



Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2019 – 10:00 AM EDT

PDB ID : 6GCU
Title : MET receptor in complex with InlB internalin domain and DARPin A3A
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Deposited on : 2018-04-19
Resolution : 6.00 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 : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

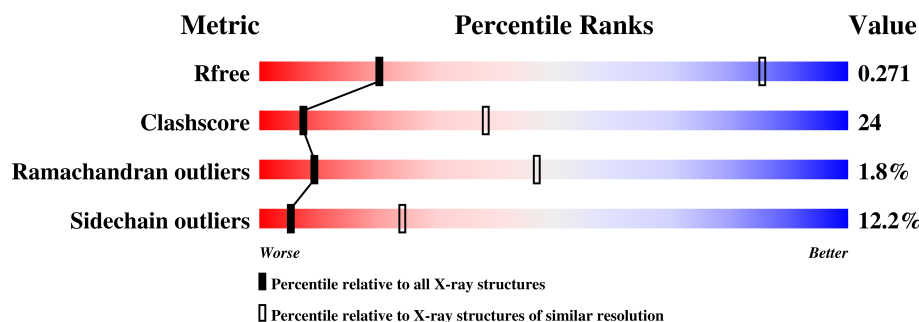
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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}	111664	1050 (8.20-3.80)
Clashscore	122126	1128 (8.20-3.80)
Ramachandran outliers	120053	1054 (8.20-3.80)
Sidechain outliers	120020	1024 (8.20-3.80)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	727	<div> <div>50%</div> <div>34%</div> <div>8%</div> <div>7%</div> </div>
1	D	727	<div> <div>52%</div> <div>32%</div> <div>9%</div> <div>7%</div> </div>
2	B	289	<div> <div>51%</div> <div>45%</div> <div>..</div> </div>
2	E	289	<div> <div>53%</div> <div>42%</div> <div>..</div> </div>
3	C	173	<div> <div>80%</div> <div>8%</div> <div>10%</div> </div>
3	F	173	<div> <div>81%</div> <div>8%</div> <div>10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17448 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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	0	0
			5314	3370	904	1002	38			
1	D	675	Total	C	N	O	S	0	0	0
			5314	3370	904	1002	38			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	-	expression tag	UNP P08581
A	23	THR	-	expression tag	UNP P08581
A	24	ARG	-	expression tag	UNP P08581
A	742	LEU	-	expression tag	UNP P08581
A	743	HIS	-	expression tag	UNP P08581
A	744	HIS	-	expression tag	UNP P08581
A	745	HIS	-	expression tag	UNP P08581
A	746	HIS	-	expression tag	UNP P08581
A	747	HIS	-	expression tag	UNP P08581
A	748	HIS	-	expression tag	UNP P08581
D	22	GLU	-	expression tag	UNP P08581
D	23	THR	-	expression tag	UNP P08581
D	24	ARG	-	expression tag	UNP P08581
D	742	LEU	-	expression tag	UNP P08581
D	743	HIS	-	expression tag	UNP P08581
D	744	HIS	-	expression tag	UNP P08581
D	745	HIS	-	expression tag	UNP P08581
D	746	HIS	-	expression tag	UNP P08581
D	747	HIS	-	expression tag	UNP P08581
D	748	HIS	-	expression tag	UNP P08581

- Molecule 2 is a protein called Internalin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	0	0
			2252	1435	378	437	2			
2	E	286	Total	C	N	O	S	0	0	0
			2252	1435	378	437	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	33	GLY	-	expression tag	UNP P25147
B	34	ALA	-	expression tag	UNP P25147
B	35	MET	-	expression tag	UNP P25147
E	33	GLY	-	expression tag	UNP P25147
E	34	ALA	-	expression tag	UNP P25147
E	35	MET	-	expression tag	UNP P25147

- Molecule 3 is a protein called DARPin A3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	155	Total	C	N	O	S	0	0	0
			1158	717	208	231	2			
3	F	155	Total	C	N	O	S	0	0	0
			1158	717	208	231	2			

3 Residue-property plots

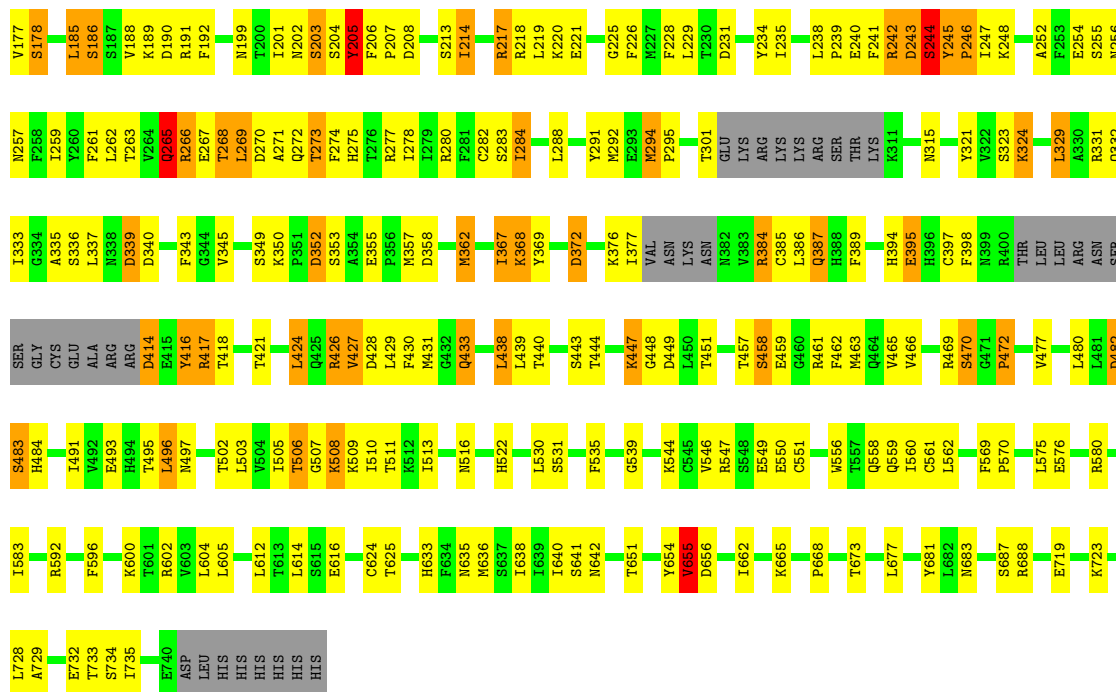
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: Hepatocyte growth factor receptor



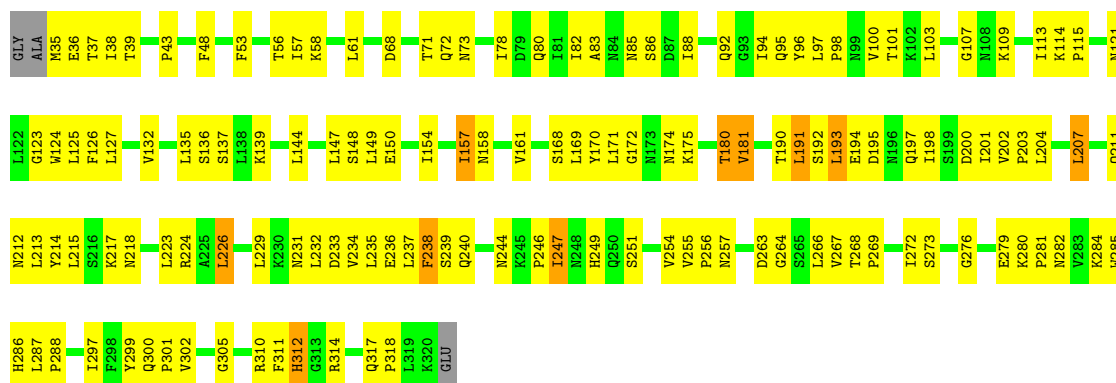
• Molecule 1: Hepatocyte growth factor receptor





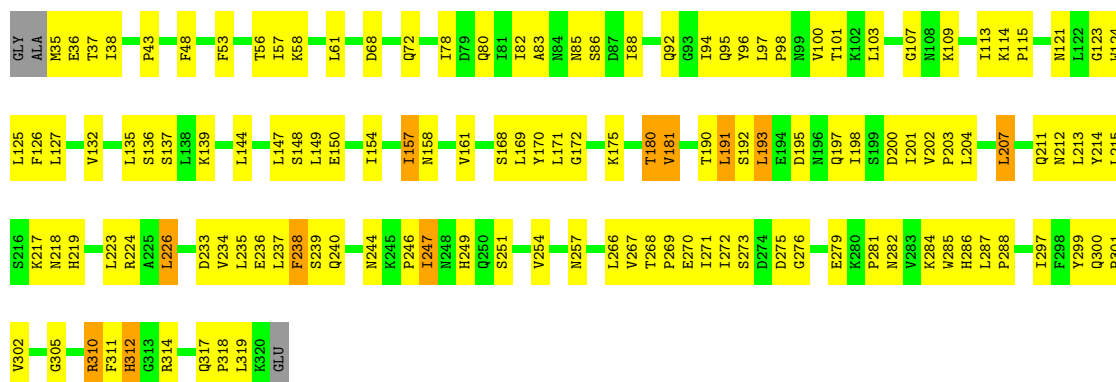
• Molecule 2: Internalin B

Chain B: 51% 45%

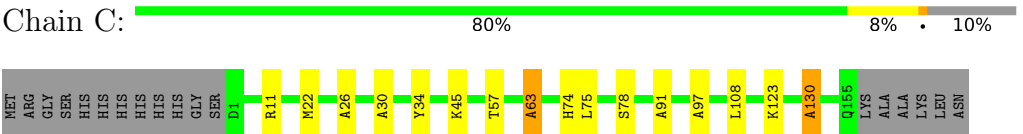


• Molecule 2: Internalin B

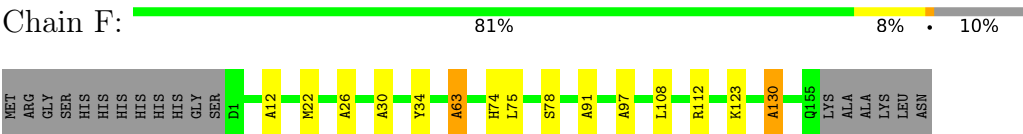
Chain E: 53% 42%



● Molecule 3: DARPin A3A



● Molecule 3: DARPin A3A



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 144.87Å 128.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.15 – 6.00 48.15 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.15-6.00) 99.8 (48.15-6.00)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 6.15Å)	Xtriage
Refinement program	PHENIX (dev_3071: ???)	Depositor
R, R_{free}	0.263 , 0.271 0.263 , 0.271	Depositor DCC
R_{free} test set	339 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	248.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 296.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.042 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	17448	wwPDB-VP
Average B, all atoms (Å ²)	317.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	2/5439 (0.0%)	0.98	23/7377 (0.3%)
1	D	0.50	1/5439 (0.0%)	0.77	17/7377 (0.2%)
2	B	0.25	0/2288	0.46	1/3105 (0.0%)
2	E	0.25	0/2288	0.52	3/3105 (0.1%)
3	C	0.93	3/1175 (0.3%)	0.82	5/1594 (0.3%)
3	F	0.94	3/1175 (0.3%)	0.83	5/1594 (0.3%)
All	All	0.54	9/17804 (0.1%)	0.79	54/24152 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	D	0	5
3	C	0	2
3	F	0	2
All	All	0	13

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	63	ALA	C-N	-17.98	0.92	1.34
3	F	63	ALA	C-N	-17.95	0.92	1.34
1	D	655	VAL	C-N	12.36	1.62	1.34
1	A	382	ASN	N-CA	-11.45	1.23	1.46
3	C	97	ALA	C-N	-10.00	1.11	1.34
3	F	97	ALA	C-N	-9.99	1.11	1.34
1	A	655	VAL	C-N	8.76	1.54	1.34
3	F	130	ALA	C-N	7.18	1.50	1.34
3	C	130	ALA	C-N	7.13	1.50	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	VAL	O-C-N	30.93	172.18	122.70
1	A	655	VAL	CA-C-N	-22.94	66.74	117.20
1	A	382	ASN	N-CA-CB	21.14	148.66	110.60
1	A	382	ASN	N-CA-C	-19.68	57.87	111.00
1	A	655	VAL	C-N-CA	-18.14	76.34	121.70
3	F	63	ALA	O-C-N	-17.44	94.80	122.70
3	C	63	ALA	O-C-N	-17.24	95.12	122.70
3	F	63	ALA	C-N-CA	13.69	155.93	121.70
3	C	63	ALA	C-N-CA	13.57	155.63	121.70
3	C	30	ALA	O-C-N	-12.47	102.75	122.70
3	F	30	ALA	O-C-N	-12.43	102.82	122.70
3	F	63	ALA	CA-C-N	11.11	141.65	117.20
3	C	63	ALA	CA-C-N	11.01	141.41	117.20
3	C	30	ALA	CA-C-N	8.76	136.46	117.20
3	F	30	ALA	CA-C-N	8.75	136.46	117.20
2	E	310	ARG	N-CA-C	8.00	132.59	111.00
2	E	238	PHE	N-CA-C	6.78	129.29	111.00
2	B	238	PHE	N-CA-C	6.77	129.28	111.00
1	D	128	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	128	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	100	ASP	CB-CG-OD1	6.34	124.01	118.30
1	D	100	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	358	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	358	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	231	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	231	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	428	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	190	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	190	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	414	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	123	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	123	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	428	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	352	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	352	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	339	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	414	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	77	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	208	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	208	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	77	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	339	ASP	CB-CG-OD2	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	243	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	372	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	243	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	482	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	153	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	127	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	482	ASP	CB-CG-OD1	5.12	122.90	118.30
1	D	372	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	153	ASP	CB-CG-OD2	5.05	122.85	118.30
2	E	310	ARG	N-CA-CB	-5.04	101.52	110.60
1	A	94	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	SER	Peptide
1	A	244	SER	Peptide
1	A	265	GLN	Peptide
1	A	274	PHE	Peptide
3	C	130	ALA	Mainchain
3	C	63	ALA	Mainchain
1	D	135	SER	Peptide
1	D	244	SER	Peptide
1	D	265	GLN	Peptide
1	D	274	PHE	Peptide
1	D	655	VAL	Mainchain
3	F	130	ALA	Mainchain
3	F	63	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5314	0	5162	311	23
1	D	5314	0	5159	322	17

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2252	0	2322	190	14
2	E	2252	0	2322	180	5
3	C	1158	0	1132	31	11
3	F	1158	0	1130	32	9
All	All	17448	0	17227	823	44

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 24.

All (823) 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:732:GLU:OE2	1:D:723:LYS:NZ	1.60	1.35
2:B:264:GLY:HA3	2:E:180:THR:CG2	1.57	1.31
1:D:602:ARG:NH2	2:E:170:TYR:OH	1.66	1.28
1:D:372:ASP:HB3	2:E:275:ASP:OD1	1.14	1.27
1:D:41:TYR:HE1	1:D:522:HIS:CD2	1.52	1.27
1:A:127:ASP:OD1	3:C:45:LYS:NZ	1.68	1.26
1:D:41:TYR:CE1	1:D:522:HIS:HD2	1.53	1.26
1:A:531:SER:OG	1:A:596:PHE:CE2	1.85	1.24
1:D:41:TYR:CE1	1:D:522:HIS:CD2	2.26	1.22
1:D:560:ILE:HG23	1:D:562:LEU:CD1	1.70	1.19
1:D:191:ARG:NH2	3:F:74:HIS:HB3	1.54	1.19
1:A:735:ILE:HG13	1:D:735:ILE:CG2	1.72	1.18
1:A:735:ILE:HG21	1:D:735:ILE:CG1	1.74	1.17
1:D:470:SER:OG	2:E:238:PHE:HB3	1.44	1.17
1:D:614:LEU:HD12	2:E:234:VAL:HG23	1.29	1.15
1:A:735:ILE:HD12	1:D:735:ILE:HD12	1.22	1.15
1:A:602:ARG:NH2	2:B:170:TYR:OH	1.80	1.14
1:D:614:LEU:CD1	2:E:234:VAL:CG2	2.26	1.12
1:D:376:LYS:HD2	2:E:275:ASP:HB3	1.18	1.12
1:D:614:LEU:HD13	2:E:234:VAL:CG2	1.79	1.11
1:D:560:ILE:HG23	1:D:562:LEU:HD11	1.17	1.11
1:D:560:ILE:CG2	1:D:562:LEU:CD1	2.28	1.10
2:B:264:GLY:HA3	2:E:180:THR:HG21	1.18	1.09
1:A:614:LEU:HB2	2:B:233:ASP:OD2	1.53	1.08
1:A:735:ILE:CG1	1:D:735:ILE:HG21	1.84	1.08
1:D:614:LEU:CD1	2:E:234:VAL:HG21	1.83	1.08
1:A:245:TYR:HB2	1:A:246:PRO:HD3	1.36	1.07
1:A:599:LYS:NZ	2:B:214:TYR:CD2	2.05	1.06
1:D:560:ILE:CG2	1:D:562:LEU:HD11	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:GLN:O	1:D:561:CYS:N	1.89	1.05
1:A:735:ILE:HG21	1:D:735:ILE:HG13	1.05	1.04
1:A:655:VAL:HG23	1:A:657:PRO:HD3	1.39	1.04
1:D:245:TYR:HB2	1:D:246:PRO:HD3	1.36	1.04
1:D:41:TYR:OH	1:D:522:HIS:NE2	1.91	1.03
1:A:602:ARG:HH21	2:B:168:SER:HB3	1.23	1.03
1:D:604:LEU:HD11	2:E:124:TRP:CZ2	1.94	1.02
2:B:224:ARG:HD3	2:E:180:THR:HG23	1.40	1.01
1:D:191:ARG:HH21	3:F:74:HIS:HB3	1.25	1.01
1:D:614:LEU:HD13	2:E:234:VAL:HG21	1.03	1.01
2:B:264:GLY:CA	2:E:180:THR:HG21	1.89	1.00
2:B:301:PRO:HB3	2:B:310:ARG:HG2	1.43	1.00
1:D:372:ASP:CB	2:E:275:ASP:OD1	2.09	1.00
1:A:191:ARG:HH22	3:C:74:HIS:C	1.65	1.00
1:A:191:ARG:HH12	3:C:75:LEU:HA	1.26	0.99
1:A:191:ARG:NH2	3:C:74:HIS:HB3	1.78	0.99
1:A:191:ARG:HH21	3:C:74:HIS:HB3	1.29	0.98
1:A:641:SER:HB3	2:B:124:TRP:CZ3	2.01	0.96
1:A:447:LYS:HD2	1:A:535:PHE:CB	1.95	0.95
1:A:604:LEU:CD1	2:B:124:TRP:CZ2	2.50	0.94
2:B:264:GLY:HA3	2:E:180:THR:HG22	1.49	0.94
1:A:600:LYS:HE3	2:B:126:PHE:CE1	2.03	0.93
1:D:191:ARG:HH22	3:F:74:HIS:C	1.69	0.93
1:A:735:ILE:CG2	1:D:735:ILE:CD1	2.46	0.93
2:B:193:LEU:HD22	2:B:198:ILE:HD11	1.51	0.93
1:A:41:TYR:OH	1:A:522:HIS:CD2	2.21	0.92
1:A:191:ARG:NH2	3:C:74:HIS:C	2.23	0.92
1:D:614:LEU:CD1	2:E:234:VAL:HG23	1.95	0.92
1:A:735:ILE:HG13	1:D:735:ILE:HG21	0.95	0.91
1:A:735:ILE:HG23	1:D:735:ILE:CD1	2.00	0.91
1:D:148:HIS:CE1	3:F:12:ALA:HA	2.06	0.91
1:A:376:LYS:O	1:A:377:ILE:C	2.09	0.91
1:A:531:SER:OG	1:A:596:PHE:HE2	1.32	0.91
1:D:85:LYS:HD2	1:D:85:LYS:H	1.35	0.91
1:D:426:ARG:CZ	2:E:271:ILE:HG23	2.00	0.91
2:E:193:LEU:HD22	2:E:198:ILE:HD11	1.51	0.90
1:A:447:LYS:HD2	1:A:535:PHE:HB3	1.50	0.90
1:A:85:LYS:H	1:A:85:LYS:HD2	1.35	0.90
1:A:735:ILE:CG2	1:D:735:ILE:HG13	1.98	0.90
2:B:301:PRO:CB	2:B:310:ARG:HG2	2.02	0.89
1:A:256:ASN:HD22	1:A:367:ILE:HD11	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:LEU:CD1	2:E:124:TRP:CZ2	2.57	0.88
1:D:427:VAL:HG23	2:E:270:GLU:OE2	1.73	0.88
1:D:469:ARG:NE	2:E:299:TYR:CE2	2.40	0.88
1:D:576:GLU:CD	1:D:729:ALA:HB2	1.95	0.88
1:D:256:ASN:HD22	1:D:367:ILE:HD11	1.38	0.87
1:A:430:PHE:O	1:A:431:MET:HG2	1.74	0.87
1:D:191:ARG:NH2	3:F:74:HIS:CB	2.37	0.87
1:D:430:PHE:O	1:D:431:MET:HG2	1.75	0.87
1:A:723:LYS:NZ	1:D:732:GLU:OE2	2.08	0.87
1:D:191:ARG:HH12	3:F:75:LEU:HA	1.39	0.86
1:A:735:ILE:HG23	1:D:735:ILE:HD12	1.58	0.86
1:D:191:ARG:CZ	3:F:108:LEU:HD13	2.05	0.86
1:A:124:THR:HG22	3:C:34:TYR:HE2	1.40	0.86
1:D:576:GLU:HB3	1:D:728:LEU:HB2	1.58	0.86
1:A:604:LEU:HD11	2:B:124:TRP:CZ2	2.10	0.85
1:A:127:ASP:CG	3:C:45:LYS:HZ1	1.79	0.85
1:A:735:ILE:CD1	1:D:735:ILE:HG23	2.07	0.85
1:A:574:PRO:HB2	1:A:729:ALA:HB2	1.57	0.84
1:D:426:ARG:NH2	2:E:271:ILE:HG23	1.93	0.84
1:D:600:LYS:HZ1	2:E:126:PHE:HE1	1.22	0.84
1:D:600:LYS:HE3	2:E:126:PHE:CE1	2.13	0.83
1:A:127:ASP:CG	3:C:45:LYS:NZ	2.30	0.83
1:A:332:GLN:NE2	1:A:469:ARG:H	1.77	0.83
1:A:614:LEU:CD1	2:B:212:ASN:OD1	2.27	0.83
1:D:332:GLN:NE2	1:D:469:ARG:H	1.77	0.82
1:A:516:ASN:O	1:A:535:PHE:HE1	1.59	0.82
1:D:531:SER:OG	1:D:596:PHE:CE2	2.32	0.82
1:A:269:LEU:CD2	1:A:269:LEU:H	1.92	0.82
1:A:614:LEU:HD11	2:B:212:ASN:OD1	1.77	0.82
1:D:41:TYR:CZ	1:D:522:HIS:CD2	2.68	0.82
1:D:560:ILE:CG2	1:D:562:LEU:HD12	2.10	0.82
1:D:269:LEU:H	1:D:269:LEU:CD2	1.92	0.81
1:D:600:LYS:NZ	2:E:126:PHE:HE1	1.77	0.81
1:A:469:ARG:NE	2:B:299:TYR:CE2	2.48	0.81
2:E:157:ILE:HG12	2:E:181:VAL:HG11	1.62	0.81
1:A:735:ILE:CG1	1:D:735:ILE:CG2	2.50	0.81
1:A:574:PRO:CB	1:A:729:ALA:HB2	2.10	0.81
2:B:157:ILE:HG12	2:B:181:VAL:HG11	1.62	0.81
1:A:735:ILE:CG2	1:D:735:ILE:CG1	2.58	0.81
1:A:239:PRO:HA	1:A:242:ARG:HD2	1.64	0.80
1:D:516:ASN:C	1:D:535:PHE:HE1	1.85	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:CG2	1:D:735:ILE:HD12	2.12	0.79
1:A:245:TYR:HB2	1:A:246:PRO:CD	2.12	0.79
1:A:735:ILE:HG21	1:D:735:ILE:CD1	2.12	0.79
2:E:226:LEU:H	2:E:226:LEU:HD12	1.48	0.79
1:D:600:LYS:CE	2:E:126:PHE:CE1	2.66	0.79
1:D:239:PRO:HA	1:D:242:ARG:HD2	1.64	0.79
1:D:530:LEU:HD12	1:D:561:CYS:SG	2.22	0.79
2:B:301:PRO:HA	2:B:310:ARG:HA	1.64	0.78
1:D:191:ARG:HH22	3:F:74:HIS:HB3	1.46	0.78
1:A:572:SER:OG	1:A:684:SER:HB3	1.83	0.78
1:D:469:ARG:NE	2:E:299:TYR:CD2	2.52	0.78
1:D:191:ARG:NH2	3:F:74:HIS:C	2.36	0.78
2:B:285:TRP:HB3	2:B:287:LEU:HD13	1.66	0.78
1:A:315:ASN:HD21	1:A:349:SER:HB2	1.49	0.78
1:D:470:SER:HG	2:E:238:PHE:HB3	1.48	0.78
1:A:431:MET:SD	2:B:310:ARG:NH1	2.57	0.78
1:D:191:ARG:NH2	3:F:108:LEU:CD1	2.47	0.78
1:A:516:ASN:O	1:A:535:PHE:CE1	2.37	0.77
1:A:602:ARG:NH2	2:B:168:SER:HB3	1.97	0.77
1:A:129:GLN:HE22	1:A:143:ARG:HE	1.31	0.77
1:A:600:LYS:CE	2:B:126:PHE:CE1	2.68	0.77
1:D:376:LYS:O	1:D:377:ILE:C	2.22	0.77
1:D:129:GLN:HE22	1:D:143:ARG:HE	1.31	0.77
1:D:655:VAL:HB	1:D:681:TYR:CG	2.20	0.77
1:A:470:SER:OG	2:B:238:PHE:HB3	1.83	0.77
2:B:247:ILE:HB	2:B:317:GLN:HE21	1.49	0.77
1:D:604:LEU:HD11	2:E:124:TRP:HZ2	1.50	0.77
1:D:516:ASN:HB3	1:D:535:PHE:CE1	2.20	0.77
2:E:247:ILE:HB	2:E:317:GLN:HE21	1.49	0.77
2:B:226:LEU:HD12	2:B:226:LEU:H	1.48	0.76
1:D:560:ILE:HG23	1:D:562:LEU:CG	2.15	0.76
1:D:245:TYR:HB2	1:D:246:PRO:CD	2.12	0.76
2:B:224:ARG:NH1	2:E:202:VAL:HB	2.00	0.76
1:D:516:ASN:O	1:D:535:PHE:CE1	2.38	0.76
1:D:315:ASN:HD21	1:D:349:SER:HB2	1.49	0.75
1:A:600:LYS:HD2	2:B:170:TYR:CZ	2.21	0.75
2:E:285:TRP:HB3	2:E:287:LEU:HD13	1.66	0.75
1:D:427:VAL:CG2	2:E:270:GLU:OE2	2.34	0.75
1:D:516:ASN:CB	1:D:535:PHE:CE1	2.70	0.75
1:D:221:GLU:OE2	3:F:112:ARG:NH2	2.18	0.75
1:A:572:SER:OG	1:A:684:SER:CB	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ILE:HG13	2:B:137:SER:HB2	1.68	0.75
1:A:162:PHE:HD1	1:A:162:PHE:C	1.89	0.75
1:D:469:ARG:HE	2:E:299:TYR:HE2	1.33	0.75
1:D:191:ARG:NE	3:F:108:LEU:CD1	2.50	0.74
1:A:516:ASN:OD1	1:A:535:PHE:CD1	2.40	0.74
1:D:162:PHE:HD1	1:D:162:PHE:C	1.89	0.74
1:A:191:ARG:NH2	3:C:74:HIS:O	2.20	0.74
1:D:505:ILE:HG13	1:D:510:ILE:HD12	1.70	0.74
1:D:426:ARG:NH1	2:E:271:ILE:CG2	2.50	0.74
1:A:505:ILE:HG13	1:A:510:ILE:HD12	1.70	0.74
1:D:191:ARG:NE	3:F:108:LEU:HD13	2.01	0.74
1:A:332:GLN:HE22	1:A:469:ARG:H	1.34	0.74
2:E:113:ILE:HG13	2:E:137:SER:HB2	1.68	0.73
1:D:560:ILE:HG22	1:D:562:LEU:HD12	1.69	0.73
2:B:224:ARG:HD3	2:E:180:THR:CG2	2.18	0.73
1:D:332:GLN:HE22	1:D:469:ARG:H	1.34	0.73
1:A:52:ILE:HD13	1:A:64:LEU:HD22	1.72	0.72
1:A:447:LYS:HD2	1:A:535:PHE:HB2	1.71	0.72
1:A:600:LYS:HD3	2:B:170:TYR:CE2	2.24	0.72
1:A:614:LEU:HD12	2:B:233:ASP:OD2	1.90	0.72
1:D:331:ARG:HG2	2:E:314:ARG:NH2	2.04	0.72
1:A:245:TYR:CB	1:A:246:PRO:HD3	2.18	0.72
1:D:600:LYS:NZ	2:E:126:PHE:CE1	2.56	0.72
1:A:600:LYS:HA	2:B:170:TYR:OH	1.89	0.71
1:D:191:ARG:HH21	3:F:108:LEU:HD11	1.55	0.71
1:A:599:LYS:HE3	2:B:234:VAL:HG11	1.72	0.71
2:B:247:ILE:HB	2:B:317:GLN:NE2	2.05	0.71
1:A:600:LYS:HE3	2:B:126:PHE:HE1	1.53	0.71
2:E:247:ILE:HB	2:E:317:GLN:NE2	2.05	0.71
1:A:191:ARG:NH2	3:C:74:HIS:CB	2.54	0.70
1:A:97:PRO:HG2	1:A:162:PHE:HE2	1.56	0.70
1:D:426:ARG:NH1	2:E:271:ILE:HG23	2.07	0.70
1:D:602:ARG:HH21	2:E:168:SER:HB3	1.57	0.70
1:D:41:TYR:OH	1:D:522:HIS:CD2	2.43	0.70
1:D:614:LEU:HD12	2:E:234:VAL:CG2	1.97	0.70
1:D:516:ASN:C	1:D:535:PHE:CE1	2.65	0.70
1:D:191:ARG:CZ	3:F:108:LEU:CD1	2.70	0.70
1:D:52:ILE:HD13	1:D:64:LEU:HD22	1.71	0.70
1:D:655:VAL:HB	1:D:681:TYR:CD1	2.27	0.69
1:D:331:ARG:CG	2:E:314:ARG:HH22	2.04	0.69
1:A:600:LYS:CE	2:B:126:PHE:HE1	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:SER:OG	1:A:596:PHE:CD2	2.44	0.69
1:A:735:ILE:CD1	1:D:735:ILE:HD12	2.13	0.69
2:B:80:GLN:HE21	2:B:82:ILE:HD11	1.58	0.69
1:D:41:TYR:CZ	1:D:522:HIS:NE2	2.61	0.69
1:A:191:ARG:HD3	3:C:78:SER:OG	1.93	0.69
1:D:600:LYS:CE	2:E:126:PHE:HE1	2.06	0.69
1:D:162:PHE:CD1	1:D:162:PHE:C	2.63	0.69
2:E:80:GLN:HE21	2:E:82:ILE:HD11	1.58	0.69
1:A:476:HIS:ND1	1:A:533:PRO:HG2	2.08	0.68
1:D:191:ARG:HH21	3:F:108:LEU:CD1	2.07	0.68
1:D:602:ARG:HH22	2:E:170:TYR:HH	1.41	0.68
1:D:97:PRO:HG2	1:D:162:PHE:HE2	1.56	0.68
1:A:162:PHE:C	1:A:162:PHE:CD1	2.63	0.68
1:D:191:ARG:HE	3:F:108:LEU:CD1	2.07	0.67
2:B:204:LEU:HA	2:B:207:LEU:HD22	1.77	0.67
1:D:275:HIS:CE1	1:D:295:PRO:HB3	2.30	0.67
1:D:191:ARG:HH22	3:F:74:HIS:CB	2.01	0.66
1:D:614:LEU:HD11	2:E:212:ASN:OD1	1.95	0.66
2:E:254:VAL:HG22	2:E:284:LYS:HG2	1.78	0.66
1:A:275:HIS:CE1	1:A:295:PRO:HB3	2.30	0.66
1:A:636:MET:HE1	1:A:654:TYR:HD2	1.61	0.66
2:B:202:VAL:HB	2:E:224:ARG:HH12	1.61	0.66
1:A:614:LEU:CB	2:B:233:ASP:OD2	2.38	0.66
1:A:735:ILE:CD1	1:D:735:ILE:CG2	2.73	0.65
2:B:192:SER:O	2:B:193:LEU:HG	1.96	0.65
1:D:576:GLU:OE2	1:D:729:ALA:CB	2.43	0.65
2:E:192:SER:O	2:E:193:LEU:HG	1.96	0.65
1:A:719:GLU:HB3	1:D:735:ILE:HG13	1.79	0.65
2:E:204:LEU:HA	2:E:207:LEU:HD22	1.77	0.65
2:B:202:VAL:CG1	2:E:224:ARG:NH1	2.60	0.65
2:B:254:VAL:HG22	2:B:284:LYS:HG2	1.77	0.65
1:D:516:ASN:O	1:D:535:PHE:CZ	2.50	0.64
1:D:138:ARG:HH11	1:D:138:ARG:HA	1.62	0.64
1:A:127:ASP:OD2	3:C:45:LYS:NZ	2.29	0.64
1:D:331:ARG:HG3	2:E:314:ARG:HH22	1.62	0.64
2:B:235:LEU:HD12	2:B:236:GLU:H	1.63	0.64
1:D:560:ILE:HG22	1:D:562:LEU:CD1	2.23	0.64
2:E:235:LEU:HD12	2:E:236:GLU:H	1.63	0.64
1:A:600:LYS:NZ	2:B:126:PHE:HE1	1.95	0.64
1:A:191:ARG:NE	3:C:108:LEU:HD13	2.12	0.64
1:A:469:ARG:HD3	2:B:299:TYR:HD2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:HD12	1:D:735:ILE:HG23	1.79	0.64
1:A:600:LYS:CD	2:B:170:TYR:CE2	2.81	0.64
2:B:236:GLU:HG2	2:B:238:PHE:CE2	2.32	0.64
1:D:470:SER:OG	2:E:238:PHE:CB	2.33	0.64
1:A:138:ARG:HA	1:A:138:ARG:HH11	1.62	0.64
1:A:604:LEU:HD12	2:B:124:TRP:CZ2	2.31	0.63
1:D:636:MET:HE1	1:D:654:TYR:HD2	1.62	0.63
1:D:426:ARG:NH1	2:E:271:ILE:HG21	2.12	0.63
1:D:457:THR:HG22	1:D:459:GLU:H	1.63	0.63
1:A:457:THR:HG22	1:A:459:GLU:H	1.63	0.63
1:A:518:LEU:O	1:A:519:GLY:O	2.17	0.63
2:E:236:GLU:HG2	2:E:238:PHE:CE2	2.33	0.63
1:A:469:ARG:HD3	2:B:299:TYR:CD2	2.34	0.63
1:A:641:SER:CB	2:B:124:TRP:CZ3	2.81	0.63
1:A:269:LEU:H	1:A:269:LEU:HD22	1.63	0.62
2:B:202:VAL:HB	2:E:224:ARG:NH1	2.14	0.62
2:B:36:GLU:HG3	2:B:95:GLN:HB3	1.80	0.62
2:B:86:SER:HB2	2:B:88:ILE:HG13	1.81	0.62
2:E:36:GLU:HG3	2:E:95:GLN:HB3	1.80	0.62
1:D:191:ARG:NH2	3:F:74:HIS:O	2.33	0.62
1:D:580:ARG:NH2	1:D:616:GLU:OE2	2.33	0.62
1:A:148:HIS:CE1	3:C:11:ARG:NH1	2.68	0.62
1:D:600:LYS:HD2	2:E:170:TYR:CZ	2.34	0.62
1:D:604:LEU:CD1	2:E:124:TRP:HZ2	2.09	0.62
1:A:580:ARG:NH2	1:A:616:GLU:OE2	2.33	0.61
2:E:94:ILE:HD12	2:E:97:LEU:HD13	1.82	0.61
2:B:94:ILE:HD12	2:B:97:LEU:HD13	1.82	0.61
1:A:476:HIS:CG	1:A:533:PRO:CG	2.84	0.61
2:B:224:ARG:HH12	2:E:202:VAL:HB	1.65	0.61
1:D:576:GLU:OE2	1:D:729:ALA:HA	2.01	0.61
1:A:482:ASP:HB2	1:A:506:THR:HG21	1.82	0.61
1:D:269:LEU:H	1:D:269:LEU:HD22	1.63	0.61
2:E:86:SER:HB2	2:E:88:ILE:HG13	1.81	0.61
1:A:476:HIS:CG	1:A:533:PRO:HG3	2.35	0.61
1:D:470:SER:HG	2:E:238:PHE:CB	2.10	0.61
2:E:246:PRO:HA	2:E:318:PRO:HB2	1.82	0.61
2:B:53:PHE:O	2:B:57:ILE:HG12	2.01	0.61
1:D:191:ARG:HH11	1:D:191:ARG:HG2	1.66	0.61
1:A:570:PRO:HD3	1:A:686:ASN:HD21	1.67	0.60
1:A:735:ILE:HG13	1:D:719:GLU:HB3	1.83	0.60
1:A:191:ARG:NH1	3:C:75:LEU:HA	2.07	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:157:ILE:HD13	2:E:157:ILE:H	1.66	0.60
1:A:269:LEU:H	1:A:269:LEU:HD23	1.66	0.60
1:A:604:LEU:HD12	2:B:124:TRP:CH2	2.37	0.60
1:D:245:TYR:CB	1:D:246:PRO:HD3	2.18	0.60
2:B:246:PRO:HA	2:B:318:PRO:HB2	1.82	0.60
1:D:256:ASN:O	1:D:257:ASN:HB2	2.00	0.60
1:D:482:ASP:HB2	1:D:506:THR:HG21	1.82	0.60
2:B:264:GLY:CA	2:E:180:THR:CG2	2.50	0.60
1:A:191:ARG:HH11	1:A:191:ARG:HG2	1.65	0.60
2:B:279:GLU:HB3	2:B:284:LYS:HE3	1.83	0.60
1:D:191:ARG:CD	3:F:108:LEU:HD22	2.32	0.60
2:E:213:LEU:HD11	2:E:215:LEU:HD21	1.84	0.60
2:E:285:TRP:HB3	2:E:287:LEU:CD1	2.32	0.60
1:A:469:ARG:NE	2:B:299:TYR:CD2	2.70	0.60
1:A:600:LYS:NZ	2:B:148:SER:HB2	2.16	0.60
1:A:68:ASN:HB3	1:A:87:GLY:HA2	1.84	0.60
2:E:53:PHE:O	2:E:57:ILE:HG12	2.01	0.60
2:B:157:ILE:HD13	2:B:157:ILE:H	1.66	0.60
2:B:56:THR:HG21	2:B:83:ALA:HB2	1.83	0.60
1:D:68:ASN:HB3	1:D:87:GLY:HA2	1.84	0.60
1:D:124:THR:HG22	3:F:34:TYR:HE2	1.65	0.60
1:A:600:LYS:HZ1	2:B:126:PHE:HE1	1.44	0.59
2:B:213:LEU:HD11	2:B:215:LEU:HD21	1.84	0.59
1:A:256:ASN:O	1:A:257:ASN:HB2	2.00	0.59
2:E:279:GLU:HB3	2:E:284:LYS:HE3	1.83	0.59
1:D:191:ARG:HE	3:F:108:LEU:HD11	1.67	0.59
1:A:384:ARG:HD3	1:A:387:GLN:HE22	1.67	0.59
1:A:516:ASN:HA	1:A:535:PHE:CE1	2.37	0.59
1:A:129:GLN:NE2	1:A:143:ARG:HE	2.01	0.59
2:E:56:THR:HG21	2:E:83:ALA:HB2	1.83	0.59
1:A:191:ARG:HE	3:C:108:LEU:CD1	2.16	0.59
2:B:285:TRP:HB3	2:B:287:LEU:CD1	2.32	0.59
1:A:331:ARG:CG	2:B:314:ARG:HH22	2.15	0.59
1:D:324:LYS:HE3	1:D:340:ASP:OD1	2.03	0.59
1:A:614:LEU:HD13	2:B:234:VAL:HG21	1.85	0.59
1:A:604:LEU:HG	2:B:124:TRP:HZ2	1.67	0.59
1:D:384:ARG:HD3	1:D:387:GLN:HE22	1.68	0.59
1:A:324:LYS:HE3	1:A:340:ASP:OD1	2.03	0.59
1:D:576:GLU:CD	1:D:729:ALA:CB	2.71	0.59
1:A:602:ARG:HH21	2:B:168:SER:CB	2.09	0.58
1:D:214:ILE:N	1:D:214:ILE:HD13	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HD13	1:A:214:ILE:N	2.18	0.58
1:A:570:PRO:HD3	1:A:686:ASN:ND2	2.18	0.58
1:D:600:LYS:HD3	2:E:170:TYR:CE2	2.39	0.58
1:A:600:LYS:NZ	2:B:126:PHE:CE1	2.70	0.58
1:D:576:GLU:OE1	1:D:729:ALA:HB2	2.03	0.58
2:E:157:ILE:CG1	2:E:181:VAL:HG11	2.33	0.58
1:A:191:ARG:CZ	3:C:108:LEU:HD13	2.33	0.58
1:A:599:LYS:HE3	2:B:234:VAL:CG1	2.34	0.58
1:A:191:ARG:HH22	3:C:75:LEU:N	2.01	0.58
1:D:64:LEU:HD11	1:D:73:LEU:HD11	1.86	0.58
2:B:299:TYR:HD1	2:B:301:PRO:HD3	1.69	0.58
1:D:416:TYR:N	1:D:416:TYR:CD1	2.71	0.58
1:A:527:SER:HA	1:A:561:CYS:SG	2.44	0.57
1:A:447:LYS:CD	1:A:535:PHE:CB	2.78	0.57
1:A:547:ARG:NH1	1:A:549:GLU:OE2	2.38	0.57
2:B:136:SER:O	2:B:139:LYS:HG3	2.04	0.57
1:A:614:LEU:HD11	2:B:212:ASN:CG	2.25	0.57
1:D:269:LEU:HD23	1:D:269:LEU:H	1.66	0.57
1:A:41:TYR:OH	1:A:522:HIS:HD2	1.81	0.57
1:A:735:ILE:HG23	1:D:735:ILE:HD11	1.85	0.57
2:B:157:ILE:CG1	2:B:181:VAL:HG11	2.33	0.57
1:D:124:THR:HG23	1:D:124:THR:O	2.04	0.57
1:A:124:THR:HG22	3:C:34:TYR:CE2	2.29	0.57
1:A:64:LEU:HD11	1:A:73:LEU:HD11	1.86	0.57
1:A:191:ARG:HD3	3:C:78:SER:CB	2.34	0.57
1:D:465:VAL:HG12	1:D:466:VAL:N	2.20	0.57
1:A:465:VAL:HG12	1:A:466:VAL:N	2.20	0.57
1:A:719:GLU:HB3	1:D:735:ILE:CG1	2.35	0.57
1:A:124:THR:O	1:A:124:THR:HG23	2.04	0.57
1:D:516:ASN:CA	1:D:535:PHE:CE1	2.87	0.57
2:E:299:TYR:HD1	2:E:301:PRO:HD3	1.69	0.57
1:D:604:LEU:HD12	2:E:124:TRP:CH2	2.40	0.57
1:D:96:PHE:HB3	1:D:97:PRO:HD3	1.87	0.57
1:A:98:CYS:SG	1:A:162:PHE:HB3	2.45	0.56
1:A:614:LEU:HD13	2:B:234:VAL:CG2	2.35	0.56
2:B:148:SER:HA	2:B:170:TYR:HB2	1.88	0.56
1:D:191:ARG:NH2	3:F:108:LEU:HD13	2.16	0.56
1:D:575:LEU:HD11	1:D:656:ASP:HB2	1.85	0.56
2:E:136:SER:O	2:E:139:LYS:HG3	2.05	0.56
1:A:96:PHE:HB3	1:A:97:PRO:HD3	1.88	0.56
1:D:531:SER:HG	1:D:596:PHE:HE2	1.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:ARG:NH1	1:D:549:GLU:OE2	2.38	0.56
1:A:332:GLN:O	2:B:297:ILE:HG21	2.06	0.56
1:D:641:SER:HB3	2:E:124:TRP:CZ3	2.41	0.56
1:D:98:CYS:SG	1:D:162:PHE:HB3	2.46	0.56
1:D:283:SER:C	1:D:284:ILE:HG12	2.27	0.56
1:D:576:GLU:OE2	1:D:729:ALA:HB2	2.05	0.56
1:D:331:ARG:CG	2:E:314:ARG:NH2	2.66	0.56
1:A:85:LYS:H	1:A:85:LYS:CD	2.08	0.56
1:A:595:LYS:HE2	2:B:236:GLU:OE2	2.05	0.56
1:D:683:ASN:HA	1:D:688:ARG:HE	1.71	0.56
1:A:604:LEU:HD11	2:B:124:TRP:CE2	2.40	0.56
2:B:180:THR:HG23	2:E:224:ARG:HD3	1.87	0.56
1:A:220:LYS:HG3	1:A:225:GLY:O	2.05	0.55
1:A:592:ARG:NH1	2:B:170:TYR:HD2	2.04	0.55
1:A:416:TYR:CD1	1:A:416:TYR:N	2.71	0.55
1:D:220:LYS:HG3	1:D:225:GLY:O	2.06	0.55
2:E:148:SER:HA	2:E:170:TYR:HB2	1.87	0.55
1:A:593:ASN:ND2	2:B:194:GLU:OE2	2.39	0.55
1:A:683:ASN:HA	1:A:688:ARG:HE	1.70	0.55
1:D:129:GLN:NE2	1:D:143:ARG:HE	2.01	0.55
1:A:602:ARG:NE	2:B:168:SER:OG	2.40	0.55
1:A:269:LEU:N	1:A:269:LEU:CD2	2.66	0.54
1:A:96:PHE:HB3	1:A:97:PRO:CD	2.37	0.54
1:D:482:ASP:HB2	1:D:506:THR:CG2	2.37	0.54
1:D:48:ALA:HB1	1:D:71:TYR:CE2	2.43	0.54
1:A:331:ARG:HG2	2:B:314:ARG:NH2	2.22	0.54
2:B:38:ILE:O	2:B:38:ILE:HG13	2.07	0.54
2:B:48:PHE:HA	2:B:92:GLN:O	2.07	0.54
1:D:469:ARG:HD3	2:E:299:TYR:HD2	1.72	0.54
2:E:48:PHE:HA	2:E:92:GLN:O	2.08	0.54
1:A:572:SER:OG	1:A:684:SER:HB2	2.07	0.54
1:A:368:LYS:HD3	1:A:369:TYR:CE1	2.43	0.54
1:A:447:LYS:CD	1:A:535:PHE:HB2	2.37	0.54
1:D:516:ASN:OD1	1:D:535:PHE:CZ	2.61	0.54
1:D:733:THR:OG1	1:D:734:SER:N	2.40	0.54
1:D:96:PHE:HB3	1:D:97:PRO:CD	2.37	0.54
1:A:283:SER:C	1:A:284:ILE:HG12	2.27	0.54
1:A:482:ASP:HB2	1:A:506:THR:CG2	2.37	0.54
2:E:299:TYR:CD1	2:E:301:PRO:HD3	2.43	0.54
2:E:94:ILE:HA	2:E:97:LEU:HD13	1.90	0.54
1:D:482:ASP:O	1:D:484:HIS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ARG:HG3	2:B:314:ARG:HH22	1.73	0.54
2:B:94:ILE:HA	2:B:97:LEU:HD13	1.90	0.54
2:E:150:GLU:HG2	2:E:172:GLY:H	1.74	0.53
2:E:150:GLU:HG2	2:E:172:GLY:N	2.23	0.53
1:A:191:ARG:NE	3:C:108:LEU:CD1	2.71	0.53
2:B:147:LEU:HD11	2:B:149:LEU:HG	1.90	0.53
2:B:150:GLU:HG2	2:B:172:GLY:H	1.74	0.53
1:D:315:ASN:ND2	1:D:349:SER:HB2	2.22	0.53
1:A:602:ARG:NH2	2:B:170:TYR:CZ	2.74	0.53
1:A:48:ALA:HB1	1:A:71:TYR:CE2	2.43	0.53
1:D:368:LYS:HD3	1:D:369:TYR:CE1	2.43	0.53
1:D:662:ILE:HG22	1:D:677:LEU:HD22	1.91	0.53
1:A:482:ASP:O	1:A:484:HIS:N	2.41	0.53
2:B:169:LEU:HG	2:B:171:LEU:HG	1.91	0.53
2:B:299:TYR:CD1	2:B:301:PRO:HD3	2.43	0.53
2:E:38:ILE:HG13	2:E:38:ILE:O	2.07	0.53
1:A:719:GLU:HB2	1:D:735:ILE:HG12	1.90	0.53
1:A:41:TYR:CZ	1:A:522:HIS:HD2	2.27	0.53
1:A:662:ILE:HG22	1:A:677:LEU:HD22	1.91	0.53
2:B:150:GLU:HG2	2:B:172:GLY:N	2.23	0.53
1:A:600:LYS:CD	2:B:170:TYR:CZ	2.92	0.53
1:D:604:LEU:HD12	2:E:124:TRP:CZ2	2.44	0.53
1:A:55:VAL:CG2	1:A:64:LEU:HD23	2.40	0.52
1:A:96:PHE:CB	1:A:97:PRO:HD3	2.39	0.52
2:B:113:ILE:HG13	2:B:137:SER:CB	2.39	0.52
2:E:113:ILE:HG13	2:E:137:SER:CB	2.39	0.52
1:A:476:HIS:CG	1:A:533:PRO:HG2	2.43	0.52
1:D:560:ILE:HG23	1:D:562:LEU:HG	1.89	0.52
2:E:147:LEU:HD11	2:E:149:LEU:HG	1.91	0.52
1:D:55:VAL:CG2	1:D:64:LEU:HD23	2.40	0.52
1:A:345:VAL:HG22	1:A:362:MET:HB2	1.92	0.52
2:E:299:TYR:HE1	2:E:301:PRO:HG3	1.74	0.52
1:A:56:ILE:HD11	1:A:120:LEU:O	2.09	0.52
1:D:426:ARG:HH12	2:E:271:ILE:CG2	2.22	0.52
1:D:583:ILE:HD13	1:D:640:ILE:HD11	1.90	0.52
1:D:191:ARG:HH22	3:F:74:HIS:CA	2.21	0.52
1:D:544:LYS:HB3	1:D:546:VAL:HG23	1.92	0.52
1:D:96:PHE:CB	1:D:97:PRO:HD3	2.39	0.52
2:B:213:LEU:HD12	2:B:214:TYR:H	1.74	0.52
1:D:600:LYS:CD	2:E:170:TYR:CE2	2.93	0.52
1:D:614:LEU:CD1	2:E:212:ASN:OD1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HB3	1:A:546:VAL:HG23	1.92	0.52
2:B:169:LEU:HD11	2:B:171:LEU:HD21	1.91	0.52
2:B:251:SER:HA	2:B:287:LEU:O	2.10	0.52
2:E:169:LEU:HD11	2:E:171:LEU:HD21	1.91	0.52
2:E:251:SER:HA	2:E:287:LEU:O	2.10	0.52
1:A:583:ILE:HD13	1:A:640:ILE:HD11	1.90	0.52
1:D:332:GLN:O	2:E:297:ILE:HG21	2.10	0.52
1:D:56:ILE:HD11	1:D:120:LEU:O	2.09	0.52
1:A:431:MET:CE	1:A:472:PRO:HA	2.40	0.51
2:B:202:VAL:CB	2:E:224:ARG:HH12	2.22	0.51
2:B:299:TYR:HE1	2:B:301:PRO:HG3	1.74	0.51
1:A:235:ILE:HG23	1:A:389:PHE:CD1	2.46	0.51
1:A:288:LEU:O	1:A:417:ARG:NH2	2.44	0.51
1:D:345:VAL:HG22	1:D:362:MET:HB2	1.92	0.51
1:A:551:CYS:SG	1:A:556:TRP:HB2	2.50	0.51
1:D:41:TYR:HH	1:D:522:HIS:CE1	2.16	0.51
1:D:551:CYS:SG	1:D:556:TRP:HB2	2.50	0.51
2:E:169:LEU:HG	2:E:171:LEU:HG	1.91	0.51
2:E:213:LEU:HD12	2:E:214:TYR:H	1.74	0.51
1:A:350:LYS:HG3	1:A:357:MET:HG3	1.93	0.51
1:A:329:LEU:HD12	1:A:451:THR:HG21	1.93	0.51
1:A:577:GLY:O	1:A:728:LEU:HB2	2.11	0.51
1:A:732:GLU:OE2	1:D:723:LYS:CE	2.54	0.51
1:A:735:ILE:HD12	1:D:735:ILE:CD1	2.16	0.51
2:E:35:MET:HE3	2:E:35:MET:HA	1.93	0.51
1:A:192:PHE:CE1	1:A:218:ARG:NH1	2.79	0.51
1:D:192:PHE:CE1	1:D:218:ARG:NH1	2.79	0.51
1:A:576:GLU:OE1	1:A:576:GLU:N	2.43	0.51
2:B:263:ASP:O	2:E:180:THR:HG22	2.10	0.51
1:D:288:LEU:O	1:D:417:ARG:NH2	2.44	0.51
1:D:447:LYS:HD2	1:D:535:PHE:HB3	1.93	0.51
2:E:223:LEU:HD11	2:E:311:PHE:CG	2.46	0.51
2:B:266:LEU:HD13	2:B:281:PRO:HB3	1.93	0.50
1:A:614:LEU:HD12	2:B:212:ASN:OD1	2.11	0.50
2:B:223:LEU:HD11	2:B:311:PHE:CG	2.46	0.50
1:D:569:PHE:CD1	1:D:570:PRO:HA	2.47	0.50
1:A:469:ARG:CD	2:B:299:TYR:CD2	2.94	0.50
1:D:235:ILE:HG23	1:D:389:PHE:CD1	2.46	0.50
1:A:569:PHE:CD1	1:A:570:PRO:HA	2.47	0.50
1:D:516:ASN:O	1:D:535:PHE:HE1	1.83	0.50
2:E:266:LEU:HD13	2:E:281:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:LEU:HD13	2:B:132:VAL:HG21	1.94	0.50
2:E:53:PHE:HB2	2:E:88:ILE:HG23	1.94	0.50
1:A:86:THR:O	1:A:87:GLY:O	2.30	0.50
2:B:125:LEU:HD12	2:B:126:PHE:N	2.27	0.50
2:E:218:ASN:O	2:E:240:GLN:HA	2.12	0.50
1:D:426:ARG:HH12	2:E:271:ILE:HG21	1.75	0.50
1:A:733:THR:OG1	1:A:734:SER:N	2.40	0.50
2:B:123:GLY:O	2:B:144:LEU:HD12	2.12	0.50
1:D:576:GLU:N	1:D:576:GLU:OE1	2.42	0.50
2:E:272:ILE:HG22	2:E:273:SER:N	2.27	0.50
1:A:191:ARG:HG2	1:A:191:ARG:NH1	2.27	0.49
1:D:118:MET:CE	1:D:118:MET:HA	2.42	0.49
1:D:124:THR:HG22	3:F:34:TYR:CE2	2.46	0.49
1:D:350:LYS:HG3	1:D:357:MET:HG3	1.93	0.49
1:D:86:THR:O	1:D:87:GLY:O	2.30	0.49
1:A:592:ARG:HH12	2:B:170:TYR:HD2	1.60	0.49
2:B:218:ASN:O	2:B:240:GLN:HA	2.12	0.49
1:D:191:ARG:NH2	3:F:74:HIS:CA	2.74	0.49
2:E:127:LEU:HD13	2:E:132:VAL:HG21	1.94	0.49
2:E:123:GLY:O	2:E:144:LEU:HD12	2.12	0.49
1:D:576:GLU:OE2	1:D:729:ALA:CA	2.59	0.49
1:D:614:LEU:HB2	2:E:233:ASP:OD2	2.12	0.49
1:D:655:VAL:CG1	1:D:681:TYR:CD1	2.96	0.49
1:D:269:LEU:HD23	1:D:269:LEU:N	2.27	0.49
1:A:118:MET:HA	1:A:118:MET:CE	2.43	0.49
1:A:559:GLN:O	1:A:561:CYS:N	2.46	0.49
2:B:272:ILE:HG22	2:B:273:SER:N	2.27	0.49
1:D:238:LEU:HD12	1:D:241:PHE:HE2	1.78	0.49
1:A:719:GLU:CB	1:D:735:ILE:CG1	2.90	0.49
2:E:85:ASN:HA	2:E:107:GLY:O	2.13	0.49
2:B:202:VAL:CB	2:E:224:ARG:NH1	2.76	0.49
2:E:244:ASN:HB2	2:E:317:GLN:OE1	2.13	0.49
1:D:51:PRO:HA	1:D:508:LYS:HB3	1.95	0.48
2:B:244:ASN:HB2	2:B:317:GLN:OE1	2.13	0.48
2:E:125:LEU:HD12	2:E:126:PHE:N	2.28	0.48
2:E:238:PHE:CE1	2:E:310:ARG:HB2	2.49	0.48
1:D:191:ARG:NH2	3:F:108:LEU:HD11	2.18	0.48
1:A:580:ARG:HG2	1:A:625:THR:HG22	1.95	0.48
2:B:235:LEU:HD12	2:B:236:GLU:N	2.27	0.48
1:D:139:GLY:O	1:D:176:VAL:N	2.45	0.48
1:A:191:ARG:HH21	3:C:108:LEU:CD1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:CG1	1:D:719:GLU:HB3	2.44	0.48
2:E:58:LYS:HD2	2:E:58:LYS:C	2.34	0.48
1:A:315:ASN:ND2	1:A:349:SER:HB2	2.22	0.48
1:A:438:LEU:HB3	1:A:458:SER:OG	2.13	0.48
1:A:92:HIS:ND1	1:A:94:ASP:HB2	2.28	0.48
1:D:191:ARG:NH1	1:D:191:ARG:HG2	2.28	0.48
1:A:55:VAL:HG22	1:A:64:LEU:HD23	1.96	0.48
2:B:114:LYS:N	2:B:115:PRO:CD	2.76	0.48
2:B:53:PHE:HB2	2:B:88:ILE:HG23	1.94	0.48
1:D:329:LEU:HD12	1:D:451:THR:HG21	1.93	0.48
1:D:85:LYS:CD	1:D:85:LYS:H	2.08	0.48
1:A:173:PRO:O	1:A:226:PHE:HB2	2.14	0.48
2:B:190:THR:HG22	2:B:191:LEU:N	2.29	0.48
2:E:114:LYS:N	2:E:115:PRO:CD	2.76	0.48
1:A:275:HIS:CD2	1:A:277:ARG:HE	2.32	0.48
1:A:530:LEU:HD22	1:A:558:GLN:HA	1.96	0.48
2:B:85:ASN:HA	2:B:107:GLY:O	2.14	0.48
1:D:416:TYR:H	1:D:416:TYR:HD1	1.60	0.48
2:B:301:PRO:CA	2:B:310:ARG:HG2	2.44	0.48
1:A:331:ARG:CG	2:B:314:ARG:NH2	2.77	0.48
1:A:148:HIS:HE1	3:C:11:ARG:NH1	2.12	0.48
1:D:592:ARG:NH1	2:E:170:TYR:HD2	2.11	0.48
1:A:329:LEU:O	1:A:333:ILE:HG13	2.14	0.48
2:B:58:LYS:C	2:B:58:LYS:HD2	2.34	0.48
1:D:140:THR:CG2	1:D:140:THR:O	2.62	0.48
1:D:503:LEU:HB3	1:D:510:ILE:HD11	1.95	0.48
2:E:235:LEU:HD12	2:E:236:GLU:N	2.27	0.48
1:D:329:LEU:O	1:D:333:ILE:HG13	2.14	0.47
1:D:655:VAL:CB	1:D:681:TYR:CD1	2.95	0.47
1:D:92:HIS:ND1	1:D:94:ASP:HB2	2.28	0.47
2:E:36:GLU:HG3	2:E:95:GLN:CB	2.44	0.47
1:A:599:LYS:CE	2:B:234:VAL:CG1	2.92	0.47
1:A:431:MET:SD	2:B:310:ARG:CZ	3.01	0.47
1:D:343:PHE:HD1	1:D:362:MET:HE1	1.78	0.47
1:D:438:LEU:HB3	1:D:458:SER:OG	2.13	0.47
1:D:173:PRO:O	1:D:226:PHE:HB2	2.14	0.47
1:A:503:LEU:HB3	1:A:510:ILE:HD11	1.96	0.47
2:E:190:THR:HG22	2:E:191:LEU:N	2.29	0.47
1:D:266:ARG:O	1:D:267:GLU:C	2.53	0.47
1:A:140:THR:CG2	1:A:140:THR:O	2.62	0.47
1:A:191:ARG:NH2	3:C:108:LEU:CD1	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD12	1:D:186:SER:N	2.30	0.47
1:A:268:THR:O	1:A:271:ALA:HB3	2.15	0.47
1:A:593:ASN:HD21	2:B:194:GLU:CD	2.18	0.47
1:D:275:HIS:CD2	1:D:277:ARG:HE	2.32	0.47
1:A:185:LEU:HD12	1:A:186:SER:N	2.30	0.47
1:A:431:MET:SD	1:A:472:PRO:HB3	2.55	0.47
1:A:614:LEU:CD1	2:B:233:ASP:OD2	2.61	0.47
2:B:158:ASN:O	2:B:161:VAL:HG12	2.14	0.47
2:B:266:LEU:CD1	2:B:281:PRO:HB3	2.45	0.47
1:A:294:MET:HE3	1:A:424:LEU:HB2	1.97	0.47
1:D:430:PHE:C	1:D:431:MET:HG2	2.34	0.47
1:D:530:LEU:HD22	1:D:558:GLN:HA	1.96	0.47
2:E:158:ASN:O	2:E:161:VAL:HG12	2.14	0.47
2:E:239:SER:HA	2:E:312:HIS:ND1	2.30	0.47
1:A:269:LEU:N	1:A:269:LEU:HD23	2.27	0.47
1:A:271:ALA:O	1:A:273:THR:N	2.48	0.47
2:B:301:PRO:HG3	2:B:310:ARG:HD3	1.97	0.47
1:D:119:ALA:HB3	1:D:133:CYS:HB2	1.97	0.47
2:E:266:LEU:CD1	2:E:281:PRO:HB3	2.45	0.47
2:B:43:PRO:HA	2:B:68:ASP:O	2.16	0.46
1:D:271:ALA:O	1:D:273:THR:N	2.48	0.46
1:A:51:PRO:HA	1:A:508:LYS:HB3	1.95	0.46
1:A:430:PHE:C	1:A:431:MET:HG2	2.34	0.46
1:A:604:LEU:CG	2:B:124:TRP:CZ2	2.97	0.46
1:A:735:ILE:HG12	1:D:719:GLU:HB2	1.97	0.46
1:D:580:ARG:HG2	1:D:625:THR:HG22	1.96	0.46
1:A:238:LEU:HD12	1:A:241:PHE:HE2	1.79	0.46
1:D:55:VAL:HG22	1:D:64:LEU:HD23	1.96	0.46
1:D:600:LYS:HA	2:E:170:TYR:OH	2.15	0.46
2:E:43:PRO:HA	2:E:68:ASP:O	2.15	0.46
1:A:447:LYS:CD	1:A:535:PHE:HB3	2.32	0.46
1:D:64:LEU:HD12	1:D:71:TYR:HB2	1.98	0.46
1:A:600:LYS:HZ1	2:B:148:SER:HB2	1.79	0.46
2:E:157:ILE:HD13	2:E:157:ILE:N	2.31	0.46
1:A:119:ALA:HB3	1:A:133:CYS:HB2	1.97	0.46
1:A:64:LEU:HD12	1:A:71:TYR:HB2	1.98	0.46
2:B:215:LEU:HB2	2:B:237:LEU:HD23	1.98	0.46
1:D:268:THR:O	1:D:271:ALA:HB3	2.15	0.46
1:A:602:ARG:HH22	2:B:170:TYR:HH	1.56	0.46
2:B:157:ILE:HD13	2:B:157:ILE:N	2.31	0.46
2:B:264:GLY:C	2:E:180:THR:HG21	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:ILE:HB	2:E:204:LEU:HD12	1.97	0.46
2:E:215:LEU:HB2	2:E:237:LEU:HD23	1.98	0.46
2:E:267:VAL:HG13	2:E:300:GLN:HB2	1.98	0.46
2:B:169:LEU:HD21	2:B:171:LEU:HD11	1.98	0.45
2:B:239:SER:HA	2:B:312:HIS:ND1	2.31	0.45
2:E:169:LEU:HD21	2:E:171:LEU:HD11	1.98	0.45
1:D:294:MET:HA	1:D:295:PRO:HD2	1.76	0.45
2:E:38:ILE:HG12	2:E:72:GLN:OE1	2.17	0.45
1:A:266:ARG:O	1:A:267:GLU:C	2.53	0.45
1:A:335:ALA:O	1:A:336:SER:HB3	2.16	0.45
2:B:267:VAL:HG22	2:B:300:GLN:HG2	1.99	0.45
2:B:36:GLU:HG3	2:B:95:GLN:CB	2.44	0.45
2:B:38:ILE:HG12	2:B:72:GLN:OE1	2.17	0.45
1:D:124:THR:CG2	1:D:124:THR:O	2.65	0.45
2:E:48:PHE:CE2	2:E:57:ILE:HG13	2.52	0.45
1:A:139:GLY:O	1:A:176:VAL:N	2.46	0.45
2:B:267:VAL:HG13	2:B:300:GLN:HB2	1.98	0.45
2:B:48:PHE:CE2	2:B:57:ILE:HG13	2.52	0.45
2:E:267:VAL:HG22	2:E:300:GLN:HG2	1.98	0.45
1:A:243:ASP:O	1:A:245:TYR:HA	2.17	0.45
1:A:687:SER:HA	1:A:688:ARG:NH1	2.32	0.45
2:B:201:ILE:HB	2:B:204:LEU:HD12	1.98	0.45
2:B:286:HIS:O	2:B:288:PRO:HD3	2.17	0.45
1:D:469:ARG:CD	2:E:299:TYR:CD2	2.99	0.45
2:E:149:LEU:HB3	2:E:154:ILE:HD11	1.99	0.45
1:A:254:GLU:HG3	1:A:259:ILE:HD13	1.99	0.45
2:B:204:LEU:CA	2:B:207:LEU:HD22	2.45	0.45
1:D:294:MET:HE3	1:D:424:LEU:HB2	1.97	0.45
1:A:491:ILE:O	1:A:502:THR:HA	2.17	0.45
1:A:574:PRO:HB3	1:A:729:ALA:HB2	1.96	0.45
1:D:335:ALA:O	1:D:336:SER:HB3	2.16	0.45
1:A:719:GLU:CB	1:D:735:ILE:HG12	2.47	0.45
1:A:496:LEU:O	1:A:497:ASN:HB2	2.17	0.45
1:A:604:LEU:CG	2:B:124:TRP:HZ2	2.30	0.45
2:B:202:VAL:N	2:B:203:PRO:CD	2.80	0.45
1:A:612:LEU:HD23	1:A:624:CYS:HB3	1.99	0.44
1:A:470:SER:HG	2:B:238:PHE:HB3	1.78	0.44
1:D:531:SER:OG	1:D:596:PHE:HE2	1.89	0.44
1:D:560:ILE:CG2	1:D:562:LEU:HG	2.45	0.44
2:E:61:LEU:HD21	2:E:78:ILE:HD11	1.99	0.44
1:A:375:ASN:O	1:A:376:LYS:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.80	0.44
2:B:202:VAL:HG11	2:E:224:ARG:NH1	2.32	0.44
1:D:254:GLU:HG3	1:D:259:ILE:HD13	1.99	0.44
1:D:687:SER:HA	1:D:688:ARG:NH1	2.32	0.44
2:E:202:VAL:N	2:E:203:PRO:CD	2.80	0.44
2:E:286:HIS:O	2:E:288:PRO:HD3	2.16	0.44
2:E:297:ILE:HD11	2:E:314:ARG:HD3	1.99	0.44
1:A:343:PHE:HD1	1:A:362:MET:CE	2.31	0.44
1:D:148:HIS:CE1	3:F:12:ALA:CA	2.89	0.44
1:D:247:ILE:HG23	1:D:265:GLN:HG2	1.99	0.44
1:D:612:LEU:HD23	1:D:624:CYS:HB3	1.99	0.44
1:A:124:THR:O	1:A:124:THR:CG2	2.65	0.44
1:A:431:MET:HE3	1:A:472:PRO:HA	1.99	0.44
1:A:600:LYS:HA	2:B:170:TYR:HH	1.81	0.44
1:D:263:THR:HG21	1:D:265:GLN:HE21	1.82	0.44
1:D:496:LEU:O	1:D:497:ASN:HB2	2.17	0.44
1:D:655:VAL:HG11	1:D:681:TYR:CD1	2.52	0.44
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.80	0.44
1:A:247:ILE:HG23	1:A:265:GLN:HG2	2.00	0.44
1:D:162:PHE:CD1	1:D:162:PHE:O	2.71	0.44
1:D:546:VAL:CG1	1:D:550:GLU:HG3	2.48	0.44
2:E:201:ILE:HD12	2:E:226:LEU:HD11	2.00	0.44
1:A:463:MET:HB2	1:A:477:VAL:O	2.18	0.44
1:D:343:PHE:HD1	1:D:362:MET:CE	2.31	0.44
1:D:463:MET:HB2	1:D:477:VAL:O	2.18	0.44
1:A:263:THR:HG21	1:A:265:GLN:HE21	1.82	0.44
1:D:243:ASP:O	1:D:245:TYR:HA	2.17	0.44
1:D:516:ASN:HB3	1:D:535:PHE:HE1	1.78	0.44
1:D:561:CYS:O	1:D:642:ASN:ND2	2.41	0.44
2:B:125:LEU:HD12	2:B:126:PHE:H	1.81	0.44
2:B:61:LEU:HD21	2:B:78:ILE:HD11	1.99	0.44
1:D:491:ILE:O	1:D:502:THR:HA	2.17	0.44
2:B:280:LYS:HA	2:B:281:PRO:HA	1.86	0.43
2:B:96:TYR:C	2:B:98:PRO:HD3	2.39	0.43
1:D:605:LEU:HD13	1:D:638:ILE:HG12	2.00	0.43
1:A:546:VAL:CG1	1:A:550:GLU:HG3	2.48	0.43
1:A:655:VAL:CG2	1:A:657:PRO:HD3	2.29	0.43
2:B:149:LEU:HB3	2:B:154:ILE:HD11	1.99	0.43
2:B:103:LEU:HD23	2:B:103:LEU:HA	1.87	0.43
1:D:343:PHE:CE2	1:D:444:THR:HG21	2.53	0.43
1:D:560:ILE:CG2	1:D:562:LEU:CG	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:204:LEU:CA	2:E:207:LEU:HD22	2.45	0.43
1:A:122:VAL:HG23	1:A:130:LEU:HD13	2.00	0.43
1:A:191:ARG:NH2	3:C:74:HIS:CA	2.81	0.43
2:B:254:VAL:HG13	2:B:282:ASN:HB3	2.00	0.43
2:E:97:LEU:O	2:E:100:VAL:HG12	2.18	0.43
1:D:191:ARG:HE	3:F:108:LEU:CD2	2.31	0.43
2:B:97:LEU:O	2:B:100:VAL:HG12	2.18	0.43
1:A:343:PHE:CE2	1:A:444:THR:HG21	2.53	0.43
1:D:191:ARG:NE	3:F:108:LEU:CD2	2.82	0.43
1:A:605:LEU:HD13	1:A:638:ILE:HG12	2.00	0.43
2:B:125:LEU:HD11	2:B:127:LEU:HG	2.01	0.43
1:D:191:ARG:HD3	3:F:78:SER:OG	2.19	0.43
1:D:217:ARG:HB3	1:D:228:PHE:CD1	2.54	0.43
2:E:254:VAL:HG13	2:E:282:ASN:HB3	2.00	0.43
2:E:257:ASN:HB3	2:E:266:LEU:HD22	2.01	0.43
2:E:96:TYR:C	2:E:98:PRO:HD3	2.39	0.43
1:D:203:SER:O	1:D:205:TYR:N	2.52	0.43
1:D:321:TYR:CE2	1:D:323:SER:HB3	2.54	0.43
1:D:431:MET:CE	1:D:472:PRO:HA	2.49	0.43
1:D:53:GLN:HE22	1:D:67:THR:N	2.17	0.43
2:E:101:THR:HG22	2:E:121:ASN:O	2.19	0.43
2:E:125:LEU:HD12	2:E:126:PHE:H	1.82	0.43
2:B:97:LEU:HD12	2:B:97:LEU:N	2.34	0.43
1:A:252:ALA:HB2	1:A:261:PHE:CE2	2.54	0.43
1:A:321:TYR:CE2	1:A:323:SER:HB3	2.54	0.43
1:A:600:LYS:HZ3	2:B:148:SER:HB2	1.81	0.43
2:B:195:ASP:H	2:B:217:LYS:HB2	1.84	0.43
2:B:231:ASN:HD22	2:B:231:ASN:HA	1.62	0.43
2:B:297:ILE:HD11	2:B:314:ARG:HD3	1.99	0.43
1:D:178:SER:HB3	1:D:199:ASN:OD1	2.19	0.43
1:A:604:LEU:HG	2:B:124:TRP:CZ2	2.48	0.42
1:D:47:THR:HG23	1:D:509:LYS:HG2	2.01	0.42
1:D:84:TYR:CD1	1:D:84:TYR:C	2.93	0.42
1:A:665:LYS:HB3	1:A:665:LYS:HE3	1.78	0.42
2:B:174:ASN:HB3	2:B:175:LYS:H	1.70	0.42
2:B:201:ILE:HD12	2:B:226:LEU:HD11	2.00	0.42
2:B:272:ILE:HG21	2:B:276:GLY:HA3	2.01	0.42
1:D:56:ILE:HD13	1:D:120:LEU:HG	2.00	0.42
1:A:162:PHE:CD1	1:A:162:PHE:O	2.71	0.42
1:A:217:ARG:HB3	1:A:228:PHE:CD1	2.54	0.42
2:B:202:VAL:CG1	2:E:224:ARG:HH12	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LEU:HB2	1:D:241:PHE:CD2	2.55	0.42
1:D:262:LEU:HD23	1:D:262:LEU:HA	1.93	0.42
1:D:665:LYS:HE3	1:D:665:LYS:HB3	1.78	0.42
1:A:178:SER:HB3	1:A:199:ASN:OD1	2.19	0.42
2:B:147:LEU:HD11	2:B:149:LEU:CG	2.49	0.42
1:D:636:MET:HB2	1:D:636:MET:HE2	1.78	0.42
2:E:195:ASP:H	2:E:217:LYS:HB2	1.84	0.42
2:E:97:LEU:N	2:E:97:LEU:HD12	2.34	0.42
1:A:239:PRO:HG3	1:A:242:ARG:NH1	2.35	0.42
1:A:416:TYR:HD1	1:A:416:TYR:H	1.60	0.42
1:A:47:THR:HG23	1:A:509:LYS:HG2	2.01	0.42
1:D:252:ALA:HB2	1:D:261:PHE:CE2	2.54	0.42
1:D:602:ARG:NH2	2:E:170:TYR:CZ	2.76	0.42
1:D:92:HIS:HB3	1:D:95:CYS:H	1.85	0.42
2:E:125:LEU:HD11	2:E:127:LEU:HG	2.01	0.42
2:E:268:THR:HA	2:E:269:PRO:HD3	1.85	0.42
1:A:53:GLN:HE22	1:A:67:THR:N	2.17	0.42
1:D:122:VAL:HG23	1:D:130:LEU:HD13	2.01	0.42
1:D:331:ARG:O	2:E:314:ARG:NH1	2.53	0.42
1:A:191:ARG:NH2	3:C:108:LEU:HD13	2.34	0.42
1:A:203:SER:O	1:A:205:TYR:N	2.52	0.42
2:B:101:THR:HG22	2:B:121:ASN:O	2.19	0.42
1:D:430:PHE:O	1:D:431:MET:CG	2.58	0.42
1:A:56:ILE:HD13	1:A:120:LEU:HG	2.00	0.42
1:D:239:PRO:HG3	1:D:242:ARG:NH1	2.35	0.42
1:D:662:ILE:HG12	1:D:734:SER:HB2	2.02	0.42
1:D:191:ARG:HD2	3:F:108:LEU:HD22	2.00	0.42
1:A:238:LEU:HB2	1:A:241:PHE:CD2	2.55	0.42
1:A:243:ASP:O	1:A:244:SER:C	2.59	0.42
1:D:245:TYR:O	1:D:266:ARG:NH1	2.53	0.42
1:D:469:ARG:HD3	2:E:299:TYR:CD2	2.51	0.42
1:A:84:TYR:C	1:A:84:TYR:CD1	2.93	0.41
2:B:147:LEU:HD12	2:B:148:SER:N	2.35	0.41
1:D:438:LEU:O	1:D:440:THR:HG23	2.20	0.41
1:A:662:ILE:HG12	1:A:734:SER:HB2	2.02	0.41
1:A:191:ARG:HH22	3:C:74:HIS:CB	2.30	0.41
2:E:147:LEU:HD12	2:E:148:SER:N	2.35	0.41
2:E:217:LYS:N	2:E:238:PHE:O	2.45	0.41
1:A:191:ARG:HE	3:C:108:LEU:HD11	1.85	0.41
1:A:599:LYS:O	2:B:170:TYR:OH	2.35	0.41
2:B:200:ASP:OD1	2:B:202:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ASP:O	1:D:244:SER:C	2.59	0.41
2:B:180:THR:CG2	2:E:224:ARG:HD3	2.49	0.41
1:A:191:ARG:HD3	3:C:78:SER:HB2	2.01	0.41
1:A:98:CYS:SG	1:A:162:PHE:CB	3.09	0.41
2:B:257:ASN:HB3	2:B:266:LEU:HD22	2.01	0.41
2:B:268:THR:HA	2:B:269:PRO:HD3	1.85	0.41
2:B:35:MET:O	2:B:35:MET:HG3	2.21	0.41
1:D:447:LYS:HD2	1:D:535:PHE:CD2	2.55	0.41
1:A:191:ARG:HH21	3:C:108:LEU:HD11	1.85	0.41
1:A:252:ALA:HB2	1:A:261:PHE:CD2	2.55	0.41
1:A:92:HIS:HB3	1:A:95:CYS:H	1.85	0.41
1:D:516:ASN:OD1	1:D:535:PHE:CE1	2.73	0.41
1:D:576:GLU:HG2	1:D:728:LEU:C	2.40	0.41
2:E:240:GLN:HG2	2:E:312:HIS:O	2.21	0.41
1:A:245:TYR:O	1:A:266:ARG:NH1	2.54	0.41
2:B:190:THR:HG22	2:B:191:LEU:H	1.85	0.41
1:D:41:TYR:CE1	1:D:522:HIS:NE2	2.80	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.93	0.41
1:A:343:PHE:HD1	1:A:362:MET:HE1	1.85	0.41
1:D:506:THR:HG22	1:D:506:THR:O	2.20	0.41
2:E:147:LEU:HD11	2:E:149:LEU:CG	2.50	0.41
1:A:462:PHE:CE2	1:A:513:ILE:HG21	2.56	0.41
1:D:252:ALA:HB2	1:D:261:PHE:CD2	2.55	0.41
1:D:291:TYR:C	1:D:292:MET:HG3	2.41	0.41
1:D:600:LYS:NZ	2:E:148:SER:HB2	2.36	0.41
2:E:318:PRO:O	2:E:319:LEU:HD23	2.21	0.41
1:A:294:MET:HA	1:A:295:PRO:HD2	1.76	0.41
2:B:229:LEU:HB3	2:B:232:LEU:HG	2.03	0.41
1:D:447:LYS:HE3	1:D:535:PHE:CB	2.50	0.41
2:E:35:MET:O	2:E:35:MET:HG3	2.21	0.41
1:D:59:GLU:O	1:D:61:HIS:HD2	2.04	0.41
2:E:103:LEU:HD23	2:E:103:LEU:HA	1.87	0.41
2:E:190:THR:HG22	2:E:191:LEU:H	1.85	0.41
1:A:561:CYS:O	1:A:642:ASN:ND2	2.41	0.40
1:A:668:PRO:HD2	1:A:673:THR:OG1	2.21	0.40
1:D:668:PRO:HD2	1:D:673:THR:OG1	2.21	0.40
1:D:92:HIS:CE1	1:D:94:ASP:HB2	2.56	0.40
2:E:272:ILE:HG21	2:E:276:GLY:HA3	2.03	0.40
1:A:438:LEU:O	1:A:440:THR:HG23	2.20	0.40
1:A:77:ASP:OD1	1:A:79:GLN:HB2	2.22	0.40
2:B:113:ILE:CG1	2:B:137:SER:HB2	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:VAL:HA	2:B:256:PRO:HD3	1.91	0.40
2:E:113:ILE:CG1	2:E:137:SER:HB2	2.43	0.40
2:E:200:ASP:OD1	2:E:202:VAL:HG23	2.20	0.40
1:A:291:TYR:C	1:A:292:MET:HG3	2.41	0.40
1:A:395:GLU:H	1:A:395:GLU:HG2	1.57	0.40
1:A:431:MET:HE1	1:A:472:PRO:HA	2.03	0.40
1:A:506:THR:HG22	1:A:506:THR:O	2.20	0.40
1:D:345:VAL:HG11	1:D:439:LEU:HB3	2.04	0.40
1:D:462:PHE:CE2	1:D:513:ILE:HG21	2.56	0.40
1:D:539:GLY:HA3	1:D:556:TRP:CE2	2.57	0.40
2:E:197:GLN:HA	2:E:219:HIS:CD2	2.56	0.40
2:E:201:ILE:CD1	2:E:226:LEU:HD11	2.52	0.40
1:A:201:ILE:HD11	1:A:211:LEU:HB2	2.04	0.40
1:A:533:PRO:HA	1:A:534:PRO:HD3	1.89	0.40
1:D:90:LEU:HB2	1:D:112:TRP:HD1	1.86	0.40

All (44) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:GLU:OE2	1:D:635:ASN:ND2[2_455]	0.86	1.34
1:D:459:GLU:OE2	1:D:635:ASN:CG[2_455]	1.00	1.20
1:A:155:GLN:OE1	2:B:71:THR:CG2[2_554]	1.06	1.14
1:A:155:GLN:CD	2:B:71:THR:CG2[2_554]	1.06	1.14
3:C:123:LYS:NZ	2:E:175:LYS:CB[3_544]	1.09	1.11
1:A:398:PHE:CE1	1:A:739:ARG:NH2[3_444]	1.09	1.11
1:A:497:ASN:OD1	3:F:26:ALA:O[3_544]	1.40	0.80
2:B:175:LYS:CG	3:F:123:LYS:NZ[3_544]	1.44	0.76
1:A:497:ASN:ND2	3:F:22:MET:CE[3_544]	1.45	0.75
3:C:26:ALA:O	1:D:497:ASN:ND2[3_544]	1.46	0.74
1:A:155:GLN:CG	2:B:71:THR:CG2[2_554]	1.48	0.72
1:A:150:HIS:ND1	2:B:39:THR:CB[2_554]	1.51	0.69
1:D:459:GLU:OE2	1:D:635:ASN:OD1[2_455]	1.53	0.67
3:C:26:ALA:O	1:D:497:ASN:CG[3_544]	1.53	0.67
3:C:26:ALA:O	1:D:497:ASN:OD1[3_544]	1.55	0.65
2:B:175:LYS:CB	3:F:123:LYS:NZ[3_544]	1.59	0.61
1:A:696:THR:OG1	1:D:207:PRO:CG[2_454]	1.59	0.61
1:D:459:GLU:CD	1:D:635:ASN:ND2[2_455]	1.64	0.56
3:C:123:LYS:NZ	2:E:175:LYS:CG[3_544]	1.65	0.55
1:A:398:PHE:CZ	1:A:739:ARG:NH2[3_444]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:ALA:O	1:D:449:ASP:OD2[3_544]	1.71	0.49
3:C:123:LYS:CG	2:E:197:GLN:NE2[3_544]	1.75	0.45
1:A:350:LYS:NZ	1:D:80:LYS:O[2_454]	1.79	0.41
1:A:696:THR:CB	1:D:207:PRO:CG[2_454]	1.79	0.41
1:A:156:SER:O	2:B:73:ASN:CB[2_554]	1.81	0.39
1:A:155:GLN:CG	2:B:71:THR:CB[2_554]	1.82	0.38
2:B:197:GLN:NE2	3:F:123:LYS:CG[3_544]	1.85	0.35
1:A:616:GLU:OE1	1:D:103:SER:OG[2_454]	1.86	0.34
1:A:696:THR:CG2	1:D:207:PRO:CB[2_454]	1.89	0.31
3:C:22:MET:CE	1:D:497:ASN:ND2[3_544]	1.90	0.30
1:A:150:HIS:ND1	2:B:39:THR:OG1[2_554]	1.90	0.30
2:B:175:LYS:CD	3:F:123:LYS:NZ[3_544]	1.91	0.29
3:C:123:LYS:CB	2:E:197:GLN:NE2[3_544]	1.92	0.28
1:A:449:ASP:OD2	3:F:91:ALA:O[3_544]	1.96	0.24
1:A:497:ASN:CG	3:F:26:ALA:O[3_544]	2.05	0.15
1:A:150:HIS:CE1	2:B:39:THR:OG1[2_554]	2.08	0.12
1:A:156:SER:O	2:B:73:ASN:CA[2_554]	2.11	0.09
3:C:57:THR:O	1:D:447:LYS:NZ[3_544]	2.11	0.09
1:A:398:PHE:CE2	1:A:666:TYR:CE2[3_444]	2.11	0.09
3:C:123:LYS:NZ	2:E:175:LYS:CD[3_544]	2.12	0.08
1:A:357:MET:CE	1:D:83:GLU:OE2[2_454]	2.13	0.07
1:D:459:GLU:OE1	1:D:635:ASN:ND2[2_455]	2.13	0.07
1:A:398:PHE:CZ	1:A:666:TYR:CE2[3_444]	2.16	0.04
2:B:197:GLN:NE2	3:F:123:LYS:CD[3_544]	2.18	0.02

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	663/727 (91%)	589 (89%)	58 (9%)	16 (2%)	6	40
1	D	663/727 (91%)	588 (89%)	60 (9%)	15 (2%)	7	41
2	B	284/289 (98%)	228 (80%)	52 (18%)	4 (1%)	12	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	284/289 (98%)	227 (80%)	53 (19%)	4 (1%)	12	52
3	C	153/173 (88%)	149 (97%)	4 (3%)	0	100	100
3	F	153/173 (88%)	149 (97%)	4 (3%)	0	100	100
All	All	2200/2378 (92%)	1930 (88%)	231 (10%)	39 (2%)	9	47

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	GLY
1	A	270	ASP
1	A	272	GLN
1	A	483	SER
2	B	193	LEU
1	D	87	GLY
1	D	270	ASP
1	D	272	GLN
1	D	483	SER
2	E	193	LEU
1	A	107	LEU
1	A	204	SER
1	A	205	TYR
1	A	266	ARG
2	B	211	GLN
1	D	107	LEU
1	D	204	SER
1	D	205	TYR
1	D	266	ARG
1	D	433	GLN
2	E	211	GLN
1	A	244	SER
1	A	395	GLU
1	A	433	GLN
1	D	244	SER
1	D	395	GLU
1	A	448	GLY
1	A	507	GLY
1	D	448	GLY
1	D	507	GLY
1	A	242	ARG
2	B	191	LEU
2	E	191	LEU

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Mol	Chain	Res	Type
1	A	246	PRO
2	B	305	GLY
1	D	246	PRO
2	E	305	GLY
1	A	472	PRO
1	D	472	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	605/654 (92%)	496 (82%)	109 (18%)	2	12
1	D	605/654 (92%)	497 (82%)	108 (18%)	2	12
2	B	264/265 (100%)	252 (96%)	12 (4%)	30	60
2	E	264/265 (100%)	252 (96%)	12 (4%)	30	60
3	C	118/132 (89%)	118 (100%)	0	100	100
3	F	118/132 (89%)	118 (100%)	0	100	100
All	All	1974/2102 (94%)	1733 (88%)	241 (12%)	5	24

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	42	GLN
1	A	45	ASN
1	A	56	ILE
1	A	78	LEU
1	A	79	GLN
1	A	83	GLU
1	A	85	LYS
1	A	86	THR
1	A	90	LEU
1	A	94	ASP
1	A	98	CYS

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Mol	Chain	Res	Type
1	A	99	GLN
1	A	100	ASP
1	A	102	SER
1	A	103	SER
1	A	104	LYS
1	A	108	SER
1	A	112	TRP
1	A	113	LYS
1	A	118	MET
1	A	123	ASP
1	A	124	THR
1	A	136	VAL
1	A	138	ARG
1	A	140	THR
1	A	142	GLN
1	A	143	ARG
1	A	149	ASN
1	A	155	GLN
1	A	162	PHE
1	A	166	ILE
1	A	170	SER
1	A	177	VAL
1	A	178	SER
1	A	185	LEU
1	A	186	SER
1	A	188	VAL
1	A	189	LYS
1	A	201	ILE
1	A	202	ASN
1	A	203	SER
1	A	205	TYR
1	A	206	PHE
1	A	213	SER
1	A	214	ILE
1	A	217	ARG
1	A	219	LEU
1	A	229	LEU
1	A	234	TYR
1	A	240	GLU
1	A	242	ARG
1	A	245	TYR
1	A	248	LYS

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Mol	Chain	Res	Type
1	A	255	SER
1	A	265	GLN
1	A	268	THR
1	A	269	LEU
1	A	273	THR
1	A	278	ILE
1	A	280	ARG
1	A	282	CYS
1	A	284	ILE
1	A	294	MET
1	A	301	THR
1	A	324	LYS
1	A	329	LEU
1	A	337	LEU
1	A	339	ASP
1	A	352	ASP
1	A	353	SER
1	A	355	GLU
1	A	362	MET
1	A	367	ILE
1	A	368	LYS
1	A	384	ARG
1	A	385	CYS
1	A	386	LEU
1	A	387	GLN
1	A	394	HIS
1	A	395	GLU
1	A	397	CYS
1	A	398	PHE
1	A	414	ASP
1	A	416	TYR
1	A	417	ARG
1	A	418	THR
1	A	421	THR
1	A	424	LEU
1	A	426	ARG
1	A	427	VAL
1	A	429	LEU
1	A	433	GLN
1	A	438	LEU
1	A	443	SER
1	A	447	LYS

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Mol	Chain	Res	Type
1	A	458	SER
1	A	461	ARG
1	A	470	SER
1	A	480	LEU
1	A	483	SER
1	A	493	GLU
1	A	495	THR
1	A	496	LEU
1	A	506	THR
1	A	508	LYS
1	A	511	THR
1	A	633	HIS
1	A	651	THR
2	B	37	THR
2	B	109	LYS
2	B	135	LEU
2	B	157	ILE
2	B	180	THR
2	B	181	VAL
2	B	207	LEU
2	B	226	LEU
2	B	247	ILE
2	B	249	HIS
2	B	302	VAL
2	B	312	HIS
1	D	40	LYS
1	D	42	GLN
1	D	45	ASN
1	D	56	ILE
1	D	78	LEU
1	D	79	GLN
1	D	83	GLU
1	D	85	LYS
1	D	86	THR
1	D	90	LEU
1	D	94	ASP
1	D	98	CYS
1	D	99	GLN
1	D	100	ASP
1	D	102	SER
1	D	103	SER
1	D	104	LYS

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Mol	Chain	Res	Type
1	D	108	SER
1	D	112	TRP
1	D	113	LYS
1	D	118	MET
1	D	123	ASP
1	D	124	THR
1	D	136	VAL
1	D	138	ARG
1	D	140	THR
1	D	142	GLN
1	D	143	ARG
1	D	155	GLN
1	D	162	PHE
1	D	166	ILE
1	D	170	SER
1	D	177	VAL
1	D	178	SER
1	D	185	LEU
1	D	186	SER
1	D	188	VAL
1	D	189	LYS
1	D	201	ILE
1	D	202	ASN
1	D	203	SER
1	D	205	TYR
1	D	206	PHE
1	D	213	SER
1	D	214	ILE
1	D	217	ARG
1	D	219	LEU
1	D	229	LEU
1	D	234	TYR
1	D	240	GLU
1	D	242	ARG
1	D	245	TYR
1	D	248	LYS
1	D	255	SER
1	D	265	GLN
1	D	268	THR
1	D	269	LEU
1	D	273	THR
1	D	278	ILE

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Mol	Chain	Res	Type
1	D	280	ARG
1	D	282	CYS
1	D	284	ILE
1	D	294	MET
1	D	301	THR
1	D	324	LYS
1	D	329	LEU
1	D	337	LEU
1	D	339	ASP
1	D	352	ASP
1	D	353	SER
1	D	355	GLU
1	D	362	MET
1	D	367	ILE
1	D	368	LYS
1	D	384	ARG
1	D	385	CYS
1	D	386	LEU
1	D	387	GLN
1	D	394	HIS
1	D	395	GLU
1	D	397	CYS
1	D	398	PHE
1	D	414	ASP
1	D	416	TYR
1	D	417	ARG
1	D	418	THR
1	D	421	THR
1	D	424	LEU
1	D	426	ARG
1	D	427	VAL
1	D	429	LEU
1	D	433	GLN
1	D	438	LEU
1	D	443	SER
1	D	447	LYS
1	D	458	SER
1	D	461	ARG
1	D	470	SER
1	D	480	LEU
1	D	483	SER
1	D	493	GLU

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Mol	Chain	Res	Type
1	D	495	THR
1	D	496	LEU
1	D	506	THR
1	D	508	LYS
1	D	511	THR
1	D	633	HIS
1	D	651	THR
2	E	37	THR
2	E	109	LYS
2	E	135	LEU
2	E	157	ILE
2	E	180	THR
2	E	181	VAL
2	E	207	LEU
2	E	226	LEU
2	E	247	ILE
2	E	249	HIS
2	E	302	VAL
2	E	312	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	61	HIS
1	A	129	GLN
1	A	148	HIS
1	A	256	ASN
1	A	275	HIS
1	A	332	GLN
1	A	387	GLN
1	A	516	ASN
1	A	522	HIS
1	A	593	ASN
1	A	686	ASN
2	B	76	ASN
2	B	121	ASN
2	B	158	ASN
2	B	173	ASN
2	B	211	GLN
2	B	231	ASN
2	B	257	ASN

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Mol	Chain	Res	Type
1	D	53	GLN
1	D	61	HIS
1	D	129	GLN
1	D	256	ASN
1	D	275	HIS
1	D	318	GLN
1	D	332	GLN
1	D	387	GLN
1	D	476	HIS
1	D	516	ASN
1	D	593	ASN
2	E	76	ASN
2	E	80	GLN
2	E	121	ASN
2	E	158	ASN
2	E	173	ASN
2	E	211	GLN
2	E	231	ASN
2	E	257	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	A	2
3	C	2
3	F	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	518:LEU	C	519:GLY	N	6.49
1	A	518:LEU	C	519:GLY	N	5.09
1	D	560:ILE	C	561:CYS	N	4.19
1	A	560:ILE	C	561:CYS	N	3.62
1	D	655:VAL	C	656:ASP	N	1.62
1	C	97:ALA	C	98:MET	N	1.11
1	F	97:ALA	C	98:MET	N	1.11
1	C	63:ALA	C	64:LYS	N	0.92
1	F	63:ALA	C	64:LYS	N	0.92

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.