:C:253:TYR:CD1	1:C:313:PHE:HD2	2.10	0.65
1:D:147:LYS:C	1:D:149:GLY:H	1.99	0.65
1:E:216:TRP:HA	1:E:295:ARG:HH21	1.61	0.65
1:A:84:ARG:HB2	1:A:84:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.77	0.65
1:D:21:ILE:O	1:D:149:GLY:HA3	1.97	0.65
1:A:21:ILE:O	1:A:149:GLY:HA3	1.97	0.65
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.61	0.65
1:B:216:TRP:HA	1:B:295:ARG:NH2	2.11	0.65
1:E:147:LYS:C	1:E:149:GLY:H	1.99	0.65
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.79	0.65
1:C:84:ARG:NH1	1:C:84:ARG:HB2	2.11	0.65
1:A:93:VAL:HG22	1:A:99:VAL:HG22	1.78	0.65
1:B:147:LYS:C	1:B:149:GLY:H	1.99	0.65
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.62	0.65
1:D:41:PHE:HE2	1:E:175:LEU:CD2	2.09	0.65
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.79	0.65
1:C:222:ALA:HB2	1:D:221:GLU:OE1	1.97	0.65
1:E:118:TYR:CE1	1:E:245:LEU:HD11	2.31	0.65
1:A:216:TRP:HA	1:A:295:ARG:NH2	2.12	0.64
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.79	0.64
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.27	0.64
1:D:84:ARG:NH1	1:D:84:ARG:HB2	2.12	0.64
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.31	0.64
1:C:21:ILE:O	1:C:149:GLY:HA3	1.98	0.64
1:A:29:LEU:HB2	1:A:156:LEU:HD11	1.80	0.64
1:C:128:TYR:O	1:C:129:LEU:HB2	1.98	0.64
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.28	0.64
1:A:219:SER:OG	1:A:222:ALA:HB3	1.98	0.64
1:A:147:LYS:C	1:A:149:GLY:H	1.99	0.64
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.33	0.64
1:D:192:GLN:OE1	1:E:249:PRO:HB3	1.98	0.64
1:D:223:ASN:O	1:D:227:VAL:HG23	1.96	0.64
1:E:128:TYR:O	1:E:129:LEU:HB2	1.98	0.64
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.28	0.64
1:A:193:TYR:O	1:A:194:PHE:HB2	1.96	0.64
1:A:221:GLU:HB3	1:B:221:GLU:CG	2.27	0.64
1:A:232:ILE:HG22	1:A:233:ALA:N	2.12	0.64
1:A:283:GLN:N	1:A:284:PRO:CD	2.60	0.64
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.32	0.64
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.63	0.64
1:D:47:LYS:HD3	1:D:49:ARG:NH2	2.13	0.64
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.63	0.64
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.79	0.64
1:E:48:ASP:O	1:E:51:LEU:HD23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ILE:HG12	1:E:172:ASN:ND2	2.12	0.64
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.33	0.63
1:C:222:ALA:HB2	1:D:221:GLU:HA	1.80	0.63
1:D:274:VAL:C	1:D:276:HIS:H	2.02	0.63
1:A:128:TYR:O	1:A:129:LEU:HB2	1.98	0.63
1:B:47:LYS:HD3	1:B:49:ARG:NH2	2.13	0.63
1:E:216:TRP:HA	1:E:295:ARG:NH2	2.13	0.63
1:B:276:HIS:O	1:B:280:VAL:HG22	1.98	0.63
1:A:104:ARG:NH1	1:B:77:PHE:O	2.29	0.63
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.80	0.63
1:B:84:ARG:HH11	1:B:84:ARG:HB2	1.64	0.63
1:C:274:VAL:C	1:C:276:HIS:H	2.02	0.63
1:D:118:TYR:CE1	1:D:245:LEU:HD11	2.32	0.63
1:A:267:VAL:HA	1:A:270:ILE:HB	1.80	0.63
1:B:274:VAL:C	1:B:276:HIS:H	2.02	0.63
1:C:149:GLY:O	1:C:164:PHE:CD1	2.51	0.63
1:D:51:LEU:HD11	1:D:70:ILE:HD12	1.79	0.63
1:D:77:PHE:H	1:D:84:ARG:HD3	1.62	0.63
1:B:193:TYR:O	1:B:194:PHE:HB2	1.97	0.63
1:C:47:LYS:HD3	1:C:49:ARG:NH2	2.14	0.63
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.34	0.63
1:C:77:PHE:H	1:C:84:ARG:HD3	1.62	0.63
1:D:232:ILE:HG22	1:D:233:ALA:N	2.13	0.63
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.64	0.63
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.61	0.63
1:A:48:ASP:O	1:A:51:LEU:HD23	1.99	0.62
1:E:144:ASP:HA	1:E:147:LYS:HB3	1.82	0.62
1:B:128:TYR:O	1:B:129:LEU:HB2	1.98	0.62
1:D:216:TRP:HA	1:D:295:ARG:NH2	2.13	0.62
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.19	0.62
1:B:118:TYR:CE1	1:B:245:LEU:HD11	2.33	0.62
1:B:283:GLN:N	1:B:284:PRO:CD	2.63	0.62
1:A:274:VAL:C	1:A:276:HIS:H	2.02	0.62
1:A:194:PHE:HE2	1:B:250:TYR:C	2.03	0.62
1:D:267:VAL:HA	1:D:270:ILE:HB	1.80	0.62
1:E:21:ILE:O	1:E:149:GLY:HA3	1.98	0.62
1:C:193:TYR:O	1:C:194:PHE:CB	2.46	0.62
1:D:84:ARG:CB	1:D:84:ARG:HH11	2.12	0.62
1:C:283:GLN:N	1:C:284:PRO:CD	2.62	0.62
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.81	0.62
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.35	0.62
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.35	0.61
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.35	0.61
1:E:283:GLN:N	1:E:284:PRO:CD	2.62	0.61
1:B:48:ASP:O	1:B:51:LEU:HD23	2.00	0.61
1:B:84:ARG:CB	1:B:84:ARG:HH11	2.13	0.61
1:D:128:TYR:O	1:D:129:LEU:HB2	1.98	0.61
1:D:283:GLN:N	1:D:284:PRO:CD	2.62	0.61
1:C:219:SER:OG	1:C:222:ALA:HB3	1.99	0.61
1:C:84:ARG:HB2	1:C:84:ARG:HH11	1.65	0.61
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.81	0.61
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.30	0.61
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.82	0.61
1:C:93:VAL:HG22	1:C:99:VAL:HG22	1.83	0.61
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.36	0.61
1:E:274:VAL:C	1:E:276:HIS:H	2.02	0.61
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.83	0.61
1:B:77:PHE:H	1:B:84:ARG:HD3	1.66	0.61
1:D:193:TYR:O	1:D:194:PHE:HB2	1.98	0.61
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.82	0.61
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.81	0.61
1:B:51:LEU:HD11	1:B:70:ILE:HD12	1.82	0.61
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.82	0.61
1:E:200:ILE:O	1:E:204:MET:HB2	2.01	0.61
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.81	0.61
1:B:281:GLU:O	1:B:283:GLN:N	2.34	0.61
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.35	0.61
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.18	0.61
1:E:94:SER:OG	1:E:95:PRO:HD2	2.01	0.61
1:A:149:GLY:O	1:A:164:PHE:CD1	2.54	0.60
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.64	0.60
1:B:144:ASP:HA	1:B:147:LYS:HB3	1.83	0.60
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.17	0.60
1:C:86:ALA:HB2	1:C:105:PHE:HB3	1.83	0.60
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.31	0.60
1:A:157:THR:HG21	1:B:34:GLU:HG3	1.84	0.60
1:B:232:ILE:HG22	1:B:233:ALA:N	2.16	0.60
1:C:84:ARG:CB	1:C:84:ARG:HH11	2.14	0.60
1:A:84:ARG:HH11	1:A:84:ARG:HB2	1.67	0.60
1:B:193:TYR:O	1:B:194:PHE:CB	2.48	0.60
1:E:193:TYR:O	1:E:194:PHE:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.37	0.60
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.83	0.60
1:B:94:SER:OG	1:B:95:PRO:HD2	2.02	0.60
1:A:225:THR:HG22	1:B:224:VAL:HG23	1.83	0.60
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.36	0.60
1:A:51:LEU:HD11	1:A:70:ILE:HD12	1.84	0.60
1:D:76:ARG:HH22	1:D:130:ILE:CD1	2.10	0.60
1:C:144:ASP:HA	1:C:147:LYS:HB3	1.84	0.59
1:C:194:PHE:HA	1:C:197:ILE:HD12	1.84	0.59
1:D:281:GLU:O	1:D:283:GLN:N	2.35	0.59
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.83	0.59
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.37	0.59
1:E:86:ALA:HB2	1:E:105:PHE:HB3	1.84	0.59
1:C:194:PHE:C	1:C:196:TYR:N	2.54	0.59
1:A:224:VAL:C	1:A:226:LEU:N	2.56	0.59
1:B:76:ARG:NH2	1:B:130:ILE:CD1	2.55	0.59
1:C:27:TYR:CB	1:D:110:LEU:HD11	2.31	0.59
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.84	0.59
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.30	0.59
1:E:224:VAL:C	1:E:226:LEU:H	2.05	0.59
1:A:193:TYR:O	1:A:194:PHE:CB	2.49	0.59
1:B:221:GLU:OE2	1:C:221:GLU:CD	2.40	0.59
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.36	0.59
1:B:200:ILE:O	1:B:204:MET:HB2	2.02	0.59
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.67	0.59
1:A:84:ARG:HH11	1:A:84:ARG:CB	2.14	0.59
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.20	0.59
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.20	0.59
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.32	0.59
1:C:194:PHE:HE2	1:D:250:TYR:O	1.86	0.59
1:C:281:GLU:O	1:C:283:GLN:N	2.36	0.59
1:B:93:VAL:HG22	1:B:99:VAL:HG22	1.85	0.59
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.37	0.59
1:C:139:ILE:HG12	1:C:172:ASN:ND2	2.14	0.59
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.32	0.59
1:B:139:ILE:HG12	1:B:172:ASN:ND2	2.16	0.58
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.85	0.58
1:E:276:HIS:O	1:E:280:VAL:HG22	2.03	0.58
1:A:86:ALA:HB2	1:A:105:PHE:HB3	1.85	0.58
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.33	0.58
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:HG22	1:E:224:VAL:CG2	2.30	0.58
1:E:194:PHE:HA	1:E:197:ILE:HD12	1.85	0.58
1:E:232:ILE:HG22	1:E:233:ALA:N	2.18	0.58
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.84	0.58
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.86	0.58
1:A:275:GLN:HG2	1:A:275:GLN:O	2.04	0.58
1:C:275:GLN:HG2	1:C:275:GLN:O	2.04	0.58
1:C:276:HIS:O	1:C:280:VAL:HG22	2.03	0.58
1:E:281:GLU:O	1:E:283:GLN:N	2.37	0.58
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.21	0.58
1:D:139:ILE:HG12	1:D:172:ASN:ND2	2.17	0.58
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.38	0.58
1:D:76:ARG:NH2	1:D:130:ILE:CD1	2.56	0.58
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.38	0.58
1:D:140:VAL:HG22	1:D:181:SER:HB3	1.86	0.58
1:E:149:GLY:O	1:E:164:PHE:CD1	2.53	0.58
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.85	0.58
1:B:86:ALA:HB2	1:B:105:PHE:HB3	1.86	0.58
1:C:200:ILE:O	1:C:204:MET:HB2	2.04	0.58
1:D:48:ASP:O	1:D:51:LEU:HD23	2.04	0.58
1:E:219:SER:OG	1:E:222:ALA:HB3	2.04	0.58
1:C:194:PHE:C	1:C:196:TYR:H	2.06	0.58
1:E:224:VAL:C	1:E:226:LEU:N	2.56	0.58
1:E:77:PHE:H	1:E:84:ARG:HD3	1.68	0.58
1:A:224:VAL:C	1:A:226:LEU:H	2.05	0.58
1:D:86:ALA:HB2	1:D:105:PHE:HB3	1.85	0.57
1:D:193:TYR:O	1:D:194:PHE:CB	2.51	0.57
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.21	0.57
1:E:275:GLN:O	1:E:275:GLN:HG2	2.04	0.57
1:E:47:LYS:CD	1:E:49:ARG:HH21	2.17	0.57
1:A:281:GLU:O	1:A:283:GLN:N	2.37	0.57
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.22	0.57
1:C:118:TYR:CD1	1:C:245:LEU:HD11	2.39	0.57
1:E:194:PHE:C	1:E:196:TYR:N	2.56	0.57
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.34	0.57
1:A:140:VAL:HG22	1:A:181:SER:HB3	1.86	0.57
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.39	0.57
1:B:275:GLN:HG2	1:B:275:GLN:O	2.04	0.57
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.39	0.57
1:B:194:PHE:C	1:B:196:TYR:N	2.57	0.57
1:A:41:PHE:HZ	1:B:76:ARG:NH2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HD12	1:C:101:TYR:CD2	2.40	0.57
1:A:47:LYS:HD3	1:A:49:ARG:NH2	2.19	0.57
1:E:93:VAL:HG22	1:E:99:VAL:HG22	1.86	0.57
1:B:224:VAL:C	1:B:226:LEU:H	2.07	0.57
1:B:47:LYS:CD	1:B:49:ARG:HH21	2.18	0.57
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.34	0.57
1:E:62:VAL:HG13	1:E:93:VAL:O	2.05	0.57
1:B:149:GLY:O	1:B:164:PHE:CD1	2.56	0.57
1:B:76:ARG:HH22	1:B:130:ILE:CD1	2.09	0.57
1:C:86:ALA:HB2	1:C:105:PHE:CB	2.35	0.57
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.26	0.56
1:D:276:HIS:O	1:D:280:VAL:HG22	2.05	0.56
1:E:29:LEU:C	1:E:29:LEU:HD23	2.25	0.56
1:B:276:HIS:C	1:B:278:LEU:H	2.09	0.56
1:C:147:LYS:HE2	1:C:165:THR:HA	1.87	0.56
1:C:76:ARG:NH2	1:C:130:ILE:CD1	2.62	0.56
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.35	0.56
1:A:139:ILE:HG12	1:A:172:ASN:ND2	2.14	0.56
1:B:194:PHE:HA	1:B:197:ILE:HD12	1.86	0.56
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.23	0.56
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.41	0.56
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.40	0.56
1:D:194:PHE:HA	1:D:197:ILE:HD12	1.86	0.56
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.23	0.56
1:A:222:ALA:O	1:A:226:LEU:HB2	2.06	0.56
1:C:224:VAL:C	1:C:226:LEU:H	2.08	0.56
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.86	0.56
1:D:37:LYS:HG2	1:D:108:ARG:HB3	1.88	0.56
1:D:149:GLY:O	1:D:164:PHE:CD1	2.57	0.56
1:D:48:ASP:O	1:D:50:ARG:N	2.39	0.56
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.86	0.56
1:A:147:LYS:O	1:A:147:LYS:HD3	2.06	0.56
1:B:147:LYS:HD3	1:B:147:LYS:O	2.06	0.56
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.24	0.56
1:D:275:GLN:O	1:D:275:GLN:HG2	2.04	0.56
1:A:147:LYS:HE2	1:A:165:THR:HA	1.86	0.56
1:A:76:ARG:NH2	1:A:130:ILE:CD1	2.60	0.56
1:C:276:HIS:C	1:C:278:LEU:H	2.09	0.56
1:E:70:ILE:HD13	1:E:70:ILE:N	2.21	0.56
1:A:194:PHE:C	1:A:196:TYR:N	2.58	0.56
1:A:25:GLU:HG3	1:B:79:ASN:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.88	0.56
1:A:253:TYR:O	1:A:256:ALA:HB3	2.06	0.56
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.35	0.56
1:B:54:ASP:HB2	1:B:57:ARG:CB	2.36	0.56
1:E:305:ALA:O	1:E:309:LEU:HB2	2.06	0.56
1:E:51:LEU:HD11	1:E:70:ILE:HD12	1.88	0.56
1:B:23:LEU:HA	1:B:40:ALA:HB2	1.87	0.55
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.71	0.55
1:B:140:VAL:HG22	1:B:181:SER:HB3	1.88	0.55
1:E:147:LYS:O	1:E:147:LYS:HD3	2.06	0.55
1:A:23:LEU:HA	1:A:40:ALA:HB2	1.87	0.55
1:B:253:TYR:O	1:B:256:ALA:HB3	2.06	0.55
1:C:147:LYS:O	1:C:147:LYS:HD3	2.06	0.55
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.88	0.55
1:D:147:LYS:O	1:D:147:LYS:HD3	2.06	0.55
1:D:276:HIS:C	1:D:278:LEU:H	2.09	0.55
1:D:23:LEU:HA	1:D:40:ALA:HB2	1.88	0.55
1:C:47:LYS:CD	1:C:49:ARG:HH21	2.20	0.55
1:A:42:LEU:HD23	1:A:103:GLU:OE1	2.06	0.55
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.35	0.55
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.94	0.55
1:D:123:GLN:NE2	1:D:123:GLN:HA	2.21	0.55
1:D:118:TYR:CE2	1:D:196:TYR:HE2	2.25	0.55
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.88	0.55
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.32	0.55
1:A:86:ALA:HB2	1:A:105:PHE:CB	2.37	0.55
1:A:276:HIS:C	1:A:278:LEU:H	2.09	0.55
1:A:240:LEU:HD13	1:B:239:ILE:CG1	2.37	0.55
1:D:84:ARG:HB2	1:D:84:ARG:HH11	1.70	0.55
1:B:118:TYR:CE2	1:B:196:TYR:HE2	2.25	0.55
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.88	0.55
1:C:29:LEU:C	1:C:29:LEU:HD23	2.27	0.55
1:A:194:PHE:HA	1:A:197:ILE:HD12	1.88	0.55
1:A:44:LEU:HD12	1:A:101:TYR:CD2	2.42	0.55
1:B:224:VAL:C	1:B:226:LEU:N	2.57	0.55
1:B:118:TYR:CE1	1:B:245:LEU:HD13	2.41	0.55
1:D:194:PHE:C	1:D:196:TYR:N	2.57	0.55
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.95	0.55
1:D:278:LEU:HD23	1:D:287:ALA:HA	1.88	0.55
1:A:276:HIS:O	1:A:280:VAL:HG22	2.06	0.55
1:D:41:PHE:CE2	1:E:175:LEU:CD2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:HIS:C	1:E:278:LEU:H	2.09	0.55
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.42	0.55
1:A:157:THR:HG21	1:B:34:GLU:OE1	2.05	0.54
1:A:278:LEU:HD23	1:A:287:ALA:HA	1.89	0.54
1:B:62:VAL:HG13	1:B:93:VAL:O	2.07	0.54
1:A:200:ILE:O	1:A:204:MET:HB2	2.07	0.54
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.42	0.54
1:C:118:TYR:CE2	1:C:196:TYR:HE2	2.25	0.54
1:E:194:PHE:C	1:E:196:TYR:H	2.10	0.54
1:C:42:LEU:HD23	1:C:103:GLU:OE1	2.06	0.54
1:C:23:LEU:CD2	1:C:38:VAL:HG21	2.37	0.54
1:D:118:TYR:CE1	1:D:245:LEU:HD13	2.41	0.54
1:E:98:THR:HG22	1:E:98:THR:O	2.07	0.54
1:C:224:VAL:C	1:C:226:LEU:N	2.60	0.54
1:D:93:VAL:HG22	1:D:99:VAL:HG22	1.88	0.54
1:A:194:PHE:CE2	1:B:250:TYR:C	2.80	0.54
1:C:215:PHE:O	1:C:291:THR:HG22	2.08	0.54
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.88	0.54
1:B:305:ALA:O	1:B:309:LEU:HB2	2.08	0.54
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.43	0.54
1:D:18:ASN:O	1:D:44:LEU:HA	2.08	0.54
1:D:222:ALA:O	1:D:226:LEU:HB2	2.08	0.54
1:E:86:ALA:HB2	1:E:105:PHE:CB	2.37	0.54
1:A:37:LYS:HG2	1:A:108:ARG:HB3	1.89	0.54
1:B:23:LEU:CD2	1:B:38:VAL:HG21	2.38	0.54
1:D:144:ASP:HA	1:D:147:LYS:HB3	1.89	0.54
1:C:41:PHE:HZ	1:D:76:ARG:NH2	2.06	0.54
1:E:278:LEU:HD23	1:E:287:ALA:HA	1.89	0.54
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.22	0.54
1:B:278:LEU:HD23	1:B:287:ALA:HA	1.89	0.54
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.42	0.54
1:E:54:ASP:HB2	1:E:57:ARG:CB	2.37	0.54
1:A:18:ASN:O	1:A:44:LEU:HA	2.07	0.53
1:C:232:ILE:HG22	1:C:233:ALA:N	2.22	0.53
1:C:155:PHE:HD1	1:D:110:LEU:CD2	2.22	0.53
1:D:86:ALA:HB2	1:D:105:PHE:CB	2.38	0.53
1:E:118:TYR:CD1	1:E:245:LEU:HD11	2.43	0.53
1:A:234:HIS:CE1	1:A:261:ILE:CG2	2.92	0.53
1:B:118:TYR:CD1	1:B:245:LEU:HD11	2.43	0.53
1:D:47:LYS:CD	1:D:49:ARG:HH21	2.21	0.53
1:C:51:LEU:HD11	1:C:70:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:VAL:C	1:D:226:LEU:H	2.11	0.53
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.91	0.53
1:B:119:PRO:O	1:B:193:TYR:HB3	2.09	0.53
1:B:219:SER:OG	1:B:222:ALA:HB3	2.09	0.53
1:B:70:ILE:HG22	1:B:71:TRP:N	2.24	0.53
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.37	0.53
1:C:62:VAL:HG13	1:C:93:VAL:O	2.08	0.53
1:D:118:TYR:CD1	1:D:245:LEU:HD11	2.43	0.53
1:D:54:ASP:HB2	1:D:57:ARG:CB	2.37	0.53
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.96	0.53
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.96	0.53
1:A:23:LEU:CD2	1:A:38:VAL:HG21	2.38	0.53
1:B:86:ALA:HB2	1:B:105:PHE:CB	2.39	0.53
1:C:76:ARG:HH22	1:C:130:ILE:CD1	2.17	0.53
1:D:119:PRO:O	1:D:193:TYR:HB3	2.09	0.53
1:D:98:THR:HG22	1:D:98:THR:O	2.09	0.53
1:C:225:THR:HG21	1:D:225:THR:OG1	2.09	0.53
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.44	0.53
1:B:147:LYS:HE2	1:B:165:THR:HA	1.90	0.53
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.91	0.53
1:A:54:ASP:HB2	1:A:57:ARG:CB	2.39	0.52
1:B:194:PHE:C	1:B:196:TYR:H	2.12	0.52
1:B:215:PHE:O	1:B:291:THR:HG22	2.09	0.52
1:C:118:TYR:CE1	1:C:245:LEU:HD13	2.43	0.52
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.44	0.52
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.38	0.52
1:E:118:TYR:CE2	1:E:196:TYR:HE2	2.27	0.52
1:A:144:ASP:HA	1:A:147:LYS:HB3	1.90	0.52
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.44	0.52
1:B:29:LEU:HD23	1:B:29:LEU:C	2.30	0.52
1:C:140:VAL:HG22	1:C:181:SER:HB3	1.91	0.52
1:C:278:LEU:HD23	1:C:287:ALA:HA	1.90	0.52
1:D:146:GLU:HG3	1:E:176:GLU:CG	2.39	0.52
1:D:225:THR:HG21	1:E:224:VAL:CG2	2.33	0.52
1:D:23:LEU:CD2	1:D:38:VAL:HG21	2.39	0.52
1:E:118:TYR:CE1	1:E:245:LEU:HD13	2.44	0.52
1:E:47:LYS:HD3	1:E:49:ARG:HH21	1.73	0.52
1:C:226:LEU:HD23	1:D:224:VAL:HG21	1.92	0.52
1:D:219:SER:OG	1:D:222:ALA:HB3	2.08	0.52
1:D:29:LEU:HD23	1:D:29:LEU:C	2.29	0.52
1:E:23:LEU:CD2	1:E:38:VAL:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PHE:C	1:A:196:TYR:H	2.12	0.52
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.96	0.52
1:D:215:PHE:O	1:D:291:THR:HG22	2.09	0.52
1:D:77:PHE:CE2	1:D:127:ILE:HG23	2.45	0.52
1:E:147:LYS:HE2	1:E:165:THR:HA	1.91	0.52
1:E:234:HIS:CE1	1:E:261:ILE:CG2	2.92	0.52
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.92	0.52
1:D:224:VAL:C	1:D:226:LEU:N	2.61	0.52
1:A:119:PRO:O	1:A:193:TYR:HB3	2.10	0.52
1:D:253:TYR:O	1:D:256:ALA:HB3	2.10	0.52
1:E:109:VAL:HG11	1:E:126:HIS:O	2.10	0.52
1:E:215:PHE:O	1:E:291:THR:HG22	2.09	0.52
1:E:70:ILE:HG22	1:E:71:TRP:N	2.25	0.52
1:A:305:ALA:O	1:A:309:LEU:HB2	2.09	0.51
1:B:222:ALA:O	1:B:226:LEU:HB2	2.10	0.51
1:E:140:VAL:HG22	1:E:181:SER:HB3	1.91	0.51
1:B:215:PHE:O	1:B:291:THR:CG2	2.58	0.51
1:C:109:VAL:HG11	1:C:126:HIS:O	2.11	0.51
1:D:123:GLN:HB2	1:D:189:ILE:HG13	1.92	0.51
1:E:212:TRP:CZ3	1:E:298:PHE:HB3	2.45	0.51
1:A:29:LEU:C	1:A:29:LEU:HD23	2.29	0.51
1:A:256:ALA:HB1	1:A:309:LEU:HD21	1.92	0.51
1:E:222:ALA:O	1:E:226:LEU:HB2	2.11	0.51
1:B:77:PHE:CE2	1:B:127:ILE:HG23	2.46	0.51
1:C:155:PHE:CD1	1:D:110:LEU:CD2	2.93	0.51
1:C:222:ALA:CB	1:D:221:GLU:OE1	2.59	0.51
1:E:23:LEU:HA	1:E:40:ALA:HB2	1.93	0.51
1:B:191:ARG:HG3	1:B:192:GLN:N	2.26	0.51
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.45	0.51
1:D:249:PRO:HD2	1:D:250:TYR:CE1	2.46	0.51
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.45	0.51
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.93	0.51
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.45	0.51
1:A:215:PHE:O	1:A:291:THR:HG22	2.09	0.51
1:C:256:ALA:HB1	1:C:309:LEU:HD21	1.92	0.51
1:E:37:LYS:HG2	1:E:108:ARG:HB3	1.91	0.51
1:A:147:LYS:O	1:A:147:LYS:CD	2.59	0.51
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.46	0.51
1:E:133:SER:HB2	1:E:137:ARG:NH1	2.25	0.51
1:A:62:VAL:HG13	1:A:93:VAL:O	2.10	0.51
1:B:147:LYS:CD	1:B:147:LYS:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LYS:HG2	1:C:108:ARG:HB3	1.92	0.51
1:C:77:PHE:CE2	1:C:127:ILE:HG23	2.46	0.51
1:D:305:ALA:O	1:D:309:LEU:HB2	2.10	0.51
1:E:77:PHE:CE2	1:E:127:ILE:HG23	2.46	0.51
1:A:18:ASN:HB2	1:A:45:SER:OG	2.11	0.51
1:A:215:PHE:O	1:A:291:THR:CG2	2.59	0.51
1:B:119:PRO:HB3	1:B:196:TYR:CD2	2.46	0.51
1:B:44:LEU:HD12	1:B:101:TYR:CD2	2.46	0.51
1:D:119:PRO:HB3	1:D:196:TYR:CD2	2.46	0.51
1:D:215:PHE:O	1:D:291:THR:CG2	2.58	0.51
1:E:147:LYS:CD	1:E:147:LYS:O	2.59	0.51
1:A:119:PRO:HB3	1:A:196:TYR:CD2	2.45	0.50
1:A:226:LEU:HD23	1:B:224:VAL:CG2	2.42	0.50
1:A:217:SER:CB	1:B:220:TYR:HE2	2.23	0.50
1:C:240:LEU:HD22	1:D:239:ILE:HD11	1.92	0.50
1:C:305:ALA:O	1:C:309:LEU:HB2	2.10	0.50
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.90	0.50
1:B:70:ILE:HG22	1:B:71:TRP:O	2.11	0.50
1:E:253:TYR:HA	1:E:313:PHE:CD2	2.46	0.50
1:B:197:ILE:CG2	1:B:202:LEU:HG	2.41	0.50
1:C:215:PHE:O	1:C:291:THR:CG2	2.59	0.50
1:C:98:THR:HG22	1:C:98:THR:O	2.10	0.50
1:B:48:ASP:O	1:B:50:ARG:N	2.44	0.50
1:D:253:TYR:HA	1:D:313:PHE:CD2	2.46	0.50
1:A:209:PHE:HB2	1:B:266:PHE:HE1	1.76	0.50
1:C:18:ASN:O	1:C:44:LEU:HA	2.12	0.50
1:D:42:LEU:HD23	1:D:103:GLU:OE1	2.11	0.50
1:E:44:LEU:HD12	1:E:101:TYR:CD2	2.47	0.50
1:E:249:PRO:HD2	1:E:250:TYR:CE1	2.46	0.50
1:C:123:GLN:NE2	1:C:123:GLN:HA	2.26	0.50
1:C:253:TYR:HA	1:C:313:PHE:CD2	2.47	0.50
1:D:194:PHE:C	1:D:196:TYR:H	2.14	0.50
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.94	0.50
1:B:79:ASN:H	1:B:79:ASN:ND2	2.02	0.50
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.47	0.50
1:C:226:LEU:HD23	1:D:224:VAL:CG2	2.42	0.50
1:D:234:HIS:CE1	1:D:261:ILE:CG2	2.93	0.50
1:A:253:TYR:HA	1:A:313:PHE:CD2	2.47	0.50
1:D:256:ALA:HB1	1:D:309:LEU:HD21	1.94	0.50
1:D:44:LEU:HD12	1:D:101:TYR:CD2	2.46	0.50
1:D:52:ALA:HA	1:D:95:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.46	0.50
1:A:76:ARG:HH22	1:A:130:ILE:CD1	2.16	0.50
1:D:197:ILE:CG2	1:D:202:LEU:HG	2.42	0.49
1:D:147:LYS:O	1:D:147:LYS:CD	2.59	0.49
1:E:268:ALA:HA	1:E:298:PHE:HE1	1.77	0.49
1:C:253:TYR:O	1:C:256:ALA:HB3	2.12	0.49
1:D:78:VAL:HB	1:D:128:TYR:HB2	1.94	0.49
1:E:215:PHE:O	1:E:291:THR:CG2	2.60	0.49
1:B:217:SER:HB3	1:B:223:ASN:OD1	2.12	0.49
1:C:78:VAL:CG2	1:C:130:ILE:HG12	2.39	0.49
1:D:78:VAL:CG2	1:D:130:ILE:HG12	2.41	0.49
1:D:200:ILE:O	1:D:204:MET:HB2	2.11	0.49
1:C:238:ASN:HA	1:C:258:ILE:HD13	1.95	0.49
1:D:153:ASP:O	1:D:154:VAL:C	2.51	0.49
1:A:77:PHE:CE2	1:A:127:ILE:HG23	2.47	0.49
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.42	0.49
1:C:27:TYR:CD1	1:D:81:GLU:OE2	2.65	0.49
1:D:147:LYS:HE2	1:D:165:THR:HA	1.94	0.49
1:E:127:ILE:HB	1:E:185:TYR:HB2	1.95	0.49
1:C:119:PRO:HB3	1:C:196:TYR:CD2	2.48	0.49
1:E:196:TYR:O	1:E:200:ILE:HB	2.13	0.49
1:A:283:GLN:H	1:A:284:PRO:HD3	1.78	0.49
1:A:240:LEU:HD22	1:B:239:ILE:HD11	1.94	0.49
1:C:119:PRO:O	1:C:193:TYR:HB3	2.13	0.49
1:C:147:LYS:CD	1:C:147:LYS:O	2.59	0.49
1:C:153:ASP:O	1:C:154:VAL:C	2.51	0.49
1:E:238:ASN:HA	1:E:258:ILE:HD13	1.93	0.49
1:A:274:VAL:C	1:A:276:HIS:N	2.66	0.49
1:B:42:LEU:HD23	1:B:103:GLU:OE1	2.13	0.49
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.77	0.49
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.47	0.49
1:E:217:SER:HB3	1:E:223:ASN:OD1	2.12	0.49
1:E:274:VAL:C	1:E:276:HIS:N	2.66	0.49
1:E:76:ARG:HH22	1:E:130:ILE:CD1	2.18	0.49
1:A:155:PHE:HE1	1:B:112:PRO:CA	2.26	0.49
1:A:27:TYR:HB2	1:B:110:LEU:HD11	1.94	0.49
1:B:212:TRP:CZ3	1:B:298:PHE:HB3	2.48	0.49
1:B:253:TYR:HA	1:B:313:PHE:CD2	2.48	0.49
1:D:217:SER:HB3	1:D:223:ASN:OD1	2.12	0.49
1:D:274:VAL:C	1:D:276:HIS:N	2.66	0.49
1:D:196:TYR:N	1:D:196:TYR:HD1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:N	1:B:70:ILE:HD13	2.27	0.48
1:B:52:ALA:HA	1:B:95:PRO:O	2.14	0.48
1:C:207:ILE:HG13	1:C:208:LEU:N	2.28	0.48
1:C:217:SER:HB3	1:C:223:ASN:OD1	2.13	0.48
1:D:196:TYR:N	1:D:196:TYR:CD1	2.80	0.48
1:D:53:PHE:HE2	1:D:63:LYS:CB	2.26	0.48
1:B:119:PRO:HB3	1:B:196:TYR:HD2	1.78	0.48
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.95	0.48
1:E:207:ILE:HG13	1:E:208:LEU:N	2.28	0.48
1:A:48:ASP:O	1:A:50:ARG:N	2.46	0.48
1:A:202:LEU:CD1	1:B:259:PHE:CZ	2.97	0.48
1:C:194:PHE:O	1:C:196:TYR:N	2.46	0.48
1:D:66:GLU:HG3	1:D:67:PRO:CD	2.40	0.48
1:E:226:LEU:HD22	1:E:226:LEU:HA	1.67	0.48
1:A:137:ARG:HD3	1:A:137:ARG:HA	1.53	0.48
1:A:19:THR:HG22	1:A:44:LEU:CD2	2.44	0.48
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.48	0.48
1:A:123:GLN:HB2	1:A:189:ILE:HG13	1.96	0.48
1:A:47:LYS:CD	1:A:49:ARG:HH21	2.27	0.48
1:C:133:SER:HB2	1:C:137:ARG:NH1	2.29	0.48
1:D:261:ILE:O	1:D:262:TYR:C	2.52	0.48
1:A:198:PRO:HA	1:B:259:PHE:CD1	2.49	0.48
1:B:238:ASN:HA	1:B:258:ILE:HD13	1.94	0.48
1:D:194:PHE:O	1:D:198:PRO:HD2	2.13	0.48
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.63	0.48
1:D:296:ILE:HD13	1:D:296:ILE:HA	1.76	0.48
1:D:48:ASP:C	1:D:50:ARG:N	2.67	0.48
1:E:119:PRO:O	1:E:193:TYR:HB3	2.13	0.48
1:E:224:VAL:O	1:E:226:LEU:N	2.47	0.48
1:E:42:LEU:HD23	1:E:103:GLU:OE1	2.14	0.48
1:A:197:ILE:CG2	1:A:202:LEU:HG	2.44	0.48
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.49	0.48
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.49	0.48
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.48	0.48
1:C:27:TYR:CE1	1:D:81:GLU:CD	2.87	0.48
1:E:70:ILE:HG22	1:E:71:TRP:O	2.13	0.48
1:B:37:LYS:HG2	1:B:108:ARG:HB3	1.96	0.48
1:D:48:ASP:C	1:D:50:ARG:H	2.17	0.48
1:D:221:GLU:OE2	1:E:221:GLU:CD	2.52	0.48
1:A:70:ILE:HG22	1:A:71:TRP:O	2.14	0.48
1:B:200:ILE:O	1:B:204:MET:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HB	1:C:198:PRO:CD	2.37	0.48
1:C:70:ILE:HG22	1:C:71:TRP:N	2.29	0.48
1:B:18:ASN:O	1:B:44:LEU:HA	2.13	0.47
1:B:79:ASN:N	1:B:79:ASN:HD22	2.01	0.47
1:D:261:ILE:HD13	1:D:302:PHE:HE1	1.79	0.47
1:E:261:ILE:HD13	1:E:302:PHE:HE1	1.79	0.47
1:B:274:VAL:C	1:B:276:HIS:N	2.66	0.47
1:B:261:ILE:HD13	1:B:302:PHE:HE1	1.79	0.47
1:B:48:ASP:C	1:B:50:ARG:N	2.68	0.47
1:C:28:SER:HB2	1:C:37:LYS:HD2	1.97	0.47
1:A:119:PRO:HB3	1:A:196:TYR:HD2	1.79	0.47
1:A:221:GLU:OE2	1:B:221:GLU:CD	2.53	0.47
1:A:226:LEU:HA	1:A:226:LEU:HD22	1.59	0.47
1:A:224:VAL:O	1:A:226:LEU:N	2.47	0.47
1:B:133:SER:HB2	1:B:137:ARG:NH1	2.29	0.47
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.96	0.47
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.80	0.47
1:B:98:THR:O	1:B:98:THR:HG22	2.14	0.47
1:C:268:ALA:HA	1:C:298:PHE:HE1	1.77	0.47
1:A:217:SER:HB3	1:A:223:ASN:OD1	2.14	0.47
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.43	0.47
1:B:234:HIS:CE1	1:B:261:ILE:CG2	2.93	0.47
1:B:296:ILE:O	1:B:300:VAL:HG23	2.13	0.47
1:C:202:LEU:HD23	1:C:202:LEU:HA	1.56	0.47
1:D:62:VAL:HG13	1:D:93:VAL:O	2.14	0.47
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.26	0.47
1:B:78:VAL:CG2	1:B:130:ILE:HG12	2.38	0.47
1:A:221:GLU:OE2	1:B:221:GLU:OE2	2.33	0.47
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.93	0.47
1:B:254:THR:HA	1:B:257:ILE:HG12	1.97	0.47
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.67	0.47
1:C:222:ALA:O	1:C:226:LEU:HB2	2.14	0.47
1:C:270:ILE:HA	1:C:270:ILE:HD13	1.64	0.47
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.26	0.47
1:B:207:ILE:HG13	1:B:208:LEU:N	2.29	0.47
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.49	0.47
1:C:123:GLN:HB2	1:C:189:ILE:HG13	1.97	0.47
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.95	0.47
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.96	0.47
1:C:46:TRP:HH2	1:C:72:ILE:HG23	1.79	0.47
1:D:261:ILE:CD1	1:D:302:PHE:HE1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:PRO:HG3	1:D:91:ILE:HD11	1.95	0.47
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.30	0.47
1:E:264:PHE:HE2	1:E:302:PHE:HB2	1.79	0.47
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.45	0.47
1:A:70:ILE:HG22	1:A:71:TRP:N	2.29	0.47
1:D:119:PRO:HB3	1:D:196:TYR:HD2	1.78	0.47
1:D:238:ASN:HA	1:D:258:ILE:HD13	1.95	0.47
1:D:89:VAL:CG1	1:E:132:ARG:HD3	2.45	0.47
1:B:123:GLN:HB2	1:B:189:ILE:HG13	1.95	0.47
1:B:196:TYR:N	1:B:196:TYR:CD1	2.83	0.47
1:B:67:PRO:HG3	1:B:91:ILE:HD11	1.95	0.47
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.97	0.47
1:E:76:ARG:NH2	1:E:130:ILE:CD1	2.62	0.47
1:A:254:THR:HA	1:A:257:ILE:HG12	1.97	0.47
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.96	0.47
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.46	0.47
1:C:274:VAL:C	1:C:276:HIS:N	2.66	0.47
1:D:70:ILE:HG22	1:D:71:TRP:N	2.30	0.47
1:E:253:TYR:O	1:E:256:ALA:HB3	2.15	0.47
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.50	0.47
1:B:153:ASP:O	1:B:154:VAL:C	2.53	0.47
1:B:18:ASN:HB2	1:B:45:SER:OG	2.15	0.47
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.65	0.47
1:D:191:ARG:HG3	1:D:192:GLN:N	2.29	0.47
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.96	0.47
1:E:147:LYS:C	1:E:149:GLY:N	2.68	0.47
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.46	0.47
1:A:70:ILE:N	1:A:70:ILE:HD13	2.29	0.47
1:C:21:ILE:HA	1:C:41:PHE:O	2.15	0.47
1:E:48:ASP:O	1:E:50:ARG:N	2.48	0.47
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.97	0.47
1:A:76:ARG:CZ	1:A:130:ILE:HD12	2.44	0.46
1:A:194:PHE:O	1:A:198:PRO:HD2	2.14	0.46
1:B:194:PHE:O	1:B:196:TYR:N	2.49	0.46
1:E:196:TYR:CD1	1:E:196:TYR:N	2.84	0.46
1:E:261:ILE:CD1	1:E:302:PHE:HE1	2.27	0.46
1:A:143:VAL:O	1:A:143:VAL:HG12	2.15	0.46
1:A:196:TYR:CD1	1:A:196:TYR:N	2.82	0.46
1:A:207:ILE:HG13	1:A:208:LEU:N	2.30	0.46
1:E:153:ASP:O	1:E:154:VAL:C	2.53	0.46
1:E:194:PHE:O	1:E:196:TYR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:VAL:CG2	1:A:130:ILE:HG12	2.42	0.46
1:A:277:TYR:O	1:A:281:GLU:HG3	2.16	0.46
1:A:268:ALA:HA	1:A:298:PHE:HE1	1.80	0.46
1:C:261:ILE:HD13	1:C:302:PHE:HE1	1.80	0.46
1:E:137:ARG:HA	1:E:137:ARG:HD3	1.58	0.46
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.50	0.46
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.62	0.46
1:A:249:PRO:HD2	1:A:250:TYR:CE1	2.50	0.46
1:A:41:PHE:CZ	1:B:76:ARG:NH2	2.82	0.46
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.46	0.46
1:C:197:ILE:CB	1:C:198:PRO:HD3	2.36	0.46
1:C:249:PRO:HD2	1:C:250:TYR:CE1	2.51	0.46
1:C:252:THR:HB	1:C:255:GLY:H	1.79	0.46
1:D:207:ILE:HG13	1:D:208:LEU:N	2.31	0.46
1:D:277:TYR:O	1:D:281:GLU:HG3	2.16	0.46
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.79	0.46
1:D:95:PRO:C	1:D:97:GLY:H	2.17	0.46
1:E:256:ALA:HB1	1:E:309:LEU:HD21	1.96	0.46
1:A:153:ASP:O	1:A:154:VAL:C	2.51	0.46
1:A:196:TYR:HD1	1:A:196:TYR:N	2.14	0.46
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.78	0.46
1:A:194:PHE:CE2	1:B:250:TYR:O	2.63	0.46
1:B:277:TYR:O	1:B:281:GLU:HG3	2.16	0.46
1:B:268:ALA:HA	1:B:298:PHE:HE1	1.80	0.46
1:C:277:TYR:O	1:C:281:GLU:HG3	2.16	0.46
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.50	0.46
1:C:104:ARG:NH2	1:D:77:PHE:O	2.40	0.46
1:E:67:PRO:HG3	1:E:91:ILE:HD11	1.97	0.46
1:A:98:THR:HG22	1:A:98:THR:O	2.14	0.46
1:B:9:PRO:HB3	1:B:48:ASP:OD1	2.15	0.46
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.31	0.46
1:C:48:ASP:O	1:C:50:ARG:N	2.48	0.46
1:D:119:PRO:HD3	1:D:254:THR:OG1	2.15	0.46
1:E:78:VAL:CG2	1:E:130:ILE:HG12	2.42	0.46
1:B:48:ASP:C	1:B:50:ARG:H	2.18	0.46
1:C:191:ARG:HG3	1:C:192:GLN:N	2.31	0.46
1:C:306:ASN:O	1:C:310:ALA:N	2.44	0.46
1:D:70:ILE:HG22	1:D:71:TRP:O	2.16	0.46
1:E:123:GLN:HB2	1:E:189:ILE:HG13	1.97	0.46
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.81	0.46
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.59	0.46
1:B:196:TYR:HD1	1:B:196:TYR:N	2.13	0.46
1:C:254:THR:HA	1:C:257:ILE:HG12	1.98	0.46
1:D:222:ALA:HA	1:D:225:THR:HB	1.97	0.46
1:D:84:ARG:NH1	1:D:84:ARG:CB	2.76	0.46
1:E:202:LEU:HB2	1:E:203:PRO:HD3	1.97	0.46
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.44	0.46
1:E:119:PRO:HB3	1:E:196:TYR:CD2	2.51	0.46
1:A:48:ASP:C	1:A:50:ARG:N	2.70	0.45
1:B:245:LEU:HD12	1:B:245:LEU:HA	1.83	0.45
1:C:70:ILE:N	1:C:70:ILE:HD13	2.31	0.45
1:D:30:ASP:HB3	1:D:33:ALA:HB3	1.98	0.45
1:D:77:PHE:CE2	1:D:127:ILE:CG2	2.99	0.45
1:A:155:PHE:HE1	1:B:112:PRO:CB	2.23	0.45
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.16	0.45
1:D:268:ALA:HA	1:D:298:PHE:HE1	1.80	0.45
1:A:19:THR:HG22	1:A:44:LEU:HD23	1.99	0.45
1:A:202:LEU:CD1	1:B:259:PHE:HZ	2.30	0.45
1:A:243:THR:HG22	1:A:244:ASN:N	2.32	0.45
1:A:88:VAL:HG12	1:A:89:VAL:N	2.31	0.45
1:C:196:TYR:O	1:C:200:ILE:HB	2.17	0.45
1:C:261:ILE:CD1	1:C:302:PHE:HE1	2.30	0.45
1:C:52:ALA:HA	1:C:95:PRO:O	2.16	0.45
1:A:175:LEU:HA	1:A:175:LEU:HD12	1.67	0.45
1:A:261:ILE:O	1:A:262:TYR:C	2.54	0.45
1:B:28:SER:HB2	1:B:37:LYS:HD2	1.99	0.45
1:C:197:ILE:CG2	1:C:202:LEU:HG	2.47	0.45
1:E:77:PHE:CE2	1:E:127:ILE:CG2	3.00	0.45
1:E:252:THR:HB	1:E:255:GLY:H	1.82	0.45
1:E:270:ILE:HA	1:E:270:ILE:HD13	1.65	0.45
1:A:28:SER:HB2	1:A:37:LYS:HD2	1.99	0.45
1:A:21:ILE:HA	1:A:41:PHE:O	2.17	0.45
1:A:67:PRO:HG3	1:A:91:ILE:HD11	1.98	0.45
1:E:76:ARG:CZ	1:E:130:ILE:HD12	2.45	0.45
1:E:243:THR:HG22	1:E:244:ASN:N	2.31	0.45
1:E:27:TYR:CE1	1:E:37:LYS:HB2	2.52	0.45
1:E:66:GLU:HG3	1:E:67:PRO:CD	2.41	0.45
1:A:223:ASN:HD22	1:A:272:VAL:HG12	1.82	0.45
1:A:30:ASP:HB3	1:A:33:ALA:HB3	1.99	0.45
1:B:127:ILE:HB	1:B:185:TYR:HB2	1.99	0.45
1:B:256:ALA:HB1	1:B:309:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:TRP:CZ3	1:C:298:PHE:HB3	2.51	0.45
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.82	0.45
1:A:240:LEU:HD22	1:B:239:ILE:CD1	2.47	0.45
1:A:27:TYR:CB	1:B:110:LEU:CD1	2.90	0.45
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.47	0.45
1:E:277:TYR:O	1:E:281:GLU:HG3	2.16	0.45
1:E:52:ALA:HA	1:E:95:PRO:O	2.17	0.45
1:A:191:ARG:HG3	1:A:192:GLN:N	2.31	0.45
1:C:147:LYS:C	1:C:149:GLY:N	2.68	0.45
1:C:179:LEU:C	1:C:179:LEU:HD12	2.38	0.45
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.46	0.45
1:A:27:TYR:CD1	1:B:81:GLU:OE2	2.70	0.45
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.17	0.45
1:C:119:PRO:HB3	1:C:196:TYR:HD2	1.82	0.45
1:E:197:ILE:CG2	1:E:202:LEU:HG	2.47	0.45
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.98	0.45
1:A:179:LEU:HD12	1:A:179:LEU:C	2.38	0.44
1:A:260:MET:CE	1:A:309:LEU:HD22	2.41	0.44
1:A:89:VAL:CG1	1:B:132:ARG:HD3	2.47	0.44
1:B:147:LYS:C	1:B:149:GLY:N	2.68	0.44
1:B:78:VAL:HB	1:B:128:TYR:HB2	1.99	0.44
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.52	0.44
1:C:216:TRP:H	1:C:216:TRP:HE3	1.65	0.44
1:C:44:LEU:HD12	1:C:101:TYR:CE2	2.51	0.44
1:D:104:ARG:HH22	1:E:78:VAL:CA	2.15	0.44
1:D:198:PRO:O	1:E:259:PHE:HD1	2.00	0.44
1:E:243:THR:HG22	1:E:244:ASN:HD22	1.82	0.44
1:C:79:ASN:OD1	1:C:109:VAL:HG12	2.18	0.44
1:C:70:ILE:HG22	1:C:71:TRP:O	2.17	0.44
1:D:254:THR:HA	1:D:257:ILE:HG12	1.99	0.44
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.49	0.44
1:E:18:ASN:O	1:E:44:LEU:HA	2.17	0.44
1:A:147:LYS:C	1:A:149:GLY:N	2.68	0.44
1:A:261:ILE:CD1	1:A:302:PHE:HE1	2.30	0.44
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.48	0.44
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.94	0.44
1:E:118:TYR:CD1	1:E:245:LEU:HD21	2.53	0.44
1:E:133:SER:HB3	1:E:137:ARG:HA	1.98	0.44
1:E:179:LEU:HD12	1:E:179:LEU:C	2.38	0.44
1:B:179:LEU:C	1:B:179:LEU:HD12	2.38	0.44
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ILE:HA	1:E:41:PHE:O	2.16	0.44
1:E:53:PHE:HE2	1:E:63:LYS:CB	2.29	0.44
1:A:109:VAL:HG11	1:A:126:HIS:O	2.17	0.44
1:A:127:ILE:HB	1:A:185:TYR:HB2	1.99	0.44
1:A:217:SER:CB	1:B:220:TYR:CE2	3.00	0.44
1:A:270:ILE:HG22	1:A:271:GLU:N	2.31	0.44
1:A:212:TRP:CZ3	1:A:298:PHE:HB3	2.52	0.44
1:B:125:LEU:HB2	1:B:187:LEU:HB3	2.00	0.44
1:C:76:ARG:CZ	1:C:130:ILE:HD12	2.46	0.44
1:C:196:TYR:N	1:C:196:TYR:CD1	2.86	0.44
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.52	0.44
1:E:197:ILE:CB	1:E:198:PRO:HD3	2.40	0.44
1:A:23:LEU:HA	1:A:40:ALA:CB	2.48	0.44
1:B:261:ILE:CD1	1:B:302:PHE:HE1	2.31	0.44
1:B:314:PHE:N	1:B:314:PHE:CD1	2.85	0.44
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.71	0.44
1:C:203:PRO:HB3	1:D:262:TYR:CZ	2.53	0.44
1:D:212:TRP:CZ3	1:D:298:PHE:HB3	2.52	0.44
1:C:274:VAL:O	1:C:278:LEU:HB3	2.18	0.44
1:D:147:LYS:C	1:D:149:GLY:N	2.68	0.44
1:C:240:LEU:HD22	1:D:239:ILE:CG1	2.48	0.44
1:D:210:ILE:CG2	1:E:269:VAL:HG11	2.37	0.44
1:E:274:VAL:O	1:E:278:LEU:HB3	2.18	0.44
1:E:276:HIS:C	1:E:278:LEU:N	2.71	0.44
1:E:9:PRO:HB3	1:E:48:ASP:OD1	2.18	0.44
1:A:290:ILE:HG22	1:A:291:THR:N	2.31	0.44
1:B:77:PHE:CE2	1:B:127:ILE:CG2	3.00	0.44
1:C:264:PHE:HE2	1:C:302:PHE:HB2	1.83	0.44
1:D:296:ILE:O	1:D:300:VAL:HG23	2.17	0.44
1:A:296:ILE:HD13	1:A:296:ILE:HA	1.78	0.44
1:A:46:TRP:HH2	1:A:72:ILE:HG23	1.82	0.44
1:B:150:LYS:HG3	1:B:154:VAL:HG21	2.00	0.44
1:B:274:VAL:O	1:B:278:LEU:HB3	2.18	0.44
1:B:95:PRO:C	1:B:97:GLY:H	2.21	0.44
1:D:150:LYS:HG3	1:D:154:VAL:HG21	2.00	0.44
1:D:179:LEU:C	1:D:179:LEU:HD12	2.38	0.44
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.47	0.44
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.18	0.44
1:A:133:SER:HB2	1:A:137:ARG:NH1	2.33	0.43
1:A:119:PRO:HD3	1:A:254:THR:OG1	2.18	0.43
1:A:52:ALA:HA	1:A:95:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:HG11	1:B:126:HIS:O	2.17	0.43
1:C:132:ARG:CA	1:C:180:GLU:HG2	2.48	0.43
1:C:200:ILE:O	1:C:204:MET:CB	2.64	0.43
1:C:77:PHE:CE2	1:C:127:ILE:CG2	3.01	0.43
1:D:9:PRO:HB3	1:D:48:ASP:OD1	2.18	0.43
1:D:49:ARG:NH1	1:D:49:ARG:HB3	2.33	0.43
1:E:150:LYS:HG3	1:E:154:VAL:HG21	2.00	0.43
1:E:194:PHE:O	1:E:198:PRO:HD2	2.17	0.43
1:E:200:ILE:O	1:E:204:MET:CB	2.66	0.43
1:E:216:TRP:H	1:E:216:TRP:HE3	1.66	0.43
1:A:150:LYS:HG3	1:A:154:VAL:HG21	2.00	0.43
1:A:197:ILE:CB	1:A:198:PRO:HD3	2.39	0.43
1:B:66:GLU:HG3	1:B:67:PRO:CD	2.41	0.43
1:B:76:ARG:NH1	1:B:130:ILE:HD11	2.33	0.43
1:C:150:LYS:HG3	1:C:154:VAL:HG21	2.00	0.43
1:C:195:SER:O	1:C:199:ASN:HB2	2.19	0.43
1:D:53:PHE:CE1	1:D:95:PRO:CA	3.01	0.43
1:D:76:ARG:NH1	1:D:130:ILE:HD11	2.33	0.43
1:A:81:GLU:HG3	1:A:108:ARG:HG3	2.00	0.43
1:A:155:PHE:CZ	1:B:112:PRO:CB	2.95	0.43
1:D:157:THR:HG21	1:E:34:GLU:OE1	2.18	0.43
1:B:132:ARG:NH2	1:B:178:ARG:HB2	2.33	0.43
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.84	0.43
1:C:23:LEU:HB2	1:C:150:LYS:HA	2.00	0.43
1:E:196:TYR:N	1:E:196:TYR:HD1	2.16	0.43
1:E:223:ASN:HD22	1:E:272:VAL:HG12	1.83	0.43
1:E:72:ILE:HA	1:E:73:PRO:HD3	1.87	0.43
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.45	0.43
1:A:27:TYR:CD2	1:B:110:LEU:HD13	2.54	0.43
1:B:224:VAL:O	1:B:228:VAL:HB	2.19	0.43
1:A:233:ALA:HB2	1:B:232:ILE:HG12	2.01	0.43
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.18	0.43
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.17	0.43
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.99	0.43
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.53	0.43
1:E:46:TRP:HH2	1:E:72:ILE:HG23	1.83	0.43
1:A:125:LEU:HB2	1:A:187:LEU:HB3	2.00	0.43
1:A:225:THR:HG22	1:A:225:THR:O	2.18	0.43
1:B:76:ARG:CZ	1:B:130:ILE:HD12	2.40	0.43
1:B:232:ILE:O	1:B:235:ILE:HB	2.19	0.43
1:C:119:PRO:HD3	1:C:254:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:PHE:O	1:D:196:TYR:N	2.51	0.43
1:D:201:ILE:HA	1:D:201:ILE:HD13	1.86	0.43
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.48	0.43
1:E:283:GLN:H	1:E:284:PRO:HD3	1.82	0.43
1:E:48:ASP:C	1:E:50:ARG:N	2.71	0.43
1:A:274:VAL:O	1:A:278:LEU:HB3	2.18	0.43
1:A:276:HIS:C	1:A:278:LEU:N	2.71	0.43
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.53	0.43
1:C:194:PHE:O	1:C:198:PRO:HD2	2.19	0.43
1:C:88:VAL:HG12	1:C:89:VAL:N	2.34	0.43
1:E:225:THR:O	1:E:225:THR:HG22	2.18	0.43
1:A:194:PHE:O	1:A:196:TYR:N	2.51	0.43
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.49	0.43
1:A:261:ILE:HD13	1:A:302:PHE:HE1	1.83	0.43
1:A:44:LEU:HD12	1:A:101:TYR:CE2	2.54	0.43
1:A:192:GLN:OE1	1:B:249:PRO:HB3	2.19	0.43
1:C:226:LEU:HA	1:C:226:LEU:HD22	1.64	0.43
1:C:283:GLN:H	1:C:284:PRO:HD3	1.80	0.43
1:D:274:VAL:O	1:D:278:LEU:HB3	2.18	0.43
1:D:296:ILE:HG22	1:D:297:ALA:N	2.33	0.43
1:D:28:SER:HB2	1:D:37:LYS:HD2	2.01	0.43
1:A:314:PHE:CD1	1:A:314:PHE:N	2.87	0.43
1:A:48:ASP:HB3	1:A:51:LEU:CD2	2.49	0.43
1:C:72:ILE:HG22	1:C:73:PRO:HD2	2.00	0.43
1:D:127:ILE:HB	1:D:185:TYR:HB2	2.01	0.43
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.50	0.43
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.84	0.43
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.54	0.43
1:B:276:HIS:C	1:B:278:LEU:N	2.71	0.43
1:C:118:TYR:CD1	1:C:245:LEU:HD21	2.53	0.43
1:C:127:ILE:HB	1:C:185:TYR:HB2	2.01	0.43
1:C:243:THR:HG22	1:C:244:ASN:HD22	1.84	0.43
1:C:194:PHE:CE2	1:D:250:TYR:O	2.70	0.43
1:D:27:TYR:CE1	1:D:37:LYS:HB2	2.54	0.43
1:D:68:GLU:H	1:D:68:GLU:CD	2.22	0.43
1:E:179:LEU:O	1:E:179:LEU:HD12	2.19	0.43
1:E:270:ILE:HG22	1:E:271:GLU:N	2.34	0.43
1:A:202:LEU:HB2	1:A:203:PRO:HD3	2.01	0.42
1:B:119:PRO:HD3	1:B:254:THR:OG1	2.19	0.42
1:B:23:LEU:HA	1:B:40:ALA:CB	2.49	0.42
1:A:192:GLN:CG	1:B:249:PRO:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:THR:HG22	1:C:244:ASN:N	2.34	0.42
1:C:66:GLU:HG3	1:C:67:PRO:CD	2.45	0.42
1:E:48:ASP:C	1:E:50:ARG:H	2.22	0.42
1:A:238:ASN:HA	1:A:258:ILE:HD13	1.97	0.42
1:A:247:LYS:HA	1:A:247:LYS:HD3	1.80	0.42
1:A:53:PHE:O	1:A:54:ASP:C	2.58	0.42
1:B:225:THR:O	1:B:225:THR:HG22	2.18	0.42
1:B:27:TYR:CE1	1:B:37:LYS:HB2	2.54	0.42
1:B:30:ASP:HB3	1:B:33:ALA:HB3	2.01	0.42
1:D:276:HIS:C	1:D:278:LEU:N	2.71	0.42
1:E:119:PRO:HD3	1:E:254:THR:OG1	2.19	0.42
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.95	0.42
1:A:179:LEU:HD12	1:A:179:LEU:O	2.19	0.42
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.84	0.42
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.54	0.42
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.48	0.42
1:C:67:PRO:HG3	1:C:91:ILE:HD11	2.00	0.42
1:D:260:MET:CE	1:D:309:LEU:HD22	2.45	0.42
1:E:133:SER:HB2	1:E:137:ARG:HH11	1.82	0.42
1:E:291:THR:O	1:E:295:ARG:HG3	2.19	0.42
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.54	0.42
1:A:155:PHE:HE1	1:B:112:PRO:HB3	1.63	0.42
1:B:232:ILE:HA	1:B:235:ILE:HD12	2.01	0.42
1:B:243:THR:HG22	1:B:244:ASN:HD22	1.84	0.42
1:C:133:SER:HB3	1:C:137:ARG:HA	2.01	0.42
1:C:210:ILE:HG21	1:D:228:VAL:HG22	2.00	0.42
1:C:225:THR:O	1:C:225:THR:HG22	2.18	0.42
1:D:286:ARG:O	1:D:289:SER:N	2.45	0.42
1:E:143:VAL:HG12	1:E:143:VAL:O	2.20	0.42
1:E:191:ARG:HG3	1:E:192:GLN:N	2.34	0.42
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.55	0.42
1:B:202:LEU:HB2	1:B:203:PRO:HD3	2.01	0.42
1:C:183:LEU:HA	1:C:183:LEU:HD23	1.88	0.42
1:E:197:ILE:HB	1:E:198:PRO:CD	2.40	0.42
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.54	0.42
1:E:28:SER:HB2	1:E:37:LYS:HD2	2.02	0.42
1:E:53:PHE:O	1:E:53:PHE:CD1	2.72	0.42
1:E:53:PHE:O	1:E:54:ASP:C	2.58	0.42
1:A:53:PHE:CD1	1:A:53:PHE:O	2.72	0.42
1:B:226:LEU:HA	1:B:226:LEU:HD22	1.74	0.42
1:B:53:PHE:O	1:B:54:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:O	1:D:225:THR:HG22	2.19	0.42
1:D:53:PHE:O	1:D:54:ASP:C	2.58	0.42
1:E:243:THR:CG2	1:E:244:ASN:N	2.81	0.42
1:A:240:LEU:HD13	1:B:239:ILE:HG13	2.00	0.42
1:C:156:LEU:HA	1:C:156:LEU:HD12	1.73	0.42
1:C:53:PHE:CD1	1:C:53:PHE:O	2.72	0.42
1:C:95:PRO:C	1:C:97:GLY:H	2.23	0.42
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.55	0.42
1:D:78:VAL:HB	1:D:128:TYR:CB	2.48	0.42
1:E:95:PRO:C	1:E:97:GLY:H	2.23	0.42
1:B:13:GLU:OE1	1:B:14:PRO:HD3	2.20	0.42
1:B:197:ILE:CB	1:B:198:PRO:HD3	2.44	0.42
1:B:21:ILE:HA	1:B:41:PHE:O	2.20	0.42
1:B:7:PRO:O	1:B:50:ARG:NH1	2.50	0.42
1:C:201:ILE:HA	1:C:201:ILE:HD13	1.91	0.42
1:C:30:ASP:HB3	1:C:33:ALA:HB3	2.01	0.42
1:D:143:VAL:O	1:D:143:VAL:HG12	2.19	0.42
1:D:243:THR:HG22	1:D:244:ASN:N	2.35	0.42
1:D:53:PHE:O	1:D:53:PHE:CD1	2.72	0.42
1:E:254:THR:HA	1:E:257:ILE:HG12	2.01	0.42
1:A:23:LEU:HB2	1:A:150:LYS:HA	2.01	0.42
1:B:179:LEU:O	1:B:179:LEU:HD12	2.19	0.42
1:B:53:PHE:CD1	1:B:53:PHE:O	2.72	0.42
1:D:21:ILE:HA	1:D:41:PHE:O	2.20	0.42
1:A:42:LEU:HB3	1:A:103:GLU:HG3	2.02	0.42
1:A:213:THR:HG22	1:A:226:LEU:CD1	2.49	0.42
1:A:27:TYR:CE1	1:A:37:LYS:HB2	2.55	0.42
1:B:270:ILE:HG22	1:B:271:GLU:N	2.35	0.42
1:C:132:ARG:HH22	1:C:176:GLU:HB2	1.85	0.42
1:C:133:SER:HB2	1:C:137:ARG:HH11	1.85	0.42
1:C:314:PHE:CD1	1:C:314:PHE:N	2.87	0.42
1:D:179:LEU:O	1:D:179:LEU:HD12	2.19	0.42
1:D:202:LEU:HB2	1:D:203:PRO:HD3	2.02	0.42
1:D:72:ILE:HA	1:D:73:PRO:HD3	1.91	0.42
1:D:77:PHE:HE2	1:D:127:ILE:CG2	2.33	0.42
1:A:233:ALA:HB1	1:B:235:ILE:HD13	2.02	0.41
1:D:76:ARG:CZ	1:D:130:ILE:HD12	2.43	0.41
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.54	0.41
1:D:95:PRO:O	1:D:97:GLY:N	2.53	0.41
1:E:30:ASP:HB3	1:E:33:ALA:HB3	2.02	0.41
1:A:47:LYS:HD3	1:A:49:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:TRP:HH2	1:B:72:ILE:HG23	1.86	0.41
1:B:49:ARG:HB3	1:B:49:ARG:NH1	2.35	0.41
1:C:53:PHE:O	1:C:54:ASP:C	2.58	0.41
1:D:232:ILE:HA	1:D:235:ILE:HD12	2.01	0.41
1:E:222:ALA:HA	1:E:225:THR:HB	2.02	0.41
1:B:243:THR:HG22	1:B:244:ASN:N	2.35	0.41
1:B:34:GLU:OE2	1:B:113:LEU:N	2.49	0.41
1:B:78:VAL:HB	1:B:128:TYR:CB	2.51	0.41
1:C:179:LEU:O	1:C:179:LEU:HD12	2.19	0.41
1:C:232:ILE:HA	1:C:235:ILE:HD12	2.02	0.41
1:C:276:HIS:C	1:C:278:LEU:N	2.71	0.41
1:C:48:ASP:C	1:C:50:ARG:N	2.72	0.41
1:D:77:PHE:HE2	1:D:127:ILE:HG23	1.85	0.41
1:D:223:ASN:HD22	1:D:272:VAL:HG12	1.85	0.41
1:E:42:LEU:HB3	1:E:103:GLU:HG3	2.01	0.41
1:A:166:ALA:HB2	1:A:185:TYR:CD2	2.55	0.41
1:A:201:ILE:HA	1:A:201:ILE:HD13	1.88	0.41
1:A:232:ILE:CG2	1:A:233:ALA:N	2.81	0.41
1:B:222:ALA:HA	1:B:225:THR:HB	2.02	0.41
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.50	0.41
1:C:270:ILE:HG22	1:C:271:GLU:N	2.35	0.41
1:D:232:ILE:O	1:D:235:ILE:HB	2.21	0.41
1:D:264:PHE:HE2	1:D:302:PHE:HB2	1.84	0.41
1:E:300:VAL:O	1:E:304:LEU:HB2	2.20	0.41
1:A:232:ILE:HA	1:A:235:ILE:HD12	2.02	0.41
1:A:79:ASN:ND2	1:A:79:ASN:H	2.10	0.41
1:A:88:VAL:CG1	1:A:89:VAL:N	2.83	0.41
1:B:175:LEU:HA	1:B:175:LEU:HD12	1.67	0.41
1:A:41:PHE:CE2	1:B:175:LEU:HD23	2.46	0.41
1:C:194:PHE:O	1:C:197:ILE:N	2.43	0.41
1:D:41:PHE:CE2	1:E:175:LEU:HD23	2.36	0.41
1:E:296:ILE:HG22	1:E:297:ALA:N	2.35	0.41
1:A:78:VAL:HB	1:A:128:TYR:CB	2.51	0.41
1:A:77:PHE:CE2	1:A:127:ILE:CG2	3.03	0.41
1:C:224:VAL:O	1:C:226:LEU:N	2.53	0.41
1:D:109:VAL:HG11	1:D:126:HIS:O	2.20	0.41
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.56	0.41
1:D:252:THR:HB	1:D:255:GLY:H	1.85	0.41
1:E:314:PHE:CD1	1:E:314:PHE:N	2.89	0.41
1:A:133:SER:HB3	1:A:137:ARG:HA	2.01	0.41
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:O	1:B:198:PRO:HD2	2.21	0.41
1:B:224:VAL:O	1:B:226:LEU:N	2.53	0.41
1:B:72:ILE:HA	1:B:73:PRO:HD3	1.85	0.41
1:D:132:ARG:NH2	1:D:178:ARG:HB2	2.35	0.41
1:E:119:PRO:HB3	1:E:196:TYR:HD2	1.84	0.41
1:E:296:ILE:HA	1:E:296:ILE:HD13	1.83	0.41
1:A:216:TRP:HE3	1:A:216:TRP:H	1.68	0.41
1:A:240:LEU:HD22	1:B:239:ILE:HG13	2.02	0.41
1:A:48:ASP:C	1:A:50:ARG:H	2.22	0.41
1:B:243:THR:CG2	1:B:244:ASN:N	2.84	0.41
1:E:221:GLU:O	1:E:221:GLU:OE1	2.39	0.41
1:E:261:ILE:O	1:E:262:TYR:C	2.59	0.41
1:C:10:ILE:HG13	1:C:10:ILE:H	1.70	0.41
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.54	0.41
1:C:222:ALA:HA	1:C:225:THR:HB	2.02	0.41
1:C:48:ASP:C	1:C:50:ARG:H	2.24	0.41
1:D:132:ARG:CA	1:D:180:GLU:HG2	2.48	0.41
1:D:278:LEU:HD23	1:D:287:ALA:CA	2.51	0.41
1:A:140:VAL:HG22	1:A:181:SER:CB	2.51	0.41
1:A:157:THR:HG21	1:B:34:GLU:CG	2.49	0.41
1:A:200:ILE:O	1:A:204:MET:CB	2.68	0.41
1:A:226:LEU:HD22	1:B:228:VAL:HG21	2.01	0.41
1:A:9:PRO:HB3	1:A:48:ASP:OD1	2.20	0.41
1:B:278:LEU:HD23	1:B:287:ALA:CA	2.51	0.41
1:B:314:PHE:N	1:B:314:PHE:HD1	2.19	0.41
1:B:25:GLU:HB2	1:B:39:ASN:HB3	2.03	0.41
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.56	0.41
1:C:72:ILE:HA	1:C:73:PRO:HD3	1.85	0.41
1:E:72:ILE:HG22	1:E:73:PRO:HD2	2.03	0.41
1:E:79:ASN:ND2	1:E:79:ASN:H	2.08	0.41
1:A:147:LYS:CE	1:A:165:THR:HA	2.51	0.41
1:A:48:ASP:HB3	1:A:51:LEU:HD21	2.02	0.41
1:A:76:ARG:NH1	1:A:130:ILE:HD11	2.35	0.41
1:B:260:MET:CE	1:B:309:LEU:HD22	2.43	0.41
1:B:44:LEU:HD12	1:B:101:TYR:CE2	2.56	0.41
1:B:48:ASP:HB3	1:B:51:LEU:HD21	2.03	0.41
1:A:27:TYR:CE1	1:B:81:GLU:CD	2.95	0.41
1:D:229:SER:CB	1:E:228:VAL:HG11	2.51	0.41
1:A:132:ARG:NH2	1:A:178:ARG:HB2	2.36	0.40
1:B:301:VAL:HG12	1:B:301:VAL:O	2.21	0.40
1:C:130:ILE:CG2	1:C:182:LYS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:VAL:HB	1:C:128:TYR:HB2	2.03	0.40
1:D:125:LEU:HB2	1:D:187:LEU:HB3	2.03	0.40
1:D:41:PHE:HD1	1:D:41:PHE:HA	1.80	0.40
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.84	0.40
1:A:72:ILE:HG22	1:A:73:PRO:HD2	2.03	0.40
1:B:269:VAL:O	1:B:273:THR:HB	2.21	0.40
1:C:76:ARG:NH1	1:C:130:ILE:HD11	2.36	0.40
1:C:18:ASN:HB2	1:C:45:SER:OG	2.21	0.40
1:C:27:TYR:CE1	1:C:37:LYS:HB2	2.56	0.40
1:D:166:ALA:HB2	1:D:185:TYR:CD2	2.56	0.40
1:D:314:PHE:N	1:D:314:PHE:CD1	2.89	0.40
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.57	0.40
1:E:202:LEU:HD23	1:E:202:LEU:HA	1.59	0.40
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.56	0.40
1:E:247:LYS:HA	1:E:247:LYS:HD3	1.89	0.40
1:E:76:ARG:NH1	1:E:130:ILE:HD11	2.36	0.40
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.55	0.40
1:B:77:PHE:HE2	1:B:127:ILE:HG23	1.87	0.40
1:C:202:LEU:HB2	1:C:203:PRO:HD3	2.02	0.40
1:C:23:LEU:HD23	1:C:38:VAL:HG21	2.02	0.40
1:A:243:THR:CG2	1:A:244:ASN:N	2.84	0.40
1:A:94:SER:HB3	1:A:98:THR:HB	2.02	0.40
1:C:218:THR:HA	1:C:275:GLN:HE22	1.86	0.40
1:E:175:LEU:HA	1:E:175:LEU:HD12	1.67	0.40
1:A:27:TYR:OH	1:B:81:GLU:HA	2.22	0.40
1:D:133:SER:HB2	1:D:137:ARG:NH1	2.37	0.40
1:D:243:THR:CG2	1:D:244:ASN:N	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/317 (97%)	244 (79%)	55 (18%)	9 (3%)	4	32
1	B	308/317 (97%)	245 (80%)	55 (18%)	8 (3%)	5	34
1	C	308/317 (97%)	246 (80%)	51 (17%)	11 (4%)	3	29
1	D	308/317 (97%)	248 (80%)	51 (17%)	9 (3%)	4	32
1	E	308/317 (97%)	243 (79%)	54 (18%)	11 (4%)	3	29
All	All	1540/1585 (97%)	1226 (80%)	266 (17%)	48 (3%)	4	32

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	PHE
1	B	118	TYR
1	B	194	PHE
1	C	118	TYR
1	C	194	PHE
1	D	118	TYR
1	D	194	PHE
1	E	118	TYR
1	E	194	PHE
1	A	118	TYR
1	A	150	LYS
1	B	150	LYS
1	C	150	LYS
1	D	49	ARG
1	D	150	LYS
1	E	150	LYS
1	A	49	ARG
1	A	225	THR
1	A	275	GLN
1	A	277	TYR
1	B	49	ARG
1	B	225	THR
1	B	275	GLN
1	B	277	TYR
1	C	49	ARG
1	C	195	SER
1	C	225	THR
1	C	275	GLN
1	C	277	TYR
1	D	275	GLN
1	D	277	TYR

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Mol	Chain	Res	Type
1	E	195	SER
1	E	225	THR
1	E	275	GLN
1	E	277	TYR
1	A	148	VAL
1	B	148	VAL
1	C	148	VAL
1	D	148	VAL
1	D	225	THR
1	E	49	ARG
1	E	148	VAL
1	E	214	ALA
1	C	131	VAL
1	C	214	ALA
1	E	131	VAL
1	D	131	VAL
1	A	131	VAL

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	278/284 (98%)	228 (82%)	50 (18%)	1	11
1	B	278/284 (98%)	227 (82%)	51 (18%)	1	10
1	C	278/284 (98%)	229 (82%)	49 (18%)	2	12
1	D	278/284 (98%)	227 (82%)	51 (18%)	1	10
1	E	278/284 (98%)	226 (81%)	52 (19%)	1	10
All	All	1390/1420 (98%)	1137 (82%)	253 (18%)	1	11

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	26	CYS

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Mol	Chain	Res	Type
1	A	32	LYS
1	A	41	PHE
1	A	51	LEU
1	A	53	PHE
1	A	54	ASP
1	A	57	ARG
1	A	64	THR
1	A	68	GLU
1	A	72	ILE
1	A	79	ASN
1	A	84	ARG
1	A	89	VAL
1	A	98	THR
1	A	100	GLN
1	A	104	ARG
1	A	113	LEU
1	A	122	SER
1	A	124	THR
1	A	140	VAL
1	A	141	LEU
1	A	151	ASN
1	A	154	VAL
1	A	155	PHE
1	A	157	THR
1	A	177	ASP
1	A	179	LEU
1	A	211	SER
1	A	212	TRP
1	A	213	THR
1	A	218	THR
1	A	221	GLU
1	A	226	LEU
1	A	232	ILE
1	A	239	ILE
1	A	243	THR
1	A	252	THR
1	A	254	THR
1	A	258	ILE
1	A	263	LEU
1	A	270	ILE
1	A	273	THR
1	A	274	VAL

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Mol	Chain	Res	Type
1	A	282	SER
1	A	292	ARG
1	A	296	ILE
1	A	304	LEU
1	A	306	ASN
1	A	314	PHE
1	B	12	ASP
1	B	26	CYS
1	B	32	LYS
1	B	49	ARG
1	B	51	LEU
1	B	53	PHE
1	B	54	ASP
1	B	57	ARG
1	B	64	THR
1	B	68	GLU
1	B	72	ILE
1	B	79	ASN
1	B	84	ARG
1	B	89	VAL
1	B	98	THR
1	B	100	GLN
1	B	104	ARG
1	B	110	LEU
1	B	113	LEU
1	B	122	SER
1	B	124	THR
1	B	140	VAL
1	B	141	LEU
1	B	151	ASN
1	B	154	VAL
1	B	155	PHE
1	B	157	THR
1	B	177	ASP
1	B	179	LEU
1	B	195	SER
1	B	211	SER
1	B	212	TRP
1	B	213	THR
1	B	218	THR
1	B	221	GLU
1	B	226	LEU

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Mol	Chain	Res	Type
1	B	232	ILE
1	B	239	ILE
1	B	243	THR
1	B	252	THR
1	B	254	THR
1	B	258	ILE
1	B	263	LEU
1	B	270	ILE
1	B	273	THR
1	B	274	VAL
1	B	282	SER
1	B	292	ARG
1	B	296	ILE
1	B	304	LEU
1	B	306	ASN
1	C	12	ASP
1	C	26	CYS
1	C	32	LYS
1	C	51	LEU
1	C	53	PHE
1	C	54	ASP
1	C	57	ARG
1	C	64	THR
1	C	68	GLU
1	C	72	ILE
1	C	79	ASN
1	C	84	ARG
1	C	89	VAL
1	C	98	THR
1	C	100	GLN
1	C	104	ARG
1	C	110	LEU
1	C	113	LEU
1	C	122	SER
1	C	124	THR
1	C	140	VAL
1	C	141	LEU
1	C	151	ASN
1	C	154	VAL
1	C	155	PHE
1	C	157	THR
1	C	177	ASP

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Mol	Chain	Res	Type
1	C	179	LEU
1	C	211	SER
1	C	212	TRP
1	C	213	THR
1	C	218	THR
1	C	221	GLU
1	C	226	LEU
1	C	232	ILE
1	C	239	ILE
1	C	243	THR
1	C	252	THR
1	C	254	THR
1	C	258	ILE
1	C	263	LEU
1	C	270	ILE
1	C	273	THR
1	C	274	VAL
1	C	282	SER
1	C	292	ARG
1	C	296	ILE
1	C	304	LEU
1	C	306	ASN
1	D	12	ASP
1	D	26	CYS
1	D	32	LYS
1	D	49	ARG
1	D	51	LEU
1	D	53	PHE
1	D	54	ASP
1	D	57	ARG
1	D	64	THR
1	D	68	GLU
1	D	72	ILE
1	D	79	ASN
1	D	84	ARG
1	D	89	VAL
1	D	98	THR
1	D	100	GLN
1	D	104	ARG
1	D	110	LEU
1	D	113	LEU
1	D	122	SER

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Mol	Chain	Res	Type
1	D	124	THR
1	D	140	VAL
1	D	141	LEU
1	D	151	ASN
1	D	154	VAL
1	D	155	PHE
1	D	157	THR
1	D	177	ASP
1	D	179	LEU
1	D	195	SER
1	D	196	TYR
1	D	211	SER
1	D	212	TRP
1	D	213	THR
1	D	218	THR
1	D	221	GLU
1	D	226	LEU
1	D	232	ILE
1	D	239	ILE
1	D	243	THR
1	D	252	THR
1	D	254	THR
1	D	258	ILE
1	D	263	LEU
1	D	270	ILE
1	D	273	THR
1	D	274	VAL
1	D	282	SER
1	D	292	ARG
1	D	296	ILE
1	D	306	ASN
1	E	12	ASP
1	E	26	CYS
1	E	32	LYS
1	E	49	ARG
1	E	51	LEU
1	E	53	PHE
1	E	54	ASP
1	E	57	ARG
1	E	64	THR
1	E	68	GLU
1	E	72	ILE

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Mol	Chain	Res	Type
1	E	79	ASN
1	E	84	ARG
1	E	89	VAL
1	E	98	THR
1	E	100	GLN
1	E	104	ARG
1	E	110	LEU
1	E	113	LEU
1	E	122	SER
1	E	124	THR
1	E	140	VAL
1	E	141	LEU
1	E	151	ASN
1	E	154	VAL
1	E	155	PHE
1	E	157	THR
1	E	177	ASP
1	E	179	LEU
1	E	195	SER
1	E	211	SER
1	E	212	TRP
1	E	213	THR
1	E	218	THR
1	E	221	GLU
1	E	226	LEU
1	E	232	ILE
1	E	239	ILE
1	E	243	THR
1	E	252	THR
1	E	254	THR
1	E	258	ILE
1	E	260	MET
1	E	263	LEU
1	E	270	ILE
1	E	273	THR
1	E	274	VAL
1	E	282	SER
1	E	292	ARG
1	E	296	ILE
1	E	304	LEU
1	E	306	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	100	GLN
1	A	151	ASN
1	A	172	ASN
1	A	244	ASN
1	B	79	ASN
1	B	100	GLN
1	B	151	ASN
1	B	172	ASN
1	B	244	ASN
1	B	275	GLN
1	C	79	ASN
1	C	100	GLN
1	C	151	ASN
1	C	172	ASN
1	C	244	ASN
1	C	275	GLN
1	D	79	ASN
1	D	100	GLN
1	D	123	GLN
1	D	151	ASN
1	D	172	ASN
1	D	244	ASN
1	D	275	GLN
1	E	79	ASN
1	E	100	GLN
1	E	151	ASN
1	E	172	ASN
1	E	244	ASN
1	E	275	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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(Å ²)	Q<0.9
1	A	310/317 (97%)	-0.25	5 (1%) 72 61	57, 98, 154, 227	0
1	B	310/317 (97%)	-0.37	1 (0%) 94 90	59, 98, 154, 227	0
1	C	310/317 (97%)	-0.26	5 (1%) 72 61	58, 98, 154, 227	0
1	D	310/317 (97%)	-0.36	2 (0%) 89 83	59, 98, 154, 227	0
1	E	310/317 (97%)	-0.31	6 (1%) 66 55	58, 99, 154, 227	0
All	All	1550/1585 (97%)	-0.31	19 (1%) 79 69	57, 98, 154, 227	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	PHE	4.3
1	A	316	PHE	4.1
1	E	59	GLY	3.8
1	A	59	GLY	3.0
1	E	315	GLY	2.8
1	C	315	GLY	2.8
1	E	316	PHE	2.7
1	A	61	ARG	2.7
1	A	58	SER	2.6
1	E	58	SER	2.6
1	D	316	PHE	2.5
1	C	59	GLY	2.3
1	D	61	ARG	2.2
1	E	57	ARG	2.2
1	E	60	VAL	2.1
1	A	60	VAL	2.1
1	B	57	ARG	2.1
1	C	61	ARG	2.1
1	C	60	VAL	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SB	E	1316	1/1	0.95	0.44	151,151,151,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.