



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:04 AM UTC

PDB ID : 6VJS / pdb_00006vjs
Title : Escherichia coli RNA polymerase and ureidothiophene-2-carboxylic acid complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2020-01-17
Resolution : 4.02 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

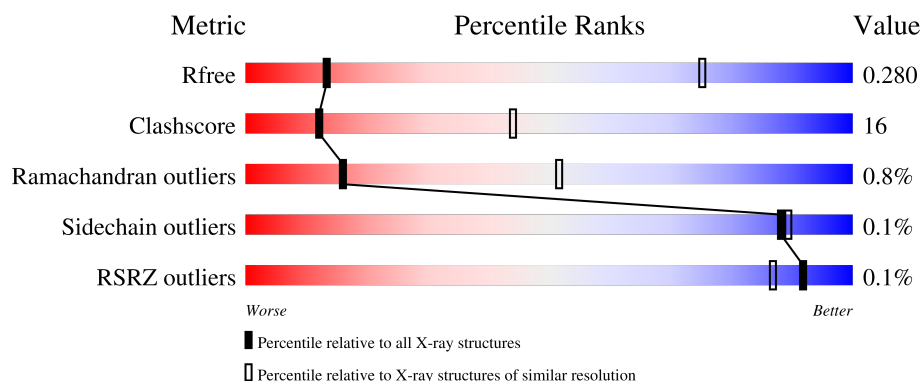
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.02 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}	180053	1095 (4.24-3.80)
Clashscore	190562	1142 (4.24-3.80)
Ramachandran outliers	187476	1074 (4.24-3.80)
Sidechain outliers	187428	1065 (4.24-3.80)
RSRZ outliers	180081	1095 (4.24-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	F	329	
1	G	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	H	1342	66%33%
3	D	1407	49%33%17%
3	I	1407	50%32%18%
4	E	91	87%12%
4	J	91	%62%21%16%
5	X	613	52%24%23%
5	Y	613	55%22%23%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56011 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1809	1126	319	357	7			
1	B	301	Total	C	N	O	S	0	0	0
			2337	1462	411	456	8			
1	F	234	Total	C	N	O	S	0	0	0
			1809	1126	319	357	7			
1	G	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1336	Total	C	N	O	S	0	0	0
			10540	6614	1836	2047	43			
2	H	1336	Total	C	N	O	S	0	0	0
			10540	6614	1836	2047	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1164	Total	C	N	O	S	0	0	0
			9093	5717	1626	1704	46			
3	I	1160	Total	C	N	O	S	0	0	0
			9061	5698	1619	1698	46			

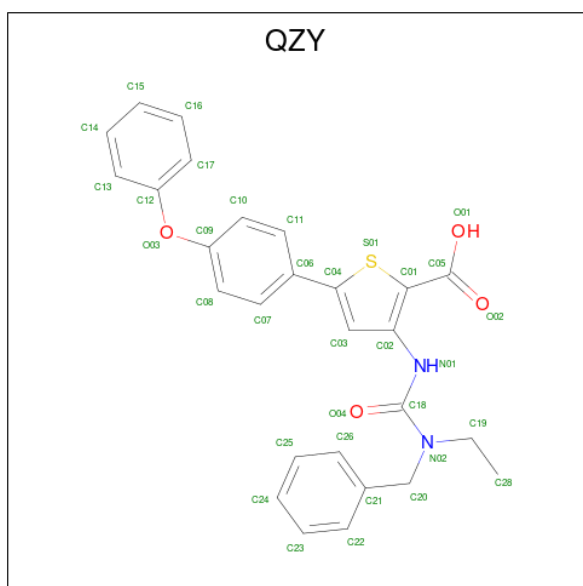
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	471	Total	C	N	O	S	0	0	0
			3832	2398	687	724	23			
5	Y	475	Total	C	N	O	S	0	0	0
			3862	2413	692	734	23			

- Molecule 6 is 3-{[benzyl(ethyl)carbamoyl]amino}-5-(4-phenoxyphenyl)thiophene-2-carboxylic acid (CCD ID: QZY) (formula: C₂₇H₂₄N₂O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			34	27	2	4	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	I	2	Total	Zn	0	0
			2	2		

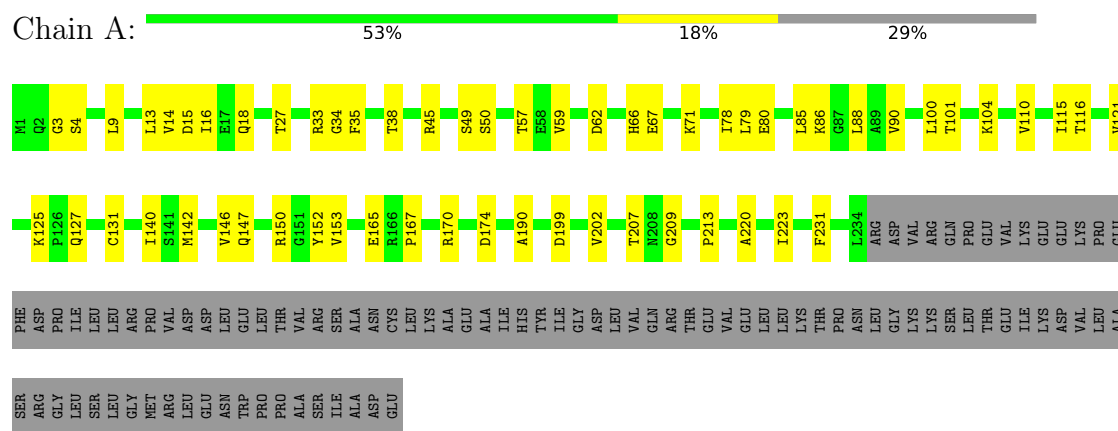
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Mg	0	0
			1	1		
8	I	1	Total	Mg	0	0
			1	1		

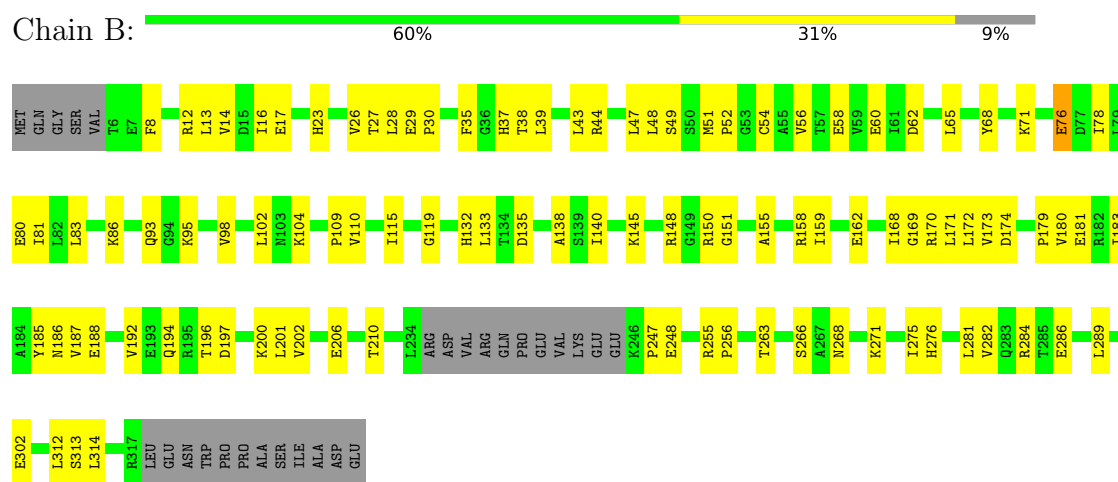
3 Residue-property plots

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

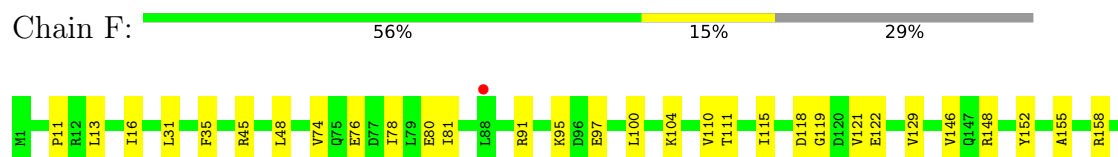
• Molecule 1: DNA-directed RNA polymerase subunit alpha

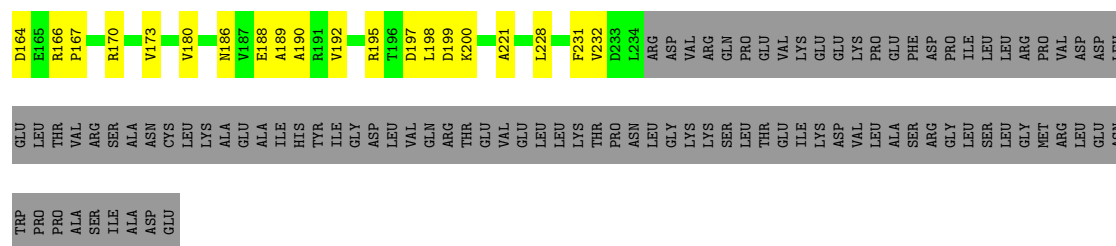


• Molecule 1: DNA-directed RNA polymerase subunit alpha

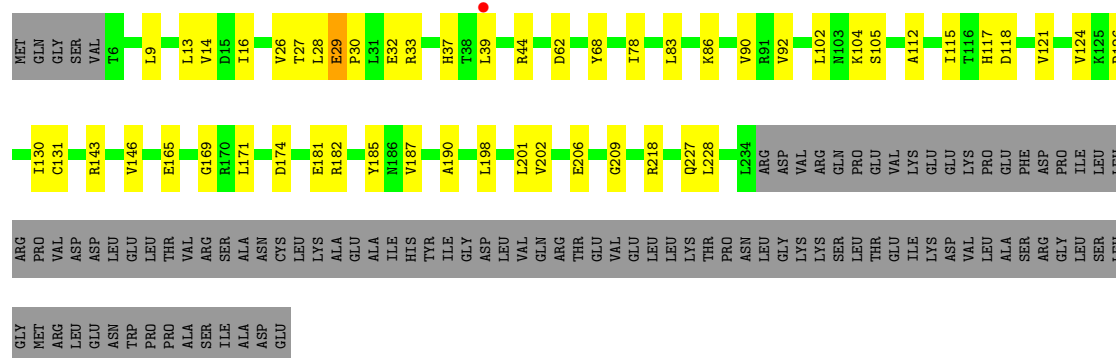


• Molecule 1: DNA-directed RNA polymerase subunit alpha

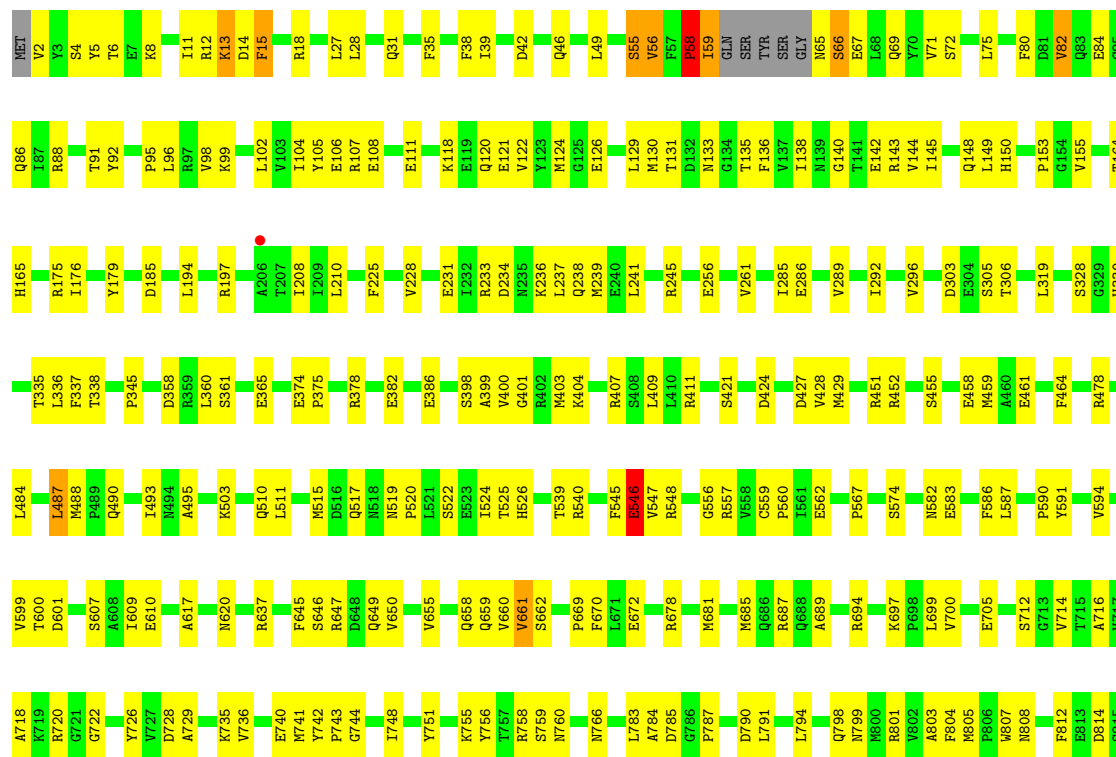


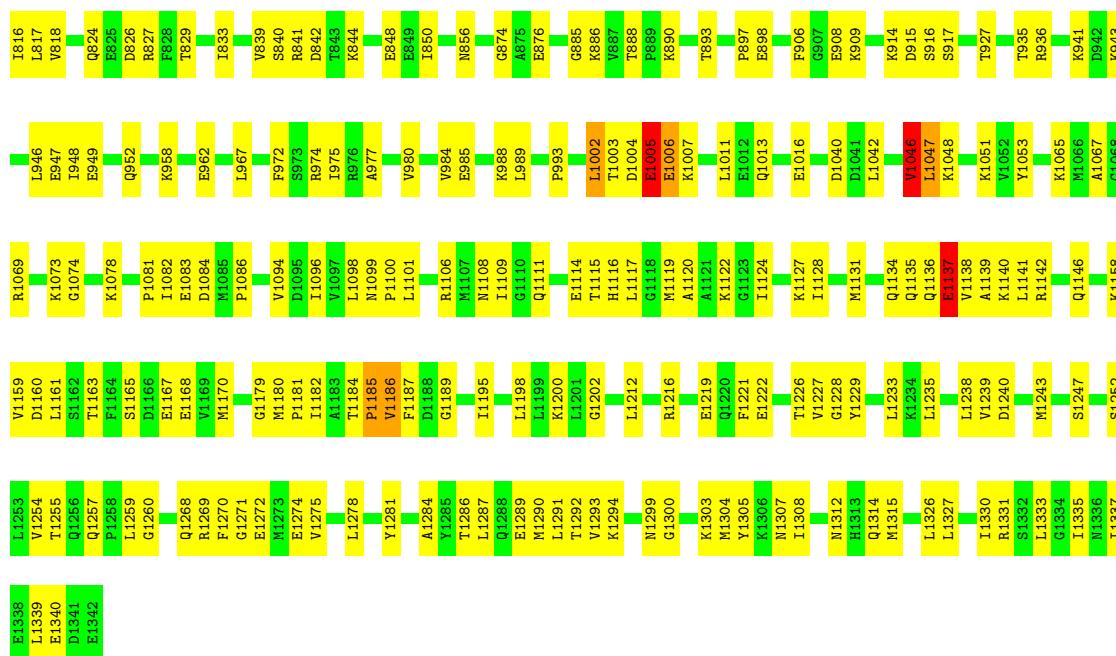


• Molecule 1: DNA-directed RNA polymerase subunit alpha

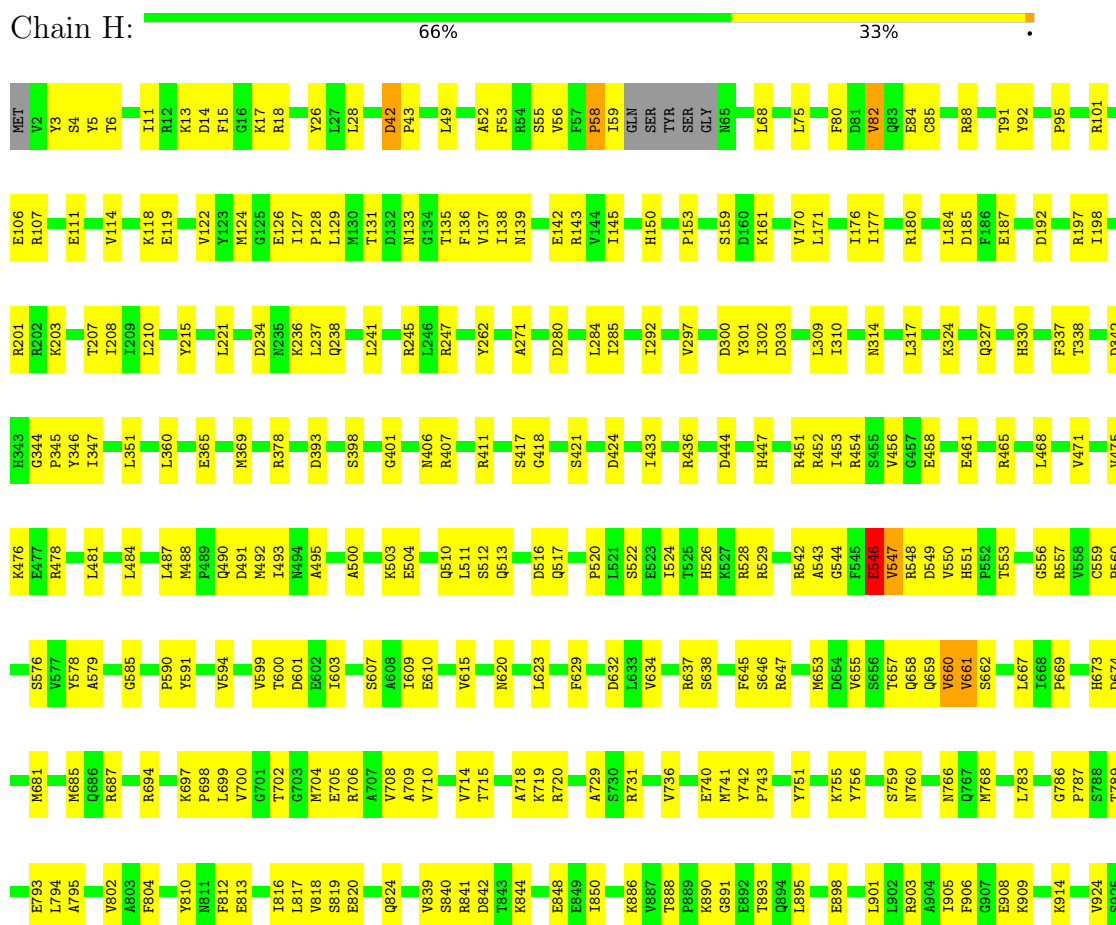


• Molecule 2: DNA-directed RNA polymerase subunit beta

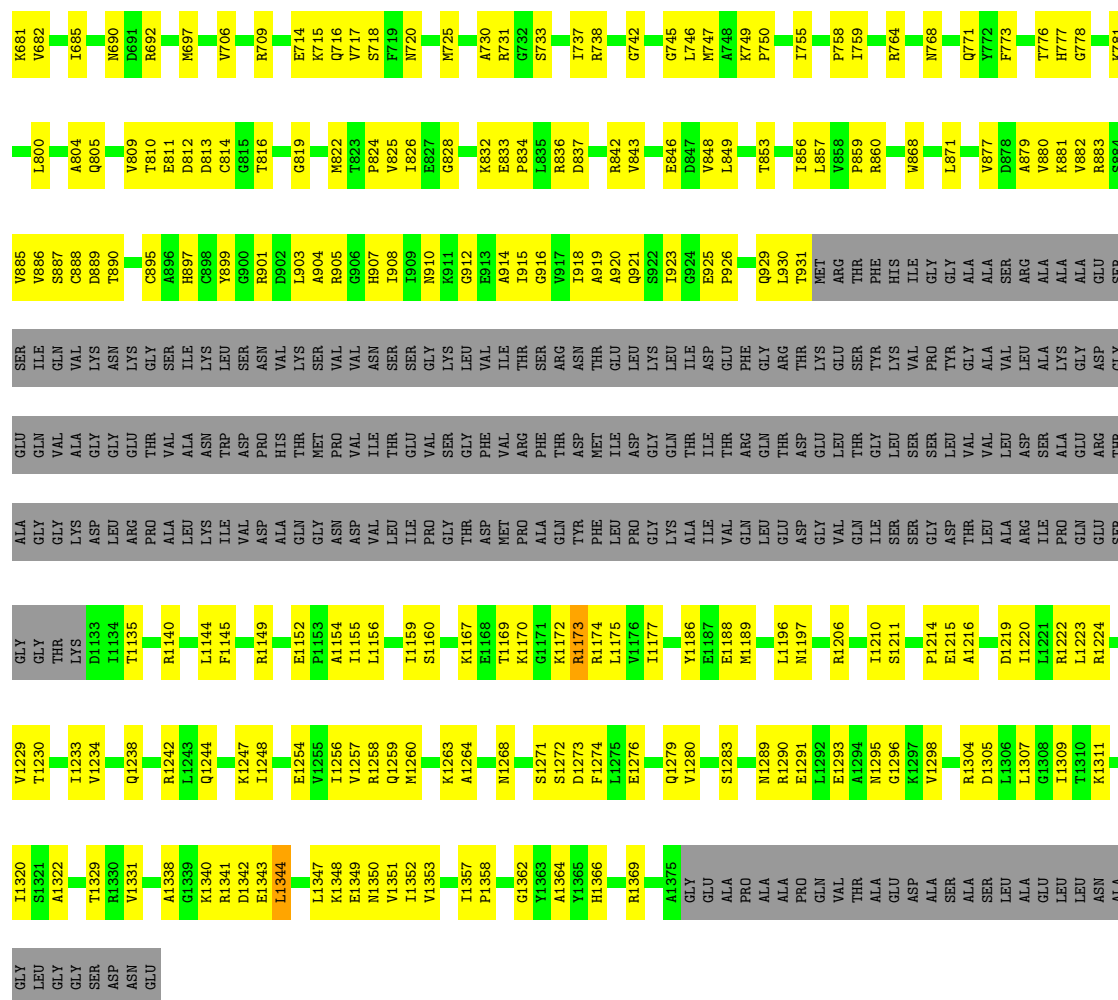




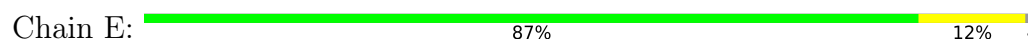
• Molecule 2: DNA-directed RNA polymerase subunit beta



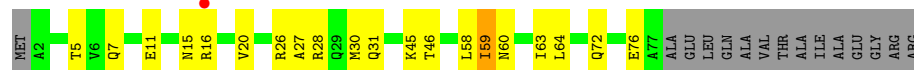




- Molecule 4: DNA-directed RNA polymerase subunit omega

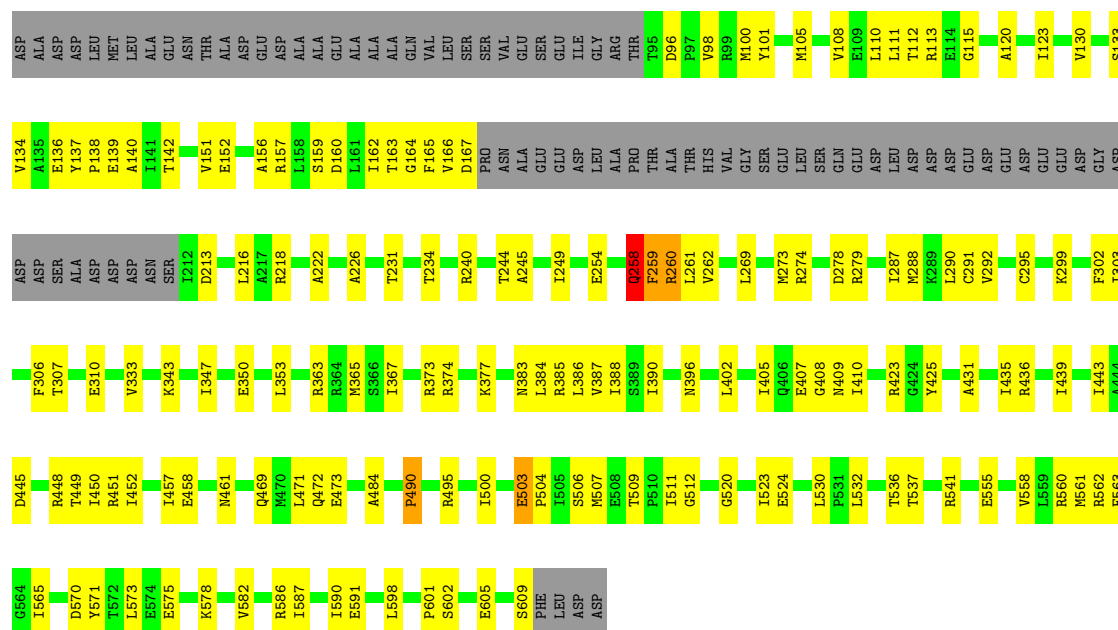


- Molecule 4: DNA-directed RNA polymerase subunit omega

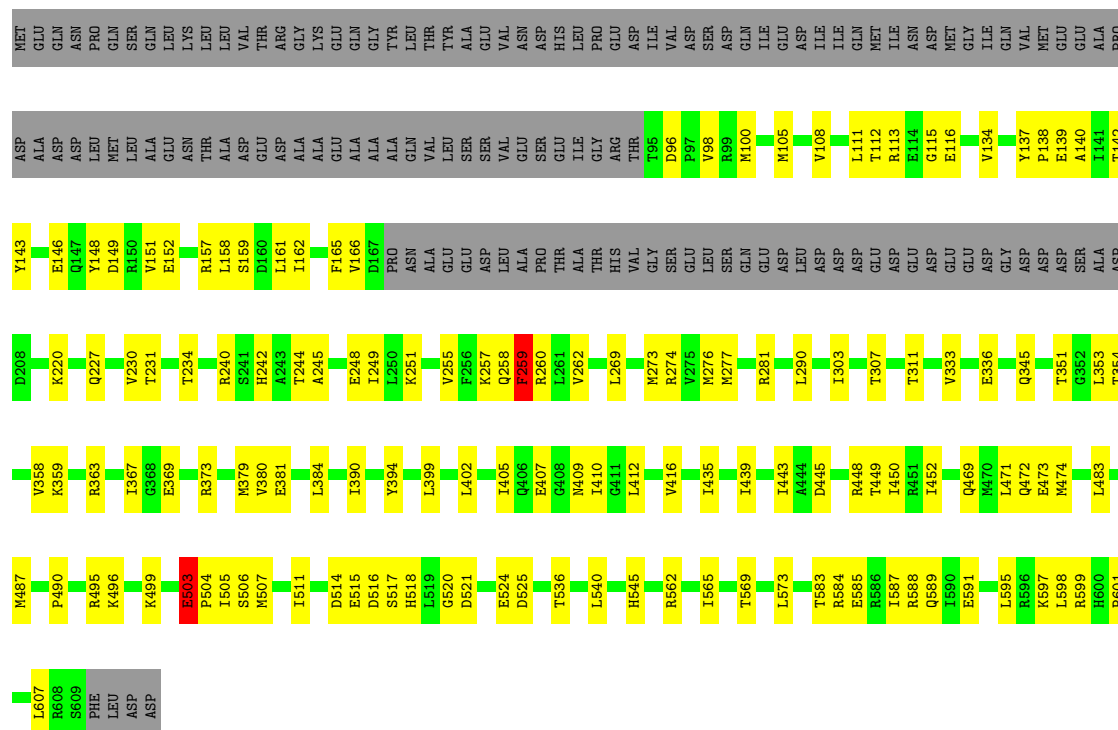


- Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.08Å 205.50Å 309.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.09 – 4.02 50.09 – 4.02	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.09-4.02) 99.4 (50.09-4.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.230 , 0.276 0.232 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	157.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 176.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	56011	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, QZY, ZN

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	0.16	0/1831	0.47	1/2481 (0.0%)
1	B	0.14	0/2365	0.37	0/3202
1	F	0.15	0/1830	0.37	0/2478
1	G	0.13	0/1797	0.34	0/2436
2	C	0.19	0/10708	0.53	8/14448 (0.1%)
2	H	0.16	0/10708	0.48	2/14448 (0.0%)
3	D	0.17	0/9231	0.49	3/12459 (0.0%)
3	I	0.16	0/9199	0.45	0/12417
4	E	0.14	0/710	0.43	0/956
4	J	0.13	0/607	0.42	0/817
5	X	0.21	0/3884	0.50	7/5220 (0.1%)
5	Y	0.15	0/3914	0.46	4/5261 (0.1%)
All	All	0.17	0/56784	0.48	25/76623 (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
2	C	0	8
2	H	0	5
3	D	0	9
3	I	0	8
5	Y	0	1
All	All	0	31

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	69	GLN	N-CA-C	7.92	120.18	110.91
1	A	9	LEU	N-CA-C	7.47	119.65	110.91
5	Y	503	GLU	CA-C-N	6.88	143.51	127.00
5	Y	503	GLU	C-N-CA	6.88	143.51	127.00
5	X	503	GLU	CA-C-N	6.54	142.71	127.00
5	X	503	GLU	C-N-CA	6.54	142.71	127.00
3	D	711	GLY	N-CA-C	-6.03	97.51	110.66
5	X	503	GLU	C-N-CD	-5.89	107.65	120.60
5	Y	259	PHE	N-CA-CB	-5.88	100.56	110.49
5	Y	503	GLU	C-N-CD	-5.80	107.83	120.60
5	X	259	PHE	N-CA-CB	-5.62	100.76	109.69
5	X	260	ARG	N-CA-C	5.38	122.26	110.80
5	X	258	GLN	CA-C-N	5.37	128.48	120.90
5	X	258	GLN	C-N-CA	5.37	128.48	120.90
3	D	848	VAL	CA-C-N	5.32	131.70	121.54
3	D	848	VAL	C-N-CA	5.32	131.70	121.54
2	C	487	LEU	CA-C-N	5.24	131.13	121.70
2	C	487	LEU	C-N-CA	5.24	131.13	121.70
2	C	65	ASN	CA-C-N	5.21	131.50	121.54
2	C	65	ASN	C-N-CA	5.21	131.50	121.54
2	C	1002	LEU	CA-CB-CG	5.20	134.50	116.30
2	C	1046	VAL	CA-C-N	5.20	131.46	121.54
2	C	1046	VAL	C-N-CA	5.20	131.46	121.54
2	H	1180	MET	CA-C-N	5.15	139.36	127.00
2	H	1180	MET	C-N-CA	5.15	139.36	127.00

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1005	GLU	Peptide
2	C	1137	GLU	Peptide
2	C	13	LYS	Peptide
2	C	42	ASP	Peptide
2	C	546	GLU	Peptide
2	C	55	SER	Peptide
2	C	58	PRO	Peptide
2	C	660	VAL	Peptide
3	D	1172	LYS	Peptide
3	D	119	SER	Peptide
3	D	1343	GLU	Peptide
3	D	1344	LEU	Peptide
3	D	152	THR	Peptide

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Mol	Chain	Res	Type	Group
3	D	588	PRO	Peptide
3	D	832	LYS	Peptide
3	D	833	GLU	Peptide
3	D	850	LYS	Peptide
2	H	1137	GLU	Peptide
2	H	42	ASP	Peptide
2	H	546	GLU	Peptide
2	H	58	PRO	Peptide
2	H	660	VAL	Peptide
3	I	1172	LYS	Peptide
3	I	119	SER	Peptide
3	I	1344	LEU	Peptide
3	I	152	THR	Peptide
3	I	588	PRO	Peptide
3	I	832	LYS	Peptide
3	I	833	GLU	Peptide
3	I	848	VAL	Peptide
5	Y	259	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1837	46	0
1	B	2337	0	2397	75	0
1	F	1809	0	1836	39	0
1	G	1775	0	1800	39	0
2	C	10540	0	10561	372	0
2	H	10540	0	10561	345	0
3	D	9093	0	9290	378	0
3	I	9061	0	9260	363	0
4	E	708	0	719	9	0
4	J	605	0	612	19	0
5	X	3832	0	3907	124	0
5	Y	3862	0	3926	119	0
6	D	34	0	0	2	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56011	0	56706	1754	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1754) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	1.82	1.13
5:X:166:VAL:H	5:X:259:PHE:HA	1.15	1.05
5:X:165:PHE:HB3	5:X:259:PHE:CD2	1.93	1.03
1:A:14:VAL:HG12	1:A:15:ASP:H	1.26	0.96
2:C:841:ARG:HA	2:C:1046:VAL:HG11	1.51	0.93
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.21	0.92
5:Y:165:PHE:HB2	5:Y:259:PHE:HB2	1.53	0.91
2:C:1330:ILE:HG13	6:D:1501:QZY:C16	2.01	0.89
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.54	0.89
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.53	0.89
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.53	0.88
2:H:106:GLU:H	2:H:107:ARG:HA	1.37	0.88
3:D:860:ARG:HE	3:D:883:ARG:HH12	1.20	0.87
3:I:1280:VAL:HA	3:I:1283:SER:HB3	1.56	0.86
5:X:165:PHE:CD1	5:X:259:PHE:HB3	2.11	0.85
2:C:1046:VAL:HG22	2:C:1047:LEU:H	1.40	0.85
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.57	0.85
3:I:1159:ILE:CD1	3:I:1186:TYR:OH	2.25	0.85
2:C:590:PRO:O	2:C:659:GLN:NE2	2.10	0.84
2:H:487:LEU:HA	2:H:488:MET:HB3	1.59	0.84
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.57	0.83
2:C:131:THR:HG23	2:C:133:ASN:H	1.42	0.82
3:I:146:VAL:HA	3:I:178:ALA:HB1	1.62	0.81
5:X:165:PHE:HB3	5:X:259:PHE:HD2	1.39	0.81
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.61	0.81
2:C:487:LEU:HA	2:C:488:MET:HB3	1.62	0.81
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.63	0.80
2:C:490:GLN:HG2	5:X:472:GLN:HB3	1.63	0.80
2:H:560:PRO:HD2	2:H:661:VAL:HG12	1.63	0.80
1:A:104:LYS:HD2	1:A:110:VAL:HG22	1.63	0.80
3:D:128:LEU:HA	3:D:192:MET:HE1	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:81:ARG:HG2	3:D:82:GLY:H	1.47	0.80
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.63	0.79
3:D:1295:ASN:HB2	3:D:1298:VAL:HG23	1.65	0.79
3:I:857:LEU:HD11	3:I:871:LEU:HD21	1.63	0.79
3:I:1159:ILE:HD12	3:I:1186:TYR:CZ	2.18	0.79
2:C:14:ASP:HA	2:C:1158:LYS:HE2	1.63	0.79
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.65	0.79
2:H:493:ILE:O	5:Y:472:GLN:NE2	2.16	0.79
3:D:278:ARG:HG2	3:D:281:ARG:HH21	1.48	0.78
2:C:106:GLU:H	2:C:107:ARG:HA	1.48	0.78
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.66	0.78
2:H:590:PRO:O	2:H:659:GLN:NE2	2.17	0.77
3:I:824:PRO:HD3	3:I:836:ARG:HE	1.50	0.77
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.64	0.77
3:I:245:LEU:O	3:I:250:ARG:NH1	2.18	0.77
2:C:1281:TYR:HE1	3:D:489:ASN:HD21	1.33	0.77
3:I:856:ILE:HG23	3:I:857:LEU:HG	1.67	0.77
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.67	0.77
2:H:1324:ASN:HA	2:H:1327:LEU:HD12	1.67	0.77
3:D:406:ALA:HA	3:D:409:TRP:HD1	1.50	0.76
2:H:1269:ARG:HD2	3:I:343:LEU:HB3	1.66	0.76
5:X:165:PHE:HD1	5:X:259:PHE:HB3	1.50	0.76
2:H:176:ILE:HD12	2:H:184:LEU:HD23	1.68	0.75
2:H:520:PRO:HB3	2:H:714:VAL:HG11	1.67	0.75
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.65	0.75
3:D:370:LYS:HG2	3:D:443:GLU:HA	1.69	0.75
1:G:90:VAL:HG11	1:G:146:VAL:HG11	1.68	0.75
1:G:83:LEU:HD11	3:I:527:LEU:HA	1.68	0.75
3:I:809:VAL:HG13	3:I:912:GLY:H	1.51	0.74
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.68	0.74
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.69	0.74
3:D:74:LYS:HD2	3:D:87:LYS:HE3	1.69	0.74
3:D:169:LEU:HD22	3:D:173:GLY:HA2	1.69	0.74
2:C:39:ILE:HD11	2:C:75:LEU:HD11	1.70	0.74
2:H:101:ARG:HG3	2:H:119:GLU:HG2	1.69	0.74
2:H:1291:LEU:HD11	3:I:1351:VAL:HG13	1.70	0.74
5:Y:149:ASP:HA	5:Y:152:GLU:HB2	1.70	0.74
3:D:1177:ILE:HD11	3:D:1196:LEU:HD21	1.69	0.73
2:C:106:GLU:HG2	2:C:111:GLU:HA	1.70	0.73
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.68	0.73
3:D:506:VAL:HG21	3:D:625:MET:HA	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1137:GLU:O	2:H:1139:ALA:N	2.21	0.73
1:F:232:VAL:HA	1:G:218:ARG:HG3	1.69	0.73
2:C:546:GLU:O	2:C:548:ARG:N	2.22	0.73
3:D:813:ASP:HB3	3:D:860:ARG:HH22	1.52	0.73
1:A:125:LYS:HE2	1:A:127:GLN:HB2	1.70	0.73
2:C:135:THR:OG1	2:C:142:GLU:O	2.07	0.73
5:X:166:VAL:N	5:X:259:PHE:HA	1.99	0.73
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.54	0.72
3:I:816:THR:HG21	3:I:888:CYS:H	1.54	0.72
3:D:207:GLU:HG2	3:D:208:THR:HG22	1.70	0.72
1:B:47:LEU:HB3	1:B:180:VAL:HG21	1.71	0.72
1:B:159:ILE:HG12	1:B:172:LEU:HD22	1.69	0.72
5:Y:165:PHE:CB	5:Y:259:PHE:HB2	2.19	0.72
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.70	0.72
3:I:517:CYS:H	3:I:545:HIS:HB2	1.53	0.72
3:I:555:TYR:H	3:I:589:TYR:HD2	1.37	0.72
5:Y:231:THR:HG23	5:Y:249:ILE:HG12	1.71	0.72
1:A:14:VAL:HG12	1:A:15:ASP:N	2.01	0.72
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.72	0.72
2:H:517:GLN:HE21	2:H:760:ASN:H	1.38	0.72
2:C:1240:ASP:HA	3:D:445:LYS:HE2	1.73	0.71
1:B:181:GLU:HA	3:D:535:ARG:HD3	1.71	0.71
5:X:165:PHE:HA	5:X:260:ARG:H	1.54	0.71
2:H:1127:LYS:HE3	2:H:1131:MET:HE3	1.72	0.71
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.23	0.71
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.71	0.71
1:A:14:VAL:CG1	1:A:15:ASP:H	2.03	0.71
2:H:106:GLU:N	2:H:107:ARG:HA	2.05	0.71
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.55	0.71
4:E:26:ARG:HE	4:E:30:MET:HE3	1.55	0.70
2:H:1275:VAL:HG12	2:H:1287:LEU:HD11	1.70	0.70
2:H:840:SER:HA	2:H:886:LYS:HD2	1.73	0.70
5:X:166:VAL:HG13	5:X:260:ARG:HG2	1.73	0.70
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.55	0.70
3:I:422:LEU:HA	3:I:436:ALA:HA	1.74	0.70
1:G:9:LEU:HD22	1:G:32:GLU:HG3	1.71	0.70
5:Y:598:LEU:HD12	5:Y:601:PRO:HB3	1.74	0.70
3:I:1159:ILE:HD11	3:I:1186:TYR:OH	1.89	0.70
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.74	0.70
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.24	0.70
2:H:516:ASP:OD1	2:H:522:SER:OG	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.74	0.69
1:G:86:LYS:NZ	1:G:174:ASP:OD2	2.23	0.69
3:I:555:TYR:HB2	3:I:589:TYR:HE2	1.55	0.69
3:I:527:LEU:HD13	3:I:532:GLU:HG3	1.73	0.69
3:I:481:ARG:HA	3:I:485:MET:HE2	1.73	0.69
2:C:804:PHE:O	3:D:638:SER:OG	2.08	0.69
2:H:546:GLU:O	2:H:548:ARG:N	2.25	0.69
3:I:1264:ALA:HA	3:I:1305:ASP:HB2	1.74	0.69
3:I:814:CYS:O	3:I:860:ARG:NH2	2.26	0.69
1:B:68:TYR:HE1	1:B:171:LEU:HD12	1.58	0.69
2:C:545:PHE:HZ	3:D:781:LYS:HB2	1.57	0.69
2:C:2:VAL:O	2:C:12:ARG:NH1	2.25	0.69
3:D:260:PHE:HB2	5:X:504:PRO:HG3	1.75	0.69
2:H:58:PRO:HB3	2:H:476:LYS:HA	1.73	0.69
3:I:846:GLU:HA	3:I:859:PRO:HA	1.74	0.69
5:X:562:ARG:NH1	5:X:591:GLU:OE1	2.26	0.69
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.75	0.68
3:D:422:LEU:HA	3:D:436:ALA:HA	1.75	0.68
3:D:1375:ALA:HB2	3:I:849:LEU:HD22	1.74	0.68
1:B:188:GLU:HB3	1:B:200:LYS:HE3	1.76	0.68
5:X:598:LEU:HD12	5:X:601:PRO:HB3	1.76	0.68
2:H:82:VAL:HA	2:H:85:CYS:HB2	1.76	0.68
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.76	0.68
5:Y:405:ILE:O	5:Y:409:ASN:ND2	2.27	0.68
2:H:971:LEU:HD21	2:H:1014:LEU:HG	1.76	0.67
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.75	0.67
2:H:1046:VAL:HG22	2:H:1047:LEU:H	1.60	0.67
5:X:112:THR:HG22	5:X:113:ARG:H	1.60	0.67
3:I:279:LEU:O	3:I:279:LEU:HD13	1.94	0.67
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.27	0.67
1:F:45:ARG:HG2	2:H:1083:GLU:HB2	1.74	0.67
5:Y:165:PHE:HB2	5:Y:259:PHE:CB	2.25	0.67
3:D:521:LYS:HB3	3:D:542:ALA:HB1	1.77	0.67
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.77	0.67
3:I:437:PHE:HZ	3:I:453:VAL:HG21	1.60	0.67
5:X:130:VAL:HG13	5:X:365:MET:HG3	1.77	0.67
5:Y:380:VAL:HG23	5:Y:412:LEU:HD23	1.76	0.66
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.76	0.66
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.78	0.66
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.76	0.66
3:D:1215:GLU:OE1	3:D:1224:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.77	0.66
5:X:111:LEU:HD22	5:X:115:GLY:HA3	1.76	0.66
5:X:165:PHE:HA	5:X:260:ARG:N	2.09	0.66
5:X:234:THR:HB	5:X:245:ALA:HB1	1.78	0.66
3:I:1215:GLU:OE1	3:I:1224:ARG:NH2	2.28	0.66
2:C:720:ARG:HH11	2:C:736:VAL:HG21	1.59	0.66
1:B:37:HIS:HE1	1:B:187:VAL:HG22	1.60	0.66
2:C:840:SER:OG	2:C:1048:LYS:O	2.14	0.66
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.77	0.66
3:I:275:ARG:HD3	3:I:298:MET:HB3	1.77	0.66
2:H:56:VAL:O	2:H:58:PRO:HD3	1.94	0.66
2:H:1124:ILE:HG21	2:H:1180:MET:HE2	1.76	0.66
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.78	0.66
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.29	0.66
3:I:1295:ASN:HB2	3:I:1298:VAL:HG23	1.76	0.66
3:I:368:LEU:HD23	3:I:439:PRO:HB3	1.78	0.65
2:C:517:GLN:HE21	2:C:760:ASN:HD22	1.41	0.65
2:H:495:ALA:HB3	5:Y:471:LEU:HD13	1.77	0.65
3:I:482:ALA:O	3:I:488:ASN:ND2	2.30	0.65
3:D:81:ARG:CG	3:D:82:GLY:H	2.08	0.65
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.77	0.65
3:I:492:SER:HB2	3:I:499:ILE:HD13	1.76	0.65
3:I:527:LEU:HD23	3:I:528:THR:H	1.62	0.65
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.79	0.65
2:H:49:LEU:HG	2:H:461:GLU:HG3	1.76	0.65
2:H:68:LEU:HD22	2:H:475:VAL:HG21	1.79	0.65
3:I:85:CYS:SG	3:I:86:GLU:N	2.69	0.65
3:I:650:LYS:NZ	3:I:742:GLY:O	2.26	0.65
2:C:398:SER:O	2:C:401:GLY:N	2.29	0.65
3:I:811:GLU:OE2	3:I:890:THR:OG1	2.12	0.65
1:B:95:LYS:HE3	1:B:98:VAL:HB	1.77	0.65
2:C:1269:ARG:HD2	3:D:343:LEU:HD21	1.77	0.65
2:H:600:THR:HG22	2:H:601:ASP:H	1.61	0.65
2:H:1134:GLN:O	2:H:1137:GLU:N	2.29	0.65
3:I:425:ARG:NH2	3:I:464:ASP:OD2	2.28	0.65
1:A:86:LYS:HE2	1:A:174:ASP:HB2	1.77	0.65
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.79	0.65
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	1.79	0.65
3:D:553:THR:HG23	3:D:567:THR:HG22	1.77	0.65
3:I:768:ASN:O	3:I:771:GLN:NE2	2.29	0.65
3:I:70:CYS:HB2	3:I:90:VAL:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:474:LEU:HD11	4:J:27:ALA:HB3	1.79	0.65
5:Y:514:ASP:C	5:Y:516:ASP:HA	2.21	0.65
5:Y:562:ARG:NH1	5:Y:591:GLU:OE1	2.30	0.65
2:C:1137:GLU:O	2:C:1139:ALA:N	2.30	0.64
1:G:83:LEU:HD13	3:I:526:VAL:HG23	1.79	0.64
2:H:607:SER:HB2	2:H:610:GLU:HG3	1.80	0.64
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.79	0.64
2:C:1304:MET:HE1	3:D:472:LEU:HD13	1.79	0.64
3:I:114:ILE:HD12	3:I:304:ASP:HB3	1.80	0.64
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.80	0.64
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.79	0.64
2:C:1013:GLN:HA	2:C:1016:GLU:HB2	1.79	0.64
1:F:11:PRO:HG3	1:G:227:GLN:HG3	1.78	0.64
3:I:1159:ILE:CD1	3:I:1186:TYR:CE2	2.74	0.64
2:C:495:ALA:HB3	5:X:471:LEU:HD13	1.79	0.64
3:I:826:ILE:HG13	3:I:828:GLY:H	1.62	0.64
2:C:560:PRO:HD2	2:C:661:VAL:HG12	1.80	0.64
2:H:935:THR:HA	2:H:1048:LYS:HB3	1.78	0.64
3:I:842:ARG:HB3	3:I:882:VAL:HG21	1.80	0.64
5:X:240:ARG:HD3	5:X:244:THR:HB	1.79	0.64
3:D:768:ASN:N	3:D:771:GLN:HE22	1.94	0.64
3:I:905:ARG:HH21	4:J:16:ARG:HG3	1.63	0.64
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.79	0.63
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.63	0.63
1:B:188:GLU:O	1:B:200:LYS:HG2	1.97	0.63
3:D:587:LEU:O	3:D:589:TYR:N	2.32	0.63
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.79	0.63
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.62	0.63
2:H:906:PHE:HZ	5:Y:601:PRO:HB2	1.63	0.63
3:I:644:MET:HG3	3:I:764:ARG:HD3	1.79	0.63
1:G:68:TYR:HE1	1:G:171:LEU:HG	1.64	0.63
2:C:138:ILE:HB	2:C:143:ARG:HD2	1.78	0.63
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.80	0.63
2:C:1002:LEU:HD13	2:C:1003:THR:H	1.64	0.63
3:D:534:GLU:HB2	3:D:578:ILE:HD13	1.80	0.63
2:H:590:PRO:HB2	2:H:655:VAL:HG21	1.81	0.63
2:C:228:VAL:N	2:C:335:THR:O	2.30	0.63
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.30	0.63
3:D:123:ARG:HD3	3:D:1337:VAL:HG21	1.79	0.63
3:D:205:LEU:HB3	3:D:217:LEU:HD13	1.78	0.63
5:X:139:GLU:HA	5:X:142:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1275:VAL:HG12	2:C:1287:LEU:HD11	1.80	0.63
2:H:1156:ARG:NH2	2:H:1194:GLU:OE1	2.27	0.63
5:Y:116:GLU:HA	5:Y:379:MET:HE1	1.81	0.63
3:I:615:LYS:HA	4:J:5:THR:HG21	1.81	0.63
2:C:66:SER:N	2:C:105:TYR:HB2	2.14	0.63
2:C:946:LEU:HA	2:C:949:GLU:HG2	1.81	0.63
3:I:649:LYS:HE2	3:I:652:GLU:HG3	1.80	0.63
5:Y:277:MET:HE1	5:Y:359:LYS:HD3	1.81	0.63
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.80	0.62
3:I:644:MET:O	3:I:764:ARG:NH1	2.32	0.62
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.81	0.62
2:H:1073:LYS:HB2	3:I:462:ASP:HB2	1.81	0.62
3:I:406:ALA:HA	3:I:409:TRP:HD1	1.64	0.62
3:D:424:ASN:HB2	3:D:434:ILE:HG13	1.79	0.62
3:I:260:PHE:HB2	5:Y:504:PRO:HG2	1.81	0.62
5:X:166:VAL:HG13	5:X:260:ARG:CG	2.29	0.62
2:C:56:VAL:O	2:C:58:PRO:HD3	2.00	0.62
2:C:66:SER:H	2:C:105:TYR:HB2	1.65	0.62
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.81	0.62
2:H:844:LYS:HE3	5:Y:496:LYS:HE3	1.81	0.62
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.82	0.62
2:H:1108:ASN:ND2	2:H:1111:GLN:OE1	2.33	0.62
3:I:709:ARG:NH1	3:I:714:GLU:OE1	2.33	0.62
2:H:207:THR:HG21	2:H:351:LEU:HG	1.82	0.62
2:H:839:VAL:HA	2:H:1049:ILE:HG22	1.82	0.62
3:I:653:ILE:HD12	3:I:692:ARG:HB3	1.81	0.62
5:Y:234:THR:HB	5:Y:245:ALA:HB1	1.82	0.62
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.82	0.62
2:H:478:ARG:NH2	2:H:491:ASP:O	2.33	0.62
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.82	0.62
1:B:158:ARG:HB2	1:B:172:LEU:HD21	1.81	0.62
2:C:400:VAL:HG11	2:C:452:ARG:HD2	1.82	0.62
2:H:903:ARG:HB3	2:H:908:GLU:HA	1.80	0.62
1:A:27:THR:HG22	1:A:202:VAL:HG22	1.81	0.61
2:H:706:ARG:NH2	2:H:793:GLU:OE2	2.32	0.61
2:H:18:ARG:NH1	2:H:620:ASN:O	2.33	0.61
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.81	0.61
2:C:1005:GLU:O	2:C:1007:LYS:N	2.33	0.61
3:D:613:GLY:O	3:D:617:THR:OG1	2.17	0.61
3:I:36:GLY:HA3	3:I:61:ILE:HG12	1.82	0.61
3:I:584:PRO:O	3:I:589:TYR:OH	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:36:GLY:HA3	3:D:61:ILE:HG12	1.82	0.61
5:Y:105:MET:HG3	5:Y:384:LEU:HD12	1.82	0.61
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.81	0.61
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.61
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.82	0.61
3:I:506:VAL:HG23	3:I:628:GLY:HA3	1.82	0.61
2:C:328:SER:OG	2:C:330:HIS:ND1	2.34	0.61
3:I:298:MET:SD	5:Y:402:LEU:HB3	2.40	0.61
5:X:560:ARG:HA	5:X:565:ILE:HG23	1.83	0.61
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.83	0.61
2:C:1287:LEU:HD23	3:D:1357:ILE:HG12	1.81	0.61
2:H:1065:LYS:HG2	2:H:1235:LEU:HD12	1.82	0.61
3:I:431:ARG:N	3:I:921:GLN:OE1	2.34	0.61
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.81	0.61
2:H:221:LEU:HD11	2:H:314:ASN:HB2	1.82	0.61
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.83	0.61
2:C:672:GLU:HB3	2:C:1187:PHE:HD1	1.66	0.61
2:H:131:THR:HG23	2:H:133:ASN:H	1.63	0.61
2:H:623:LEU:HD11	2:H:653:MET:HE1	1.83	0.61
3:I:555:TYR:HD2	3:I:563:LEU:HB3	1.66	0.61
5:X:303:ILE:O	5:X:307:THR:OG1	2.15	0.61
2:C:1268:GLN:HE22	3:D:352:ARG:HE	1.48	0.60
2:C:1327:LEU:HB3	2:C:1331:ARG:HH12	1.66	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.33	0.60
2:C:817:LEU:HD21	2:C:1078:LYS:HB3	1.83	0.60
3:D:677:GLU:HB2	3:D:680:ASN:HB2	1.83	0.60
1:F:91:ARG:HB3	1:F:122:GLU:HB3	1.83	0.60
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.83	0.60
2:C:99:LYS:HG2	2:C:121:GLU:HG3	1.82	0.60
2:C:559:CYS:HB2	2:C:662:SER:H	1.66	0.60
3:I:415:VAL:O	4:J:45:LYS:NZ	2.35	0.60
5:X:157:ARG:HB3	5:X:160:ASP:OD2	2.01	0.60
3:I:1291:GLU:HA	3:I:1296:GLY:HA2	1.84	0.60
3:I:1159:ILE:CD1	3:I:1186:TYR:CZ	2.84	0.60
2:H:559:CYS:HB2	2:H:662:SER:H	1.67	0.60
2:H:1287:LEU:HD23	3:I:1357:ILE:HG12	1.84	0.60
3:I:146:VAL:HA	3:I:178:ALA:CB	2.31	0.60
2:C:104:ILE:HD12	2:C:484:LEU:HD13	1.84	0.60
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.20	0.60
3:D:389:GLY:O	3:D:391:ALA:N	2.35	0.59
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.84	0.59
1:B:58:GLU:HB2	1:B:145:LYS:HB3	1.83	0.59
2:H:1293:VAL:HG21	2:H:1304:MET:HG3	1.83	0.59
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.37	0.59
2:C:106:GLU:HB2	2:C:108:GLU:H	1.67	0.59
2:H:557:ARG:NH2	2:H:607:SER:O	2.35	0.59
1:A:45:ARG:HH12	2:C:1084:ASP:HB3	1.67	0.59
2:C:148:GLN:HB2	2:C:511:LEU:HD21	1.84	0.59
3:D:345:LYS:HE3	6:D:1501:QZY:C19	2.32	0.59
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.18	0.59
2:H:135:THR:OG1	2:H:142:GLU:O	2.20	0.59
3:I:697:MET:HE1	3:I:738:ARG:HA	1.83	0.59
4:J:72:GLN:NE2	4:J:76:GLU:OE2	2.36	0.59
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	1.83	0.59
1:B:110:VAL:HG21	1:B:140:ILE:HD11	1.85	0.59
2:H:1159:VAL:HB	2:H:1160:ASP:HB2	1.84	0.59
3:D:517:CYS:HA	3:D:716:GLN:OE1	2.02	0.59
3:D:576:ARG:NH2	3:D:594:GLN:O	2.36	0.59
3:D:839:VAL:HG12	3:D:863:LEU:HD12	1.84	0.59
3:D:849:LEU:O	3:D:850:LYS:HB2	2.02	0.59
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.68	0.59
2:H:14:ASP:O	2:H:1158:LYS:HD3	2.03	0.59
1:B:104:LYS:HD2	1:B:110:VAL:HG12	1.85	0.59
2:H:615:VAL:HA	2:H:638:SER:HB2	1.85	0.59
2:H:669:PRO:HA	2:H:702:THR:HG22	1.85	0.59
3:D:849:LEU:HA	3:D:856:ILE:H	1.67	0.59
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.85	0.59
3:I:514:THR:HG21	3:I:596:LEU:HA	1.85	0.59
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.84	0.58
2:C:1252:SER:HA	5:X:524:GLU:HA	1.85	0.58
2:C:1326:LEU:O	2:C:1330:ILE:HG12	2.03	0.58
3:D:930:LEU:HD11	3:D:1241:TYR:HE2	1.68	0.58
2:H:685:MET:HE3	2:H:1235:LEU:HD11	1.85	0.58
2:C:107:ARG:O	2:C:107:ARG:NE	2.21	0.58
2:C:681:MET:O	2:C:685:MET:HG2	2.04	0.58
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.85	0.58
5:X:165:PHE:CB	5:X:259:PHE:HD2	2.14	0.58
3:D:186:GLN:HG3	3:D:238:ILE:HD11	1.84	0.58
2:H:766:ASN:HD21	2:H:768:MET:HE3	1.67	0.58
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.85	0.58
3:I:513:MET:O	3:I:575:GLY:HA3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.85	0.58
2:H:1341:ASP:OD1	2:H:1341:ASP:N	2.37	0.58
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.36	0.58
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.67	0.58
3:D:527:LEU:HB2	3:D:532:GLU:CD	2.28	0.58
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.86	0.58
2:H:95:PRO:HA	2:H:126:GLU:HG2	1.85	0.58
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.84	0.58
1:A:33:ARG:N	1:A:34:GLY:HA3	2.18	0.58
2:H:1252:SER:OG	2:H:1255:THR:O	2.21	0.58
2:H:632:ASP:HA	2:H:647:ARG:HE	1.68	0.58
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.37	0.58
2:H:992:LEU:HB3	2:H:996:ARG:HB3	1.86	0.58
2:C:18:ARG:NH1	2:C:620:ASN:O	2.37	0.58
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.68	0.58
5:Y:248:GLU:HA	5:Y:251:LYS:HB2	1.86	0.58
3:I:584:PRO:HD2	3:I:587:LEU:HD22	1.86	0.57
4:J:60:ASN:H	4:J:63:ILE:HB	1.69	0.57
3:D:527:LEU:HD13	3:D:535:ARG:HH21	1.67	0.57
2:H:1308:ILE:HG21	3:I:379:PRO:HB2	1.86	0.57
3:I:207:GLU:HG2	3:I:208:THR:HG22	1.85	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.86	0.57
2:H:1078:LYS:HD3	2:H:1080:ASN:HD22	1.69	0.57
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.86	0.57
1:B:133:LEU:HD21	1:B:140:ILE:HD13	1.84	0.57
3:D:151:MET:HB3	3:D:152:THR:HG23	1.86	0.57
5:Y:149:ASP:OD2	5:Y:149:ASP:N	2.32	0.57
2:C:2:VAL:N	2:C:1158:LYS:HZ2	2.02	0.57
3:D:311:ARG:HB3	3:D:312:ARG:HG3	1.86	0.57
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.84	0.57
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.84	0.57
3:I:1344:LEU:O	3:I:1350:ASN:ND2	2.37	0.57
3:D:650:LYS:HE3	3:D:654:ILE:HD11	1.86	0.57
2:H:971:LEU:HD12	2:H:1018:TYR:CD1	2.39	0.57
3:I:587:LEU:O	3:I:589:TYR:N	2.37	0.57
2:C:524:ILE:HG13	2:C:712:SER:HB2	1.86	0.57
1:G:92:VAL:HG22	1:G:121:VAL:HG22	1.87	0.57
3:D:156:ARG:NH2	3:D:191:SER:OG	2.38	0.57
2:H:238:GLN:HB3	2:H:284:LEU:HD11	1.86	0.57
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.87	0.57
1:A:66:HIS:HB3	2:C:874:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.87	0.57
2:C:1271:GLY:HA2	3:D:344:GLY:N	2.20	0.57
3:D:81:ARG:O	3:D:83:VAL:N	2.37	0.57
3:D:214:ARG:HD3	3:D:1275:LEU:HD21	1.86	0.57
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.87	0.57
3:I:613:GLY:O	3:I:617:THR:OG1	2.17	0.57
5:Y:157:ARG:NH1	5:Y:159:SER:H	2.02	0.57
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.87	0.56
2:H:731:ARG:NH2	2:H:962:GLU:OE2	2.38	0.56
2:H:1253:LEU:HA	5:Y:525:ASP:HB2	1.87	0.56
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.70	0.56
3:I:353:SER:HB3	3:I:447:ILE:HG22	1.87	0.56
3:I:514:THR:HG22	3:I:515:ARG:H	1.70	0.56
2:H:818:VAL:HA	2:H:1096:ILE:HG22	1.86	0.56
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.87	0.56
1:B:12:ARG:H	1:B:30:PRO:HD2	1.70	0.56
2:C:80:PHE:CE2	2:C:84:GLU:HG2	2.39	0.56
2:C:886:LYS:HE2	2:C:916:SER:HB3	1.86	0.56
2:C:1140:LYS:HG2	2:C:1142:ARG:HE	1.70	0.56
3:D:849:LEU:HB3	3:D:854:ALA:O	2.05	0.56
3:D:851:PRO:HG3	3:D:875:ASN:HB2	1.86	0.56
3:D:871:LEU:HB3	3:D:877:VAL:HG21	1.87	0.56
2:H:1072:ASN:HD22	2:H:1111:GLN:NE2	2.03	0.56
3:I:553:THR:HG23	3:I:567:THR:HG22	1.87	0.56
5:Y:157:ARG:HH11	5:Y:159:SER:H	1.53	0.56
1:B:44:ARG:HA	1:B:183:ILE:HG21	1.88	0.56
3:D:145:VAL:HG22	3:D:159:ILE:HG13	1.86	0.56
2:H:159:SER:HB3	2:H:161:LYS:HG3	1.88	0.56
2:H:720:ARG:HD2	2:H:736:VAL:HG22	1.86	0.56
2:H:28:LEU:HD21	2:H:524:ILE:HG12	1.87	0.56
2:H:1117:LEU:HD21	2:H:1182:ILE:HD13	1.88	0.56
3:I:37:GLU:HG2	3:I:39:LYS:HG2	1.87	0.56
3:I:836:ARG:HH22	3:I:880:VAL:HG22	1.71	0.56
2:C:15:PHE:H	2:C:15:PHE:HD2	1.53	0.56
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.87	0.56
3:D:515:ARG:NH2	3:D:718:SER:O	2.36	0.56
1:F:95:LYS:O	1:F:148:ARG:NH2	2.39	0.56
1:G:169:GLY:O	1:G:171:LEU:HD22	2.05	0.56
2:H:487:LEU:HD13	2:H:492:MET:HE2	1.88	0.56
3:I:416:ILE:HD12	3:I:439:PRO:HB2	1.88	0.56
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1002:LEU:HG	2:C:1007:LYS:HB2	1.87	0.56
3:D:125:GLY:O	3:D:129:ASP:N	2.38	0.56
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.88	0.56
2:H:700:VAL:O	2:H:1069:ARG:NH1	2.33	0.56
3:I:1256:ILE:HA	3:I:1259:GLN:NE2	2.21	0.56
5:Y:134:VAL:HG22	5:Y:273:MET:HE1	1.87	0.56
5:Y:161:LEU:O	5:Y:262:VAL:HG22	2.06	0.56
3:D:127:LEU:HD21	3:D:234:PRO:HB3	1.88	0.56
5:Y:562:ARG:HH21	5:Y:587:ILE:HG23	1.71	0.56
3:D:169:LEU:C	3:D:169:LEU:HD13	2.31	0.56
3:D:515:ARG:HH22	3:D:717:VAL:C	2.14	0.56
2:H:52:ALA:HB2	2:H:465:ARG:HE	1.71	0.56
2:H:810:TYR:HB3	2:H:817:LEU:HD23	1.88	0.56
3:I:718:SER:HB3	3:I:720:ASN:HB2	1.88	0.56
5:X:530:LEU:HD12	5:X:530:LEU:H	1.70	0.56
2:C:699:LEU:HB2	2:C:799:ASN:ND2	2.20	0.56
1:F:80:GLU:HA	2:H:694:ARG:HH12	1.71	0.56
1:G:190:ALA:N	1:G:198:LEU:O	2.35	0.56
2:H:91:THR:HG22	2:H:139:ASN:H	1.71	0.56
2:H:300:ASP:HB2	2:H:309:LEU:HD21	1.87	0.56
5:X:101:TYR:OH	5:X:409:ASN:ND2	2.38	0.56
5:X:575:GLU:HA	5:X:578:LYS:HD2	1.87	0.56
2:C:517:GLN:NE2	2:C:760:ASN:HD22	2.03	0.55
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.87	0.55
2:H:347:ILE:HD11	2:H:433:ILE:HD11	1.89	0.55
2:H:842:ASP:N	2:H:1046:VAL:HG11	2.21	0.55
2:H:924:VAL:HG12	2:H:1058:ARG:HH22	1.72	0.55
3:D:877:VAL:O	3:D:879:ALA:N	2.36	0.55
2:H:517:GLN:HE21	2:H:760:ASN:N	2.03	0.55
3:I:108:ALA:CB	3:I:279:LEU:HD12	2.37	0.55
3:I:489:ASN:HA	3:I:904:ALA:HB1	1.89	0.55
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.86	0.55
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.34	0.55
2:C:798:GLN:HB3	2:C:827:ARG:HH21	1.71	0.55
3:D:596:LEU:HD11	3:D:598:LYS:HZ1	1.72	0.55
3:D:1165:PHE:CD2	3:D:1168:GLU:HG3	2.42	0.55
3:D:1347:LEU:HD22	3:D:1357:ILE:HG22	1.87	0.55
2:H:556:GLY:HA2	2:H:659:GLN:O	2.07	0.55
2:H:1151:LEU:HD12	2:H:1201:LEU:HD22	1.87	0.55
3:D:169:LEU:HD13	3:D:169:LEU:O	2.06	0.55
1:F:167:PRO:HG2	1:F:170:ARG:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:841:ARG:NH1	3:I:256:ASP:HB3	2.21	0.55
1:B:255:ARG:HG2	1:B:256:PRO:HD2	1.89	0.55
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.42	0.55
5:X:469:GLN:NE2	5:X:473:GLU:OE2	2.31	0.55
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.88	0.55
2:H:300:ASP:OD1	2:H:300:ASP:N	2.37	0.55
2:H:755:LYS:HB3	2:H:756:TYR:HD2	1.71	0.55
1:B:159:ILE:HA	1:B:162:GLU:HG2	1.88	0.55
3:D:825:VAL:HB	3:D:834:PRO:HB2	1.88	0.55
2:H:971:LEU:HD12	2:H:1018:TYR:HD1	1.72	0.55
3:I:1159:ILE:HD12	3:I:1186:TYR:OH	2.01	0.55
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.89	0.55
5:Y:583:THR:HG22	5:Y:584:ARG:H	1.72	0.55
1:B:49:SER:O	1:B:151:GLY:HA2	2.07	0.55
3:D:245:LEU:O	3:D:250:ARG:NH1	2.39	0.55
2:H:80:PHE:CE2	2:H:84:GLU:HG2	2.42	0.55
3:I:931:THR:HG23	3:I:1244:GLN:HE22	1.72	0.55
1:B:155:ALA:N	1:B:174:ASP:OD1	2.39	0.54
5:X:157:ARG:HG3	5:X:159:SER:HB2	1.89	0.54
5:Y:412:LEU:HB2	5:Y:435:ILE:HD11	1.88	0.54
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.40	0.54
3:I:612:LEU:HB3	3:I:616:PRO:HB2	1.89	0.54
3:I:800:LEU:HB3	3:I:920:ALA:HB1	1.88	0.54
3:I:1349:GLU:OE1	3:I:1349:GLU:N	2.31	0.54
4:J:7:GLN:NE2	4:J:11:GLU:OE1	2.39	0.54
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.22	0.54
1:A:207:THR:HG23	1:A:209:GLY:H	1.72	0.54
2:C:231:GLU:HB3	2:C:233:ARG:HG3	1.89	0.54
2:C:1284:ALA:HA	3:D:1357:ILE:HD13	1.89	0.54
3:D:285:LEU:HD12	5:X:410:ILE:HD11	1.89	0.54
3:D:856:ILE:HG23	3:D:857:LEU:HG	1.89	0.54
1:G:68:TYR:HB3	1:G:78:ILE:HB	1.89	0.54
2:H:1295:SER:HB2	3:I:347:VAL:HG12	1.89	0.54
2:H:1313:HIS:HD2	3:I:477:GLN:HE22	1.53	0.54
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.88	0.54
2:C:935:THR:HG21	2:C:941:LYS:HG2	1.88	0.54
3:D:771:GLN:HA	3:D:774:ILE:HB	1.88	0.54
3:I:528:THR:HG21	3:I:551:ARG:HE	1.73	0.54
3:I:1268:ASN:O	3:I:1274:PHE:HB3	2.07	0.54
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.43	0.54
2:C:545:PHE:CZ	3:D:781:LYS:HB2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.90	0.54
2:H:4:SER:HA	2:H:1159:VAL:HG21	1.88	0.54
2:H:344:GLY:HA3	2:H:346:TYR:CZ	2.42	0.54
2:H:452:ARG:HH11	2:H:585:GLY:HA3	1.71	0.54
2:H:484:LEU:HD23	2:H:484:LEU:H	1.72	0.54
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.89	0.54
5:Y:545:HIS:ND1	5:Y:545:HIS:O	2.40	0.54
2:C:13:LYS:HG2	2:C:1181:PRO:HG2	1.88	0.54
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.36	0.54
3:I:643:ASP:O	3:I:720:ASN:ND2	2.41	0.54
3:D:884:SER:OG	3:D:885:VAL:N	2.41	0.54
2:H:80:PHE:CE2	2:H:88:ARG:HD3	2.42	0.54
3:I:825:VAL:HB	3:I:834:PRO:HB2	1.89	0.54
3:I:843:VAL:HG12	3:I:883:ARG:HD3	1.90	0.54
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.88	0.54
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.16	0.54
2:C:1159:VAL:HB	2:C:1160:ASP:HB2	1.89	0.54
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.89	0.54
2:H:1281:TYR:CD2	3:I:484:MET:HG2	2.43	0.54
3:I:156:ARG:NH1	3:I:157:GLN:OE1	2.41	0.54
3:I:245:LEU:HD23	3:I:250:ARG:HG2	1.89	0.54
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.88	0.54
2:C:1180:MET:HG3	2:C:1181:PRO:O	2.07	0.54
2:H:11:ILE:HD13	2:H:697:LYS:NZ	2.23	0.54
2:H:444:ASP:HB3	2:H:447:HIS:HB2	1.90	0.54
2:H:591:TYR:OH	2:H:637:ARG:NH2	2.40	0.54
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.72	0.54
5:X:165:PHE:H	5:X:260:ARG:NH1	2.05	0.54
1:B:197:ASP:OD1	1:B:197:ASP:N	2.36	0.53
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.72	0.53
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.89	0.53
1:F:118:ASP:OD1	1:F:119:GLY:N	2.40	0.53
2:H:13:LYS:HG2	2:H:1181:PRO:HG2	1.90	0.53
2:H:131:THR:HG22	2:H:135:THR:H	1.73	0.53
3:I:201:LEU:HB3	3:I:221:ILE:HG22	1.89	0.53
1:B:51:MET:H	1:B:150:ARG:HG3	1.73	0.53
1:F:158:ARG:NH1	1:F:173:VAL:O	2.41	0.53
2:C:1139:ALA:O	2:C:1140:LYS:HB2	2.08	0.53
3:D:822:MET:HE1	3:D:842:ARG:HH21	1.73	0.53
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.90	0.53
2:H:972:PHE:HA	2:H:975:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1209:GLN:HB3	2:H:1224:PRO:HB2	1.90	0.53
2:C:839:VAL:O	2:C:886:LYS:NZ	2.25	0.53
3:D:1289:ASN:HD22	3:D:1290:ARG:HG3	1.73	0.53
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.41	0.53
3:I:1362:GLY:C	3:I:1364:ALA:H	2.16	0.53
2:C:150:HIS:HE2	2:C:452:ARG:HE	1.55	0.53
3:I:515:ARG:NH2	3:I:718:SER:O	2.42	0.53
5:X:582:VAL:HG12	5:X:586:ARG:HB2	1.91	0.53
1:B:282:VAL:HG21	1:B:312:LEU:HD23	1.90	0.53
2:C:1073:LYS:HB2	3:D:462:ASP:HB2	1.90	0.53
3:D:516:ASP:H	3:D:576:ARG:HH11	1.55	0.53
3:D:587:LEU:HD12	3:D:611:ILE:HD11	1.91	0.53
3:D:773:PHE:O	3:D:776:THR:HG22	2.09	0.53
1:G:68:TYR:CE1	1:G:171:LEU:HG	2.44	0.53
1:G:104:LYS:HD3	1:G:105:SER:N	2.24	0.53
5:Y:469:GLN:NE2	5:Y:473:GLU:OE2	2.37	0.53
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.74	0.53
2:C:908:GLU:HG2	2:C:909:LYS:H	1.72	0.53
3:D:88:CYS:SG	3:D:89:GLY:N	2.81	0.53
2:H:53:PHE:CE1	2:H:68:LEU:HB3	2.43	0.53
2:H:718:ALA:HB2	2:H:783:LEU:HG	1.91	0.53
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.42	0.53
3:I:18:ASP:OD1	3:I:1369:ARG:NH2	2.40	0.53
3:I:655:SER:HA	3:I:658:GLU:HG2	1.91	0.53
3:I:901:ARG:HB3	3:I:908:ILE:HA	1.90	0.53
5:X:445:ASP:OD1	5:X:445:ASP:N	2.36	0.53
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.91	0.53
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.91	0.53
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.90	0.53
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.44	0.53
5:X:162:ILE:HA	5:X:262:VAL:HG23	1.91	0.53
5:Y:585:GLU:O	5:Y:589:GLN:HG2	2.09	0.53
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.91	0.53
2:H:698:PRO:HD3	2:H:795:ALA:HB2	1.92	0.53
3:I:1341:ARG:NH2	3:I:1343:GLU:OE1	2.42	0.53
4:J:26:ARG:HD3	4:J:64:LEU:HD21	1.91	0.53
5:X:105:MET:CG	5:X:384:LEU:HD12	2.32	0.53
2:C:510:GLN:O	2:C:511:LEU:HB2	2.09	0.52
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.91	0.52
3:D:871:LEU:HD12	3:D:877:VAL:HG21	1.90	0.52
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.90	0.52
1:B:44:ARG:HD2	3:D:538:ARG:HH11	1.74	0.52
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.09	0.52
2:C:1134:GLN:O	2:C:1137:GLU:N	2.27	0.52
2:C:1238:LEU:HD23	2:C:1238:LEU:H	1.73	0.52
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.41	0.52
3:I:871:LEU:HD12	3:I:877:VAL:HG21	1.90	0.52
1:B:268:ASN:HA	1:B:271:LYS:HB3	1.90	0.52
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.73	0.52
2:H:906:PHE:CZ	5:Y:601:PRO:HB2	2.44	0.52
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.91	0.52
2:C:1051:LYS:HB3	2:C:1053:TYR:HE1	1.75	0.52
3:D:154:LEU:HD11	3:D:160:LEU:HD21	1.91	0.52
3:D:1353:VAL:HG13	3:D:1355:ARG:HG3	1.91	0.52
2:H:1238:LEU:HD23	2:H:1238:LEU:H	1.74	0.52
1:B:37:HIS:HD2	2:C:1216:ARG:HB3	1.74	0.52
2:H:106:GLU:HG2	2:H:111:GLU:HA	1.91	0.52
2:H:942:ASP:OD1	2:H:944:ARG:N	2.42	0.52
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.92	0.52
2:C:898:GLU:HG3	5:X:565:ILE:HD12	1.92	0.52
2:C:1330:ILE:HD11	3:D:331:ILE:HG21	1.92	0.52
5:Y:495:ARG:HA	5:Y:495:ARG:HE	1.75	0.52
3:D:849:LEU:H	3:D:856:ILE:HG22	1.74	0.52
3:D:1362:GLY:C	3:D:1364:ALA:H	2.17	0.52
3:I:213:LYS:O	3:I:217:LEU:HG	2.09	0.52
2:C:980:VAL:HG22	2:C:984:VAL:HG22	1.90	0.52
3:D:146:VAL:HA	3:D:178:ALA:HB1	1.91	0.52
2:H:342:ASP:OD1	2:H:342:ASP:N	2.41	0.52
2:H:452:ARG:NH1	2:H:585:GLY:HA3	2.25	0.52
5:X:166:VAL:H	5:X:259:PHE:CA	2.05	0.52
5:X:602:SER:HA	5:X:605:GLU:HB3	1.91	0.52
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.92	0.52
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.90	0.52
2:C:1200:LYS:C	2:C:1202:GLY:H	2.18	0.52
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.92	0.52
3:I:536:LEU:HG	3:I:541:LEU:O	2.09	0.52
3:I:665:GLN:HG2	3:I:678:ARG:NH1	2.25	0.52
3:I:813:ASP:HA	3:I:895:CYS:SG	2.50	0.52
5:X:167:ASP:HA	5:X:259:PHE:CZ	2.45	0.52
5:Y:597:LYS:O	5:Y:598:LEU:HD13	2.10	0.52
1:A:57:THR:HG21	1:A:147:GLN:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:THR:HG22	2:C:12:ARG:HH21	1.75	0.52
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.33	0.52
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.75	0.52
2:H:80:PHE:HB3	2:H:85:CYS:SG	2.50	0.52
2:H:247:ARG:HH12	2:H:271:ALA:HB2	1.75	0.52
3:I:1160:SER:H	3:I:1206:ARG:HG2	1.74	0.52
2:C:658:GLN:HB3	2:C:1186:VAL:HG11	1.92	0.51
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.92	0.51
3:D:1237:VAL:HG11	3:D:1253:ILE:HD12	1.91	0.51
1:F:164:ASP:C	1:F:166:ARG:H	2.16	0.51
2:H:549:ASP:OD1	2:H:550:VAL:N	2.43	0.51
2:H:905:ILE:HG12	5:Y:595:LEU:HD22	1.91	0.51
3:I:57:PHE:HB3	3:I:98:ARG:NH1	2.24	0.51
3:I:527:LEU:HD23	3:I:528:THR:N	2.23	0.51
3:I:919:ALA:O	3:I:923:ILE:HG12	2.10	0.51
5:Y:165:PHE:CA	5:Y:259:PHE:HB2	2.39	0.51
2:C:958:LYS:O	2:C:962:GLU:HG2	2.09	0.51
3:I:79:LYS:HG3	5:Y:569:THR:HG22	1.92	0.51
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.92	0.51
2:C:814:ASP:OD2	2:C:1106:ARG:NH2	2.43	0.51
1:G:165:GLU:O	1:G:165:GLU:CD	2.54	0.51
2:H:1200:LYS:C	2:H:1202:GLY:H	2.18	0.51
1:A:45:ARG:HD2	1:B:38:THR:OG1	2.10	0.51
1:B:186:ASN:HB2	1:B:202:VAL:HB	1.92	0.51
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.75	0.51
5:Y:599:ARG:C	5:Y:601:PRO:HD3	2.36	0.51
2:C:748:ILE:HD11	2:C:967:LEU:HA	1.91	0.51
2:C:785:ASP:OD1	2:C:791:LEU:N	2.39	0.51
3:D:9:LYS:HG3	3:D:11:GLN:HG2	1.92	0.51
3:D:94:GLN:HB2	3:D:97:VAL:HG23	1.93	0.51
3:D:482:ALA:HA	4:E:6:VAL:HG11	1.93	0.51
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.74	0.51
2:H:819:SER:HB2	2:H:1085:MET:SD	2.50	0.51
3:I:145:VAL:HG22	3:I:159:ILE:HG13	1.91	0.51
5:Y:161:LEU:HG	5:Y:162:ILE:HG23	1.92	0.51
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.93	0.51
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.92	0.51
3:D:849:LEU:N	3:D:856:ILE:HG22	2.25	0.51
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.26	0.51
2:H:741:MET:N	2:H:741:MET:SD	2.84	0.51
2:H:1246:ARG:NH2	2:H:1258:PRO:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:72:CYS:SG	3:I:73:GLY:N	2.84	0.51
3:I:552:ILE:HD13	3:I:570:LYS:HB2	1.92	0.51
3:I:930:LEU:HD23	3:I:1244:GLN:HG3	1.92	0.51
1:A:100:LEU:HB3	1:A:115:ILE:HD11	1.92	0.51
2:C:697:LYS:HE2	2:C:790:ASP:OD2	2.11	0.51
2:C:1291:LEU:O	3:D:345:LYS:NZ	2.38	0.51
1:G:112:ALA:HB3	1:G:126:PRO:HA	1.91	0.51
3:I:589:TYR:O	3:I:590:SER:HB2	2.09	0.51
3:I:843:VAL:HG11	3:I:897:HIS:HB3	1.93	0.51
3:I:1271:SER:HB2	3:I:1290:ARG:CZ	2.41	0.51
2:C:1270:PHE:CZ	2:C:1290:MET:HG2	2.45	0.51
3:D:809:VAL:HG13	3:D:912:GLY:H	1.75	0.51
2:H:542:ARG:O	2:H:544:GLY:N	2.44	0.51
3:I:42:GLU:O	3:I:55:GLY:HA3	2.11	0.51
3:I:306:LEU:HD23	3:I:307:LEU:HD23	1.91	0.51
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.92	0.51
5:X:374:ARG:NH2	5:X:377:LYS:HD2	2.25	0.51
2:C:539:THR:HG22	2:C:540:ARG:H	1.75	0.51
2:C:842:ASP:N	2:C:1046:VAL:HG21	2.25	0.51
3:D:512:TYR:HD2	3:D:724:MET:HE1	1.76	0.51
2:H:75:LEU:HD21	2:H:127:ILE:HD11	1.93	0.51
2:H:118:LYS:HG2	2:H:488:MET:H	1.74	0.51
2:H:898:GLU:HG3	5:Y:565:ILE:HD12	1.93	0.51
3:I:93:THR:O	3:I:94:GLN:HG2	2.11	0.51
3:I:1219:ASP:HA	3:I:1222:ARG:HB3	1.93	0.51
2:C:102:LEU:HD12	2:C:118:LYS:HD3	1.92	0.51
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.93	0.51
1:F:186:ASN:HB3	1:F:188:GLU:HG3	1.93	0.51
2:H:1240:ASP:HA	3:I:445:LYS:HE2	1.93	0.51
3:I:389:GLY:O	3:I:391:ALA:N	2.44	0.51
5:X:452:ILE:HD11	5:X:500:ILE:HG22	1.92	0.51
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.76	0.50
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.92	0.50
2:C:646:SER:O	2:C:647:ARG:HB3	2.11	0.50
3:D:334:LYS:HE3	3:D:1324:SER:O	2.11	0.50
3:D:1264:ALA:HA	3:D:1305:ASP:HB2	1.93	0.50
3:I:501:VAL:HG21	3:I:602:SER:HB2	1.92	0.50
3:I:733:SER:O	3:I:737:ILE:HG12	2.11	0.50
5:X:423:ARG:HB3	5:X:425:TYR:HD1	1.75	0.50
2:C:517:GLN:HE21	2:C:760:ASN:H	1.58	0.50
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:309:ASN:HB2	3:D:326:SER:HB3	1.93	0.50
3:D:530:PRO:HB2	3:D:581:MET:HG2	1.93	0.50
4:E:38:LEU:HD11	4:E:67:ARG:HH12	1.75	0.50
1:F:78:ILE:HD13	1:F:81:ILE:HD12	1.93	0.50
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.92	0.50
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.76	0.50
5:Y:143:TYR:HA	5:Y:146:GLU:HB2	1.94	0.50
1:A:190:ALA:H	1:A:199:ASP:HA	1.77	0.50
2:C:71:VAL:HG12	2:C:72:SER:HB3	1.91	0.50
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.93	0.50
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.46	0.50
1:F:197:ASP:O	1:F:198:LEU:HD23	2.11	0.50
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.92	0.50
2:H:1259:LEU:HD12	3:I:346:ARG:NH1	2.25	0.50
3:I:311:ARG:HH22	3:I:1329:THR:HG21	1.75	0.50
5:Y:511:ILE:HG23	5:Y:517:SER:HB3	1.93	0.50
1:B:17:GLU:HG3	1:B:17:GLU:O	2.10	0.50
2:C:360:LEU:HD11	2:C:378:ARG:HG2	1.92	0.50
3:D:914:ALA:O	3:D:918:ILE:HG22	2.11	0.50
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.11	0.50
3:D:1333:THR:O	3:D:1337:VAL:HG23	2.11	0.50
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.47	0.50
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.93	0.50
2:H:3:TYR:HD2	2:H:6:THR:HG21	1.75	0.50
2:H:594:VAL:HG22	2:H:599:VAL:HG22	1.93	0.50
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.93	0.50
5:X:157:ARG:NH1	5:X:159:SER:H	2.10	0.50
5:Y:157:ARG:HG3	5:Y:159:SER:HB2	1.92	0.50
2:C:1167:GLU:HA	2:C:1170:MET:HB2	1.94	0.50
3:D:44:ILE:HG22	5:X:450:ILE:HG22	1.93	0.50
3:D:205:LEU:HD13	3:D:217:LEU:HB3	1.93	0.50
3:D:381:ILE:HG21	3:D:408:VAL:HG23	1.94	0.50
3:D:842:ARG:HB3	3:D:882:VAL:CG2	2.41	0.50
4:J:26:ARG:HB2	4:J:64:LEU:HD11	1.92	0.50
2:C:106:GLU:N	2:C:107:ARG:HA	2.14	0.50
2:C:289:VAL:HG13	2:C:319:LEU:HD22	1.94	0.50
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.94	0.50
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.94	0.50
3:D:1280:VAL:HA	3:D:1283:SER:HB3	1.93	0.50
2:H:187:GLU:OE2	2:H:197:ARG:NE	2.38	0.50
2:H:1119:MET:HE2	2:H:1227:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HG3	1:B:183:ILE:HG22	1.93	0.50
2:C:1247:SER:HB3	3:D:375:GLU:O	2.12	0.50
3:D:1372:ARG:HG3	3:I:853:THR:OG1	2.11	0.50
2:H:478:ARG:HA	2:H:481:LEU:HD12	1.94	0.50
2:H:1219:GLU:OE2	3:I:634:ARG:NH1	2.44	0.50
2:C:890:LYS:HE2	2:C:893:THR:HG21	1.93	0.50
2:C:1222:GLU:OE1	3:D:537:TYR:OH	2.21	0.50
3:D:230:SER:HB2	3:D:1339:GLY:H	1.77	0.50
3:D:308:ASP:OD1	3:D:311:ARG:NH1	2.44	0.50
3:I:205:LEU:HD13	3:I:217:LEU:HB3	1.93	0.50
2:C:6:THR:HG22	2:C:12:ARG:NH2	2.27	0.49
2:C:153:PRO:HG2	2:C:179:TYR:HD1	1.76	0.49
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.47	0.49
2:C:1002:LEU:HD13	2:C:1003:THR:N	2.27	0.49
3:D:46:TYR:HB3	5:X:451:ARG:O	2.12	0.49
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.27	0.49
3:I:804:ALA:O	3:I:916:GLY:HA3	2.12	0.49
2:C:487:LEU:HA	2:C:488:MET:CB	2.37	0.49
2:C:935:THR:HA	2:C:1048:LYS:HB3	1.94	0.49
3:D:282:LEU:HD13	3:D:291:ILE:HG22	1.94	0.49
1:G:13:LEU:O	1:G:28:LEU:HA	2.12	0.49
2:H:812:PHE:HB2	3:I:357:VAL:HG21	1.94	0.49
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.47	0.49
5:X:165:PHE:HB3	5:X:259:PHE:CG	2.45	0.49
2:C:1335:ILE:HD12	3:D:22:ILE:HD11	1.94	0.49
3:D:339:ARG:O	3:D:340:GLN:NE2	2.44	0.49
2:H:131:THR:HG21	2:H:135:THR:HG22	1.95	0.49
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.44	0.49
3:I:1177:ILE:HD11	3:I:1196:LEU:HD11	1.95	0.49
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.93	0.49
1:B:263:THR:HG22	1:B:302:GLU:HG2	1.94	0.49
2:C:144:VAL:HG23	2:C:515:MET:HG3	1.94	0.49
2:C:540:ARG:HD3	2:C:567:PRO:HB2	1.93	0.49
1:G:37:HIS:HE1	1:G:187:VAL:HG22	1.78	0.49
2:H:197:ARG:NH1	2:H:201:ARG:O	2.44	0.49
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.43	0.49
5:X:231:THR:HG23	5:X:249:ILE:HG12	1.94	0.49
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.93	0.49
3:D:262:THR:OG1	3:D:263:SER:N	2.46	0.49
3:D:910:ASN:HB3	4:E:15:ASN:ND2	2.27	0.49
3:D:1344:LEU:O	3:D:1350:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:GLU:HB2	2:H:694:ARG:HH22	1.76	0.49
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.95	0.49
2:H:1270:PHE:CE1	2:H:1290:MET:HG2	2.48	0.49
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.47	0.49
3:I:877:VAL:O	3:I:879:ALA:N	2.40	0.49
5:X:96:ASP:O	5:X:100:MET:HB2	2.11	0.49
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.45	0.49
3:D:1286:LYS:HA	3:D:1289:ASN:HB3	1.94	0.49
1:F:195:ARG:O	1:F:198:LEU:HG	2.12	0.49
3:I:714:GLU:HG3	3:I:715:LYS:H	1.77	0.49
5:X:292:VAL:HG11	5:X:299:LYS:HG2	1.94	0.49
1:B:14:VAL:HG22	1:B:28:LEU:HD22	1.93	0.49
2:C:59:ILE:H	2:C:59:ILE:HD12	1.77	0.49
2:C:493:ILE:O	5:X:472:GLN:NE2	2.46	0.49
3:D:1250:ASP:O	3:D:1254:GLU:HG3	2.12	0.49
2:H:15:PHE:CE2	2:H:1182:ILE:HD11	2.48	0.49
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.95	0.49
5:X:163:THR:OG1	5:X:261:LEU:O	2.27	0.49
5:Y:255:VAL:HA	5:Y:258:GLN:HG3	1.93	0.49
5:Y:290:LEU:HD13	5:Y:336:GLU:HB3	1.94	0.49
2:C:338:THR:HB	2:C:345:PRO:HG3	1.94	0.49
2:C:718:ALA:HA	2:C:751:TYR:CE1	2.48	0.49
2:C:729:ALA:O	2:C:755:LYS:HD2	2.12	0.49
2:C:758:ARG:HA	2:C:833:ILE:HD12	1.94	0.49
3:D:423:LEU:HB3	3:D:466:MET:HE2	1.93	0.49
2:H:1038:GLN:HG2	2:H:1039:GLY:H	1.77	0.49
5:X:165:PHE:C	5:X:259:PHE:HD2	2.20	0.49
3:D:584:PRO:HD2	3:D:587:LEU:HD22	1.94	0.49
3:D:733:SER:OG	3:D:736:GLN:OE1	2.29	0.49
5:X:105:MET:O	5:X:108:VAL:HG13	2.13	0.49
5:X:279:ARG:NH2	5:X:347:ILE:HG12	2.28	0.49
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.94	0.49
1:B:313:SER:OG	1:B:314:LEU:N	2.42	0.49
3:D:493:PRO:HB3	3:D:918:ILE:HD11	1.94	0.49
3:D:811:GLU:OE2	3:D:890:THR:OG1	2.17	0.49
3:D:890:THR:HG21	3:D:894:VAL:HA	1.94	0.49
1:G:181:GLU:HA	3:I:535:ARG:HD3	1.93	0.49
2:H:992:LEU:HG	2:H:996:ARG:HG2	1.95	0.49
2:H:1180:MET:HG3	2:H:1181:PRO:O	2.12	0.49
3:I:205:LEU:HB3	3:I:217:LEU:HD13	1.94	0.49
3:I:615:LYS:HE3	4:J:5:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:306:PHE:O	5:X:310:GLU:HG2	2.13	0.49
1:A:167:PRO:HB2	1:A:170:ARG:HG3	1.94	0.48
3:D:144:TYR:CD2	3:D:180:MET:HB3	2.48	0.48
3:D:744:ARG:HD2	3:D:763:PHE:CZ	2.48	0.48
3:D:1291:GLU:HA	3:D:1296:GLY:HA2	1.95	0.48
2:H:1267:GLY:HA3	3:I:347:VAL:O	2.13	0.48
3:I:262:THR:O	5:Y:507:MET:N	2.34	0.48
3:I:506:VAL:HG21	3:I:625:MET:HA	1.94	0.48
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.94	0.48
1:A:67:GLU:HA	1:A:78:ILE:HG21	1.94	0.48
2:C:102:LEU:HB3	2:C:118:LYS:HB2	1.94	0.48
2:C:722:GLY:HA3	2:C:735:LYS:O	2.13	0.48
2:C:975:ILE:HD11	2:C:1011:LEU:HD21	1.95	0.48
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	1.95	0.48
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.28	0.48
1:G:104:LYS:HD3	1:G:105:SER:H	1.78	0.48
2:H:956:ALA:HB3	2:H:1032:LYS:HE3	1.95	0.48
2:H:1072:ASN:OD1	2:H:1072:ASN:N	2.45	0.48
2:C:672:GLU:HG2	2:C:1186:VAL:O	2.12	0.48
2:C:1299:ASN:HB3	2:C:1303:LYS:HE3	1.95	0.48
3:D:270:ARG:HE	5:X:449:THR:HG22	1.78	0.48
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.95	0.48
1:B:196:THR:HB	3:D:443:GLU:HG3	1.95	0.48
2:C:98:VAL:HG11	2:C:124:MET:SD	2.54	0.48
2:C:1290:MET:HG3	3:D:347:VAL:HG11	1.95	0.48
1:F:189:ALA:HA	1:F:199:ASP:HA	1.95	0.48
2:H:131:THR:HG22	2:H:135:THR:N	2.28	0.48
3:I:94:GLN:HB2	3:I:97:VAL:HG23	1.94	0.48
3:I:128:LEU:HA	3:I:192:MET:HE1	1.96	0.48
3:I:286:ALA:HB2	5:Y:373:ARG:NH2	2.29	0.48
5:X:458:GLU:HA	5:X:461:ASN:HD22	1.79	0.48
5:Y:112:THR:HG22	5:Y:113:ARG:N	2.29	0.48
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.29	0.48
2:C:856:ASN:ND2	5:X:609:SER:O	2.45	0.48
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	1.93	0.48
2:C:1339:LEU:HD23	3:D:17:PHE:CD2	2.49	0.48
2:H:941:LYS:NZ	2:H:949:GLU:OE1	2.40	0.48
2:H:1333:LEU:HB2	2:H:1335:ILE:HG22	1.96	0.48
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.12	0.48
1:A:50:SER:HA	1:A:150:ARG:HD2	1.96	0.48
2:C:164:THR:HG23	2:C:165:HIS:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:234:ASP:HB2	2:C:236:LYS:HE2	1.95	0.48
2:C:1141:LEU:C	2:C:1141:LEU:HD12	2.39	0.48
3:D:370:LYS:HD3	3:D:443:GLU:CD	2.39	0.48
2:H:153:PRO:HA	2:H:177:ILE:HG22	1.95	0.48
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.12	0.48
3:I:849:LEU:HD12	3:I:849:LEU:H	1.79	0.48
2:C:1293:VAL:HG23	2:C:1300:GLY:C	2.38	0.48
3:D:701:LEU:HD23	3:D:723:TYR:HB2	1.95	0.48
5:Y:412:LEU:HD13	5:Y:435:ILE:HD11	1.95	0.48
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.48	0.48
2:C:120:GLN:CD	2:C:490:GLN:HB2	2.39	0.48
2:C:358:ASP:OD1	2:C:361:SER:OG	2.21	0.48
2:C:848:GLU:HG2	2:C:888:THR:HA	1.95	0.48
3:I:837:ASP:HA	3:I:868:TRP:HE1	1.79	0.48
3:I:1173:ARG:HA	3:I:1174:ARG:C	2.38	0.48
5:Y:151:VAL:HG11	5:Y:158:LEU:HB2	1.96	0.48
5:Y:277:MET:HE3	5:Y:281:ARG:HE	1.78	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:NH2	2.29	0.48
2:H:198:ILE:H	2:H:369:MET:HE1	1.78	0.48
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.79	0.48
3:I:1135:THR:HB	3:I:1140:ARG:HD3	1.96	0.48
5:X:105:MET:O	5:X:105:MET:HG2	2.14	0.48
5:X:287:ILE:HG22	5:X:302:PHE:HZ	1.79	0.48
5:X:511:ILE:HG23	5:X:512:GLY:H	1.78	0.48
5:Y:162:ILE:C	5:Y:262:VAL:HG13	2.39	0.48
2:C:1136:GLN:O	2:C:1139:ALA:HB2	2.14	0.47
3:D:298:MET:SD	5:X:402:LEU:HB3	2.54	0.47
5:X:98:VAL:HB	5:X:402:LEU:HD21	1.96	0.47
2:C:756:TYR:H	2:C:766:ASN:HB2	1.79	0.47
2:C:906:PHE:HZ	5:X:601:PRO:HB2	1.78	0.47
2:C:985:GLU:HG3	2:C:988:LYS:HB2	1.94	0.47
3:D:430:HIS:NE2	3:D:432:LEU:HB2	2.29	0.47
3:D:1289:ASN:ND2	3:D:1293:GLU:OE1	2.47	0.47
1:F:104:LYS:HG3	1:F:110:VAL:HG13	1.95	0.47
2:H:407:ARG:HH22	2:H:609:ILE:HG21	1.79	0.47
2:H:629:PHE:CE2	2:H:634:VAL:HG21	2.49	0.47
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.38	0.47
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.95	0.47
2:C:1271:GLY:HA2	3:D:344:GLY:H	1.79	0.47
3:D:201:LEU:HB3	3:D:221:ILE:HG22	1.96	0.47
3:D:515:ARG:NH1	3:D:717:VAL:HB	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:536:LEU:HG	3:D:541:LEU:O	2.13	0.47
1:F:152:TYR:CZ	2:H:824:GLN:HA	2.49	0.47
1:F:190:ALA:H	1:F:199:ASP:HA	1.79	0.47
1:G:16:ILE:HG12	1:G:26:VAL:HG13	1.97	0.47
3:I:56:LEU:O	3:I:250:ARG:NH2	2.39	0.47
3:I:576:ARG:NH2	3:I:594:GLN:O	2.47	0.47
3:I:1289:ASN:ND2	3:I:1293:GLU:OE1	2.47	0.47
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.79	0.47
3:D:173:GLY:O	3:D:175:GLU:HG3	2.14	0.47
3:D:747:MET:O	3:D:755:ILE:HG22	2.14	0.47
3:D:860:ARG:HH21	3:D:883:ARG:HH22	1.61	0.47
3:D:1247:LYS:H	3:D:1247:LYS:HG2	1.51	0.47
2:H:490:GLN:NE2	5:Y:472:GLN:O	2.47	0.47
3:I:1197:ASN:HB3	3:I:1210:ILE:HA	1.96	0.47
5:X:105:MET:HE3	5:X:385:ARG:NH1	2.30	0.47
5:X:134:VAL:HG22	5:X:273:MET:HE1	1.96	0.47
2:C:808:ASN:H	3:D:633:ALA:HB2	1.79	0.47
2:C:1108:ASN:ND2	2:C:1111:GLN:OE1	2.47	0.47
2:H:82:VAL:HG23	2:H:137:VAL:HG21	1.97	0.47
2:H:170:VAL:HG23	2:H:171:LEU:H	1.80	0.47
2:H:673:HIS:O	2:H:1109:ILE:HG22	2.15	0.47
2:H:1067:ALA:HB2	2:H:1073:LYS:HA	1.97	0.47
2:H:1108:ASN:ND2	2:H:1108:ASN:O	2.46	0.47
3:I:161:THR:O	3:I:165:TYR:N	2.43	0.47
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.96	0.47
3:I:1152:GLU:HG3	3:I:1214:PRO:HD2	1.97	0.47
3:I:1358:PRO:HB3	3:I:1366:HIS:CG	2.49	0.47
5:Y:166:VAL:HG13	5:Y:260:ARG:HG2	1.97	0.47
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.15	0.47
3:D:1369:ARG:HA	3:D:1372:ARG:HB2	1.95	0.47
2:H:360:LEU:HD11	2:H:378:ARG:HG2	1.95	0.47
1:A:35:PHE:HA	1:A:38:THR:HB	1.96	0.47
2:C:130:MET:HE3	2:C:136:PHE:CZ	2.50	0.47
2:C:587:LEU:HD12	2:C:587:LEU:HA	1.73	0.47
2:C:818:VAL:HA	2:C:1096:ILE:HG22	1.96	0.47
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.50	0.47
3:D:514:THR:HG21	3:D:596:LEU:HA	1.96	0.47
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.47
3:D:1166:GLY:N	3:D:1176:VAL:O	2.35	0.47
3:D:1173:ARG:HA	3:D:1174:ARG:C	2.39	0.47
1:G:44:ARG:HD3	1:G:185:TYR:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:314:ASN:O	2:H:314:ASN:ND2	2.48	0.47
2:H:1110:GLY:HA2	2:H:1113:LEU:HD13	1.97	0.47
2:H:1131:MET:SD	2:H:1141:LEU:HD12	2.55	0.47
3:I:518:VAL:HA	3:I:547:ARG:HH12	1.78	0.47
3:I:528:THR:HA	3:I:529:GLY:HA2	1.59	0.47
3:I:716:GLN:O	3:I:717:VAL:HG23	2.14	0.47
2:C:672:GLU:O	3:D:767:LEU:HB2	2.15	0.47
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.95	0.47
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.96	0.47
2:C:8:LYS:HE3	2:C:8:LYS:HB3	1.54	0.47
2:C:805:MET:HE1	2:C:1221:PHE:CD1	2.49	0.47
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.97	0.47
3:D:394:ILE:HG21	5:X:536:THR:HA	1.96	0.47
3:D:1175:LEU:H	3:D:1175:LEU:HD12	1.80	0.47
2:H:187:GLU:OE2	2:H:203:LYS:HD3	2.14	0.47
2:H:303:ASP:OD1	2:H:310:ILE:HD11	2.15	0.47
2:H:513:GLN:OE1	2:H:526:HIS:NE2	2.48	0.47
3:I:528:THR:HG22	3:I:551:ARG:HB2	1.97	0.47
3:I:537:TYR:CE1	3:I:544:LEU:HG	2.49	0.47
3:I:1350:ASN:HA	3:I:1353:VAL:HG12	1.97	0.47
5:X:383:ASN:HB3	5:X:386:LEU:HD12	1.97	0.47
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.97	0.47
2:C:718:ALA:HA	2:C:751:TYR:HE1	1.80	0.47
3:D:107:LEU:HD23	3:D:299:LEU:HD21	1.97	0.47
3:D:819:GLY:H	3:D:881:LYS:HE2	1.79	0.47
2:H:91:THR:HG21	2:H:503:LYS:HE3	1.96	0.47
2:H:180:ARG:CZ	2:H:465:ARG:HD2	2.45	0.47
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.50	0.47
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.15	0.47
2:C:55:SER:O	2:C:67:GLU:HB3	2.16	0.46
3:D:268:LEU:HD22	3:D:324:LEU:HD23	1.98	0.46
3:D:678:ARG:O	3:D:682:VAL:HG13	2.14	0.46
2:H:135:THR:HG21	2:H:142:GLU:OE1	2.15	0.46
2:H:657:THR:OG1	2:H:1187:PHE:HB2	2.15	0.46
3:I:156:ARG:HD3	3:I:157:GLN:HG3	1.96	0.46
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.97	0.46
3:I:1167:LYS:HB3	3:I:1170:LYS:HB2	1.97	0.46
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.15	0.46
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.80	0.46
2:C:803:ALA:HB2	2:C:1094:VAL:HG11	1.97	0.46
2:C:1106:ARG:HE	3:D:731:ARG:HH22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.49	0.46
2:H:1007:LYS:HA	2:H:1010:GLN:HE21	1.80	0.46
3:I:62:PHE:CD1	3:I:247:PRO:HD3	2.50	0.46
3:I:149:GLY:HA2	3:I:176:PHE:HB2	1.96	0.46
3:I:1238:GLN:HE22	3:I:1248:ILE:HG23	1.81	0.46
2:C:407:ARG:HH22	2:C:609:ILE:CD1	2.28	0.46
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	1.97	0.46
2:C:1337:ILE:HG22	3:D:22:ILE:HG13	1.97	0.46
2:H:14:ASP:HA	2:H:1158:LYS:HE2	1.96	0.46
2:H:529:ARG:HH22	2:H:687:ARG:NH2	2.12	0.46
2:H:646:SER:O	2:H:647:ARG:HB3	2.14	0.46
2:H:759:SER:OG	2:H:760:ASN:N	2.46	0.46
3:I:261:ALA:HA	5:Y:505:ILE:O	2.15	0.46
3:I:591:ILE:HD12	3:I:592:VAL:HG13	1.98	0.46
5:X:555:GLU:HG2	5:X:590:ILE:HG23	1.97	0.46
2:C:856:ASN:HD21	5:X:609:SER:C	2.24	0.46
3:D:75:TYR:HD2	3:D:80:HIS:CG	2.34	0.46
3:D:161:THR:HB	3:D:164:GLN:HG3	1.97	0.46
3:D:292:VAL:O	3:D:296:LYS:HG3	2.16	0.46
3:D:555:TYR:H	3:D:589:TYR:HD2	1.64	0.46
2:H:1313:HIS:CE1	4:J:31:GLN:HE22	2.32	0.46
3:I:1156:LEU:HB2	3:I:1223:LEU:HD23	1.98	0.46
2:C:75:LEU:HD23	2:C:96:LEU:HD13	1.96	0.46
2:C:672:GLU:HB3	2:C:1187:PHE:CD1	2.50	0.46
2:C:678:ARG:HH21	2:C:1106:ARG:HG2	1.80	0.46
2:C:687:ARG:HE	2:C:687:ARG:HB2	1.60	0.46
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.97	0.46
2:C:826:ASP:OD1	2:C:829:THR:HG21	2.15	0.46
2:C:897:PRO:HB3	5:X:563:PHE:O	2.15	0.46
2:C:1243:MET:SD	3:D:445:LYS:HG2	2.55	0.46
3:D:255:LEU:HB2	3:D:259:ARG:O	2.16	0.46
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.98	0.46
3:D:813:ASP:HA	3:D:895:CYS:HB2	1.96	0.46
3:D:1322:ALA:O	3:D:1326:GLN:HG2	2.16	0.46
2:H:324:LYS:HA	2:H:327:GLN:HB3	1.97	0.46
2:H:1105:SER:HB2	3:I:731:ARG:HB2	1.96	0.46
3:I:590:SER:O	3:I:594:GLN:HB2	2.16	0.46
5:Y:148:TYR:HE2	5:Y:152:GLU:HG2	1.80	0.46
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.79	0.46
1:B:12:ARG:HB2	1:B:30:PRO:HG2	1.98	0.46
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:805:GLN:OE1	3:D:1348:LYS:HE2	2.15	0.46
2:H:124:MET:HE2	2:H:124:MET:HB3	1.87	0.46
2:H:302:ILE:HG22	2:H:309:LEU:HA	1.96	0.46
3:I:169:LEU:HD22	3:I:173:GLY:HA2	1.98	0.46
3:I:423:LEU:O	3:I:434:ILE:HA	2.16	0.46
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.97	0.46
2:C:82:VAL:HB	2:C:92:TYR:CD2	2.50	0.46
2:C:239:MET:HE2	2:C:285:ILE:HD11	1.98	0.46
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.49	0.46
2:C:756:TYR:H	2:C:766:ASN:CB	2.29	0.46
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.81	0.46
2:C:1330:ILE:CG2	2:C:1335:ILE:HD11	2.46	0.46
2:H:122:VAL:HG21	2:H:493:ILE:CG2	2.46	0.46
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	1.98	0.46
3:I:1272:SER:HB3	3:I:1276:GLU:OE1	2.16	0.46
2:C:1278:LEU:HD21	2:C:1286:THR:HG22	1.98	0.46
3:D:93:THR:O	3:D:94:GLN:HG2	2.15	0.46
3:D:530:PRO:HG3	3:D:580:TRP:CE3	2.51	0.46
3:D:885:VAL:O	3:D:1258:ARG:HD3	2.16	0.46
2:H:710:VAL:HA	2:H:715:THR:HG21	1.97	0.46
2:H:1222:GLU:OE1	3:I:537:TYR:OH	2.27	0.46
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.51	0.46
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.98	0.46
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.45	0.46
3:D:21:LYS:HG2	3:D:22:ILE:N	2.31	0.46
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.80	0.46
2:H:106:GLU:O	2:H:114:VAL:HG23	2.16	0.46
2:H:131:THR:CG2	2:H:135:THR:HG22	2.45	0.46
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.98	0.46
2:H:660:VAL:HG22	2:H:661:VAL:H	1.81	0.46
3:I:363:LEU:O	3:I:486:SER:OG	2.24	0.46
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.15	0.46
5:Y:276:MET:HE2	5:Y:276:MET:HB2	1.85	0.46
3:D:1206:ARG:NH1	3:I:1298:VAL:HG11	2.31	0.46
2:H:551:HIS:CE1	2:H:553:THR:HG1	2.34	0.46
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.98	0.46
2:H:1043:ALA:C	2:H:1045:GLY:H	2.24	0.46
3:I:11:GLN:HE21	3:I:11:GLN:HB3	1.62	0.46
3:I:572:THR:OG1	3:I:573:THR:N	2.49	0.46
3:I:706:VAL:HA	3:I:714:GLU:O	2.16	0.46
3:I:931:THR:O	3:I:931:THR:OG1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1154:ALA:HB1	3:I:1211:SER:HB3	1.97	0.46
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.51	0.46
2:C:1135:GLN:HA	2:C:1136:GLN:HA	1.64	0.45
3:D:427:PRO:O	3:D:429:LEU:HD22	2.15	0.45
3:D:747:MET:HE3	3:D:775:SER:HB2	1.97	0.45
3:D:1156:LEU:HD11	3:D:1224:ARG:HH21	1.81	0.45
3:D:1262:ARG:HD3	3:D:1279:GLN:OE1	2.16	0.45
1:G:130:ILE:HG22	1:G:131:CYS:SG	2.55	0.45
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.98	0.45
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.98	0.45
3:I:475:GLU:OE2	4:J:28:ARG:NH2	2.49	0.45
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.49	0.45
5:X:506:SER:O	5:X:509:THR:OG1	2.28	0.45
5:Y:112:THR:HG22	5:Y:113:ARG:HG2	1.97	0.45
1:B:52:PRO:O	1:B:179:PRO:HD3	2.16	0.45
2:C:409:LEU:HD12	2:C:427:ASP:HB3	1.99	0.45
2:C:705:GLU:HB2	2:C:794:LEU:H	1.82	0.45
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.97	0.45
2:C:914:LYS:HG2	2:C:915:ASP:H	1.81	0.45
2:C:1270:PHE:CE2	2:C:1290:MET:HG2	2.51	0.45
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.98	0.45
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.52	0.45
3:D:514:THR:HG22	3:D:515:ARG:H	1.80	0.45
3:D:583:VAL:HG21	3:D:593:ASN:OD1	2.16	0.45
1:F:111:THR:HG22	1:F:129:VAL:HG22	1.99	0.45
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.98	0.45
2:H:700:VAL:HA	2:H:1182:ILE:HG22	1.98	0.45
3:I:1170:LYS:O	3:I:1173:ARG:HD2	2.17	0.45
3:I:1247:LYS:H	3:I:1247:LYS:HG2	1.56	0.45
5:Y:162:ILE:C	5:Y:162:ILE:HD12	2.42	0.45
5:Y:474:MET:HE3	5:Y:474:MET:HB3	1.84	0.45
3:D:146:VAL:HA	3:D:178:ALA:CB	2.45	0.45
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.50	0.45
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.98	0.45
3:D:1157:ALA:O	3:D:1207:GLY:N	2.49	0.45
2:H:234:ASP:HB2	2:H:236:LYS:HE2	1.99	0.45
2:H:804:PHE:HE1	2:H:1115:THR:HG21	1.80	0.45
3:I:413:ASP:O	3:I:417:ARG:HG2	2.16	0.45
5:X:457:ILE:O	5:X:461:ASN:ND2	2.49	0.45
5:Y:105:MET:O	5:Y:108:VAL:HG13	2.16	0.45
5:Y:448:ARG:HD2	5:Y:452:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:O	1:B:28:LEU:HA	2.16	0.45
2:C:582:ASN:HB3	2:C:586:PHE:N	2.32	0.45
3:D:81:ARG:CG	3:D:82:GLY:N	2.76	0.45
3:D:1170:LYS:O	3:D:1173:ARG:HD2	2.16	0.45
3:D:1258:ARG:HG3	3:D:1259:GLN:N	2.32	0.45
1:F:166:ARG:O	1:F:167:PRO:C	2.60	0.45
1:B:35:PHE:O	1:B:39:LEU:HG	2.17	0.45
2:C:600:THR:HG22	2:C:601:ASP:H	1.81	0.45
2:C:886:LYS:HE2	2:C:916:SER:CB	2.46	0.45
3:D:849:LEU:HA	3:D:856:ILE:N	2.31	0.45
2:H:1115:THR:HG22	2:H:1228:GLY:HA3	1.97	0.45
3:I:74:LYS:HD2	3:I:87:LYS:HE3	1.97	0.45
3:I:518:VAL:HA	3:I:547:ARG:NH1	2.30	0.45
1:A:3:GLY:HA3	1:A:4:SER:HA	1.59	0.45
1:A:90:VAL:HG11	1:A:146:VAL:HG11	1.99	0.45
2:C:744:GLY:HA2	2:C:974:ARG:HH11	1.82	0.45
2:C:814:ASP:OD1	2:C:1106:ARG:NH1	2.50	0.45
3:D:437:PHE:HZ	3:D:453:VAL:HG21	1.81	0.45
1:G:181:GLU:O	3:I:535:ARG:NH1	2.48	0.45
2:H:145:ILE:HG22	2:H:456:VAL:HG22	1.98	0.45
2:H:510:GLN:O	2:H:511:LEU:HB2	2.16	0.45
2:H:1292:THR:OG1	2:H:1293:VAL:N	2.49	0.45
3:I:587:LEU:H	3:I:611:ILE:HD11	1.81	0.45
3:I:914:ALA:O	3:I:918:ILE:HG22	2.17	0.45
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.52	0.45
5:Y:157:ARG:NH1	5:Y:159:SER:N	2.65	0.45
2:C:105:TYR:HA	2:C:106:GLU:HA	1.47	0.45
2:C:841:ARG:HB2	2:C:848:GLU:CD	2.42	0.45
2:H:1135:GLN:HA	2:H:1136:GLN:HA	1.62	0.45
5:Y:311:THR:O	5:Y:345:GLN:NE2	2.49	0.45
2:C:28:LEU:HD21	2:C:524:ILE:HG12	1.98	0.45
2:C:88:ARG:NH2	2:C:1040:ASP:HA	2.31	0.45
2:C:685:MET:CE	2:C:1073:LYS:HG2	2.47	0.45
3:D:704:GLU:O	3:D:705:THR:OG1	2.32	0.45
3:D:1134:ILE:HD12	3:D:1134:ILE:O	2.16	0.45
3:D:1140:ARG:NH2	3:D:1144:LEU:HD21	2.30	0.45
2:H:53:PHE:CZ	2:H:68:LEU:HB3	2.52	0.45
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	1.99	0.45
2:H:901:LEU:O	2:H:905:ILE:HG13	2.17	0.45
3:I:193:ASP:HB3	3:I:196:GLN:HB2	1.98	0.45
3:I:370:LYS:HA	3:I:441:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:479:GLU:HG3	4:J:20:VAL:HG11	1.98	0.45
5:X:288:MET:HE1	5:X:303:ILE:HD11	1.99	0.45
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.16	0.45
1:B:65:LEU:HB3	1:B:168:ILE:HG21	1.98	0.45
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.98	0.45
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.52	0.45
4:J:59:ILE:HG23	4:J:64:LEU:HG	1.99	0.45
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.79	0.45
1:A:142:MET:HE2	1:A:142:MET:HB3	1.89	0.45
3:D:343:LEU:HG	3:D:344:GLY:N	2.31	0.45
3:D:504:GLN:HA	3:D:730:ALA:HA	1.99	0.45
3:D:1323:ALA:HA	3:D:1331:VAL:HG11	1.97	0.45
2:H:393:ASP:N	2:H:393:ASP:OD1	2.46	0.45
2:H:985:GLU:HG3	2:H:988:LYS:HB2	1.99	0.45
3:I:538:ARG:HA	3:I:539:SER:HA	1.64	0.45
3:I:777:HIS:NE2	3:I:781:LYS:HD3	2.32	0.45
3:I:819:GLY:H	3:I:881:LYS:HE2	1.81	0.45
3:I:1169:THR:HA	3:I:1173:ARG:O	2.17	0.45
3:I:1175:LEU:H	3:I:1175:LEU:HD12	1.82	0.45
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.99	0.45
5:Y:562:ARG:HD3	5:Y:573:LEU:HG	1.99	0.45
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.52	0.44
2:C:844:LYS:HD3	2:C:844:LYS:HA	1.77	0.44
2:C:943:LYS:O	2:C:947:GLU:HG2	2.17	0.44
2:C:1289:GLU:HA	2:C:1293:VAL:HG12	1.98	0.44
3:D:186:GLN:CG	3:D:238:ILE:HD11	2.46	0.44
3:D:841:GLY:HA3	3:D:901:ARG:HD3	2.00	0.44
2:H:338:THR:HB	2:H:345:PRO:HG3	1.99	0.44
2:H:1247:SER:O	3:I:348:ASP:HB3	2.17	0.44
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.82	0.44
3:I:251:PRO:HD2	5:Y:507:MET:HE1	1.99	0.44
5:X:151:VAL:HG22	5:X:156:ALA:HB3	1.99	0.44
5:Y:105:MET:SD	5:Y:384:LEU:HD12	2.57	0.44
2:C:807:TRP:HE1	2:C:1086:PRO:HD3	1.82	0.44
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.97	0.44
3:D:527:LEU:H	3:D:550:VAL:HG12	1.82	0.44
3:D:528:THR:HA	3:D:529:GLY:HA2	1.55	0.44
3:D:796:LEU:HG	3:D:800:LEU:HD23	1.99	0.44
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.82	0.44
2:H:895:LEU:HD13	2:H:895:LEU:HA	1.79	0.44
2:H:1011:LEU:HA	2:H:1014:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1137:GLU:C	2:H:1139:ALA:N	2.74	0.44
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.99	0.44
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.82	0.44
3:I:516:ASP:OD1	3:I:516:ASP:N	2.49	0.44
5:X:108:VAL:HG23	5:X:110:LEU:HG	1.99	0.44
5:X:222:ALA:O	5:X:226:ALA:N	2.45	0.44
2:C:4:SER:O	2:C:5:TYR:HB2	2.16	0.44
2:C:726:TYR:OH	2:C:728:ASP:OD1	2.35	0.44
3:D:316:ILE:HD11	3:D:321:LYS:C	2.42	0.44
3:D:608:CYS:O	3:D:612:LEU:HB2	2.17	0.44
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.31	0.44
2:H:136:PHE:CE1	2:H:456:VAL:HG11	2.52	0.44
2:H:1004:ASP:N	2:H:1004:ASP:OD1	2.50	0.44
2:H:1272:GLU:HG2	3:I:342:LEU:H	1.83	0.44
3:I:366:CYS:HB3	3:I:437:PHE:CD2	2.52	0.44
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.99	0.44
3:I:544:LEU:HD22	3:I:575:GLY:HA2	1.99	0.44
3:I:690:ASN:OD1	3:I:738:ARG:NH1	2.50	0.44
3:I:1280:VAL:HG21	3:I:1304:ARG:CZ	2.46	0.44
5:X:448:ARG:HD3	5:X:450:ILE:HG13	1.98	0.44
2:C:759:SER:OG	2:C:760:ASN:N	2.50	0.44
3:D:515:ARG:HH12	3:D:717:VAL:HB	1.83	0.44
3:I:524:GLY:HA2	3:I:548:VAL:HA	1.99	0.44
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.52	0.44
1:A:152:TYR:O	1:A:153:VAL:C	2.61	0.44
2:C:38:PHE:CE2	2:C:46:GLN:HG2	2.53	0.44
2:C:122:VAL:HG23	5:X:472:GLN:HG2	2.00	0.44
2:C:382:GLU:O	2:C:386:GLU:HG2	2.17	0.44
2:C:1106:ARG:O	2:C:1108:ASN:N	2.46	0.44
3:D:828:GLY:HA2	3:D:829:GLY:HA2	1.52	0.44
2:H:848:GLU:HG2	2:H:888:THR:HA	2.00	0.44
2:H:972:PHE:HE1	2:H:998:LEU:HD23	1.82	0.44
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	2.00	0.44
3:I:1188:GLU:HG3	3:I:1189:MET:H	1.83	0.44
3:I:1320:ILE:HD12	3:I:1342:ASP:OD2	2.17	0.44
5:X:138:PRO:HD2	5:X:353:LEU:HD11	2.00	0.44
5:X:439:ILE:O	5:X:443:ILE:HG13	2.18	0.44
5:Y:166:VAL:HG22	5:Y:259:PHE:HA	1.99	0.44
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.53	0.44
2:C:1286:THR:N	3:D:479:GLU:OE2	2.48	0.44
3:D:63:GLY:O	3:D:98:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:431:ARG:N	3:D:921:GLN:OE1	2.50	0.44
3:D:591:ILE:HG13	3:D:592:VAL:N	2.33	0.44
2:H:645:PHE:HA	2:H:646:SER:HA	1.61	0.44
2:H:704:MET:HA	2:H:704:MET:HE3	1.98	0.44
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.99	0.44
5:X:166:VAL:N	5:X:259:PHE:CD2	2.86	0.44
1:B:275:ILE:HG21	1:B:281:LEU:HB2	1.99	0.44
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.53	0.44
2:C:155:VAL:HB	2:C:176:ILE:HG12	2.00	0.44
2:C:1069:ARG:H	2:C:1069:ARG:HG2	1.38	0.44
3:D:37:GLU:HG2	3:D:39:LYS:HG2	2.00	0.44
3:D:1169:THR:HA	3:D:1173:ARG:O	2.17	0.44
3:D:1371:ARG:HG2	3:I:849:LEU:CD2	2.48	0.44
2:H:301:TYR:HD1	2:H:330:HIS:CD2	2.36	0.44
2:H:755:LYS:HE3	2:H:756:TYR:CE2	2.52	0.44
3:I:161:THR:HB	3:I:164:GLN:HG3	2.00	0.44
3:I:309:ASN:HB2	3:I:326:SER:HB3	1.99	0.44
3:I:596:LEU:HD11	3:I:598:LYS:NZ	2.32	0.44
3:I:1260:MET:HG3	3:I:1307:LEU:O	2.18	0.44
1:B:62:ASP:O	1:B:71:LYS:HE2	2.17	0.44
2:C:118:LYS:HG2	2:C:488:MET:H	1.83	0.44
2:C:1212:LEU:HD21	2:C:1227:VAL:HG21	1.99	0.44
3:D:266:ASN:O	3:D:270:ARG:HB2	2.18	0.44
3:D:544:LEU:HD22	3:D:575:GLY:HA2	1.99	0.44
3:D:789:LYS:HD2	3:D:930:LEU:O	2.18	0.44
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	2.00	0.44
4:E:5:THR:C	4:E:7:GLN:H	2.25	0.44
4:E:5:THR:C	4:E:7:GLN:N	2.76	0.44
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.99	0.44
2:H:720:ARG:HD2	2:H:736:VAL:CG2	2.46	0.44
2:H:740:GLU:HB2	2:H:741:MET:SD	2.58	0.44
2:H:802:VAL:HG11	2:H:1230:MET:HB2	1.99	0.44
5:X:140:ALA:HB1	5:X:269:LEU:HD13	1.99	0.44
2:C:92:TYR:CE1	2:C:129:LEU:HB2	2.53	0.44
2:C:556:GLY:HA2	2:C:659:GLN:O	2.17	0.44
2:C:1073:LYS:H	2:C:1073:LYS:HG3	1.57	0.44
3:D:720:ASN:C	3:D:722:ILE:H	2.25	0.44
2:H:192:ASP:OD2	2:H:436:ARG:NH2	2.51	0.44
2:H:908:GLU:HG2	2:H:909:LYS:H	1.82	0.44
3:I:504:GLN:HA	3:I:730:ALA:HA	1.99	0.44
5:X:254:GLU:O	5:X:258:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:537:THR:O	5:X:541:ARG:HG3	2.18	0.44
5:X:561:MET:O	5:X:571:TYR:HB2	2.18	0.44
5:Y:483:LEU:O	5:Y:487:MET:HG2	2.18	0.44
2:C:645:PHE:HA	2:C:646:SER:HA	1.65	0.43
3:D:169:LEU:C	3:D:169:LEU:CD1	2.91	0.43
1:G:27:THR:HG22	1:G:202:VAL:HG22	2.00	0.43
3:I:412:LEU:HA	3:I:415:VAL:HG22	2.00	0.43
3:I:925:GLU:HB3	3:I:926:PRO:HD3	2.00	0.43
5:X:164:GLY:C	5:X:165:PHE:CG	2.96	0.43
5:X:402:LEU:HD13	5:X:405:ILE:HD11	2.00	0.43
5:X:407:GLU:O	5:X:410:ILE:HG22	2.18	0.43
1:B:192:VAL:HG12	1:B:194:GLN:HG2	2.00	0.43
2:C:1007:LYS:O	2:C:1011:LEU:HB2	2.18	0.43
2:C:1101:LEU:HD21	3:D:508:LEU:HD13	2.00	0.43
2:C:1272:GLU:O	2:C:1275:VAL:HG22	2.18	0.43
3:D:555:TYR:HB2	3:D:585:LYS:O	2.18	0.43
3:D:671:GLY:C	3:D:673:VAL:H	2.26	0.43
3:D:781:LYS:NZ	3:D:785:ASP:OD1	2.51	0.43
3:D:822:MET:HG2	3:D:839:VAL:HG23	2.00	0.43
1:F:74:VAL:HG12	1:F:76:GLU:H	1.83	0.43
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.00	0.43
2:H:842:ASP:CB	2:H:1046:VAL:HG21	2.48	0.43
4:J:58:LEU:HD12	4:J:58:LEU:HA	1.79	0.43
5:Y:220:LYS:HB3	5:Y:259:PHE:CE2	2.53	0.43
5:Y:379:MET:HB3	5:Y:416:VAL:HG21	2.00	0.43
1:A:13:LEU:HD11	1:A:16:ILE:HD11	2.01	0.43
1:B:284:ARG:HA	1:B:284:ARG:HD2	1.73	0.43
2:C:91:THR:HG21	2:C:503:LYS:HE3	2.01	0.43
3:D:389:GLY:C	3:D:391:ALA:H	2.26	0.43
3:D:646:ILE:C	3:D:646:ILE:HD12	2.43	0.43
3:D:724:MET:HE2	3:D:724:MET:HB3	1.71	0.43
2:H:417:SER:OG	2:H:418:GLY:N	2.50	0.43
2:H:1151:LEU:HD23	2:H:1151:LEU:HA	1.90	0.43
2:H:1340:GLU:CD	3:I:1341:ARG:HH11	2.26	0.43
3:I:671:GLY:C	3:I:673:VAL:H	2.26	0.43
3:I:738:ARG:NH2	3:I:745:GLY:H	2.16	0.43
2:C:38:PHE:CG	2:C:38:PHE:O	2.71	0.43
2:C:1046:VAL:CG2	2:C:1047:LEU:H	2.20	0.43
2:C:1106:ARG:HE	3:D:731:ARG:NH2	2.16	0.43
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.83	0.43
2:H:143:ARG:HA	2:H:513:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:716:GLN:HE21	3:I:716:GLN:HB3	1.59	0.43
3:I:1230:THR:O	3:I:1234:VAL:HG12	2.19	0.43
5:Y:96:ASP:O	5:Y:100:MET:HB2	2.18	0.43
5:Y:231:THR:OG1	5:Y:248:GLU:O	2.37	0.43
5:Y:303:ILE:O	5:Y:307:THR:OG1	2.21	0.43
1:B:135:ASP:OD1	1:B:138:ALA:HB2	2.17	0.43
2:C:303:ASP:C	2:C:305:SER:H	2.27	0.43
2:C:409:LEU:HD21	2:C:428:VAL:HG22	1.99	0.43
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.01	0.43
2:C:756:TYR:CE2	2:C:766:ASN:ND2	2.87	0.43
2:C:885:GLY:HA2	2:C:917:SER:HB3	2.01	0.43
2:C:898:GLU:OE1	2:C:898:GLU:N	2.41	0.43
2:C:1106:ARG:HH21	3:D:731:ARG:HH22	1.65	0.43
3:D:145:VAL:CG2	3:D:159:ILE:HG13	2.48	0.43
1:F:152:TYR:O	1:F:152:TYR:CG	2.70	0.43
2:H:603:ILE:HD12	2:H:603:ILE:O	2.19	0.43
2:H:1192:GLU:O	2:H:1196:LYS:HD3	2.19	0.43
3:I:279:LEU:HD13	3:I:279:LEU:C	2.42	0.43
3:I:513:MET:SD	3:I:579:LEU:HD23	2.59	0.43
3:I:682:VAL:HA	3:I:685:ILE:HD12	2.00	0.43
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.82	0.43
1:A:101:THR:OG1	1:A:116:THR:OG1	2.29	0.43
1:A:165:GLU:O	1:A:165:GLU:HG3	2.18	0.43
2:C:421:SER:H	2:C:424:ASP:HB2	1.83	0.43
2:C:455:SER:O	2:C:459:MET:HG3	2.19	0.43
2:C:607:SER:HB2	2:C:610:GLU:HG3	1.99	0.43
2:C:678:ARG:HD3	2:C:681:MET:HG3	2.00	0.43
2:C:1124:ILE:O	2:C:1128:ILE:HD13	2.19	0.43
2:C:1305:TYR:CZ	3:D:379:PRO:HG3	2.54	0.43
3:D:141:PHE:CZ	3:D:296:LYS:HD2	2.53	0.43
3:D:1181:ASP:OD2	3:D:1203:ARG:NH2	2.52	0.43
3:I:489:ASN:HA	3:I:904:ALA:CB	2.48	0.43
3:I:810:THR:O	3:I:811:GLU:HG2	2.18	0.43
3:I:905:ARG:NH2	4:J:16:ARG:HG3	2.32	0.43
5:Y:165:PHE:HA	5:Y:259:PHE:HB2	1.99	0.43
2:C:303:ASP:HB2	2:C:306:THR:OG1	2.19	0.43
2:C:1042:LEU:HD11	2:C:1047:LEU:O	2.18	0.43
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.00	0.43
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.34	0.43
4:E:58:LEU:HD12	4:E:58:LEU:HA	1.77	0.43
2:H:890:LYS:HB2	2:H:914:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:84:ILE:H	3:I:84:ILE:HG13	1.61	0.43
3:I:910:ASN:OD1	4:J:15:ASN:HA	2.19	0.43
2:C:669:PRO:HG2	2:C:670:PHE:H	1.83	0.43
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.34	0.43
3:D:253:VAL:HG11	5:X:523:ILE:HG21	1.99	0.43
3:D:355:ILE:HG12	3:D:464:ASP:O	2.18	0.43
3:D:840:LEU:C	3:D:842:ARG:H	2.27	0.43
3:D:1173:ARG:HA	3:D:1174:ARG:O	2.19	0.43
1:G:37:HIS:CE1	1:G:187:VAL:HG22	2.54	0.43
2:H:681:MET:HE3	2:H:681:MET:HB3	1.79	0.43
2:H:844:LYS:HE2	5:Y:499:LYS:HZ3	1.84	0.43
2:H:890:LYS:HG2	2:H:891:GLY:H	1.84	0.43
2:H:1154:ASP:HB2	2:H:1156:ARG:HE	1.83	0.43
1:B:78:ILE:HA	1:B:81:ILE:HD12	2.00	0.43
2:C:1340:GLU:CD	3:D:1341:ARG:HH11	2.27	0.43
3:D:213:LYS:O	3:D:217:LEU:HG	2.18	0.43
3:D:334:LYS:HG3	3:D:335:GLN:N	2.33	0.43
3:D:716:GLN:HG2	3:D:717:VAL:H	1.84	0.43
2:H:1200:LYS:HE2	2:H:1206:THR:HB	2.00	0.43
3:I:179:LYS:HE2	3:I:179:LYS:HB2	1.80	0.43
3:I:294:ASN:ND2	3:I:298:MET:SD	2.92	0.43
3:I:527:LEU:H	3:I:550:VAL:HG12	1.82	0.43
5:X:343:LYS:O	5:X:347:ILE:HG13	2.18	0.43
5:X:373:ARG:HG3	5:X:377:LYS:HE3	2.01	0.43
5:X:390:ILE:HD13	5:X:436:ARG:HG3	2.01	0.43
5:Y:105:MET:CG	5:Y:384:LEU:HD12	2.48	0.43
5:Y:540:LEU:HB2	5:Y:607:LEU:HD12	2.01	0.43
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.80	0.43
2:C:399:ALA:O	2:C:403:MET:N	2.46	0.43
2:C:459:MET:HE2	2:C:459:MET:HB3	1.86	0.43
2:C:714:VAL:HG23	2:C:787:PRO:HD2	2.00	0.43
3:D:518:VAL:HA	3:D:547:ARG:HH12	1.82	0.43
3:D:521:LYS:HD2	3:D:542:ALA:O	2.19	0.43
3:D:903:LEU:HG	3:D:909:ILE:HG22	2.00	0.43
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	2.01	0.43
2:H:210:LEU:O	2:H:215:TYR:HB2	2.19	0.43
2:H:500:ALA:O	2:H:504:GLU:HB2	2.19	0.43
2:H:578:TYR:CE2	2:H:658:GLN:HG3	2.50	0.43
5:X:274:ARG:O	5:X:278:ASP:N	2.50	0.43
5:X:291:CYS:O	5:X:295:CYS:HB2	2.19	0.43
5:Y:399:LEU:HD12	5:Y:399:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:HG12	1:B:173:VAL:HG11	2.01	0.42
1:B:60:GLU:HA	1:B:169:GLY:O	2.19	0.42
2:C:237:LEU:O	2:C:286:GLU:HG3	2.19	0.42
2:C:296:VAL:HB	2:C:336:LEU:HD12	2.01	0.42
2:C:740:GLU:HB2	2:C:741:MET:SD	2.59	0.42
2:C:841:ARG:HA	2:C:1046:VAL:CG1	2.35	0.42
2:C:1333:LEU:HD13	3:D:115:TRP:CH2	2.54	0.42
3:D:317:THR:O	3:D:324:LEU:HD11	2.19	0.42
2:H:1192:GLU:CD	3:I:764:ARG:HE	2.27	0.42
3:I:62:PHE:O	3:I:101:ARG:HG3	2.19	0.42
3:I:363:LEU:HD12	3:I:450:HIS:CE1	2.54	0.42
3:I:647:PRO:HG3	3:I:697:MET:HB2	2.02	0.42
3:I:747:MET:O	3:I:755:ILE:HG22	2.19	0.42
4:J:26:ARG:HE	4:J:30:MET:HE3	1.84	0.42
5:X:213:ASP:HB2	5:X:216:LEU:HB3	2.01	0.42
5:X:448:ARG:HD2	5:X:452:ILE:HD12	2.00	0.42
5:Y:390:ILE:HD11	5:Y:435:ILE:CG2	2.48	0.42
5:Y:407:GLU:O	5:Y:410:ILE:HG22	2.19	0.42
1:B:109:PRO:HB3	1:B:132:HIS:NE2	2.34	0.42
2:C:225:PHE:CD2	2:C:336:LEU:HD13	2.54	0.42
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.52	0.42
2:C:1146:GLN:HA	2:C:1161:LEU:HD13	2.00	0.42
3:D:197:GLU:O	3:D:201:LEU:HD23	2.19	0.42
3:D:506:VAL:HG23	3:D:628:GLY:HA3	2.02	0.42
3:D:849:LEU:HA	3:D:855:ASP:HA	2.01	0.42
2:H:510:GLN:C	2:H:512:SER:H	2.27	0.42
3:I:491:LEU:HB2	3:I:904:ALA:HA	2.01	0.42
3:I:1140:ARG:NH2	3:I:1144:LEU:HD21	2.34	0.42
3:I:1173:ARG:HA	3:I:1174:ARG:O	2.20	0.42
5:X:570:ASP:N	5:X:570:ASP:OD1	2.52	0.42
2:C:256:GLU:HB3	2:C:261:VAL:HG22	2.01	0.42
2:C:720:ARG:HD2	2:C:736:VAL:HG21	2.00	0.42
3:D:381:ILE:HD11	3:D:412:LEU:HD13	2.01	0.42
3:D:521:LYS:HB3	3:D:542:ALA:CB	2.49	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.54	0.42
2:H:660:VAL:HG22	2:H:661:VAL:N	2.34	0.42
3:I:901:ARG:CB	3:I:908:ILE:HA	2.48	0.42
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.20	0.42
2:C:210:LEU:HD11	2:C:429:MET:HE1	2.00	0.42
2:C:948:ILE:HG13	2:C:949:GLU:N	2.33	0.42
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1268:GLN:H	3:D:350:SER:HB2	1.84	0.42
3:D:154:LEU:HD23	3:D:154:LEU:HA	1.72	0.42
2:H:714:VAL:HG22	2:H:787:PRO:HD2	2.00	0.42
2:H:956:ALA:CB	2:H:1032:LYS:HE3	2.50	0.42
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	2.01	0.42
3:I:361:LEU:HD21	3:I:366:CYS:HA	2.02	0.42
5:Y:148:TYR:C	5:Y:148:TYR:CD2	2.98	0.42
1:B:48:LEU:HD22	3:D:535:ARG:HA	2.00	0.42
2:C:11:ILE:CD1	2:C:697:LYS:HD3	2.49	0.42
2:C:55:SER:O	2:C:56:VAL:C	2.62	0.42
2:C:407:ARG:HH22	2:C:609:ILE:HD12	1.84	0.42
2:C:985:GLU:HB3	2:C:989:LEU:HD22	2.01	0.42
3:D:526:VAL:HG12	3:D:549:LYS:O	2.19	0.42
1:F:228:LEU:HD23	1:F:231:PHE:HE2	1.83	0.42
2:H:453:ILE:O	2:H:453:ILE:HG23	2.18	0.42
2:H:1252:SER:HA	5:Y:524:GLU:HA	2.02	0.42
2:H:1299:ASN:HB3	2:H:1303:LYS:HE3	2.00	0.42
3:I:264:ASP:OD1	5:Y:506:SER:HB2	2.20	0.42
3:I:681:LYS:HE3	3:I:681:LYS:HB2	1.86	0.42
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.20	0.42
5:Y:105:MET:HE2	5:Y:105:MET:HB3	1.92	0.42
1:B:54:CYS:SG	1:B:148:ARG:HD3	2.59	0.42
1:B:93:GLN:HG3	1:B:276:HIS:HB3	2.01	0.42
3:D:546:ALA:N	3:D:573:THR:OG1	2.52	0.42
3:D:1238:GLN:O	3:D:1241:TYR:N	2.52	0.42
4:E:12:LYS:HD3	4:E:12:LYS:HA	1.85	0.42
2:H:687:ARG:HE	2:H:687:ARG:HB2	1.49	0.42
2:H:844:LYS:HE2	5:Y:499:LYS:NZ	2.35	0.42
2:H:1313:HIS:CD2	3:I:477:GLN:HE22	2.35	0.42
2:H:1326:LEU:HA	2:H:1326:LEU:HD23	1.76	0.42
3:I:534:GLU:HB2	3:I:578:ILE:HD13	2.02	0.42
3:I:639:VAL:HG13	3:I:725:MET:HE1	2.01	0.42
1:A:100:LEU:HD11	1:A:121:VAL:HG11	2.00	0.42
2:C:1082:ILE:H	2:C:1082:ILE:HG13	1.59	0.42
3:D:514:THR:HG23	3:D:576:ARG:HG2	2.01	0.42
3:D:644:MET:HE2	3:D:644:MET:HB3	1.91	0.42
3:D:714:GLU:HG3	3:D:715:LYS:N	2.35	0.42
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	2.01	0.42
3:D:1372:ARG:HE	3:I:853:THR:HG23	1.85	0.42
1:G:83:LEU:HD12	1:G:83:LEU:HA	1.83	0.42
2:H:122:VAL:HG21	2:H:493:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:719:LYS:HE2	2:H:751:TYR:HE2	1.83	0.42
3:I:85:CYS:SG	3:I:87:LYS:N	2.93	0.42
3:I:405:GLU:C	3:I:407:VAL:H	2.28	0.42
3:I:810:THR:C	3:I:812:ASP:H	2.28	0.42
1:A:220:ALA:HA	1:A:223:ILE:HD12	2.01	0.42
2:C:86:GLN:HA	2:C:140:GLY:HA2	2.01	0.42
2:C:525:THR:HG21	2:C:687:ARG:HD2	2.02	0.42
2:C:646:SER:HB3	2:C:649:GLN:HG3	2.02	0.42
2:C:1083:GLU:HG2	2:C:1083:GLU:H	1.63	0.42
3:D:102:MET:HE3	3:D:102:MET:HB3	1.77	0.42
3:D:1362:GLY:O	3:D:1364:ALA:N	2.51	0.42
2:H:4:SER:O	2:H:5:TYR:HB2	2.19	0.42
2:H:91:THR:HG22	2:H:139:ASN:N	2.35	0.42
2:H:1279:GLU:OE2	3:I:1347:LEU:HB3	2.19	0.42
3:I:805:GLN:OE1	3:I:1348:LYS:HE2	2.20	0.42
1:B:76:GLU:HB2	1:B:80:GLU:HB2	2.01	0.42
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.87	0.42
3:D:521:LYS:O	3:D:542:ALA:HB3	2.20	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HG23	2.55	0.42
3:D:1272:SER:HB3	3:D:1276:GLU:OE1	2.20	0.42
1:F:13:LEU:HD21	1:F:16:ILE:HD11	2.00	0.42
3:I:288:PRO:O	3:I:292:VAL:HG12	2.20	0.42
3:I:1167:LYS:HB2	3:I:1167:LYS:HE3	1.78	0.42
3:I:1272:SER:H	3:I:1290:ARG:HH12	1.67	0.42
5:X:396:ASN:ND2	5:X:396:ASN:O	2.52	0.42
1:A:62:ASP:O	1:A:71:LYS:NZ	2.33	0.42
1:B:16:ILE:HG12	1:B:26:VAL:HG13	2.02	0.42
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.00	0.42
1:B:263:THR:HG23	1:B:266:SER:H	1.84	0.42
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.55	0.42
2:C:1268:GLN:H	3:D:350:SER:CB	2.33	0.42
3:D:809:VAL:HG23	3:D:894:VAL:O	2.20	0.42
3:D:825:VAL:O	3:D:834:PRO:HB2	2.20	0.42
3:D:1271:SER:HB2	3:D:1290:ARG:CZ	2.50	0.42
2:H:128:PRO:O	2:H:129:LEU:HD23	2.20	0.42
2:H:421:SER:H	2:H:424:ASP:HB2	1.84	0.42
2:H:528:ARG:NH2	2:H:576:SER:O	2.52	0.42
2:H:542:ARG:C	2:H:544:GLY:H	2.27	0.42
3:I:286:ALA:C	3:I:288:PRO:HD3	2.45	0.42
5:X:112:THR:HG22	5:X:113:ARG:N	2.29	0.42
5:Y:354:THR:O	5:Y:358:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.19	0.42
5:Y:585:GLU:O	5:Y:588:ARG:N	2.53	0.42
2:C:35:PHE:CE1	2:C:136:PHE:HE2	2.37	0.41
2:C:478:ARG:HE	2:C:487:LEU:HD11	1.85	0.41
2:C:583:GLU:H	2:C:583:GLU:HG3	1.69	0.41
2:C:741:MET:SD	2:C:741:MET:N	2.93	0.41
2:C:1099:ASN:OD1	2:C:1100:PRO:HD2	2.19	0.41
2:C:1141:LEU:C	2:C:1141:LEU:CD1	2.93	0.41
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.53	0.41
3:D:745:GLY:C	3:D:758:PRO:HB3	2.45	0.41
3:D:762:ASN:OD1	3:D:765:GLU:HG3	2.20	0.41
1:F:48:LEU:HD23	1:F:180:VAL:HG12	2.01	0.41
1:G:182:ARG:HG2	1:G:206:GLU:HB3	2.02	0.41
2:H:1146:GLN:HA	2:H:1161:LEU:HD13	2.02	0.41
2:H:1319:MET:HE3	2:H:1324:ASN:HB2	2.01	0.41
3:I:57:PHE:HZ	3:I:266:ASN:ND2	2.18	0.41
3:I:146:VAL:HG12	3:I:158:GLN:O	2.20	0.41
5:Y:257:LYS:HB3	5:Y:257:LYS:HE2	1.82	0.41
1:B:247:PRO:HA	1:B:248:GLU:HA	1.75	0.41
2:C:49:LEU:HD12	2:C:461:GLU:HB2	2.01	0.41
2:C:404:LYS:HD3	2:C:586:PHE:HZ	1.85	0.41
2:C:1069:ARG:HD3	2:C:1114:GLU:OE1	2.21	0.41
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.85	0.41
1:F:97:GLU:HA	1:F:146:VAL:O	2.19	0.41
2:H:542:ARG:H	2:H:542:ARG:HG3	1.50	0.41
2:H:839:VAL:HG11	2:H:841:ARG:NH2	2.35	0.41
3:I:20:ILE:O	3:I:20:ILE:HG13	2.20	0.41
5:X:431:ALA:O	5:X:435:ILE:HG13	2.20	0.41
3:D:388:ARG:HB2	3:D:390:LEU:HD13	2.02	0.41
2:H:17:LYS:HD3	2:H:1154:ASP:OD2	2.21	0.41
2:H:406:ASN:HB3	2:H:411:ARG:HB2	2.02	0.41
2:H:931:VAL:HG21	2:H:944:ARG:NH2	2.34	0.41
2:H:954:LYS:HE3	2:H:954:LYS:HB3	1.90	0.41
2:H:1332:SER:O	3:I:243:PRO:HG2	2.20	0.41
3:I:134:ASP:O	3:I:138:VAL:HG23	2.19	0.41
5:X:279:ARG:HH22	5:X:350:GLU:CD	2.29	0.41
5:X:558:VAL:HG21	5:X:587:ILE:HD11	2.03	0.41
1:B:145:LYS:NZ	1:B:170:ARG:HH21	2.18	0.41
2:C:1255:THR:C	2:C:1257:GLN:H	2.28	0.41
3:D:527:LEU:HD13	3:D:535:ARG:NH2	2.33	0.41
3:D:1221:LEU:HB2	3:D:1229:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.56	0.41
2:H:398:SER:O	2:H:401:GLY:N	2.53	0.41
2:H:600:THR:HG22	2:H:601:ASP:N	2.30	0.41
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	2.03	0.41
2:H:1119:MET:O	2:H:1123:GLY:N	2.52	0.41
2:H:1254:VAL:O	3:I:99:ARG:NH1	2.53	0.41
3:I:510:LEU:HD12	3:I:601:ILE:HD13	2.02	0.41
3:I:901:ARG:HA	3:I:908:ILE:HA	2.03	0.41
3:I:1311:LYS:HE3	3:I:1311:LYS:HB3	1.90	0.41
5:Y:139:GLU:HG3	5:Y:351:THR:HA	2.02	0.41
2:C:38:PHE:CD2	2:C:46:GLN:HG2	2.56	0.41
2:C:398:SER:O	2:C:400:VAL:N	2.54	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.95	0.41
3:D:271:ARG:HD2	3:D:275:ARG:NH2	2.35	0.41
2:H:667:LEU:HD11	2:H:708:VAL:HG21	2.01	0.41
2:H:697:LYS:HB3	2:H:697:LYS:HE2	1.77	0.41
3:I:576:ARG:H	3:I:576:ARG:HG3	1.64	0.41
3:I:856:ILE:O	3:I:857:LEU:HD23	2.21	0.41
5:X:507:MET:HB3	5:X:520:GLY:HA3	2.02	0.41
1:B:289:LEU:HD12	1:B:314:LEU:HD21	2.01	0.41
2:C:374:GLU:H	2:C:374:GLU:HG3	1.74	0.41
2:C:805:MET:HE1	2:C:1221:PHE:CE1	2.55	0.41
2:C:1307:ASN:HB3	2:C:1312:ASN:HB3	2.03	0.41
3:D:30:ILE:HD13	3:D:33:TRP:CZ3	2.56	0.41
3:D:584:PRO:O	3:D:589:TYR:OH	2.38	0.41
3:D:1167:LYS:HE3	3:D:1167:LYS:HB2	1.80	0.41
3:D:1167:LYS:HE3	3:D:1173:ARG:NH1	2.33	0.41
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.21	0.41
3:D:1327:GLU:H	3:D:1327:GLU:HG3	1.61	0.41
1:F:100:LEU:HB3	1:F:115:ILE:HD11	2.01	0.41
1:G:117:HIS:HD2	1:G:118:ASP:CG	2.28	0.41
2:H:176:ILE:HB	2:H:184:LEU:HB3	2.03	0.41
2:H:576:SER:HB3	2:H:579:ALA:HB2	2.02	0.41
2:H:709:ALA:HB2	2:H:794:LEU:HB2	2.03	0.41
2:H:1184:THR:OG1	2:H:1189:GLY:HA3	2.21	0.41
3:I:601:ILE:HD12	3:I:604:MET:HE2	2.03	0.41
3:I:813:ASP:OD1	3:I:897:HIS:ND1	2.53	0.41
3:I:903:LEU:HB2	3:I:905:ARG:O	2.20	0.41
5:X:407:GLU:HA	5:X:410:ILE:HG22	2.03	0.41
1:A:50:SER:HB3	1:B:8:PHE:CE2	2.56	0.41
1:B:23:HIS:HD2	1:B:206:GLU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:562:GLU:O	2:C:562:GLU:HG3	2.21	0.41
2:C:1051:LYS:HB3	2:C:1053:TYR:CE1	2.53	0.41
1:F:11:PRO:HD3	1:G:227:GLN:NE2	2.35	0.41
1:F:221:ALA:HB1	1:G:228:LEU:HD13	2.03	0.41
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	2.03	0.41
2:H:1294:LYS:HE2	3:I:348:ASP:O	2.21	0.41
3:I:128:LEU:HD13	3:I:189:LEU:HD23	2.03	0.41
3:I:416:ILE:HD13	3:I:441:LEU:CD2	2.50	0.41
2:C:948:ILE:O	2:C:952:GLN:HG3	2.21	0.41
3:D:343:LEU:HG	3:D:344:GLY:H	1.84	0.41
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.02	0.41
3:D:857:LEU:HD11	3:D:871:LEU:HD21	2.01	0.41
1:F:192:VAL:HG21	1:F:198:LEU:HD12	2.02	0.41
2:H:262:TYR:OH	2:H:280:ASP:OD2	2.27	0.41
2:H:1128:ILE:HG21	2:H:1176:LEU:HB2	2.02	0.41
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	2.03	0.41
3:I:166:LEU:HD12	3:I:167:ASP:N	2.36	0.41
1:B:14:VAL:HA	1:B:28:LEU:HD23	2.03	0.41
1:B:37:HIS:CD2	2:C:1216:ARG:HH21	2.38	0.41
2:C:736:VAL:HG11	2:C:740:GLU:HB3	2.03	0.41
2:C:801:ARG:HD2	2:C:1229:TYR:OH	2.20	0.41
2:C:1004:ASP:O	2:C:1005:GLU:O	2.39	0.41
2:C:1161:LEU:C	2:C:1163:THR:H	2.29	0.41
3:D:58:CYS:SG	3:D:59:ALA:N	2.94	0.41
3:D:355:ILE:HG22	3:D:447:ILE:HG23	2.01	0.41
3:D:362:ARG:HG2	3:D:364:HIS:CE1	2.56	0.41
3:D:405:GLU:C	3:D:407:VAL:H	2.29	0.41
3:D:552:ILE:HG23	3:D:580:TRP:CZ2	2.56	0.41
3:D:810:THR:C	3:D:812:ASP:H	2.29	0.41
3:D:1167:LYS:HB3	3:D:1170:LYS:HD2	2.02	0.41
1:F:31:LEU:HD22	1:F:35:PHE:HB2	2.03	0.41
1:F:228:LEU:HD23	1:F:231:PHE:CE2	2.56	0.41
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.56	0.41
2:H:150:HIS:CE1	2:H:454:ARG:HB2	2.56	0.41
2:H:719:LYS:HG3	2:H:751:TYR:CE2	2.55	0.41
2:H:729:ALA:O	2:H:755:LYS:HD2	2.20	0.41
3:I:169:LEU:C	3:I:169:LEU:HD13	2.45	0.41
3:I:437:PHE:CZ	3:I:453:VAL:HG21	2.48	0.41
3:I:541:LEU:HA	3:I:542:ALA:HA	1.85	0.41
3:I:822:MET:HE2	3:I:822:MET:HB2	1.98	0.41
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:157:ARG:HH11	5:X:159:SER:H	1.68	0.41
5:X:484:ALA:HB1	5:X:490:PRO:O	2.21	0.41
5:Y:140:ALA:HB1	5:Y:269:LEU:HD13	2.03	0.41
5:Y:240:ARG:O	5:Y:242:HIS:N	2.53	0.41
2:C:817:LEU:CD2	2:C:1078:LYS:HB3	2.49	0.41
2:C:841:ARG:C	2:C:1046:VAL:HG21	2.46	0.41
3:D:12:THR:C	3:D:13:LYS:HD2	2.46	0.41
3:D:129:ASP:HB2	3:D:220:ARG:CZ	2.51	0.41
3:D:268:LEU:HB3	3:D:306:LEU:HD12	2.01	0.41
2:H:681:MET:O	2:H:685:MET:HG2	2.21	0.41
2:H:786:GLY:H	2:H:789:THR:CG2	2.34	0.41
2:H:1069:ARG:H	2:H:1069:ARG:HG3	1.61	0.41
2:H:1140:LYS:C	2:H:1142:ARG:H	2.28	0.41
3:I:308:ASP:OD1	3:I:311:ARG:NH1	2.54	0.41
3:I:1338:ALA:O	3:I:1340:LYS:N	2.48	0.41
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.55	0.41
5:X:562:ARG:HD3	5:X:573:LEU:HG	2.01	0.41
1:B:179:PRO:HB3	1:B:210:THR:HB	2.02	0.40
2:C:136:PHE:CE1	2:C:145:ILE:HD12	2.56	0.40
2:C:519:ASN:OD1	2:C:522:SER:N	2.48	0.40
2:C:699:LEU:HD23	2:C:799:ASN:OD1	2.22	0.40
2:C:812:PHE:CE1	3:D:451:PRO:HB2	2.56	0.40
2:C:1106:ARG:NE	3:D:731:ARG:HH22	2.19	0.40
2:C:1127:LYS:HE3	2:C:1131:MET:HE3	2.04	0.40
2:C:1184:THR:O	2:C:1184:THR:HG23	2.22	0.40
2:C:1281:TYR:CE1	3:D:484:MET:HA	2.56	0.40
3:D:123:ARG:HD2	3:D:1333:THR:HG22	2.01	0.40
3:D:759:ILE:HG12	3:D:771:GLN:HB2	2.03	0.40
2:H:237:LEU:HD13	2:H:292:ILE:HD12	2.04	0.40
2:H:1101:LEU:O	2:H:1104:PRO:HD2	2.21	0.40
3:I:773:PHE:O	3:I:776:THR:HG22	2.20	0.40
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.36	0.40
1:B:286:GLU:HA	1:B:289:LEU:HB2	2.02	0.40
2:C:646:SER:O	2:C:646:SER:OG	2.31	0.40
2:C:1100:PRO:HG3	3:D:637:ALA:O	2.21	0.40
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.21	0.40
3:D:1363:TYR:O	3:D:1367:GLN:HB2	2.22	0.40
2:H:1289:GLU:O	2:H:1294:LYS:HB2	2.21	0.40
2:H:1296:ASP:OD1	3:I:345:LYS:HD3	2.21	0.40
3:I:108:ALA:HB1	3:I:279:LEU:HD12	2.03	0.40
3:I:846:GLU:HA	3:I:859:PRO:CA	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.86	0.40
5:X:120:ALA:HA	5:X:123:ILE:HD12	2.02	0.40
5:Y:394:TYR:CD2	5:Y:439:ILE:HD11	2.56	0.40
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.21	0.40
1:A:49:SER:OG	1:A:50:SER:N	2.53	0.40
2:C:122:VAL:HG21	2:C:493:ILE:CG2	2.52	0.40
2:C:557:ARG:HD3	2:C:587:LEU:HB3	2.02	0.40
2:C:817:LEU:HD23	2:C:817:LEU:HA	1.82	0.40
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.55	0.40
2:H:451:ARG:NH2	2:H:547:VAL:HG11	2.36	0.40
2:H:840:SER:HB3	2:H:850:ILE:HD11	2.03	0.40
2:H:1328:LYS:O	2:H:1332:SER:N	2.54	0.40
3:I:644:MET:HE2	3:I:644:MET:HB3	1.88	0.40
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	2.03	0.40
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.56	0.40
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.93	0.40
1:B:119:GLY:HA3	1:B:271:LYS:HD3	2.03	0.40
2:C:459:MET:HE1	2:C:511:LEU:HD22	2.03	0.40
2:C:1259:LEU:HA	2:C:1260:GLY:HA3	1.87	0.40
2:C:1294:LYS:NZ	3:D:470:VAL:O	2.55	0.40
3:D:245:LEU:HD12	3:D:246:PRO:HD2	2.04	0.40
1:F:155:ALA:HA	1:F:158:ARG:HB2	2.03	0.40
2:H:55:SER:O	2:H:56:VAL:C	2.64	0.40
2:H:1142:ARG:NH2	2:H:1164:PHE:O	2.29	0.40
2:H:1255:THR:O	2:H:1257:GLN:N	2.49	0.40
3:I:149:GLY:CA	3:I:176:PHE:HB2	2.52	0.40
5:X:133:SER:HA	5:X:136:GLU:OE2	2.21	0.40
5:X:363:ARG:O	5:X:367:ILE:HG12	2.21	0.40
5:Y:311:THR:HB	5:Y:345:GLN:HG2	2.03	0.40
2:C:27:LEU:HD12	2:C:524:ILE:HD13	2.03	0.40
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.96	0.40
2:C:617:ALA:HB2	2:C:650:VAL:HG11	2.03	0.40
2:C:977:ALA:O	2:C:980:VAL:HG12	2.21	0.40
3:D:128:LEU:HD13	3:D:189:LEU:HD23	2.02	0.40
3:D:547:ARG:H	3:D:573:THR:HG1	1.69	0.40
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.57	0.40
1:G:14:VAL:HG22	1:G:28:LEU:HD22	2.04	0.40
2:H:468:LEU:O	2:H:471:VAL:HG22	2.22	0.40
3:I:290:ILE:HD12	5:Y:381:GLU:HG2	2.03	0.40
3:I:825:VAL:O	3:I:834:PRO:HB2	2.21	0.40
3:I:929:GLN:H	3:I:929:GLN:HG2	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:111:LEU:HD22	5:Y:115:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/329 (70%)	201 (87%)	31 (13%)	0	100	100
1	B	297/329 (90%)	269 (91%)	28 (9%)	0	100	100
1	F	230/329 (70%)	203 (88%)	27 (12%)	0	100	100
1	G	227/329 (69%)	201 (88%)	26 (12%)	0	100	100
2	C	1334/1342 (99%)	1130 (85%)	186 (14%)	18 (1%)	9	41
2	H	1334/1342 (99%)	1127 (84%)	192 (14%)	15 (1%)	11	44
3	D	1158/1407 (82%)	983 (85%)	166 (14%)	9 (1%)	16	51
3	I	1154/1407 (82%)	955 (83%)	192 (17%)	7 (1%)	21	57
4	E	88/91 (97%)	75 (85%)	12 (14%)	1 (1%)	11	44
4	J	74/91 (81%)	64 (86%)	9 (12%)	1 (1%)	9	39
5	X	467/613 (76%)	425 (91%)	39 (8%)	3 (1%)	21	57
5	Y	471/613 (77%)	431 (92%)	37 (8%)	3 (1%)	21	57
All	All	7066/8222 (86%)	6064 (86%)	945 (13%)	57 (1%)	16	51

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	15	PHE
2	C	66	SER
2	C	547	VAL

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Mol	Chain	Res	Type
2	C	661	VAL
2	C	1005	GLU
2	C	1006	GLU
2	C	1138	VAL
2	H	547	VAL
2	H	661	VAL
2	H	1047	LEU
2	H	1138	VAL
2	C	546	GLU
2	C	993	PRO
2	C	1185	PRO
3	D	82	GLY
3	D	1273	ASP
2	H	993	PRO
3	I	588	PRO
3	I	889	ASP
3	I	1273	ASP
5	X	490	PRO
2	C	1137	GLU
3	D	588	PRO
3	D	889	ASP
3	D	1173	ARG
2	H	543	ALA
2	H	546	GLU
2	H	893	THR
2	H	1185	PRO
3	I	1173	ARG
5	Y	259	PHE
5	Y	490	PRO
3	D	887	SER
2	H	82	VAL
2	H	813	GLU
3	I	887	SER
2	C	59	ILE
2	C	82	VAL
2	C	1047	LEU
2	H	59	ILE
3	I	587	LEU
5	X	258	GLN
5	Y	503	GLU
3	D	587	LEU
3	D	850	LYS

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Mol	Chain	Res	Type
2	H	42	ASP
2	H	43	PRO
3	I	595	ALA
2	C	1046	VAL
4	J	59	ILE
5	X	503	GLU
2	C	56	VAL
2	C	58	PRO
2	C	1186	VAL
2	H	1046	VAL
3	D	834	PRO
4	E	59	ILE

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	201/286 (70%)	201 (100%)	0	100	100
1	B	261/286 (91%)	260 (100%)	1 (0%)	84	84
1	F	201/286 (70%)	201 (100%)	0	100	100
1	G	197/286 (69%)	196 (100%)	1 (0%)	81	82
2	C	1152/1157 (100%)	1152 (100%)	0	100	100
2	H	1152/1157 (100%)	1152 (100%)	0	100	100
3	D	975/1168 (84%)	973 (100%)	2 (0%)	87	87
3	I	972/1168 (83%)	972 (100%)	0	100	100
4	E	74/75 (99%)	74 (100%)	0	100	100
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	418/540 (77%)	418 (100%)	0	100	100
5	Y	422/540 (78%)	422 (100%)	0	100	100
All	All	6090/7024 (87%)	6086 (100%)	4 (0%)	88	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	GLU
3	D	422	LEU
3	D	1351	VAL
1	G	29	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	18	GLN
1	A	75	GLN
1	A	137	ASN
1	B	37	HIS
1	B	41	ASN
1	B	132	HIS
1	B	160	HIS
1	B	268	ASN
1	B	276	HIS
2	C	20	GLN
2	C	139	ASN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	573	ASN
2	C	580	GLN
2	C	622	ASN
2	C	688	GLN
2	C	922	ASN
2	C	1108	ASN
2	C	1236	ASN
2	C	1237	HIS
2	C	1268	GLN
2	C	1288	GLN
3	D	94	GLN
3	D	164	GLN
3	D	209	ASN
3	D	294	ASN
3	D	320	ASN
3	D	469	HIS
3	D	477	GLN
3	D	560	ASN
3	D	680	ASN
3	D	690	ASN

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Mol	Chain	Res	Type
3	D	716	GLN
3	D	768	ASN
3	D	771	GLN
3	D	1289	ASN
4	E	15	ASN
1	F	66	HIS
1	F	84	ASN
1	F	147	GLN
1	F	186	ASN
1	G	23	HIS
1	G	84	ASN
1	G	117	HIS
1	G	227	GLN
2	H	65	ASN
2	H	133	ASN
2	H	517	GLN
2	H	554	HIS
2	H	582	ASN
2	H	684	ASN
2	H	688	GLN
2	H	737	ASN
2	H	760	ASN
2	H	766	ASN
2	H	808	ASN
2	H	824	GLN
2	H	932	GLN
2	H	1010	GLN
2	H	1080	ASN
2	H	1108	ASN
2	H	1111	GLN
2	H	1256	GLN
2	H	1257	GLN
2	H	1313	HIS
3	I	11	GLN
3	I	153	ASN
3	I	164	GLN
3	I	206	ASN
3	I	309	ASN
3	I	488	ASN
3	I	504	GLN
3	I	560	ASN
3	I	680	ASN

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Mol	Chain	Res	Type
3	I	720	ASN
3	I	768	ASN
3	I	771	GLN
3	I	1227	HIS
3	I	1244	GLN
3	I	1366	HIS
4	J	15	ASN
4	J	31	GLN
5	X	283	GLN
5	X	331	HIS
5	X	406	GLN
5	X	446	GLN
5	X	461	ASN
5	X	518	HIS
5	Y	283	GLN
5	Y	331	HIS
5	Y	362	ASN
5	Y	406	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	QZY	D	1501	-	37,37,37	2.58	10 (27%)	47,50,50	3.95	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	QZY	D	1501	-	-	11/26/26/26	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1501	QZY	C01-S01	-8.40	1.56	1.74
6	D	1501	QZY	C03-C02	7.80	1.59	1.42
6	D	1501	QZY	C02-C01	5.45	1.45	1.38
6	D	1501	QZY	C18-N02	5.14	1.45	1.36
6	D	1501	QZY	C04-S01	-3.97	1.56	1.73
6	D	1501	QZY	C05-C01	2.62	1.53	1.48
6	D	1501	QZY	C18-N01	2.62	1.45	1.39
6	D	1501	QZY	C06-C04	2.54	1.52	1.47
6	D	1501	QZY	C03-C04	2.48	1.44	1.37
6	D	1501	QZY	O04-C18	-2.30	1.19	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1501	QZY	C04-S01-C01	19.21	107.08	91.75
6	D	1501	QZY	C02-N01-C18	-13.62	114.21	124.87
6	D	1501	QZY	C01-C02-N01	7.70	128.96	121.17
6	D	1501	QZY	C03-C02-C01	-4.77	108.69	113.80
6	D	1501	QZY	C02-C01-S01	-4.42	107.44	111.20
6	D	1501	QZY	C06-C04-S01	3.36	129.59	121.02
6	D	1501	QZY	C09-O03-C12	-3.31	111.23	118.78
6	D	1501	QZY	C20-N02-C19	3.07	120.22	116.36
6	D	1501	QZY	C05-C01-S01	2.87	126.63	115.13
6	D	1501	QZY	O01-C05-O02	2.42	129.65	123.90
6	D	1501	QZY	C06-C04-C03	-2.06	122.18	127.97
6	D	1501	QZY	C02-C03-C04	-2.05	108.58	111.72

There are no chirality outliers.

All (11) torsion outliers are listed below:

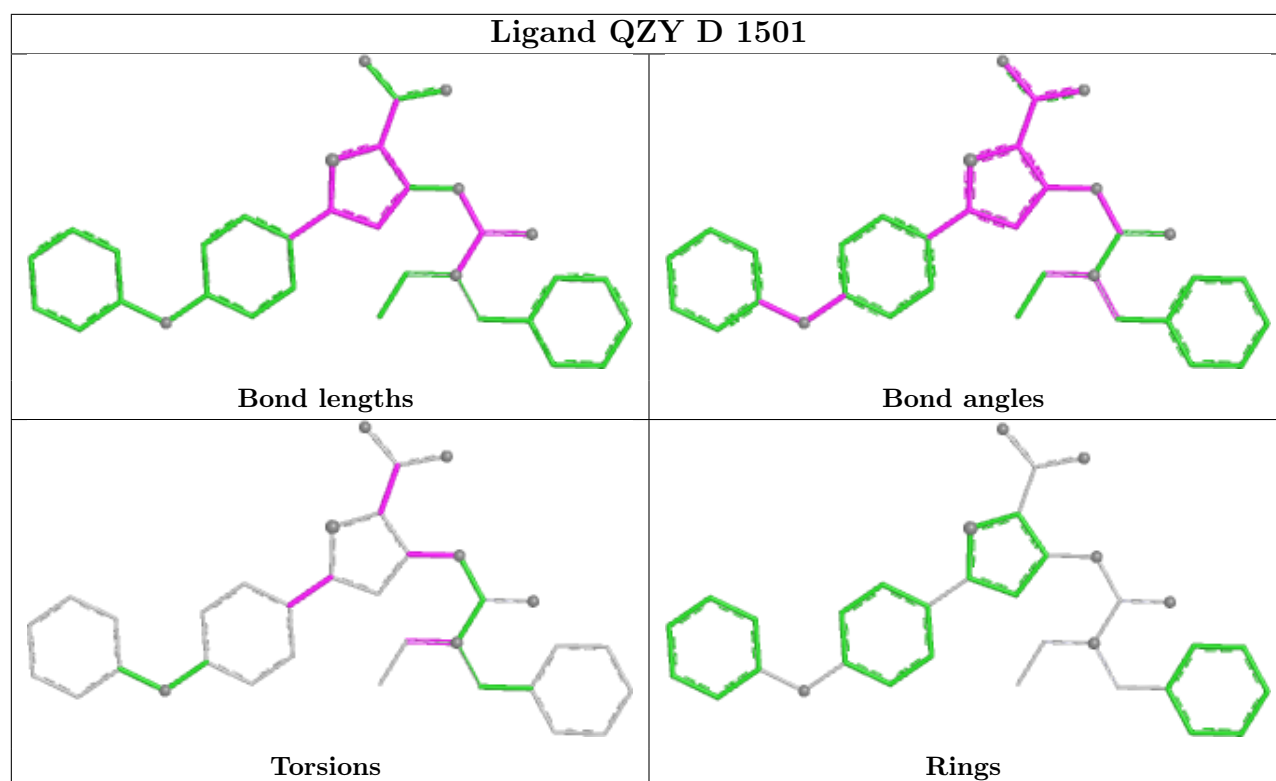
Mol	Chain	Res	Type	Atoms
6	D	1501	QZY	C03-C02-N01-C18
6	D	1501	QZY	C03-C04-C06-C11
6	D	1501	QZY	C03-C04-C06-C07
6	D	1501	QZY	S01-C04-C06-C11
6	D	1501	QZY	S01-C04-C06-C07
6	D	1501	QZY	C28-C19-N02-C18
6	D	1501	QZY	S01-C01-C05-O01
6	D	1501	QZY	S01-C01-C05-O02
6	D	1501	QZY	C28-C19-N02-C20
6	D	1501	QZY	C01-C02-N01-C18
6	D	1501	QZY	C02-C01-C05-O02

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1501	QZY	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	2:GLN	C	3:GLY	N	3.61

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	234/329 (71%)	-0.52	0	100	100	118, 170, 244, 287	0
1	B	301/329 (91%)	-0.54	0	100	100	127, 224, 319, 341	0
1	F	234/329 (71%)	-0.48	1 (0%)	88	75	188, 241, 284, 351	0
1	G	229/329 (69%)	-0.23	1 (0%)	88	75	199, 303, 339, 364	0
2	C	1336/1342 (99%)	-0.55	1 (0%)	92	87	95, 160, 263, 327	0
2	H	1336/1342 (99%)	-0.56	0	100	100	137, 195, 310, 420	0
3	D	1164/1407 (82%)	-0.51	0	100	100	90, 154, 258, 314	0
3	I	1160/1407 (82%)	-0.43	0	100	100	130, 203, 302, 360	0
4	E	90/91 (98%)	-0.55	0	100	100	141, 198, 256, 300	0
4	J	76/91 (83%)	-0.46	1 (1%)	75	57	277, 333, 432, 451	0
5	X	471/613 (76%)	-0.57	0	100	100	135, 226, 364, 410	0
5	Y	475/613 (77%)	-0.55	0	100	100	149, 240, 364, 394	0
All	All	7106/8222 (86%)	-0.51	4 (0%)	92	87	90, 194, 319, 451	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	16	ARG	2.7
1	G	39	LEU	2.6
1	F	88	LEU	2.4
2	C	206	ALA	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

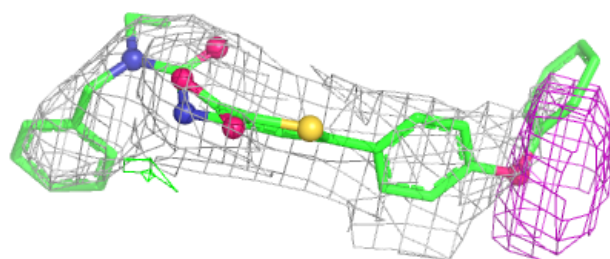
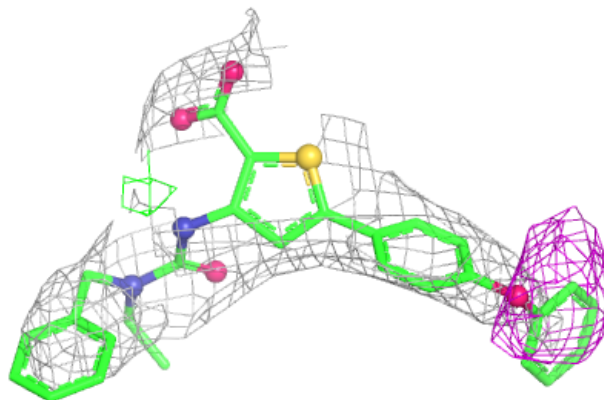
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	QZY	D	1501	34/34	0.92	0.13	112,133,149,170	0
7	ZN	I	1502	1/1	0.97	0.04	149,149,149,149	0
8	MG	I	1503	1/1	0.98	0.07	135,135,135,135	0
7	ZN	D	1502	1/1	0.99	0.04	171,171,171,171	0
8	MG	D	1504	1/1	0.99	0.02	58,58,58,58	0
7	ZN	D	1503	1/1	0.99	0.10	179,179,179,179	0
7	ZN	I	1501	1/1	1.00	0.03	168,168,168,168	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QZY D 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.