Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:59 AM GMT

PDB ID	:	3QOE
Title	:	Crystal Structure of Heterocyst Differentiation Protein, HetR from Fischerella mv11
Authors	:	Kim, Y.; Joachimiak, G.; Gornicki, P.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2011-02-09
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

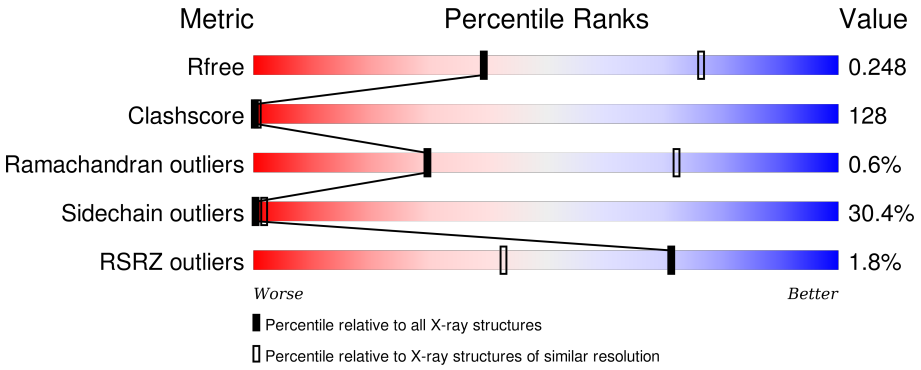
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	302	2% 14% 57% 22% 7%
1	B	302	% 20% 49% 23% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4589 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 Heterocyst differentiation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2305	1467	408	414	16			
1	B	278	Total	C	N	O	S	0	0	0
			2283	1453	403	411	16			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q2ACK9
A	-1	ASN	-	EXPRESSION TAG	UNP Q2ACK9
A	0	ALA	-	EXPRESSION TAG	UNP Q2ACK9
A	1	MET	-	EXPRESSION TAG	UNP Q2ACK9
A	2	SER	-	EXPRESSION TAG	UNP Q2ACK9
A	3	ASN	-	EXPRESSION TAG	UNP Q2ACK9
A	4	ASP	-	EXPRESSION TAG	UNP Q2ACK9
A	5	VAL	-	EXPRESSION TAG	UNP Q2ACK9
A	6	ASP	-	EXPRESSION TAG	UNP Q2ACK9
A	7	LEU	-	EXPRESSION TAG	UNP Q2ACK9
A	8	ILE	-	EXPRESSION TAG	UNP Q2ACK9
A	9	LYS	-	EXPRESSION TAG	UNP Q2ACK9
A	10	ARG	-	EXPRESSION TAG	UNP Q2ACK9
A	11	LEU	-	EXPRESSION TAG	UNP Q2ACK9
A	12	GLY	-	EXPRESSION TAG	UNP Q2ACK9
A	13	PRO	-	EXPRESSION TAG	UNP Q2ACK9
A	14	SER	-	EXPRESSION TAG	UNP Q2ACK9
A	15	ALA	-	EXPRESSION TAG	UNP Q2ACK9
A	16	MET	-	EXPRESSION TAG	UNP Q2ACK9
A	17	ASP	-	EXPRESSION TAG	UNP Q2ACK9
A	18	GLN	-	EXPRESSION TAG	UNP Q2ACK9
A	19	ILE	-	EXPRESSION TAG	UNP Q2ACK9
A	20	MET	-	EXPRESSION TAG	UNP Q2ACK9
A	21	LEU	-	EXPRESSION TAG	UNP Q2ACK9
A	22	TYR	-	EXPRESSION TAG	UNP Q2ACK9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	-	EXPRESSION TAG	UNP Q2ACK9
A	24	ALA	-	EXPRESSION TAG	UNP Q2ACK9
A	25	PHE	-	EXPRESSION TAG	UNP Q2ACK9
A	26	SER	-	EXPRESSION TAG	UNP Q2ACK9
A	27	ALA	-	EXPRESSION TAG	UNP Q2ACK9
A	28	MET	-	EXPRESSION TAG	UNP Q2ACK9
A	276	TRP	-	EXPRESSION TAG	UNP Q2ACK9
A	277	ALA	-	EXPRESSION TAG	UNP Q2ACK9
A	278	ASP	-	EXPRESSION TAG	UNP Q2ACK9
A	278A	LYS	-	EXPRESSION TAG	UNP Q2ACK9
A	278B	TYR	-	EXPRESSION TAG	UNP Q2ACK9
A	278C	HIS	-	EXPRESSION TAG	UNP Q2ACK9
A	278D	GLN	-	EXPRESSION TAG	UNP Q2ACK9
A	278E	ASP	-	EXPRESSION TAG	UNP Q2ACK9
A	278F	ASP	-	EXPRESSION TAG	UNP Q2ACK9
A	278G	GLY	-	EXPRESSION TAG	UNP Q2ACK9
A	278H	VAL	-	EXPRESSION TAG	UNP Q2ACK9
A	286	PRO	-	EXPRESSION TAG	UNP Q2ACK9
A	287	VAL	-	EXPRESSION TAG	UNP Q2ACK9
A	288	VAL	-	EXPRESSION TAG	UNP Q2ACK9
A	289	LEU	-	EXPRESSION TAG	UNP Q2ACK9
A	290	GLN	-	EXPRESSION TAG	UNP Q2ACK9
A	291	MET	-	EXPRESSION TAG	UNP Q2ACK9
A	292	VAL	-	EXPRESSION TAG	UNP Q2ACK9
A	293	PHE	-	EXPRESSION TAG	UNP Q2ACK9
A	294	GLY	-	EXPRESSION TAG	UNP Q2ACK9
A	295	LYS	-	EXPRESSION TAG	UNP Q2ACK9
A	296	LYS	-	EXPRESSION TAG	UNP Q2ACK9
A	297	GLU	-	EXPRESSION TAG	UNP Q2ACK9
A	298	ASP	-	EXPRESSION TAG	UNP Q2ACK9
B	-2	SER	-	EXPRESSION TAG	UNP Q2ACK9
B	-1	ASN	-	EXPRESSION TAG	UNP Q2ACK9
B	0	ALA	-	EXPRESSION TAG	UNP Q2ACK9
B	1	MET	-	EXPRESSION TAG	UNP Q2ACK9
B	2	SER	-	EXPRESSION TAG	UNP Q2ACK9
B	3	ASN	-	EXPRESSION TAG	UNP Q2ACK9
B	4	ASP	-	EXPRESSION TAG	UNP Q2ACK9
B	5	VAL	-	EXPRESSION TAG	UNP Q2ACK9
B	6	ASP	-	EXPRESSION TAG	UNP Q2ACK9
B	7	LEU	-	EXPRESSION TAG	UNP Q2ACK9
B	8	ILE	-	EXPRESSION TAG	UNP Q2ACK9
B	9	LYS	-	EXPRESSION TAG	UNP Q2ACK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ARG	-	EXPRESSION TAG	UNP Q2ACK9
B	11	LEU	-	EXPRESSION TAG	UNP Q2ACK9
B	12	GLY	-	EXPRESSION TAG	UNP Q2ACK9
B	13	PRO	-	EXPRESSION TAG	UNP Q2ACK9
B	14	SER	-	EXPRESSION TAG	UNP Q2ACK9
B	15	ALA	-	EXPRESSION TAG	UNP Q2ACK9
B	16	MET	-	EXPRESSION TAG	UNP Q2ACK9
B	17	ASP	-	EXPRESSION TAG	UNP Q2ACK9
B	18	GLN	-	EXPRESSION TAG	UNP Q2ACK9
B	19	ILE	-	EXPRESSION TAG	UNP Q2ACK9
B	20	MET	-	EXPRESSION TAG	UNP Q2ACK9
B	21	LEU	-	EXPRESSION TAG	UNP Q2ACK9
B	22	TYR	-	EXPRESSION TAG	UNP Q2ACK9
B	23	LEU	-	EXPRESSION TAG	UNP Q2ACK9
B	24	ALA	-	EXPRESSION TAG	UNP Q2ACK9
B	25	PHE	-	EXPRESSION TAG	UNP Q2ACK9
B	26	SER	-	EXPRESSION TAG	UNP Q2ACK9
B	27	ALA	-	EXPRESSION TAG	UNP Q2ACK9
B	28	MET	-	EXPRESSION TAG	UNP Q2ACK9
B	276	TRP	-	EXPRESSION TAG	UNP Q2ACK9
B	277	ALA	-	EXPRESSION TAG	UNP Q2ACK9
B	278	ASP	-	EXPRESSION TAG	UNP Q2ACK9
B	278A	LYS	-	EXPRESSION TAG	UNP Q2ACK9
B	278B	TYR	-	EXPRESSION TAG	UNP Q2ACK9
B	278C	HIS	-	EXPRESSION TAG	UNP Q2ACK9
B	278D	GLN	-	EXPRESSION TAG	UNP Q2ACK9
B	278E	ASP	-	EXPRESSION TAG	UNP Q2ACK9
B	278F	ASP	-	EXPRESSION TAG	UNP Q2ACK9
B	278G	GLY	-	EXPRESSION TAG	UNP Q2ACK9
B	278H	VAL	-	EXPRESSION TAG	UNP Q2ACK9
B	286	PRO	-	EXPRESSION TAG	UNP Q2ACK9
B	287	VAL	-	EXPRESSION TAG	UNP Q2ACK9
B	288	VAL	-	EXPRESSION TAG	UNP Q2ACK9
B	289	LEU	-	EXPRESSION TAG	UNP Q2ACK9
B	290	GLN	-	EXPRESSION TAG	UNP Q2ACK9
B	291	MET	-	EXPRESSION TAG	UNP Q2ACK9
B	292	VAL	-	EXPRESSION TAG	UNP Q2ACK9
B	293	PHE	-	EXPRESSION TAG	UNP Q2ACK9
B	294	GLY	-	EXPRESSION TAG	UNP Q2ACK9
B	295	LYS	-	EXPRESSION TAG	UNP Q2ACK9
B	296	LYS	-	EXPRESSION TAG	UNP Q2ACK9
B	297	GLU	-	EXPRESSION TAG	UNP Q2ACK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	298	ASP	-	EXPRESSION TAG	UNP Q2ACK9

- Molecule 2 is water.

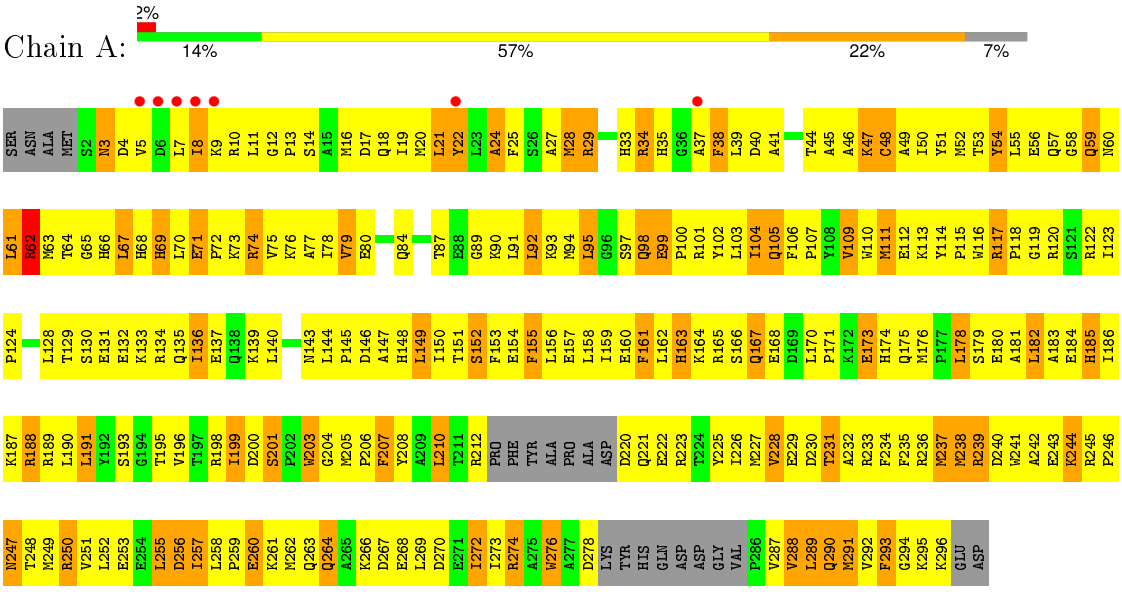
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

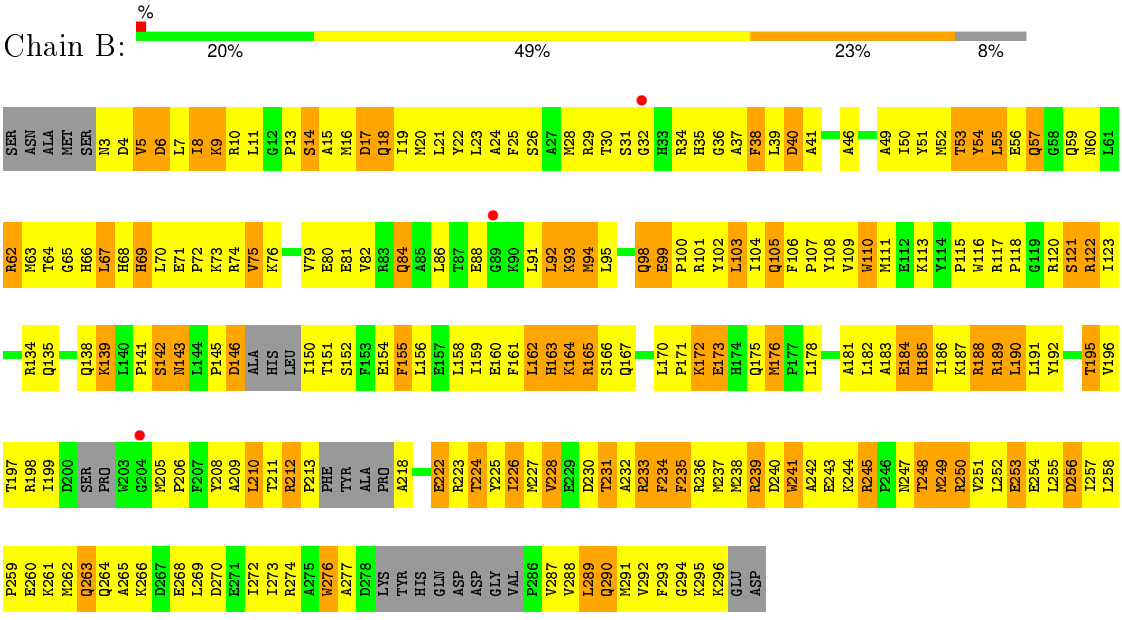
- Molecule 1: Heterocyst differentiation protein

Chain A:



- Molecule 1: Heterocyst differentiation protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	92.93Å 92.93Å 97.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.47 – 3.00 46.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.47-3.00) 100.0 (46.47-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.179 , 0.247 0.178 , 0.248	Depositor DCC
R_{free} test set	963 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 86.9	EDS
Estimated twinning fraction	0.370 for -h,-k,l 0.376 for h,-h-k,-l 0.467 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Outliers	0 of 18786 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4589	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.42	0/2356	0.69	0/3173
1	B	0.45	0/2331	0.69	1/3136 (0.0%)
All	All	0.43	0/4687	0.69	1/6309 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	14	SER	N-CA-C	-5.25	96.81	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2305	0	2321	720	0
1	B	2283	0	2295	658	0
2	A	1	0	0	0	0
All	All	4589	0	4616	1180	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 128.

All (1180) 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:184:GLU:O	1:A:188:ARG:HB2	1.33	1.28
1:B:57:GLN:OE1	1:B:64:THR:HG22	1.34	1.25
1:A:244:LYS:HB3	1:A:248:THR:HG21	1.20	1.19
1:B:150:ILE:HG23	1:B:154:GLU:HB2	1.25	1.17
1:A:295:LYS:HA	1:B:287:VAL:HG22	1.27	1.16
1:A:198:ARG:HG3	1:A:206:PRO:HB3	1.20	1.15
1:A:182:LEU:HB2	1:B:69:HIS:NE2	1.65	1.10
1:A:130:SER:HA	1:A:133:LYS:HE3	1.27	1.10
1:B:160:GLU:HA	1:B:178:LEU:HD22	1.12	1.10
1:B:13:PRO:HG2	1:B:18:GLN:HG2	1.29	1.10
1:B:72:PRO:HA	1:B:75:VAL:HB	1.33	1.10
1:A:62:ARG:HA	1:A:72:PRO:HG3	1.34	1.10
1:B:163:HIS:CE1	1:B:178:LEU:HD21	1.87	1.08
1:A:201:SER:HB2	1:A:204:GLY:H	0.94	1.08
1:B:261:LYS:HA	1:B:264:GLN:HE21	1.10	1.07
1:A:190:LEU:HA	1:A:193:SER:HB2	1.35	1.07
1:A:72:PRO:O	1:A:76:LYS:HB2	1.56	1.06
1:A:128:LEU:HD21	1:A:136:ILE:HD12	1.37	1.06
1:A:181:ALA:O	1:A:185:HIS:HB3	1.54	1.05
1:A:227:MET:HB3	1:B:242:ALA:CB	1.86	1.05
1:A:25:PHE:HD1	1:A:29:ARG:HB2	1.21	1.05
1:A:251:VAL:HB	1:B:291:MET:HB3	1.34	1.05
1:B:187:LYS:HD2	1:B:188:ARG:HH21	1.20	1.04
1:A:182:LEU:HG	1:A:186:ILE:HD12	1.41	1.03
1:A:182:LEU:CB	1:B:69:HIS:HE2	1.73	1.02
1:B:250:ARG:HH11	1:B:250:ARG:HG2	0.88	1.02
1:B:164:LYS:HD3	1:B:167:GLN:HB2	1.41	1.02
1:B:53:THR:HG21	1:B:68:HIS:CE1	1.94	1.01
1:A:100:PRO:HG2	1:A:103:LEU:HD12	1.41	1.01
1:A:11:LEU:HD11	1:B:92:LEU:HD11	1.42	1.01
1:B:240:ASP:HA	1:B:243:GLU:HB2	1.40	1.00
1:A:37:ALA:HB1	1:A:101:ARG:HH22	1.25	1.00
1:B:51:TYR:CE2	1:B:55:LEU:HD21	1.94	1.00
1:B:65:GLY:HA2	1:B:68:HIS:HD2	1.26	0.99
1:B:65:GLY:HA2	1:B:68:HIS:CD2	1.96	0.99
1:A:201:SER:HB2	1:A:204:GLY:N	1.76	0.99
1:B:205:MET:HG3	1:B:206:PRO:HD2	1.44	0.98
1:A:182:LEU:HB2	1:B:69:HIS:HE2	0.84	0.97
1:B:160:GLU:HA	1:B:178:LEU:CD2	1.93	0.97
1:A:122:ARG:HG3	1:A:148:HIS:HA	1.45	0.97
1:A:248:THR:HA	1:B:293:PHE:O	1.62	0.97
1:A:289:LEU:O	1:B:252:LEU:HB2	1.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HH21	1:B:56:GLU:HB3	1.29	0.96
1:A:200:ASP:HA	1:A:206:PRO:HA	1.49	0.95
1:A:116:TRP:CD1	1:A:122:ARG:HB2	2.01	0.94
1:A:130:SER:O	1:A:134:ARG:HB2	1.67	0.94
1:A:131:GLU:CD	1:A:135:GLN:HE22	1.69	0.94
1:A:231:THR:CG2	1:B:238:MET:HG2	1.99	0.93
1:A:139:LYS:HB3	1:A:199:ILE:HG21	1.50	0.93
1:A:124:PRO:HG3	1:A:148:HIS:HD2	1.33	0.93
1:A:106:PHE:CD2	1:A:162:LEU:HD22	2.03	0.92
1:A:167:GLN:HA	1:A:170:LEU:HD12	1.50	0.92
1:B:250:ARG:NH1	1:B:250:ARG:HG2	1.67	0.92
1:B:110:TRP:CZ2	1:B:150:ILE:HB	2.04	0.92
1:B:241:TRP:HA	1:B:248:THR:CG2	2.01	0.91
1:B:35:HIS:HA	1:B:38:PHE:HB3	1.50	0.90
1:B:264:GLN:O	1:B:268:GLU:HB3	1.71	0.90
1:A:245:ARG:HG3	1:A:246:PRO:HD2	1.52	0.90
1:A:25:PHE:CD1	1:A:29:ARG:HB2	2.06	0.90
1:A:235:PHE:HA	1:A:238:MET:HB2	1.53	0.90
1:A:122:ARG:HA	1:A:148:HIS:HB2	1.53	0.89
1:B:63:MET:HA	1:B:66:HIS:HB2	1.55	0.89
1:A:182:LEU:O	1:A:186:ILE:HB	1.71	0.89
1:A:3:ASN:HB2	1:B:56:GLU:HA	1.51	0.89
1:A:250:ARG:HG2	1:A:251:VAL:N	1.88	0.88
1:A:231:THR:HG23	1:B:238:MET:HG2	1.54	0.88
1:B:241:TRP:HA	1:B:248:THR:HG23	1.54	0.88
1:A:62:ARG:CA	1:A:72:PRO:HG3	2.03	0.88
1:A:93:LYS:HA	1:A:170:LEU:HD21	1.54	0.88
1:A:28:MET:HE2	1:B:68:HIS:HA	1.55	0.88
1:A:227:MET:HB3	1:B:242:ALA:HB1	1.52	0.88
1:A:33:HIS:HA	1:A:100:PRO:HG3	1.56	0.88
1:A:117:ARG:HB3	1:A:120:ARG:HB2	1.56	0.87
1:A:203:TRP:CE3	1:A:203:TRP:HA	2.08	0.86
1:B:117:ARG:HB3	1:B:120:ARG:HG3	1.56	0.86
1:B:226:ILE:HG23	1:B:230:ASP:HB2	1.54	0.86
1:B:5:VAL:HA	1:B:8:ILE:HB	1.56	0.86
1:A:243:GLU:HG2	1:A:244:LYS:H	1.41	0.86
1:A:52:MET:HE1	1:B:8:ILE:HA	1.56	0.85
1:A:233:ARG:HG2	1:A:237:MET:SD	2.17	0.85
1:A:240:ASP:HA	1:A:245:ARG:HH22	1.41	0.85
1:A:28:MET:CE	1:B:68:HIS:HA	2.06	0.85
1:A:63:MET:HE1	1:A:67:LEU:HD21	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:HA	1:A:274:ARG:NE	1.89	0.85
1:A:249:MET:H	1:B:293:PHE:HB3	1.39	0.85
1:B:261:LYS:HA	1:B:264:GLN:NE2	1.91	0.85
1:A:114:TYR:HA	1:A:148:HIS:HE1	1.42	0.85
1:A:274:ARG:HA	1:A:274:ARG:HE	1.39	0.85
1:B:212:ARG:HA	1:B:213:PRO:O	1.78	0.84
1:A:159:ILE:HA	1:A:162:LEU:HB3	1.58	0.84
1:B:64:THR:O	1:B:68:HIS:CD2	2.30	0.84
1:B:110:TRP:HZ2	1:B:208:TYR:O	1.61	0.84
1:A:54:TYR:HB2	1:A:64:THR:HG21	1.60	0.84
1:A:257:ILE:HD11	1:B:287:VAL:HG23	1.60	0.84
1:A:201:SER:CB	1:A:204:GLY:H	1.85	0.84
1:A:263:GLN:HE22	1:A:266:LYS:HE3	1.41	0.84
1:A:233:ARG:O	1:A:237:MET:SD	2.36	0.83
1:B:289:LEU:HD12	1:B:290:GLN:N	1.93	0.83
1:B:13:PRO:HG2	1:B:18:GLN:CG	2.09	0.83
1:A:37:ALA:HB1	1:A:101:ARG:NH2	1.92	0.83
1:A:116:TRP:O	1:A:146:ASP:HB3	1.78	0.83
1:A:62:ARG:HA	1:A:72:PRO:CG	2.08	0.83
1:A:106:PHE:CE2	1:A:158:LEU:HG	2.14	0.83
1:A:187:LYS:HD3	1:A:191:LEU:HD13	1.60	0.82
1:A:236:ARG:HA	1:A:239:ARG:HG2	1.60	0.82
1:B:13:PRO:CG	1:B:18:GLN:HG2	2.09	0.82
1:A:102:TYR:CE1	1:A:186:ILE:HG12	2.15	0.82
1:B:92:LEU:H	1:B:92:LEU:HD12	1.45	0.81
1:A:122:ARG:HG2	1:A:149:LEU:HG	1.61	0.81
1:A:114:TYR:CD1	1:A:148:HIS:CE1	2.68	0.81
1:B:152:SER:HA	1:B:155:PHE:HB2	1.61	0.81
1:B:224:THR:O	1:B:228:VAL:HG22	1.81	0.81
1:A:41:ALA:HB2	1:A:94:MET:HA	1.61	0.80
1:B:212:ARG:HA	1:B:213:PRO:C	1.99	0.80
1:A:290:GLN:HA	1:B:252:LEU:CB	2.10	0.80
1:B:35:HIS:HD2	1:B:35:HIS:O	1.64	0.80
1:A:198:ARG:HD2	1:A:206:PRO:HG3	1.62	0.80
1:A:41:ALA:HA	1:A:94:MET:CE	2.12	0.80
1:B:57:GLN:OE1	1:B:64:THR:CG2	2.23	0.80
1:A:22:TYR:OH	1:B:236:ARG:HA	1.82	0.80
1:A:198:ARG:HG3	1:A:206:PRO:CB	2.07	0.80
1:B:171:PRO:HB2	1:B:173:GLU:HG2	1.64	0.80
1:B:35:HIS:HA	1:B:38:PHE:CB	2.12	0.80
1:A:228:VAL:HG23	1:A:229:GLU:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:TYR:CE1	1:A:186:ILE:HG23	2.17	0.80
1:B:107:PRO:HA	1:B:210:LEU:HD11	1.63	0.79
1:A:106:PHE:HD2	1:A:162:LEU:HD22	1.44	0.79
1:A:34:ARG:NH2	1:A:186:ILE:HD11	1.96	0.79
1:B:101:ARG:O	1:B:105:GLN:HG2	1.82	0.79
1:B:54:TYR:CD1	1:B:55:LEU:HG	2.18	0.79
1:A:114:TYR:CD1	1:A:148:HIS:HE1	1.99	0.79
1:A:244:LYS:HB3	1:A:248:THR:CG2	2.08	0.79
1:A:14:SER:O	1:A:17:ASP:HB2	1.82	0.79
1:A:231:THR:HG21	1:B:235:PHE:CE2	2.17	0.79
1:A:14:SER:HB3	1:A:17:ASP:OD1	1.83	0.79
1:B:32:GLY:O	1:B:100:PRO:HG3	1.84	0.78
1:A:173:GLU:HG2	1:A:174:HIS:N	1.98	0.78
1:A:128:LEU:HD21	1:A:136:ILE:CD1	2.14	0.78
1:A:255:LEU:HD22	1:A:256:ASP:H	1.46	0.78
1:B:158:LEU:O	1:B:162:LEU:HB2	1.83	0.78
1:A:22:TYR:CZ	1:B:236:ARG:HA	2.19	0.78
1:B:51:TYR:O	1:B:54:TYR:HD1	1.65	0.78
1:B:65:GLY:CA	1:B:68:HIS:HD2	1.95	0.78
1:B:110:TRP:HZ3	1:B:155:PHE:CD1	2.02	0.78
1:B:116:TRP:HD1	1:B:122:ARG:CA	1.97	0.78
1:B:152:SER:HA	1:B:155:PHE:CB	2.14	0.78
1:A:102:TYR:CZ	1:A:186:ILE:HG12	2.19	0.78
1:B:191:LEU:HG	1:B:196:VAL:O	1.83	0.78
1:B:4:ASP:HB2	1:B:25:PHE:CD1	2.19	0.78
1:B:205:MET:HG3	1:B:206:PRO:CD	2.14	0.78
1:A:57:GLN:NE2	1:A:67:LEU:HD11	1.98	0.77
1:A:165:ARG:HG3	1:A:166:SER:N	1.98	0.77
1:A:187:LYS:HZ2	1:A:188:ARG:HD3	1.49	0.77
1:B:163:HIS:CE1	1:B:178:LEU:CD2	2.65	0.77
1:B:25:PHE:HA	1:B:29:ARG:HB2	1.65	0.77
1:A:74:ARG:HD2	1:A:74:ARG:C	2.05	0.77
1:A:110:TRP:CZ3	1:A:196:VAL:HG22	2.19	0.77
1:A:35:HIS:HA	1:A:38:PHE:CE1	2.20	0.77
1:B:71:GLU:H	1:B:71:GLU:CD	1.86	0.77
1:A:161:PHE:HA	1:A:164:LYS:HD2	1.66	0.76
1:B:198:ARG:HG3	1:B:198:ARG:O	1.83	0.76
1:A:239:ARG:HH12	1:B:8:ILE:HG21	1.49	0.76
1:A:182:LEU:CB	1:B:69:HIS:NE2	2.41	0.76
1:A:250:ARG:HG2	1:A:251:VAL:H	1.48	0.76
1:A:110:TRP:CZ3	1:A:155:PHE:CZ	2.72	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:HA	1:A:245:ARG:NH2	2.00	0.76
1:A:47:LYS:HB3	1:A:50:ILE:HD12	1.67	0.76
1:B:116:TRP:HD1	1:B:122:ARG:HA	1.50	0.76
1:B:57:GLN:HE22	1:B:64:THR:HA	1.51	0.76
1:A:291:MET:SD	1:B:251:VAL:HB	2.26	0.76
1:A:250:ARG:HA	1:B:291:MET:O	1.86	0.76
1:A:171:PRO:O	1:A:175:GLN:HG3	1.86	0.76
1:B:241:TRP:CZ3	1:B:250:ARG:HD3	2.19	0.76
1:B:269:LEU:O	1:B:272:ILE:HG22	1.86	0.76
1:B:241:TRP:HD1	1:B:249:MET:HA	1.51	0.76
1:B:110:TRP:CE2	1:B:150:ILE:HB	2.20	0.76
1:B:68:HIS:HB3	1:B:70:LEU:HB2	1.68	0.75
1:B:110:TRP:CZ2	1:B:208:TYR:O	2.39	0.75
1:B:53:THR:HG21	1:B:68:HIS:HE1	1.51	0.75
1:A:222:GLU:O	1:A:226:ILE:HG13	1.87	0.75
1:B:116:TRP:CB	1:B:122:ARG:NH2	2.49	0.75
1:A:47:LYS:HB3	1:A:50:ILE:CD1	2.17	0.75
1:B:163:HIS:HE1	1:B:178:LEU:HD21	1.52	0.75
1:A:251:VAL:CB	1:B:291:MET:HB3	2.14	0.75
1:B:189:ARG:HA	1:B:192:TYR:HB3	1.68	0.75
1:A:294:GLY:O	1:B:287:VAL:HG13	1.87	0.75
1:A:129:THR:OG1	1:A:132:GLU:HB3	1.85	0.75
1:A:251:VAL:HB	1:B:291:MET:CB	2.16	0.75
1:A:198:ARG:CG	1:A:206:PRO:HB3	2.09	0.75
1:B:100:PRO:O	1:B:104:ILE:HB	1.87	0.75
1:A:41:ALA:HA	1:A:94:MET:HE2	1.67	0.75
1:A:122:ARG:HA	1:A:148:HIS:CB	2.17	0.74
1:B:54:TYR:CE1	1:B:55:LEU:HG	2.23	0.74
1:B:59:GLN:O	1:B:59:GLN:HG3	1.87	0.74
1:A:73:LYS:O	1:A:77:ALA:N	2.21	0.74
1:B:236:ARG:HB2	1:B:236:ARG:NH1	2.01	0.74
1:B:250:ARG:HH11	1:B:250:ARG:CG	1.82	0.74
1:B:265:ALA:HA	1:B:268:GLU:CD	2.07	0.74
1:A:29:ARG:NH2	1:B:57:GLN:OE1	2.21	0.74
1:A:235:PHE:O	1:A:239:ARG:N	2.21	0.74
1:A:249:MET:HG2	1:B:293:PHE:CB	2.17	0.74
1:A:182:LEU:HD23	1:A:183:ALA:N	2.03	0.74
1:A:190:LEU:HA	1:A:193:SER:CB	2.17	0.74
1:A:117:ARG:HE	1:A:120:ARG:HG2	1.52	0.74
1:B:234:PHE:HE2	1:B:238:MET:HB2	1.53	0.73
1:B:186:ILE:O	1:B:190:LEU:HD12	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:O	1:B:59:GLN:HA	1.88	0.73
1:A:238:MET:HA	1:A:241:TRP:HB3	1.70	0.73
1:B:116:TRP:CG	1:B:122:ARG:NH2	2.57	0.73
1:A:109:VAL:O	1:A:113:LYS:HB2	1.87	0.73
1:A:247:ASN:O	1:B:294:GLY:HA2	1.88	0.73
1:A:114:TYR:HA	1:A:148:HIS:CE1	2.23	0.73
1:B:99:GLU:O	1:B:104:ILE:HD12	1.89	0.73
1:B:4:ASP:HB2	1:B:25:PHE:CG	2.23	0.73
1:A:93:LYS:HA	1:A:170:LEU:CD2	2.18	0.72
1:A:231:THR:CG2	1:B:234:PHE:HZ	2.02	0.72
1:B:227:MET:O	1:B:231:THR:HB	1.89	0.72
1:A:116:TRP:NE1	1:A:122:ARG:HB2	2.05	0.72
1:B:51:TYR:HE2	1:B:55:LEU:HD21	1.53	0.72
1:A:239:ARG:HB3	1:B:22:TYR:CZ	2.23	0.72
1:A:72:PRO:O	1:A:76:LYS:CB	2.37	0.72
1:A:101:ARG:HE	1:A:170:LEU:HD11	1.54	0.72
1:B:51:TYR:CD1	1:B:79:VAL:HG13	2.25	0.72
1:A:114:TYR:CA	1:A:148:HIS:HE1	2.01	0.72
1:A:61:LEU:HD11	1:A:79:VAL:HG21	1.70	0.72
1:B:241:TRP:CD2	1:B:250:ARG:HB2	2.25	0.72
1:A:170:LEU:HB3	1:A:171:PRO:CD	2.20	0.72
1:A:295:LYS:HA	1:B:287:VAL:CG2	2.15	0.71
1:A:203:TRP:HA	1:A:203:TRP:HE3	1.50	0.71
1:A:76:LYS:HA	1:A:79:VAL:HB	1.70	0.71
1:A:110:TRP:CZ3	1:A:155:PHE:HZ	2.09	0.71
1:A:231:THR:HG23	1:B:238:MET:CG	2.20	0.71
1:B:55:LEU:HA	1:B:59:GLN:OE1	1.91	0.71
1:B:240:ASP:HA	1:B:243:GLU:CB	2.17	0.71
1:B:187:LYS:HD2	1:B:188:ARG:NH2	2.00	0.71
1:B:35:HIS:CA	1:B:38:PHE:HB3	2.20	0.71
1:B:116:TRP:CD1	1:B:122:ARG:CA	2.74	0.71
1:A:34:ARG:HH12	1:A:163:HIS:HD2	1.38	0.71
1:A:239:ARG:HG3	1:A:240:ASP:H	1.55	0.71
1:A:52:MET:CE	1:B:8:ILE:HA	2.21	0.71
1:A:139:LYS:HB3	1:A:199:ILE:CG2	2.21	0.71
1:A:179:SER:N	1:A:182:LEU:HD22	2.06	0.70
1:A:249:MET:HG2	1:B:293:PHE:HB2	1.71	0.70
1:B:116:TRP:CD1	1:B:122:ARG:HB2	2.25	0.70
1:B:158:LEU:O	1:B:162:LEU:N	2.22	0.70
1:A:263:GLN:NE2	1:A:267:ASP:OD2	2.24	0.70
1:A:114:TYR:CA	1:A:148:HIS:CE1	2.75	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HG3	1:A:166:SER:H	1.55	0.70
1:A:287:VAL:HB	1:B:254:GLU:O	1.90	0.70
1:A:110:TRP:CH2	1:A:196:VAL:HG22	2.27	0.70
1:A:231:THR:HG21	1:B:235:PHE:HE2	1.56	0.70
1:A:110:TRP:CH2	1:A:155:PHE:HZ	2.09	0.70
1:B:62:ARG:O	1:B:66:HIS:N	2.24	0.70
1:A:290:GLN:HB2	1:B:250:ARG:CZ	2.22	0.70
1:B:163:HIS:HE1	1:B:178:LEU:CD2	2.04	0.70
1:B:164:LYS:HE2	1:B:167:GLN:NE2	2.07	0.70
1:A:140:LEU:HD13	1:A:144:LEU:HD11	1.72	0.70
1:A:102:TYR:CD1	1:A:186:ILE:HG23	2.27	0.69
1:A:28:MET:SD	1:A:38:PHE:CE1	2.85	0.69
1:A:29:ARG:HH22	1:B:64:THR:HG22	1.57	0.69
1:A:182:LEU:O	1:A:186:ILE:N	2.21	0.69
1:A:35:HIS:O	1:A:39:LEU:HB2	1.92	0.69
1:B:265:ALA:HA	1:B:268:GLU:CG	2.23	0.69
1:B:245:ARG:O	1:B:248:THR:HB	1.93	0.69
1:A:117:ARG:HB3	1:A:120:ARG:CB	2.21	0.69
1:A:75:VAL:HA	1:A:78:ILE:HG22	1.75	0.69
1:A:295:LYS:CA	1:B:287:VAL:HG22	2.17	0.69
1:A:92:LEU:H	1:A:92:LEU:HD13	1.56	0.69
1:B:68:HIS:CB	1:B:70:LEU:HB2	2.23	0.69
1:A:66:HIS:O	1:A:69:HIS:HA	1.93	0.69
1:B:25:PHE:HA	1:B:29:ARG:HD3	1.74	0.69
1:B:35:HIS:CD2	1:B:38:PHE:CD1	2.81	0.69
1:B:259:PRO:O	1:B:262:MET:HG2	1.92	0.69
1:A:153:PHE:O	1:A:157:GLU:HG2	1.92	0.69
1:A:114:TYR:CG	1:A:148:HIS:CE1	2.81	0.68
1:A:249:MET:N	1:B:293:PHE:HB3	2.08	0.68
1:A:99:GLU:HG3	1:A:104:ILE:HB	1.75	0.68
1:B:241:TRP:CE3	1:B:250:ARG:HD3	2.28	0.68
1:A:253:GLU:HB2	1:B:277:ALA:HB2	1.74	0.68
1:B:5:VAL:CA	1:B:8:ILE:HB	2.24	0.68
1:A:110:TRP:CH2	1:A:155:PHE:CZ	2.82	0.68
1:A:104:ILE:HG23	1:A:105:GLN:HE21	1.58	0.68
1:A:234:PHE:CE1	1:B:234:PHE:CE1	2.81	0.68
1:A:239:ARG:HH22	1:B:5:VAL:HG22	1.57	0.68
1:A:270:ASP:O	1:A:273:ILE:HG13	1.93	0.68
1:A:124:PRO:HG2	1:A:150:ILE:HD11	1.76	0.68
1:A:29:ARG:NH2	1:B:53:THR:O	2.26	0.68
1:B:68:HIS:HB2	1:B:70:LEU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LYS:H	1:B:287:VAL:HA	1.57	0.68
1:A:245:ARG:CG	1:A:246:PRO:HD2	2.21	0.68
1:A:57:GLN:HE22	1:A:67:LEU:HD11	1.59	0.68
1:B:191:LEU:HD11	1:B:198:ARG:N	2.09	0.68
1:B:54:TYR:HA	1:B:64:THR:OG1	1.93	0.67
1:B:35:HIS:O	1:B:35:HIS:CD2	2.47	0.67
1:B:187:LYS:CD	1:B:188:ARG:HH21	2.00	0.67
1:A:101:ARG:NE	1:A:170:LEU:HD11	2.09	0.67
1:A:182:LEU:CG	1:A:186:ILE:HD12	2.22	0.67
1:A:236:ARG:O	1:A:240:ASP:CG	2.33	0.67
1:B:98:GLN:HG2	1:B:228:VAL:HG21	1.77	0.67
1:B:263:GLN:HA	1:B:263:GLN:HE21	1.59	0.67
1:A:249:MET:SD	1:B:269:LEU:HD12	2.34	0.67
1:A:143:ASN:O	1:A:144:LEU:HG	1.95	0.67
1:A:114:TYR:CB	1:A:148:HIS:CE1	2.76	0.67
1:B:218:ALA:O	1:B:222:GLU:HB3	1.93	0.67
1:A:106:PHE:CE1	1:A:110:TRP:HE3	2.11	0.67
1:A:198:ARG:HH11	1:A:198:ARG:HB3	1.59	0.67
1:A:92:LEU:N	1:A:92:LEU:HD13	2.10	0.67
1:A:7:LEU:HD22	1:A:10:ARG:HD2	1.75	0.67
1:A:236:ARG:NH1	1:B:296:LYS:HE2	2.10	0.67
1:B:46:ALA:O	1:B:50:ILE:HD13	1.95	0.67
1:A:245:ARG:HG3	1:A:246:PRO:CD	2.24	0.67
1:A:117:ARG:HB3	1:A:120:ARG:CG	2.25	0.67
1:A:104:ILE:HG23	1:A:105:GLN:H	1.59	0.66
1:A:233:ARG:C	1:A:237:MET:SD	2.74	0.66
1:B:6:ASP:O	1:B:10:ARG:HG3	1.95	0.66
1:A:117:ARG:HE	1:A:120:ARG:HE	1.43	0.66
1:A:263:GLN:HE21	1:A:267:ASP:CG	1.98	0.66
1:A:185:HIS:CE1	1:B:69:HIS:ND1	2.63	0.66
1:A:155:PHE:CD2	1:A:208:TYR:HD2	2.13	0.66
1:B:68:HIS:HB2	1:B:70:LEU:CB	2.25	0.66
1:A:239:ARG:HG3	1:A:240:ASP:N	2.10	0.66
1:B:151:THR:O	1:B:155:PHE:HB2	1.95	0.66
1:A:50:ILE:HD11	1:B:38:PHE:HE1	1.59	0.66
1:A:102:TYR:CE1	1:A:103:LEU:HG	2.30	0.66
1:A:34:ARG:HB2	1:B:69:HIS:ND1	2.10	0.66
1:A:28:MET:HG2	1:B:68:HIS:ND1	2.10	0.66
1:A:117:ARG:NE	1:A:120:ARG:HE	1.92	0.66
1:A:187:LYS:NZ	1:A:188:ARG:HD3	2.09	0.66
1:B:38:PHE:O	1:B:41:ALA:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLN:HA	1:B:175:GLN:OE1	1.96	0.66
1:A:184:GLU:O	1:A:188:ARG:CB	2.27	0.66
1:A:289:LEU:H	1:B:254:GLU:HG2	1.60	0.66
1:B:116:TRP:CD1	1:B:122:ARG:N	2.63	0.66
1:A:54:TYR:O	1:A:59:GLN:HA	1.96	0.66
1:B:8:ILE:HG13	1:B:25:PHE:HE1	1.59	0.66
1:A:76:LYS:O	1:A:79:VAL:HB	1.96	0.66
1:A:223:ARG:HH11	1:A:226:ILE:HD12	1.60	0.66
1:A:179:SER:HB2	1:A:182:LEU:HB3	1.78	0.66
1:B:226:ILE:O	1:B:230:ASP:N	2.28	0.66
1:A:227:MET:CB	1:B:242:ALA:CB	2.71	0.66
1:B:198:ARG:HA	1:B:208:TYR:CE1	2.31	0.65
1:A:264:GLN:HA	1:A:264:GLN:NE2	2.11	0.65
1:A:167:GLN:HA	1:A:170:LEU:CD1	2.26	0.65
1:A:34:ARG:HE	1:A:37:ALA:HB2	1.61	0.65
1:A:291:MET:SD	1:B:251:VAL:O	2.54	0.65
1:B:35:HIS:CD2	1:B:38:PHE:HD1	2.13	0.65
1:B:258:LEU:HD12	1:B:258:LEU:N	2.11	0.65
1:A:12:GLY:N	1:A:13:PRO:HD3	2.11	0.65
1:A:29:ARG:CZ	1:B:53:THR:HB	2.26	0.65
1:A:35:HIS:HA	1:A:38:PHE:CD1	2.32	0.65
1:A:245:ARG:O	1:A:248:THR:HB	1.96	0.65
1:B:53:THR:HG21	1:B:68:HIS:NE2	2.11	0.65
1:B:161:PHE:O	1:B:164:LYS:HB3	1.97	0.65
1:B:13:PRO:CB	1:B:17:ASP:HB2	2.26	0.65
1:B:191:LEU:O	1:B:191:LEU:HD23	1.96	0.65
1:B:261:LYS:HG2	1:B:264:GLN:NE2	2.12	0.65
1:A:294:GLY:HA2	1:B:247:ASN:O	1.97	0.65
1:A:188:ARG:HH22	1:A:191:LEU:HD22	1.60	0.65
1:B:191:LEU:HD11	1:B:198:ARG:H	1.62	0.65
1:B:239:ARG:HE	1:B:243:GLU:HG3	1.62	0.65
1:A:129:THR:O	1:A:133:LYS:HG2	1.95	0.65
1:B:265:ALA:HA	1:B:268:GLU:HG2	1.78	0.65
1:A:292:VAL:HG12	1:A:293:PHE:N	2.12	0.65
1:B:16:MET:O	1:B:19:ILE:HD13	1.96	0.65
1:B:265:ALA:O	1:B:268:GLU:HG2	1.97	0.65
1:A:57:GLN:HG2	1:A:64:THR:OG1	1.97	0.65
1:A:124:PRO:CG	1:A:148:HIS:HD2	2.09	0.64
1:A:244:LYS:CB	1:A:248:THR:HG21	2.13	0.64
1:B:240:ASP:CA	1:B:243:GLU:HB2	2.21	0.64
1:B:51:TYR:CE2	1:B:54:TYR:HE1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:HG23	1:B:230:ASP:CB	2.26	0.64
1:A:231:THR:HG23	1:B:238:MET:HE3	1.78	0.64
1:A:185:HIS:CG	1:A:186:ILE:N	2.63	0.64
1:A:290:GLN:HA	1:B:252:LEU:HB3	1.77	0.64
1:B:289:LEU:HD12	1:B:289:LEU:C	2.17	0.64
1:A:264:GLN:O	1:A:268:GLU:HB2	1.97	0.64
1:A:9:LYS:O	1:A:12:GLY:N	2.31	0.64
1:A:227:MET:HB3	1:B:242:ALA:HB2	1.77	0.64
1:A:235:PHE:CE2	1:B:234:PHE:HE1	2.16	0.64
1:A:263:GLN:HE22	1:A:266:LYS:CE	2.11	0.64
1:A:29:ARG:NH1	1:B:53:THR:HB	2.12	0.64
1:A:3:ASN:CB	1:B:56:GLU:HA	2.24	0.64
1:A:252:LEU:HD12	1:A:253:GLU:N	2.12	0.64
1:A:104:ILE:HG23	1:A:105:GLN:NE2	2.12	0.64
1:A:28:MET:HE1	1:A:35:HIS:ND1	2.12	0.64
1:A:34:ARG:HG2	1:A:37:ALA:HB3	1.78	0.64
1:A:28:MET:SD	1:A:38:PHE:HE1	2.20	0.64
1:A:234:PHE:O	1:A:238:MET:N	2.30	0.64
1:B:150:ILE:HG23	1:B:154:GLU:CB	2.15	0.64
1:A:69:HIS:HB3	1:B:182:LEU:CD1	2.28	0.64
1:B:117:ARG:HB3	1:B:120:ARG:CG	2.27	0.64
1:A:38:PHE:CD2	1:A:38:PHE:C	2.71	0.64
1:A:181:ALA:O	1:A:185:HIS:CB	2.39	0.63
1:A:190:LEU:CA	1:A:193:SER:HB2	2.22	0.63
1:A:117:ARG:NE	1:A:120:ARG:HG2	2.13	0.63
1:B:122:ARG:O	1:B:122:ARG:HG3	1.98	0.63
1:A:124:PRO:HG3	1:A:148:HIS:CD2	2.25	0.63
1:A:296:LYS:O	1:B:288:VAL:HG22	1.99	0.63
1:A:187:LYS:HZ2	1:A:188:ARG:NH2	1.96	0.63
1:A:41:ALA:CA	1:A:94:MET:HE2	2.29	0.63
1:B:38:PHE:CD2	1:B:38:PHE:C	2.69	0.63
1:A:162:LEU:HG	1:A:163:HIS:N	2.14	0.63
1:A:253:GLU:HG3	1:B:276:TRP:HB3	1.81	0.63
1:B:13:PRO:HB2	1:B:17:ASP:HB2	1.79	0.63
1:A:296:LYS:N	1:B:287:VAL:HA	2.12	0.63
1:A:234:PHE:O	1:A:237:MET:HB2	1.97	0.63
1:B:101:ARG:O	1:B:104:ILE:HG22	1.97	0.63
1:B:225:TYR:O	1:B:228:VAL:HG23	1.99	0.63
1:A:178:LEU:HA	1:A:182:LEU:HD22	1.81	0.63
1:A:240:ASP:HB3	1:A:245:ARG:HH21	1.62	0.63
1:B:261:LYS:CA	1:B:264:GLN:HE21	2.00	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:MET:CG	1:B:206:PRO:HD2	2.26	0.63
1:B:155:PHE:O	1:B:158:LEU:HB2	1.99	0.63
1:A:131:GLU:CD	1:A:135:GLN:NE2	2.50	0.63
1:A:16:MET:HE3	1:B:95:LEU:O	1.99	0.63
1:B:8:ILE:HG12	1:B:21:LEU:HD11	1.81	0.63
1:A:111:MET:O	1:A:115:PRO:N	2.32	0.62
1:A:123:ILE:HG23	1:A:207:PHE:CZ	2.34	0.62
1:B:51:TYR:CE1	1:B:79:VAL:HG13	2.34	0.62
1:A:67:LEU:O	1:A:69:HIS:CE1	2.52	0.62
1:A:57:GLN:CD	1:A:64:THR:HG23	2.19	0.62
1:B:163:HIS:HE1	1:B:178:LEU:CG	2.13	0.62
1:A:296:LYS:O	1:B:288:VAL:HG13	1.99	0.62
1:A:101:ARG:CZ	1:A:101:ARG:HB2	2.29	0.62
1:B:57:GLN:O	1:B:60:ASN:HB2	1.99	0.62
1:B:188:ARG:O	1:B:192:TYR:N	2.31	0.62
1:B:259:PRO:HA	1:B:262:MET:SD	2.40	0.62
1:A:140:LEU:O	1:A:140:LEU:HD12	1.99	0.62
1:B:231:THR:O	1:B:234:PHE:HB3	1.99	0.62
1:B:234:PHE:HA	1:B:237:MET:CE	2.29	0.62
1:B:237:MET:SD	1:B:288:VAL:HG23	2.40	0.62
1:A:235:PHE:HA	1:A:238:MET:CB	2.27	0.62
1:A:243:GLU:HG2	1:A:244:LYS:N	2.12	0.62
1:A:68:HIS:C	1:A:69:HIS:CG	2.72	0.62
1:B:6:ASP:O	1:B:9:LYS:HG3	1.98	0.62
1:A:110:TRP:CH2	1:A:195:THR:O	2.53	0.62
1:B:51:TYR:CZ	1:B:54:TYR:CE1	2.87	0.62
1:B:63:MET:HA	1:B:66:HIS:CB	2.28	0.62
1:A:75:VAL:O	1:A:79:VAL:HG23	2.00	0.62
1:B:191:LEU:HD11	1:B:198:ARG:HB3	1.80	0.62
1:A:248:THR:N	1:B:266:LYS:HE3	2.15	0.62
1:B:63:MET:SD	1:B:66:HIS:CD2	2.93	0.62
1:A:95:LEU:HD12	1:A:97:SER:O	1.99	0.61
1:B:75:VAL:O	1:B:79:VAL:HG23	2.00	0.61
1:A:41:ALA:HA	1:A:94:MET:HE3	1.82	0.61
1:A:292:VAL:HG11	1:B:237:MET:O	1.99	0.61
1:B:250:ARG:HH22	1:B:252:LEU:CD2	2.13	0.61
1:B:3:ASN:HA	1:B:6:ASP:HB3	1.82	0.61
1:A:161:PHE:O	1:A:164:LYS:HB2	2.00	0.61
1:A:179:SER:H	1:A:182:LEU:HD22	1.63	0.61
1:A:198:ARG:HB2	1:A:208:TYR:HE1	1.65	0.61
1:A:235:PHE:CZ	1:B:234:PHE:HE1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:HIS:NE2	1:B:178:LEU:HD11	2.15	0.61
1:B:151:THR:O	1:B:155:PHE:N	2.32	0.61
1:B:91:LEU:HG	1:B:92:LEU:O	2.00	0.61
1:A:51:TYR:CZ	1:A:55:LEU:HD11	2.35	0.61
1:A:231:THR:OG1	1:B:238:MET:HG2	2.00	0.61
1:A:239:ARG:HH12	1:B:8:ILE:CG2	2.13	0.61
1:B:111:MET:HB3	1:B:210:LEU:HD22	1.82	0.61
1:A:69:HIS:HB3	1:B:182:LEU:HD13	1.83	0.61
1:A:244:LYS:HD3	1:B:223:ARG:HH22	1.64	0.61
1:A:289:LEU:N	1:B:254:GLU:HG2	2.16	0.61
1:B:54:TYR:CE1	1:B:55:LEU:CD2	2.83	0.60
1:A:276:TRP:CD1	1:A:276:TRP:C	2.73	0.60
1:A:182:LEU:HA	1:B:69:HIS:NE2	2.16	0.60
1:B:31:SER:OG	1:B:98:GLN:NE2	2.29	0.60
1:B:116:TRP:CE3	1:B:146:ASP:OD1	2.54	0.60
1:A:107:PRO:O	1:A:110:TRP:HB3	2.02	0.60
1:A:182:LEU:O	1:A:186:ILE:CB	2.49	0.60
1:B:35:HIS:CG	1:B:38:PHE:HD1	2.20	0.60
1:B:241:TRP:CD1	1:B:249:MET:C	2.75	0.60
1:A:160:GLU:O	1:A:164:LYS:HG3	2.01	0.60
1:A:264:GLN:HA	1:A:264:GLN:HE21	1.65	0.60
1:A:233:ARG:HG2	1:A:237:MET:CE	2.31	0.60
1:B:8:ILE:HG22	1:B:9:LYS:N	2.17	0.60
1:B:164:LYS:HA	1:B:167:GLN:HG3	1.84	0.60
1:A:57:GLN:OE1	1:A:64:THR:HG23	2.02	0.59
1:B:241:TRP:CD1	1:B:249:MET:HA	2.34	0.59
1:A:128:LEU:HD23	1:A:133:LYS:HB2	1.83	0.59
1:B:93:LYS:HE2	1:B:170:LEU:HD22	1.84	0.59
1:B:107:PRO:HB3	1:B:210:LEU:HD21	1.83	0.59
1:A:185:HIS:N	1:B:66:HIS:CE1	2.71	0.59
1:B:54:TYR:HE1	1:B:55:LEU:CD2	2.15	0.59
1:A:29:ARG:HH12	1:B:64:THR:HA	1.66	0.59
1:A:18:GLN:HA	1:A:21:LEU:HB2	1.83	0.59
1:A:130:SER:HA	1:A:133:LYS:CE	2.18	0.59
1:B:163:HIS:CE1	1:B:178:LEU:HD11	2.37	0.59
1:A:122:ARG:NE	1:A:147:ALA:O	2.35	0.59
1:A:155:PHE:CE2	1:A:208:TYR:HD2	2.21	0.59
1:A:190:LEU:HD12	1:A:193:SER:HB2	1.85	0.59
1:B:50:ILE:HA	1:B:53:THR:HG23	1.84	0.59
1:A:114:TYR:CG	1:A:148:HIS:HE1	2.20	0.59
1:A:53:THR:OG1	1:B:29:ARG:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:TRP:CD1	1:B:122:ARG:CB	2.86	0.59
1:A:239:ARG:HB3	1:B:22:TYR:CE1	2.37	0.59
1:A:182:LEU:HA	1:B:69:HIS:CE1	2.38	0.59
1:A:68:HIS:O	1:A:70:LEU:HD12	2.03	0.59
1:A:293:PHE:O	1:B:248:THR:HA	2.02	0.59
1:B:295:LYS:O	1:B:296:LYS:HB2	2.03	0.59
1:A:210:LEU:HD11	1:A:212:ARG:O	2.02	0.59
1:A:185:HIS:ND1	1:B:69:HIS:ND1	2.49	0.59
1:A:257:ILE:HD11	1:B:287:VAL:CG2	2.33	0.58
1:A:259:PRO:HA	1:A:262:MET:HG2	1.85	0.58
1:A:198:ARG:NH1	1:A:198:ARG:HB3	2.18	0.58
1:A:255:LEU:HG	1:B:277:ALA:O	2.03	0.58
1:A:143:ASN:C	1:A:144:LEU:HG	2.24	0.58
1:B:64:THR:O	1:B:68:HIS:HD2	1.83	0.58
1:A:235:PHE:CZ	1:B:234:PHE:CE1	2.91	0.58
1:A:260:GLU:HG2	1:A:261:LYS:HG2	1.84	0.58
1:B:113:LYS:O	1:B:115:PRO:HD3	2.02	0.58
1:B:54:TYR:HA	1:B:64:THR:CB	2.33	0.58
1:B:68:HIS:CB	1:B:70:LEU:CB	2.81	0.58
1:A:231:THR:HG22	1:B:234:PHE:HZ	1.68	0.58
1:A:54:TYR:HD2	1:A:59:GLN:HA	1.68	0.58
1:A:112:GLU:C	1:A:115:PRO:HD3	2.23	0.58
1:B:15:ALA:HA	1:B:18:GLN:CD	2.23	0.58
1:B:234:PHE:HA	1:B:237:MET:HE3	1.85	0.58
1:A:296:LYS:C	1:B:288:VAL:HG22	2.24	0.58
1:A:84:GLN:HB3	1:A:90:LYS:H	1.69	0.58
1:A:34:ARG:NH2	1:A:182:LEU:HD12	2.18	0.58
1:A:293:PHE:HD2	1:B:249:MET:HG3	1.69	0.58
1:A:106:PHE:HE2	1:A:158:LEU:HG	1.64	0.58
1:A:61:LEU:HB3	1:A:72:PRO:HB3	1.84	0.58
1:B:52:MET:HA	1:B:55:LEU:HD12	1.84	0.58
1:A:233:ARG:O	1:A:237:MET:N	2.35	0.58
1:A:68:HIS:HB3	1:B:35:HIS:ND1	2.19	0.58
1:A:69:HIS:NE2	1:B:35:HIS:N	2.47	0.58
1:B:145:PRO:HD3	1:B:211:THR:O	2.04	0.58
1:A:290:GLN:HB2	1:B:250:ARG:NH2	2.19	0.58
1:A:253:GLU:OE2	1:B:276:TRP:CE3	2.57	0.58
1:B:116:TRP:CB	1:B:122:ARG:HH22	2.16	0.58
1:A:240:ASP:OD2	1:B:296:LYS:HD2	2.04	0.58
1:A:54:TYR:HB2	1:A:64:THR:CG2	2.34	0.58
1:A:234:PHE:HE1	1:B:234:PHE:CE1	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:CG	1:A:104:ILE:HB	2.33	0.57
1:B:106:PHE:HA	1:B:162:LEU:CD2	2.33	0.57
1:B:171:PRO:HB2	1:B:173:GLU:CG	2.33	0.57
1:A:116:TRP:CD1	1:A:122:ARG:CB	2.83	0.57
1:A:178:LEU:HD12	1:A:182:LEU:HD21	1.87	0.57
1:A:245:ARG:H	1:A:248:THR:HB	1.69	0.57
1:A:54:TYR:CB	1:A:64:THR:HG21	2.32	0.57
1:A:292:VAL:CG1	1:A:293:PHE:N	2.66	0.57
1:B:291:MET:HG3	1:B:292:VAL:H	1.70	0.57
1:A:28:MET:HE3	1:A:33:HIS:O	2.04	0.57
1:A:29:ARG:HD2	1:B:67:LEU:HD12	1.86	0.57
1:B:92:LEU:HD13	1:B:94:MET:SD	2.44	0.57
1:B:262:MET:N	1:B:262:MET:SD	2.78	0.57
1:A:166:SER:O	1:A:170:LEU:HD12	2.04	0.57
1:A:28:MET:HE1	1:A:35:HIS:N	2.19	0.57
1:B:63:MET:SD	1:B:66:HIS:HD2	2.28	0.57
1:A:65:GLY:O	1:A:70:LEU:N	2.36	0.57
1:B:198:ARG:CB	1:B:208:TYR:HE1	2.17	0.57
1:A:28:MET:HE2	1:B:68:HIS:CA	2.32	0.57
1:A:76:LYS:CA	1:A:79:VAL:HB	2.35	0.57
1:A:50:ILE:HD11	1:B:38:PHE:CE1	2.40	0.57
1:A:28:MET:CE	1:A:33:HIS:O	2.52	0.57
1:A:34:ARG:HG3	1:A:37:ALA:H	1.69	0.57
1:A:236:ARG:CA	1:A:239:ARG:HG2	2.33	0.57
1:A:62:ARG:C	1:A:62:ARG:CD	2.73	0.57
1:A:190:LEU:HG	1:A:195:THR:HG22	1.86	0.57
1:B:51:TYR:HD1	1:B:79:VAL:HG13	1.69	0.57
1:A:50:ILE:O	1:A:53:THR:HG22	2.05	0.56
1:A:128:LEU:HB3	1:A:133:LYS:HB3	1.86	0.56
1:B:163:HIS:CE1	1:B:178:LEU:CG	2.88	0.56
1:A:139:LYS:CE	1:A:199:ILE:HG22	2.35	0.56
1:A:187:LYS:HZ2	1:A:188:ARG:CD	2.18	0.56
1:A:60:ASN:HB3	1:A:63:MET:H	1.70	0.56
1:B:258:LEU:HD12	1:B:258:LEU:H	1.69	0.56
1:A:155:PHE:CE2	1:A:208:TYR:CD2	2.94	0.56
1:A:29:ARG:NH2	1:B:56:GLU:HB3	2.09	0.56
1:A:122:ARG:HD3	1:A:149:LEU:HD21	1.87	0.56
1:A:232:ALA:HA	1:A:235:PHE:HD1	1.71	0.56
1:B:110:TRP:HZ3	1:B:155:PHE:CG	2.23	0.56
1:A:114:TYR:CB	1:A:148:HIS:HE1	2.17	0.56
1:A:75:VAL:O	1:A:78:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:HA	1:B:175:GLN:HB2	1.88	0.56
1:A:158:LEU:O	1:A:158:LEU:HD12	2.06	0.56
1:B:241:TRP:HA	1:B:248:THR:HG21	1.82	0.56
1:B:4:ASP:O	1:B:8:ILE:HB	2.05	0.56
1:A:152:SER:O	1:A:155:PHE:HB2	2.04	0.56
1:A:182:LEU:CA	1:B:69:HIS:NE2	2.69	0.56
1:B:103:LEU:HG	1:B:190:LEU:CD2	2.36	0.56
1:B:103:LEU:HA	1:B:190:LEU:HD21	1.87	0.56
1:B:234:PHE:CE2	1:B:238:MET:HB2	2.37	0.56
1:A:119:GLY:O	1:A:120:ARG:CZ	2.54	0.56
1:A:106:PHE:CE1	1:A:110:TRP:CE3	2.93	0.56
1:A:198:ARG:CB	1:A:208:TYR:HE1	2.19	0.56
1:B:167:GLN:NE2	1:B:176:MET:O	2.28	0.56
1:A:156:LEU:O	1:A:160:GLU:HB2	2.05	0.56
1:A:99:GLU:HG3	1:A:104:ILE:CB	2.36	0.56
1:B:209:ALA:O	1:B:211:THR:HG23	2.05	0.56
1:A:288:VAL:HA	1:B:254:GLU:HG2	1.86	0.56
1:B:261:LYS:HG2	1:B:264:GLN:HE22	1.70	0.56
1:A:117:ARG:HB3	1:A:120:ARG:HG2	1.88	0.56
1:A:40:ASP:HB3	1:A:92:LEU:HB2	1.88	0.55
1:B:35:HIS:C	1:B:35:HIS:CD2	2.80	0.55
1:A:162:LEU:O	1:A:165:ARG:HG2	2.05	0.55
1:B:110:TRP:CH2	1:B:150:ILE:HG22	2.41	0.55
1:A:228:VAL:HG23	1:A:229:GLU:N	2.17	0.55
1:A:123:ILE:HD12	1:A:123:ILE:N	2.21	0.55
1:B:98:GLN:CG	1:B:228:VAL:HG21	2.36	0.55
1:B:171:PRO:CB	1:B:173:GLU:HG2	2.34	0.55
1:B:184:GLU:O	1:B:188:ARG:HB2	2.07	0.55
1:A:28:MET:SD	1:A:35:HIS:CE1	3.00	0.55
1:A:247:ASN:HA	1:B:266:LYS:HE3	1.88	0.55
1:A:248:THR:O	1:B:266:LYS:NZ	2.30	0.55
1:B:234:PHE:CG	1:B:235:PHE:N	2.75	0.55
1:B:250:ARG:HH22	1:B:252:LEU:HD23	1.71	0.55
1:A:116:TRP:HE1	1:A:122:ARG:N	2.04	0.55
1:B:49:ALA:O	1:B:53:THR:HG23	2.07	0.55
1:A:231:THR:CB	1:B:238:MET:HG2	2.37	0.55
1:A:54:TYR:HE2	1:A:59:GLN:HB2	1.72	0.55
1:A:46:ALA:HA	1:B:20:MET:CE	2.37	0.55
1:B:295:LYS:O	1:B:296:LYS:CB	2.55	0.55
1:B:31:SER:CB	1:B:98:GLN:HE22	2.18	0.55
1:A:187:LYS:HZ2	1:A:188:ARG:HH21	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:MET:HE2	1:B:67:LEU:O	2.07	0.55
1:B:51:TYR:CZ	1:B:54:TYR:HE1	2.24	0.55
1:A:230:ASP:HA	1:A:233:ARG:HH21	1.71	0.55
1:A:62:ARG:C	1:A:62:ARG:HD2	2.28	0.55
1:A:75:VAL:CA	1:A:78:ILE:HG22	2.37	0.55
1:B:190:LEU:O	1:B:195:THR:HB	2.07	0.55
1:A:74:ARG:O	1:A:77:ALA:HB3	2.07	0.54
1:B:231:THR:HG22	1:B:232:ALA:N	2.21	0.54
1:A:5:VAL:HG12	1:A:5:VAL:O	2.06	0.54
1:B:116:TRP:CZ2	1:B:120:ARG:O	2.60	0.54
1:A:200:ASP:CA	1:A:206:PRO:HA	2.31	0.54
1:A:235:PHE:HB3	1:B:22:TYR:HE2	1.72	0.54
1:B:186:ILE:O	1:B:190:LEU:CD1	2.55	0.54
1:B:191:LEU:CG	1:B:196:VAL:O	2.53	0.54
1:A:29:ARG:HH11	1:B:67:LEU:HD12	1.73	0.54
1:A:257:ILE:HD13	1:A:295:LYS:NZ	2.23	0.54
1:B:122:ARG:NH2	1:B:122:ARG:HB2	2.22	0.54
1:A:50:ILE:HD13	1:B:35:HIS:CE1	2.43	0.54
1:A:71:GLU:HG2	1:A:74:ARG:H	1.73	0.54
1:B:107:PRO:HG3	1:B:195:THR:HG21	1.90	0.54
1:B:163:HIS:O	1:B:166:SER:HB2	2.07	0.54
1:B:291:MET:CG	1:B:292:VAL:N	2.70	0.54
1:A:34:ARG:CG	1:A:37:ALA:H	2.21	0.54
1:A:231:THR:CG2	1:B:234:PHE:CZ	2.88	0.54
1:B:116:TRP:HB2	1:B:122:ARG:HH21	1.73	0.54
1:A:190:LEU:HD12	1:A:190:LEU:O	2.08	0.54
1:B:51:TYR:CD2	1:B:55:LEU:HD11	2.43	0.54
1:B:76:LYS:HA	1:B:79:VAL:HB	1.89	0.54
1:B:13:PRO:O	1:B:14:SER:C	2.45	0.54
1:B:145:PRO:HB3	1:B:213:PRO:HD2	1.90	0.54
1:A:234:PHE:HA	1:A:237:MET:HB2	1.91	0.53
1:B:226:ILE:HG22	1:B:227:MET:N	2.22	0.53
1:B:25:PHE:CB	1:B:29:ARG:HD3	2.36	0.53
1:B:25:PHE:CA	1:B:29:ARG:HD3	2.38	0.53
1:A:29:ARG:HH12	1:B:64:THR:CA	2.20	0.53
1:B:230:ASP:O	1:B:233:ARG:HB3	2.09	0.53
1:B:31:SER:HB3	1:B:98:GLN:O	2.08	0.53
1:A:117:ARG:O	1:A:120:ARG:N	2.40	0.53
1:A:106:PHE:HE1	1:A:110:TRP:CE3	2.26	0.53
1:A:167:GLN:O	1:A:170:LEU:HB2	2.08	0.53
1:B:25:PHE:O	1:B:29:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:HG2	1:B:123:ILE:HG13	1.91	0.53
1:B:79:VAL:O	1:B:82:VAL:HB	2.09	0.53
1:A:54:TYR:CE2	1:A:59:GLN:CB	2.92	0.53
1:B:110:TRP:C	1:B:110:TRP:CD1	2.82	0.53
1:B:291:MET:HG3	1:B:292:VAL:N	2.24	0.53
1:B:258:LEU:H	1:B:258:LEU:CD1	2.21	0.53
1:A:62:ARG:CG	1:A:63:MET:N	2.72	0.53
1:A:76:LYS:HA	1:A:79:VAL:CG2	2.39	0.53
1:B:25:PHE:CD2	1:B:29:ARG:HD3	2.43	0.53
1:A:245:ARG:CD	1:B:295:LYS:O	2.56	0.53
1:B:57:GLN:HE22	1:B:64:THR:CA	2.19	0.53
1:B:76:LYS:O	1:B:80:GLU:HG3	2.09	0.53
1:B:6:ASP:OD2	1:B:6:ASP:C	2.46	0.53
1:B:256:ASP:O	1:B:257:ILE:HD12	2.09	0.53
1:A:107:PRO:HA	1:A:110:TRP:HB3	1.91	0.53
1:A:29:ARG:HD2	1:B:67:LEU:CD1	2.39	0.53
1:A:95:LEU:N	1:A:95:LEU:CD2	2.71	0.53
1:A:291:MET:N	1:B:251:VAL:O	2.42	0.53
1:B:110:TRP:CZ2	1:B:150:ILE:CB	2.87	0.53
1:A:52:MET:HE1	1:B:21:LEU:HD11	1.91	0.53
1:B:8:ILE:HG13	1:B:25:PHE:CE1	2.41	0.53
1:A:195:THR:OG1	1:A:210:LEU:HB2	2.08	0.53
1:A:188:ARG:HG3	1:B:63:MET:CE	2.39	0.53
1:B:181:ALA:O	1:B:184:GLU:HB2	2.09	0.53
1:B:241:TRP:CD1	1:B:250:ARG:N	2.77	0.53
1:A:123:ILE:HG23	1:A:207:PHE:CE2	2.43	0.53
1:B:104:ILE:HG22	1:B:105:GLN:HG2	1.91	0.53
1:B:239:ARG:O	1:B:243:GLU:N	2.42	0.53
1:B:163:HIS:HE1	1:B:178:LEU:HG	1.74	0.53
1:A:95:LEU:HA	1:A:101:ARG:HG3	1.91	0.52
1:A:291:MET:O	1:B:251:VAL:N	2.42	0.52
1:A:230:ASP:OD2	1:B:241:TRP:CH2	2.61	0.52
1:B:160:GLU:OE2	1:B:178:LEU:HD13	2.09	0.52
1:A:178:LEU:CD1	1:A:182:LEU:HD21	2.39	0.52
1:B:68:HIS:C	1:B:70:LEU:N	2.59	0.52
1:A:11:LEU:HD13	1:B:92:LEU:HD21	1.91	0.52
1:B:110:TRP:HE3	1:B:158:LEU:HD12	1.74	0.52
1:B:53:THR:O	1:B:64:THR:CG2	2.58	0.52
1:A:231:THR:HG22	1:A:235:PHE:CE1	2.44	0.52
1:A:122:ARG:O	1:A:149:LEU:N	2.42	0.52
1:B:54:TYR:CE1	1:B:55:LEU:CG	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ALA:HA	1:B:18:GLN:OE1	2.10	0.52
1:B:18:GLN:O	1:B:22:TYR:CG	2.62	0.52
1:A:227:MET:SD	1:B:242:ALA:HB1	2.50	0.52
1:A:159:ILE:HA	1:A:162:LEU:CB	2.35	0.52
1:A:180:GLU:O	1:A:184:GLU:HB2	2.09	0.52
1:A:234:PHE:HA	1:A:237:MET:SD	2.49	0.52
1:A:54:TYR:CD2	1:A:54:TYR:C	2.83	0.52
1:A:253:GLU:OE2	1:B:289:LEU:HD23	2.10	0.52
1:A:25:PHE:CD1	1:A:29:ARG:CB	2.89	0.52
1:B:65:GLY:O	1:B:68:HIS:HB2	2.10	0.52
1:A:239:ARG:NE	1:B:22:TYR:HE1	2.08	0.52
1:A:22:TYR:CE1	1:B:239:ARG:HB3	2.45	0.52
1:B:253:GLU:OE2	1:B:255:LEU:HG	2.10	0.52
1:A:291:MET:O	1:B:250:ARG:HA	2.10	0.52
1:B:25:PHE:CA	1:B:29:ARG:HB2	2.35	0.52
1:A:187:LYS:C	1:A:187:LYS:HD2	2.30	0.51
1:A:187:LYS:NZ	1:A:188:ARG:NH2	2.58	0.51
1:B:241:TRP:CD1	1:B:249:MET:CA	2.92	0.51
1:B:25:PHE:HD2	1:B:29:ARG:CD	2.23	0.51
1:A:56:GLU:OE1	1:B:4:ASP:HA	2.09	0.51
1:B:54:TYR:CD1	1:B:55:LEU:N	2.79	0.51
1:A:239:ARG:NE	1:B:22:TYR:CE1	2.78	0.51
1:B:287:VAL:HG12	1:B:288:VAL:N	2.24	0.51
1:A:263:GLN:NE2	1:A:267:ASP:CG	2.63	0.51
1:A:110:TRP:CZ3	1:A:195:THR:HG23	2.46	0.51
1:B:167:GLN:OE1	1:B:176:MET:N	2.44	0.51
1:A:225:TYR:CD1	1:A:225:TYR:O	2.63	0.51
1:A:152:SER:HB3	1:A:208:TYR:HE2	1.75	0.51
1:A:28:MET:SD	1:A:35:HIS:ND1	2.84	0.51
1:A:29:ARG:O	1:A:189:ARG:NH1	2.44	0.51
1:A:239:ARG:CZ	1:A:239:ARG:HB2	2.41	0.51
1:A:66:HIS:C	1:A:69:HIS:H	2.14	0.51
1:B:152:SER:HA	1:B:155:PHE:HB3	1.92	0.51
1:B:92:LEU:N	1:B:92:LEU:HD12	2.22	0.51
1:A:190:LEU:CG	1:A:195:THR:HG22	2.41	0.51
1:A:287:VAL:HG12	1:A:288:VAL:N	2.24	0.51
1:A:46:ALA:HA	1:B:20:MET:HE2	1.92	0.51
1:B:134:ARG:HE	1:B:135:GLN:HG3	1.76	0.51
1:A:112:GLU:O	1:A:115:PRO:HD3	2.10	0.51
1:A:185:HIS:O	1:A:188:ARG:N	2.44	0.51
1:B:50:ILE:N	1:B:50:ILE:HD12	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PHE:CE2	1:B:234:PHE:CE1	2.98	0.51
1:B:143:ASN:HD21	1:B:213:PRO:C	2.14	0.51
1:B:117:ARG:CB	1:B:120:ARG:HG3	2.34	0.51
1:A:34:ARG:HD3	1:B:69:HIS:ND1	2.26	0.51
1:A:236:ARG:NH1	1:B:296:LYS:CE	2.74	0.51
1:B:102:TYR:CD1	1:B:186:ILE:HG23	2.45	0.51
1:B:158:LEU:HB3	1:B:162:LEU:HD13	1.92	0.51
1:B:20:MET:O	1:B:23:LEU:N	2.44	0.51
1:B:99:GLU:HB2	1:B:104:ILE:HG13	1.91	0.51
1:B:173:GLU:OE1	1:B:173:GLU:HA	2.11	0.51
1:A:249:MET:HG2	1:B:293:PHE:HB3	1.93	0.51
1:B:101:ARG:HA	1:B:105:GLN:HE21	1.76	0.51
1:B:182:LEU:HD11	1:B:185:HIS:CD2	2.46	0.51
1:A:92:LEU:N	1:A:92:LEU:CD1	2.73	0.51
1:A:37:ALA:HA	1:A:93:LYS:HE3	1.93	0.51
1:A:106:PHE:HB3	1:A:107:PRO:HD3	1.92	0.50
1:A:292:VAL:HA	1:B:249:MET:O	2.10	0.50
1:B:198:ARG:HA	1:B:208:TYR:HE1	1.75	0.50
1:A:57:GLN:CD	1:A:67:LEU:HD11	2.30	0.50
1:A:61:LEU:O	1:A:72:PRO:HG3	2.11	0.50
1:A:48:CYS:O	1:A:51:TYR:HB3	2.11	0.50
1:A:128:LEU:O	1:A:133:LYS:HD3	2.11	0.50
1:A:174:HIS:ND1	1:A:174:HIS:O	2.42	0.50
1:B:37:ALA:HA	1:B:40:ASP:HB2	1.94	0.50
1:A:100:PRO:HG2	1:A:103:LEU:CD1	2.29	0.50
1:A:140:LEU:HD22	1:A:144:LEU:HD11	1.93	0.50
1:B:173:GLU:N	1:B:173:GLU:CD	2.65	0.50
1:A:195:THR:O	1:A:210:LEU:HA	2.12	0.50
1:B:3:ASN:O	1:B:7:LEU:N	2.36	0.50
1:B:5:VAL:O	1:B:9:LYS:N	2.36	0.50
1:A:34:ARG:CZ	1:A:186:ILE:HD11	2.42	0.50
1:A:200:ASP:HA	1:A:206:PRO:CA	2.32	0.50
1:A:76:LYS:HA	1:A:79:VAL:CB	2.38	0.50
1:B:18:GLN:O	1:B:22:TYR:CD1	2.65	0.50
1:A:239:ARG:HE	1:B:22:TYR:HE1	1.60	0.50
1:B:234:PHE:CD1	1:B:235:PHE:N	2.79	0.50
1:B:35:HIS:O	1:B:38:PHE:HB3	2.11	0.50
1:A:95:LEU:HD23	1:A:95:LEU:O	2.12	0.50
1:A:245:ARG:HD3	1:B:295:LYS:O	2.12	0.50
1:A:55:LEU:HA	1:A:59:GLN:OE1	2.11	0.50
1:A:62:ARG:HD2	1:A:63:MET:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TRP:H	1:A:146:ASP:C	2.15	0.50
1:B:185:HIS:CD2	1:B:186:ILE:HG12	2.47	0.50
1:A:52:MET:SD	1:B:25:PHE:HZ	2.35	0.50
1:B:28:MET:SD	1:B:38:PHE:CD1	3.05	0.50
1:B:35:HIS:C	1:B:38:PHE:H	2.15	0.50
1:B:257:ILE:CG2	1:B:261:LYS:HB2	2.42	0.50
1:A:195:THR:C	1:A:210:LEU:HA	2.32	0.50
1:B:116:TRP:HE3	1:B:146:ASP:CG	2.14	0.50
1:B:51:TYR:CD1	1:B:79:VAL:HG22	2.47	0.49
1:A:61:LEU:HD12	1:A:76:LYS:HD3	1.94	0.49
1:B:116:TRP:CE3	1:B:146:ASP:CG	2.85	0.49
1:A:89:GLY:O	1:A:91:LEU:HG	2.12	0.49
1:A:19:ILE:HD13	1:B:235:PHE:HD1	1.76	0.49
1:A:241:TRP:CZ3	1:B:231:THR:OG1	2.65	0.49
1:B:106:PHE:O	1:B:107:PRO:C	2.49	0.49
1:A:170:LEU:HD23	1:A:171:PRO:HD3	1.93	0.49
1:B:110:TRP:HB2	1:B:158:LEU:CD1	2.43	0.49
1:B:183:ALA:O	1:B:187:LYS:HB2	2.12	0.49
1:A:295:LYS:HD3	1:B:247:ASN:ND2	2.27	0.49
1:A:47:LYS:HG2	1:B:39:LEU:HD21	1.94	0.49
1:A:116:TRP:NE1	1:A:122:ARG:N	2.60	0.49
1:A:190:LEU:HD21	1:A:195:THR:HG21	1.93	0.49
1:A:266:LYS:CG	1:A:267:ASP:N	2.76	0.49
1:A:188:ARG:NH2	1:A:191:LEU:HD22	2.27	0.49
1:B:107:PRO:O	1:B:111:MET:HG2	2.12	0.49
1:B:20:MET:O	1:B:21:LEU:C	2.48	0.49
1:A:37:ALA:HB2	1:A:101:ARG:HH12	1.78	0.49
1:A:107:PRO:HA	1:A:110:TRP:CB	2.42	0.49
1:B:105:GLN:O	1:B:108:TYR:HB2	2.13	0.49
1:B:25:PHE:CD2	1:B:29:ARG:CD	2.95	0.49
1:B:258:LEU:N	1:B:258:LEU:CD1	2.75	0.49
1:A:116:TRP:NE1	1:A:122:ARG:CB	2.74	0.49
1:A:145:PRO:O	1:A:147:ALA:N	2.46	0.49
1:A:178:LEU:HG	1:A:182:LEU:CD2	2.42	0.49
1:A:28:MET:SD	1:B:68:HIS:HA	2.52	0.49
1:B:198:ARG:CA	1:B:208:TYR:HE1	2.26	0.49
1:A:244:LYS:HB2	1:A:244:LYS:NZ	2.28	0.49
1:A:122:ARG:C	1:A:123:ILE:HD12	2.33	0.49
1:A:257:ILE:C	1:A:258:LEU:HD12	2.32	0.49
1:B:17:ASP:OD2	1:B:17:ASP:N	2.46	0.49
1:B:150:ILE:O	1:B:208:TYR:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HB2	1:B:236:ARG:HH11	1.76	0.49
1:B:270:ASP:O	1:B:273:ILE:N	2.46	0.49
1:B:116:TRP:HB3	1:B:122:ARG:HH22	1.78	0.49
1:A:176:MET:SD	1:A:182:LEU:CD1	3.01	0.48
1:A:240:ASP:CA	1:A:245:ARG:NH2	2.73	0.48
1:A:117:ARG:CD	1:A:120:ARG:HG2	2.43	0.48
1:B:116:TRP:CD1	1:B:121:SER:C	2.86	0.48
1:A:104:ILE:HG23	1:A:105:GLN:N	2.25	0.48
1:A:50:ILE:CD1	1:B:38:PHE:HE1	2.26	0.48
1:A:261:LYS:O	1:A:264:GLN:HB2	2.12	0.48
1:B:51:TYR:CZ	1:B:55:LEU:HD21	2.45	0.48
1:A:249:MET:O	1:B:293:PHE:N	2.46	0.48
1:B:122:ARG:HB2	1:B:122:ARG:CZ	2.43	0.48
1:A:198:ARG:HB2	1:A:208:TYR:CE1	2.47	0.48
1:A:110:TRP:C	1:A:110:TRP:CD1	2.87	0.48
1:A:37:ALA:CB	1:A:101:ARG:HH12	2.26	0.48
1:A:34:ARG:HD3	1:B:69:HIS:CE1	2.49	0.48
1:A:54:TYR:CE2	1:A:59:GLN:HB2	2.49	0.48
1:B:13:PRO:HB3	1:B:17:ASP:HB2	1.95	0.48
1:A:116:TRP:HB2	1:A:147:ALA:N	2.28	0.48
1:A:124:PRO:CG	1:A:148:HIS:CD2	2.92	0.48
1:A:155:PHE:HD1	1:A:159:ILE:HD11	1.78	0.48
1:A:95:LEU:HD22	1:A:95:LEU:H	1.78	0.48
1:B:51:TYR:CE2	1:B:54:TYR:CE1	2.98	0.48
1:A:234:PHE:CE1	1:B:234:PHE:CD1	3.02	0.48
1:B:14:SER:O	1:B:15:ALA:C	2.51	0.48
1:A:117:ARG:NH2	1:A:120:ARG:HH21	2.12	0.48
1:A:190:LEU:CD1	1:A:193:SER:HB2	2.44	0.48
1:A:54:TYR:HE2	1:A:59:GLN:CB	2.27	0.48
1:A:68:HIS:CE1	1:B:28:MET:HE1	2.49	0.48
1:A:75:VAL:C	1:A:78:ILE:HG22	2.34	0.48
1:B:28:MET:O	1:B:28:MET:CG	2.62	0.48
1:A:116:TRP:HB3	1:A:146:ASP:HA	1.95	0.48
1:A:110:TRP:CZ2	1:A:195:THR:O	2.67	0.48
1:A:51:TYR:CE1	1:A:55:LEU:HD11	2.49	0.47
1:B:106:PHE:HA	1:B:162:LEU:HD21	1.96	0.47
1:A:66:HIS:HE1	1:B:184:GLU:OE1	1.97	0.47
1:B:241:TRP:HD1	1:B:249:MET:CA	2.22	0.47
1:B:164:LYS:HD3	1:B:167:GLN:CB	2.28	0.47
1:A:41:ALA:O	1:A:94:MET:HE2	2.14	0.47
1:B:51:TYR:CE1	1:B:54:TYR:CE1	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HH22	1:B:5:VAL:CG2	2.26	0.47
1:B:110:TRP:CZ3	1:B:155:PHE:CD1	2.93	0.47
1:A:253:GLU:HB3	1:B:273:ILE:HG23	1.95	0.47
1:A:117:ARG:CZ	1:A:120:ARG:HE	2.27	0.47
1:B:34:ARG:HG2	1:B:36:GLY:N	2.29	0.47
1:B:110:TRP:CE3	1:B:158:LEU:HD12	2.50	0.47
1:B:103:LEU:HG	1:B:190:LEU:HG	1.96	0.47
1:B:19:ILE:N	1:B:19:ILE:HD12	2.30	0.47
1:A:236:ARG:O	1:A:240:ASP:OD2	2.32	0.47
1:A:293:PHE:CD1	1:A:294:GLY:N	2.83	0.47
1:B:233:ARG:HG2	1:B:290:GLN:HE22	1.79	0.47
1:B:4:ASP:O	1:B:8:ILE:N	2.47	0.47
1:B:7:LEU:CD1	1:B:7:LEU:N	2.77	0.47
1:B:116:TRP:HB3	1:B:122:ARG:NH2	2.29	0.47
1:A:34:ARG:HH21	1:A:182:LEU:HD12	1.80	0.47
1:A:290:GLN:HA	1:B:252:LEU:HB2	1.91	0.47
1:B:53:THR:O	1:B:64:THR:HG21	2.15	0.47
1:A:95:LEU:CD2	1:A:95:LEU:H	2.27	0.47
1:A:67:LEU:O	1:A:69:HIS:ND1	2.48	0.47
1:B:182:LEU:HD11	1:B:185:HIS:HD2	1.79	0.47
1:B:4:ASP:CB	1:B:25:PHE:CG	2.97	0.47
1:A:129:THR:O	1:A:133:LYS:CG	2.60	0.47
1:A:7:LEU:HD22	1:A:10:ARG:CD	2.44	0.47
1:B:165:ARG:NH1	1:B:165:ARG:HB3	2.30	0.47
1:A:29:ARG:HH22	1:B:64:THR:CG2	2.24	0.47
1:A:293:PHE:CG	1:A:294:GLY:N	2.83	0.47
1:A:287:VAL:C	1:B:254:GLU:HB3	2.34	0.47
1:A:102:TYR:OH	1:A:185:HIS:CE1	2.68	0.47
1:B:51:TYR:CE2	1:B:55:LEU:CD2	2.85	0.47
1:B:54:TYR:O	1:B:64:THR:HG21	2.15	0.47
1:A:28:MET:HG3	1:B:67:LEU:O	2.15	0.47
1:B:160:GLU:O	1:B:164:LYS:HB2	2.14	0.47
1:A:12:GLY:H	1:A:13:PRO:HD3	1.77	0.47
1:A:61:LEU:C	1:A:72:PRO:HG3	2.35	0.47
1:B:156:LEU:O	1:B:159:ILE:N	2.47	0.47
1:B:160:GLU:OE2	1:B:178:LEU:HD22	2.15	0.47
1:B:26:SER:O	1:B:30:THR:HB	2.15	0.47
1:A:290:GLN:HA	1:B:252:LEU:CA	2.45	0.46
1:A:290:GLN:HA	1:B:252:LEU:HA	1.97	0.46
1:A:54:TYR:HA	1:A:64:THR:HG21	1.97	0.46
1:B:103:LEU:HG	1:B:190:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASP:OD2	1:B:274:ARG:HG2	2.15	0.46
1:A:54:TYR:CE2	1:A:59:GLN:HB3	2.50	0.46
1:A:63:MET:O	1:A:66:HIS:CB	2.63	0.46
1:B:108:TYR:O	1:B:111:MET:HG2	2.14	0.46
1:B:236:ARG:CB	1:B:236:ARG:HH11	2.27	0.46
1:A:52:MET:SD	1:B:8:ILE:HA	2.54	0.46
1:A:111:MET:O	1:A:115:PRO:CA	2.64	0.46
1:A:179:SER:O	1:A:182:LEU:HB3	2.15	0.46
1:B:57:GLN:CD	1:B:64:THR:HG22	2.25	0.46
1:A:227:MET:SD	1:B:239:ARG:HD2	2.56	0.46
1:B:159:ILE:O	1:B:160:GLU:C	2.54	0.46
1:A:178:LEU:CA	1:A:182:LEU:HD22	2.45	0.46
1:A:240:ASP:CB	1:A:245:ARG:NH2	2.77	0.46
1:B:236:ARG:HB2	1:B:236:ARG:CZ	2.45	0.46
1:A:117:ARG:HE	1:A:120:ARG:CG	2.24	0.46
1:A:76:LYS:C	1:A:79:VAL:HB	2.36	0.46
1:B:189:ARG:HD2	1:B:189:ARG:HA	1.50	0.46
1:A:236:ARG:HH12	1:B:296:LYS:CE	2.29	0.46
1:A:139:LYS:HE3	1:A:199:ILE:HG22	1.97	0.46
1:B:51:TYR:O	1:B:54:TYR:CD1	2.55	0.46
1:A:62:ARG:HG3	1:A:63:MET:N	2.31	0.46
1:A:253:GLU:HG3	1:B:277:ALA:N	2.31	0.46
1:A:50:ILE:HG12	1:B:28:MET:HE2	1.98	0.46
1:B:178:LEU:N	1:B:178:LEU:HD12	2.31	0.46
1:A:205:MET:HB3	1:A:206:PRO:HD2	1.96	0.46
1:A:18:GLN:O	1:A:22:TYR:N	2.48	0.46
1:A:287:VAL:CG1	1:A:288:VAL:N	2.79	0.46
1:A:179:SER:O	1:A:183:ALA:N	2.32	0.46
1:B:68:HIS:O	1:B:69:HIS:C	2.52	0.46
1:B:75:VAL:O	1:B:79:VAL:CG2	2.64	0.46
1:B:161:PHE:O	1:B:164:LYS:N	2.47	0.46
1:A:149:LEU:HB2	1:A:207:PHE:CD2	2.50	0.46
1:A:93:LYS:HE3	1:A:93:LYS:HB3	1.60	0.46
1:B:212:ARG:CA	1:B:213:PRO:C	2.80	0.46
1:A:244:LYS:CD	1:B:223:ARG:HH22	2.29	0.46
1:A:263:GLN:HG3	1:A:263:GLN:O	2.15	0.46
1:A:151:THR:OG1	1:A:152:SER:N	2.48	0.46
1:A:35:HIS:ND1	1:A:38:PHE:HE1	2.14	0.46
1:A:50:ILE:HD13	1:B:35:HIS:HE1	1.81	0.46
1:B:236:ARG:CB	1:B:236:ARG:NH1	2.77	0.46
1:B:250:ARG:CG	1:B:250:ARG:NH1	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HE	1:A:120:ARG:NE	2.11	0.46
1:B:116:TRP:CZ3	1:B:118:PRO:HA	2.52	0.46
1:A:210:LEU:HG	1:A:210:LEU:O	2.15	0.45
1:A:295:LYS:H	1:A:295:LYS:HG2	1.53	0.45
1:B:14:SER:O	1:B:17:ASP:OD2	2.34	0.45
1:B:31:SER:O	1:B:99:GLU:HG2	2.16	0.45
1:A:168:GLU:HA	1:A:175:GLN:NE2	2.30	0.45
1:A:196:VAL:HG13	1:A:208:TYR:HB3	1.98	0.45
1:A:29:ARG:NH1	1:B:64:THR:HA	2.28	0.45
1:A:29:ARG:NH2	1:B:64:THR:HG22	2.26	0.45
1:B:250:ARG:HH22	1:B:252:LEU:HD22	1.82	0.45
1:A:154:GLU:CD	1:A:154:GLU:N	2.69	0.45
1:A:238:MET:CA	1:A:241:TRP:HB3	2.44	0.45
1:B:139:LYS:HB3	1:B:199:ILE:HD13	1.98	0.45
1:B:28:MET:SD	1:B:38:PHE:CE1	3.09	0.45
1:A:34:ARG:NH2	1:A:182:LEU:CD1	2.80	0.45
1:A:230:ASP:OD2	1:B:241:TRP:HH2	1.99	0.45
1:A:62:ARG:N	1:A:72:PRO:HG3	2.31	0.45
1:A:139:LYS:HE2	1:A:199:ILE:HG22	1.99	0.45
1:B:122:ARG:NH2	1:B:146:ASP:HA	2.32	0.45
1:A:170:LEU:HB3	1:A:171:PRO:HD2	1.94	0.45
1:A:184:GLU:OE2	1:A:184:GLU:HA	2.16	0.45
1:A:237:MET:O	1:A:241:TRP:HB2	2.16	0.45
1:B:234:PHE:HA	1:B:237:MET:HE1	1.97	0.45
1:B:239:ARG:HH21	1:B:243:GLU:CD	2.19	0.45
1:A:185:HIS:CA	1:B:66:HIS:CE1	2.99	0.45
1:B:241:TRP:CG	1:B:250:ARG:HB2	2.51	0.45
1:A:109:VAL:O	1:A:113:LYS:CB	2.61	0.45
1:B:191:LEU:HG	1:B:197:THR:HA	1.99	0.45
1:B:8:ILE:HG12	1:B:21:LEU:CD1	2.47	0.45
1:A:252:LEU:HD13	1:B:289:LEU:O	2.17	0.45
1:B:105:GLN:O	1:B:109:VAL:HG23	2.17	0.45
1:B:158:LEU:O	1:B:162:LEU:CB	2.61	0.45
1:B:155:PHE:CE2	1:B:208:TYR:CG	3.05	0.45
1:A:116:TRP:HB2	1:A:147:ALA:C	2.37	0.44
1:A:143:ASN:O	1:A:144:LEU:CG	2.63	0.44
1:A:145:PRO:O	1:A:146:ASP:C	2.54	0.44
1:A:168:GLU:C	1:A:170:LEU:N	2.70	0.44
1:A:178:LEU:HA	1:A:182:LEU:CD2	2.45	0.44
1:A:178:LEU:HG	1:A:182:LEU:HD21	1.99	0.44
1:B:51:TYR:CE2	1:B:55:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:TYR:O	1:B:55:LEU:HG	2.17	0.44
1:A:263:GLN:OE1	1:A:266:LYS:HD3	2.16	0.44
1:A:157:GLU:HA	1:A:160:GLU:HB2	1.99	0.44
1:B:104:ILE:O	1:B:108:TYR:CE2	2.70	0.44
1:A:269:LEU:O	1:A:272:ILE:HB	2.17	0.44
1:A:163:HIS:NE2	1:A:167:GLN:NE2	2.65	0.44
1:A:68:HIS:CE1	1:B:28:MET:CE	2.99	0.44
1:A:74:ARG:CD	1:A:74:ARG:C	2.83	0.44
1:A:263:GLN:NE2	1:A:266:LYS:HG2	2.33	0.44
1:A:150:ILE:CG2	1:A:151:THR:N	2.81	0.44
1:A:28:MET:CE	1:B:68:HIS:CA	2.90	0.44
1:A:44:THR:HG23	1:A:45:ALA:N	2.33	0.44
1:A:195:THR:OG1	1:A:210:LEU:HD13	2.17	0.44
1:A:41:ALA:HB1	1:A:94:MET:HG3	2.00	0.44
1:B:256:ASP:C	1:B:257:ILE:HD12	2.38	0.44
1:B:116:TRP:HE3	1:B:146:ASP:OD2	2.00	0.44
1:A:101:ARG:HH21	1:A:101:ARG:HG3	1.82	0.44
1:A:98:GLN:HE21	1:A:98:GLN:HB3	1.62	0.44
1:B:54:TYR:HE1	1:B:55:LEU:HD21	1.80	0.44
1:B:273:ILE:CG2	1:B:273:ILE:O	2.66	0.44
1:A:266:LYS:HG2	1:A:267:ASP:OD2	2.17	0.44
1:A:156:LEU:O	1:A:160:GLU:N	2.45	0.44
1:B:64:THR:C	1:B:68:HIS:HD2	2.20	0.44
1:B:100:PRO:O	1:B:104:ILE:N	2.42	0.44
1:B:14:SER:O	1:B:16:MET:N	2.51	0.44
1:B:165:ARG:CZ	1:B:165:ARG:HB3	2.47	0.44
1:A:114:TYR:HB3	1:A:148:HIS:CE1	2.52	0.44
1:A:110:TRP:HZ3	1:A:155:PHE:CZ	2.32	0.44
1:A:182:LEU:CB	1:B:69:HIS:CE1	3.01	0.44
1:A:68:HIS:O	1:A:69:HIS:CD2	2.70	0.44
1:B:152:SER:CA	1:B:155:PHE:HB2	2.39	0.44
1:B:210:LEU:HD23	1:B:212:ARG:O	2.18	0.44
1:A:128:LEU:HD23	1:A:133:LYS:CB	2.47	0.44
1:A:68:HIS:O	1:A:69:HIS:CG	2.71	0.44
1:B:230:ASP:O	1:B:231:THR:C	2.55	0.44
1:A:100:PRO:O	1:A:104:ILE:HG22	2.17	0.43
1:A:287:VAL:O	1:B:254:GLU:HB3	2.18	0.43
1:A:122:ARG:NH2	1:A:144:LEU:HD13	2.32	0.43
1:A:234:PHE:HA	1:A:290:GLN:HE22	1.83	0.43
1:A:115:PRO:HA	1:A:147:ALA:HA	1.99	0.43
1:A:3:ASN:H	1:B:56:GLU:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:HE2	1:B:208:TYR:CG	2.37	0.43
1:A:131:GLU:HG2	1:A:134:ARG:HH21	1.83	0.43
1:B:161:PHE:O	1:B:164:LYS:CB	2.65	0.43
1:B:34:ARG:HB3	1:B:37:ALA:HB3	1.99	0.43
1:A:49:ALA:HB3	1:B:24:ALA:HB2	1.98	0.43
1:B:84:GLN:HE21	1:B:84:GLN:CA	2.30	0.43
1:B:107:PRO:CB	1:B:210:LEU:HD21	2.48	0.43
1:A:180:GLU:H	1:A:180:GLU:CD	2.22	0.43
1:A:210:LEU:HD11	1:A:212:ARG:C	2.38	0.43
1:A:245:ARG:CG	1:A:246:PRO:CD	2.93	0.43
1:A:290:GLN:HB2	1:B:250:ARG:NH1	2.32	0.43
1:B:210:LEU:HD23	1:B:213:PRO:HD3	2.00	0.43
1:B:163:HIS:C	1:B:166:SER:H	2.21	0.43
1:A:155:PHE:CD2	1:A:208:TYR:CD2	3.01	0.43
1:B:92:LEU:H	1:B:92:LEU:CD1	2.13	0.43
1:A:116:TRP:CD1	1:A:122:ARG:CA	3.02	0.43
1:B:63:MET:O	1:B:67:LEU:HG	2.19	0.43
1:A:234:PHE:CE1	1:B:234:PHE:CZ	3.07	0.43
1:B:109:VAL:CG1	1:B:162:LEU:HD11	2.48	0.43
1:B:54:TYR:C	1:B:64:THR:HG21	2.38	0.43
1:A:238:MET:HE3	1:A:241:TRP:CE3	2.53	0.43
1:A:93:LYS:HD2	1:A:170:LEU:HD22	2.00	0.43
1:A:28:MET:CE	1:A:35:HIS:N	2.81	0.43
1:B:51:TYR:C	1:B:51:TYR:CD2	2.91	0.43
1:A:235:PHE:C	1:A:238:MET:H	2.22	0.43
1:A:245:ARG:O	1:A:246:PRO:C	2.57	0.43
1:A:47:LYS:HB3	1:A:50:ILE:HD11	2.00	0.43
1:A:75:VAL:HA	1:A:78:ILE:CG2	2.45	0.43
1:B:101:ARG:CG	1:B:105:GLN:HE21	2.31	0.43
1:A:33:HIS:CE1	1:A:98:GLN:O	2.72	0.43
1:B:51:TYR:CD2	1:B:51:TYR:O	2.71	0.43
1:B:60:ASN:ND2	1:B:63:MET:HB2	2.34	0.43
1:A:231:THR:O	1:A:234:PHE:HB3	2.18	0.43
1:A:238:MET:O	1:A:242:ALA:N	2.52	0.43
1:A:248:THR:HG23	1:A:248:THR:O	2.19	0.43
1:B:105:GLN:HG2	1:B:105:GLN:H	1.69	0.43
1:A:69:HIS:HD1	1:B:185:HIS:CG	2.37	0.43
1:B:240:ASP:HA	1:B:243:GLU:CG	2.48	0.43
1:A:144:LEU:HA	1:A:145:PRO:HD3	1.74	0.42
1:A:292:VAL:HG13	1:B:241:TRP:HB2	2.01	0.42
1:A:117:ARG:HD2	1:A:118:PRO:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:TRP:CE2	1:B:120:ARG:O	2.72	0.42
1:A:230:ASP:O	1:A:233:ARG:HB3	2.20	0.42
1:B:249:MET:C	1:B:249:MET:SD	2.98	0.42
1:A:180:GLU:CD	1:A:180:GLU:N	2.73	0.42
1:A:190:LEU:CD1	1:A:195:THR:HG22	2.49	0.42
1:A:37:ALA:HB1	1:A:101:ARG:CZ	2.49	0.42
1:A:236:ARG:HH12	1:B:296:LYS:HE3	1.83	0.42
1:B:50:ILE:N	1:B:50:ILE:CD1	2.82	0.42
1:A:247:ASN:CA	1:B:266:LYS:HE3	2.48	0.42
1:A:156:LEU:O	1:A:160:GLU:CB	2.67	0.42
1:A:154:GLU:OE2	1:A:154:GLU:N	2.53	0.42
1:A:27:ALA:O	1:A:33:HIS:N	2.41	0.42
1:A:41:ALA:CB	1:A:94:MET:HG3	2.50	0.42
1:A:92:LEU:CD2	1:A:94:MET:HB2	2.50	0.42
1:B:250:ARG:HH12	1:B:252:LEU:HB3	1.85	0.42
1:B:4:ASP:O	1:B:8:ILE:CB	2.67	0.42
1:A:131:GLU:OE2	1:A:131:GLU:C	2.58	0.42
1:A:101:ARG:HB3	1:A:166:SER:HB3	2.01	0.42
1:A:102:TYR:CE1	1:A:186:ILE:CG1	2.96	0.42
1:A:154:GLU:O	1:A:158:LEU:HB2	2.20	0.42
1:A:22:TYR:CB	1:B:235:PHE:CE1	3.03	0.42
1:A:234:PHE:CA	1:A:290:GLN:HE22	2.32	0.42
1:A:190:LEU:HD11	1:A:195:THR:HG22	2.01	0.42
1:B:226:ILE:HA	1:B:230:ASP:OD1	2.19	0.42
1:A:253:GLU:OE1	1:B:273:ILE:HD12	2.20	0.42
1:B:25:PHE:C	1:B:29:ARG:HB2	2.40	0.42
1:A:128:LEU:HB3	1:A:133:LYS:CB	2.49	0.42
1:A:185:HIS:CD2	1:A:185:HIS:C	2.86	0.42
1:A:52:MET:SD	1:B:25:PHE:CZ	3.13	0.42
1:B:163:HIS:CD2	1:B:163:HIS:C	2.92	0.42
1:A:100:PRO:HD2	1:A:103:LEU:HB2	2.02	0.41
1:B:99:GLU:CB	1:B:104:ILE:HG13	2.51	0.41
1:B:142:SER:OG	1:B:143:ASN:N	2.52	0.41
1:B:4:ASP:CB	1:B:25:PHE:CD2	3.03	0.41
1:B:258:LEU:HA	1:B:259:PRO:HD3	1.89	0.41
1:A:152:SER:HB3	1:A:208:TYR:CE2	2.55	0.41
1:B:51:TYR:O	1:B:55:LEU:CD1	2.68	0.41
1:A:235:PHE:O	1:A:239:ARG:HG2	2.20	0.41
1:A:71:GLU:O	1:A:75:VAL:HG22	2.20	0.41
1:A:247:ASN:C	1:B:266:LYS:HE3	2.40	0.41
1:B:109:VAL:HG11	1:B:162:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:MET:N	1:B:176:MET:SD	2.92	0.41
1:A:117:ARG:HH21	1:A:120:ARG:NE	2.18	0.41
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.90	0.41
1:A:296:LYS:O	1:B:288:VAL:N	2.54	0.41
1:B:241:TRP:CE2	1:B:250:ARG:CB	3.03	0.41
1:B:5:VAL:HA	1:B:8:ILE:CB	2.39	0.41
1:A:274:ARG:CA	1:A:274:ARG:HE	2.21	0.41
1:B:253:GLU:CA	1:B:253:GLU:OE1	2.68	0.41
1:A:94:MET:O	1:A:101:ARG:HD3	2.21	0.41
1:A:170:LEU:HB3	1:A:171:PRO:HD3	2.02	0.41
1:B:104:ILE:CG2	1:B:105:GLN:N	2.83	0.41
1:A:22:TYR:HE1	1:B:239:ARG:HB3	1.84	0.41
1:B:240:ASP:HA	1:B:243:GLU:HG3	2.02	0.41
1:B:287:VAL:CG1	1:B:288:VAL:N	2.83	0.41
1:B:57:GLN:O	1:B:60:ASN:N	2.52	0.41
1:A:69:HIS:HB3	1:B:182:LEU:HD12	2.01	0.41
1:B:191:LEU:HD11	1:B:198:ARG:CB	2.50	0.41
1:B:265:ALA:CA	1:B:268:GLU:HG2	2.49	0.41
1:A:257:ILE:HD13	1:A:295:LYS:HZ2	1.84	0.41
1:B:25:PHE:HA	1:B:29:ARG:CB	2.43	0.41
1:B:35:HIS:HA	1:B:38:PHE:HB2	1.99	0.41
1:B:6:ASP:OD2	1:B:10:ARG:NE	2.50	0.41
1:B:163:HIS:CE1	1:B:178:LEU:CD1	3.03	0.41
1:B:159:ILE:HG22	1:B:163:HIS:HD1	1.85	0.41
1:A:9:LYS:O	1:A:10:ARG:C	2.58	0.41
1:A:102:TYR:CE1	1:A:186:ILE:CG2	2.97	0.41
1:A:167:GLN:NE2	1:A:176:MET:H	2.19	0.41
1:A:188:ARG:HG3	1:B:63:MET:HE1	2.02	0.41
1:A:239:ARG:NH2	1:A:239:ARG:HB2	2.36	0.41
1:A:21:LEU:O	1:A:24:ALA:HB2	2.21	0.41
1:A:257:ILE:O	1:A:258:LEU:HD12	2.21	0.41
1:B:7:LEU:N	1:B:7:LEU:HD12	2.36	0.41
1:B:84:GLN:CA	1:B:84:GLN:NE2	2.84	0.41
1:A:102:TYR:OH	1:A:185:HIS:NE2	2.54	0.41
1:A:63:MET:O	1:A:66:HIS:N	2.51	0.41
1:A:66:HIS:CE1	1:B:184:GLU:OE1	2.73	0.41
1:B:38:PHE:CD2	1:B:38:PHE:O	2.73	0.41
1:A:65:GLY:O	1:A:69:HIS:N	2.54	0.41
1:B:163:HIS:O	1:B:166:SER:N	2.54	0.41
1:B:122:ARG:NH2	1:B:146:ASP:C	2.74	0.41
1:B:139:LYS:O	1:B:141:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLN:N	1:B:84:GLN:CD	2.75	0.41
1:A:99:GLU:HG3	1:A:104:ILE:HA	2.02	0.41
1:B:210:LEU:HD23	1:B:213:PRO:CD	2.51	0.41
1:B:241:TRP:CE2	1:B:250:ARG:HB3	2.56	0.41
1:A:234:PHE:C	1:A:237:MET:HB2	2.42	0.40
1:A:292:VAL:HA	1:B:250:ARG:HA	2.03	0.40
1:B:13:PRO:CG	1:B:18:GLN:CG	2.85	0.40
1:B:19:ILE:HD12	1:B:19:ILE:H	1.86	0.40
1:A:230:ASP:OD2	1:B:241:TRP:CZ3	2.74	0.40
1:A:247:ASN:O	1:B:294:GLY:CA	2.65	0.40
1:A:69:HIS:CE1	1:B:185:HIS:CE1	3.09	0.40
1:B:234:PHE:CZ	1:B:235:PHE:HA	2.57	0.40
1:B:3:ASN:O	1:B:4:ASP:C	2.58	0.40
1:B:265:ALA:HA	1:B:268:GLU:OE1	2.21	0.40
1:B:117:ARG:HB3	1:B:120:ARG:HB2	2.03	0.40
1:A:7:LEU:C	1:A:8:ILE:HG12	2.41	0.40
1:A:111:MET:O	1:A:114:TYR:C	2.59	0.40
1:A:116:TRP:CE2	1:A:122:ARG:HB2	2.55	0.40
1:A:188:ARG:HG3	1:B:63:MET:HE2	2.03	0.40
1:B:54:TYR:CE1	1:B:55:LEU:HD23	2.55	0.40
1:B:103:LEU:HG	1:B:190:LEU:CG	2.51	0.40
1:A:195:THR:HA	1:A:210:LEU:HA	2.04	0.40
1:A:34:ARG:O	1:A:38:PHE:CD1	2.74	0.40
1:A:58:GLY:O	1:A:59:GLN:HG2	2.21	0.40
1:A:34:ARG:HB3	1:A:185:HIS:HE1	1.86	0.40
1:A:54:TYR:CA	1:A:64:THR:HG21	2.52	0.40
1:B:28:MET:HG3	1:B:28:MET:O	2.21	0.40
1:B:164:LYS:HA	1:B:167:GLN:HB2	2.02	0.40
1:A:117:ARG:NH2	1:A:120:ARG:HE	2.19	0.40
1:B:116:TRP:HB2	1:B:122:ARG:NH2	2.28	0.40
1:A:157:GLU:OE1	1:A:160:GLU:OE1	2.38	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	275/302 (91%)	250 (91%)	22 (8%)	3 (1%)	17 58
1	B	268/302 (89%)	250 (93%)	18 (7%)	0	100 100
All	All	543/604 (90%)	500 (92%)	40 (7%)	3 (1%)	30 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ALA
1	A	62	ARG
1	A	228	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	248/265 (94%)	174 (70%)	74 (30%)	0 2
1	B	245/265 (92%)	169 (69%)	76 (31%)	0 2
All	All	493/530 (93%)	343 (70%)	150 (30%)	0 2

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	ASP
1	A	8	ILE
1	A	20	MET
1	A	21	LEU
1	A	22	TYR
1	A	28	MET
1	A	29	ARG
1	A	34	ARG
1	A	38	PHE

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Mol	Chain	Res	Type
1	A	47	LYS
1	A	48	CYS
1	A	54	TYR
1	A	59	GLN
1	A	61	LEU
1	A	62	ARG
1	A	67	LEU
1	A	69	HIS
1	A	71	GLU
1	A	74	ARG
1	A	79	VAL
1	A	80	GLU
1	A	87	THR
1	A	92	LEU
1	A	95	LEU
1	A	98	GLN
1	A	99	GLU
1	A	104	ILE
1	A	105	GLN
1	A	109	VAL
1	A	111	MET
1	A	117	ARG
1	A	136	ILE
1	A	137	GLU
1	A	149	LEU
1	A	152	SER
1	A	155	PHE
1	A	161	PHE
1	A	163	HIS
1	A	167	GLN
1	A	173	GLU
1	A	178	LEU
1	A	182	LEU
1	A	185	HIS
1	A	188	ARG
1	A	191	LEU
1	A	199	ILE
1	A	201	SER
1	A	203	TRP
1	A	207	PHE
1	A	210	LEU
1	A	220	ASP

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Mol	Chain	Res	Type
1	A	221	GLN
1	A	231	THR
1	A	237	MET
1	A	238	MET
1	A	239	ARG
1	A	244	LYS
1	A	247	ASN
1	A	250	ARG
1	A	255	LEU
1	A	256	ASP
1	A	257	ILE
1	A	260	GLU
1	A	264	GLN
1	A	272	ILE
1	A	274	ARG
1	A	276	TRP
1	A	278	ASP
1	A	288	VAL
1	A	289	LEU
1	A	290	GLN
1	A	291	MET
1	A	293	PHE
1	B	5	VAL
1	B	6	ASP
1	B	8	ILE
1	B	9	LYS
1	B	11	LEU
1	B	17	ASP
1	B	18	GLN
1	B	38	PHE
1	B	40	ASP
1	B	53	THR
1	B	54	TYR
1	B	55	LEU
1	B	57	GLN
1	B	62	ARG
1	B	67	LEU
1	B	69	HIS
1	B	73	LYS
1	B	74	ARG
1	B	75	VAL
1	B	81	GLU

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Mol	Chain	Res	Type
1	B	84	GLN
1	B	86	LEU
1	B	88	GLU
1	B	92	LEU
1	B	93	LYS
1	B	94	MET
1	B	98	GLN
1	B	99	GLU
1	B	103	LEU
1	B	105	GLN
1	B	110	TRP
1	B	121	SER
1	B	122	ARG
1	B	138	GLN
1	B	139	LYS
1	B	142	SER
1	B	143	ASN
1	B	146	ASP
1	B	155	PHE
1	B	162	LEU
1	B	163	HIS
1	B	164	LYS
1	B	165	ARG
1	B	172	LYS
1	B	173	GLU
1	B	176	MET
1	B	184	GLU
1	B	185	HIS
1	B	188	ARG
1	B	189	ARG
1	B	190	LEU
1	B	195	THR
1	B	210	LEU
1	B	212	ARG
1	B	222	GLU
1	B	224	THR
1	B	226	ILE
1	B	228	VAL
1	B	231	THR
1	B	233	ARG
1	B	234	PHE
1	B	235	PHE

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Mol	Chain	Res	Type
1	B	239	ARG
1	B	241	TRP
1	B	244	LYS
1	B	245	ARG
1	B	248	THR
1	B	249	MET
1	B	250	ARG
1	B	253	GLU
1	B	256	ASP
1	B	260	GLU
1	B	263	GLN
1	B	276	TRP
1	B	289	LEU
1	B	290	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	57	GLN
1	A	68	HIS
1	A	98	GLN
1	A	105	GLN
1	A	135	GLN
1	A	138	GLN
1	A	148	HIS
1	A	185	HIS
1	A	263	GLN
1	A	264	GLN
1	B	35	HIS
1	B	66	HIS
1	B	84	GLN
1	B	98	GLN
1	B	105	GLN
1	B	138	GLN
1	B	163	HIS
1	B	221	GLN
1	B	263	GLN
1	B	264	GLN
1	B	290	GLN

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	281/302 (93%)	-0.32	7 (2%) 61 30	18, 51, 94, 281	0
1	B	278/302 (92%)	-0.55	3 (1%) 82 58	15, 47, 80, 127	0
All	All	559/604 (92%)	-0.44	10 (1%) 71 43	15, 49, 89, 281	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	9.1
1	A	9	LYS	5.4
1	A	22	TYR	5.2
1	B	204	GLY	4.7
1	A	7	LEU	4.6
1	A	5	VAL	4.3
1	A	37	ALA	3.9
1	B	32	GLY	2.6
1	A	8	ILE	2.1
1	B	89	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.