



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:59 PM GMT

PDB ID : 3LIB
Title : Crystal Structure of the extracellular domain of the putative histidine kinase
mmHK1S-Z3
Authors : Zhang, Z.; Hendrickson, W.A.
Deposited on : 2010-01-24
Resolution : 2.99 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

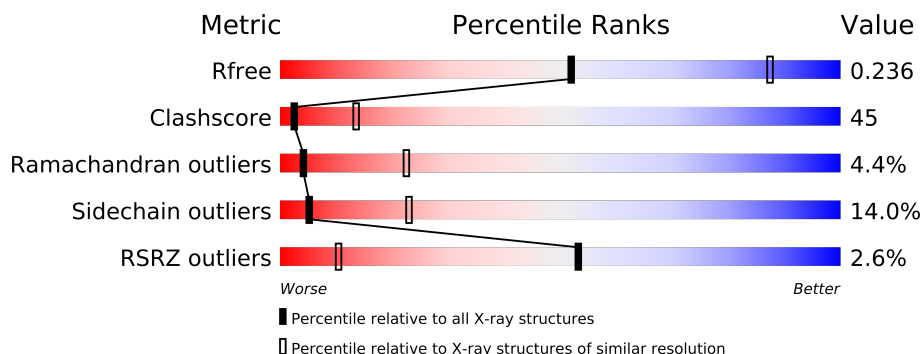
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.99 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	290	
1	B	290	
1	C	290	
1	D	290	
1	E	290	
1	F	290	
1	G	290	
1	H	290	
1	I	290	
1	J	290	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	K	A	1	-	X
2	K	B	10	-	X
2	K	C	3	-	X
2	K	D	5	-	X
2	K	E	6	-	X
2	K	F	8	-	X
2	K	G	4	-	X
2	K	H	7	-	X
2	K	I	9	-	X
2	K	J	2	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21176 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hypothetical sensory transduction histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	B	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	C	268	Total	C	N	O	S	0	0	0
			2092	1333	329	422	8			
1	D	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	E	268	Total	C	N	O	S	0	0	0
			2094	1335	329	422	8			
1	F	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	G	270	Total	C	N	O	S	0	0	0
			2113	1347	334	424	8			
1	H	267	Total	C	N	O	S	0	0	0
			2086	1331	328	419	8			
1	I	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	J	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
A	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
A	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
A	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
B	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
B	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
B	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
C	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
C	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
C	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
D	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
D	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
D	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
E	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
E	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
E	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
F	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
F	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
F	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1

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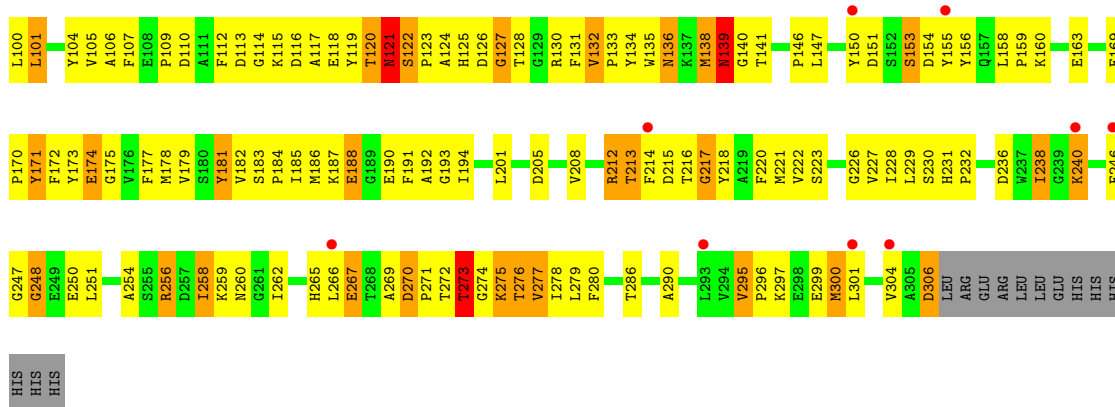
Chain	Residue	Modelled	Actual	Comment	Reference
F	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
G	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
G	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
G	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
H	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
H	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
H	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
I	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
I	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
I	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
J	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
J	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
J	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	I	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

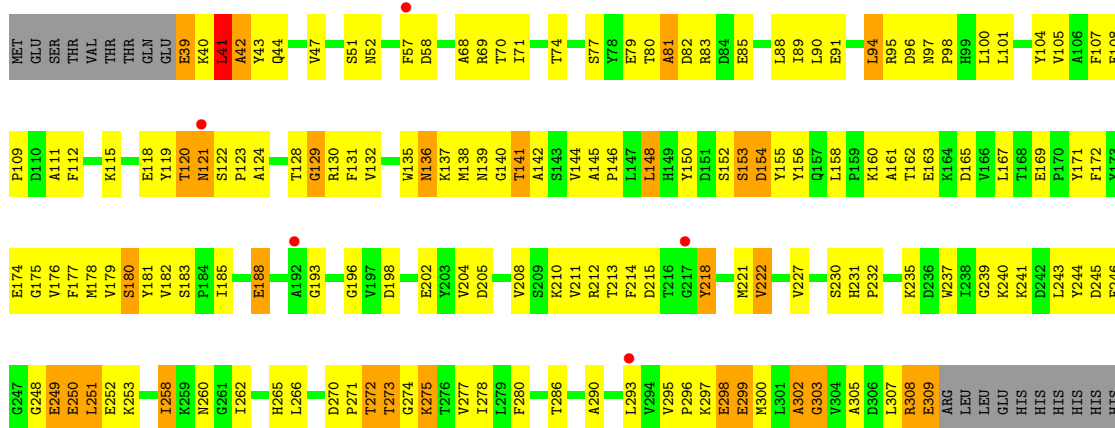
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	C	7	Total O 7 7	0	0
3	D	7	Total O 7 7	0	0
3	E	6	Total O 6 6	0	0
3	F	8	Total O 8 8	0	0
3	G	3	Total O 3 3	0	0
3	H	3	Total O 3 3	0	0
3	I	2	Total O 2 2	0	0
3	J	8	Total O 8 8	0	0



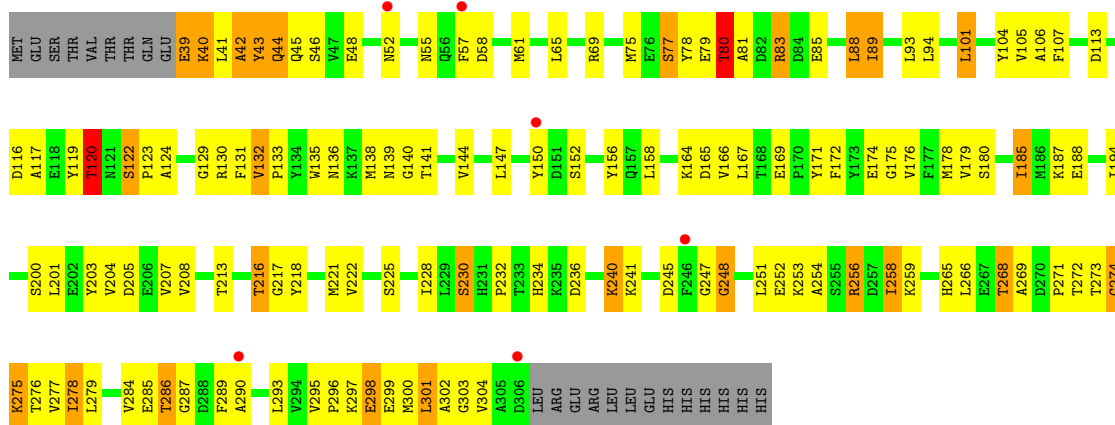
• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain D:



• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain E:

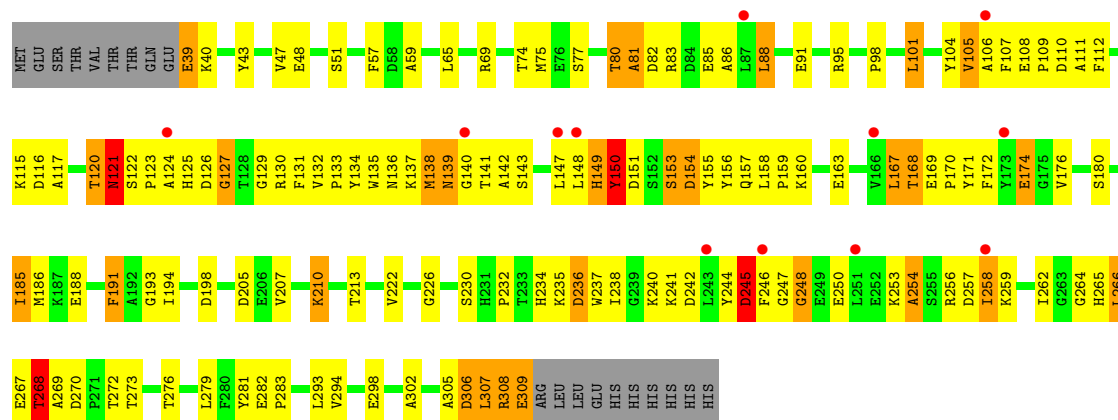


• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain F:

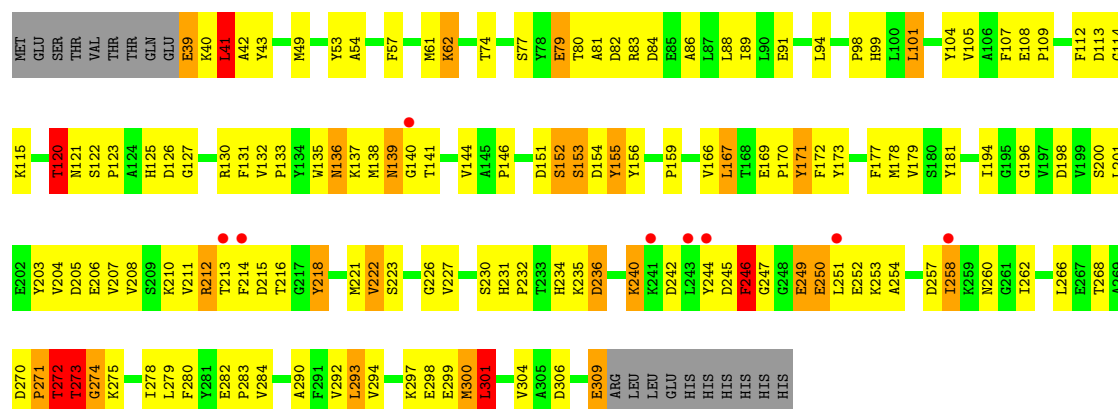






• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.52Å 129.52Å 404.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.72 – 2.99 46.12 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.72-2.99) 99.4 (46.12-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.197 , 0.272 0.194 , 0.236	Depositor DCC
R_{free} test set	3839 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 76427 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21176	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.75	0/2172	0.83	0/2950
1	B	0.70	0/2172	0.77	0/2950
1	C	0.83	1/2142 (0.0%)	0.86	1/2910 (0.0%)
1	D	0.75	0/2172	0.84	1/2950 (0.0%)
1	E	0.77	1/2144 (0.0%)	0.85	0/2913
1	F	0.74	0/2172	0.83	1/2950 (0.0%)
1	G	0.73	0/2163	0.84	1/2938 (0.0%)
1	H	0.80	0/2136	0.84	2/2902 (0.1%)
1	I	0.68	0/2172	0.74	0/2950
1	J	0.77	0/2172	0.84	0/2950
All	All	0.75	2/21617 (0.0%)	0.83	6/29363 (0.0%)

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	D	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	52	ASN	CG-OD1	5.32	1.35	1.24
1	C	139	ASN	CG-OD1	5.01	1.34	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	GLN	N-CA-C	6.15	127.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	178	MET	CB-CG-SD	-5.24	96.67	112.40
1	F	274	GLY	N-CA-C	-5.24	100.00	113.10
1	H	75	MET	CG-SD-CE	-5.12	92.00	100.20
1	D	303	GLY	N-CA-C	-5.03	100.52	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	297	LYS	Peptide
1	D	298	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2122	0	2022	192	0
1	B	2122	0	2022	200	0
1	C	2092	0	1985	235	0
1	D	2122	0	2022	197	0
1	E	2094	0	1991	158	0
1	F	2122	0	2022	142	0
1	G	2113	0	2016	193	0
1	H	2086	0	1988	215	0
1	I	2122	0	2022	172	0
1	J	2122	0	2022	222	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	5	0	0	1	0
3	C	7	0	0	4	0
3	D	7	0	0	0	0
3	E	6	0	0	0	0
3	F	8	0	0	1	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	2	0	0	0	0
3	J	8	0	0	0	0
All	All	21176	0	20112	1852	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 45.

All (1852) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:41:LEU:CD2	1:D:42:ALA:H	1.17	1.56
1:D:39:GLU:N	1:D:40:LYS:CG	1.71	1.50
1:C:270:ASP:CB	1:C:271:PRO:HA	1.32	1.44
1:E:39:GLU:N	1:E:40:LYS:HB3	1.31	1.42
1:D:41:LEU:CD2	1:D:42:ALA:N	1.77	1.41
1:A:39:GLU:HA	1:A:40:LYS:CB	1.41	1.39
1:D:41:LEU:HD22	1:D:42:ALA:N	1.05	1.35
1:F:39:GLU:CA	1:F:40:LYS:HB2	1.60	1.32
1:F:39:GLU:HA	1:F:40:LYS:CB	1.54	1.31
1:H:231:HIS:ND1	1:H:232:PRO:HD2	1.48	1.28
1:C:270:ASP:CB	1:C:271:PRO:CA	2.14	1.26
1:C:39:GLU:HB3	1:C:40:LYS:CB	1.64	1.25
1:D:41:LEU:O	1:D:43:TYR:N	1.70	1.23
1:C:91:GLU:HG3	1:C:135:TRP:CE2	1.75	1.21
1:A:39:GLU:OE2	1:A:40:LYS:HD3	1.07	1.21
1:B:307:LEU:CD2	1:B:307:LEU:N	2.05	1.19
1:E:273:THR:HG23	1:E:274:GLY:N	1.41	1.19
1:E:273:THR:CG2	1:E:274:GLY:H	1.50	1.18
1:G:136:ASN:OD1	1:G:138:MET:HB2	1.43	1.18
1:C:91:GLU:HG3	1:C:135:TRP:CZ2	1.78	1.18
1:A:39:GLU:CA	1:A:40:LYS:HB2	1.72	1.17
1:J:214:PHE:CD2	1:J:299:GLU:HB3	1.79	1.17
1:G:43:TYR:CE1	1:G:300:MET:HE2	1.79	1.17
1:D:298:GLU:N	1:D:299:GLU:HB2	1.60	1.16

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:273:THR:HG23	1:F:274:GLY:N	1.59	1.16
1:E:273:THR:HG21	1:E:275:LYS:CG	1.76	1.15
1:I:39:GLU:N	1:I:40:LYS:HB2	1.62	1.14
1:J:273:THR:OG1	1:J:274:GLY:N	1.70	1.14
1:H:39:GLU:HA	1:H:41:LEU:H	1.02	1.14
1:C:277:VAL:HG12	1:C:296:PRO:HA	1.21	1.14
1:E:273:THR:HG21	1:E:275:LYS:HG3	1.29	1.13
1:E:273:THR:HG21	1:E:275:LYS:CD	1.78	1.13
1:E:43:TYR:O	1:E:45:GLN:N	1.82	1.12
1:J:249:GLU:HB2	1:J:252:GLU:N	1.64	1.12
1:C:270:ASP:HB3	1:C:271:PRO:HA	1.16	1.12
1:A:308:ARG:HH11	1:A:308:ARG:HG2	1.00	1.12
1:C:39:GLU:HB3	1:C:40:LYS:HB3	1.25	1.11
1:J:245:ASP:O	1:J:247:GLY:N	1.82	1.11
1:A:173:TYR:HB3	1:A:178:MET:HE3	1.23	1.11
1:E:273:THR:HG21	1:E:275:LYS:HD2	1.32	1.11
1:C:270:ASP:HB2	1:C:271:PRO:CA	1.80	1.10
1:B:307:LEU:HD22	1:B:307:LEU:N	1.63	1.10
1:E:77:SER:HB3	1:F:88:LEU:HD13	1.15	1.10
1:B:249:GLU:O	1:B:251:LEU:N	1.85	1.10
1:D:39:GLU:N	1:D:40:LYS:HG3	0.77	1.10
1:G:270:ASP:OD2	1:G:273:THR:HG23	1.48	1.09
1:J:249:GLU:CG	1:J:252:GLU:HB2	1.82	1.09
1:D:298:GLU:H	1:D:299:GLU:HB2	0.94	1.07
1:C:272:THR:O	1:C:273:THR:HB	1.53	1.07
1:I:270:ASP:OD2	1:I:273:THR:HG23	1.51	1.07
1:A:298:GLU:OE1	1:H:121:ASN:HB3	1.54	1.07
1:A:39:GLU:OE2	1:A:40:LYS:CD	2.02	1.07
1:J:249:GLU:CB	1:J:252:GLU:H	1.65	1.07
1:C:120:THR:O	1:C:121:ASN:HB2	1.51	1.07
1:J:173:TYR:HB3	1:J:178:MET:CE	1.82	1.06
1:J:309:GLU:OE2	1:J:309:GLU:N	1.88	1.06
1:H:39:GLU:OE2	1:H:39:GLU:N	1.88	1.06
1:A:260:ASN:HB2	1:A:262:ILE:HD12	1.36	1.06
1:I:222:VAL:HG13	1:I:226:GLY:HA2	1.33	1.06
1:F:273:THR:HG21	1:F:275:LYS:HB3	1.37	1.06
1:J:249:GLU:HA	1:J:250:GLU:HG3	1.36	1.06
1:F:273:THR:CG2	1:F:274:GLY:H	1.64	1.06
1:H:39:GLU:N	1:H:40:LYS:HB2	1.71	1.06
1:J:298:GLU:HA	1:J:301:LEU:CD2	1.86	1.05
1:F:273:THR:HG23	1:F:275:LYS:N	1.71	1.05
1:J:40:LYS:O	1:J:42:ALA:N	1.89	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:240:LYS:HA	1:B:240:LYS:HE2	1.35	1.05
1:J:249:GLU:CA	1:J:250:GLU:HG3	1.87	1.04
1:H:91:GLU:HG3	1:H:135:TRP:CE2	1.92	1.04
1:F:273:THR:HG23	1:F:275:LYS:H	1.16	1.04
1:J:249:GLU:HG3	1:J:252:GLU:HB2	1.10	1.03
1:J:251:LEU:HD23	1:J:266:LEU:CD1	1.88	1.03
1:H:250:GLU:HB3	1:H:266:LEU:CD2	1.89	1.03
1:F:301:LEU:HA	1:F:304:VAL:CG2	1.88	1.03
1:C:273:THR:CG2	1:C:275:LYS:HG3	1.88	1.02
1:B:222:VAL:HG13	1:B:226:GLY:HA2	1.39	1.02
1:I:306:ASP:O	1:I:308:ARG:N	1.93	1.02
1:H:91:GLU:HG3	1:H:135:TRP:CZ2	1.94	1.02
1:G:40:LYS:HA	1:G:42:ALA:H	1.24	1.02
1:A:308:ARG:HH11	1:A:308:ARG:CG	1.73	1.02
1:G:272:THR:HG22	1:G:273:THR:H	1.19	1.02
1:B:307:LEU:H	1:B:307:LEU:HD23	1.24	1.02
1:D:41:LEU:HD22	1:D:42:ALA:CA	1.90	1.01
1:J:214:PHE:HB3	1:J:299:GLU:HG2	1.40	1.01
1:D:270:ASP:OD1	1:D:277:VAL:CG2	2.07	1.01
1:D:135:TRP:CE2	1:D:144:VAL:HG23	1.94	1.01
1:C:270:ASP:OD2	1:C:274:GLY:HA2	1.59	1.01
1:H:231:HIS:ND1	1:H:232:PRO:CD	2.22	1.01
1:D:39:GLU:N	1:D:39:GLU:OE1	1.93	1.01
1:H:39:GLU:CD	1:H:39:GLU:N	2.14	1.01
1:D:298:GLU:HG3	1:D:299:GLU:CG	1.91	1.00
1:F:273:THR:HG23	1:F:274:GLY:H	0.85	1.00
1:J:91:GLU:HB2	1:J:135:TRP:CE2	1.96	1.00
1:C:270:ASP:HB2	1:C:271:PRO:HA	1.01	1.00
1:E:273:THR:CG2	1:E:275:LYS:HD2	1.92	1.00
1:J:297:LYS:C	1:J:301:LEU:HD22	1.83	0.99
1:J:173:TYR:HB3	1:J:178:MET:HE2	1.41	0.99
1:B:120:THR:O	1:B:121:ASN:HB2	1.61	0.99
1:E:278:ILE:HD12	1:E:278:ILE:N	1.77	0.99
1:H:231:HIS:CE1	1:H:232:PRO:HD2	1.98	0.98
1:J:249:GLU:HB2	1:J:252:GLU:H	0.82	0.98
1:H:136:ASN:OD1	1:H:138:MET:HB2	1.63	0.98
1:I:122:SER:HB2	1:I:123:PRO:HD2	1.41	0.98
1:G:135:TRP:CD2	1:G:144:VAL:HG23	1.99	0.98
1:G:43:TYR:CD1	1:G:300:MET:CE	2.47	0.98
1:J:298:GLU:HA	1:J:301:LEU:HD23	1.45	0.98
1:F:300:MET:O	1:F:304:VAL:HG22	1.61	0.98
1:B:39:GLU:N	1:B:39:GLU:OE2	1.97	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:39:GLU:N	1:E:40:LYS:CB	2.27	0.97
1:C:270:ASP:HB3	1:C:271:PRO:CA	1.83	0.97
1:D:270:ASP:OD1	1:D:277:VAL:HG21	1.62	0.97
1:A:173:TYR:HB3	1:A:178:MET:CE	1.95	0.97
1:G:272:THR:HG22	1:G:273:THR:N	1.77	0.96
1:A:231:HIS:ND1	1:A:232:PRO:HD2	1.79	0.96
1:I:75:MET:HE2	1:I:75:MET:HA	1.44	0.96
1:B:191:PHE:O	1:B:191:PHE:HD2	1.49	0.96
1:A:39:GLU:HA	1:A:40:LYS:CG	1.95	0.95
1:D:273:THR:OG1	1:D:274:GLY:HA2	1.64	0.95
1:C:39:GLU:HB3	1:C:40:LYS:HB2	1.46	0.95
1:I:205:ASP:HA	1:I:230:SER:HB2	1.47	0.95
1:A:91:GLU:HG3	1:A:135:TRP:CZ2	2.00	0.95
1:G:273:THR:HG21	1:G:275:LYS:HE3	1.48	0.94
1:A:39:GLU:CA	1:A:40:LYS:CB	2.33	0.94
1:E:273:THR:HG23	1:E:275:LYS:H	1.28	0.94
1:J:300:MET:CA	1:J:301:LEU:HB2	1.97	0.94
1:G:135:TRP:CE2	1:G:144:VAL:HG23	2.00	0.94
1:I:191:PHE:O	1:I:191:PHE:HD2	1.49	0.94
1:D:39:GLU:CA	1:D:40:LYS:HG3	1.97	0.94
1:J:240:LYS:HA	1:J:240:LYS:HE2	1.49	0.94
1:C:160:LYS:HG3	1:C:191:PHE:CE2	2.02	0.94
1:C:132:VAL:O	1:C:132:VAL:HG23	1.65	0.94
1:F:303:GLY:O	1:F:307:LEU:HG	1.68	0.93
1:C:39:GLU:CB	1:C:40:LYS:HB3	1.96	0.93
1:H:39:GLU:HA	1:H:41:LEU:N	1.82	0.93
1:J:298:GLU:CA	1:J:301:LEU:CD2	2.47	0.93
1:B:48:GLU:O	1:B:51:SER:HB3	1.69	0.93
1:B:163:GLU:HB3	1:B:186:MET:HE1	1.49	0.93
1:J:231:HIS:ND1	1:J:232:PRO:HD2	1.82	0.93
1:I:309:GLU:C	1:I:309:GLU:OE1	2.07	0.93
1:J:260:ASN:HB2	1:J:262:ILE:HD12	1.49	0.92
1:I:307:LEU:HD11	1:J:41:LEU:HD21	1.50	0.92
1:I:191:PHE:O	1:I:191:PHE:CD2	2.23	0.92
1:E:188:GLU:O	1:E:188:GLU:HG3	1.69	0.92
1:F:234:HIS:CE1	1:F:272:THR:HG23	2.04	0.92
1:C:277:VAL:HG12	1:C:296:PRO:CA	1.98	0.92
1:F:222:VAL:HG12	1:F:290:ALA:HB3	1.50	0.92
1:F:41:LEU:HD12	1:F:41:LEU:C	1.91	0.92
1:J:271:PRO:O	1:J:273:THR:N	2.02	0.91
1:D:277:VAL:HG12	1:D:296:PRO:HA	1.50	0.91
1:H:250:GLU:HB3	1:H:266:LEU:HD21	1.52	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.31	0.91
1:D:39:GLU:HA	1:D:40:LYS:HB2	1.53	0.91
1:H:250:GLU:C	1:H:266:LEU:HD11	1.91	0.91
1:C:163:GLU:HB3	1:E:259:LYS:NZ	1.85	0.91
1:J:298:GLU:CA	1:J:301:LEU:HD22	2.00	0.90
1:G:39:GLU:CA	1:G:40:LYS:HB2	1.99	0.90
1:J:297:LYS:O	1:J:301:LEU:HD22	1.71	0.90
1:A:58:ASP:OD2	1:A:286:THR:HG23	1.71	0.90
1:I:39:GLU:N	1:I:39:GLU:OE2	2.03	0.90
1:D:309:GLU:HA	1:D:309:GLU:OE1	1.72	0.90
1:E:204:VAL:O	1:E:208:VAL:HG23	1.72	0.90
1:J:79:GLU:OE2	1:J:79:GLU:HA	1.70	0.90
1:D:265:HIS:O	1:D:266:LEU:HD23	1.72	0.90
1:E:77:SER:CB	1:F:88:LEU:HD13	2.02	0.89
1:F:41:LEU:CD1	1:F:41:LEU:C	2.40	0.89
1:E:273:THR:HG23	1:E:275:LYS:N	1.86	0.89
1:J:298:GLU:N	1:J:301:LEU:HD22	1.87	0.89
1:G:122:SER:HB2	1:G:123:PRO:HD2	1.52	0.89
1:J:300:MET:N	1:J:301:LEU:HB2	1.88	0.88
1:E:247:GLY:O	1:E:248:GLY:O	1.91	0.88
1:D:296:PRO:O	1:D:299:GLU:HB3	1.73	0.88
1:A:43:TYR:HE1	1:A:300:MET:HE1	1.37	0.88
1:E:302:ALA:N	1:E:303:GLY:HA3	1.87	0.88
1:G:205:ASP:HA	1:G:230:SER:HB2	1.56	0.88
1:J:249:GLU:HA	1:J:251:LEU:H	1.38	0.88
1:C:273:THR:HG21	1:C:275:LYS:HG3	1.53	0.88
1:H:273:THR:OG1	1:H:275:LYS:HG2	1.74	0.88
1:E:117:ALA:O	1:E:120:THR:HG22	1.74	0.88
1:E:39:GLU:CA	1:E:40:LYS:HB3	2.03	0.88
1:H:117:ALA:O	1:H:120:THR:HG22	1.74	0.87
1:G:245:ASP:O	1:G:247:GLY:N	2.07	0.87
1:G:39:GLU:N	1:G:40:LYS:HB2	1.90	0.87
1:D:58:ASP:OD2	1:D:286:THR:HG23	1.73	0.87
1:G:218:TYR:CD2	1:G:232:PRO:HG2	2.10	0.87
1:F:139:ASN:O	1:F:141:THR:N	2.07	0.87
1:B:191:PHE:O	1:B:191:PHE:CD2	2.27	0.87
1:C:231:HIS:ND1	1:C:232:PRO:HD2	1.90	0.86
1:D:177:PHE:CZ	1:D:240:LYS:HD2	2.10	0.86
1:B:248:GLY:O	1:B:249:GLU:HB2	1.73	0.86
1:H:275:LYS:HB3	1:H:275:LYS:NZ	1.90	0.86
1:A:305:ALA:HA	1:A:308:ARG:HH12	1.40	0.86
1:G:77:SER:OG	1:H:92:ASN:OD1	1.92	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:43:TYR:CE1	1:G:300:MET:CE	2.57	0.86
1:E:48:GLU:HG3	1:F:48:GLU:HG3	1.57	0.86
1:C:120:THR:O	1:C:121:ASN:CB	2.24	0.86
1:A:308:ARG:HG2	1:A:308:ARG:NH1	1.83	0.86
1:B:177:PHE:HB3	1:B:201:LEU:HD12	1.56	0.86
1:I:136:ASN:OD1	1:I:138:MET:HB2	1.76	0.86
1:D:41:LEU:HD23	1:D:42:ALA:N	1.91	0.86
1:E:58:ASP:OD1	1:E:286:THR:HG23	1.74	0.86
1:F:234:HIS:HE1	1:F:272:THR:HG23	1.41	0.85
1:E:172:PHE:CZ	1:E:175:GLY:HA2	2.09	0.85
1:A:296:PRO:HB2	1:A:299:GLU:HG3	1.56	0.85
1:H:247:GLY:O	1:H:248:GLY:O	1.94	0.85
1:E:273:THR:CG2	1:E:275:LYS:HG3	2.05	0.85
1:I:39:GLU:CA	1:I:40:LYS:HB2	2.06	0.85
1:A:231:HIS:CE1	1:A:232:PRO:HD2	2.10	0.85
1:B:128:THR:OG1	1:B:130:ARG:HG3	1.77	0.85
1:D:135:TRP:CD2	1:D:144:VAL:HG23	2.11	0.85
1:B:104:TYR:HE2	1:B:198:ASP:OD2	1.60	0.84
1:G:58:ASP:OD2	1:G:286:THR:HG23	1.76	0.84
1:H:39:GLU:CA	1:H:41:LEU:H	1.88	0.84
1:F:273:THR:CG2	1:F:275:LYS:H	1.89	0.84
1:A:260:ASN:CB	1:A:262:ILE:HD12	2.07	0.84
1:C:273:THR:HG23	1:C:275:LYS:HG3	1.59	0.84
1:H:214:PHE:HE2	1:H:300:MET:HA	1.43	0.84
1:B:83:ARG:O	1:B:87:LEU:HD12	1.77	0.84
1:J:249:GLU:HG3	1:J:252:GLU:CB	2.03	0.83
1:C:277:VAL:CG1	1:C:296:PRO:HA	2.06	0.83
1:C:273:THR:HG23	1:C:275:LYS:CG	2.08	0.83
1:G:120:THR:O	1:G:121:ASN:HB2	1.77	0.83
1:E:88:LEU:HD13	1:F:77:SER:HB3	1.57	0.83
1:J:156:TYR:O	1:J:159:PRO:HD2	1.77	0.83
1:C:278:ILE:HG22	1:C:280:PHE:CE1	2.12	0.83
1:I:222:VAL:CG1	1:I:226:GLY:HA2	2.08	0.83
1:A:43:TYR:CE1	1:A:300:MET:HE1	2.12	0.83
1:F:204:VAL:O	1:F:208:VAL:HG23	1.77	0.83
1:E:273:THR:HG23	1:E:274:GLY:H	0.68	0.83
1:H:188:GLU:O	1:H:188:GLU:HG2	1.76	0.83
1:G:272:THR:HG22	1:G:273:THR:HG22	1.58	0.83
1:F:41:LEU:HD12	1:F:42:ALA:N	1.94	0.83
1:A:39:GLU:HA	1:A:40:LYS:HB2	0.84	0.82
1:D:39:GLU:CA	1:D:40:LYS:CB	2.57	0.82
1:G:43:TYR:CD1	1:G:300:MET:HE2	2.10	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:136:ASN:HD22	1:A:138:MET:HB2	1.42	0.82
1:J:245:ASP:C	1:J:247:GLY:N	2.32	0.82
1:I:120:THR:O	1:I:120:THR:HG23	1.78	0.82
1:A:77:SER:OG	1:B:92:ASN:OD1	1.97	0.82
1:D:270:ASP:O	1:D:274:GLY:HA3	1.80	0.82
1:I:191:PHE:C	1:I:191:PHE:CD2	2.53	0.82
1:F:122:SER:HB2	1:F:123:PRO:HD2	1.62	0.82
1:E:273:THR:CG2	1:E:275:LYS:H	1.92	0.82
1:J:139:ASN:O	1:J:141:THR:HG22	1.78	0.82
1:B:163:GLU:HB3	1:B:186:MET:CE	2.09	0.82
1:C:273:THR:CG2	1:C:275:LYS:CG	2.57	0.81
1:C:136:ASN:OD1	1:C:138:MET:HB2	1.79	0.81
1:D:136:ASN:OD1	1:D:138:MET:HB2	1.79	0.81
1:D:298:GLU:HG3	1:D:299:GLU:HG2	1.62	0.81
1:G:273:THR:HG21	1:G:275:LYS:CE	2.09	0.81
1:I:75:MET:CE	1:I:75:MET:HA	2.10	0.81
1:H:240:LYS:CE	1:H:240:LYS:HA	2.11	0.81
1:G:273:THR:OG1	1:G:274:GLY:N	2.08	0.81
1:G:213:THR:O	1:G:217:GLY:HA3	1.81	0.81
1:C:91:GLU:HG3	1:C:135:TRP:CH2	2.15	0.81
1:H:39:GLU:N	1:H:40:LYS:HD2	1.95	0.81
1:D:91:GLU:OE1	1:D:135:TRP:CZ2	2.34	0.81
1:B:39:GLU:HB3	1:B:40:LYS:O	1.80	0.81
1:J:260:ASN:CB	1:J:262:ILE:HD12	2.10	0.81
1:J:122:SER:HB2	1:J:123:PRO:HD2	1.61	0.81
1:D:270:ASP:OD1	1:D:277:VAL:HG22	1.79	0.81
1:A:173:TYR:CB	1:A:178:MET:HE3	2.07	0.81
1:C:205:ASP:HA	1:C:230:SER:HB2	1.62	0.81
1:C:121:ASN:O	1:C:122:SER:HB2	1.79	0.81
1:B:191:PHE:CD2	1:B:191:PHE:C	2.54	0.81
1:C:218:TYR:CD2	1:C:232:PRO:HG2	2.16	0.81
1:H:174:GLU:HA	1:H:174:GLU:OE2	1.77	0.81
1:B:257:ASP:HB3	1:B:262:ILE:O	1.81	0.80
1:B:39:GLU:CB	1:B:40:LYS:O	2.30	0.80
1:I:120:THR:O	1:I:121:ASN:HB2	1.80	0.80
1:C:91:GLU:CG	1:C:135:TRP:CZ2	2.62	0.80
1:A:41:LEU:HD11	1:B:307:LEU:CD1	2.11	0.80
1:G:43:TYR:CD1	1:G:300:MET:HE1	2.14	0.80
1:B:246:PHE:O	1:B:251:LEU:HD13	1.82	0.80
1:C:119:TYR:O	1:C:121:ASN:N	2.14	0.80
1:H:214:PHE:CE2	1:H:300:MET:HA	2.17	0.80
1:H:39:GLU:N	1:H:40:LYS:CB	2.45	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:298:GLU:O	1:J:301:LEU:HB3	1.80	0.80
1:D:107:PHE:O	1:D:130:ARG:HD2	1.82	0.80
1:I:43:TYR:O	1:I:47:VAL:HG23	1.80	0.80
1:E:273:THR:CG2	1:E:274:GLY:N	2.17	0.80
1:E:278:ILE:CD1	1:E:278:ILE:N	2.44	0.80
1:D:208:VAL:O	1:D:211:VAL:HG23	1.81	0.80
1:I:258:ILE:HG13	1:I:259:LYS:N	1.95	0.80
1:J:300:MET:CB	1:J:301:LEU:HB2	2.12	0.79
1:H:246:PHE:O	1:H:251:LEU:HD12	1.83	0.79
1:B:120:THR:O	1:B:120:THR:HG23	1.82	0.79
1:B:101:LEU:O	1:B:101:LEU:HD22	1.81	0.79
1:D:296:PRO:HB2	1:D:299:GLU:HG3	1.64	0.79
1:J:249:GLU:N	1:J:249:GLU:OE1	2.14	0.79
1:F:222:VAL:CG1	1:F:290:ALA:HB3	2.11	0.79
1:I:306:ASP:C	1:I:308:ARG:H	1.85	0.79
1:H:83:ARG:NH1	1:H:113:ASP:OD2	2.16	0.79
1:A:298:GLU:O	1:A:300:MET:N	2.16	0.79
1:H:91:GLU:HG3	1:H:135:TRP:CH2	2.18	0.79
1:F:203:TYR:O	1:F:207:VAL:HG23	1.83	0.79
1:A:203:TYR:O	1:A:207:VAL:HG23	1.83	0.79
1:H:95:ARG:NH1	1:J:253:LYS:HG3	1.98	0.79
1:E:234:HIS:NE2	1:E:272:THR:HG23	1.97	0.78
1:C:91:GLU:HG3	1:C:135:TRP:CD2	2.18	0.78
1:I:270:ASP:OD2	1:I:273:THR:CG2	2.31	0.78
1:A:91:GLU:HG3	1:A:135:TRP:CE2	2.18	0.78
1:C:174:GLU:OE2	1:C:174:GLU:HA	1.84	0.78
1:A:244:TYR:CE2	1:A:252:GLU:HG2	2.19	0.78
1:H:278:ILE:HG21	1:H:280:PHE:CE1	2.19	0.78
1:B:95:ARG:CZ	1:D:253:LYS:HB3	2.13	0.78
1:C:177:PHE:HB3	1:C:201:LEU:HD12	1.64	0.78
1:E:203:TYR:O	1:E:207:VAL:HG23	1.83	0.78
1:D:39:GLU:HA	1:D:40:LYS:CB	2.13	0.78
1:A:39:GLU:OE2	1:A:39:GLU:N	2.17	0.78
1:C:174:GLU:CA	1:C:174:GLU:OE2	2.32	0.78
1:D:39:GLU:CD	1:D:39:GLU:N	2.36	0.78
1:H:277:VAL:HG12	1:H:296:PRO:HA	1.64	0.78
1:D:270:ASP:HB3	1:D:272:THR:HG22	1.67	0.77
1:J:177:PHE:HB3	1:J:201:LEU:HD12	1.66	0.77
1:J:215:ASP:HB2	1:J:299:GLU:OE2	1.84	0.77
1:H:278:ILE:CG2	1:H:280:PHE:CE1	2.67	0.77
1:I:83:ARG:NH1	1:I:125:HIS:CD2	2.52	0.77
1:G:89:ILE:HD13	1:H:74:THR:HG23	1.66	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:278:ILE:HD11	1:E:297:LYS:HD3	1.66	0.77
1:C:278:ILE:HD12	1:C:300:MET:HE1	1.67	0.77
1:F:139:ASN:O	1:F:141:THR:HG22	1.85	0.77
1:E:85:GLU:OE1	1:F:79:GLU:HB2	1.83	0.77
1:G:277:VAL:HG12	1:G:296:PRO:HA	1.67	0.77
1:J:91:GLU:HB2	1:J:135:TRP:NE1	1.99	0.76
1:H:132:VAL:HG23	1:H:132:VAL:O	1.81	0.76
1:A:79:GLU:OE2	1:A:79:GLU:HA	1.84	0.76
1:G:135:TRP:CE2	1:G:144:VAL:CG2	2.67	0.76
1:D:80:THR:HG22	1:D:80:THR:O	1.85	0.76
1:H:130:ARG:O	1:H:132:VAL:HG13	1.86	0.76
1:I:39:GLU:N	1:I:39:GLU:CD	2.32	0.76
1:B:246:PHE:O	1:B:251:LEU:CD1	2.34	0.76
1:G:39:GLU:HA	1:G:40:LYS:HB2	1.67	0.76
1:E:132:VAL:HG23	1:E:147:LEU:H	1.51	0.76
1:H:57:PHE:O	1:H:61:MET:HG3	1.85	0.76
1:C:213:THR:HG21	1:C:295:VAL:HG23	1.67	0.76
1:I:256:ARG:HG3	1:I:256:ARG:HH11	1.50	0.76
1:H:277:VAL:CG1	1:H:296:PRO:HA	2.16	0.75
1:F:107:PHE:O	1:F:130:ARG:HD2	1.86	0.75
1:F:298:GLU:CD	1:F:298:GLU:H	1.90	0.75
1:C:125:HIS:O	1:C:146:PRO:HG2	1.86	0.75
1:A:231:HIS:ND1	1:A:232:PRO:CD	2.49	0.75
1:F:43:TYR:O	1:F:45:GLN:N	2.20	0.75
1:H:122:SER:HB2	1:H:123:PRO:HD2	1.69	0.75
1:E:188:GLU:CG	1:E:188:GLU:O	2.33	0.75
1:G:120:THR:HG23	1:G:120:THR:O	1.86	0.75
1:B:222:VAL:CG1	1:B:226:GLY:HA2	2.16	0.75
1:D:94:LEU:HD13	1:D:137:LYS:HE3	1.69	0.75
1:D:260:ASN:HB2	1:D:262:ILE:HD12	1.69	0.75
1:F:273:THR:HG21	1:F:275:LYS:CE	2.16	0.75
1:E:132:VAL:O	1:E:132:VAL:HG23	1.86	0.75
1:J:250:GLU:O	1:J:253:LYS:HB2	1.85	0.74
1:H:160:LYS:HG3	1:H:191:PHE:CE2	2.22	0.74
1:H:188:GLU:CG	1:H:188:GLU:O	2.33	0.74
1:A:136:ASN:ND2	1:A:138:MET:HB2	2.01	0.74
1:H:91:GLU:HG3	1:H:135:TRP:CD2	2.23	0.74
1:A:305:ALA:HA	1:A:308:ARG:NH1	2.02	0.74
1:F:41:LEU:O	1:F:41:LEU:HD13	1.87	0.74
1:H:105:VAL:HG13	1:H:107:PHE:HE1	1.52	0.74
1:H:95:ARG:CZ	1:J:253:LYS:HG3	2.17	0.74
1:C:91:GLU:CG	1:C:135:TRP:CE2	2.66	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:39:GLU:N	1:D:40:LYS:CB	2.51	0.74
1:A:91:GLU:HG3	1:A:135:TRP:CH2	2.23	0.74
1:H:80:THR:HG22	1:H:82:ASP:H	1.51	0.74
1:C:92:ASN:OD1	1:D:77:SER:OG	2.06	0.74
1:A:246:PHE:HB3	1:A:251:LEU:HD12	1.69	0.74
1:E:167:LEU:HD23	1:E:287:GLY:HA3	1.70	0.74
1:B:148:LEU:O	1:B:149:HIS:HB2	1.86	0.74
1:D:214:PHE:CD1	1:D:295:VAL:HG13	2.23	0.74
1:J:231:HIS:CE1	1:J:232:PRO:HD2	2.23	0.74
1:J:120:THR:O	1:J:120:THR:HG23	1.87	0.74
1:G:218:TYR:HD2	1:G:232:PRO:HG2	1.53	0.73
1:F:306:ASP:O	1:F:309:GLU:OE2	2.06	0.73
1:C:231:HIS:ND1	1:C:232:PRO:CD	2.51	0.73
1:G:100:LEU:HD22	1:G:197:VAL:HB	1.70	0.73
1:J:300:MET:N	1:J:301:LEU:CB	2.51	0.73
1:J:249:GLU:CG	1:J:252:GLU:CB	2.63	0.73
1:E:83:ARG:HD2	1:E:113:ASP:OD1	1.88	0.73
1:C:278:ILE:CG2	1:C:280:PHE:CE1	2.72	0.73
1:B:61:MET:CE	1:B:284:VAL:HG11	2.19	0.73
1:D:273:THR:OG1	1:D:274:GLY:CA	2.37	0.73
1:F:273:THR:HG21	1:F:275:LYS:CB	2.17	0.73
1:A:246:PHE:HB3	1:A:251:LEU:CD1	2.18	0.73
1:A:139:ASN:O	1:A:141:THR:HG22	1.89	0.73
1:J:251:LEU:CD2	1:J:266:LEU:CD1	2.67	0.73
1:D:296:PRO:O	1:D:299:GLU:CB	2.36	0.73
1:B:107:PHE:O	1:B:130:ARG:HD2	1.88	0.73
1:F:273:THR:HG21	1:F:275:LYS:HE2	1.70	0.72
1:A:298:GLU:OE1	1:H:121:ASN:CB	2.35	0.72
1:J:231:HIS:ND1	1:J:232:PRO:CD	2.52	0.72
1:J:122:SER:HB2	1:J:123:PRO:CD	2.19	0.72
1:J:251:LEU:HD23	1:J:266:LEU:HD11	1.69	0.72
1:J:57:PHE:O	1:J:61:MET:HG3	1.88	0.72
1:C:250:GLU:O	1:C:266:LEU:HD11	1.88	0.72
1:D:91:GLU:HB2	1:D:135:TRP:NE1	2.04	0.72
1:I:104:TYR:HD2	1:I:134:TYR:CE2	2.08	0.72
1:J:156:TYR:C	1:J:159:PRO:HD2	2.10	0.72
1:F:301:LEU:HA	1:F:304:VAL:HG23	1.70	0.72
1:C:178:MET:HE1	3:C:8:HOH:O	1.88	0.72
1:H:240:LYS:HE2	1:H:240:LYS:HA	1.72	0.72
1:E:136:ASN:OD1	1:E:138:MET:HB2	1.88	0.72
1:C:267:GLU:OE1	1:C:297:LYS:NZ	2.19	0.72
1:J:300:MET:HB2	1:J:301:LEU:HB2	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:91:GLU:CG	1:H:135:TRP:CZ2	2.72	0.72
1:B:69:ARG:HG2	1:B:69:ARG:NH1	2.04	0.72
1:F:122:SER:CB	1:F:123:PRO:HD2	2.19	0.72
1:H:82:ASP:OD1	1:H:84:ASP:HB2	1.90	0.72
1:A:154:ASP:O	1:A:156:TYR:N	2.23	0.72
1:H:240:LYS:HE2	1:H:240:LYS:CA	2.19	0.72
1:D:39:GLU:CA	1:D:40:LYS:CG	2.60	0.71
1:C:273:THR:HG23	1:C:275:LYS:H	1.53	0.71
1:J:240:LYS:HA	1:J:240:LYS:CE	2.19	0.71
1:B:104:TYR:CE2	1:B:198:ASP:OD2	2.43	0.71
1:B:185:ILE:HG13	1:B:194:ILE:N	2.05	0.71
1:B:205:ASP:HA	1:B:230:SER:HB2	1.71	0.71
1:G:271:PRO:O	1:G:272:THR:C	2.29	0.71
1:J:171:TYR:N	1:J:171:TYR:CD1	2.57	0.71
1:B:39:GLU:CA	1:B:40:LYS:O	2.39	0.71
1:J:249:GLU:HA	1:J:251:LEU:N	2.05	0.71
1:J:173:TYR:CB	1:J:178:MET:CE	2.67	0.71
1:D:250:GLU:HG3	1:D:266:LEU:HD13	1.73	0.71
1:D:41:LEU:CG	1:D:42:ALA:H	2.02	0.71
1:A:298:GLU:O	1:A:301:LEU:N	2.23	0.71
1:H:275:LYS:HB3	1:H:275:LYS:HZ3	1.54	0.71
1:C:231:HIS:CE1	1:C:232:PRO:HD2	2.26	0.71
1:G:204:VAL:O	1:G:208:VAL:HG23	1.90	0.71
1:H:136:ASN:OD1	1:H:138:MET:CB	2.39	0.71
1:B:148:LEU:O	1:B:149:HIS:CB	2.38	0.71
1:C:75:MET:CE	1:C:105:VAL:HG21	2.21	0.71
1:J:171:TYR:HD1	1:J:171:TYR:N	1.89	0.70
1:I:168:THR:HG23	1:I:180:SER:O	1.91	0.70
1:A:218:TYR:N	1:A:218:TYR:CD1	2.57	0.70
1:H:238:ILE:HG22	1:H:238:ILE:O	1.92	0.70
1:J:214:PHE:HD2	1:J:299:GLU:HB3	1.47	0.70
1:J:139:ASN:O	1:J:141:THR:N	2.23	0.70
1:H:124:ALA:O	1:H:146:PRO:HB3	1.91	0.70
1:H:109:PRO:CD	1:H:130:ARG:HD3	2.22	0.70
1:G:80:THR:HG22	1:G:80:THR:O	1.88	0.70
1:J:245:ASP:C	1:J:247:GLY:H	1.94	0.70
1:D:218:TYR:CD2	1:D:232:PRO:HG2	2.27	0.70
1:G:222:VAL:HG12	1:G:290:ALA:HB3	1.74	0.70
1:A:39:GLU:CA	1:A:40:LYS:CG	2.66	0.70
1:H:174:GLU:CA	1:H:174:GLU:OE2	2.39	0.70
1:J:120:THR:O	1:J:120:THR:CG2	2.38	0.70
1:C:270:ASP:HB3	1:C:271:PRO:C	2.12	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:272:THR:CG2	1:G:273:THR:H	1.98	0.70
1:H:139:ASN:O	1:H:141:THR:N	2.18	0.70
1:J:278:ILE:HG22	1:J:280:PHE:CE1	2.26	0.70
1:E:277:VAL:C	1:E:278:ILE:HD12	2.11	0.70
1:C:139:ASN:O	1:C:141:THR:N	2.23	0.70
1:D:95:ARG:CZ	1:E:253:LYS:HD2	2.22	0.70
1:B:250:GLU:HA	1:B:253:LYS:HE2	1.72	0.70
1:J:240:LYS:CA	1:J:240:LYS:HE2	2.21	0.70
1:J:154:ASP:O	1:J:156:TYR:N	2.25	0.70
1:H:277:VAL:HG12	1:H:296:PRO:CA	2.21	0.70
1:D:205:ASP:HA	1:D:230:SER:HB2	1.74	0.70
1:F:301:LEU:HA	1:F:304:VAL:HG22	1.72	0.69
1:I:149:HIS:C	1:I:151:ASP:H	1.96	0.69
1:F:109:PRO:N	1:F:130:ARG:HD3	2.07	0.69
1:B:272:THR:O	1:B:272:THR:HG22	1.92	0.69
1:A:107:PHE:O	1:A:130:ARG:NH1	2.25	0.69
1:D:298:GLU:HG3	1:D:299:GLU:HG3	1.72	0.69
1:J:214:PHE:CD2	1:J:299:GLU:CB	2.70	0.69
1:E:41:LEU:O	1:E:42:ALA:C	2.31	0.69
1:H:120:THR:O	1:H:121:ASN:HB2	1.93	0.69
1:A:205:ASP:HA	1:A:230:SER:HB2	1.75	0.69
1:D:139:ASN:C	1:D:141:THR:H	1.95	0.69
1:F:218:TYR:CD2	1:F:232:PRO:HG2	2.27	0.69
1:B:74:THR:O	1:B:77:SER:N	2.25	0.69
1:C:39:GLU:CB	1:C:40:LYS:CB	2.56	0.69
1:H:250:GLU:CB	1:H:266:LEU:CD1	2.70	0.69
1:H:109:PRO:HD3	1:H:130:ARG:HD3	1.74	0.69
1:C:82:ASP:OD1	1:C:84:ASP:HB2	1.92	0.69
1:H:43:TYR:HA	1:H:300:MET:HE1	1.73	0.69
1:F:273:THR:CG2	1:F:275:LYS:HB3	2.19	0.69
1:D:91:GLU:HB2	1:D:135:TRP:CE2	2.28	0.69
1:B:83:ARG:NH1	1:B:125:HIS:CD2	2.61	0.69
1:E:116:ASP:OD2	1:E:130:ARG:HG2	1.92	0.69
1:C:188:GLU:HB3	1:E:252:GLU:OE2	1.93	0.69
1:B:83:ARG:HH11	1:B:125:HIS:CD2	2.11	0.69
1:A:250:GLU:HB2	1:A:266:LEU:HD22	1.75	0.69
1:E:222:VAL:CG2	1:E:290:ALA:HB3	2.22	0.69
1:J:249:GLU:HA	1:J:250:GLU:CG	2.17	0.68
1:C:132:VAL:CG2	1:C:132:VAL:O	2.41	0.68
1:D:248:GLY:O	1:D:251:LEU:HB2	1.93	0.68
1:I:83:ARG:HH11	1:I:125:HIS:CD2	2.09	0.68
1:I:65:LEU:O	1:I:69:ARG:HG3	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:272:THR:O	1:C:272:THR:HG23	1.93	0.68
1:H:65:LEU:O	1:H:69:ARG:HG3	1.93	0.68
1:G:273:THR:CG2	1:G:275:LYS:HE3	2.21	0.68
1:G:305:ALA:O	1:G:308:ARG:HG3	1.93	0.68
1:H:301:LEU:O	1:H:304:VAL:HG23	1.93	0.68
1:G:43:TYR:HD1	1:G:300:MET:HE1	1.59	0.68
1:C:278:ILE:HD12	1:C:300:MET:CE	2.23	0.68
1:C:214:PHE:CE2	1:C:300:MET:HA	2.29	0.68
1:B:39:GLU:HA	1:B:40:LYS:CB	2.24	0.68
1:J:254:ALA:O	1:J:258:ILE:HG23	1.94	0.68
1:C:267:GLU:HG2	1:C:278:ILE:HG12	1.76	0.67
1:H:105:VAL:HG13	1:H:107:PHE:CE1	2.30	0.67
1:J:222:VAL:HA	1:J:227:VAL:O	1.94	0.67
1:D:174:GLU:OE2	1:D:174:GLU:HA	1.94	0.67
1:G:45:GLN:H	1:G:46:SER:HB2	1.59	0.67
1:D:302:ALA:O	1:D:305:ALA:HB3	1.94	0.67
1:F:278:ILE:CD1	1:F:300:MET:HG3	2.24	0.67
1:H:231:HIS:CD2	1:H:237:TRP:HE3	2.13	0.67
1:A:218:TYR:CD2	1:A:232:PRO:HG2	2.29	0.67
1:A:43:TYR:HE1	1:A:300:MET:CE	2.05	0.67
1:D:139:ASN:O	1:D:141:THR:N	2.27	0.67
1:C:222:VAL:HG22	1:C:226:GLY:HA2	1.77	0.67
1:J:167:LEU:HD22	1:J:181:TYR:CE2	2.29	0.67
1:J:101:LEU:HD22	1:J:101:LEU:O	1.94	0.67
1:G:272:THR:CG2	1:G:273:THR:N	2.49	0.67
1:A:214:PHE:HB3	1:A:299:GLU:OE1	1.94	0.67
1:I:74:THR:O	1:I:77:SER:N	2.26	0.67
1:C:131:PHE:CE1	1:C:133:PRO:HG3	2.29	0.67
1:H:105:VAL:CG1	1:H:107:PHE:HE1	2.08	0.67
1:D:132:VAL:O	1:D:132:VAL:HG23	1.93	0.67
1:C:139:ASN:C	1:C:141:THR:H	1.99	0.67
1:H:151:ASP:O	1:H:152:SER:HB3	1.93	0.67
1:F:58:ASP:OD1	1:F:286:THR:HG23	1.95	0.67
1:D:165:ASP:OD1	1:D:183:SER:OG	2.09	0.67
1:E:43:TYR:O	1:E:44:GLN:C	2.34	0.66
1:J:173:TYR:HB3	1:J:178:MET:HE3	1.75	0.66
1:J:218:TYR:N	1:J:218:TYR:CD1	2.62	0.66
1:G:122:SER:HB2	1:G:123:PRO:CD	2.25	0.66
1:G:135:TRP:HZ3	1:G:142:ALA:O	1.78	0.66
1:I:265:HIS:O	1:I:266:LEU:HD23	1.96	0.66
1:F:123:PRO:O	1:F:124:ALA:HB3	1.95	0.66
1:I:105:VAL:HG12	1:I:133:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:213:THR:HG21	1:J:293:LEU:HD21	1.77	0.66
1:F:41:LEU:O	1:F:41:LEU:CD1	2.44	0.66
1:G:214:PHE:CD1	1:G:295:VAL:HG13	2.31	0.66
1:B:157:GLN:HE21	1:B:157:GLN:HA	1.59	0.66
1:C:75:MET:HE2	1:C:105:VAL:HG21	1.78	0.66
1:D:120:THR:HG23	1:D:120:THR:O	1.96	0.66
1:J:105:VAL:CG1	1:J:107:PHE:CE1	2.79	0.66
1:C:74:THR:HG23	1:D:89:ILE:HG12	1.78	0.66
1:I:57:PHE:HE2	1:I:207:VAL:CG1	2.09	0.66
1:D:41:LEU:CD2	1:D:42:ALA:CA	2.62	0.65
1:E:222:VAL:HG23	1:E:290:ALA:HB3	1.78	0.65
1:F:244:TYR:CE2	1:F:252:GLU:HG3	2.31	0.65
1:D:120:THR:O	1:D:121:ASN:HB2	1.94	0.65
1:B:40:LYS:O	1:B:42:ALA:N	2.24	0.65
1:G:245:ASP:C	1:G:247:GLY:N	2.48	0.65
1:I:107:PHE:O	1:I:130:ARG:HD2	1.96	0.65
1:I:155:TYR:O	1:I:159:PRO:HG2	1.96	0.65
1:I:307:LEU:HD11	1:J:41:LEU:CD2	2.23	0.65
1:H:109:PRO:HD3	1:H:130:ARG:CD	2.26	0.65
1:G:80:THR:O	1:G:82:ASP:N	2.29	0.65
1:G:182:VAL:HG12	1:G:183:SER:N	2.10	0.65
1:I:39:GLU:N	1:I:40:LYS:CB	2.52	0.65
1:D:177:PHE:CE1	1:D:240:LYS:HD2	2.32	0.65
1:F:205:ASP:HA	1:F:230:SER:HB2	1.79	0.65
1:C:178:MET:CE	3:C:8:HOH:O	2.44	0.65
1:H:158:LEU:HB2	1:H:159:PRO:HD3	1.79	0.65
1:J:297:LYS:HD2	1:J:301:LEU:HD13	1.78	0.65
1:I:131:PHE:CE1	1:I:133:PRO:HG3	2.32	0.65
1:J:105:VAL:HG11	1:J:107:PHE:HE1	1.61	0.65
1:J:136:ASN:OD1	1:J:138:MET:HB2	1.96	0.65
1:H:185:ILE:HG13	1:H:193:GLY:O	1.97	0.65
1:A:39:GLU:N	1:A:40:LYS:HD3	2.12	0.64
1:C:273:THR:HG21	1:C:275:LYS:CG	2.25	0.64
1:J:113:ASP:O	1:J:115:LYS:HG3	1.97	0.64
1:B:259:LYS:HG2	1:B:259:LYS:O	1.96	0.64
1:D:135:TRP:CE2	1:D:144:VAL:CG2	2.78	0.64
1:G:248:GLY:O	1:G:251:LEU:HB2	1.97	0.64
1:C:41:LEU:HD23	1:C:44:GLN:OE1	1.97	0.64
1:D:300:MET:O	1:D:303:GLY:HA3	1.98	0.64
1:A:308:ARG:CG	1:A:308:ARG:NH1	2.42	0.64
1:E:276:THR:O	1:E:297:LYS:CB	2.46	0.64
1:J:204:VAL:O	1:J:208:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:83:ARG:O	1:F:87:LEU:HD12	1.97	0.64
1:F:270:ASP:OD2	1:F:272:THR:HB	1.98	0.64
1:D:237:TRP:CD1	1:D:241:LYS:HD2	2.33	0.64
1:J:249:GLU:CA	1:J:250:GLU:CG	2.73	0.64
1:H:250:GLU:HB3	1:H:266:LEU:HD22	1.78	0.64
1:D:96:ASP:HB2	1:E:256:ARG:HH22	1.62	0.64
1:E:298:GLU:O	1:E:301:LEU:HB3	1.98	0.64
1:J:249:GLU:CA	1:J:251:LEU:H	2.10	0.64
1:B:39:GLU:N	1:B:39:GLU:CD	2.51	0.64
1:F:244:TYR:HE2	1:F:252:GLU:HG3	1.63	0.64
1:B:110:ASP:H	1:B:116:ASP:CG	2.01	0.64
1:B:306:ASP:C	1:B:307:LEU:HD22	2.18	0.64
1:H:250:GLU:CB	1:H:266:LEU:HD11	2.28	0.64
1:J:105:VAL:CG1	1:J:107:PHE:HE1	2.11	0.64
1:A:43:TYR:CE1	1:A:300:MET:CE	2.81	0.64
1:H:278:ILE:HG21	1:H:280:PHE:CZ	2.33	0.64
1:I:257:ASP:HB3	1:I:262:ILE:O	1.98	0.64
1:A:169:GLU:HB3	1:A:170:PRO:HD2	1.79	0.63
1:D:158:LEU:O	1:D:162:THR:HG23	1.97	0.63
1:B:122:SER:HB2	1:B:123:PRO:HD2	1.80	0.63
1:B:82:ASP:OD1	1:B:82:ASP:C	2.36	0.63
1:A:244:TYR:CD2	1:A:252:GLU:HG2	2.34	0.63
1:B:136:ASN:OD1	1:B:138:MET:HB2	1.98	0.63
1:C:163:GLU:HG2	1:C:186:MET:HE1	1.80	0.63
1:B:267:GLU:OE1	1:B:297:LYS:HE3	1.97	0.63
1:J:39:GLU:HG2	1:J:40:LYS:N	2.14	0.63
1:I:75:MET:CE	1:I:75:MET:CA	2.76	0.63
1:E:136:ASN:OD1	1:E:138:MET:CB	2.46	0.63
1:B:110:ASP:OD1	1:B:116:ASP:HB2	1.98	0.63
1:J:83:ARG:HG3	1:J:112:PHE:HE1	1.64	0.63
1:J:298:GLU:CA	1:J:301:LEU:HD23	2.18	0.63
1:G:40:LYS:N	1:G:41:LEU:HB3	2.14	0.63
1:G:253:LYS:HB3	1:I:95:ARG:CZ	2.29	0.63
1:H:250:GLU:HB2	1:H:266:LEU:HD13	1.81	0.63
1:G:139:ASN:C	1:G:141:THR:H	2.00	0.63
1:I:309:GLU:C	1:I:309:GLU:CD	2.56	0.63
1:G:279:LEU:CD2	1:G:294:VAL:HG22	2.28	0.63
1:A:139:ASN:O	1:A:141:THR:N	2.30	0.63
1:G:173:TYR:HB3	1:G:178:MET:HE3	1.79	0.63
1:C:260:ASN:CB	1:C:262:ILE:HD12	2.29	0.63
1:B:307:LEU:N	1:B:307:LEU:HD23	1.85	0.63
1:A:222:VAL:HG22	1:A:226:GLY:HA2	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:177:PHE:HB3	1:J:201:LEU:CD1	2.28	0.63
1:E:43:TYR:C	1:E:45:GLN:N	2.52	0.62
1:H:250:GLU:HB3	1:H:266:LEU:CD1	2.29	0.62
1:D:299:GLU:O	1:D:302:ALA:CB	2.46	0.62
1:I:160:LYS:HG2	1:I:160:LYS:O	2.00	0.62
1:I:135:TRP:CZ3	1:I:143:SER:HA	2.34	0.62
1:E:300:MET:O	1:E:304:VAL:HG23	1.98	0.62
1:I:259:LYS:HG2	1:I:259:LYS:O	1.99	0.62
1:A:244:TYR:HE2	1:A:252:GLU:HG2	1.63	0.62
1:H:83:ARG:HH11	1:H:113:ASP:CG	2.02	0.62
1:E:40:LYS:O	1:E:40:LYS:HD2	1.99	0.62
1:D:298:GLU:CA	1:D:299:GLU:HB2	2.28	0.62
1:C:121:ASN:O	1:C:122:SER:CB	2.46	0.62
1:C:124:ALA:C	1:C:146:PRO:HG3	2.19	0.62
1:B:120:THR:O	1:B:121:ASN:CB	2.43	0.62
1:A:62:LYS:HD3	1:B:59:ALA:HB1	1.81	0.62
1:D:222:VAL:CG1	1:D:258:ILE:HD13	2.30	0.62
1:I:267:GLU:C	1:I:268:THR:HG22	2.20	0.62
1:F:172:PHE:CZ	1:F:175:GLY:HA2	2.35	0.62
1:C:269:ALA:HA	1:C:276:THR:HA	1.82	0.62
1:G:40:LYS:HA	1:G:42:ALA:N	2.07	0.62
1:I:91:GLU:HB2	1:I:135:TRP:NE1	2.15	0.62
1:I:105:VAL:HG12	1:I:133:PRO:CD	2.30	0.62
1:C:213:THR:HG22	1:C:217:GLY:HA3	1.82	0.62
1:G:120:THR:O	1:G:120:THR:CG2	2.47	0.62
1:E:254:ALA:O	1:E:258:ILE:HG23	2.00	0.62
1:E:164:LYS:O	1:E:166:VAL:HG23	1.99	0.62
1:B:212:ARG:NH1	1:C:212:ARG:NH2	2.47	0.62
1:B:248:GLY:O	1:B:249:GLU:CB	2.45	0.61
1:I:91:GLU:HB2	1:I:135:TRP:CE2	2.35	0.61
1:C:256:ARG:HD3	3:C:321:HOH:O	2.00	0.61
1:E:79:GLU:O	1:E:81:ALA:N	2.33	0.61
1:C:213:THR:HG21	1:C:295:VAL:CG2	2.30	0.61
1:G:218:TYR:HD2	1:G:232:PRO:CG	2.13	0.61
1:E:48:GLU:CG	1:F:48:GLU:HG3	2.30	0.61
1:E:172:PHE:CE2	1:E:175:GLY:HA2	2.34	0.61
1:G:306:ASP:O	1:G:308:ARG:N	2.33	0.61
1:D:222:VAL:HG12	1:D:290:ALA:HB3	1.81	0.61
1:C:306:ASP:OD1	1:C:306:ASP:N	2.34	0.61
1:D:249:GLU:HG3	1:D:249:GLU:O	2.00	0.61
1:H:275:LYS:HB3	1:H:275:LYS:HZ2	1.64	0.61
1:D:85:GLU:O	1:D:89:ILE:HD12	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:245:ASP:O	1:J:246:PHE:C	2.38	0.61
1:H:231:HIS:CD2	1:H:237:TRP:CE3	2.88	0.61
1:B:84:ASP:HA	1:B:87:LEU:HD12	1.83	0.61
1:I:265:HIS:HA	1:I:279:LEU:O	2.00	0.61
1:B:105:VAL:HG12	1:B:133:PRO:HD2	1.81	0.61
1:A:57:PHE:O	1:A:61:MET:HG3	2.01	0.61
1:F:254:ALA:O	1:F:258:ILE:HG23	2.00	0.61
1:J:120:THR:OG1	1:J:127:GLY:O	2.17	0.61
1:I:234:HIS:CE1	1:I:272:THR:HG23	2.36	0.61
1:I:108:GLU:O	1:I:111:ALA:CB	2.49	0.61
1:E:41:LEU:O	1:E:43:TYR:N	2.34	0.60
1:A:214:PHE:HE2	1:A:299:GLU:O	1.83	0.60
1:I:57:PHE:HE2	1:I:207:VAL:HG12	1.65	0.60
1:C:110:ASP:OD1	1:C:114:GLY:C	2.39	0.60
1:H:216:THR:OG1	1:H:299:GLU:OE2	2.20	0.60
1:G:135:TRP:CD2	1:G:144:VAL:CG2	2.81	0.60
1:I:104:TYR:HD2	1:I:134:TYR:HE2	1.49	0.60
1:A:105:VAL:CG1	1:A:107:PHE:HE1	2.13	0.60
1:C:115:LYS:O	1:C:116:ASP:C	2.39	0.60
1:J:300:MET:CA	1:J:301:LEU:CB	2.78	0.60
1:B:177:PHE:CZ	1:B:240:LYS:HD2	2.37	0.60
1:E:228:ILE:HD12	1:E:241:LYS:O	2.01	0.60
1:H:275:LYS:CB	1:H:275:LYS:NZ	2.60	0.60
1:F:79:GLU:OE2	1:F:79:GLU:HA	2.01	0.60
1:H:186:MET:HE2	1:H:191:PHE:HD1	1.67	0.60
1:G:165:ASP:C	1:G:166:VAL:HG23	2.21	0.60
1:F:104:TYR:HB3	1:F:134:TYR:HD2	1.66	0.60
1:H:91:GLU:CG	1:H:135:TRP:CE2	2.80	0.60
1:F:139:ASN:C	1:F:141:THR:H	2.01	0.60
1:G:185:ILE:HG13	1:G:193:GLY:C	2.21	0.60
1:C:172:PHE:CZ	1:C:175:GLY:HA2	2.36	0.60
1:F:211:VAL:HG12	1:F:212:ARG:N	2.15	0.60
1:G:43:TYR:HE1	1:G:300:MET:HE2	1.57	0.60
1:G:271:PRO:O	1:G:272:THR:O	2.20	0.60
1:F:250:GLU:O	1:F:266:LEU:HD11	2.02	0.60
1:C:163:GLU:HB3	1:E:259:LYS:HZ3	1.64	0.60
1:H:43:TYR:HA	1:H:300:MET:CE	2.32	0.60
1:D:105:VAL:HG13	1:D:107:PHE:HE1	1.65	0.60
1:G:307:LEU:HD23	1:G:307:LEU:N	2.17	0.60
1:C:150:TYR:HB3	1:C:155:TYR:OH	2.01	0.60
1:E:117:ALA:O	1:E:120:THR:CG2	2.49	0.60
1:F:117:ALA:O	1:F:120:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:106:ALA:HB3	1:I:194:ILE:HG12	1.84	0.60
1:H:273:THR:OG1	1:H:274:GLY:N	2.34	0.60
1:H:278:ILE:HG22	1:H:280:PHE:CE1	2.37	0.60
1:I:120:THR:O	1:I:121:ASN:CB	2.50	0.60
1:H:130:ARG:NH2	1:H:150:TYR:HE1	2.00	0.60
1:D:94:LEU:HD11	1:D:137:LYS:HG3	1.84	0.60
1:A:105:VAL:HG11	1:A:107:PHE:HE1	1.67	0.60
1:A:171:TYR:N	1:A:171:TYR:CD1	2.70	0.59
1:J:278:ILE:CG2	1:J:280:PHE:CE1	2.85	0.59
1:E:276:THR:O	1:E:297:LYS:HB3	2.02	0.59
1:J:54:ALA:O	1:J:284:VAL:HG22	2.02	0.59
1:C:247:GLY:O	1:C:248:GLY:O	2.19	0.59
1:I:59:ALA:HB1	1:J:62:LYS:HD2	1.84	0.59
1:G:104:TYR:OH	1:G:180:SER:HB3	2.01	0.59
1:D:250:GLU:CG	1:D:266:LEU:HD13	2.32	0.59
1:F:172:PHE:CE2	1:F:175:GLY:HA2	2.37	0.59
1:H:106:ALA:HB3	1:H:194:ILE:HG12	1.84	0.59
1:I:110:ASP:H	1:I:116:ASP:CG	2.05	0.59
1:C:185:ILE:HD11	1:C:194:ILE:O	2.01	0.59
1:B:281:TYR:HB3	1:B:292:VAL:HG22	1.84	0.59
1:G:101:LEU:O	1:G:101:LEU:HD23	2.02	0.59
1:A:101:LEU:HD22	1:A:101:LEU:O	2.01	0.59
1:J:270:ASP:OD2	1:J:273:THR:HG23	2.03	0.59
1:J:249:GLU:HB2	1:J:251:LEU:N	2.17	0.59
1:D:105:VAL:HG13	1:D:107:PHE:CE1	2.37	0.59
1:D:105:VAL:CG1	1:D:107:PHE:HE1	2.15	0.59
1:C:130:ARG:O	1:C:132:VAL:HG13	2.02	0.59
1:H:130:ARG:C	1:H:132:VAL:HG13	2.22	0.59
1:I:256:ARG:HG3	1:I:256:ARG:NH1	2.14	0.59
1:F:116:ASP:OD2	1:F:130:ARG:HG2	2.02	0.59
1:D:245:ASP:O	1:D:246:PHE:HD2	1.85	0.59
1:D:80:THR:O	1:D:81:ALA:C	2.40	0.59
1:I:147:LEU:O	1:I:150:TYR:CE2	2.56	0.59
1:A:245:ASP:C	1:A:247:GLY:N	2.56	0.59
1:H:212:ARG:NH1	1:I:232:PRO:O	2.36	0.59
1:G:253:LYS:HD3	1:I:95:ARG:NH1	2.18	0.59
1:B:168:THR:HG23	1:B:180:SER:O	2.01	0.59
1:H:167:LEU:HD11	1:H:179:VAL:HG13	1.84	0.59
1:J:169:GLU:HB3	1:J:170:PRO:HD2	1.84	0.59
1:H:205:ASP:HA	1:H:230:SER:HB2	1.85	0.59
1:G:45:GLN:N	1:G:46:SER:HB2	2.17	0.59
1:G:41:LEU:O	1:G:41:LEU:HD13	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:GLU:CG	1:A:135:TRP:CZ2	2.82	0.59
1:C:131:PHE:CD1	1:C:133:PRO:HD3	2.38	0.59
1:C:101:LEU:HD22	1:C:101:LEU:O	2.01	0.59
1:E:43:TYR:O	1:E:46:SER:N	2.36	0.59
1:G:270:ASP:OD2	1:G:273:THR:CG2	2.37	0.59
1:E:48:GLU:HG3	1:F:48:GLU:CG	2.32	0.59
1:J:249:GLU:CA	1:J:251:LEU:N	2.65	0.59
1:F:136:ASN:OD1	1:F:138:MET:HB2	2.03	0.58
1:G:249:GLU:O	1:G:249:GLU:HG2	2.02	0.58
1:I:85:GLU:O	1:I:86:ALA:C	2.41	0.58
1:H:208:VAL:HG11	1:H:230:SER:OG	2.03	0.58
1:B:117:ALA:O	1:B:120:THR:HG22	2.03	0.58
1:J:177:PHE:CZ	1:J:240:LYS:HD2	2.38	0.58
1:C:265:HIS:HA	1:C:279:LEU:O	2.03	0.58
1:C:297:LYS:HE2	1:C:301:LEU:HD11	1.84	0.58
1:B:158:LEU:HB2	1:B:159:PRO:HD3	1.86	0.58
1:H:126:ASP:O	1:H:127:GLY:C	2.41	0.58
1:A:270:ASP:HB3	1:A:273:THR:O	2.04	0.58
1:H:110:ASP:OD1	1:H:114:GLY:C	2.42	0.58
1:A:82:ASP:OD1	1:A:84:ASP:N	2.33	0.58
1:D:231:HIS:ND1	1:D:232:PRO:HD2	2.19	0.58
1:F:270:ASP:HB3	1:F:273:THR:HG22	1.86	0.58
1:G:270:ASP:OD1	1:G:271:PRO:N	2.37	0.58
1:I:308:ARG:HA	1:I:309:GLU:C	2.24	0.58
1:G:305:ALA:HA	1:G:308:ARG:NH1	2.19	0.58
1:G:43:TYR:HD1	1:G:300:MET:CE	2.09	0.58
1:C:125:HIS:O	1:C:146:PRO:CG	2.52	0.58
1:B:39:GLU:HA	1:B:40:LYS:O	2.04	0.58
1:B:185:ILE:HG13	1:B:193:GLY:C	2.23	0.58
1:I:48:GLU:O	1:I:51:SER:HB3	2.04	0.58
1:B:120:THR:CG2	1:B:120:THR:O	2.52	0.58
1:B:108:GLU:O	1:B:111:ALA:CB	2.52	0.58
1:A:254:ALA:O	1:A:258:ILE:HG23	2.04	0.58
1:J:173:TYR:CB	1:J:178:MET:HE3	2.31	0.58
1:B:177:PHE:HZ	1:B:240:LYS:HD2	1.68	0.58
1:A:218:TYR:N	1:A:218:TYR:HD1	1.99	0.57
1:C:250:GLU:CD	1:C:250:GLU:H	2.07	0.57
1:A:104:TYR:OH	1:A:180:SER:HB3	2.03	0.57
1:G:136:ASN:HD22	1:G:136:ASN:H	1.51	0.57
1:C:214:PHE:HE2	1:C:300:MET:HA	1.69	0.57
1:A:262:ILE:CD1	1:C:98:PRO:HG3	2.34	0.57
1:A:222:VAL:HG23	1:A:227:VAL:O	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:211:VAL:CG1	1:F:212:ARG:N	2.67	0.57
1:D:41:LEU:CD2	1:D:41:LEU:C	2.67	0.57
1:C:91:GLU:CG	1:C:135:TRP:CH2	2.86	0.57
1:G:43:TYR:C	1:G:45:GLN:H	2.08	0.57
1:B:155:TYR:O	1:B:159:PRO:HG2	2.04	0.57
1:I:120:THR:CG2	1:I:120:THR:O	2.49	0.57
1:B:149:HIS:C	1:B:151:ASP:H	2.05	0.57
1:F:306:ASP:O	1:F:309:GLU:HG3	2.03	0.57
1:D:39:GLU:CA	1:D:40:LYS:HB2	2.22	0.57
1:E:83:ARG:HD3	1:E:119:TYR:CZ	2.39	0.57
1:H:109:PRO:HD3	1:H:130:ARG:NH1	2.20	0.57
1:J:171:TYR:H	1:J:171:TYR:HD1	1.53	0.57
1:B:306:ASP:C	1:B:308:ARG:H	2.08	0.57
1:D:177:PHE:HZ	1:D:240:LYS:HD2	1.64	0.57
1:B:53:TYR:O	1:B:54:ALA:C	2.42	0.57
1:J:271:PRO:C	1:J:273:THR:H	2.02	0.57
1:B:149:HIS:C	1:B:151:ASP:N	2.58	0.57
1:A:145:ALA:HB1	1:A:146:PRO:HD2	1.85	0.57
1:E:122:SER:CB	1:E:123:PRO:HD2	2.34	0.57
1:B:302:ALA:O	1:B:305:ALA:HB3	2.05	0.57
1:A:262:ILE:HG12	1:C:98:PRO:HG3	1.85	0.57
1:B:108:GLU:O	1:B:111:ALA:HB3	2.05	0.57
1:A:105:VAL:CG1	1:A:107:PHE:CE1	2.88	0.57
1:I:108:GLU:HB2	1:I:111:ALA:HB2	1.86	0.57
1:H:39:GLU:N	1:H:40:LYS:CD	2.68	0.57
1:J:105:VAL:HG13	1:J:107:PHE:CE1	2.40	0.57
1:G:80:THR:O	1:G:81:ALA:C	2.43	0.57
1:C:260:ASN:HB2	1:C:262:ILE:HD12	1.87	0.57
1:E:123:PRO:O	1:E:124:ALA:HB3	2.05	0.57
1:B:188:GLU:C	1:B:190:GLU:H	2.08	0.57
1:C:240:LYS:HE2	1:C:240:LYS:HA	1.85	0.57
1:D:41:LEU:C	1:D:43:TYR:H	2.03	0.56
1:E:39:GLU:CA	1:E:40:LYS:CB	2.82	0.56
1:E:274:GLY:O	1:E:275:LYS:C	2.44	0.56
1:A:214:PHE:HD2	1:A:299:GLU:HB3	1.68	0.56
1:I:185:ILE:HG13	1:I:193:GLY:C	2.26	0.56
1:J:203:TYR:O	1:J:207:VAL:HG23	2.05	0.56
1:H:157:GLN:HA	1:H:157:GLN:OE1	2.05	0.56
1:C:295:VAL:HG11	1:C:300:MET:HG3	1.87	0.56
1:E:41:LEU:C	1:E:43:TYR:N	2.58	0.56
1:H:250:GLU:HB2	1:H:266:LEU:CD1	2.34	0.56
1:G:185:ILE:HG13	1:G:193:GLY:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:104:TYR:CZ	1:G:196:GLY:HA3	2.39	0.56
1:F:273:THR:CG2	1:F:275:LYS:N	2.53	0.56
1:F:273:THR:HG21	1:F:275:LYS:CD	2.35	0.56
1:J:249:GLU:N	1:J:250:GLU:HG3	2.21	0.56
1:J:249:GLU:CB	1:J:251:LEU:N	2.68	0.56
1:H:123:PRO:O	1:H:124:ALA:HB3	2.05	0.56
1:F:43:TYR:O	1:F:44:GLN:C	2.44	0.56
1:D:122:SER:HB3	1:D:123:PRO:HD2	1.85	0.56
1:B:108:GLU:HA	1:B:130:ARG:NH1	2.20	0.56
1:I:105:VAL:O	1:I:133:PRO:HD2	2.05	0.56
1:H:57:PHE:O	1:H:61:MET:CG	2.52	0.56
1:G:306:ASP:C	1:G:308:ARG:H	2.08	0.56
1:G:165:ASP:C	1:G:166:VAL:CG2	2.73	0.56
1:I:106:ALA:O	1:I:193:GLY:HA3	2.05	0.56
1:G:151:ASP:HA	1:G:157:GLN:OE1	2.06	0.56
1:J:205:ASP:HA	1:J:230:SER:HB2	1.86	0.56
1:A:122:SER:HB2	1:A:123:PRO:HD2	1.85	0.56
1:I:108:GLU:O	1:I:111:ALA:HB3	2.05	0.56
1:D:302:ALA:HB3	1:D:303:GLY:CA	2.36	0.56
1:I:104:TYR:CD2	1:I:134:TYR:CE2	2.93	0.56
1:B:234:HIS:CE1	1:B:272:THR:HG23	2.40	0.56
1:F:160:LYS:HG3	1:F:191:PHE:CE2	2.41	0.56
1:A:120:THR:HG23	1:A:120:THR:O	2.06	0.56
1:J:172:PHE:HB2	1:J:177:PHE:CE2	2.40	0.56
1:J:260:ASN:CB	1:J:262:ILE:CD1	2.83	0.56
1:E:89:ILE:HD13	1:F:74:THR:HG23	1.88	0.56
1:E:132:VAL:O	1:E:132:VAL:CG2	2.54	0.56
1:D:95:ARG:NE	1:E:253:LYS:HD2	2.21	0.56
1:G:253:LYS:HD3	1:I:95:ARG:HH12	1.71	0.56
1:I:153:SER:O	1:I:157:GLN:HG2	2.06	0.56
1:G:43:TYR:O	1:G:45:GLN:N	2.39	0.56
1:C:273:THR:HG23	1:C:275:LYS:HG2	1.87	0.56
1:E:122:SER:CB	1:E:123:PRO:CD	2.84	0.56
1:E:65:LEU:O	1:E:69:ARG:HG3	2.06	0.56
1:H:234:HIS:HB2	1:H:237:TRP:CE3	2.41	0.56
1:E:43:TYR:C	1:E:45:GLN:H	2.10	0.56
1:J:251:LEU:CD2	1:J:266:LEU:HD12	2.36	0.56
1:E:296:PRO:HB2	1:E:299:GLU:HG3	1.88	0.56
1:A:245:ASP:C	1:A:247:GLY:H	2.07	0.56
1:A:41:LEU:CD1	1:B:307:LEU:CD1	2.84	0.56
1:J:246:PHE:HB3	1:J:251:LEU:CD1	2.36	0.56
1:C:163:GLU:HB3	1:E:259:LYS:HZ1	1.68	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:246:PHE:HB3	1:G:251:LEU:CD1	2.35	0.56
1:A:222:VAL:HA	1:A:227:VAL:O	2.06	0.56
1:E:169:GLU:OE2	1:E:225:SER:OG	2.24	0.56
1:E:41:LEU:HD22	1:E:44:GLN:OE1	2.06	0.56
1:J:249:GLU:C	1:J:250:GLU:CG	2.74	0.56
1:C:186:MET:CE	1:C:191:PHE:HD1	2.19	0.56
1:G:101:LEU:CD2	1:G:101:LEU:O	2.54	0.56
1:A:39:GLU:CA	1:A:39:GLU:OE2	2.54	0.55
1:J:245:ASP:O	1:J:247:GLY:CA	2.54	0.55
1:C:132:VAL:HG23	1:C:147:LEU:H	1.71	0.55
1:B:57:PHE:HE2	1:B:207:VAL:CG1	2.19	0.55
1:D:104:TYR:OH	1:D:180:SER:HB3	2.06	0.55
1:H:185:ILE:HG13	1:H:193:GLY:C	2.26	0.55
1:F:176:VAL:HA	3:F:6:HOH:O	2.05	0.55
1:G:91:GLU:HB2	1:G:135:TRP:NE1	2.21	0.55
1:H:80:THR:HG22	1:H:82:ASP:N	2.21	0.55
1:J:167:LEU:C	1:J:167:LEU:HD12	2.26	0.55
1:C:105:VAL:HG13	1:C:107:PHE:CE1	2.41	0.55
1:C:158:LEU:HB2	1:C:159:PRO:HD3	1.87	0.55
1:J:104:TYR:CZ	1:J:196:GLY:HA3	2.41	0.55
1:H:250:GLU:O	1:H:266:LEU:HD11	2.06	0.55
1:A:131:PHE:CE1	1:A:133:PRO:HG3	2.41	0.55
1:G:139:ASN:O	1:G:141:THR:N	2.28	0.55
1:D:83:ARG:HG2	1:D:112:PHE:HE1	1.70	0.55
1:H:122:SER:HB2	1:H:123:PRO:CD	2.36	0.55
1:D:124:ALA:HB2	1:D:144:VAL:HG11	1.89	0.55
1:E:83:ARG:HD3	1:E:119:TYR:CE1	2.41	0.55
1:H:42:ALA:C	1:H:300:MET:CE	2.75	0.55
1:I:258:ILE:CG1	1:I:259:LYS:N	2.68	0.55
1:I:156:TYR:O	1:I:159:PRO:HD2	2.06	0.55
1:A:39:GLU:N	1:A:40:LYS:CD	2.70	0.55
1:G:41:LEU:CD1	1:G:41:LEU:O	2.54	0.55
1:J:82:ASP:OD1	1:J:82:ASP:C	2.45	0.55
1:E:273:THR:CG2	1:E:275:LYS:CG	2.66	0.55
1:D:299:GLU:O	1:D:302:ALA:HB2	2.07	0.55
1:F:123:PRO:O	1:F:124:ALA:CB	2.55	0.55
1:A:297:LYS:HD2	1:A:297:LYS:O	2.06	0.55
1:A:260:ASN:CB	1:A:262:ILE:CD1	2.82	0.55
1:E:301:LEU:C	1:E:301:LEU:HD23	2.26	0.55
1:H:222:VAL:HG12	1:H:290:ALA:HB3	1.89	0.55
1:D:273:THR:CB	1:D:274:GLY:HA2	2.37	0.54
1:J:297:LYS:O	1:J:301:LEU:CD2	2.51	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:154:ASP:O	1:J:155:TYR:C	2.46	0.54
1:H:185:ILE:HD11	1:H:194:ILE:O	2.07	0.54
1:C:57:PHE:O	1:C:61:MET:CG	2.55	0.54
1:F:182:VAL:HG11	1:F:194:ILE:HD12	1.89	0.54
1:D:265:HIS:C	1:D:266:LEU:HD23	2.27	0.54
1:J:153:SER:HB3	1:J:155:TYR:CD1	2.42	0.54
1:A:250:GLU:H	1:A:250:GLU:CD	2.09	0.54
1:F:167:LEU:HD23	1:F:287:GLY:HA3	1.88	0.54
1:G:266:LEU:HD23	1:G:266:LEU:H	1.72	0.54
1:E:273:THR:HG22	1:E:275:LYS:HD2	1.86	0.54
1:A:215:ASP:N	1:A:299:GLU:OE1	2.36	0.54
1:I:306:ASP:C	1:I:308:ARG:N	2.50	0.54
1:E:130:ARG:NH2	1:E:150:TYR:HE1	2.04	0.54
1:E:273:THR:CG2	1:E:275:LYS:CD	2.63	0.54
1:D:296:PRO:HB2	1:D:299:GLU:CG	2.36	0.54
1:D:298:GLU:N	1:D:299:GLU:CB	2.52	0.54
1:B:240:LYS:HE2	1:B:240:LYS:CA	2.18	0.54
1:D:104:TYR:CZ	1:D:196:GLY:HA3	2.42	0.54
1:I:242:ASP:OD2	1:I:245:ASP:OD2	2.26	0.54
1:J:249:GLU:CB	1:J:252:GLU:N	2.42	0.54
1:I:122:SER:HB2	1:I:123:PRO:CD	2.26	0.54
1:J:177:PHE:CB	1:J:201:LEU:HD12	2.35	0.54
1:C:187:LYS:HG3	1:C:192:ALA:HB2	1.89	0.54
1:F:301:LEU:HD23	1:F:304:VAL:HG21	1.90	0.54
1:F:42:ALA:HB3	1:F:300:MET:HE1	1.89	0.54
1:E:79:GLU:O	1:E:80:THR:C	2.45	0.54
1:B:188:GLU:O	1:B:190:GLU:N	2.39	0.54
1:C:254:ALA:O	1:C:258:ILE:HG23	2.08	0.54
1:G:93:LEU:HD23	1:H:73:THR:HG21	1.89	0.54
1:G:45:GLN:CA	1:G:46:SER:HB2	2.38	0.54
1:E:187:LYS:O	1:E:188:GLU:HG2	2.08	0.54
1:C:248:GLY:HA3	1:C:250:GLU:OE2	2.08	0.54
1:B:213:THR:CG2	1:B:217:GLY:HA3	2.38	0.54
1:C:109:PRO:HD3	1:C:130:ARG:NH1	2.23	0.54
1:A:250:GLU:N	1:A:250:GLU:OE1	2.30	0.54
1:A:167:LEU:HD23	1:A:287:GLY:HA3	1.90	0.54
1:C:222:VAL:CG2	1:C:226:GLY:HA2	2.38	0.54
1:I:108:GLU:HB2	1:I:111:ALA:CB	2.38	0.54
1:G:137:LYS:HA	1:G:141:THR:O	2.08	0.54
1:G:266:LEU:HD23	1:G:266:LEU:N	2.22	0.54
1:E:139:ASN:O	1:E:141:THR:N	2.33	0.54
1:F:43:TYR:HD1	1:F:300:MET:HE1	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:90:LEU:HD11	1:D:105:VAL:HB	1.90	0.53
1:I:258:ILE:C	1:I:258:ILE:HD12	2.29	0.53
1:F:120:THR:O	1:F:121:ASN:HB2	2.08	0.53
1:A:270:ASP:OD1	1:A:271:PRO:N	2.41	0.53
1:G:107:PHE:O	1:G:130:ARG:HD2	2.08	0.53
1:C:79:GLU:OE2	1:C:79:GLU:HA	2.09	0.53
1:H:109:PRO:HD3	1:H:130:ARG:CZ	2.38	0.53
1:H:185:ILE:N	1:H:193:GLY:O	2.33	0.53
1:C:126:ASP:O	1:C:127:GLY:C	2.45	0.53
1:G:273:THR:CG2	1:G:275:LYS:CE	2.83	0.53
1:C:75:MET:HE3	1:C:105:VAL:HG21	1.88	0.53
1:I:213:THR:HG21	1:I:293:LEU:HD21	1.91	0.53
1:A:275:LYS:HB3	1:H:122:SER:HB3	1.91	0.53
1:D:94:LEU:CD1	1:D:137:LYS:HE3	2.36	0.53
1:C:115:LYS:O	1:C:117:ALA:N	2.42	0.53
1:B:265:HIS:HA	1:B:279:LEU:O	2.09	0.53
1:E:273:THR:CG2	1:E:275:LYS:N	2.62	0.53
1:J:214:PHE:HD2	1:J:299:GLU:CB	2.18	0.53
1:B:230:SER:HA	1:B:238:ILE:HG12	1.90	0.53
1:C:222:VAL:HG13	1:C:290:ALA:HB3	1.89	0.53
1:C:61:MET:HB2	1:C:286:THR:OG1	2.09	0.53
1:D:273:THR:HG1	1:D:274:GLY:HA2	1.70	0.53
1:B:104:TYR:HB3	1:B:134:TYR:HD2	1.74	0.53
1:G:213:THR:O	1:G:217:GLY:CA	2.53	0.53
1:I:157:GLN:HA	1:I:157:GLN:OE1	2.09	0.53
1:C:277:VAL:HA	1:C:297:LYS:H	1.72	0.53
1:J:249:GLU:C	1:J:250:GLU:HG3	2.29	0.53
1:B:108:GLU:HA	1:B:130:ARG:HH11	1.73	0.53
1:H:105:VAL:CG1	1:H:107:PHE:CE1	2.89	0.53
1:J:120:THR:O	1:J:121:ASN:HB2	2.09	0.53
1:E:122:SER:OG	1:E:123:PRO:HD2	2.09	0.53
1:J:249:GLU:O	1:J:249:GLU:CD	2.48	0.53
1:E:83:ARG:NH2	1:E:129:GLY:O	2.42	0.53
1:A:281:TYR:N	1:A:281:TYR:CD2	2.77	0.53
1:F:63:ALA:O	1:F:67:ILE:HG13	2.09	0.53
1:G:145:ALA:HB1	1:G:146:PRO:HD2	1.91	0.53
1:H:131:PHE:C	1:H:132:VAL:CG1	2.77	0.53
1:J:207:VAL:O	1:J:210:LYS:CG	2.56	0.53
1:J:94:LEU:HD11	1:J:137:LYS:HG3	1.91	0.53
1:F:42:ALA:HB3	1:F:300:MET:CE	2.39	0.52
1:B:69:ARG:CG	1:B:69:ARG:NH1	2.70	0.52
1:B:104:TYR:HE2	1:B:198:ASP:CG	2.12	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:88:LEU:HD22	1:C:92:ASN:OD1	2.10	0.52
1:E:297:LYS:O	1:E:300:MET:HB2	2.08	0.52
1:A:205:ASP:OD2	1:A:209:SER:OG	2.25	0.52
1:H:173:TYR:O	1:H:174:GLU:C	2.48	0.52
1:D:80:THR:O	1:D:80:THR:CG2	2.55	0.52
1:F:268:THR:HG23	1:F:269:ALA:N	2.24	0.52
1:D:97:ASN:HB2	1:D:100:LEU:HD12	1.92	0.52
1:C:163:GLU:CB	1:E:259:LYS:NZ	2.68	0.52
1:I:104:TYR:HE2	1:I:198:ASP:CG	2.12	0.52
1:I:159:PRO:O	1:I:163:GLU:N	2.40	0.52
1:B:127:GLY:O	1:B:129:GLY:N	2.43	0.52
1:H:177:PHE:HB3	1:H:201:LEU:HD12	1.89	0.52
1:D:178:MET:CE	1:D:198:ASP:OD1	2.58	0.52
1:B:159:PRO:O	1:B:163:GLU:N	2.42	0.52
1:H:278:ILE:HG22	1:H:280:PHE:CD1	2.45	0.52
1:F:308:ARG:O	1:F:309:GLU:C	2.48	0.52
1:D:169:GLU:HA	1:D:169:GLU:OE2	2.08	0.52
1:A:41:LEU:CD1	1:B:307:LEU:HD11	2.39	0.52
1:G:91:GLU:HB2	1:G:135:TRP:CE2	2.44	0.52
1:I:104:TYR:HB3	1:I:134:TYR:HD2	1.74	0.52
1:A:59:ALA:HA	1:B:59:ALA:HA	1.91	0.52
1:G:272:THR:HG22	1:G:273:THR:CG2	2.34	0.52
1:J:39:GLU:O	1:J:304:VAL:HG21	2.10	0.52
1:B:240:LYS:HA	1:B:240:LYS:CE	2.21	0.52
1:A:218:TYR:HD1	1:A:218:TYR:H	1.56	0.52
1:B:186:MET:SD	1:B:191:PHE:HB2	2.50	0.52
1:D:80:THR:O	1:D:82:ASP:N	2.42	0.52
1:D:139:ASN:C	1:D:141:THR:N	2.61	0.52
1:C:248:GLY:CA	1:C:250:GLU:OE2	2.58	0.52
1:J:107:PHE:O	1:J:130:ARG:NH1	2.40	0.52
1:G:139:ASN:C	1:G:141:THR:N	2.63	0.52
1:G:101:LEU:CD2	1:G:101:LEU:C	2.78	0.52
1:I:247:GLY:O	1:I:248:GLY:O	2.27	0.52
1:I:149:HIS:C	1:I:151:ASP:N	2.59	0.52
1:C:185:ILE:N	1:C:193:GLY:O	2.39	0.52
1:H:170:PRO:HG3	1:H:229:LEU:HD21	1.90	0.52
1:G:188:GLU:HG3	1:G:188:GLU:O	2.10	0.52
1:B:95:ARG:NH1	1:D:253:LYS:HB3	2.25	0.52
1:C:105:VAL:HG13	1:C:107:PHE:HE1	1.74	0.52
1:I:150:TYR:H	1:I:150:TYR:HD2	1.48	0.52
1:J:99:HIS:HD1	1:J:203:TYR:HE1	1.57	0.52
1:D:215:ASP:HB2	1:D:299:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:299:GLU:O	1:D:302:ALA:HB3	2.09	0.52
1:H:125:HIS:N	1:H:125:HIS:HD1	2.07	0.52
1:D:214:PHE:HD1	1:D:295:VAL:HG13	1.71	0.52
1:H:139:ASN:OD1	1:H:139:ASN:N	2.43	0.52
1:H:119:TYR:O	1:H:120:THR:C	2.48	0.51
1:J:298:GLU:O	1:J:301:LEU:HD23	2.10	0.51
1:B:272:THR:CG2	1:B:272:THR:O	2.57	0.51
1:A:105:VAL:O	1:A:133:PRO:HD2	2.11	0.51
1:I:158:LEU:N	1:I:159:PRO:CD	2.72	0.51
1:D:115:LYS:HD3	1:D:118:GLU:OE2	2.10	0.51
1:D:41:LEU:O	1:D:43:TYR:HB2	2.11	0.51
1:B:39:GLU:HA	1:B:40:LYS:HB3	1.92	0.51
1:B:90:LEU:HD13	1:B:104:TYR:HA	1.90	0.51
1:I:258:ILE:HG13	1:I:259:LYS:H	1.71	0.51
1:A:264:GLY:C	1:A:281:TYR:CE2	2.84	0.51
1:F:148:LEU:HD12	1:F:174:GLU:OE2	2.10	0.51
1:D:153:SER:HB2	1:D:155:TYR:CD1	2.45	0.51
1:G:83:ARG:HG2	1:G:112:PHE:HE1	1.74	0.51
1:A:214:PHE:CE2	1:A:299:GLU:O	2.61	0.51
1:A:156:TYR:O	1:A:159:PRO:HD2	2.10	0.51
1:B:265:HIS:O	1:B:266:LEU:HD23	2.10	0.51
1:B:268:THR:HG23	1:B:269:ALA:O	2.11	0.51
1:G:206:GLU:C	1:G:206:GLU:OE1	2.48	0.51
1:D:271:PRO:CD	1:D:272:THR:H	2.24	0.51
1:D:272:THR:HG22	1:D:273:THR:HG23	1.93	0.51
1:C:273:THR:HG23	1:C:275:LYS:N	2.22	0.51
1:F:43:TYR:CD1	1:F:300:MET:HE1	2.45	0.51
1:E:300:MET:O	1:E:304:VAL:N	2.43	0.51
1:G:123:PRO:O	1:G:124:ALA:HB3	2.11	0.51
1:J:154:ASP:C	1:J:156:TYR:N	2.62	0.51
1:A:278:ILE:HD11	1:A:297:LYS:HD3	1.93	0.51
1:C:296:PRO:O	1:C:297:LYS:C	2.48	0.51
1:B:251:LEU:C	1:B:254:ALA:HB3	2.30	0.51
1:C:174:GLU:OE2	1:C:174:GLU:N	2.42	0.51
1:D:119:TYR:O	1:D:121:ASN:N	2.43	0.51
1:F:265:HIS:HA	1:F:279:LEU:O	2.10	0.51
1:H:72:SER:O	1:H:76:GLU:HG3	2.10	0.51
1:D:41:LEU:CD2	1:D:42:ALA:HA	2.40	0.51
1:G:43:TYR:C	1:G:45:GLN:N	2.63	0.51
1:G:218:TYR:CD2	1:G:232:PRO:CG	2.88	0.51
1:G:177:PHE:HZ	1:G:240:LYS:HD2	1.76	0.51
1:J:49:MET:CE	1:J:53:TYR:HE1	2.24	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:270:ASP:OD2	1:C:274:GLY:CA	2.46	0.51
1:G:136:ASN:OD1	1:G:138:MET:CE	2.59	0.51
1:I:309:GLU:O	1:I:309:GLU:OE1	2.29	0.51
1:A:267:GLU:OE1	1:A:297:LYS:NZ	2.44	0.51
1:H:91:GLU:CG	1:H:135:TRP:CH2	2.91	0.51
1:H:91:GLU:HG3	1:H:135:TRP:CZ3	2.45	0.51
1:I:117:ALA:O	1:I:120:THR:HG22	2.10	0.51
1:F:105:VAL:O	1:F:133:PRO:HD2	2.10	0.51
1:E:205:ASP:HA	1:E:230:SER:HB2	1.92	0.51
1:A:39:GLU:CB	1:A:40:LYS:HB2	2.38	0.51
1:B:82:ASP:OD1	1:B:83:ARG:N	2.44	0.51
1:A:203:TYR:CE2	1:A:207:VAL:HG21	2.46	0.51
1:C:169:GLU:HB3	1:C:170:PRO:CD	2.40	0.51
1:D:41:LEU:O	1:D:43:TYR:CA	2.55	0.51
1:J:40:LYS:C	1:J:42:ALA:N	2.63	0.51
1:F:266:LEU:O	1:F:278:ILE:HG23	2.11	0.51
1:F:43:TYR:O	1:F:46:SER:N	2.42	0.51
1:D:91:GLU:OE1	1:D:135:TRP:HZ2	1.93	0.51
1:B:83:ARG:O	1:B:87:LEU:CD1	2.53	0.51
1:C:139:ASN:OD1	1:C:139:ASN:N	2.43	0.51
1:A:105:VAL:HG13	1:A:107:PHE:CE1	2.46	0.51
1:A:83:ARG:HG2	1:A:112:PHE:HE1	1.76	0.51
1:E:165:ASP:C	1:E:166:VAL:HG23	2.31	0.51
1:C:76:GLU:HG3	1:C:185:ILE:HG23	1.93	0.51
1:A:279:LEU:HD22	1:A:292:VAL:HG11	1.93	0.51
1:J:272:THR:O	1:J:273:THR:HG22	2.10	0.50
1:J:246:PHE:HB3	1:J:251:LEU:HD12	1.93	0.50
1:G:270:ASP:C	1:G:270:ASP:OD1	2.49	0.50
1:B:157:GLN:O	1:B:160:LYS:N	2.44	0.50
1:A:156:TYR:C	1:A:159:PRO:HD2	2.31	0.50
1:D:154:ASP:N	1:D:154:ASP:OD1	2.44	0.50
1:J:74:THR:O	1:J:77:SER:N	2.44	0.50
1:D:136:ASN:HD22	1:D:136:ASN:H	1.59	0.50
1:E:269:ALA:O	1:E:271:PRO:HD3	2.11	0.50
1:J:218:TYR:N	1:J:218:TYR:HD1	2.07	0.50
1:B:230:SER:O	1:B:231:HIS:HB2	2.11	0.50
1:E:106:ALA:HB3	1:E:194:ILE:HG12	1.93	0.50
1:D:272:THR:CG2	1:D:273:THR:HG23	2.41	0.50
1:J:40:LYS:C	1:J:42:ALA:H	2.14	0.50
1:A:218:TYR:CD2	1:A:232:PRO:CG	2.95	0.50
1:I:110:ASP:N	1:I:116:ASP:OD2	2.37	0.50
1:J:82:ASP:OD1	1:J:84:ASP:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:ALA:HB2	1:A:147:LEU:HD12	1.93	0.50
1:J:279:LEU:HD23	1:J:294:VAL:HG22	1.93	0.50
1:A:109:PRO:HA	1:A:130:ARG:HD3	1.92	0.50
1:G:188:GLU:O	1:G:188:GLU:CG	2.59	0.50
1:H:241:LYS:HA	1:H:245:ASP:OD2	2.10	0.50
1:G:122:SER:CB	1:G:123:PRO:CD	2.90	0.50
1:I:104:TYR:HE2	1:I:198:ASP:OD2	1.95	0.50
1:G:165:ASP:O	1:G:166:VAL:HG22	2.11	0.50
1:B:249:GLU:C	1:B:251:LEU:N	2.61	0.50
1:D:204:VAL:O	1:D:208:VAL:HG23	2.12	0.50
1:B:75:MET:HE2	1:B:75:MET:HA	1.93	0.50
1:D:107:PHE:O	1:D:130:ARG:CD	2.57	0.50
1:J:109:PRO:HA	1:J:130:ARG:HD3	1.94	0.50
1:D:172:PHE:CZ	1:D:175:GLY:HA2	2.47	0.50
1:C:123:PRO:O	1:C:124:ALA:HB3	2.12	0.50
1:H:213:THR:O	1:H:214:PHE:HB2	2.10	0.50
1:H:131:PHE:CE1	1:H:133:PRO:HG3	2.47	0.50
1:I:282:GLU:OE2	1:I:283:PRO:HD2	2.11	0.50
1:D:124:ALA:HB2	1:D:144:VAL:CG1	2.42	0.49
1:G:122:SER:CB	1:G:123:PRO:HD2	2.34	0.49
1:F:278:ILE:HD11	1:F:300:MET:HG3	1.93	0.49
1:F:45:GLN:O	1:F:45:GLN:HG2	2.12	0.49
1:C:170:PRO:HG3	1:C:229:LEU:HD21	1.94	0.49
1:C:139:ASN:C	1:C:141:THR:N	2.65	0.49
1:J:108:GLU:HA	1:J:130:ARG:NH1	2.27	0.49
1:G:136:ASN:OD1	1:G:138:MET:CB	2.37	0.49
1:I:123:PRO:O	1:I:124:ALA:HB3	2.12	0.49
1:C:86:ALA:CB	1:C:131:PHE:CZ	2.95	0.49
1:B:48:GLU:O	1:B:51:SER:CB	2.51	0.49
1:B:108:GLU:HB2	1:B:111:ALA:HB2	1.94	0.49
1:F:49:MET:CE	1:F:293:LEU:HD11	2.42	0.49
1:G:262:ILE:CD1	1:I:98:PRO:HG3	2.41	0.49
1:G:221:MET:HE3	1:G:229:LEU:HD12	1.94	0.49
1:D:41:LEU:HD22	1:D:42:ALA:H	0.38	0.49
1:J:270:ASP:OD1	1:J:271:PRO:N	2.45	0.49
1:H:98:PRO:HG3	1:J:262:ILE:CD1	2.43	0.49
1:G:246:PHE:HB3	1:G:251:LEU:HD12	1.94	0.49
1:I:104:TYR:HD2	1:I:134:TYR:CD2	2.30	0.49
1:C:260:ASN:HB3	1:C:262:ILE:HD12	1.94	0.49
1:C:65:LEU:O	1:C:69:ARG:HG3	2.12	0.49
1:B:65:LEU:HD12	1:B:65:LEU:O	2.13	0.49
1:C:295:VAL:HG12	1:C:295:VAL:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:78:TYR:OH	1:C:85:GLU:HB3	2.13	0.49
1:H:277:VAL:HG12	1:H:296:PRO:N	2.27	0.49
1:A:305:ALA:C	1:A:307:LEU:H	2.16	0.49
1:H:267:GLU:OE1	1:H:297:LYS:HD3	2.13	0.49
1:C:222:VAL:CG1	1:C:290:ALA:HB3	2.43	0.49
1:G:165:ASP:O	1:G:166:VAL:CG2	2.60	0.49
1:G:172:PHE:CE2	1:G:175:GLY:HA2	2.47	0.49
1:B:50:ALA:HA	1:B:293:LEU:HD12	1.94	0.49
1:F:270:ASP:C	1:F:272:THR:H	2.14	0.49
1:C:275:LYS:CB	1:C:275:LYS:NZ	2.76	0.49
1:B:39:GLU:OE2	1:B:39:GLU:CA	2.60	0.49
1:C:80:THR:O	1:C:81:ALA:C	2.51	0.49
1:C:208:VAL:HG11	1:C:220:PHE:HA	1.93	0.49
1:H:277:VAL:HG12	1:H:295:VAL:C	2.32	0.49
1:I:112:PHE:CD1	1:I:131:PHE:CD2	3.00	0.49
1:C:115:LYS:C	1:C:117:ALA:N	2.63	0.49
1:H:254:ALA:O	1:H:258:ILE:HG23	2.13	0.49
1:G:39:GLU:CA	1:G:40:LYS:CB	2.75	0.49
1:C:80:THR:O	1:C:80:THR:HG22	2.10	0.49
1:E:130:ARG:NH2	1:E:150:TYR:CE1	2.80	0.49
1:H:186:MET:CE	1:H:191:PHE:HD1	2.25	0.49
1:I:267:GLU:O	1:I:268:THR:HG22	2.11	0.49
1:D:154:ASP:O	1:D:156:TYR:N	2.45	0.49
1:B:49:MET:HG2	1:B:293:LEU:HD11	1.95	0.49
1:G:273:THR:OG1	1:G:275:LYS:HD2	2.13	0.49
1:C:86:ALA:CB	1:C:131:PHE:HZ	2.25	0.49
1:G:77:SER:CB	1:H:88:LEU:HD13	2.43	0.49
1:I:120:THR:HA	1:I:129:GLY:HA3	1.94	0.49
1:B:297:LYS:O	1:B:301:LEU:HG	2.13	0.49
1:E:75:MET:HB2	1:E:185:ILE:HD13	1.95	0.49
1:J:125:HIS:O	1:J:146:PRO:HG3	2.12	0.49
1:D:185:ILE:HG13	1:D:193:GLY:O	2.13	0.49
1:J:309:GLU:OE2	1:J:309:GLU:CA	2.59	0.49
1:D:177:PHE:CE2	1:D:239:GLY:O	2.66	0.49
1:G:302:ALA:O	1:G:305:ALA:HB3	2.13	0.49
1:G:177:PHE:HB3	1:G:201:LEU:HD22	1.94	0.49
1:E:55:ASN:ND2	1:F:52:ASN:OD1	2.42	0.49
1:H:49:MET:O	1:H:50:ALA:C	2.50	0.49
1:A:115:LYS:HD3	1:A:118:GLU:OE2	2.11	0.49
1:D:298:GLU:HG3	1:D:299:GLU:CB	2.42	0.48
1:J:298:GLU:C	1:J:301:LEU:CD2	2.82	0.48
1:B:148:LEU:O	1:B:149:HIS:CG	2.66	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:234:HIS:HB3	1:I:237:TRP:CD1	2.47	0.48
1:I:185:ILE:HG13	1:I:194:ILE:CA	2.43	0.48
1:H:169:GLU:HB3	1:H:170:PRO:HD2	1.93	0.48
1:A:200:SER:O	1:A:204:VAL:HG23	2.12	0.48
1:H:122:SER:CB	1:H:123:PRO:HD2	2.40	0.48
1:J:309:GLU:CD	1:J:309:GLU:H	2.15	0.48
1:J:300:MET:HB2	1:J:301:LEU:HD13	1.95	0.48
1:B:40:LYS:C	1:B:42:ALA:H	2.12	0.48
1:E:48:GLU:CG	1:F:48:GLU:CG	2.91	0.48
1:D:137:LYS:HA	1:D:141:THR:O	2.13	0.48
1:A:109:PRO:O	1:A:110:ASP:HB2	2.12	0.48
1:I:150:TYR:CD2	1:I:150:TYR:N	2.68	0.48
1:G:173:TYR:CD2	1:G:178:MET:HE3	2.48	0.48
1:A:171:TYR:N	1:A:171:TYR:HD1	2.08	0.48
1:C:130:ARG:NH2	1:C:150:TYR:HE1	2.12	0.48
1:C:171:TYR:OH	1:C:178:MET:HE3	2.13	0.48
1:A:154:ASP:O	1:A:155:TYR:C	2.52	0.48
1:C:57:PHE:O	1:C:61:MET:HG2	2.13	0.48
1:C:187:LYS:HG3	1:C:192:ALA:CB	2.43	0.48
1:H:171:TYR:OH	1:H:178:MET:HE3	2.13	0.48
1:J:260:ASN:HB3	1:J:262:ILE:CD1	2.43	0.48
1:E:302:ALA:N	1:E:303:GLY:CA	2.69	0.48
1:H:130:ARG:NH2	1:H:150:TYR:CE1	2.81	0.48
1:I:57:PHE:CE2	1:I:207:VAL:HG12	2.48	0.48
1:C:49:MET:O	1:C:50:ALA:C	2.50	0.48
1:I:254:ALA:O	1:I:258:ILE:HG23	2.14	0.48
1:D:214:PHE:CD1	1:D:295:VAL:CG1	2.94	0.48
1:I:108:GLU:OE2	1:I:160:LYS:HE3	2.14	0.48
1:I:185:ILE:HG13	1:I:194:ILE:N	2.29	0.48
1:E:213:THR:HG22	1:E:217:GLY:HA3	1.94	0.48
1:D:182:VAL:HG12	1:D:183:SER:N	2.27	0.48
1:E:79:GLU:C	1:E:81:ALA:N	2.63	0.48
1:C:115:LYS:HB3	1:C:118:GLU:HG3	1.96	0.48
1:J:151:ASP:O	1:J:152:SER:HB3	2.13	0.48
1:I:39:GLU:HA	1:I:40:LYS:HB2	1.93	0.48
1:H:98:PRO:HG3	1:J:262:ILE:HD11	1.94	0.48
1:H:273:THR:HG1	1:H:275:LYS:HG2	1.73	0.48
1:H:42:ALA:O	1:H:300:MET:HE3	2.13	0.48
1:A:154:ASP:C	1:A:156:TYR:N	2.66	0.48
1:C:256:ARG:HH22	1:F:92:ASN:CG	2.17	0.48
1:C:258:ILE:HG13	1:C:259:LYS:N	2.22	0.48
1:F:122:SER:CB	1:F:123:PRO:CD	2.88	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:105:VAL:HG11	1:J:107:PHE:CE1	2.44	0.48
1:C:70:THR:HB	1:D:70:THR:HG21	1.95	0.48
1:F:158:LEU:HD23	1:F:158:LEU:HA	1.56	0.48
1:H:91:GLU:HG3	1:H:135:TRP:CE3	2.49	0.48
1:J:61:MET:SD	1:J:284:VAL:HG11	2.54	0.48
1:A:83:ARG:HG2	1:A:112:PHE:CE1	2.49	0.48
1:F:182:VAL:CG1	1:F:194:ILE:HD12	2.43	0.48
1:D:188:GLU:CG	1:D:188:GLU:O	2.61	0.48
1:F:132:VAL:O	1:F:132:VAL:HG23	2.14	0.48
1:J:173:TYR:CG	1:J:178:MET:HE3	2.49	0.48
1:B:237:TRP:CE2	1:B:241:LYS:NZ	2.82	0.48
1:G:306:ASP:C	1:G:308:ARG:N	2.67	0.48
1:H:208:VAL:HG21	1:H:221:MET:HG3	1.95	0.48
1:D:145:ALA:HB1	1:D:146:PRO:HD2	1.94	0.48
1:A:41:LEU:HD11	1:B:307:LEU:HD11	1.94	0.47
1:J:251:LEU:HD23	1:J:266:LEU:HD13	1.85	0.47
1:G:272:THR:CG2	1:G:273:THR:HG22	2.37	0.47
1:E:295:VAL:CG1	1:E:300:MET:HG2	2.44	0.47
1:B:104:TYR:HD2	1:B:134:TYR:CE2	2.32	0.47
1:A:132:VAL:N	1:A:133:PRO:HD3	2.28	0.47
1:H:125:HIS:O	1:H:146:PRO:HG3	2.13	0.47
1:C:218:TYR:CD2	1:C:232:PRO:CG	2.94	0.47
1:H:43:TYR:N	1:H:300:MET:HE2	2.29	0.47
1:J:222:VAL:HG22	1:J:226:GLY:C	2.35	0.47
1:B:279:LEU:CD2	1:B:294:VAL:HG22	2.45	0.47
1:E:265:HIS:HA	1:E:279:LEU:O	2.14	0.47
1:C:112:PHE:CG	1:C:131:PHE:HD2	2.33	0.47
1:C:169:GLU:HB3	1:C:170:PRO:HD2	1.97	0.47
1:G:79:GLU:C	1:G:81:ALA:H	2.17	0.47
1:F:49:MET:HE1	1:F:293:LEU:HD11	1.95	0.47
1:I:150:TYR:HB2	1:I:156:TYR:CD1	2.49	0.47
1:I:154:ASP:OD2	1:I:158:LEU:HD11	2.14	0.47
1:C:256:ARG:CD	3:C:321:HOH:O	2.61	0.47
1:A:135:TRP:HZ3	1:A:142:ALA:O	1.97	0.47
1:J:113:ASP:O	1:J:115:LYS:N	2.47	0.47
1:H:182:VAL:HG11	1:H:194:ILE:HD12	1.97	0.47
1:J:200:SER:O	1:J:204:VAL:HG23	2.14	0.47
1:C:273:THR:CG2	1:C:275:LYS:HG2	2.43	0.47
1:D:214:PHE:CE1	1:D:295:VAL:HG11	2.49	0.47
1:G:172:PHE:CZ	1:G:175:GLY:HA2	2.50	0.47
1:E:83:ARG:HH11	1:E:113:ASP:CG	2.15	0.47
1:C:105:VAL:CG1	1:C:107:PHE:HE1	2.27	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:279:LEU:HD22	1:B:294:VAL:HG22	1.97	0.47
1:A:39:GLU:CA	1:A:40:LYS:HG3	2.42	0.47
1:H:250:GLU:CB	1:H:266:LEU:HD13	2.42	0.47
1:E:295:VAL:HG11	1:E:300:MET:HG2	1.96	0.47
1:C:186:MET:HE2	1:C:191:PHE:HD1	1.80	0.47
1:H:302:ALA:C	1:H:304:VAL:H	2.18	0.47
1:G:182:VAL:CG1	1:G:183:SER:N	2.76	0.47
1:B:131:PHE:CE1	1:B:133:PRO:HG3	2.49	0.47
1:A:61:MET:SD	1:A:284:VAL:HG11	2.55	0.47
1:D:172:PHE:CE2	1:D:175:GLY:HA2	2.50	0.47
1:B:91:GLU:HB2	1:B:135:TRP:CE2	2.50	0.47
1:E:93:LEU:CD2	1:F:70:THR:HG23	2.45	0.47
1:E:93:LEU:HD21	1:F:70:THR:HG23	1.96	0.47
1:D:71:ILE:O	1:D:74:THR:HB	2.15	0.47
1:J:234:HIS:O	1:J:236:ASP:N	2.48	0.47
1:F:240:LYS:HE3	1:F:240:LYS:HB3	1.61	0.47
1:B:89:ILE:O	1:B:90:LEU:C	2.51	0.47
1:A:251:LEU:HD23	1:A:266:LEU:CD1	2.45	0.47
1:I:104:TYR:CD2	1:I:134:TYR:HE2	2.29	0.47
1:F:85:GLU:O	1:F:89:ILE:HG13	2.15	0.47
1:D:249:GLU:CG	1:D:249:GLU:O	2.62	0.47
1:G:249:GLU:O	1:G:249:GLU:CG	2.63	0.47
1:G:128:THR:C	1:G:130:ARG:H	2.18	0.47
1:G:154:ASP:OD1	1:G:154:ASP:N	2.47	0.47
1:G:273:THR:HG21	1:G:275:LYS:HE2	1.94	0.47
1:B:160:LYS:HA	1:B:191:PHE:CE1	2.50	0.47
1:B:130:ARG:NH2	1:B:150:TYR:CD1	2.83	0.47
1:I:88:LEU:HD13	1:J:77:SER:HB3	1.97	0.47
1:B:50:ALA:CA	1:B:293:LEU:HD12	2.45	0.47
1:J:278:ILE:HD11	1:J:297:LYS:HD3	1.97	0.47
1:D:136:ASN:HD22	1:D:136:ASN:N	2.12	0.47
1:I:107:PHE:HB3	1:I:111:ALA:HB3	1.97	0.47
1:C:301:LEU:HA	1:C:304:VAL:HG23	1.96	0.46
1:B:39:GLU:HA	1:B:40:LYS:C	2.35	0.46
1:A:99:HIS:ND1	1:A:203:TYR:CE1	2.83	0.46
1:E:107:PHE:O	1:E:130:ARG:HD2	2.15	0.46
1:A:250:GLU:N	1:A:250:GLU:CD	2.67	0.46
1:I:156:TYR:C	1:I:159:PRO:HD2	2.35	0.46
1:B:122:SER:CB	1:B:123:PRO:HD2	2.45	0.46
1:J:169:GLU:CB	1:J:170:PRO:HD2	2.43	0.46
1:H:126:ASP:O	1:H:129:GLY:N	2.47	0.46
1:D:188:GLU:O	1:D:188:GLU:HG3	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:101:LEU:HD22	1:H:101:LEU:O	2.15	0.46
1:G:45:GLN:H	1:G:46:SER:CB	2.26	0.46
1:B:39:GLU:CA	1:B:40:LYS:CB	2.92	0.46
1:C:80:THR:CG2	1:C:80:THR:O	2.60	0.46
1:G:245:ASP:O	1:G:246:PHE:C	2.51	0.46
1:F:298:GLU:CD	1:F:298:GLU:N	2.65	0.46
1:H:215:ASP:HB2	1:H:299:GLU:OE1	2.15	0.46
1:F:193:GLY:O	1:F:194:ILE:HG22	2.15	0.46
1:F:273:THR:CG2	1:F:274:GLY:N	2.33	0.46
1:A:262:ILE:CG1	1:C:98:PRO:HG3	2.44	0.46
1:I:222:VAL:HG13	1:I:226:GLY:CA	2.25	0.46
1:H:231:HIS:HD2	1:H:237:TRP:HE3	1.62	0.46
1:C:278:ILE:HG22	1:C:280:PHE:CD1	2.49	0.46
1:A:300:MET:O	1:A:304:VAL:HG23	2.16	0.46
1:D:108:GLU:O	1:D:111:ALA:CB	2.63	0.46
1:H:277:VAL:HG13	1:H:296:PRO:HA	1.96	0.46
1:E:85:GLU:O	1:E:89:ILE:HG13	2.15	0.46
1:B:106:ALA:HB3	1:B:194:ILE:HG12	1.96	0.46
1:C:97:ASN:HB2	1:C:100:LEU:HD12	1.97	0.46
1:D:272:THR:HG23	1:D:273:THR:HG22	1.97	0.46
1:C:213:THR:O	1:C:217:GLY:HA3	2.15	0.46
1:D:136:ASN:OD1	1:D:138:MET:CB	2.58	0.46
1:G:80:THR:CG2	1:G:80:THR:O	2.59	0.46
1:B:138:MET:CE	1:B:174:GLU:HG2	2.45	0.46
1:J:83:ARG:HG3	1:J:112:PHE:CE1	2.46	0.46
1:J:98:PRO:HA	1:J:137:LYS:NZ	2.31	0.46
1:F:247:GLY:HA3	1:F:251:LEU:HD12	1.98	0.46
1:A:73:THR:HG21	1:B:93:LEU:HD23	1.97	0.46
1:A:187:LYS:NZ	3:A:7:HOH:O	2.48	0.46
1:C:85:GLU:O	1:C:86:ALA:C	2.54	0.46
1:A:201:LEU:O	1:A:204:VAL:N	2.49	0.46
1:H:39:GLU:N	1:H:40:LYS:CG	2.79	0.46
1:C:85:GLU:O	1:C:89:ILE:HG13	2.15	0.46
1:A:79:GLU:OE2	1:A:79:GLU:CA	2.60	0.46
1:A:222:VAL:HG12	1:A:290:ALA:O	2.15	0.46
1:C:57:PHE:O	1:C:61:MET:HG3	2.15	0.46
1:J:249:GLU:N	1:J:249:GLU:CD	2.68	0.46
1:A:298:GLU:C	1:A:300:MET:N	2.69	0.46
1:D:109:PRO:N	1:D:130:ARG:HD3	2.31	0.46
1:A:242:ASP:O	1:A:244:TYR:N	2.49	0.46
1:E:78:TYR:OH	1:E:85:GLU:HB3	2.16	0.46
1:D:231:HIS:O	1:D:235:LYS:HD3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:213:THR:HG23	1:B:217:GLY:HA3	1.98	0.46
1:D:178:MET:HE3	1:D:198:ASP:OD1	2.15	0.46
1:A:41:LEU:HD11	1:B:307:LEU:HD12	1.95	0.46
1:H:135:TRP:CD2	1:H:144:VAL:HB	2.51	0.46
1:G:77:SER:HB3	1:H:88:LEU:HD13	1.96	0.46
1:I:171:TYR:N	1:I:171:TYR:CD1	2.84	0.46
1:E:80:THR:O	1:E:81:ALA:C	2.53	0.46
1:E:131:PHE:CE1	1:E:133:PRO:HG3	2.51	0.46
1:C:91:GLU:HG3	1:C:135:TRP:CZ3	2.50	0.46
1:C:120:THR:HG23	1:C:120:THR:O	2.16	0.46
1:F:43:TYR:C	1:F:45:GLN:N	2.70	0.46
1:J:80:THR:O	1:J:81:ALA:HB3	2.16	0.46
1:C:208:VAL:HG21	1:C:221:MET:HG3	1.98	0.46
1:I:147:LEU:O	1:I:150:TYR:CD2	2.69	0.46
1:B:109:PRO:HA	1:B:116:ASP:OD2	2.16	0.46
1:B:57:PHE:HE2	1:B:207:VAL:HG11	1.80	0.46
1:C:83:ARG:NH2	1:C:113:ASP:OD2	2.34	0.46
1:G:273:THR:OG1	1:G:275:LYS:HE2	2.15	0.45
1:A:99:HIS:ND1	1:A:203:TYR:HE1	2.14	0.45
1:I:57:PHE:HE2	1:I:207:VAL:HG11	1.80	0.45
1:H:182:VAL:HG12	1:H:194:ILE:HB	1.98	0.45
1:B:126:ASP:O	1:B:127:GLY:C	2.54	0.45
1:B:287:GLY:O	1:B:288:ASP:C	2.54	0.45
1:G:265:HIS:ND1	1:G:265:HIS:O	2.48	0.45
1:J:215:ASP:H	1:J:299:GLU:HG2	1.81	0.45
1:F:270:ASP:C	1:F:272:THR:N	2.70	0.45
1:H:98:PRO:HG3	1:J:262:ILE:HG12	1.97	0.45
1:I:131:PHE:C	1:I:132:VAL:HG13	2.36	0.45
1:E:132:VAL:HG23	1:E:147:LEU:HB2	1.98	0.45
1:A:88:LEU:HD22	1:A:92:ASN:OD1	2.16	0.45
1:J:214:PHE:HE2	1:J:299:GLU:O	1.98	0.45
1:G:41:LEU:C	1:G:41:LEU:CD1	2.85	0.45
1:G:135:TRP:CE3	1:G:144:VAL:HG23	2.50	0.45
1:C:134:TYR:O	1:C:136:ASN:ND2	2.46	0.45
1:G:177:PHE:CZ	1:G:240:LYS:HD2	2.51	0.45
1:I:250:GLU:OE1	1:I:250:GLU:HA	2.15	0.45
1:B:308:ARG:O	1:B:309:GLU:HB2	2.17	0.45
1:H:120:THR:O	1:H:121:ASN:CB	2.62	0.45
1:H:246:PHE:O	1:H:251:LEU:CD1	2.60	0.45
1:B:117:ALA:O	1:B:120:THR:CG2	2.64	0.45
1:E:83:ARG:CD	1:E:119:TYR:CE1	2.99	0.45
1:A:258:ILE:HG22	1:A:281:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:GLU:HB2	1:B:135:TRP:NE1	2.32	0.45
1:H:117:ALA:O	1:H:120:THR:CG2	2.56	0.45
1:I:307:LEU:C	1:I:308:ARG:HG3	2.30	0.45
1:I:136:ASN:OD1	1:I:138:MET:CB	2.57	0.45
1:J:156:TYR:CD1	1:J:194:ILE:HD13	2.52	0.45
1:A:82:ASP:OD1	1:A:82:ASP:C	2.55	0.45
1:G:154:ASP:O	1:G:156:TYR:N	2.49	0.45
1:I:302:ALA:O	1:I:305:ALA:HB3	2.16	0.45
1:I:244:TYR:C	1:I:246:PHE:H	2.19	0.45
1:C:213:THR:CG2	1:C:295:VAL:CG2	2.95	0.45
1:J:246:PHE:CD1	1:J:251:LEU:HD11	2.51	0.45
1:B:130:ARG:NH2	1:B:150:TYR:HD1	2.15	0.45
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.72	0.45
1:C:182:VAL:HG12	1:C:194:ILE:HB	1.99	0.45
1:J:104:TYR:CE1	1:J:196:GLY:HA3	2.50	0.45
1:D:272:THR:HG23	1:D:273:THR:CG2	2.47	0.45
1:B:182:VAL:HG11	1:B:194:ILE:HD12	1.97	0.45
1:B:112:PHE:CE1	1:B:131:PHE:CD2	3.04	0.45
1:C:126:ASP:O	1:C:128:THR:N	2.50	0.45
1:E:218:TYR:CD2	1:E:232:PRO:HG2	2.52	0.45
1:D:160:LYS:O	1:D:161:ALA:C	2.54	0.45
1:J:282:GLU:OE2	1:J:282:GLU:HA	2.17	0.45
1:E:298:GLU:HG2	1:E:299:GLU:N	2.31	0.45
1:C:110:ASP:OD1	1:C:114:GLY:O	2.34	0.45
1:H:178:MET:HE3	1:H:198:ASP:OD1	2.16	0.45
1:A:240:LYS:HA	1:A:240:LYS:HE2	1.98	0.45
1:A:150:TYR:CD1	1:A:150:TYR:C	2.90	0.45
1:B:172:PHE:O	1:B:172:PHE:CG	2.69	0.45
1:G:275:LYS:HD2	1:G:275:LYS:N	2.31	0.45
1:G:279:LEU:HD21	1:G:294:VAL:HG22	1.99	0.45
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.57	0.45
1:D:95:ARG:CZ	1:E:253:LYS:CD	2.93	0.45
1:J:213:THR:HG21	1:J:293:LEU:CD2	2.44	0.45
1:A:169:GLU:CB	1:A:170:PRO:HD2	2.46	0.45
1:B:105:VAL:O	1:B:133:PRO:HD2	2.17	0.45
1:D:83:ARG:HD3	1:D:131:PHE:CD1	2.52	0.45
1:I:264:GLY:HA3	1:I:281:TYR:CZ	2.52	0.45
1:A:126:ASP:N	1:A:126:ASP:OD2	2.50	0.45
1:F:270:ASP:O	1:F:272:THR:N	2.50	0.45
1:G:273:THR:OG1	1:G:275:LYS:CE	2.65	0.45
1:E:130:ARG:HH21	1:E:150:TYR:HE1	1.65	0.45
1:F:84:ASP:HA	1:F:87:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:256:ARG:NH2	1:F:92:ASN:CG	2.71	0.45
1:A:282:GLU:OE2	1:A:283:PRO:HD2	2.16	0.45
1:E:275:LYS:HG3	1:E:275:LYS:H	1.55	0.44
1:B:254:ALA:O	1:B:258:ILE:HG23	2.17	0.44
1:B:159:PRO:O	1:B:163:GLU:HA	2.17	0.44
1:H:275:LYS:CB	1:H:275:LYS:HZ2	2.28	0.44
1:I:86:ALA:CB	1:I:131:PHE:HE2	2.30	0.44
1:D:308:ARG:HA	1:D:308:ARG:HE	1.81	0.44
1:A:94:LEU:HD21	1:A:100:LEU:O	2.17	0.44
1:F:88:LEU:HD23	1:F:88:LEU:HA	1.67	0.44
1:B:40:LYS:C	1:B:42:ALA:N	2.71	0.44
1:C:205:ASP:HB2	1:C:238:ILE:HD13	2.00	0.44
1:C:201:LEU:HD21	1:C:229:LEU:HD22	1.99	0.44
1:H:139:ASN:C	1:H:141:THR:N	2.71	0.44
1:B:123:PRO:O	1:B:124:ALA:HB3	2.17	0.44
1:H:212:ARG:HH22	1:I:235:LYS:NZ	2.15	0.44
1:D:185:ILE:HG13	1:D:193:GLY:C	2.38	0.44
1:G:215:ASP:HB2	1:G:299:GLU:CD	2.38	0.44
1:B:169:GLU:HB3	1:B:170:PRO:HD2	2.00	0.44
1:A:208:VAL:HG11	1:A:220:PHE:HA	1.99	0.44
1:J:212:ARG:HA	1:J:212:ARG:HD3	1.71	0.44
1:G:270:ASP:OD1	1:G:272:THR:HB	2.17	0.44
1:C:273:THR:O	1:C:275:LYS:N	2.47	0.44
1:H:150:TYR:HB3	1:H:155:TYR:OH	2.17	0.44
1:I:104:TYR:CE2	1:I:198:ASP:OD2	2.70	0.44
1:H:167:LEU:CD1	1:H:179:VAL:HG13	2.45	0.44
1:C:154:ASP:O	1:C:156:TYR:N	2.50	0.44
1:H:125:HIS:N	1:H:125:HIS:ND1	2.63	0.44
1:G:39:GLU:HA	1:G:40:LYS:CB	2.34	0.44
1:H:276:THR:OG1	1:H:297:LYS:HB3	2.18	0.44
1:H:132:VAL:N	1:H:133:PRO:HD3	2.32	0.44
1:D:120:THR:O	1:D:120:THR:CG2	2.65	0.44
1:D:104:TYR:CE2	1:D:196:GLY:C	2.91	0.44
1:F:193:GLY:C	1:F:194:ILE:CG2	2.85	0.44
1:A:177:PHE:HB3	1:A:201:LEU:HD12	1.99	0.44
1:E:135:TRP:CE2	1:E:144:VAL:HB	2.53	0.44
1:G:108:GLU:HB2	1:G:111:ALA:HB2	2.00	0.44
1:G:136:ASN:OD1	1:G:138:MET:HE2	2.17	0.44
1:J:91:GLU:OE1	1:J:135:TRP:CZ2	2.71	0.44
1:C:94:LEU:HD11	1:C:136:ASN:HA	1.99	0.44
1:B:105:VAL:HG12	1:B:133:PRO:CD	2.45	0.44
1:C:240:LYS:HA	1:C:240:LYS:CE	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:203:TYR:O	1:J:206:GLU:HB3	2.18	0.44
1:E:61:MET:SD	1:E:284:VAL:HG11	2.58	0.44
1:D:213:THR:HG21	1:D:293:LEU:HD22	2.00	0.44
1:I:167:LEU:HD12	1:I:167:LEU:C	2.38	0.44
1:G:43:TYR:O	1:G:46:SER:HB3	2.18	0.44
1:G:275:LYS:HD2	1:G:275:LYS:H	1.83	0.44
1:A:262:ILE:HD11	1:C:98:PRO:HG3	2.00	0.44
1:J:213:THR:CG2	1:J:293:LEU:HD21	2.46	0.44
1:H:97:ASN:CB	1:H:100:LEU:HD12	2.47	0.44
1:G:158:LEU:HD23	1:G:158:LEU:HA	1.80	0.44
1:H:108:GLU:O	1:H:111:ALA:HB3	2.17	0.44
1:H:108:GLU:O	1:H:111:ALA:CB	2.65	0.44
1:C:215:ASP:HB2	1:C:299:GLU:OE1	2.18	0.44
1:A:216:THR:OG1	1:A:299:GLU:OE2	2.28	0.44
1:C:86:ALA:HB3	1:C:131:PHE:HZ	1.82	0.44
1:C:78:TYR:CE1	1:C:80:THR:HB	2.53	0.44
1:F:305:ALA:O	1:F:308:ARG:CB	2.66	0.44
1:I:272:THR:O	1:I:272:THR:HG22	2.18	0.44
1:B:53:TYR:HB3	1:B:291:PHE:CE1	2.52	0.44
1:J:203:TYR:CE2	1:J:207:VAL:HG21	2.52	0.44
1:H:293:LEU:HD23	1:H:293:LEU:HA	1.83	0.44
1:F:39:GLU:HA	1:F:40:LYS:HB2	0.64	0.44
1:J:39:GLU:HG2	1:J:40:LYS:H	1.82	0.44
1:D:266:LEU:O	1:D:278:ILE:HA	2.18	0.44
1:G:245:ASP:C	1:G:247:GLY:H	2.20	0.44
1:B:101:LEU:O	1:B:101:LEU:CD2	2.60	0.44
1:B:211:VAL:CG1	1:B:212:ARG:N	2.80	0.44
1:A:269:ALA:O	1:A:270:ASP:C	2.55	0.44
1:G:221:MET:CE	1:G:229:LEU:HD12	2.48	0.44
1:G:44:GLN:NE2	1:H:45:GLN:OE1	2.50	0.44
1:D:299:GLU:HA	1:D:299:GLU:OE1	2.17	0.44
1:B:244:TYR:C	1:B:246:PHE:H	2.22	0.44
1:A:209:SER:HB3	1:A:232:PRO:HA	1.99	0.44
1:J:218:TYR:CD2	1:J:232:PRO:HG2	2.53	0.44
1:F:222:VAL:CG1	1:F:258:ILE:HD12	2.48	0.44
1:D:57:PHE:CE2	1:D:208:VAL:HG22	2.53	0.44
1:B:61:MET:SD	1:B:284:VAL:HG11	2.58	0.44
1:I:207:VAL:O	1:I:210:LYS:HB2	2.17	0.44
1:B:57:PHE:HE2	1:B:207:VAL:HG12	1.83	0.44
1:F:193:GLY:C	1:F:194:ILE:HG23	2.39	0.44
1:I:98:PRO:HA	1:I:137:LYS:NZ	2.33	0.44
1:C:53:TYR:O	1:C:54:ALA:C	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:273:THR:OG1	1:D:275:LYS:N	2.50	0.43
1:C:173:TYR:CD2	1:C:178:MET:HE1	2.53	0.43
1:E:122:SER:HB2	1:E:123:PRO:HD2	2.00	0.43
1:G:105:VAL:HG13	1:G:107:PHE:CE1	2.52	0.43
1:J:282:GLU:OE2	1:J:283:PRO:HD2	2.17	0.43
1:E:57:PHE:O	1:E:61:MET:HG3	2.18	0.43
1:C:181:TYR:CD1	1:C:181:TYR:N	2.86	0.43
1:I:148:LEU:HD12	1:I:174:GLU:OE2	2.17	0.43
1:J:242:ASP:OD2	1:J:242:ASP:C	2.56	0.43
1:C:295:VAL:CG1	1:C:300:MET:HG3	2.48	0.43
1:J:244:TYR:HE2	1:J:252:GLU:HG2	1.83	0.43
1:C:272:THR:O	1:C:272:THR:CG2	2.64	0.43
1:J:231:HIS:ND1	1:J:232:PRO:N	2.65	0.43
1:G:119:TYR:O	1:G:121:ASN:N	2.49	0.43
1:H:132:VAL:O	1:H:132:VAL:CG2	2.56	0.43
1:B:148:LEU:C	1:B:149:HIS:CG	2.91	0.43
1:C:250:GLU:HB2	1:C:266:LEU:HD13	2.00	0.43
1:I:171:TYR:OH	1:I:180:SER:OG	2.30	0.43
1:H:68:ALA:O	1:H:69:ARG:C	2.56	0.43
1:J:166:VAL:HG12	1:J:167:LEU:N	2.33	0.43
1:J:207:VAL:O	1:J:210:LYS:HG3	2.17	0.43
1:J:279:LEU:HD22	1:J:292:VAL:HG11	1.99	0.43
1:A:253:LYS:HD3	1:C:95:ARG:NH2	2.34	0.43
1:B:79:GLU:O	1:B:80:THR:C	2.57	0.43
1:B:250:GLU:C	1:B:252:GLU:H	2.22	0.43
1:J:300:MET:N	1:J:301:LEU:HB3	2.33	0.43
1:A:135:TRP:CD2	1:A:144:VAL:HB	2.53	0.43
1:I:186:MET:SD	1:I:191:PHE:HB2	2.58	0.43
1:C:238:ILE:O	1:C:238:ILE:HG22	2.18	0.43
1:I:81:ALA:HA	1:I:112:PHE:CE2	2.54	0.43
1:H:131:PHE:CD1	1:H:133:PRO:HD3	2.53	0.43
1:F:148:LEU:HD12	1:F:174:GLU:CD	2.39	0.43
1:H:178:MET:CE	1:H:198:ASP:OD1	2.66	0.43
1:H:265:HIS:HA	1:H:279:LEU:O	2.18	0.43
1:C:273:THR:C	1:C:275:LYS:H	2.21	0.43
1:J:40:LYS:CG	1:J:41:LEU:H	2.32	0.43
1:B:201:LEU:HA	1:B:201:LEU:HD23	1.65	0.43
1:G:40:LYS:H	1:G:41:LEU:HB3	1.81	0.43
1:G:218:TYR:CE1	1:G:294:VAL:HG11	2.54	0.43
1:F:105:VAL:HG13	1:F:107:PHE:CE1	2.54	0.43
1:A:222:VAL:HG22	1:A:226:GLY:CA	2.47	0.43
1:J:298:GLU:C	1:J:301:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:119:TYR:O	1:E:120:THR:C	2.57	0.43
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.57	0.43
1:I:86:ALA:CB	1:I:131:PHE:CE2	3.01	0.43
1:I:149:HIS:O	1:I:151:ASP:N	2.51	0.43
1:G:214:PHE:CE1	1:G:295:VAL:CG1	3.02	0.43
1:C:158:LEU:HB2	1:C:159:PRO:CD	2.49	0.43
1:F:167:LEU:HD11	1:F:179:VAL:HG13	1.99	0.43
1:I:88:LEU:HA	1:I:88:LEU:HD23	1.76	0.43
1:J:131:PHE:CD1	1:J:133:PRO:HD3	2.53	0.43
1:B:258:ILE:HG13	1:B:259:LYS:N	2.33	0.43
1:B:156:TYR:C	1:B:159:PRO:HD2	2.38	0.43
1:B:61:MET:HE1	1:B:284:VAL:HG11	2.00	0.43
1:D:307:LEU:O	1:D:308:ARG:C	2.56	0.43
1:B:139:ASN:C	1:B:141:THR:H	2.21	0.43
1:D:68:ALA:O	1:D:69:ARG:C	2.57	0.43
1:D:41:LEU:C	1:D:43:TYR:N	2.54	0.43
1:F:39:GLU:CA	1:F:40:LYS:CB	2.46	0.43
1:C:276:THR:O	1:C:297:LYS:HB3	2.19	0.43
1:H:250:GLU:HB3	1:H:266:LEU:HD11	1.99	0.43
1:J:177:PHE:HZ	1:J:240:LYS:HD2	1.80	0.43
1:C:208:VAL:HG11	1:C:230:SER:OG	2.18	0.43
1:C:170:PRO:HG2	1:C:227:VAL:HG11	2.00	0.43
1:I:148:LEU:O	1:I:149:HIS:HB2	2.19	0.43
1:H:110:ASP:OD1	1:H:114:GLY:HA2	2.19	0.43
1:A:212:ARG:HG3	1:A:217:GLY:O	2.18	0.43
1:D:296:PRO:O	1:D:299:GLU:HB2	2.19	0.43
1:C:130:ARG:HH21	1:C:150:TYR:HE1	1.66	0.43
1:I:83:ARG:HH12	1:I:125:HIS:CD2	2.36	0.43
1:D:79:GLU:C	1:D:81:ALA:H	2.21	0.43
1:H:75:MET:CE	1:H:105:VAL:HG21	2.48	0.43
1:B:110:ASP:N	1:B:116:ASP:OD2	2.49	0.43
1:G:253:LYS:HB3	1:I:95:ARG:NH1	2.32	0.43
1:I:169:GLU:HB3	1:I:170:PRO:HD2	2.01	0.43
1:D:148:LEU:HD12	1:D:148:LEU:HA	1.73	0.43
1:C:216:THR:OG1	1:C:299:GLU:OE2	2.26	0.43
1:A:171:TYR:CE2	1:A:173:TYR:HB2	2.53	0.43
1:B:249:GLU:HB2	1:B:250:GLU:OE2	2.18	0.43
1:G:77:SER:HB3	1:H:88:LEU:HB3	2.01	0.43
1:J:122:SER:CB	1:J:123:PRO:CD	2.91	0.43
1:B:151:ASP:O	1:B:152:SER:HB3	2.18	0.43
1:A:169:GLU:OE2	1:A:170:PRO:HD2	2.18	0.43
1:F:173:TYR:O	1:F:174:GLU:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:103:THR:C	1:H:104:TYR:CD2	2.93	0.43
1:C:132:VAL:N	1:C:133:PRO:HD3	2.34	0.42
1:E:245:ASP:C	1:E:247:GLY:H	2.23	0.42
1:B:101:LEU:HD22	1:B:101:LEU:C	2.40	0.42
1:D:218:TYR:N	1:D:218:TYR:CD1	2.86	0.42
1:B:227:VAL:HA	1:B:242:ASP:HB3	2.01	0.42
1:B:94:LEU:HD13	1:B:137:LYS:HE3	2.01	0.42
1:A:206:GLU:O	1:A:210:LYS:HG2	2.19	0.42
1:I:101:LEU:HD23	1:I:101:LEU:HA	1.78	0.42
1:C:91:GLU:HG3	1:C:135:TRP:CE3	2.53	0.42
1:C:278:ILE:HG21	1:C:280:PHE:CE1	2.53	0.42
1:C:112:PHE:CD2	1:C:131:PHE:HD2	2.36	0.42
1:E:216:THR:OG1	1:E:299:GLU:OE2	2.36	0.42
1:F:120:THR:HG23	1:F:120:THR:O	2.19	0.42
1:A:78:TYR:CE2	1:A:81:ALA:N	2.87	0.42
1:H:41:LEU:HA	1:H:41:LEU:HD23	1.80	0.42
1:C:295:VAL:HA	1:C:296:PRO:HD3	1.79	0.42
1:C:153:SER:HB3	1:C:155:TYR:CD1	2.54	0.42
1:I:109:PRO:CA	1:I:130:ARG:HD3	2.49	0.42
1:A:104:TYR:HH	1:A:180:SER:HB3	1.84	0.42
1:J:234:HIS:O	1:J:235:LYS:C	2.57	0.42
1:B:72:SER:O	1:B:73:THR:C	2.57	0.42
1:G:245:ASP:O	1:G:247:GLY:CA	2.68	0.42
1:H:295:VAL:HA	1:H:296:PRO:HD3	1.83	0.42
1:C:246:PHE:HB2	1:C:251:LEU:HD13	2.01	0.42
1:E:240:LYS:HE2	1:E:240:LYS:CA	2.50	0.42
1:C:296:PRO:HB2	1:C:299:GLU:HG3	2.01	0.42
1:A:218:TYR:HD2	1:A:232:PRO:CG	2.32	0.42
1:A:231:HIS:HA	1:A:232:PRO:HD3	1.89	0.42
1:C:160:LYS:HG3	1:C:191:PHE:CD2	2.53	0.42
1:E:245:ASP:C	1:E:247:GLY:N	2.73	0.42
1:E:248:GLY:N	1:E:251:LEU:HD12	2.34	0.42
1:D:107:PHE:HB3	1:D:111:ALA:HB3	2.00	0.42
1:I:112:PHE:CE1	1:I:131:PHE:CD2	3.07	0.42
1:A:227:VAL:CG1	1:A:228:ILE:N	2.82	0.42
1:J:169:GLU:OE2	1:J:223:SER:OG	2.24	0.42
1:A:212:ARG:HB2	1:A:212:ARG:HE	1.53	0.42
1:G:171:TYR:N	1:G:171:TYR:CD1	2.88	0.42
1:D:167:LEU:HD13	1:D:181:TYR:CD2	2.54	0.42
1:D:298:GLU:CG	1:D:299:GLU:HB2	2.48	0.42
1:G:97:ASN:HB2	1:G:100:LEU:HD12	2.01	0.42
1:C:105:VAL:CG1	1:C:107:PHE:CE1	3.03	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:268:THR:OG1	1:I:269:ALA:N	2.53	0.42
1:F:104:TYR:HE1	1:F:198:ASP:OD2	2.02	0.42
1:A:172:PHE:CE1	1:A:175:GLY:O	2.72	0.42
1:C:90:LEU:HD13	1:C:104:TYR:HA	2.02	0.42
1:H:120:THR:O	1:H:120:THR:HG23	2.19	0.42
1:E:203:TYR:CE2	1:E:207:VAL:HG21	2.55	0.42
1:I:65:LEU:HG	1:I:69:ARG:HD2	2.02	0.42
1:I:130:ARG:NH2	1:I:150:TYR:CD1	2.88	0.42
1:J:104:TYR:N	1:J:104:TYR:CD2	2.87	0.42
1:B:213:THR:HG22	1:B:217:GLY:HA3	2.02	0.42
1:E:240:LYS:HA	1:E:240:LYS:CE	2.48	0.42
1:G:273:THR:OG1	1:G:275:LYS:CD	2.67	0.42
1:B:201:LEU:HD21	1:B:229:LEU:HD22	2.01	0.42
1:A:246:PHE:CD1	1:A:251:LEU:HD11	2.55	0.42
1:E:165:ASP:C	1:E:166:VAL:CG2	2.88	0.42
1:E:79:GLU:HB2	1:F:85:GLU:OE1	2.19	0.42
1:G:105:VAL:CG1	1:G:107:PHE:HE1	2.33	0.42
1:H:241:LYS:HD2	1:H:245:ASP:OD2	2.20	0.42
1:H:93:LEU:O	1:H:94:LEU:C	2.57	0.42
1:B:273:THR:HB	1:B:274:GLY:H	1.77	0.42
1:E:158:LEU:HA	1:E:158:LEU:HD23	1.35	0.42
1:I:139:ASN:N	1:I:139:ASN:OD1	2.52	0.42
1:I:241:LYS:HD3	1:I:241:LYS:HA	1.89	0.42
1:H:218:TYR:CD2	1:H:232:PRO:CG	3.03	0.42
1:B:306:ASP:C	1:B:308:ARG:N	2.72	0.42
1:J:40:LYS:O	1:J:43:TYR:N	2.46	0.42
1:A:222:VAL:CG2	1:A:227:VAL:O	2.66	0.42
1:I:115:LYS:O	1:I:116:ASP:C	2.57	0.42
1:J:86:ALA:O	1:J:89:ILE:HB	2.20	0.42
1:B:88:LEU:HA	1:B:88:LEU:HD23	1.68	0.42
1:B:245:ASP:N	1:B:245:ASP:OD2	2.52	0.42
1:E:201:LEU:HD23	1:E:201:LEU:HA	1.61	0.42
1:E:40:LYS:O	1:E:40:LYS:CD	2.67	0.42
1:H:233:THR:OG1	1:H:234:HIS:HD2	2.02	0.42
1:H:119:TYR:HB3	1:H:125:HIS:CD2	2.55	0.42
1:C:119:TYR:O	1:C:120:THR:C	2.58	0.42
1:G:89:ILE:CD1	1:H:74:THR:HG23	2.42	0.42
1:C:88:LEU:HD13	1:D:77:SER:HB3	2.02	0.42
1:F:305:ALA:O	1:F:308:ARG:HB3	2.20	0.42
1:I:130:ARG:NH2	1:I:150:TYR:HD1	2.17	0.42
1:G:128:THR:C	1:G:130:ARG:N	2.72	0.42
1:G:131:PHE:CD1	1:G:133:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:80:THR:O	1:I:82:ASP:N	2.53	0.42
1:E:171:TYR:CD1	1:E:171:TYR:N	2.88	0.42
1:D:251:LEU:HD23	1:D:266:LEU:HD12	2.01	0.41
1:C:231:HIS:ND1	1:C:232:PRO:N	2.68	0.41
1:E:130:ARG:O	1:E:132:VAL:HG13	2.20	0.41
1:H:75:MET:HE3	1:H:105:VAL:HG21	2.02	0.41
1:G:214:PHE:CE1	1:G:295:VAL:HG13	2.55	0.41
1:A:104:TYR:CD2	1:A:104:TYR:N	2.87	0.41
1:H:53:TYR:O	1:H:54:ALA:C	2.58	0.41
1:F:243:LEU:HA	1:F:243:LEU:HD23	1.82	0.41
1:E:285:GLU:O	1:E:285:GLU:HG2	2.19	0.41
1:E:156:TYR:CD2	1:E:156:TYR:C	2.93	0.41
1:J:298:GLU:N	1:J:301:LEU:CD2	2.70	0.41
1:B:156:TYR:O	1:B:159:PRO:HD2	2.21	0.41
1:H:42:ALA:C	1:H:300:MET:HE2	2.40	0.41
1:F:115:LYS:O	1:F:116:ASP:C	2.58	0.41
1:B:234:HIS:HB3	1:B:237:TRP:CD1	2.55	0.41
1:J:135:TRP:CE2	1:J:144:VAL:HB	2.56	0.41
1:E:276:THR:O	1:E:297:LYS:HB2	2.19	0.41
1:A:231:HIS:CG	1:A:232:PRO:CD	3.03	0.41
1:H:278:ILE:HD12	1:H:300:MET:SD	2.60	0.41
1:J:141:THR:O	1:J:141:THR:HG23	2.19	0.41
1:H:296:PRO:O	1:H:297:LYS:C	2.57	0.41
1:I:83:ARG:HG2	1:I:112:PHE:HE1	1.85	0.41
1:G:97:ASN:HA	1:G:98:PRO:HD2	1.69	0.41
1:I:168:THR:CG2	1:I:180:SER:HB2	2.50	0.41
1:B:131:PHE:C	1:B:132:VAL:HG13	2.40	0.41
1:G:104:TYR:N	1:G:104:TYR:CD2	2.88	0.41
1:E:123:PRO:O	1:E:124:ALA:CB	2.68	0.41
1:J:104:TYR:CE2	1:J:198:ASP:OD2	2.73	0.41
1:D:83:ARG:HG2	1:D:112:PHE:CE1	2.54	0.41
1:I:293:LEU:HD23	1:I:294:VAL:N	2.35	0.41
1:G:262:ILE:HD13	1:I:98:PRO:HG3	2.02	0.41
1:A:158:LEU:HA	1:A:158:LEU:HD23	1.80	0.41
1:B:249:GLU:C	1:B:251:LEU:H	2.18	0.41
1:D:123:PRO:O	1:D:124:ALA:HB3	2.20	0.41
1:H:138:MET:HB3	1:H:138:MET:HE3	1.83	0.41
1:D:171:TYR:OH	1:D:178:MET:HE3	2.20	0.41
1:G:108:GLU:O	1:G:111:ALA:CB	2.67	0.41
1:G:258:ILE:HG21	1:G:258:ILE:HD13	1.62	0.41
1:D:135:TRP:NE1	1:D:144:VAL:CG2	2.84	0.41
1:D:91:GLU:HB2	1:D:135:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:268:THR:HG23	1:B:269:ALA:N	2.35	0.41
1:G:154:ASP:O	1:G:155:TYR:C	2.58	0.41
1:H:97:ASN:HB2	1:H:100:LEU:HD12	2.03	0.41
1:E:156:TYR:CD2	1:E:156:TYR:O	2.73	0.41
1:E:104:TYR:OH	1:E:180:SER:HB3	2.20	0.41
1:D:244:TYR:CE2	1:D:252:GLU:HG2	2.55	0.41
1:A:298:GLU:O	1:A:299:GLU:C	2.59	0.41
1:A:244:TYR:CD2	1:A:252:GLU:CG	3.03	0.41
1:H:80:THR:O	1:H:81:ALA:C	2.57	0.41
1:C:250:GLU:HG2	1:C:251:LEU:N	2.35	0.41
1:G:106:ALA:O	1:G:193:GLY:HA3	2.21	0.41
1:A:122:SER:CB	1:A:123:PRO:HD2	2.50	0.41
1:E:101:LEU:CD1	1:E:178:MET:HE2	2.51	0.41
1:F:135:TRP:CE2	1:F:144:VAL:HB	2.55	0.41
1:C:122:SER:HA	1:C:123:PRO:HA	1.81	0.41
1:J:278:ILE:CD1	1:J:297:LYS:HD3	2.51	0.41
1:B:61:MET:HE2	1:B:284:VAL:HG11	2.01	0.41
1:A:112:PHE:CD1	1:A:131:PHE:CD2	3.09	0.41
1:I:237:TRP:O	1:I:238:ILE:C	2.57	0.41
1:A:101:LEU:O	1:A:101:LEU:CD2	2.67	0.41
1:C:223:SER:O	1:C:258:ILE:HD11	2.20	0.41
1:G:177:PHE:CE2	1:G:239:GLY:O	2.74	0.41
1:J:126:ASP:OD2	1:J:126:ASP:N	2.54	0.41
1:J:132:VAL:O	1:J:132:VAL:HG23	2.21	0.41
1:F:201:LEU:HD23	1:F:201:LEU:HA	1.65	0.41
1:H:132:VAL:N	1:H:133:PRO:CD	2.84	0.41
1:A:153:SER:HB3	1:A:155:TYR:CD1	2.56	0.41
1:D:231:HIS:NE2	1:D:237:TRP:HZ3	2.19	0.41
1:D:222:VAL:HG22	1:D:227:VAL:O	2.21	0.41
1:C:256:ARG:HG3	1:C:256:ARG:NH1	2.35	0.41
1:J:49:MET:HE2	1:J:53:TYR:HE1	1.85	0.41
1:C:270:ASP:HA	1:C:274:GLY:N	2.36	0.41
1:D:272:THR:CG2	1:D:273:THR:N	2.83	0.41
1:H:251:LEU:HD23	1:H:266:LEU:HD12	2.03	0.41
1:C:130:ARG:C	1:C:132:VAL:HG13	2.41	0.41
1:J:79:GLU:O	1:J:80:THR:C	2.58	0.41
1:D:231:HIS:CD2	1:D:237:TRP:CE3	3.09	0.41
1:H:298:GLU:HA	1:H:301:LEU:HB2	2.02	0.41
1:I:135:TRP:HZ3	1:I:142:ALA:O	2.03	0.41
1:F:103:THR:O	1:F:104:TYR:HB3	2.20	0.41
1:G:101:LEU:C	1:G:101:LEU:HD23	2.42	0.41
1:A:272:THR:C	1:A:273:THR:HG22	2.40	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:213:THR:HG22	1:B:217:GLY:C	2.41	0.41
1:A:167:LEU:HD11	1:A:179:VAL:CG1	2.50	0.41
1:H:172:PHE:CD1	1:H:177:PHE:CE2	3.08	0.41
1:E:268:THR:HG23	1:E:269:ALA:N	2.35	0.41
1:G:108:GLU:O	1:G:109:PRO:C	2.58	0.41
1:J:214:PHE:CE2	1:J:299:GLU:O	2.74	0.41
1:D:135:TRP:HZ3	1:D:142:ALA:O	2.04	0.41
1:J:81:ALA:HB1	1:J:113:ASP:HB3	2.02	0.41
1:G:222:VAL:HG22	1:G:227:VAL:O	2.21	0.41
1:C:240:LYS:HE2	1:C:240:LYS:CA	2.47	0.41
1:D:97:ASN:HA	1:D:98:PRO:HD2	1.84	0.41
1:C:63:ALA:O	1:C:66:ALA:HB3	2.20	0.41
1:I:172:PHE:O	1:I:172:PHE:CG	2.74	0.41
1:A:308:ARG:HA	1:A:308:ARG:HD3	1.60	0.40
1:B:40:LYS:O	1:B:41:LEU:HG	2.20	0.40
1:I:75:MET:N	1:I:75:MET:HE3	2.36	0.40
1:B:158:LEU:CB	1:B:159:PRO:HD3	2.51	0.40
1:C:106:ALA:HB2	1:C:147:LEU:HD12	2.03	0.40
1:D:231:HIS:ND1	1:D:232:PRO:CD	2.84	0.40
1:J:222:VAL:HG12	1:J:290:ALA:HB3	2.03	0.40
1:F:119:TYR:O	1:F:120:THR:C	2.60	0.40
1:H:222:VAL:CG1	1:H:290:ALA:HB3	2.51	0.40
1:G:128:THR:O	1:G:130:ARG:N	2.53	0.40
1:I:236:ASP:O	1:I:240:LYS:HG2	2.21	0.40
1:A:235:LYS:H	1:A:235:LYS:HG2	1.53	0.40
1:C:91:GLU:CD	1:C:135:TRP:CZ2	2.94	0.40
1:J:249:GLU:O	1:J:249:GLU:OE2	2.39	0.40
1:E:241:LYS:HD2	1:E:245:ASP:OD2	2.21	0.40
1:H:173:TYR:O	1:H:175:GLY:N	2.54	0.40
1:A:132:VAL:N	1:A:133:PRO:CD	2.85	0.40
1:I:185:ILE:HD11	1:I:194:ILE:C	2.42	0.40
1:G:112:PHE:CD1	1:G:131:PHE:CD2	3.10	0.40
1:G:153:SER:HB2	1:G:155:TYR:CD2	2.56	0.40
1:I:82:ASP:OD1	1:I:82:ASP:C	2.58	0.40
1:D:47:VAL:HG23	1:D:280:PHE:HE2	1.85	0.40
1:C:184:PRO:HB2	1:C:186:MET:CE	2.51	0.40
1:F:222:VAL:HG23	1:F:227:VAL:O	2.21	0.40
1:C:201:LEU:CD2	1:C:229:LEU:HD22	2.52	0.40
1:D:128:THR:O	1:D:129:GLY:C	2.59	0.40
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.81	0.40
1:B:303:GLY:O	1:B:306:ASP:HB2	2.21	0.40
1:F:278:ILE:HD11	1:F:297:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:113:ASP:C	1:J:115:LYS:H	2.24	0.40
1:F:218:TYR:O	1:F:293:LEU:HD23	2.21	0.40
1:B:211:VAL:HG12	1:B:212:ARG:N	2.35	0.40
1:J:207:VAL:O	1:J:210:LYS:HG2	2.21	0.40
1:D:154:ASP:O	1:D:155:TYR:C	2.60	0.40
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.73	0.40
1:I:126:ASP:O	1:I:127:GLY:C	2.59	0.40
1:G:167:LEU:HD11	1:G:179:VAL:HG13	2.02	0.40
1:A:76:GLU:HG2	1:A:186:MET:O	2.21	0.40
1:H:63:ALA:O	1:H:66:ALA:HB3	2.21	0.40
1:D:302:ALA:CB	1:D:303:GLY:CA	2.98	0.40
1:H:123:PRO:O	1:H:124:ALA:CB	2.70	0.40
1:I:138:MET:HB3	1:I:138:MET:HE3	1.80	0.40
1:C:134:TYR:CE1	1:C:173:TYR:HE2	2.40	0.40
1:I:86:ALA:HB3	1:I:131:PHE:CZ	2.57	0.40
1:F:193:GLY:O	1:F:194:ILE:CG2	2.68	0.40
1:H:172:PHE:HD1	1:H:177:PHE:CD2	2.38	0.40
1:A:177:PHE:HB3	1:A:201:LEU:CD1	2.52	0.40
1:A:73:THR:CG2	1:B:93:LEU:HD23	2.52	0.40
1:E:101:LEU:HG	1:E:200:SER:HB3	2.04	0.40
1:G:169:GLU:OE2	1:G:225:SER:OG	2.38	0.40
1:F:282:GLU:HA	1:F:283:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/290 (93%)	230 (86%)	29 (11%)	10 (4%)	5	28
1	B	269/290 (93%)	209 (78%)	46 (17%)	14 (5%)	3	18
1	C	266/290 (92%)	221 (83%)	33 (12%)	12 (4%)	4	22
1	D	269/290 (93%)	224 (83%)	34 (13%)	11 (4%)	4	24
1	E	266/290 (92%)	221 (83%)	34 (13%)	11 (4%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	269/290 (93%)	231 (86%)	30 (11%)	8 (3%)	7	34
1	G	268/290 (92%)	225 (84%)	28 (10%)	15 (6%)	3	16
1	H	265/290 (91%)	219 (83%)	37 (14%)	9 (3%)	6	31
1	I	269/290 (93%)	217 (81%)	38 (14%)	14 (5%)	3	18
1	J	269/290 (93%)	222 (82%)	32 (12%)	15 (6%)	3	16
All	All	2679/2900 (92%)	2219 (83%)	341 (13%)	119 (4%)	4	22

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	299	GLU
1	B	120	THR
1	B	149	HIS
1	B	188	GLU
1	B	250	GLU
1	C	120	THR
1	C	121	ASN
1	C	248	GLY
1	C	270	ASP
1	C	273	THR
1	D	42	ALA
1	D	81	ALA
1	D	120	THR
1	D	121	ASN
1	D	302	ALA
1	E	43	TYR
1	E	44	GLN
1	E	248	GLY
1	F	43	TYR
1	F	44	GLN
1	G	81	ALA
1	G	121	ASN
1	G	246	PHE
1	G	272	THR
1	G	273	THR
1	H	152	SER
1	H	248	GLY
1	I	81	ALA
1	I	248	GLY

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Mol	Chain	Res	Type
1	I	307	LEU
1	J	41	LEU
1	J	152	SER
1	J	246	PHE
1	J	272	THR
1	J	301	LEU
1	A	140	GLY
1	A	155	TYR
1	A	306	ASP
1	B	41	LEU
1	B	127	GLY
1	B	152	SER
1	B	249	GLU
1	C	80	THR
1	C	127	GLY
1	C	140	GLY
1	C	188	GLU
1	D	140	GLY
1	D	152	SER
1	E	42	ALA
1	E	80	THR
1	E	140	GLY
1	F	140	GLY
1	F	248	GLY
1	G	44	GLN
1	G	140	GLY
1	G	271	PRO
1	G	307	LEU
1	H	127	GLY
1	H	140	GLY
1	H	238	ILE
1	I	120	THR
1	I	188	GLU
1	I	245	ASP
1	J	114	GLY
1	J	140	GLY
1	J	271	PRO
1	J	273	THR
1	A	40	LYS
1	A	243	LEU
1	B	128	THR
1	B	189	GLY

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Mol	Chain	Res	Type
1	D	188	GLU
1	D	299	GLU
1	F	40	LYS
1	F	120	THR
1	F	124	ALA
1	G	188	GLU
1	G	274	GLY
1	H	120	THR
1	I	121	ASN
1	I	149	HIS
1	I	150	TYR
1	J	120	THR
1	J	211	VAL
1	J	250	GLU
1	J	306	ASP
1	B	254	ALA
1	B	288	ASP
1	D	41	LEU
1	E	120	THR
1	E	274	GLY
1	E	289	PHE
1	F	188	GLU
1	G	46	SER
1	G	80	THR
1	I	127	GLY
1	I	268	THR
1	J	274	GLY
1	A	152	SER
1	B	121	ASN
1	C	122	SER
1	C	217	GLY
1	H	137	LYS
1	I	80	THR
1	B	40	LYS
1	E	40	LYS
1	G	51	SER
1	I	140	GLY
1	I	254	ALA
1	J	155	TYR
1	A	271	PRO
1	G	175	GLY
1	H	109	PRO

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Mol	Chain	Res	Type
1	D	129	GLY
1	C	238	ILE
1	A	109	PRO
1	E	89	ILE
1	H	122	SER

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	227/246 (92%)	197 (87%)	30 (13%)	6	25
1	B	227/246 (92%)	194 (86%)	33 (14%)	5	22
1	C	223/246 (91%)	187 (84%)	36 (16%)	3	17
1	D	227/246 (92%)	194 (86%)	33 (14%)	5	22
1	E	224/246 (91%)	193 (86%)	31 (14%)	5	24
1	F	227/246 (92%)	202 (89%)	25 (11%)	9	34
1	G	226/246 (92%)	192 (85%)	34 (15%)	4	20
1	H	223/246 (91%)	189 (85%)	34 (15%)	4	20
1	I	227/246 (92%)	198 (87%)	29 (13%)	6	27
1	J	227/246 (92%)	195 (86%)	32 (14%)	5	23
All	All	2258/2460 (92%)	1941 (86%)	317 (14%)	5	23

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	LEU
1	A	60	ASP
1	A	88	LEU
1	A	94	LEU
1	A	101	LEU
1	A	105	VAL
1	A	138	MET
1	A	139	ASN

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Mol	Chain	Res	Type
1	A	144	VAL
1	A	150	TYR
1	A	153	SER
1	A	171	TYR
1	A	176	VAL
1	A	179	VAL
1	A	202	GLU
1	A	207	VAL
1	A	212	ARG
1	A	216	THR
1	A	218	TYR
1	A	221	MET
1	A	236	ASP
1	A	246	PHE
1	A	258	ILE
1	A	268	THR
1	A	272	THR
1	A	273	THR
1	A	275	LYS
1	A	293	LEU
1	A	308	ARG
1	B	39	GLU
1	B	40	LYS
1	B	41	LEU
1	B	49	MET
1	B	74	THR
1	B	88	LEU
1	B	101	LEU
1	B	105	VAL
1	B	118	GLU
1	B	122	SER
1	B	128	THR
1	B	150	TYR
1	B	154	ASP
1	B	157	GLN
1	B	176	VAL
1	B	179	VAL
1	B	182	VAL
1	B	185	ILE
1	B	191	PHE
1	B	210	LYS
1	B	212	ARG

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Mol	Chain	Res	Type
1	B	234	HIS
1	B	236	ASP
1	B	240	LYS
1	B	245	ASP
1	B	256	ARG
1	B	258	ILE
1	B	266	LEU
1	B	268	THR
1	B	273	THR
1	B	276	THR
1	B	300	MET
1	B	307	LEU
1	C	39	GLU
1	C	44	GLN
1	C	45	GLN
1	C	61	MET
1	C	65	LEU
1	C	88	LEU
1	C	94	LEU
1	C	101	LEU
1	C	121	ASN
1	C	132	VAL
1	C	136	ASN
1	C	138	MET
1	C	139	ASN
1	C	151	ASP
1	C	153	SER
1	C	171	TYR
1	C	174	GLU
1	C	179	VAL
1	C	181	TYR
1	C	183	SER
1	C	190	GLU
1	C	212	ARG
1	C	213	THR
1	C	228	ILE
1	C	236	ASP
1	C	240	LYS
1	C	256	ARG
1	C	258	ILE
1	C	267	GLU
1	C	273	THR

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Mol	Chain	Res	Type
1	C	275	LYS
1	C	276	THR
1	C	277	VAL
1	C	295	VAL
1	C	300	MET
1	C	306	ASP
1	D	39	GLU
1	D	41	LEU
1	D	44	GLN
1	D	51	SER
1	D	52	ASN
1	D	88	LEU
1	D	94	LEU
1	D	101	LEU
1	D	136	ASN
1	D	141	THR
1	D	148	LEU
1	D	150	TYR
1	D	153	SER
1	D	154	ASP
1	D	163	GLU
1	D	176	VAL
1	D	179	VAL
1	D	180	SER
1	D	202	GLU
1	D	210	LYS
1	D	212	ARG
1	D	218	TYR
1	D	221	MET
1	D	222	VAL
1	D	249	GLU
1	D	250	GLU
1	D	251	LEU
1	D	258	ILE
1	D	272	THR
1	D	273	THR
1	D	275	LYS
1	D	308	ARG
1	D	309	GLU
1	E	39	GLU
1	E	77	SER
1	E	80	THR

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Mol	Chain	Res	Type
1	E	83	ARG
1	E	88	LEU
1	E	94	LEU
1	E	101	LEU
1	E	105	VAL
1	E	120	THR
1	E	122	SER
1	E	132	VAL
1	E	152	SER
1	E	174	GLU
1	E	176	VAL
1	E	179	VAL
1	E	185	ILE
1	E	216	THR
1	E	221	MET
1	E	230	SER
1	E	236	ASP
1	E	240	LYS
1	E	256	ARG
1	E	258	ILE
1	E	266	LEU
1	E	268	THR
1	E	275	LYS
1	E	278	ILE
1	E	286	THR
1	E	293	LEU
1	E	298	GLU
1	E	301	LEU
1	F	41	LEU
1	F	46	SER
1	F	60	ASP
1	F	77	SER
1	F	85	GLU
1	F	88	LEU
1	F	94	LEU
1	F	95	ARG
1	F	101	LEU
1	F	105	VAL
1	F	138	MET
1	F	152	SER
1	F	179	VAL
1	F	212	ARG

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Mol	Chain	Res	Type
1	F	221	MET
1	F	240	LYS
1	F	250	GLU
1	F	258	ILE
1	F	266	LEU
1	F	268	THR
1	F	275	LYS
1	F	286	THR
1	F	293	LEU
1	F	304	VAL
1	F	308	ARG
1	G	39	GLU
1	G	41	LEU
1	G	46	SER
1	G	51	SER
1	G	52	ASN
1	G	88	LEU
1	G	94	LEU
1	G	101	LEU
1	G	120	THR
1	G	122	SER
1	G	130	ARG
1	G	136	ASN
1	G	144	VAL
1	G	153	SER
1	G	154	ASP
1	G	171	TYR
1	G	179	VAL
1	G	180	SER
1	G	185	ILE
1	G	201	LEU
1	G	206	GLU
1	G	210	LYS
1	G	212	ARG
1	G	213	THR
1	G	221	MET
1	G	222	VAL
1	G	236	ASP
1	G	246	PHE
1	G	251	LEU
1	G	258	ILE
1	G	266	LEU

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Mol	Chain	Res	Type
1	G	273	THR
1	G	275	LYS
1	G	293	LEU
1	H	39	GLU
1	H	44	GLN
1	H	45	GLN
1	H	61	MET
1	H	83	ARG
1	H	88	LEU
1	H	94	LEU
1	H	101	LEU
1	H	109	PRO
1	H	120	THR
1	H	122	SER
1	H	125	HIS
1	H	132	VAL
1	H	139	ASN
1	H	174	GLU
1	H	179	VAL
1	H	182	VAL
1	H	185	ILE
1	H	188	GLU
1	H	208	VAL
1	H	210	LYS
1	H	216	THR
1	H	221	MET
1	H	222	VAL
1	H	225	SER
1	H	240	LYS
1	H	258	ILE
1	H	268	THR
1	H	273	THR
1	H	275	LYS
1	H	276	THR
1	H	277	VAL
1	H	295	VAL
1	H	301	LEU
1	I	39	GLU
1	I	88	LEU
1	I	101	LEU
1	I	105	VAL
1	I	121	ASN

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Mol	Chain	Res	Type
1	I	138	MET
1	I	139	ASN
1	I	141	THR
1	I	150	TYR
1	I	153	SER
1	I	154	ASP
1	I	167	LEU
1	I	168	THR
1	I	174	GLU
1	I	176	VAL
1	I	185	ILE
1	I	191	PHE
1	I	210	LYS
1	I	236	ASP
1	I	245	ASP
1	I	253	LYS
1	I	258	ILE
1	I	266	LEU
1	I	268	THR
1	I	276	THR
1	I	298	GLU
1	I	306	ASP
1	I	308	ARG
1	I	309	GLU
1	J	39	GLU
1	J	41	LEU
1	J	62	LYS
1	J	79	GLU
1	J	88	LEU
1	J	101	LEU
1	J	120	THR
1	J	136	ASN
1	J	139	ASN
1	J	153	SER
1	J	167	LEU
1	J	171	TYR
1	J	179	VAL
1	J	212	ARG
1	J	216	THR
1	J	218	TYR
1	J	221	MET
1	J	222	VAL

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Mol	Chain	Res	Type
1	J	236	ASP
1	J	240	LYS
1	J	246	PHE
1	J	249	GLU
1	J	257	ASP
1	J	258	ILE
1	J	268	THR
1	J	272	THR
1	J	273	THR
1	J	275	LYS
1	J	293	LEU
1	J	300	MET
1	J	301	LEU
1	J	309	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	271/290 (93%)	0.40	6 (2%)	59	12	57, 74, 97, 127	0
1	B	271/290 (93%)	0.42	5 (1%)	65	14	62, 80, 102, 115	0
1	C	268/290 (92%)	0.38	10 (3%)	39	8	50, 70, 100, 113	0
1	D	271/290 (93%)	0.39	5 (1%)	65	14	20, 71, 97, 113	0
1	E	268/290 (92%)	0.39	6 (2%)	59	12	43, 66, 98, 119	0
1	F	271/290 (93%)	0.36	5 (1%)	65	14	42, 67, 96, 130	0
1	G	270/290 (93%)	0.41	7 (2%)	53	10	48, 71, 94, 107	0
1	H	267/290 (92%)	0.38	7 (2%)	53	10	51, 70, 97, 108	0
1	I	271/290 (93%)	0.41	12 (4%)	33	7	62, 80, 103, 113	0
1	J	271/290 (93%)	0.43	8 (2%)	48	9	58, 74, 97, 123	0
All	All	2699/2900 (93%)	0.40	71 (2%)	53	10	20, 73, 99, 130	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	305	ALA	5.2
1	I	251	LEU	3.9
1	A	293	LEU	3.4
1	E	246	PHE	3.1
1	C	240	LYS	3.1
1	B	147	LEU	3.0
1	G	57	PHE	3.0
1	I	140	GLY	2.8
1	F	57	PHE	2.8
1	C	40	LYS	2.7
1	D	293	LEU	2.7
1	E	52	ASN	2.7
1	I	124	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	243	LEU	2.7
1	B	189	GLY	2.6
1	B	173	TYR	2.6
1	H	41	LEU	2.6
1	G	268	THR	2.6
1	J	244	TYR	2.5
1	H	150	TYR	2.5
1	C	304	VAL	2.5
1	I	243	LEU	2.5
1	E	57	PHE	2.5
1	H	172	PHE	2.5
1	I	106	ALA	2.5
1	J	213	THR	2.5
1	D	217	GLY	2.5
1	H	215	ASP	2.4
1	F	172	PHE	2.4
1	C	155	TYR	2.4
1	I	173	TYR	2.4
1	D	121	ASN	2.4
1	J	214	PHE	2.4
1	D	57	PHE	2.4
1	A	258	ILE	2.4
1	B	258	ILE	2.4
1	F	48	GLU	2.3
1	E	306	ASP	2.3
1	G	293	LEU	2.3
1	B	156	TYR	2.2
1	I	258	ILE	2.2
1	G	241	LYS	2.2
1	E	290	ALA	2.2
1	A	243	LEU	2.2
1	G	214	PHE	2.2
1	G	294	VAL	2.2
1	D	192	ALA	2.2
1	C	266	LEU	2.2
1	I	246	PHE	2.2
1	A	44	GLN	2.2
1	C	293	LEU	2.1
1	I	166	VAL	2.1
1	A	214	PHE	2.1
1	I	87	LEU	2.1
1	H	244	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	253	LYS	2.1
1	I	147	LEU	2.1
1	I	148	LEU	2.1
1	J	241	LYS	2.1
1	C	246	PHE	2.1
1	J	140	GLY	2.1
1	G	278	ILE	2.1
1	E	150	TYR	2.1
1	C	301	LEU	2.1
1	H	293	LEU	2.1
1	J	258	ILE	2.0
1	J	251	LEU	2.0
1	A	123	PRO	2.0
1	F	118	GLU	2.0
1	C	214	PHE	2.0
1	C	150	TYR	2.0

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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	K	J	2	1/1	0.40	97.50	85,85,85,85	0
2	K	H	7	1/1	0.42	23.19	119,119,119,119	0
2	K	A	1	1/1	0.36	15.00	91,91,91,91	0
2	K	F	8	1/1	0.40	9.63	107,107,107,107	0
2	K	G	4	1/1	0.41	6.67	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	K	C	3	1/1	0.41	6.57	112,112,112,112	0
2	K	E	6	1/1	0.27	2.57	104,104,104,104	0
2	K	I	9	1/1	0.35	2.19	113,113,113,113	0
2	K	B	10	1/1	0.38	2.12	130,130,130,130	0
2	K	D	5	1/1	0.34	2.08	131,131,131,131	0

6.5 Other polymers ⓘ

There are no such residues in this entry.