Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 05:45 pm BST

PDB ID	:	5NG5 / pdb_00005ng5
EMDB ID	:	EMD-3636
Title	:	multi-drug efflux; membrane transport; RND superfamily; Drug resistance
Authors	:	Wang, Z.; Fan, G.; Hryc, C.F.; Blaza, J.N.; Serysheva, I.I.; Schmid, M.F.; Chiu, W.; Luisi, B.F.; Du, D.
Deposited on	:	2017-03-16
Resolution	:	6.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

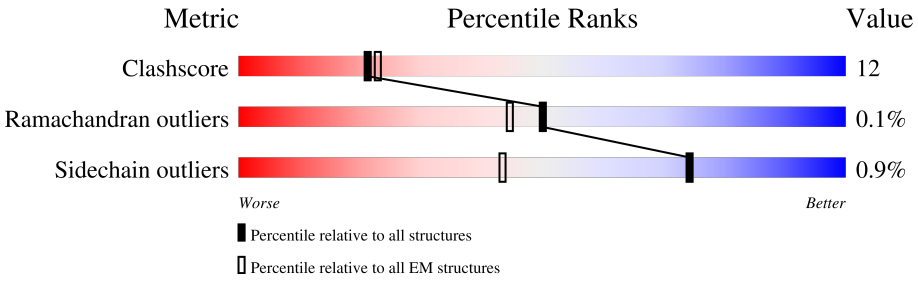
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	373	69% 21% • 9%
1	B	373	69% 21% • 9%
1	D	373	60% 28% • 9%
1	E	373	63% 25% • 9%
1	G	373	61% 28% • 9%
1	H	373	67% 23% • 9%
2	C	493	66% 21% 13%
2	F	493	66% 21% 13%
2	I	493	63% 24% 13%

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Mol	Chain	Length	Quality of chain
3	J	1049	71% 27%
3	K	1049	73% 26%
3	L	1049	74% 24%
4	M	54	69% 17% 15%
4	N	54	74% 11% 15%
4	O	54	70% 15% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	5QF	J	1101	-	-	X	-
5	5QF	K	1101	-	-	X	-
5	5QF	L	1101	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 49920 atoms, of which 114 are hydrogens and 0 are deuteriums.

In the tables below, 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 Multidrug efflux pump subunit AcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	340	Total	C	N	O	S	0	0
			2553	1591	451	506	5		
1	D	340	Total	C	N	O	S	0	0
			2553	1591	451	506	5		
1	G	340	Total	C	N	O	S	0	0
			2553	1591	451	506	5		
1	H	340	Total	C	N	O	S	0	0
			2553	1591	451	506	5		
1	A	340	Total	C	N	O	S	0	0
			2553	1591	451	506	5		
1	B	340	Total	C	N	O	S	0	0
			2553	1591	451	506	5		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	223	MET	PHE	conflict	UNP P0AE06
E	224	MET	LEU	conflict	UNP P0AE06
E	287	MET	LEU	conflict	UNP P0AE06
E	288	MET	LEU	conflict	UNP P0AE06
D	223	MET	PHE	conflict	UNP P0AE06
D	224	MET	LEU	conflict	UNP P0AE06
D	287	MET	LEU	conflict	UNP P0AE06
D	288	MET	LEU	conflict	UNP P0AE06
G	223	MET	PHE	conflict	UNP P0AE06
G	224	MET	LEU	conflict	UNP P0AE06
G	287	MET	LEU	conflict	UNP P0AE06
G	288	MET	LEU	conflict	UNP P0AE06
H	223	MET	PHE	conflict	UNP P0AE06
H	224	MET	LEU	conflict	UNP P0AE06
H	287	MET	LEU	conflict	UNP P0AE06
H	288	MET	LEU	conflict	UNP P0AE06
A	223	MET	PHE	conflict	UNP P0AE06
A	224	MET	LEU	conflict	UNP P0AE06

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Chain	Residue	Modelled	Actual	Comment	Reference
A	287	MET	LEU	conflict	UNP P0AE06
A	288	MET	LEU	conflict	UNP P0AE06
B	223	MET	PHE	conflict	UNP P0AE06
B	224	MET	LEU	conflict	UNP P0AE06
B	287	MET	LEU	conflict	UNP P0AE06
B	288	MET	LEU	conflict	UNP P0AE06

- Molecule 2 is a protein called Outer membrane protein TolC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	428	Total	C	N	O	S	0	0
			3304	2037	586	676	5		
2	I	428	Total	C	N	O	S	0	0
			3304	2037	586	676	5		
2	C	428	Total	C	N	O	S	0	0
			3304	2037	586	676	5		

- Molecule 3 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	1037	Total	C	N	O	S	0	0
			7819	5032	1290	1453	44		
3	L	1037	Total	C	N	O	S	0	0
			7819	5032	1290	1453	44		
3	J	1033	Total	C	N	O	S	0	0
			7849	5052	1295	1458	44		

- Molecule 4 is a protein called Multidrug efflux pump accessory protein AcrZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	46	Total	C	N	O	S	0	0
			326	219	48	56	3		
4	N	46	Total	C	N	O	S	0	0
			326	219	48	56	3		
4	O	46	Total	C	N	O	S	0	0
			326	219	48	56	3		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	50	HIS	-	expression tag	UNP P0AAW9
M	51	HIS	-	expression tag	UNP P0AAW9

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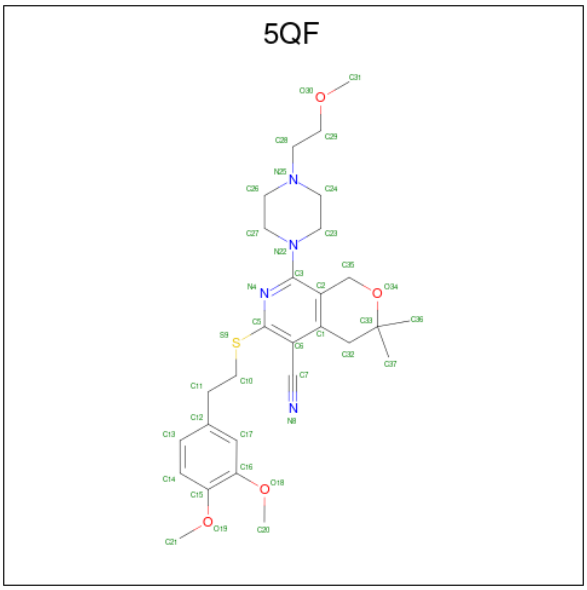
Chain	Residue	Modelled	Actual	Comment	Reference
M	52	HIS	-	expression tag	UNP P0AAW9
M	53	HIS	-	expression tag	UNP P0AAW9
M	54	HIS	-	expression tag	UNP P0AAW9
N	50	HIS	-	expression tag	UNP P0AAW9
N	51	HIS	-	expression tag	UNP P0AAW9
N	52	HIS	-	expression tag	UNP P0AAW9
N	53	HIS	-	expression tag	UNP P0AAW9
N	54	HIS	-	expression tag	UNP P0AAW9
O	50	HIS	-	expression tag	UNP P0AAW9
O	51	HIS	-	expression tag	UNP P0AAW9
O	52	HIS	-	expression tag	UNP P0AAW9
O	53	HIS	-	expression tag	UNP P0AAW9
O	54	HIS	-	expression tag	UNP P0AAW9

- Molecule 5 is 6-[2-(3,4-dimethoxyphenyl)ethylsulfanyl]-8-[4-(2-methoxyethyl)piperazin-1-yl]-3,3-dimethyl-1,4-dihydropyrano[3,4-c]pyridine-5-carbonitrile (CCD ID: 5QF) (formula: $C_{28}H_{38}N_4O_4S$).



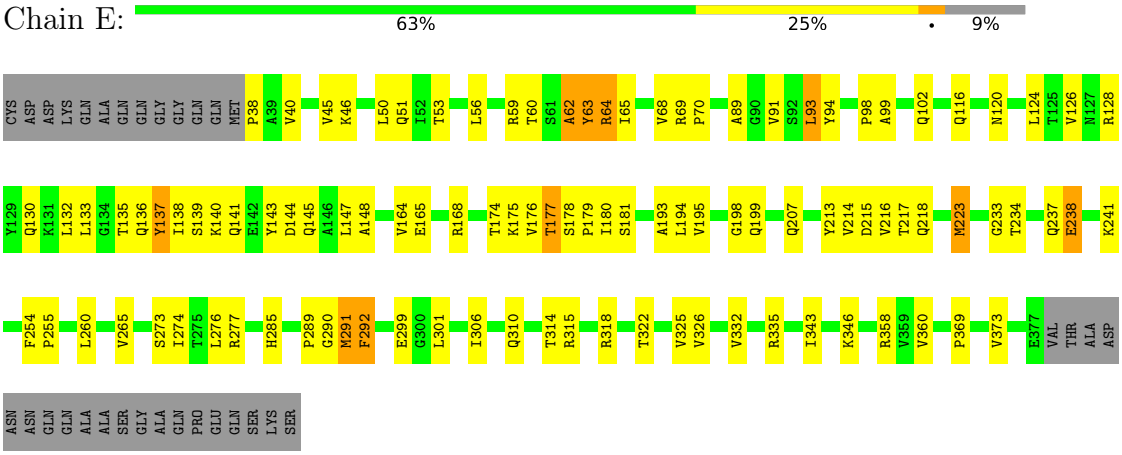
Mol	Chain	Residues	Atoms						AltConf
5	K	1	Total	C	H	N	O	S	0
			75	28	38	4	4	1	
5	L	1	Total	C	H	N	O	S	0
			75	28	38	4	4	1	
5	J	1	Total	C	H	N	O	S	0
			75	28	38	4	4	1	

3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

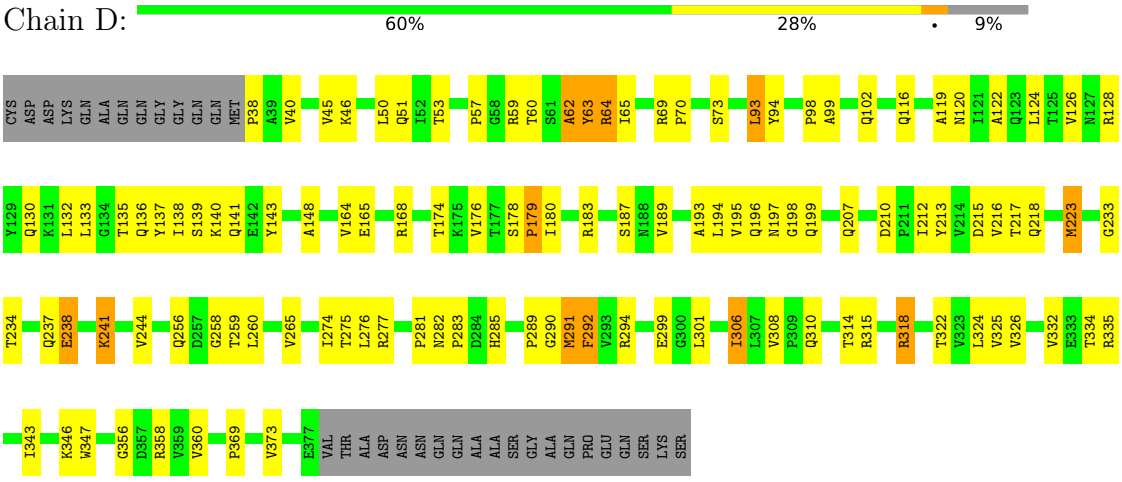
• Molecule 1: Multidrug efflux pump subunit AcrA

Chain E:



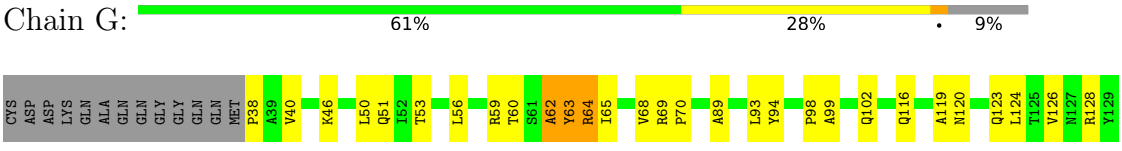
• Molecule 1: Multidrug efflux pump subunit AcrA

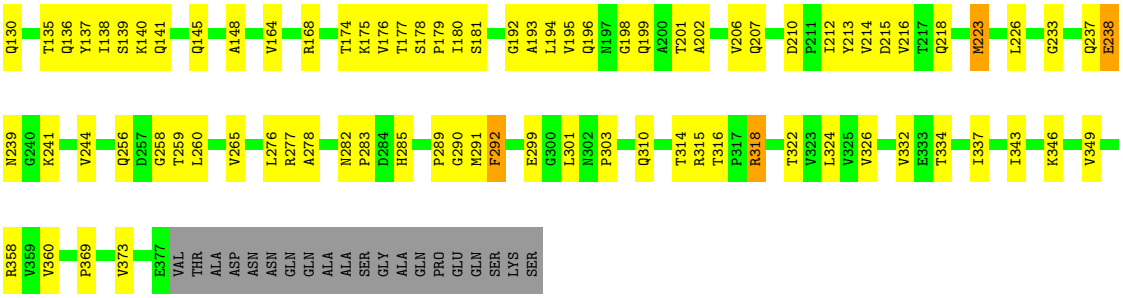
Chain D:



• Molecule 1: Multidrug efflux pump subunit AcrA

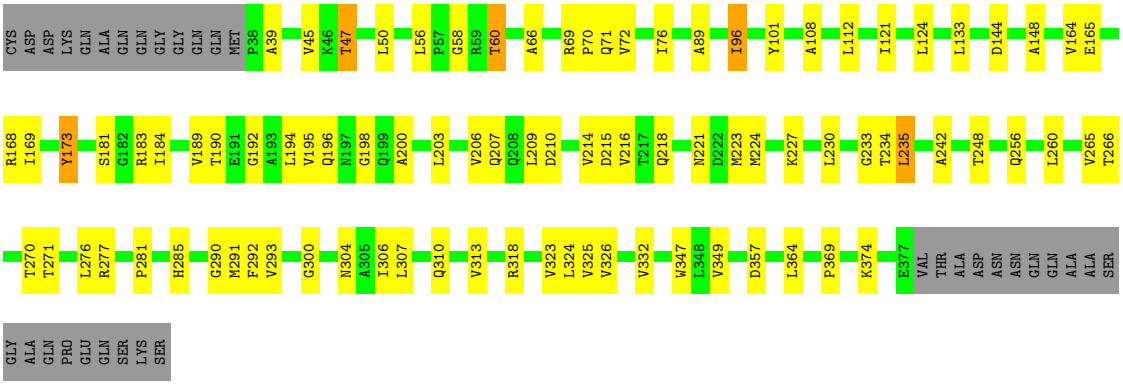
Chain G:





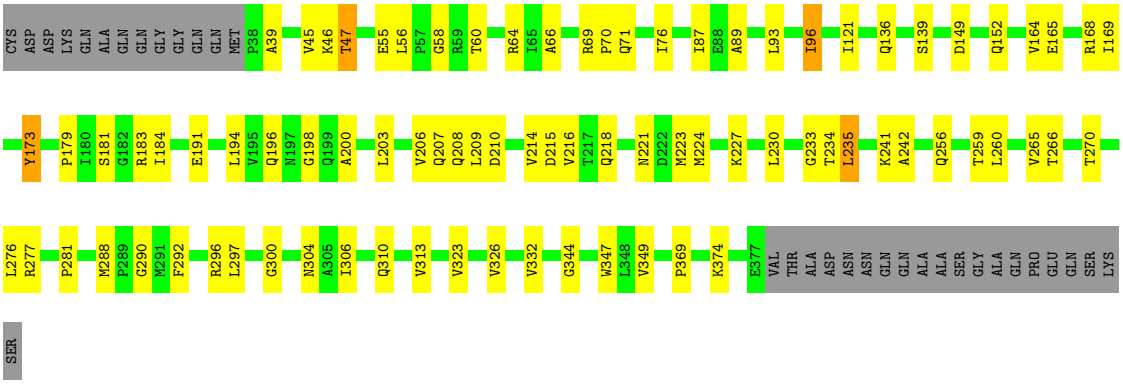
• Molecule 1: Multidrug efflux pump subunit AcrA

Chain H:



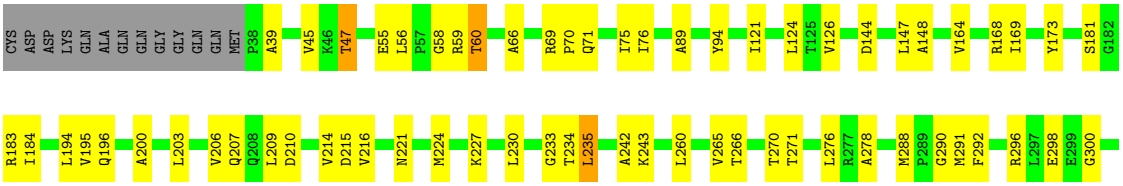
• Molecule 1: Multidrug efflux pump subunit AcrA

Chain A:



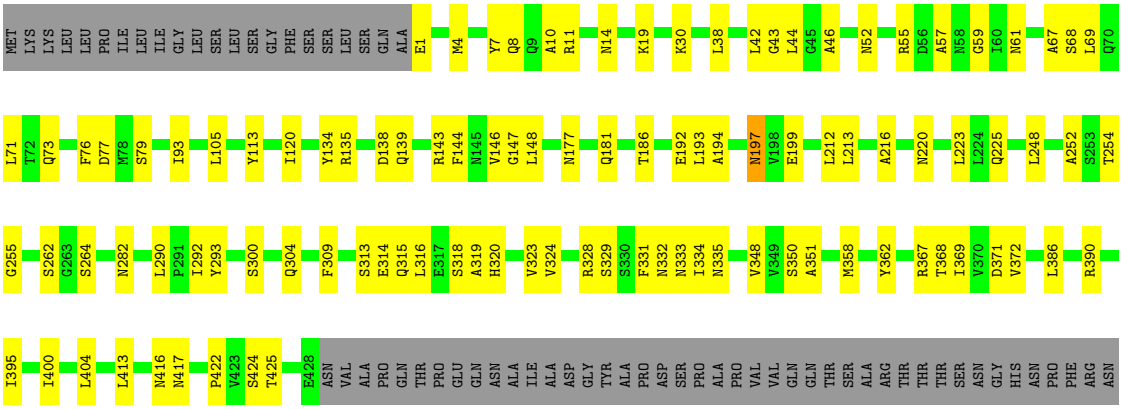
• Molecule 1: Multidrug efflux pump subunit AcrA

Chain B:



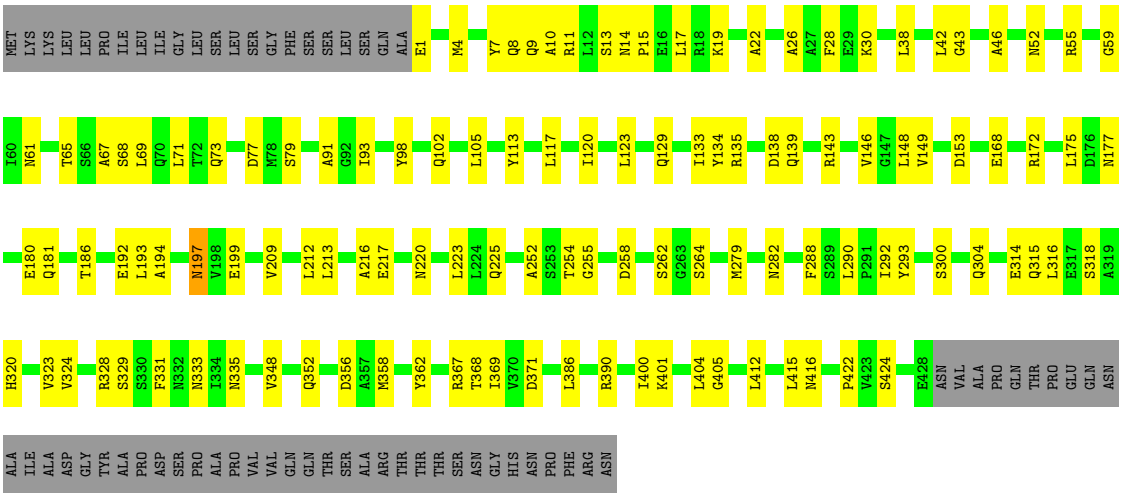
• Molecule 2: Outer membrane protein TolC

Chain F:



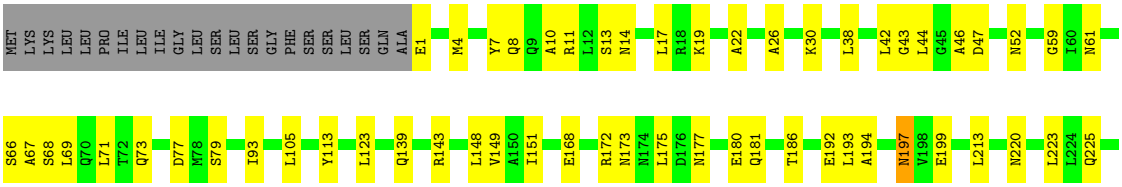
• Molecule 2: Outer membrane protein TolC

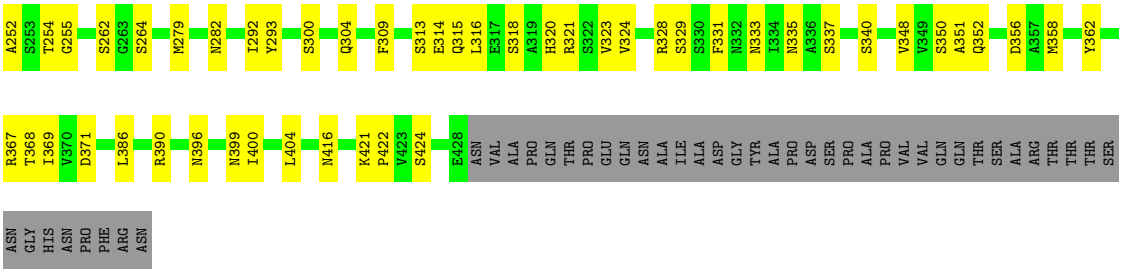
Chain I:



• Molecule 2: Outer membrane protein TolC

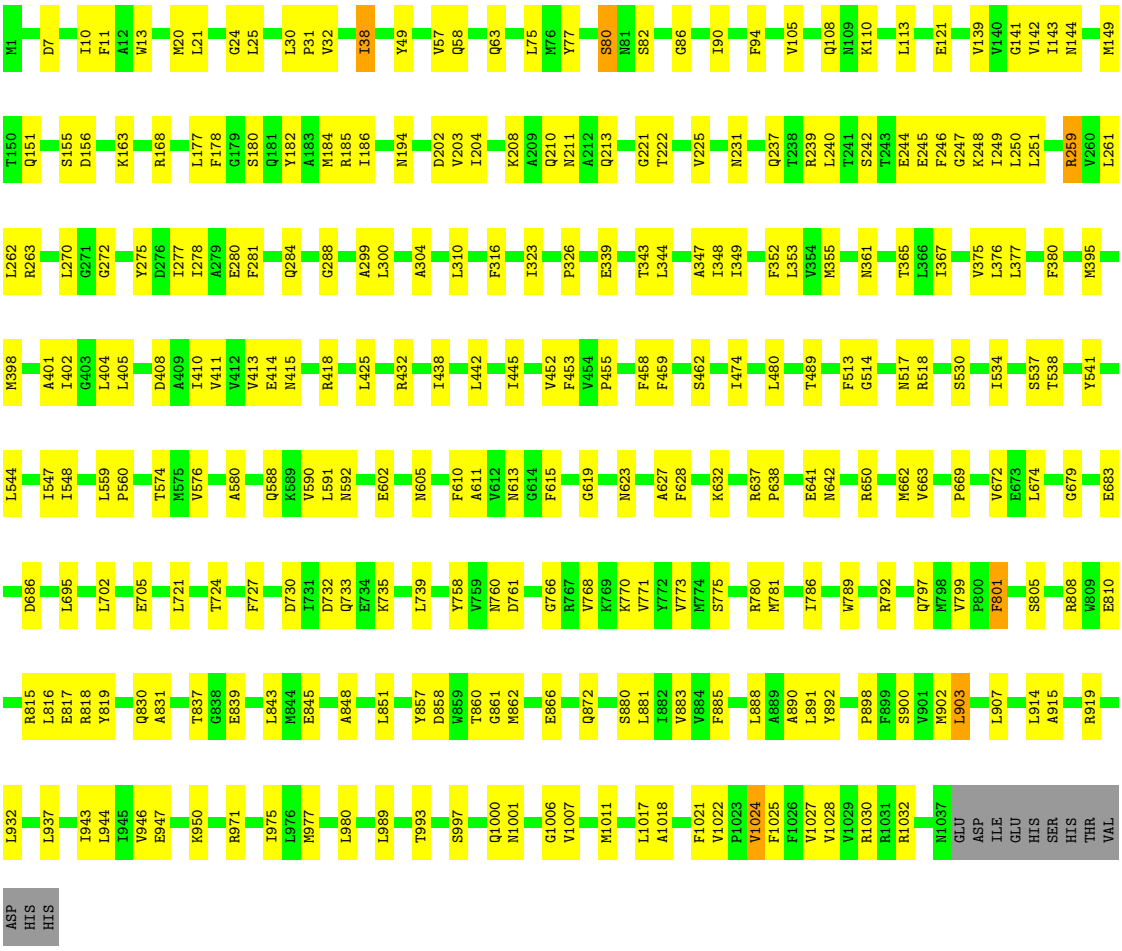
Chain C:





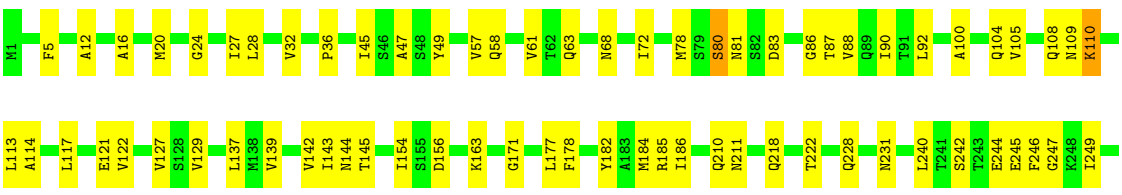
• Molecule 3: Multidrug efflux pump subunit AcrB

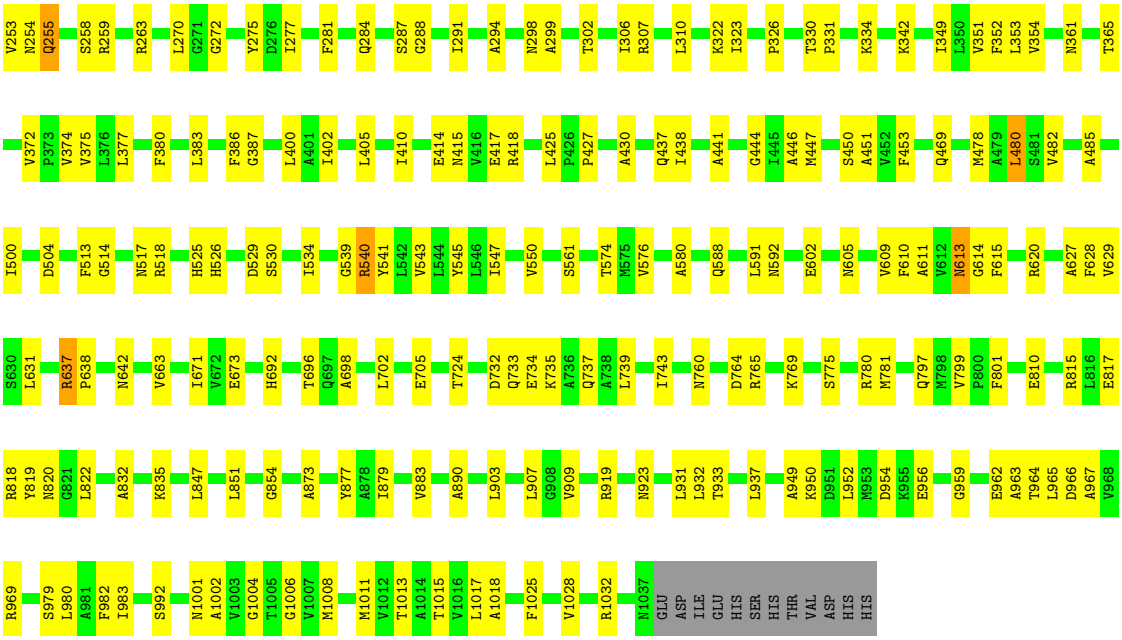
Chain K:



• Molecule 3: Multidrug efflux pump subunit AcrB

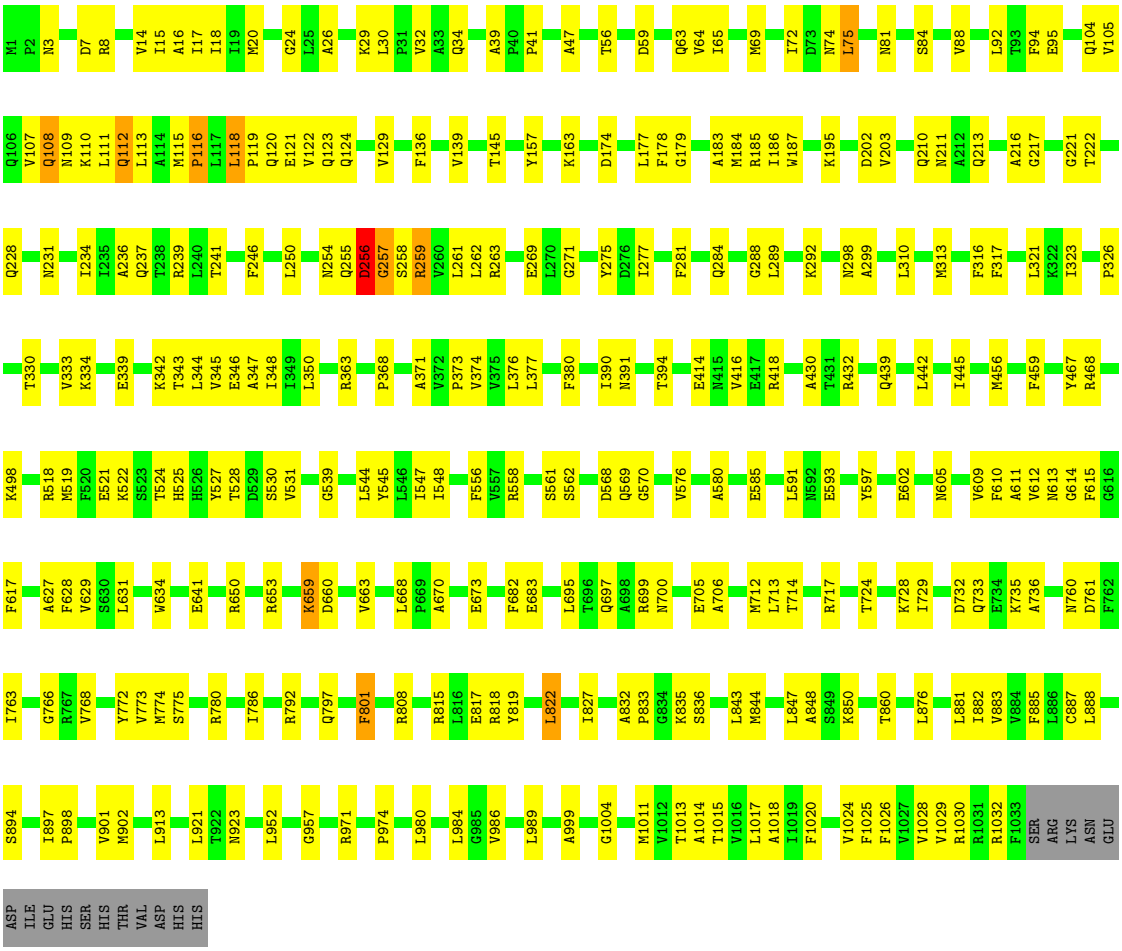
Chain L:





• Molecule 3: Multidrug efflux pump subunit AcrB

Chain J:

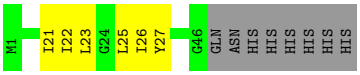


• Molecule 4: Multidrug efflux pump accessory protein AcrZ

Chain M:

• Molecule 4: Multidrug efflux pump accessory protein AcrZ

Chain N:



• Molecule 4: Multidrug efflux pump accessory protein AcrZ

Chain O:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5QF

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	0.57	0/2585	0.74	1/3512 (0.0%)
1	B	0.58	0/2585	0.75	1/3512 (0.0%)
1	D	0.56	0/2585	0.79	3/3512 (0.1%)
1	E	0.59	1/2585 (0.0%)	0.78	3/3512 (0.1%)
1	G	0.57	1/2585 (0.0%)	0.80	3/3512 (0.1%)
1	H	0.57	0/2585	0.76	2/3512 (0.1%)
2	C	0.43	0/3345	0.60	0/4544
2	F	0.44	1/3345 (0.0%)	0.60	0/4544
2	I	0.43	0/3345	0.60	0/4544
3	J	0.49	0/7999	0.71	10/10863 (0.1%)
3	K	0.51	2/7968 (0.0%)	0.69	7/10826 (0.1%)
3	L	0.49	0/7968	0.68	2/10826 (0.0%)
4	M	0.29	0/330	0.61	0/448
4	N	0.30	0/330	0.62	0/448
4	O	0.31	0/330	0.61	0/448
All	All	0.51	5/50470 (0.0%)	0.70	32/68563 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
1	D	0	10
1	E	0	10
1	G	0	6
1	H	0	5
3	J	0	9
3	K	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	3
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	68	VAL	C-N	-7.85	1.16	1.34
3	K	805	SER	CA-CB	-7.13	1.42	1.52
1	G	68	VAL	C-N	-5.13	1.22	1.34
3	K	789	TRP	CB-CG	-5.05	1.41	1.50
2	F	146	VAL	CB-CG1	-5.04	1.42	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	256	ASP	CB-CG-OD1	12.60	129.64	118.30
1	H	56	LEU	CB-CG-CD1	-8.22	97.02	111.00
1	A	56	LEU	CB-CG-CD1	-7.29	98.62	111.00
3	J	113	LEU	CA-CB-CG	7.00	131.40	115.30
1	B	56	LEU	CB-CG-CD1	-6.76	99.51	111.00
3	J	256	ASP	CB-CG-OD2	-6.70	112.27	118.30
3	J	258	SER	N-CA-C	-6.68	92.95	111.00
1	E	63	TYR	C-N-CA	6.68	138.41	121.70
1	D	63	TYR	C-N-CA	6.43	137.79	121.70
3	J	75	LEU	CA-CB-CG	6.37	129.94	115.30
3	J	344	LEU	CA-CB-CG	6.35	129.90	115.30
1	G	63	TYR	C-N-CA	6.34	137.56	121.70
3	K	425	LEU	CA-CB-CG	6.25	129.66	115.30
3	L	425	LEU	CA-CB-CG	6.11	129.36	115.30
3	K	38	ILE	CG1-CB-CG2	-6.05	98.08	111.40
3	K	1017	LEU	CA-CB-CG	6.00	129.10	115.30
3	J	822	LEU	CA-CB-CG	5.94	128.96	115.30
3	J	289	LEU	CA-CB-CG	5.76	128.56	115.30
1	G	56	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	E	64	ARG	N-CA-C	5.64	126.24	111.00
1	E	50	LEU	CA-CB-CG	5.59	128.16	115.30
1	H	133	LEU	CA-CB-CG	5.58	128.12	115.30
3	J	876	LEU	CA-CB-CG	5.55	128.07	115.30
3	K	310	LEU	CA-CB-CG	5.49	127.93	115.30
3	J	695	LEU	CA-CB-CG	5.39	127.69	115.30
1	D	50	LEU	CA-CB-CG	5.37	127.65	115.30
3	K	480	LEU	CA-CB-CG	5.30	127.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	64	ARG	N-CA-C	5.30	125.30	111.00
3	K	376	LEU	CA-CB-CG	5.26	127.39	115.30
3	K	914	LEU	CA-CB-CG	5.24	127.36	115.30
3	L	480	LEU	CA-CB-CG	5.21	127.29	115.30
1	G	64	ARG	N-CA-C	5.08	124.73	111.00

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	TYR	Peptide
1	A	210	ASP	Peptide
1	A	235	LEU	Peptide
1	A	300	GLY	Peptide
1	A	46	LYS	Peptide
1	A	47	THR	Peptide
1	B	210	ASP	Peptide
1	B	235	LEU	Peptide
1	B	300	GLY	Peptide
1	B	47	THR	Peptide
1	D	135	THR	Peptide
1	D	174	THR	Peptide
1	D	223	MET	Peptide
1	D	238	GLU	Peptide
1	D	241	LYS	Peptide
1	D	291	MET	Peptide
1	D	292	PHE	Peptide
1	D	306	ILE	Peptide
1	D	62	ALA	Peptide
1	D	93	LEU	Peptide
1	E	135	THR	Peptide
1	E	174	THR	Peptide
1	E	177	THR	Peptide
1	E	223	MET	Peptide
1	E	238	GLU	Peptide
1	E	241	LYS	Peptide
1	E	291	MET	Peptide
1	E	292	PHE	Peptide
1	E	62	ALA	Peptide
1	E	93	LEU	Peptide
1	G	135	THR	Peptide
1	G	174	THR	Peptide

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Mol	Chain	Res	Type	Group
1	G	223	MET	Peptide
1	G	238	GLU	Peptide
1	G	292	PHE	Peptide
1	G	62	ALA	Peptide
1	H	173	TYR	Peptide
1	H	210	ASP	Peptide
1	H	235	LEU	Peptide
1	H	300	GLY	Peptide
1	H	47	THR	Peptide
3	J	108	GLN	Peptide
3	J	112	GLN	Peptide
3	J	116	PRO	Peptide
3	J	118	LEU	Peptide
3	J	119	PRO	Peptide
3	J	255	GLN	Peptide
3	J	256	ASP	Peptide
3	J	257	GLY	Peptide
3	J	732	ASP	Peptide
3	K	1024	VAL	Peptide
3	K	38	ILE	Peptide
3	K	80	SER	Peptide
3	K	903	LEU	Peptide
3	L	110	LYS	Peptide
3	L	80	SER	Peptide
3	L	879	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2610	59	0
1	B	2553	0	2610	55	0
1	D	2553	0	2610	80	0
1	E	2553	0	2609	68	0
1	G	2553	0	2610	76	0
1	H	2553	0	2610	61	0
2	C	3304	0	3254	78	0
2	F	3304	0	3254	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	3304	0	3254	88	0
3	J	7849	0	8001	226	0
3	K	7819	0	7919	207	0
3	L	7819	0	7919	204	0
4	M	326	0	346	7	0
4	N	326	0	346	4	0
4	O	326	0	346	6	0
5	J	37	38	0	49	0
5	K	37	38	0	43	0
5	L	37	38	0	42	0
All	All	49806	114	50298	1161	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 12.

All (1161) 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:J:628:PHE:HE2	5:J:1101:5QF:C5	1.07	1.64
3:J:628:PHE:CE2	5:J:1101:5QF:C5	1.84	1.59
3:K:277:ILE:HG21	5:K:1101:5QF:C16	1.31	1.57
3:L:178:PHE:HB3	5:L:1101:5QF:C15	1.39	1.49
3:J:628:PHE:HE2	5:J:1101:5QF:N4	1.18	1.39
3:L:277:ILE:CG2	5:L:1101:5QF:O19	1.70	1.38
3:J:628:PHE:CD2	5:J:1101:5QF:C6	2.09	1.35
3:K:277:ILE:CG2	5:K:1101:5QF:C16	2.05	1.34
3:J:628:PHE:CE2	5:J:1101:5QF:C6	2.08	1.33
3:K:277:ILE:HG21	5:K:1101:5QF:O18	1.17	1.32
3:K:610:PHE:HE2	5:K:1101:5QF:S9	1.55	1.29
3:L:277:ILE:HG21	5:L:1101:5QF:C15	1.61	1.28
3:K:277:ILE:CG2	5:K:1101:5QF:O18	1.81	1.25
3:J:628:PHE:CE2	5:J:1101:5QF:N4	1.96	1.25
3:L:178:PHE:CB	5:L:1101:5QF:C14	2.00	1.24
3:K:610:PHE:CE2	5:K:1101:5QF:S9	2.32	1.21
3:K:139:VAL:HG11	5:K:1101:5QF:C7	1.68	1.21
3:J:615:PHE:CE2	5:J:1101:5QF:C26	2.23	1.21
3:K:615:PHE:CZ	5:K:1101:5QF:C26	2.24	1.20
3:J:615:PHE:CZ	5:J:1101:5QF:C26	2.26	1.19
3:L:277:ILE:HG13	5:L:1101:5QF:C20	1.74	1.16
3:J:628:PHE:CE2	5:J:1101:5QF:C3	2.26	1.16
3:J:277:ILE:HD13	5:J:1101:5QF:C20	1.75	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:615:PHE:CE1	5:K:1101:5QF:C26	2.29	1.15
3:J:628:PHE:CZ	5:J:1101:5QF:C3	2.29	1.14
3:K:277:ILE:HG13	5:K:1101:5QF:C20	1.77	1.13
3:J:326:PRO:HB2	5:J:1101:5QF:N8	1.61	1.13
3:L:178:PHE:HB3	5:L:1101:5QF:C14	1.52	1.11
3:L:277:ILE:HG21	5:L:1101:5QF:C16	1.81	1.10
3:K:277:ILE:CB	5:K:1101:5QF:O18	2.00	1.08
3:L:277:ILE:HG21	5:L:1101:5QF:O19	1.36	1.07
3:J:628:PHE:CE2	5:J:1101:5QF:C1	2.38	1.06
3:L:178:PHE:O	5:L:1101:5QF:C21	2.10	0.99
3:J:628:PHE:CE2	5:J:1101:5QF:C2	2.46	0.99
3:J:610:PHE:CE2	5:J:1101:5QF:S9	2.58	0.97
3:L:178:PHE:HB3	5:L:1101:5QF:C16	1.68	0.95
3:K:178:PHE:HB3	5:K:1101:5QF:C12	1.96	0.95
3:J:139:VAL:HG11	5:J:1101:5QF:C5	1.96	0.95
3:K:277:ILE:HG21	5:K:1101:5QF:C17	1.99	0.91
3:J:628:PHE:HD2	5:J:1101:5QF:C7	1.83	0.91
3:J:628:PHE:CD2	5:J:1101:5QF:C1	2.54	0.90
3:K:277:ILE:HG13	5:K:1101:5QF:O18	1.72	0.89
3:L:277:ILE:HG22	5:L:1101:5QF:O19	1.70	0.89
3:L:277:ILE:CB	5:L:1101:5QF:O19	2.20	0.88
3:K:277:ILE:CG1	5:K:1101:5QF:O18	2.21	0.88
3:L:178:PHE:CB	5:L:1101:5QF:C15	2.33	0.88
3:L:277:ILE:HB	5:L:1101:5QF:C21	2.02	0.88
3:J:610:PHE:HE2	5:J:1101:5QF:C10	1.87	0.88
3:L:178:PHE:CE1	5:L:1101:5QF:C27	2.57	0.87
3:J:628:PHE:CD2	5:J:1101:5QF:C7	2.57	0.87
3:J:628:PHE:CZ	5:J:1101:5QF:C2	2.58	0.86
3:J:628:PHE:HD2	5:J:1101:5QF:C6	1.87	0.85
3:L:277:ILE:CG2	5:L:1101:5QF:C15	2.39	0.84
3:J:668:LEU:HD11	5:J:1101:5QF:C36	2.07	0.84
3:J:139:VAL:HG11	5:J:1101:5QF:C6	2.07	0.83
3:K:178:PHE:O	5:K:1101:5QF:C15	2.26	0.83
3:J:628:PHE:CD2	5:J:1101:5QF:C5	2.46	0.83
3:J:277:ILE:CD1	5:J:1101:5QF:C20	2.56	0.82
3:L:277:ILE:HG21	5:L:1101:5QF:O18	1.79	0.81
3:K:178:PHE:HB3	5:K:1101:5QF:C11	2.10	0.80
3:J:139:VAL:HG12	5:J:1101:5QF:S9	2.21	0.80
3:J:610:PHE:CE2	5:J:1101:5QF:C10	2.65	0.79
3:L:222:THR:HB	3:J:275:TYR:HB2	1.65	0.78
3:L:615:PHE:CZ	5:L:1101:5QF:C26	2.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:610:PHE:HE2	5:J:1101:5QF:S9	2.07	0.78
3:K:277:ILE:CG2	5:K:1101:5QF:C15	2.65	0.75
1:G:148:ALA:HB2	1:H:121:ILE:HG13	1.68	0.75
3:L:143:ILE:HD11	3:L:284:GLN:HG3	1.70	0.74
3:K:277:ILE:HG22	5:K:1101:5QF:C16	2.17	0.73
3:K:178:PHE:O	5:K:1101:5QF:C14	2.37	0.72
3:K:178:PHE:O	5:K:1101:5QF:C16	2.38	0.71
1:D:148:ALA:HB2	1:B:121:ILE:HG13	1.71	0.71
3:K:139:VAL:HG11	5:K:1101:5QF:N8	2.01	0.71
2:F:52:ASN:HB3	2:I:282:ASN:HB2	1.73	0.71
1:G:218:GLN:HG2	1:G:223:MET:HG3	1.73	0.70
2:F:282:ASN:HB2	2:C:52:ASN:HB3	1.72	0.70
3:L:277:ILE:HB	5:L:1101:5QF:O19	1.90	0.70
1:E:148:ALA:HB2	1:A:121:ILE:HG13	1.72	0.70
3:J:185:ARG:NH2	3:J:774:MET:SD	2.65	0.70
3:J:139:VAL:CG1	5:J:1101:5QF:C5	2.69	0.70
3:K:259:ARG:NH1	3:L:734:GLU:OE2	2.26	0.69
3:K:139:VAL:CG1	5:K:1101:5QF:C7	2.60	0.69
3:J:326:PRO:CB	5:J:1101:5QF:N8	2.50	0.69
1:A:60:THR:HG23	1:A:290:GLY:H	1.58	0.68
1:D:93:LEU:H	1:D:176:VAL:HB	1.58	0.68
2:I:52:ASN:HB3	2:C:282:ASN:HB2	1.74	0.68
4:M:45:PRO:HB2	3:J:1032:ARG:HH12	1.59	0.67
3:J:178:PHE:CD2	5:J:1101:5QF:C11	2.78	0.67
3:L:5:PHE:HB3	3:L:12:ALA:HB2	1.77	0.67
1:E:69:ARG:HD2	1:A:194:LEU:HB3	1.75	0.67
3:K:610:PHE:HE2	5:K:1101:5QF:C10	2.08	0.67
3:L:671:ILE:HG22	3:L:673:GLU:H	1.60	0.67
3:L:576:VAL:HG23	3:L:663:VAL:HG22	1.77	0.67
3:L:139:VAL:HG11	5:L:1101:5QF:S9	2.34	0.66
1:G:216:VAL:HB	1:G:276:LEU:HB2	1.78	0.66
1:A:230:LEU:HD23	1:A:235:LEU:H	1.60	0.66
3:J:610:PHE:CZ	5:J:1101:5QF:C11	2.79	0.66
3:K:139:VAL:HG11	5:K:1101:5QF:C6	2.25	0.66
3:K:277:ILE:HB	5:K:1101:5QF:O19	1.96	0.66
3:L:775:SER:HB3	3:L:780:ARG:HD3	1.78	0.66
3:K:628:PHE:CE2	5:K:1101:5QF:C5	2.68	0.65
3:K:349:ILE:HA	3:K:352:PHE:HB3	1.77	0.65
3:L:539:GLY:HA3	4:O:40:GLY:H	1.62	0.65
3:J:72:ILE:HA	3:J:110:LYS:HE2	1.77	0.65
3:K:574:THR:HB	3:K:627:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:THR:HG23	1:H:290:GLY:H	1.62	0.65
3:J:254:ASN:ND2	3:J:256:ASP:OD1	2.30	0.65
1:B:60:THR:HG23	1:B:290:GLY:H	1.63	0.64
3:K:890:ALA:HB1	3:J:8:ARG:HD3	1.78	0.64
3:J:277:ILE:HG21	5:J:1101:5QF:O18	1.92	0.64
3:K:628:PHE:CD2	5:K:1101:5QF:C6	2.68	0.64
3:K:178:PHE:CD2	5:K:1101:5QF:S9	2.91	0.63
3:J:277:ILE:CG2	5:J:1101:5QF:O18	2.46	0.63
1:B:230:LEU:HD23	1:B:235:LEU:H	1.63	0.63
3:K:375:VAL:HG11	3:K:405:LEU:HD11	1.81	0.63
3:J:178:PHE:HD2	5:J:1101:5QF:C11	2.12	0.63
3:J:211:ASN:O	3:J:760:ASN:ND2	2.31	0.63
3:K:178:PHE:CB	5:K:1101:5QF:C11	2.77	0.63
1:D:216:VAL:HB	1:D:276:LEU:HB2	1.81	0.63
3:K:143:ILE:HD11	3:K:284:GLN:HG3	1.81	0.63
3:K:185:ARG:NH2	3:K:272:GLY:O	2.30	0.63
3:J:174:ASP:HB3	3:J:292:LYS:HB2	1.81	0.62
3:L:326:PRO:HB2	5:L:1101:5QF:N8	2.14	0.62
1:G:93:LEU:H	1:G:176:VAL:HB	1.64	0.62
1:H:230:LEU:HD23	1:H:235:LEU:H	1.64	0.62
3:K:733:GLN:OE1	3:J:237:GLN:NE2	2.33	0.62
2:I:223:LEU:HD22	2:I:323:VAL:HG11	1.82	0.62
3:J:64:VAL:HG11	3:J:118:LEU:HA	1.81	0.62
3:J:628:PHE:HZ	5:J:1101:5QF:C3	2.02	0.62
1:D:63:TYR:HB3	1:D:64:ARG:HB2	1.82	0.61
1:B:243:LYS:NZ	1:B:298:GLU:OE1	2.33	0.61
3:K:277:ILE:HB	5:K:1101:5QF:O18	1.98	0.61
1:G:215:ASP:OD1	1:G:277:ARG:NH1	2.33	0.61
1:H:60:THR:HB	1:H:214:VAL:HG22	1.82	0.61
2:F:304:GLN:HE21	2:C:30:LYS:HA	1.64	0.61
3:L:108:GLN:NE2	3:J:112:GLN:O	2.33	0.61
2:C:1:GLU:N	2:C:192:GLU:O	2.34	0.61
1:B:58:GLY:HA2	1:B:216:VAL:HA	1.82	0.61
2:I:30:LYS:HA	2:C:304:GLN:HE21	1.65	0.61
2:C:143:ARG:HB3	2:C:148:LEU:HB2	1.82	0.61
3:J:888:LEU:HB2	3:J:898:PRO:HG3	1.83	0.61
1:B:69:ARG:NH1	1:B:200:ALA:O	2.34	0.61
2:F:30:LYS:HA	2:I:304:GLN:HE21	1.65	0.61
1:B:306:ILE:HB	1:B:349:VAL:HB	1.83	0.61
3:K:377:LEU:HA	3:K:380:PHE:HD2	1.65	0.61
2:F:10:ALA:HB2	2:F:186:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:414:GLU:HB3	3:J:974:PRO:HG3	1.84	0.60
2:I:1:GLU:N	2:I:192:GLU:O	2.34	0.60
3:K:222:THR:HB	3:L:275:TYR:HB2	1.83	0.60
3:K:538:THR:HA	3:K:541:TYR:HB2	1.83	0.60
3:J:277:ILE:HD13	5:J:1101:5QF:O18	2.01	0.60
3:J:610:PHE:HZ	5:J:1101:5QF:C11	2.14	0.60
1:D:207:GLN:NE2	1:H:266:THR:OG1	2.35	0.60
1:H:306:ILE:HB	1:H:349:VAL:HB	1.82	0.60
3:K:213:GLN:HB2	3:K:239:ARG:HG3	1.82	0.60
1:B:326:VAL:HA	1:B:332:VAL:HA	1.83	0.60
3:J:136:PHE:CE2	5:J:1101:5QF:C23	2.85	0.60
3:K:277:ILE:HG22	5:K:1101:5QF:C15	2.31	0.60
1:D:69:ARG:NH1	1:D:199:GLN:O	2.34	0.60
3:K:781:MET:SD	3:J:228:GLN:NE2	2.75	0.60
3:J:139:VAL:CG1	5:J:1101:5QF:S9	2.89	0.60
1:D:51:GLN:NE2	1:D:301:LEU:O	2.35	0.60
1:D:289:PRO:HD2	1:H:265:VAL:HG12	1.84	0.60
1:A:306:ILE:HB	1:A:349:VAL:HB	1.84	0.60
2:I:10:ALA:HB2	2:I:186:THR:HG22	1.84	0.60
3:K:186:ILE:HB	3:K:773:VAL:HA	1.83	0.60
2:F:368:THR:OG1	2:F:369:ILE:N	2.35	0.59
3:J:628:PHE:CZ	5:J:1101:5QF:N4	2.57	0.59
2:F:386:LEU:HD21	2:F:390:ARG:HH21	1.67	0.59
3:L:178:PHE:C	5:L:1101:5QF:C21	2.71	0.59
1:H:318:ARG:NH2	3:L:810:GLU:OE1	2.36	0.59
3:K:108:GLN:NE2	3:L:109:ASN:O	2.35	0.59
3:J:65:ILE:HG23	3:J:111:LEU:HD13	1.84	0.59
3:K:361:ASN:HB2	3:K:365:THR:HG23	1.85	0.59
1:G:69:ARG:NH1	1:G:199:GLN:O	2.34	0.59
1:H:58:GLY:HA2	1:H:216:VAL:HA	1.85	0.59
3:L:602:GLU:OE1	3:L:605:ASN:ND2	2.36	0.59
1:E:69:ARG:NH1	1:E:199:GLN:O	2.36	0.59
3:L:615:PHE:CE2	5:L:1101:5QF:C26	2.85	0.59
1:B:60:THR:HB	1:B:214:VAL:HG22	1.85	0.59
3:K:459:PHE:HE1	3:K:872:GLN:H	1.49	0.59
3:L:80:SER:HA	3:L:90:ILE:HA	1.85	0.59
3:J:1020:PHE:O	3:J:1024:VAL:N	2.32	0.58
2:F:194:ALA:HA	2:F:422:PRO:HA	1.85	0.58
3:K:576:VAL:HG23	3:K:663:VAL:HG22	1.85	0.58
3:L:414:GLU:HA	3:L:417:GLU:HB3	1.85	0.58
3:J:216:ALA:HB2	3:J:236:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:GLN:HE22	1:D:283:PRO:HD3	1.69	0.58
3:K:534:ILE:HA	3:K:537:SER:HB2	1.86	0.58
3:K:679:GLY:HA2	3:K:830:GLN:HA	1.86	0.58
1:D:215:ASP:OD1	1:D:277:ARG:NH1	2.37	0.58
1:G:292:PHE:HB3	3:J:735:LYS:HE2	1.86	0.58
3:L:702:LEU:HD12	3:L:705:GLU:HB3	1.86	0.58
1:E:289:PRO:HD2	1:B:265:VAL:HG12	1.86	0.58
1:G:69:ARG:HD2	1:H:194:LEU:HB3	1.85	0.58
1:A:326:VAL:HA	1:A:332:VAL:HA	1.85	0.58
3:K:240:LEU:HD23	3:K:245:GLU:HB3	1.85	0.58
3:L:142:VAL:HG12	3:L:323:ILE:HG12	1.85	0.58
3:L:326:PRO:HG2	5:L:1101:5QF:N8	2.18	0.58
1:D:38:PRO:HB2	1:D:373:VAL:HA	1.85	0.57
2:C:348:VAL:HG21	2:C:386:LEU:HD22	1.86	0.57
3:J:202:ASP:OD2	3:J:792:ARG:NH2	2.37	0.57
3:J:459:PHE:O	3:J:468:ARG:NH1	2.37	0.57
3:J:524:THR:HA	3:J:527:TYR:HB3	1.86	0.57
1:E:51:GLN:NE2	1:E:301:LEU:O	2.37	0.57
1:E:198:GLY:O	1:A:196:GLN:NE2	2.36	0.57
2:C:192:GLU:HA	2:C:424:SER:HA	1.85	0.57
2:C:223:LEU:HD22	2:C:323:VAL:HG11	1.84	0.57
3:K:156:ASP:HB3	3:K:182:TYR:HB2	1.84	0.57
3:J:39:ALA:HB2	3:J:673:GLU:HB3	1.85	0.57
3:J:239:ARG:HB2	3:J:763:ILE:HG12	1.86	0.57
3:J:699:ARG:HG2	3:J:827:ILE:HD11	1.87	0.57
1:G:51:GLN:NE2	1:G:301:LEU:O	2.36	0.57
1:G:63:TYR:HB3	1:G:64:ARG:HB2	1.84	0.57
2:I:192:GLU:HA	2:I:424:SER:HA	1.85	0.57
3:K:610:PHE:CE2	5:K:1101:5QF:C10	2.85	0.57
3:K:632:LYS:O	3:K:637:ARG:NH1	2.38	0.57
3:J:342:LYS:O	3:J:346:GLU:N	2.32	0.57
2:F:220:ASN:HD22	2:F:323:VAL:HG23	1.69	0.57
1:E:93:LEU:H	1:E:176:VAL:HB	1.69	0.57
1:B:318:ARG:NH2	3:K:810:GLU:OE1	2.35	0.57
3:K:602:GLU:OE1	3:K:605:ASN:ND2	2.38	0.57
3:L:178:PHE:HE1	5:L:1101:5QF:C27	2.17	0.57
3:J:254:ASN:HD22	3:J:259:ARG:HA	1.70	0.57
2:F:358:MET:O	2:F:362:TYR:N	2.38	0.57
3:J:986:VAL:HG21	3:J:1004:GLY:HA3	1.87	0.57
2:I:300:SER:O	2:I:304:GLN:N	2.36	0.57
2:C:386:LEU:HD21	2:C:390:ARG:HH21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ARG:NH1	3:L:255:GLN:OE1	2.38	0.57
3:L:427:PRO:HA	3:L:430:ALA:HB3	1.86	0.57
3:K:514:GLY:O	3:K:518:ARG:NH1	2.38	0.57
3:J:705:GLU:OE2	3:J:850:LYS:NZ	2.38	0.57
3:K:971:ARG:O	3:K:975:ILE:N	2.38	0.57
3:L:100:ALA:O	3:L:104:GLN:N	2.36	0.57
1:D:57:PRO:HB3	1:D:294:ARG:HG2	1.87	0.56
3:L:105:VAL:HG23	3:J:109:ASN:HD21	1.70	0.56
1:G:332:VAL:HG23	1:G:369:PRO:HA	1.87	0.56
3:K:278:ILE:HB	3:K:613:ASN:HB3	1.85	0.56
3:K:1007:VAL:HG22	3:K:1011:MET:HG2	1.87	0.56
1:D:179:PRO:HD2	1:B:75:ILE:HG21	1.86	0.56
2:F:76:PHE:HB3	2:F:248:LEU:HB3	1.87	0.56
2:F:197:ASN:ND2	2:F:199:GLU:OE1	2.38	0.56
2:F:300:SER:O	2:F:304:GLN:N	2.36	0.56
2:I:71:LEU:HB3	2:I:252:ALA:HB3	1.86	0.56
2:I:143:ARG:HB3	2:I:148:LEU:HB2	1.86	0.56
2:C:358:MET:O	2:C:362:TYR:N	2.39	0.56
3:K:453:PHE:HB3	3:K:932:LEU:HD13	1.86	0.56
3:K:943:ILE:O	3:K:947:GLU:N	2.37	0.56
3:L:349:ILE:O	3:L:353:LEU:N	2.34	0.56
2:F:68:SER:HA	2:F:255:GLY:HA3	1.86	0.56
3:K:1025:PHE:HA	3:K:1028:VAL:HG12	1.87	0.56
3:J:952:LEU:O	3:J:957:GLY:N	2.33	0.56
1:E:63:TYR:HB3	1:E:64:ARG:HB2	1.86	0.56
2:F:1:GLU:H2	2:F:193:LEU:HA	1.70	0.56
3:K:591:LEU:HD23	3:K:611:ALA:HB1	1.86	0.56
3:L:114:ALA:HB1	3:L:117:LEU:HB2	1.87	0.56
3:L:815:ARG:NH1	3:L:817:GLU:OE2	2.35	0.56
2:C:10:ALA:HB2	2:C:186:THR:HG22	1.88	0.56
3:K:775:SER:HB3	3:K:780:ARG:HD3	1.88	0.56
2:I:139:GLN:O	2:I:143:ARG:N	2.39	0.56
3:L:574:THR:HB	3:L:627:ALA:HB3	1.86	0.56
3:J:342:LYS:NZ	3:J:346:GLU:OE2	2.38	0.56
1:D:70:PRO:HG3	1:D:195:VAL:HB	1.88	0.56
3:K:404:LEU:HG	3:K:937:LEU:HD21	1.88	0.56
3:K:845:GLU:HG2	3:K:857:TYR:HE2	1.71	0.56
3:L:108:GLN:O	3:J:112:GLN:NE2	2.36	0.56
1:B:183:ARG:O	1:B:207:GLN:N	2.39	0.56
3:K:7:ASP:OD1	3:K:432:ARG:NH2	2.39	0.56
1:H:164:VAL:O	1:H:168:ARG:N	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:139:VAL:HG11	5:L:1101:5QF:C7	2.35	0.55
2:F:71:LEU:HB3	2:F:252:ALA:HB3	1.87	0.55
2:F:19:LYS:HE2	2:I:315:GLN:HE21	1.71	0.55
3:K:211:ASN:O	3:K:760:ASN:ND2	2.39	0.55
3:L:444:GLY:HA2	3:L:447:MET:HB2	1.87	0.55
1:E:136:GLN:O	2:I:368:THR:OG1	2.22	0.55
1:B:60:THR:HA	1:B:214:VAL:HA	1.89	0.55
2:C:197:ASN:ND2	2:C:199:GLU:OE1	2.40	0.55
3:K:277:ILE:HB	5:K:1101:5QF:C21	2.37	0.55
3:J:576:VAL:HG13	3:J:663:VAL:HG22	1.89	0.55
3:K:548:ILE:HD13	3:K:907:LEU:HD21	1.89	0.55
3:K:989:LEU:O	3:K:1001:ASN:ND2	2.40	0.55
3:L:952:LEU:HA	3:L:956:GLU:HB3	1.88	0.55
1:G:99:ALA:HB1	1:A:169:ILE:HD13	1.87	0.55
3:K:326:PRO:HG2	5:K:1101:5QF:N8	2.22	0.55
3:K:686:ASP:HB2	3:K:695:LEU:HD13	1.88	0.55
3:K:730:ASP:OD2	3:K:808:ARG:NH1	2.39	0.55
3:K:892:TYR:OH	3:K:946:VAL:O	2.24	0.55
3:K:900:SER:HA	3:K:903:LEU:HD13	1.89	0.55
1:D:310:GLN:O	1:D:315:ARG:NH1	2.40	0.55
2:I:386:LEU:HD21	2:I:390:ARG:HH21	1.70	0.55
3:K:178:PHE:HB3	5:K:1101:5QF:C17	2.36	0.55
3:L:451:ALA:HB1	3:L:883:VAL:HG13	1.89	0.55
3:J:69:MET:HB3	3:J:72:ILE:HD11	1.89	0.55
1:E:218:GLN:HB3	1:E:274:ILE:HB	1.89	0.55
1:D:136:GLN:O	2:C:368:THR:OG1	2.24	0.55
1:D:218:GLN:HG2	1:D:223:MET:HG3	1.89	0.55
2:C:400:ILE:O	2:C:404:LEU:N	2.36	0.55
3:J:16:ALA:HB1	3:J:374:VAL:HG21	1.88	0.55
1:A:60:THR:HB	1:A:214:VAL:HG22	1.89	0.54
2:I:400:ILE:O	2:I:404:LEU:N	2.38	0.54
2:F:1:GLU:N	2:F:192:GLU:O	2.40	0.54
2:F:139:GLN:O	2:F:143:ARG:N	2.38	0.54
2:C:71:LEU:HB3	2:C:252:ALA:HB3	1.89	0.54
3:L:72:ILE:HG22	3:L:110:LYS:HD2	1.89	0.54
3:J:187:TRP:NE1	3:J:269:GLU:OE2	2.38	0.54
1:H:60:THR:HA	1:H:214:VAL:HA	1.90	0.54
3:K:339:GLU:O	3:K:343:THR:N	2.35	0.54
3:L:277:ILE:CG1	5:L:1101:5QF:C20	2.68	0.54
3:J:3:ASN:ND2	3:J:439:GLN:OE1	2.41	0.54
3:J:330:THR:HA	3:J:333:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:O	1:A:207:GLN:N	2.39	0.54
2:I:194:ALA:HA	2:I:422:PRO:HA	1.90	0.54
3:K:395:MET:HA	3:K:398:MET:HG2	1.88	0.54
3:L:58:GLN:HE21	3:L:818:ARG:HD2	1.73	0.54
3:J:617:PHE:CZ	5:J:1101:5QF:C24	2.90	0.54
3:J:775:SER:HB3	3:J:780:ARG:HD3	1.89	0.54
1:E:56:LEU:HD11	1:E:216:VAL:HG13	1.90	0.54
1:B:71:GLN:HB2	1:B:173:TYR:HB3	1.90	0.54
3:K:105:VAL:HG21	3:L:105:VAL:HG22	1.90	0.54
3:L:310:LEU:HD11	3:L:323:ILE:HG21	1.87	0.54
3:L:980:LEU:HA	3:L:983:ILE:HG22	1.90	0.54
3:K:275:TYR:HB2	3:J:222:THR:HB	1.89	0.54
4:O:10:PHE:HA	4:O:13:ILE:HG22	1.88	0.54
3:J:518:ARG:O	3:J:522:LYS:N	2.39	0.54
1:E:137:TYR:H	2:I:139:GLN:HG2	1.71	0.54
1:D:57:PRO:HD2	3:K:259:ARG:HH12	1.71	0.54
1:D:139:SER:HB3	2:C:368:THR:HB	1.88	0.54
1:A:71:GLN:HB2	1:A:173:TYR:HB3	1.90	0.54
2:C:194:ALA:HA	2:C:422:PRO:HA	1.89	0.54
3:K:442:LEU:HA	3:K:445:ILE:HG12	1.90	0.54
3:L:513:PHE:O	3:L:517:ASN:N	2.39	0.54
3:J:391:ASN:OD1	3:J:394:THR:N	2.37	0.54
1:E:218:GLN:HG2	1:E:223:MET:HG3	1.90	0.54
1:E:332:VAL:HG23	1:E:369:PRO:HA	1.90	0.54
2:I:368:THR:OG1	2:I:369:ILE:N	2.40	0.54
1:D:237:GLN:HG3	1:D:238:GLU:HG3	1.90	0.54
2:F:143:ARG:HB3	2:F:148:LEU:HB2	1.89	0.54
3:K:32:VAL:O	3:K:299:ALA:N	2.39	0.54
3:K:63:GLN:NE2	3:J:766:GLY:O	2.40	0.54
4:M:34:ASN:HD21	3:J:530:SER:HA	1.72	0.54
3:J:26:ALA:HA	3:J:29:LYS:HG2	1.89	0.54
1:H:76:ILE:HD13	1:H:96:ILE:HG13	1.90	0.54
2:C:220:ASN:HD22	2:C:323:VAL:HG23	1.73	0.54
3:L:377:LEU:HA	3:L:380:PHE:HD2	1.73	0.54
1:H:326:VAL:HA	1:H:332:VAL:HA	1.90	0.53
3:K:80:SER:HB3	3:K:818:ARG:H	1.72	0.53
3:J:47:ALA:HB3	3:J:88:VAL:HB	1.90	0.53
1:D:99:ALA:HB1	1:H:169:ILE:HD13	1.90	0.53
2:F:331:PHE:O	2:F:335:ASN:ND2	2.42	0.53
1:E:98:PRO:O	1:E:102:GLN:N	2.35	0.53
1:D:40:VAL:HG11	1:D:360:VAL:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:LEU:O	1:G:128:ARG:N	2.37	0.53
2:F:120:ILE:HD11	2:F:425:THR:HG22	1.91	0.53
2:C:316:LEU:O	2:C:320:HIS:N	2.37	0.53
2:C:368:THR:OG1	2:C:369:ILE:N	2.41	0.53
1:D:332:VAL:HG23	1:D:369:PRO:HA	1.90	0.53
1:A:139:SER:OG	2:F:147:GLY:O	2.27	0.53
3:L:27:ILE:HG21	3:L:377:LEU:HB2	1.90	0.53
2:C:68:SER:HA	2:C:255:GLY:HA3	1.91	0.53
3:L:832:ALA:HB3	3:L:835:LYS:HD3	1.89	0.53
3:J:1013:THR:HA	3:J:1017:LEU:HD13	1.91	0.53
1:D:294:ARG:NH2	3:L:732:ASP:OD2	2.35	0.53
3:K:57:VAL:HG21	3:K:86:GLY:HA2	1.89	0.53
3:K:344:LEU:HA	3:K:347:ALA:HB3	1.91	0.53
3:L:966:ASP:OD1	3:L:969:ARG:NH2	2.40	0.53
3:J:615:PHE:CZ	5:J:1101:5QF:N25	2.76	0.53
1:E:207:GLN:NE2	1:B:266:THR:OG1	2.41	0.53
3:K:410:ILE:HA	3:K:413:VAL:HG22	1.91	0.53
3:L:139:VAL:HG11	5:L:1101:5QF:C5	2.39	0.53
3:L:615:PHE:CE1	5:L:1101:5QF:C26	2.92	0.53
4:M:18:VAL:HG11	3:J:984:LEU:HD21	1.91	0.53
3:J:377:LEU:HA	3:J:380:PHE:HD2	1.73	0.53
3:J:1014:ALA:HA	3:J:1018:ALA:HB3	1.90	0.53
1:B:164:VAL:O	1:B:168:ARG:N	2.36	0.53
1:B:313:VAL:HG22	1:B:323:VAL:HG22	1.91	0.53
3:K:143:ILE:HD13	3:K:281:PHE:HB3	1.91	0.53
3:K:638:PRO:O	3:K:642:ASN:ND2	2.40	0.53
1:G:136:GLN:O	2:F:368:THR:OG1	2.24	0.53
1:G:194:LEU:HD23	1:A:69:ARG:HD2	1.90	0.53
1:H:69:ARG:NH1	1:H:200:ALA:O	2.42	0.53
3:J:561:SER:HA	3:J:923:ASN:HB3	1.91	0.53
3:J:815:ARG:NH2	3:J:817:GLU:OE2	2.41	0.53
1:E:60:THR:HG23	1:E:290:GLY:H	1.73	0.52
2:F:42:LEU:HB3	2:I:293:TYR:HB3	1.92	0.52
3:L:58:GLN:HE21	3:L:818:ARG:HH11	1.56	0.52
3:L:185:ARG:NH2	3:L:272:GLY:O	2.42	0.52
3:J:34:GLN:HB2	3:J:333:VAL:HG22	1.89	0.52
3:J:894:SER:HB3	3:J:897:ILE:HG12	1.91	0.52
1:G:207:GLN:NE2	1:A:266:THR:OG1	2.42	0.52
2:F:358:MET:HB3	2:F:372:VAL:HG22	1.91	0.52
2:C:314:GLU:O	2:C:318:SER:N	2.34	0.52
1:E:165:GLU:OE2	1:E:168:ARG:NH2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:NH1	1:A:208:GLN:OE1	2.40	0.52
3:K:58:GLN:HE21	3:K:818:ARG:HH11	1.56	0.52
3:J:213:GLN:HB2	3:J:239:ARG:HG2	1.91	0.52
2:I:331:PHE:O	2:I:335:ASN:ND2	2.42	0.52
3:J:92:LEU:HD22	3:J:107:VAL:HG22	1.91	0.52
3:J:602:GLU:OE1	3:J:605:ASN:ND2	2.42	0.52
1:A:69:ARG:NH1	1:A:200:ALA:O	2.42	0.52
2:F:38:LEU:O	2:F:73:GLN:NE2	2.35	0.52
2:F:46:ALA:HB3	2:I:288:PHE:HB3	1.91	0.52
2:C:93:ILE:HG23	2:C:225:GLN:HG3	1.90	0.52
3:K:58:GLN:HE21	3:K:818:ARG:HD2	1.75	0.52
3:L:277:ILE:CB	5:L:1101:5QF:C21	2.79	0.52
1:H:256:GLN:HG3	1:H:281:PRO:HG2	1.91	0.52
3:L:186:ILE:HD11	3:L:246:PHE:HD2	1.73	0.52
3:L:240:LEU:HD23	3:L:245:GLU:HB3	1.91	0.52
3:L:342:LYS:HE3	4:O:3:GLU:HB2	1.91	0.52
3:J:121:GLU:HA	3:J:124:GLN:HB2	1.91	0.52
1:D:260:LEU:HD21	1:D:276:LEU:HB3	1.92	0.52
1:A:218:GLN:HG2	1:A:223:MET:HB2	1.92	0.52
2:I:197:ASN:ND2	2:I:199:GLU:OE1	2.42	0.52
3:K:462:SER:OG	3:K:862:MET:SD	2.67	0.52
1:D:62:ALA:HB3	1:D:65:ILE:HG23	1.92	0.52
3:L:330:THR:O	3:L:334:LYS:N	2.42	0.52
3:L:526:HIS:O	3:L:530:SER:N	2.42	0.52
1:E:38:PRO:HB2	1:E:373:VAL:HA	1.92	0.51
1:G:289:PRO:HD2	1:A:265:VAL:HG12	1.91	0.51
3:K:139:VAL:CG1	5:K:1101:5QF:N8	2.68	0.51
3:K:202:ASP:OD2	3:K:792:ARG:NH2	2.39	0.51
1:D:164:VAL:O	1:D:168:ARG:N	2.42	0.51
3:L:16:ALA:HB1	3:L:374:VAL:HG11	1.92	0.51
3:J:56:THR:HG23	3:J:59:ASP:HB2	1.91	0.51
3:J:145:THR:O	3:J:284:GLN:NE2	2.43	0.51
3:J:418:ARG:HD3	3:J:971:ARG:HE	1.75	0.51
1:H:60:THR:O	1:H:290:GLY:N	2.43	0.51
1:H:313:VAL:HG22	1:H:323:VAL:HG22	1.92	0.51
1:A:45:VAL:HG12	1:A:47:THR:HG22	1.91	0.51
1:A:260:LEU:HD12	1:A:297:LEU:HD11	1.92	0.51
3:J:525:HIS:HA	3:J:528:THR:HG23	1.92	0.51
3:J:713:LEU:HG	3:J:843:LEU:HD23	1.91	0.51
3:L:143:ILE:HG23	3:L:322:LYS:HB3	1.92	0.51
3:J:556:PHE:HD1	3:J:913:LEU:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:882:ILE:HA	3:J:885:PHE:HB3	1.91	0.51
1:G:326:VAL:HA	1:G:332:VAL:HA	1.91	0.51
1:A:164:VAL:O	1:A:168:ARG:N	2.36	0.51
3:K:615:PHE:CE2	5:K:1101:5QF:C26	2.90	0.51
3:K:766:GLY:O	3:L:63:GLN:NE2	2.44	0.51
3:L:178:PHE:O	5:L:1101:5QF:C14	2.59	0.51
1:G:256:GLN:HE22	1:G:283:PRO:HD3	1.75	0.51
2:F:400:ILE:O	2:F:404:LEU:N	2.43	0.51
3:K:141:GLY:HA2	3:K:288:GLY:HA2	1.93	0.51
3:K:221:GLY:HA3	3:L:780:ARG:HH12	1.76	0.51
3:J:20:MET:O	3:J:24:GLY:N	2.42	0.51
3:J:241:THR:HG22	3:J:763:ILE:HB	1.92	0.51
3:J:368:PRO:HA	3:J:371:ALA:HB3	1.92	0.51
1:E:164:VAL:O	1:E:168:ARG:N	2.44	0.51
1:E:285:HIS:O	1:B:227:LYS:NZ	2.42	0.51
1:B:39:ALA:HA	1:B:374:LYS:HB2	1.93	0.51
3:L:78:MET:HG3	3:L:92:LEU:HG	1.93	0.51
1:D:69:ARG:HD2	1:B:194:LEU:HB3	1.92	0.51
1:D:137:TYR:CD2	2:C:143:ARG:HD2	2.46	0.51
1:D:194:LEU:HD23	1:H:69:ARG:HD2	1.93	0.51
1:A:89:ALA:N	1:A:181:SER:OG	2.44	0.51
3:K:178:PHE:O	5:K:1101:5QF:C13	2.59	0.51
3:L:437:GLN:HG2	3:L:438:ILE:HG23	1.92	0.51
3:L:737:GLN:HE21	3:L:743:ILE:HG12	1.74	0.51
1:D:265:VAL:HG21	1:B:209:LEU:HD11	1.93	0.51
1:G:137:TYR:H	2:F:139:GLN:HG2	1.76	0.51
1:A:60:THR:HA	1:A:214:VAL:HA	1.91	0.51
3:K:619:GLY:HA3	3:K:815:ARG:HD2	1.93	0.51
1:G:198:GLY:O	1:H:196:GLN:NE2	2.45	0.50
2:F:309:PHE:O	2:F:313:SER:N	2.39	0.50
3:L:615:PHE:CZ	5:L:1101:5QF:N25	2.79	0.50
3:J:203:VAL:HG13	3:J:262:LEU:HD11	1.91	0.50
1:E:326:VAL:HA	1:E:332:VAL:HA	1.93	0.50
3:K:415:ASN:HD22	3:K:438:ILE:HD13	1.76	0.50
3:L:20:MET:HA	3:L:377:LEU:HD11	1.93	0.50
3:L:32:VAL:O	3:L:299:ALA:N	2.45	0.50
3:L:156:ASP:OD2	3:L:765:ARG:NH2	2.43	0.50
3:L:609:VAL:HG22	3:L:629:VAL:HG22	1.93	0.50
1:G:126:VAL:O	1:G:130:GLN:N	2.44	0.50
1:G:285:HIS:O	1:A:227:LYS:NZ	2.44	0.50
2:I:134:TYR:O	2:I:138:ASP:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:155:SER:HB3	3:K:180:SER:H	1.77	0.50
3:K:1007:VAL:O	3:K:1011:MET:N	2.43	0.50
3:L:354:VAL:HG11	3:L:410:ILE:HD12	1.94	0.50
1:G:60:THR:HG23	1:G:289:PRO:HA	1.92	0.50
3:L:907:LEU:HD13	3:L:1018:ALA:HA	1.93	0.50
1:D:198:GLY:O	1:B:196:GLN:NE2	2.44	0.50
1:D:213:TYR:CG	1:D:277:ARG:HD2	2.47	0.50
1:D:285:HIS:O	1:H:227:LYS:NZ	2.40	0.50
1:H:39:ALA:HA	1:H:374:LYS:HB2	1.94	0.50
2:F:42:LEU:HD13	2:F:71:LEU:HD12	1.94	0.50
2:I:38:LEU:O	2:I:73:GLN:NE2	2.35	0.50
2:I:220:ASN:HD22	2:I:323:VAL:HG23	1.75	0.50
3:K:144:ASN:ND2	3:K:149:MET:O	2.38	0.50
1:G:241:LYS:HE3	1:G:259:THR:HG21	1.94	0.50
1:H:271:THR:HA	3:L:799:VAL:HG22	1.93	0.50
2:F:113:TYR:HE1	2:F:193:LEU:HD22	1.76	0.50
3:L:950:LYS:O	3:L:954:ASP:N	2.42	0.50
3:J:112:GLN:HA	3:J:115:MET:HG2	1.93	0.50
3:J:545:TYR:HA	3:J:548:ILE:HD12	1.93	0.50
3:J:611:ALA:HA	3:J:627:ALA:HA	1.94	0.50
1:D:45:VAL:HG11	1:D:306:ILE:HG23	1.92	0.50
1:D:294:ARG:HH22	3:L:734:GLU:HB3	1.76	0.50
1:A:60:THR:O	1:A:290:GLY:N	2.45	0.50
2:F:316:LEU:O	2:F:320:HIS:N	2.37	0.50
2:F:348:VAL:HG21	2:F:386:LEU:HD22	1.93	0.50
3:K:513:PHE:O	3:K:517:ASN:N	2.40	0.50
3:J:185:ARG:HD2	3:J:772:TYR:HB2	1.93	0.50
3:L:277:ILE:CG2	5:L:1101:5QF:O18	2.56	0.50
1:A:310:GLN:NE2	1:A:344:GLY:O	2.44	0.49
2:F:55:ARG:NH2	2:I:279:MET:O	2.43	0.49
2:F:77:ASP:OD2	2:F:79:SER:OG	2.29	0.49
2:C:4:MET:O	2:C:8:GLN:N	2.39	0.49
2:C:331:PHE:O	2:C:335:ASN:ND2	2.45	0.49
1:E:99:ALA:HB1	1:B:169:ILE:HD13	1.94	0.49
1:D:124:LEU:O	1:D:128:ARG:N	2.37	0.49
1:G:53:THR:OG1	1:G:299:GLU:N	2.45	0.49
1:G:196:GLN:NE2	1:A:198:GLY:O	2.45	0.49
1:G:343:ILE:N	1:G:346:LYS:O	2.44	0.49
1:A:184:ILE:HA	1:A:206:VAL:HA	1.94	0.49
2:F:59:GLY:HA2	2:F:264:SER:H	1.76	0.49
3:K:702:LEU:HD12	3:K:705:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:LEU:HD13	1:H:307:LEU:HD11	1.93	0.49
1:A:292:PHE:H	3:J:195:LYS:HG3	1.77	0.49
1:B:365:GLN:HG2	3:K:662:MET:HB2	1.93	0.49
2:F:192:GLU:HA	2:F:424:SER:HA	1.94	0.49
2:I:7:TYR:O	2:I:11:ARG:N	2.43	0.49
2:I:14:ASN:HB3	2:I:17:LEU:HB3	1.94	0.49
3:L:638:PRO:O	3:L:642:ASN:ND2	2.45	0.49
3:J:32:VAL:HG22	3:J:390:ILE:HB	1.94	0.49
3:J:186:ILE:HB	3:J:773:VAL:HA	1.94	0.49
3:J:414:GLU:O	3:J:418:ARG:N	2.45	0.49
1:E:343:ILE:N	1:E:346:LYS:O	2.46	0.49
2:C:309:PHE:O	2:C:313:SER:N	2.37	0.49
2:I:358:MET:O	2:I:362:TYR:N	2.34	0.49
3:K:20:MET:O	3:K:24:GLY:N	2.44	0.49
3:L:877:TYR:HE1	3:L:932:LEU:HD11	1.76	0.49
3:L:1002:ALA:O	3:L:1006:GLY:N	2.45	0.49
2:I:177:ASN:O	2:I:181:GLN:N	2.42	0.49
2:I:314:GLU:O	2:I:318:SER:N	2.43	0.49
4:M:40:GLY:H	3:J:539:GLY:HA3	1.76	0.49
1:E:310:GLN:HB3	1:E:315:ARG:HH22	1.77	0.49
2:I:352:GLN:NE2	2:I:356:ASP:OD2	2.44	0.49
2:C:300:SER:O	2:C:304:GLN:N	2.39	0.49
4:N:21:ILE:O	4:N:25:LEU:N	2.43	0.49
2:I:77:ASP:OD2	2:I:79:SER:OG	2.29	0.49
3:K:445:ILE:HD13	3:K:944:LEU:HD21	1.95	0.49
3:L:530:SER:O	3:L:534:ILE:N	2.40	0.49
1:D:63:TYR:HD2	1:D:64:ARG:HD3	1.78	0.49
1:B:310:GLN:HA	1:B:347:TRP:CD1	2.47	0.49
3:L:27:ILE:HG22	3:L:380:PHE:HB2	1.95	0.49
3:J:659:LYS:HD2	3:J:660:ASP:HB2	1.95	0.49
3:J:729:ILE:HD12	3:J:786:ILE:HD12	1.94	0.49
1:G:216:VAL:O	1:G:276:LEU:N	2.38	0.49
2:F:93:ILE:HG23	2:F:225:GLN:HG3	1.95	0.49
2:C:177:ASN:O	2:C:181:GLN:N	2.46	0.49
3:K:225:VAL:HG12	3:L:781:MET:HG2	1.94	0.49
3:K:997:SER:O	3:K:1000:GLN:NE2	2.38	0.49
3:L:500:ILE:HD12	3:L:504:ASP:HB3	1.94	0.49
3:L:541:TYR:OH	4:O:33:PHE:O	2.25	0.49
1:G:141:GLN:O	1:G:145:GLN:N	2.44	0.48
1:B:60:THR:O	1:B:290:GLY:N	2.46	0.48
2:F:134:TYR:O	2:F:138:ASP:N	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:292:ILE:H	2:C:43:GLY:HA2	1.78	0.48
2:I:42:LEU:HB3	2:C:293:TYR:HB3	1.95	0.48
2:C:352:GLN:NE2	2:C:356:ASP:OD2	2.43	0.48
3:L:330:THR:HB	3:L:334:LYS:HE2	1.95	0.48
3:J:346:GLU:O	3:J:350:LEU:N	2.37	0.48
1:D:165:GLU:OE2	1:D:168:ARG:NH2	2.36	0.48
1:H:70:PRO:HG3	1:H:195:VAL:HB	1.94	0.48
1:H:332:VAL:HG23	1:H:369:PRO:HA	1.95	0.48
1:A:76:ILE:HD13	1:A:96:ILE:HG13	1.96	0.48
1:B:216:VAL:O	1:B:276:LEU:N	2.46	0.48
1:B:271:THR:HA	3:K:799:VAL:HG22	1.95	0.48
3:L:211:ASN:O	3:L:760:ASN:ND2	2.46	0.48
3:J:921:LEU:HD13	3:J:999:ALA:HA	1.95	0.48
1:A:58:GLY:HA2	1:A:216:VAL:HA	1.94	0.48
2:I:117:LEU:HD23	2:I:120:ILE:HD12	1.94	0.48
2:C:14:ASN:HB3	2:C:17:LEU:HB3	1.95	0.48
3:K:919:ARG:NH1	3:K:1001:ASN:OD1	2.46	0.48
1:D:216:VAL:O	1:D:276:LEU:N	2.39	0.48
1:D:326:VAL:HA	1:D:332:VAL:HA	1.94	0.48
2:C:42:LEU:HD13	2:C:71:LEU:HD12	1.95	0.48
3:L:68:ASN:HB3	3:L:113:LEU:HD12	1.94	0.48
1:G:38:PRO:HB2	1:G:373:VAL:HA	1.96	0.48
1:G:63:TYR:HD2	1:G:64:ARG:HD3	1.78	0.48
1:H:60:THR:HG23	1:H:290:GLY:N	2.29	0.48
1:A:39:ALA:HA	1:A:374:LYS:HB2	1.95	0.48
2:C:59:GLY:HA2	2:C:264:SER:H	1.79	0.48
3:K:452:VAL:HB	3:K:932:LEU:HD22	1.95	0.48
3:L:326:PRO:CG	5:L:1101:5QF:N8	2.76	0.48
3:L:963:ALA:O	3:L:967:ALA:N	2.46	0.48
2:I:71:LEU:N	2:I:252:ALA:O	2.46	0.48
2:I:316:LEU:O	2:I:320:HIS:N	2.38	0.48
2:C:77:ASP:OD2	2:C:79:SER:OG	2.29	0.48
3:K:178:PHE:O	5:K:1101:5QF:C17	2.61	0.48
3:K:242:SER:OG	3:K:244:GLU:OE1	2.32	0.48
3:L:349:ILE:HA	3:L:352:PHE:HB3	1.96	0.48
3:J:641:GLU:O	3:J:650:ARG:NH2	2.37	0.48
3:J:1025:PHE:HB3	3:J:1029:VAL:HB	1.96	0.48
1:A:233:GLY:HA3	1:A:234:THR:HA	1.58	0.48
2:F:334:ILE:HG21	2:F:400:ILE:HD11	1.95	0.48
3:K:247:GLY:HA2	3:K:263:ARG:HB3	1.95	0.48
3:L:218:GLN:NE2	3:J:84:SER:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:733:GLN:HA	3:J:736:ALA:HB3	1.96	0.48
1:E:139:SER:HB3	2:I:368:THR:HB	1.96	0.48
1:D:116:GLN:O	1:D:120:ASN:N	2.41	0.48
1:A:332:VAL:HG23	1:A:369:PRO:HA	1.95	0.48
3:K:880:SER:HA	3:K:883:VAL:HG12	1.95	0.48
3:L:57:VAL:HG21	3:L:86:GLY:HA2	1.95	0.48
1:D:60:THR:HG23	1:D:289:PRO:HA	1.94	0.48
1:D:187:SER:OG	1:D:189:VAL:O	2.32	0.48
1:B:332:VAL:HG23	1:B:369:PRO:HA	1.95	0.48
2:C:46:ALA:HA	2:C:67:ALA:HA	1.95	0.48
3:K:151:GLN:HE22	3:K:278:ILE:HG23	1.78	0.48
3:J:81:ASN:OD1	3:J:81:ASN:N	2.46	0.48
3:J:569:GLN:NE2	3:J:670:ALA:O	2.47	0.48
3:J:615:PHE:HE2	5:J:1101:5QF:C26	2.13	0.48
3:K:367:ILE:HG21	3:K:413:VAL:HG11	1.96	0.48
3:K:860:THR:OG1	3:K:861:GLY:N	2.45	0.48
3:K:1028:VAL:O	3:K:1032:ARG:N	2.45	0.48
3:J:712:MET:HA	3:J:832:ALA:HB2	1.95	0.48
1:E:53:THR:OG1	1:E:299:GLU:N	2.46	0.47
2:I:93:ILE:HG23	2:I:225:GLN:HG3	1.96	0.47
3:K:11:PHE:HD1	3:L:890:ALA:HB1	1.79	0.47
3:K:77:TYR:OH	3:K:683:GLU:OE2	2.32	0.47
3:L:24:GLY:HA2	3:L:27:ILE:HG12	1.95	0.47
3:J:288:GLY:HA3	5:J:1101:5QF:C11	2.43	0.47
1:E:194:LEU:HD23	1:B:69:ARG:HD2	1.96	0.47
2:F:223:LEU:HD22	2:F:323:VAL:HG11	1.96	0.47
3:K:1024:VAL:HA	3:K:1027:VAL:HG22	1.96	0.47
3:L:143:ILE:HD13	3:L:281:PHE:HB3	1.95	0.47
3:L:372:VAL:HG13	3:L:405:LEU:HD11	1.95	0.47
3:J:519:MET:HA	3:J:522:LYS:HB3	1.96	0.47
1:G:213:TYR:CG	1:G:277:ARG:HD2	2.48	0.47
2:F:61:ASN:O	2:F:262:SER:N	2.47	0.47
2:F:213:LEU:HD11	2:F:324:VAL:HG22	1.96	0.47
2:I:368:THR:HG23	2:I:371:ASP:H	1.78	0.47
3:K:559:LEU:HD12	3:K:560:PRO:HD2	1.96	0.47
3:L:139:VAL:HG11	5:L:1101:5QF:C6	2.44	0.47
1:E:124:LEU:O	1:E:128:ARG:N	2.41	0.47
1:E:326:VAL:HG11	1:E:358:ARG:HD2	1.96	0.47
1:A:165:GLU:HG3	1:A:168:ARG:HH21	1.79	0.47
3:K:881:LEU:HA	3:K:902:MET:HG3	1.96	0.47
1:B:270:THR:OG1	3:K:797:GLN:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:68:SER:HA	2:I:255:GLY:HA3	1.95	0.47
2:C:368:THR:HG23	2:C:371:ASP:H	1.79	0.47
3:L:61:VAL:HG22	3:L:122:VAL:HG11	1.97	0.47
3:L:81:ASN:HA	3:L:817:GLU:HA	1.96	0.47
3:L:1004:GLY:O	3:L:1008:MET:N	2.42	0.47
1:H:218:GLN:HG2	1:H:223:MET:HB2	1.95	0.47
3:L:692:HIS:O	3:L:696:THR:N	2.48	0.47
3:J:210:GLN:OE1	3:J:250:LEU:N	2.45	0.47
1:D:53:THR:OG1	1:D:299:GLU:N	2.44	0.47
1:D:193:ALA:HB2	1:H:66:ALA:HA	1.96	0.47
1:D:326:VAL:HG11	1:D:358:ARG:HD2	1.95	0.47
1:G:60:THR:HG23	1:G:290:GLY:H	1.79	0.47
1:H:108:ALA:O	1:H:112:LEU:N	2.46	0.47
1:A:310:GLN:HA	1:A:347:TRP:CD1	2.49	0.47
1:B:184:ILE:HA	1:B:206:VAL:HA	1.97	0.47
2:I:212:LEU:O	2:I:216:ALA:N	2.47	0.47
3:L:144:ASN:HB2	3:L:154:ILE:HD11	1.96	0.47
3:L:698:ALA:HB1	3:L:851:LEU:HD23	1.96	0.47
3:J:310:LEU:HD12	3:J:323:ILE:HG13	1.95	0.47
3:J:593:GLU:O	3:J:597:TYR:N	2.45	0.47
1:E:237:GLN:HG3	1:E:238:GLU:HG3	1.97	0.47
1:E:260:LEU:HD21	1:E:276:LEU:HB3	1.97	0.47
1:D:70:PRO:HD2	1:D:199:GLN:HG2	1.97	0.47
1:D:212:ILE:HD11	1:D:289:PRO:HB3	1.96	0.47
1:G:139:SER:HB3	2:F:368:THR:HB	1.97	0.47
3:L:105:VAL:HG21	3:J:105:VAL:HG13	1.97	0.47
1:D:314:THR:OG1	1:D:322:THR:OG1	2.29	0.47
1:G:214:VAL:HB	1:G:278:ALA:HB3	1.96	0.47
1:H:144:ASP:O	1:H:148:ALA:N	2.39	0.47
1:B:70:PRO:HG3	1:B:195:VAL:HB	1.97	0.47
2:I:348:VAL:O	2:I:352:GLN:N	2.38	0.47
2:C:139:GLN:O	2:C:143:ARG:N	2.48	0.47
3:K:623:ASN:HD21	3:K:721:LEU:HD23	1.80	0.47
3:K:1022:VAL:HA	3:K:1025:PHE:HB2	1.97	0.47
3:L:80:SER:OG	3:L:81:ASN:N	2.48	0.47
3:L:400:LEU:HD13	3:L:933:THR:HG21	1.96	0.47
3:J:706:ALA:HA	3:J:847:LEU:HD13	1.96	0.47
3:K:237:GLN:NE2	3:L:733:GLN:HE22	2.13	0.47
3:K:891:LEU:HB3	3:K:950:LYS:HD3	1.96	0.47
3:L:171:GLY:O	3:L:294:ALA:N	2.45	0.47
3:L:702:LEU:HB2	3:L:851:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:32:VAL:O	3:J:299:ALA:N	2.41	0.47
3:J:521:GLU:O	3:J:525:HIS:ND1	2.42	0.47
3:J:883:VAL:O	3:J:887:CYS:N	2.48	0.47
3:K:401:ALA:HB2	3:K:474:ILE:HG22	1.98	0.46
3:K:758:TYR:HE1	3:K:770:LYS:HG3	1.79	0.46
1:D:310:GLN:HB3	1:D:315:ARG:HH22	1.81	0.46
1:A:216:VAL:O	1:A:276:LEU:N	2.48	0.46
2:F:282:ASN:O	2:C:52:ASN:N	2.49	0.46
2:C:7:TYR:O	2:C:11:ARG:N	2.43	0.46
3:L:580:ALA:HB1	3:L:724:THR:HG22	1.98	0.46
3:J:568:ASP:OD2	3:J:634:TRP:NE1	2.48	0.46
2:I:46:ALA:HA	2:I:67:ALA:HA	1.98	0.46
3:J:528:THR:HA	3:J:531:VAL:HB	1.97	0.46
3:J:609:VAL:HG13	3:J:629:VAL:HG22	1.97	0.46
1:E:70:PRO:HG3	1:E:195:VAL:HB	1.98	0.46
1:G:164:VAL:O	1:G:168:ARG:N	2.48	0.46
1:G:316:THR:OG1	1:G:318:ARG:NH1	2.49	0.46
2:F:290:LEU:O	2:C:44:LEU:N	2.48	0.46
3:K:10:ILE:HA	3:K:13:TRP:HD1	1.81	0.46
3:K:1018:ALA:HA	3:K:1021:PHE:HD2	1.80	0.46
1:G:226:LEU:HD13	1:G:226:LEU:HA	1.82	0.46
1:H:242:ALA:HB3	1:H:260:LEU:HB3	1.98	0.46
1:B:59:ARG:N	1:B:215:ASP:O	2.45	0.46
2:F:7:TYR:O	2:F:11:ARG:N	2.43	0.46
2:I:401:LYS:O	2:I:405:GLY:N	2.48	0.46
3:K:110:LYS:HB2	3:K:113:LEU:HD12	1.98	0.46
3:K:919:ARG:HH22	3:K:993:THR:HG21	1.81	0.46
3:J:628:PHE:HZ	5:J:1101:5QF:C27	2.29	0.46
3:K:588:GLN:HB2	3:K:613:ASN:ND2	2.31	0.46
3:K:732:ASP:HB3	3:K:735:LYS:HB3	1.98	0.46
3:K:1027:VAL:HA	3:K:1030:ARG:HB2	1.98	0.46
1:E:128:ARG:NH1	2:I:146:VAL:O	2.49	0.46
1:G:326:VAL:HG11	1:G:358:ARG:HD2	1.97	0.46
1:B:45:VAL:HG12	1:B:47:THR:HG22	1.98	0.46
2:I:19:LYS:HE2	2:C:315:GLN:HE21	1.80	0.46
3:J:348:ILE:HD13	3:J:373:PRO:HG3	1.96	0.46
3:J:714:THR:HG21	3:J:833:PRO:HD3	1.98	0.46
1:E:178:SER:O	1:E:180:ILE:N	2.49	0.46
2:I:61:ASN:O	2:I:262:SER:N	2.49	0.46
2:I:135:ARG:HH21	2:I:369:ILE:HG21	1.81	0.46
3:L:591:LEU:HD23	3:L:611:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:VAL:HG11	1:E:360:VAL:HG13	1.97	0.46
1:E:215:ASP:O	1:E:217:THR:OG1	2.33	0.46
1:E:314:THR:OG1	1:E:322:THR:OG1	2.32	0.46
2:F:177:ASN:O	2:F:181:GLN:N	2.44	0.46
3:K:408:ASP:HA	3:K:411:VAL:HG22	1.98	0.46
3:L:302:THR:O	3:L:306:ILE:N	2.44	0.46
1:G:265:VAL:HG21	1:H:209:LEU:HD11	1.98	0.45
3:K:280:GLU:HB3	3:K:611:ALA:HB3	1.98	0.45
3:K:455:PRO:HA	3:K:458:PHE:HD2	1.81	0.45
1:E:274:ILE:HD12	1:A:288:MET:HE2	1.98	0.45
1:A:242:ALA:H	1:A:259:THR:HG23	1.81	0.45
2:C:329:SER:O	2:C:333:ASN:N	2.49	0.45
3:K:300:LEU:O	3:K:304:ALA:N	2.32	0.45
3:L:127:VAL:HG22	3:J:116:PRO:HG3	1.97	0.45
3:J:330:THR:HB	3:J:334:LYS:HE3	1.98	0.45
3:J:343:THR:O	3:J:347:ALA:N	2.41	0.45
3:J:819:TYR:N	3:J:822:LEU:O	2.49	0.45
3:J:844:MET:O	3:J:848:ALA:N	2.49	0.45
1:D:196:GLN:NE2	1:H:198:GLY:O	2.49	0.45
1:H:165:GLU:HG3	1:H:168:ARG:HH21	1.82	0.45
1:H:248:THR:HB	1:H:293:VAL:HG23	1.98	0.45
1:H:270:THR:OG1	3:L:797:GLN:OE1	2.35	0.45
2:F:69:LEU:N	2:F:254:THR:O	2.36	0.45
2:I:113:TYR:HE1	2:I:193:LEU:HD22	1.82	0.45
3:J:277:ILE:HG23	3:J:612:VAL:HG13	1.98	0.45
3:J:570:GLY:O	3:J:631:LEU:N	2.46	0.45
3:J:885:PHE:HD1	3:J:902:MET:HG3	1.81	0.45
1:D:98:PRO:O	1:D:102:GLN:N	2.35	0.45
2:I:213:LEU:HD11	2:I:324:VAL:HG22	1.98	0.45
3:K:349:ILE:O	3:K:353:LEU:N	2.45	0.45
3:J:363:ARG:HD3	3:J:498:LYS:HE3	1.98	0.45
2:F:314:GLU:O	2:F:318:SER:N	2.45	0.45
3:K:210:GLN:HE22	3:K:250:LEU:HB3	1.82	0.45
3:K:251:LEU:HD23	3:K:251:LEU:HA	1.84	0.45
3:L:171:GLY:HA2	3:L:298:ASN:HD22	1.82	0.45
3:L:383:LEU:HA	3:L:386:PHE:HB2	1.99	0.45
3:L:732:ASP:HB3	3:L:735:LYS:HB3	1.98	0.45
3:L:873:ALA:HA	3:L:877:TYR:HD2	1.81	0.45
3:L:919:ARG:HD3	3:L:1002:ALA:HB2	1.97	0.45
1:E:63:TYR:HD2	1:E:64:ARG:HD3	1.81	0.45
1:G:237:GLN:HG3	1:G:238:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:ALA:N	1:H:181:SER:OG	2.49	0.45
3:L:104:GLN:NE2	3:L:129:VAL:O	2.49	0.45
3:J:580:ALA:HB1	3:J:724:THR:HG22	1.99	0.45
4:N:23:LEU:O	4:N:27:TYR:N	2.49	0.45
1:G:310:GLN:HB3	1:G:315:ARG:HH22	1.81	0.45
1:H:216:VAL:O	1:H:276:LEU:N	2.45	0.45
1:A:270:THR:OG1	3:J:797:GLN:OE1	2.35	0.45
1:A:326:VAL:HB	1:A:332:VAL:HG12	1.98	0.45
2:I:123:LEU:HD22	2:I:175:LEU:HD22	1.99	0.45
3:L:246:PHE:HA	3:L:249:ILE:HG13	1.99	0.45
3:L:351:VAL:HG13	3:L:410:ILE:HD13	1.99	0.45
3:L:959:GLY:O	3:L:963:ALA:N	2.36	0.45
3:J:339:GLU:OE2	3:J:343:THR:OG1	2.35	0.45
3:J:544:LEU:HD13	3:J:547:ILE:HD12	1.99	0.45
1:E:141:GLN:O	1:E:145:GLN:N	2.49	0.45
1:D:138:ILE:HD12	1:D:138:ILE:HA	1.75	0.45
1:D:241:LYS:HE3	1:D:259:THR:HG21	1.99	0.45
1:G:192:GLY:HA2	1:A:179:PRO:HB2	1.99	0.45
1:B:60:THR:HG23	1:B:290:GLY:N	2.30	0.45
2:C:143:ARG:HE	2:C:149:VAL:HG13	1.82	0.45
2:C:337:SER:HA	2:C:340:SER:HB3	1.99	0.45
1:G:137:TYR:CD2	2:F:143:ARG:HD2	2.52	0.45
1:H:45:VAL:HG12	1:H:47:THR:HG22	1.99	0.45
2:F:52:ASN:N	2:I:282:ASN:O	2.50	0.45
2:I:69:LEU:N	2:I:254:THR:O	2.37	0.45
2:I:348:VAL:HG21	2:I:386:LEU:HD22	1.99	0.45
3:K:888:LEU:HD23	3:K:891:LEU:HD12	1.99	0.45
3:J:14:VAL:HG13	3:J:17:ILE:HD12	1.98	0.45
3:J:832:ALA:HB3	3:J:835:LYS:HB2	1.99	0.45
1:E:193:ALA:HB2	1:B:66:ALA:HA	1.99	0.44
1:D:210:ASP:HA	1:D:282:ASN:HB3	1.99	0.44
1:G:62:ALA:HB2	1:G:289:PRO:HG3	1.99	0.44
1:H:184:ILE:HA	1:H:206:VAL:HA	1.98	0.44
1:H:216:VAL:HB	1:H:276:LEU:HB2	1.99	0.44
1:B:242:ALA:HB3	1:B:260:LEU:HB3	1.99	0.44
2:I:386:LEU:O	2:I:390:ARG:N	2.44	0.44
2:I:412:LEU:HD12	2:I:415:LEU:HD12	1.99	0.44
3:K:163:LYS:HD2	3:K:177:LEU:HB2	1.99	0.44
3:K:277:ILE:CG1	5:K:1101:5QF:C20	2.68	0.44
3:K:344:LEU:HD21	3:K:402:ILE:HG21	1.99	0.44
3:L:446:ALA:HB1	3:L:478:MET:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:610:PHE:HB3	3:L:628:PHE:HB2	1.97	0.44
3:J:986:VAL:HG12	3:J:989:LEU:HD12	2.00	0.44
1:E:132:LEU:HD22	2:I:139:GLN:HE21	1.81	0.44
1:D:244:VAL:N	1:D:258:GLY:O	2.48	0.44
1:G:310:GLN:O	1:G:315:ARG:NH1	2.49	0.44
1:A:221:ASN:HA	1:A:224:MET:HB3	1.99	0.44
3:L:247:GLY:HA2	3:L:263:ARG:HB3	1.99	0.44
4:O:6:LYS:HG2	4:O:10:PHE:HB2	1.98	0.44
3:J:281:PHE:N	3:J:284:GLN:O	2.51	0.44
1:E:138:ILE:HD12	1:E:138:ILE:HA	1.70	0.44
1:G:324:LEU:HD12	1:G:334:THR:HB	1.99	0.44
2:I:180:GLU:HG3	2:C:328:ARG:HD3	1.99	0.44
3:K:413:VAL:HG12	3:K:489:THR:HG23	1.99	0.44
3:J:317:PHE:HB3	3:J:321:LEU:HB3	1.98	0.44
3:J:345:VAL:HA	3:J:348:ILE:HD12	2.00	0.44
3:J:888:LEU:HD13	3:J:901:VAL:HB	2.00	0.44
1:E:213:TYR:CG	1:E:277:ARG:HD3	2.53	0.44
1:E:325:VAL:HG21	1:E:335:ARG:HE	1.81	0.44
3:K:588:GLN:O	3:K:592:ASN:N	2.49	0.44
3:J:728:LYS:HG2	3:J:808:ARG:HE	1.82	0.44
1:E:60:THR:HG23	1:E:289:PRO:HA	1.99	0.44
1:E:144:ASP:HA	1:E:147:LEU:HB3	2.00	0.44
1:D:217:THR:HA	1:D:275:THR:HA	2.00	0.44
1:G:119:ALA:O	1:G:123:GLN:N	2.51	0.44
1:G:238:GLU:HB2	1:G:239:ASN:HB2	2.00	0.44
1:B:221:ASN:HA	1:B:224:MET:HB3	1.99	0.44
2:F:212:LEU:O	2:F:216:ALA:N	2.50	0.44
3:K:674:LEU:HD21	3:K:862:MET:HB2	2.00	0.44
3:K:848:ALA:HA	3:K:851:LEU:HD13	2.00	0.44
3:J:32:VAL:H	3:J:298:ASN:HA	1.82	0.44
3:J:525:HIS:O	3:J:528:THR:OG1	2.27	0.44
3:J:544:LEU:HA	3:J:547:ILE:HD12	2.00	0.44
1:E:126:VAL:O	1:E:130:GLN:N	2.48	0.44
1:D:233:GLY:HA3	1:D:234:THR:HA	1.82	0.44
2:F:395:ILE:HD13	2:F:395:ILE:HA	1.86	0.44
2:I:168:GLU:OE2	2:I:172:ARG:NE	2.50	0.44
3:L:561:SER:HA	3:L:923:ASN:HB3	1.99	0.44
1:E:314:THR:HG1	1:E:322:THR:HG1	1.64	0.44
1:D:343:ILE:N	1:D:346:LYS:O	2.51	0.44
1:G:70:PRO:HG3	1:G:195:VAL:HB	2.00	0.44
1:G:314:THR:OG1	1:G:322:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:293:TYR:HB3	2:C:42:LEU:HB3	1.99	0.44
2:F:413:LEU:O	2:F:417:ASN:N	2.48	0.44
2:I:98:TYR:HE2	2:I:102:GLN:HE21	1.66	0.44
1:D:59:ARG:HD2	1:D:292:PHE:HA	1.99	0.44
1:D:183:ARG:N	1:D:207:GLN:O	2.41	0.44
1:G:116:GLN:O	1:G:120:ASN:N	2.38	0.44
1:A:149:ASP:HA	1:A:152:GLN:HG2	1.99	0.44
2:F:44:LEU:N	2:I:290:LEU:O	2.48	0.44
2:C:61:ASN:O	2:C:262:SER:N	2.50	0.44
3:K:641:GLU:O	3:K:650:ARG:NH2	2.42	0.44
3:L:331:PRO:HA	3:L:334:LYS:HB2	1.98	0.44
1:E:89:ALA:N	1:E:181:SER:OG	2.51	0.44
1:G:193:ALA:HB2	1:A:66:ALA:HA	2.00	0.43
1:H:233:GLY:HA3	1:H:234:THR:HA	1.58	0.43
1:A:55:GLU:HA	1:A:296:ARG:HA	2.00	0.43
1:B:76:ILE:HG23	1:B:94:TYR:HB3	1.99	0.43
2:F:4:MET:H	2:F:416:ASN:ND2	2.16	0.43
2:F:135:ARG:HH21	2:F:369:ILE:HG21	1.83	0.43
2:I:4:MET:O	2:I:8:GLN:N	2.39	0.43
2:I:43:GLY:HA2	2:C:292:ILE:H	1.83	0.43
2:C:113:TYR:HE1	2:C:193:LEU:HD22	1.83	0.43
2:C:348:VAL:O	2:C:352:GLN:N	2.42	0.43
3:K:316:PHE:HE1	3:L:854:GLY:H	1.66	0.43
3:L:992:SER:O	3:L:1001:ASN:ND2	2.40	0.43
3:J:343:THR:HA	3:J:346:GLU:HB2	1.99	0.43
3:L:49:TYR:HE1	3:L:121:GLU:HB2	1.83	0.43
3:L:326:PRO:CB	5:L:1101:5QF:N8	2.81	0.43
1:D:60:THR:HG23	1:D:290:GLY:H	1.83	0.43
1:G:50:LEU:H	1:G:301:LEU:HD12	1.84	0.43
2:I:42:LEU:HD13	2:I:71:LEU:HD12	1.99	0.43
2:I:254:THR:HA	2:I:282:ASN:HA	1.99	0.43
3:K:203:VAL:HG13	3:K:262:LEU:HD11	2.00	0.43
3:J:347:ALA:HA	3:J:350:LEU:HB2	1.99	0.43
3:J:650:ARG:HG2	3:J:653:ARG:NH2	2.34	0.43
1:E:62:ALA:HB3	1:E:65:ILE:HG23	2.00	0.43
2:F:46:ALA:HA	2:F:67:ALA:HA	2.01	0.43
2:C:168:GLU:OE2	2:C:172:ARG:NE	2.51	0.43
3:K:815:ARG:NH1	3:K:817:GLU:OE2	2.40	0.43
3:L:819:TYR:O	3:L:822:LEU:N	2.50	0.43
1:D:45:VAL:O	1:D:356:GLY:N	2.46	0.43
1:G:139:SER:O	1:G:141:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:326:VAL:HB	1:H:332:VAL:HG12	1.99	0.43
1:A:310:GLN:HA	1:A:347:TRP:HD1	1.84	0.43
2:I:217:GLU:HA	2:I:223:LEU:HD23	2.00	0.43
2:C:421:LYS:HA	2:C:422:PRO:HD3	1.88	0.43
3:K:544:LEU:HD12	3:K:547:ILE:HD11	2.00	0.43
1:H:71:GLN:HB2	1:H:173:TYR:HB3	1.99	0.43
2:I:22:ALA:O	2:I:26:ALA:N	2.52	0.43
2:C:4:MET:H	2:C:416:ASN:ND2	2.16	0.43
3:K:75:LEU:HA	3:K:94:PHE:HA	2.00	0.43
3:K:819:TYR:HE2	3:K:858:ASP:HB3	1.83	0.43
3:L:402:ILE:HA	3:L:405:LEU:HG	2.01	0.43
1:G:50:LEU:HG	1:G:301:LEU:HD11	2.01	0.43
1:G:314:THR:HG1	1:G:322:THR:HG1	1.60	0.43
1:B:326:VAL:HB	1:B:332:VAL:HG12	2.00	0.43
2:F:113:TYR:OH	2:F:194:ALA:N	2.49	0.43
2:F:350:SER:OG	2:F:351:ALA:N	2.51	0.43
2:I:329:SER:O	2:I:333:ASN:N	2.52	0.43
2:C:350:SER:OG	2:C:351:ALA:N	2.51	0.43
3:K:355:MET:HB3	3:K:365:THR:HG22	2.01	0.43
3:J:881:LEU:HB3	3:J:902:MET:HE1	2.01	0.43
3:J:980:LEU:HA	3:J:984:LEU:HD23	2.00	0.43
1:D:119:ALA:HA	1:D:122:ALA:HB3	2.01	0.43
1:H:310:GLN:HA	1:H:347:TRP:CD1	2.53	0.43
2:I:4:MET:H	2:I:416:ASN:ND2	2.17	0.43
3:K:30:LEU:HD12	3:K:31:PRO:HD2	1.99	0.43
3:K:248:LYS:HA	3:K:261:LEU:HD23	2.01	0.43
3:L:45:ILE:HG12	3:L:129:VAL:HG13	2.01	0.43
3:L:242:SER:OG	3:L:244:GLU:OE1	2.37	0.43
3:L:547:ILE:HA	3:L:550:VAL:HG13	2.01	0.43
3:J:63:GLN:HG2	3:J:818:ARG:HH12	1.84	0.43
3:J:104:GLN:HG2	3:J:129:VAL:HG12	2.00	0.43
2:I:59:GLY:HA2	2:I:264:SER:H	1.84	0.43
2:C:113:TYR:OH	2:C:194:ALA:N	2.52	0.43
3:K:326:PRO:CG	5:K:1101:5QF:N8	2.82	0.43
3:L:613:ASN:HD22	3:L:614:GLY:N	2.16	0.43
3:J:118:LEU:HD22	3:J:122:VAL:HG11	1.99	0.43
1:E:233:GLY:HA3	1:E:234:THR:HA	1.81	0.43
1:G:65:ILE:HG13	1:H:190:THR:HG21	2.01	0.43
1:H:183:ARG:HH21	1:H:285:HIS:CE1	2.37	0.43
1:B:233:GLY:HA3	1:B:234:THR:HA	1.63	0.43
2:F:43:GLY:HA2	2:I:292:ILE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:GLN:O	2:I:13:SER:OG	2.37	0.43
2:C:38:LEU:O	2:C:73:GLN:NE2	2.35	0.43
3:K:246:PHE:HA	3:K:249:ILE:HG13	2.00	0.43
1:D:62:ALA:HB2	1:D:289:PRO:HG3	2.01	0.42
1:B:126:VAL:HG11	1:B:147:LEU:HD13	2.01	0.42
2:F:329:SER:O	2:F:333:ASN:N	2.52	0.42
2:C:71:LEU:N	2:C:252:ALA:O	2.44	0.42
3:L:228:GLN:N	3:J:585:GLU:OE1	2.48	0.42
3:L:482:VAL:HA	3:L:485:ALA:HB3	2.00	0.42
1:G:98:PRO:O	1:G:102:GLN:N	2.35	0.42
1:H:304:ASN:OD1	1:H:304:ASN:N	2.52	0.42
2:F:328:ARG:HD3	2:C:180:GLU:HG3	2.00	0.42
3:L:438:ILE:HB	3:L:441:ALA:HB3	1.99	0.42
3:L:525:HIS:O	3:L:529:ASP:N	2.38	0.42
4:N:23:LEU:HA	4:N:26:ILE:HG12	2.00	0.42
1:E:265:VAL:HG21	1:A:209:LEU:HD11	2.01	0.42
1:G:138:ILE:HA	1:G:138:ILE:HD12	1.70	0.42
1:G:176:VAL:HA	1:G:177:THR:HA	1.68	0.42
1:A:215:ASP:OD1	1:A:277:ARG:NH1	2.52	0.42
1:B:144:ASP:O	1:B:148:ALA:N	2.43	0.42
2:F:71:LEU:N	2:F:252:ALA:O	2.45	0.42
2:C:22:ALA:O	2:C:26:ALA:N	2.50	0.42
3:K:801:PHE:HD1	3:K:801:PHE:HA	1.68	0.42
3:L:178:PHE:HD1	5:L:1101:5QF:C16	2.25	0.42
3:L:254:ASN:OD1	3:L:258:SER:OG	2.36	0.42
3:L:361:ASN:HB2	3:L:365:THR:HG23	2.02	0.42
3:L:514:GLY:O	3:L:518:ARG:NH1	2.52	0.42
3:L:964:THR:HA	3:L:967:ALA:HB3	2.01	0.42
1:D:274:ILE:HD12	1:B:288:MET:HE2	2.01	0.42
2:C:254:THR:HA	2:C:282:ASN:HA	2.01	0.42
3:K:280:GLU:N	3:K:611:ALA:O	2.53	0.42
3:K:977:MET:HA	3:K:980:LEU:HB3	2.01	0.42
3:L:27:ILE:HG13	3:L:28:LEU:HD12	2.00	0.42
3:L:949:ALA:HA	3:L:952:LEU:HB2	2.00	0.42
4:O:32:VAL:HG12	4:O:35:ILE:HD12	2.02	0.42
3:J:157:TYR:OH	3:J:316:PHE:O	2.35	0.42
1:E:133:LEU:HD11	1:E:143:TYR:CZ	2.55	0.42
1:D:60:THR:OG1	1:D:213:TYR:O	2.30	0.42
1:A:70:PRO:HD3	1:A:203:LEU:HG	2.01	0.42
2:F:14:ASN:ND2	2:F:105:LEU:HD13	2.35	0.42
3:K:414:GLU:O	3:K:418:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:177:LEU:HD22	3:J:178:PHE:H	1.85	0.42
3:J:416:VAL:HA	3:J:430:ALA:HB1	2.00	0.42
3:J:610:PHE:HZ	5:J:1101:5QF:C12	2.33	0.42
1:E:137:TYR:CD2	2:I:143:ARG:HD2	2.54	0.42
1:H:324:LEU:HD13	1:H:364:LEU:HD22	2.02	0.42
2:I:1:GLU:H2	2:I:193:LEU:HA	1.84	0.42
2:C:14:ASN:ND2	2:C:105:LEU:HD13	2.34	0.42
3:K:761:ASP:HB3	3:K:768:VAL:HG13	2.02	0.42
3:L:210:GLN:HB3	3:J:733:GLN:HE22	1.85	0.42
3:L:982:PHE:HE2	3:L:1011:MET:HG3	1.84	0.42
3:J:120:GLN:OE1	3:J:123:GLN:NE2	2.41	0.42
3:J:1011:MET:O	3:J:1015:THR:N	2.52	0.42
1:E:116:GLN:O	1:E:120:ASN:N	2.47	0.42
1:D:218:GLN:HB3	1:D:274:ILE:HB	2.01	0.42
1:D:256:GLN:HE21	1:D:281:PRO:HG2	1.84	0.42
1:D:308:VAL:HG13	1:D:347:TRP:HB2	2.00	0.42
1:G:210:ASP:HA	1:G:282:ASN:HB3	2.02	0.42
1:G:233:GLY:HA2	1:G:303:PRO:HD3	2.02	0.42
1:A:256:GLN:HG3	1:A:281:PRO:HG2	2.02	0.42
2:F:57:ALA:HB2	2:I:279:MET:HB3	2.02	0.42
2:I:55:ARG:NH2	2:C:279:MET:O	2.52	0.42
2:I:149:VAL:HB	2:I:153:ASP:HB2	2.01	0.42
2:C:213:LEU:HD11	2:C:324:VAL:HG22	2.00	0.42
2:C:213:LEU:HD21	2:C:324:VAL:HG22	2.02	0.42
3:K:727:PHE:HD2	3:J:234:ILE:HG12	1.84	0.42
3:K:885:PHE:HE1	3:K:898:PRO:HD2	1.85	0.42
3:L:145:THR:HG21	3:L:322:LYS:HE2	2.02	0.42
3:L:383:LEU:O	3:L:387:GLY:N	2.52	0.42
3:J:41:PRO:HG2	3:J:94:PHE:HB2	2.00	0.42
3:J:163:LYS:HD2	3:J:177:LEU:HB2	2.02	0.42
3:J:178:PHE:HA	3:J:179:GLY:HA2	1.78	0.42
1:D:318:ARG:HD3	3:K:270:LEU:HD12	2.01	0.42
1:H:189:VAL:HG11	1:H:203:LEU:HD22	2.02	0.42
1:H:215:ASP:OD1	1:H:277:ARG:NH1	2.53	0.42
1:B:291:MET:H	1:B:292:PHE:HA	1.85	0.42
2:I:15:PRO:HG3	2:C:321:ARG:HD2	2.02	0.42
2:C:47:ASP:N	2:C:66:SER:O	2.52	0.42
3:L:163:LYS:HD2	3:L:177:LEU:HD13	2.01	0.42
3:L:253:VAL:HG12	3:L:259:ARG:HA	2.01	0.42
3:L:588:GLN:O	3:L:592:ASN:N	2.52	0.42
1:D:139:SER:O	1:D:141:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:ASN:HA	2:C:399:ASN:HB2	2.00	0.42
3:K:184:MET:HB3	3:K:771:VAL:HG22	2.02	0.42
3:K:669:PRO:HD2	3:K:672:VAL:HA	2.02	0.42
3:L:184:MET:HA	3:L:270:LEU:HD23	2.01	0.42
3:L:375:VAL:HG13	3:L:480:LEU:HD12	2.01	0.42
3:L:1013:THR:HA	3:L:1017:LEU:HB3	2.00	0.42
3:J:108:GLN:O	3:J:112:GLN:HB3	2.20	0.42
3:J:442:LEU:HA	3:J:445:ILE:HB	2.02	0.42
3:J:697:GLN:HA	3:J:700:ASN:HB2	2.02	0.42
1:E:273:SER:HA	3:J:256:ASP:HB2	2.02	0.42
1:D:126:VAL:O	1:D:130:GLN:N	2.51	0.42
2:F:4:MET:O	2:F:8:GLN:N	2.39	0.42
2:F:42:LEU:N	2:I:293:TYR:O	2.45	0.42
3:K:77:TYR:CE1	3:K:860:THR:HB	2.55	0.42
3:L:631:LEU:HD13	3:L:637:ARG:HH22	1.85	0.42
3:L:979:SER:HB3	3:L:1015:THR:HB	2.01	0.42
3:J:15:ILE:HG12	3:J:18:ILE:HD12	2.02	0.42
3:J:801:PHE:HD1	3:J:801:PHE:HA	1.70	0.42
1:E:60:THR:HA	1:E:214:VAL:HA	2.02	0.41
1:G:244:VAL:N	1:G:258:GLY:O	2.43	0.41
3:K:610:PHE:CZ	5:K:1101:5QF:S9	3.05	0.41
3:K:786:ILE:HG22	3:K:801:PHE:HB3	2.02	0.41
3:J:7:ASP:OD2	3:J:432:ARG:NH2	2.53	0.41
3:J:613:ASN:OD1	3:J:614:GLY:N	2.53	0.41
1:E:91:VAL:HG12	1:E:93:LEU:HG	2.03	0.41
1:A:234:THR:OG1	1:A:235:LEU:O	2.35	0.41
2:F:315:GLN:HE21	2:C:19:LYS:HE2	1.85	0.41
2:I:14:ASN:ND2	2:I:105:LEU:HD13	2.34	0.41
3:K:142:VAL:HG12	3:K:323:ILE:HA	2.02	0.41
3:L:909:VAL:HG12	3:L:931:LEU:HG	2.01	0.41
3:J:74:ASN:O	3:J:95:GLU:N	2.37	0.41
3:J:683:GLU:HG3	3:J:860:THR:HG22	2.01	0.41
1:D:132:LEU:HD22	2:C:139:GLN:NE2	2.36	0.41
1:D:178:SER:O	1:D:180:ILE:N	2.52	0.41
1:D:325:VAL:HG21	1:D:335:ARG:HE	1.85	0.41
1:A:60:THR:HG23	1:A:290:GLY:N	2.29	0.41
1:A:87:ILE:HG21	1:A:93:LEU:HD21	2.02	0.41
1:B:323:VAL:HG11	1:B:353:LEU:HD11	2.00	0.41
3:K:184:MET:HA	3:K:270:LEU:HD23	2.01	0.41
3:L:47:ALA:HB3	3:L:88:VAL:HB	2.02	0.41
3:L:178:PHE:CB	5:L:1101:5QF:C16	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:937:LEU:HA	3:L:937:LEU:HD23	1.86	0.41
1:E:216:VAL:HG12	1:E:276:LEU:HD12	2.02	0.41
1:D:133:LEU:HD21	1:D:143:TYR:CG	2.55	0.41
1:G:337:ILE:HD12	1:G:349:VAL:HG22	2.03	0.41
1:A:241:LYS:HA	1:A:242:ALA:HA	1.92	0.41
3:K:1021:PHE:O	3:K:1025:PHE:N	2.53	0.41
4:M:15:VAL:HG13	3:J:980:LEU:HD12	2.02	0.41
3:J:217:GLY:O	3:J:234:ILE:N	2.49	0.41
3:J:527:TYR:O	3:J:531:VAL:N	2.50	0.41
3:J:591:LEU:HD23	3:J:591:LEU:HA	1.92	0.41
1:E:213:TYR:CD2	1:E:277:ARG:HD3	2.55	0.41
1:H:221:ASN:HA	1:H:224:MET:HB3	2.02	0.41
1:B:55:GLU:HA	1:B:296:ARG:HA	2.01	0.41
3:K:80:SER:HA	3:K:90:ILE:HG22	2.03	0.41
3:K:168:ARG:NH1	3:L:820:ASN:O	2.53	0.41
3:L:182:TYR:HB3	3:L:270:LEU:HD22	2.02	0.41
3:J:705:GLU:HG3	3:J:847:LEU:HD22	2.01	0.41
1:A:304:ASN:OD1	1:A:304:ASN:N	2.52	0.41
2:I:209:VAL:HG21	2:I:328:ARG:HG2	2.01	0.41
2:C:13:SER:OG	2:C:186:THR:O	2.39	0.41
2:C:69:LEU:HB3	2:C:254:THR:HG23	2.02	0.41
3:K:862:MET:O	3:K:866:GLU:N	2.45	0.41
3:J:183:ALA:N	3:J:271:GLY:O	2.54	0.41
3:J:373:PRO:HA	3:J:376:LEU:HD12	2.03	0.41
1:A:136:GLN:HG2	2:F:144:PHE:HE1	1.85	0.41
3:K:204:ILE:HG22	3:K:208:LYS:HE2	2.02	0.41
3:K:576:VAL:HG21	3:K:590:VAL:HG11	2.01	0.41
3:L:137:LEU:N	3:L:291:ILE:O	2.50	0.41
3:L:287:SER:OG	3:L:288:GLY:N	2.54	0.41
3:J:1026:PHE:HA	3:J:1030:ARG:HB2	2.01	0.41
1:E:176:VAL:HA	1:E:177:THR:HA	1.63	0.41
1:G:89:ALA:N	1:G:181:SER:OG	2.53	0.41
1:G:175:LYS:HD2	1:G:175:LYS:HA	1.84	0.41
2:I:129:GLN:HE21	2:I:133:ILE:HD12	1.85	0.41
2:I:213:LEU:HD21	2:I:324:VAL:HG22	2.03	0.41
2:C:123:LEU:HD22	2:C:175:LEU:HD22	2.01	0.41
3:L:299:ALA:HB1	3:L:330:THR:HG22	2.01	0.41
3:J:72:ILE:HB	3:J:75:LEU:HG	2.03	0.41
3:J:81:ASN:HD22	3:J:815:ARG:NH2	2.18	0.41
1:E:45:VAL:HG11	1:E:306:ILE:HG23	2.03	0.41
1:E:64:ARG:NH1	1:A:191:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:VAL:HG11	1:H:306:ILE:HG23	2.03	0.41
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.89	0.41
1:B:308:VAL:HG23	1:B:359:VAL:HG11	2.02	0.41
3:K:151:GLN:NE2	3:K:278:ILE:HG23	2.36	0.41
3:K:184:MET:HG2	3:K:246:PHE:CD2	2.55	0.41
3:K:530:SER:O	3:K:534:ILE:N	2.53	0.41
3:K:580:ALA:HB1	3:K:724:THR:HA	2.02	0.41
3:K:780:ARG:HH12	3:J:221:GLY:HA3	1.85	0.41
3:K:839:GLU:O	3:K:843:LEU:N	2.53	0.41
3:L:45:ILE:HG12	3:L:129:VAL:HG22	2.03	0.41
3:L:139:VAL:HG21	5:L:1101:5QF:C6	2.51	0.41
3:L:450:SER:HA	3:L:453:PHE:HE1	1.86	0.41
4:M:10:PHE:HA	4:M:13:ILE:HG22	2.02	0.41
4:N:22:ILE:HA	4:N:25:LEU:HD12	2.02	0.41
3:J:682:PHE:HD2	3:J:827:ILE:HB	1.86	0.41
1:G:180:ILE:HD11	1:G:206:VAL:HB	2.03	0.41
3:K:344:LEU:O	3:K:348:ILE:N	2.48	0.41
4:M:29:LEU:O	4:M:33:PHE:N	2.53	0.41
1:G:40:VAL:HG11	1:G:360:VAL:HG13	2.03	0.40
1:G:201:THR:OG1	1:G:202:ALA:N	2.53	0.40
1:H:72:VAL:HG13	1:H:101:TYR:CZ	2.56	0.40
1:A:313:VAL:HG22	1:A:323:VAL:HG22	2.02	0.40
2:F:332:ASN:HB3	2:C:173:ASN:HB3	2.03	0.40
2:F:368:THR:HG23	2:F:371:ASP:H	1.86	0.40
2:I:28:PHE:CD1	2:I:91:ALA:HB1	2.57	0.40
2:I:65:THR:N	2:I:258:ASP:O	2.48	0.40
3:K:915:ALA:HB3	3:K:1006:GLY:HA2	2.03	0.40
3:L:178:PHE:HE1	5:L:1101:5QF:C28	2.34	0.40
3:L:764:ASP:HB3	3:L:769:LYS:HD2	2.02	0.40
3:J:30:LEU:HD23	3:J:30:LEU:HA	1.93	0.40
3:J:184:MET:HG2	3:J:246:PHE:CD2	2.56	0.40
3:J:628:PHE:HZ	5:J:1101:5QF:N22	2.19	0.40
1:E:59:ARG:HD2	1:E:292:PHE:HA	2.02	0.40
1:E:175:LYS:HD2	1:E:175:LYS:HA	1.88	0.40
1:E:254:PHE:HA	1:E:255:PRO:HD3	1.96	0.40
1:G:260:LEU:HD21	1:G:276:LEU:HB3	2.04	0.40
1:G:265:VAL:O	1:H:207:GLN:NE2	2.35	0.40
1:H:124:LEU:HD23	1:H:124:LEU:HA	1.89	0.40
1:H:291:MET:H	1:H:292:PHE:HA	1.85	0.40
2:F:319:ALA:O	2:F:323:VAL:N	2.47	0.40
3:L:83:ASP:OD1	3:L:87:THR:OG1	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1028:VAL:O	3:J:1032:ARG:N	2.49	0.40
1:G:178:SER:OG	1:H:192:GLY:O	2.32	0.40
1:H:325:VAL:HG11	1:H:357:ASP:HB3	2.03	0.40
1:B:89:ALA:N	1:B:181:SER:OG	2.54	0.40
3:K:49:TYR:HE1	3:K:121:GLU:HB2	1.87	0.40
3:K:210:GLN:OE1	3:K:250:LEU:N	2.54	0.40
3:L:540:ARG:HA	3:L:543:VAL:HG22	2.03	0.40
3:L:620:ARG:HD2	5:L:1101:5QF:C31	2.52	0.40
3:J:120:GLN:O	3:J:124:GLN:HG2	2.22	0.40
3:J:261:LEU:HB3	3:J:263:ARG:HG2	2.03	0.40
1:G:212:ILE:HD11	1:G:289:PRO:HB3	2.02	0.40
1:B:214:VAL:N	1:B:278:ALA:O	2.44	0.40
1:B:315:ARG:NH1	1:B:321:ALA:HB2	2.36	0.40
3:K:21:LEU:O	3:K:25:LEU:N	2.54	0.40
3:L:545:TYR:OH	3:L:903:LEU:O	2.34	0.40
3:L:962:GLU:HA	3:L:965:LEU:HB2	2.03	0.40
3:J:313:MET:HA	3:J:316:PHE:HD2	1.87	0.40
3:J:562:SER:HB3	3:J:836:SER:HB2	2.03	0.40
1:D:73:SER:OG	1:D:197:ASN:N	2.55	0.40
1:D:324:LEU:HD12	1:D:334:THR:HB	2.03	0.40
1:B:70:PRO:HD3	1:B:203:LEU:HG	2.04	0.40
2:I:52:ASN:N	2:C:282:ASN:O	2.54	0.40
2:C:151:ILE:HD12	2:C:151:ILE:HA	1.94	0.40
3:K:82:SER:O	3:K:816:LEU:N	2.46	0.40
3:K:831:ALA:HB2	3:K:837:THR:HB	2.02	0.40
3:L:36:PRO:HG3	3:L:469:GLN:HG3	2.03	0.40
3:L:620:ARG:CZ	5:L:1101:5QF:C31	2.98	0.40
3:L:705:GLU:HG3	3:L:847:LEU:HD13	2.03	0.40
3:L:1025:PHE:HA	3:L:1028:VAL:HG12	2.03	0.40
3:J:456:MET:HB2	3:J:467:TYR:HB3	2.04	0.40
3:J:761:ASP:HB3	3:J:768:VAL:HG13	2.02	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 PDB entries followed by that with respect to all EM entries.

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	338/373 (91%)	299 (88%)	39 (12%)	0	100	100
1	B	338/373 (91%)	300 (89%)	38 (11%)	0	100	100
1	D	338/373 (91%)	288 (85%)	48 (14%)	2 (1%)	22	60
1	E	338/373 (91%)	286 (85%)	50 (15%)	2 (1%)	22	60
1	G	338/373 (91%)	283 (84%)	53 (16%)	2 (1%)	22	60
1	H	338/373 (91%)	297 (88%)	41 (12%)	0	100	100
2	C	426/493 (86%)	407 (96%)	19 (4%)	0	100	100
2	F	426/493 (86%)	407 (96%)	19 (4%)	0	100	100
2	I	426/493 (86%)	408 (96%)	18 (4%)	0	100	100
3	J	1031/1049 (98%)	937 (91%)	93 (9%)	1 (0%)	48	83
3	K	1035/1049 (99%)	925 (89%)	110 (11%)	0	100	100
3	L	1035/1049 (99%)	935 (90%)	100 (10%)	0	100	100
4	M	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
4	N	44/54 (82%)	40 (91%)	4 (9%)	0	100	100
4	O	44/54 (82%)	41 (93%)	3 (7%)	0	100	100
All	All	6539/7026 (93%)	5892 (90%)	640 (10%)	7 (0%)	50	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	140	LYS
1	D	140	LYS
1	G	140	LYS
1	D	179	PRO
3	J	257	GLY
1	E	179	PRO
1	G	179	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	274/299 (92%)	273 (100%)	1 (0%)	89 91
1	B	274/299 (92%)	273 (100%)	1 (0%)	89 91
1	D	274/299 (92%)	270 (98%)	4 (2%)	60 75
1	E	274/299 (92%)	269 (98%)	5 (2%)	54 71
1	G	274/299 (92%)	270 (98%)	4 (2%)	60 75
1	H	274/299 (92%)	272 (99%)	2 (1%)	81 87
2	C	358/412 (87%)	356 (99%)	2 (1%)	84 88
2	F	358/412 (87%)	356 (99%)	2 (1%)	84 88
2	I	358/412 (87%)	356 (99%)	2 (1%)	84 88
3	J	839/855 (98%)	832 (99%)	7 (1%)	79 85
3	K	826/855 (97%)	821 (99%)	5 (1%)	84 88
3	L	826/855 (97%)	815 (99%)	11 (1%)	65 77
4	M	34/46 (74%)	34 (100%)	0	100 100
4	N	34/46 (74%)	34 (100%)	0	100 100
4	O	34/46 (74%)	34 (100%)	0	100 100
All	All	5311/5733 (93%)	5265 (99%)	46 (1%)	74 83

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	46	LYS
1	E	94	TYR
1	E	137	TYR
1	E	291	MET
1	E	318	ARG
1	D	46	LYS
1	D	94	TYR
1	D	291	MET
1	D	318	ARG
1	G	46	LYS
1	G	94	TYR
1	G	291	MET
1	G	318	ARG
1	H	60	THR
1	H	96	ILE
1	A	96	ILE

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Mol	Chain	Res	Type
1	B	60	THR
2	F	197	ASN
2	F	367	ARG
2	I	197	ASN
2	I	367	ARG
2	C	197	ASN
2	C	367	ARG
3	K	194	ASN
3	K	231	ASN
3	K	259	ARG
3	K	739	LEU
3	K	801	PHE
3	L	231	ASN
3	L	255	GLN
3	L	307	ARG
3	L	415	ASN
3	L	418	ARG
3	L	540	ARG
3	L	613	ASN
3	L	637	ARG
3	L	739	LEU
3	L	801	PHE
3	L	1032	ARG
3	J	231	ASN
3	J	256	ASP
3	J	259	ARG
3	J	558	ARG
3	J	659	LYS
3	J	717	ARG
3	J	801	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	207	GLN
1	G	207	GLN
2	F	197	ASN
2	F	225	GLN
2	I	127	GLN
2	I	129	GLN
2	I	197	ASN
2	I	225	GLN

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Mol	Chain	Res	Type
2	I	315	GLN
2	I	325	GLN
2	C	197	ASN
2	C	315	GLN
2	C	332	ASN
3	K	58	GLN
3	K	108	GLN
3	K	161	ASN
3	K	176	GLN
3	K	213	GLN
3	K	228	GLN
3	K	237	GLN
3	K	254	ASN
3	K	415	ASN
3	K	588	GLN
3	L	125	GLN
3	L	176	GLN
3	L	254	ASN
3	L	737	GLN
3	J	109	ASN
3	J	237	GLN
3	J	733	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)

3 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	5QF	K	1101	3	40,40,40	1.96	10 (25%)	49,56,56	2.09	12 (24%)
5	5QF	L	1101	3	40,40,40	1.94	12 (30%)	49,56,56	2.43	15 (30%)
5	5QF	J	1101	-	40,40,40	2.03	10 (25%)	49,56,56	2.15	12 (24%)

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
5	5QF	K	1101	3	-	12/19/41/41	0/4/4/4
5	5QF	L	1101	3	-	11/19/41/41	0/4/4/4
5	5QF	J	1101	-	-	10/19/41/41	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1101	5QF	C5-S9	4.77	1.83	1.76
5	K	1101	5QF	C3-N22	4.74	1.49	1.37
5	J	1101	5QF	C3-N22	4.42	1.48	1.37
5	L	1101	5QF	C2-C1	-4.37	1.33	1.40
5	K	1101	5QF	C6-C7	4.25	1.51	1.44
5	L	1101	5QF	C3-N22	4.18	1.48	1.37
5	J	1101	5QF	C32-C33	-4.13	1.48	1.52
5	L	1101	5QF	C5-S9	4.12	1.82	1.76
5	K	1101	5QF	C35-C2	4.02	1.57	1.51
5	J	1101	5QF	C6-C1	-3.98	1.36	1.40
5	L	1101	5QF	C6-C7	3.92	1.51	1.44
5	K	1101	5QF	C32-C33	-3.90	1.48	1.52
5	J	1101	5QF	C6-C7	3.88	1.50	1.44
5	J	1101	5QF	C5-S9	3.83	1.81	1.76
5	J	1101	5QF	C2-C1	-3.78	1.34	1.40
5	J	1101	5QF	C35-C2	3.73	1.57	1.51
5	J	1101	5QF	C6-C5	-3.68	1.37	1.41
5	L	1101	5QF	C6-C1	-3.64	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1101	5QF	C2-C1	-3.56	1.35	1.40
5	L	1101	5QF	C32-C33	-3.41	1.49	1.52
5	L	1101	5QF	C35-C2	3.38	1.56	1.51
5	K	1101	5QF	O34-C33	-3.14	1.43	1.45
5	K	1101	5QF	C6-C1	-2.95	1.37	1.40
5	L	1101	5QF	O34-C33	-2.83	1.43	1.45
5	J	1101	5QF	O34-C33	-2.72	1.43	1.45
5	J	1101	5QF	O18-C16	2.35	1.40	1.37
5	K	1101	5QF	O19-C15	2.27	1.40	1.37
5	L	1101	5QF	C23-N22	-2.26	1.43	1.46
5	L	1101	5QF	C6-C5	-2.25	1.38	1.41
5	L	1101	5QF	O18-C16	2.22	1.40	1.37
5	K	1101	5QF	C23-N22	-2.09	1.43	1.46
5	L	1101	5QF	C27-N22	-2.08	1.43	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1101	5QF	C10-C11-C12	-7.65	100.22	113.97
5	K	1101	5QF	C10-S9-C5	7.01	112.87	101.82
5	L	1101	5QF	C10-S9-C5	6.81	112.55	101.82
5	J	1101	5QF	O18-C16-C15	6.59	124.60	115.41
5	K	1101	5QF	C6-C5-N4	-4.94	119.37	123.12
5	K	1101	5QF	C6-C5-S9	4.74	123.05	117.75
5	L	1101	5QF	O19-C15-C16	4.54	121.73	115.41
5	L	1101	5QF	O19-C15-C14	-4.35	116.92	124.37
5	L	1101	5QF	C6-C5-N4	-4.22	119.92	123.12
5	L	1101	5QF	C21-O19-C15	-4.22	111.17	117.53
5	J	1101	5QF	O34-C35-C2	4.20	118.94	111.72
5	L	1101	5QF	C36-C33-C32	-4.07	106.18	111.13
5	K	1101	5QF	O34-C35-C2	4.03	118.66	111.72
5	J	1101	5QF	C36-C33-C32	-3.96	106.30	111.13
5	J	1101	5QF	O19-C15-C16	3.88	120.81	115.41
5	J	1101	5QF	O18-C16-C17	-3.79	117.59	124.12
5	J	1101	5QF	C1-C6-C7	3.77	124.50	119.57
5	L	1101	5QF	O18-C16-C15	3.71	120.57	115.41
5	J	1101	5QF	C21-O19-C15	-3.69	111.96	117.53
5	K	1101	5QF	C36-C33-C32	-3.58	106.76	111.13
5	J	1101	5QF	C5-C6-C7	-3.52	115.87	119.79
5	K	1101	5QF	O19-C15-C16	3.50	120.28	115.41
5	J	1101	5QF	O19-C15-C14	-3.44	118.47	124.37
5	J	1101	5QF	C26-C27-N22	-3.37	104.16	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1101	5QF	C6-C5-S9	3.23	121.36	117.75
5	L	1101	5QF	C24-C23-N22	-3.09	104.69	110.70
5	K	1101	5QF	O18-C16-C15	3.05	119.66	115.41
5	L	1101	5QF	O34-C35-C2	3.02	116.92	111.72
5	K	1101	5QF	C27-N22-C3	-2.88	109.02	119.05
5	J	1101	5QF	C6-C5-N4	-2.82	120.98	123.12
5	K	1101	5QF	C21-O19-C15	-2.69	113.47	117.53
5	K	1101	5QF	O18-C16-C17	-2.59	119.66	124.12
5	K	1101	5QF	O19-C15-C14	-2.45	120.17	124.37
5	L	1101	5QF	C27-N22-C23	2.29	116.58	111.52
5	L	1101	5QF	C26-C27-N22	-2.27	106.28	110.70
5	L	1101	5QF	O18-C16-C17	-2.17	120.39	124.12
5	J	1101	5QF	C32-C1-C6	2.10	122.42	119.87
5	K	1101	5QF	C3-N4-C5	2.03	121.80	116.30
5	L	1101	5QF	C20-O18-C16	-2.00	114.51	117.53

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	1101	5QF	C11-C10-S9-C5
5	J	1101	5QF	S9-C10-C11-C12
5	L	1101	5QF	C16-C15-O19-C21
5	K	1101	5QF	C15-C16-O18-C20
5	J	1101	5QF	C14-C15-O19-C21
5	L	1101	5QF	C14-C15-O19-C21
5	K	1101	5QF	C17-C16-O18-C20
5	J	1101	5QF	C16-C15-O19-C21
5	J	1101	5QF	C15-C16-O18-C20
5	K	1101	5QF	N25-C28-C29-O30
5	J	1101	5QF	C17-C16-O18-C20
5	L	1101	5QF	C17-C16-O18-C20
5	K	1101	5QF	C14-C15-O19-C21
5	L	1101	5QF	C15-C16-O18-C20
5	L	1101	5QF	N25-C28-C29-O30
5	K	1101	5QF	C16-C15-O19-C21
5	L	1101	5QF	C2-C3-N22-C27
5	L	1101	5QF	N4-C3-N22-C27
5	K	1101	5QF	C10-C11-C12-C17
5	J	1101	5QF	C10-C11-C12-C17
5	J	1101	5QF	C10-C11-C12-C13
5	K	1101	5QF	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	K	1101	5QF	N4-C5-S9-C10
5	K	1101	5QF	C6-C5-S9-C10
5	J	1101	5QF	N25-C28-C29-O30
5	K	1101	5QF	N4-C3-N22-C23
5	J	1101	5QF	N4-C3-N22-C23
5	L	1101	5QF	S9-C10-C11-C12
5	L	1101	5QF	C29-C28-N25-C24
5	K	1101	5QF	C28-C29-O30-C31
5	L	1101	5QF	C29-C28-N25-C26
5	K	1101	5QF	C1-C6-C7-N8
5	J	1101	5QF	C2-C3-N22-C23

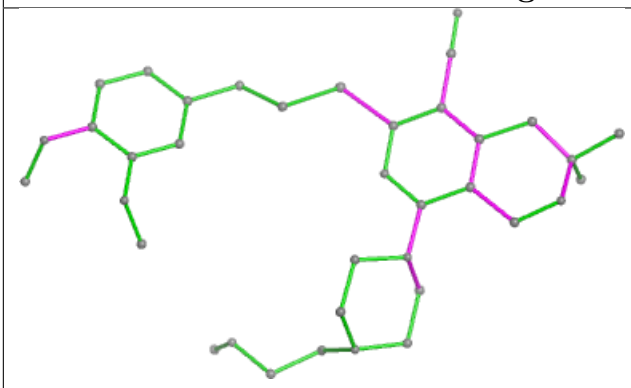
There are no ring outliers.

3 monomers are involved in 134 short contacts:

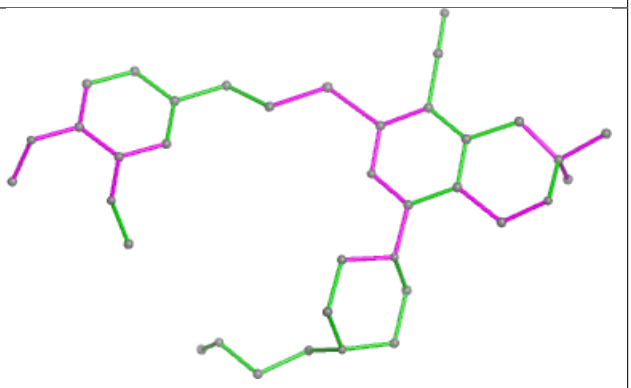
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1101	5QF	43	0
5	L	1101	5QF	42	0
5	J	1101	5QF	49	0

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 then 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.

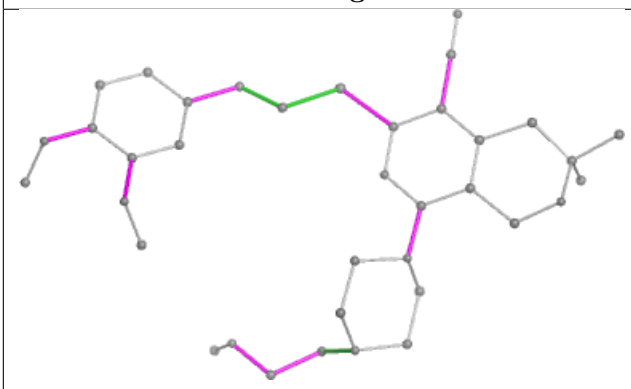
Ligand 5QF K 1101



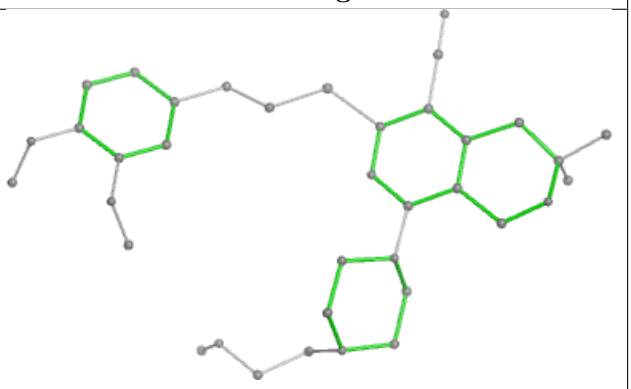
Bond lengths



Bond angles

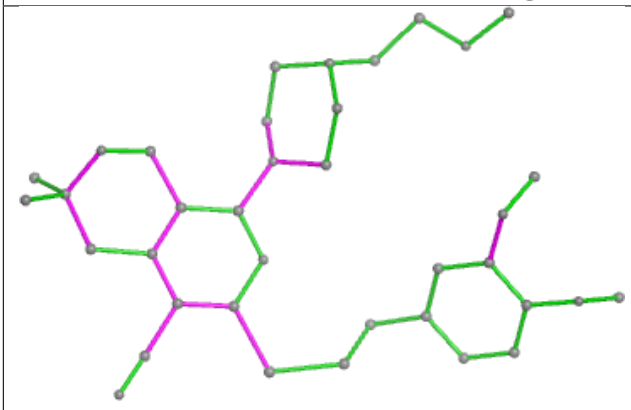


Torsions

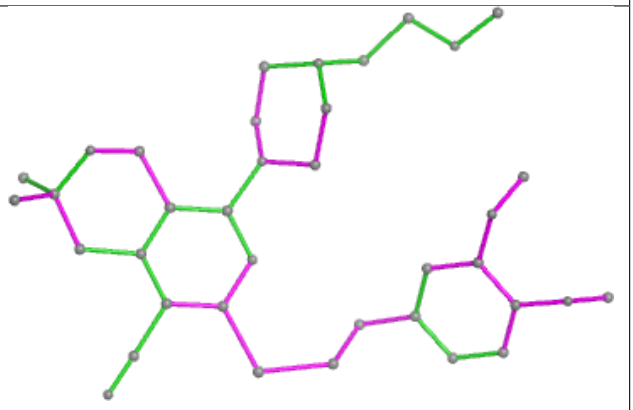


Rings

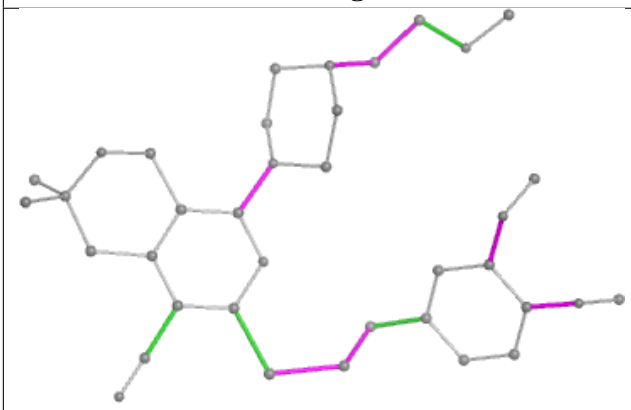
Ligand 5QF L 1101



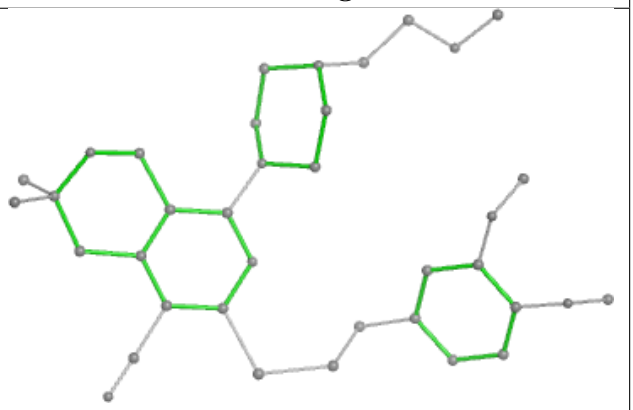
Bond lengths



Bond angles

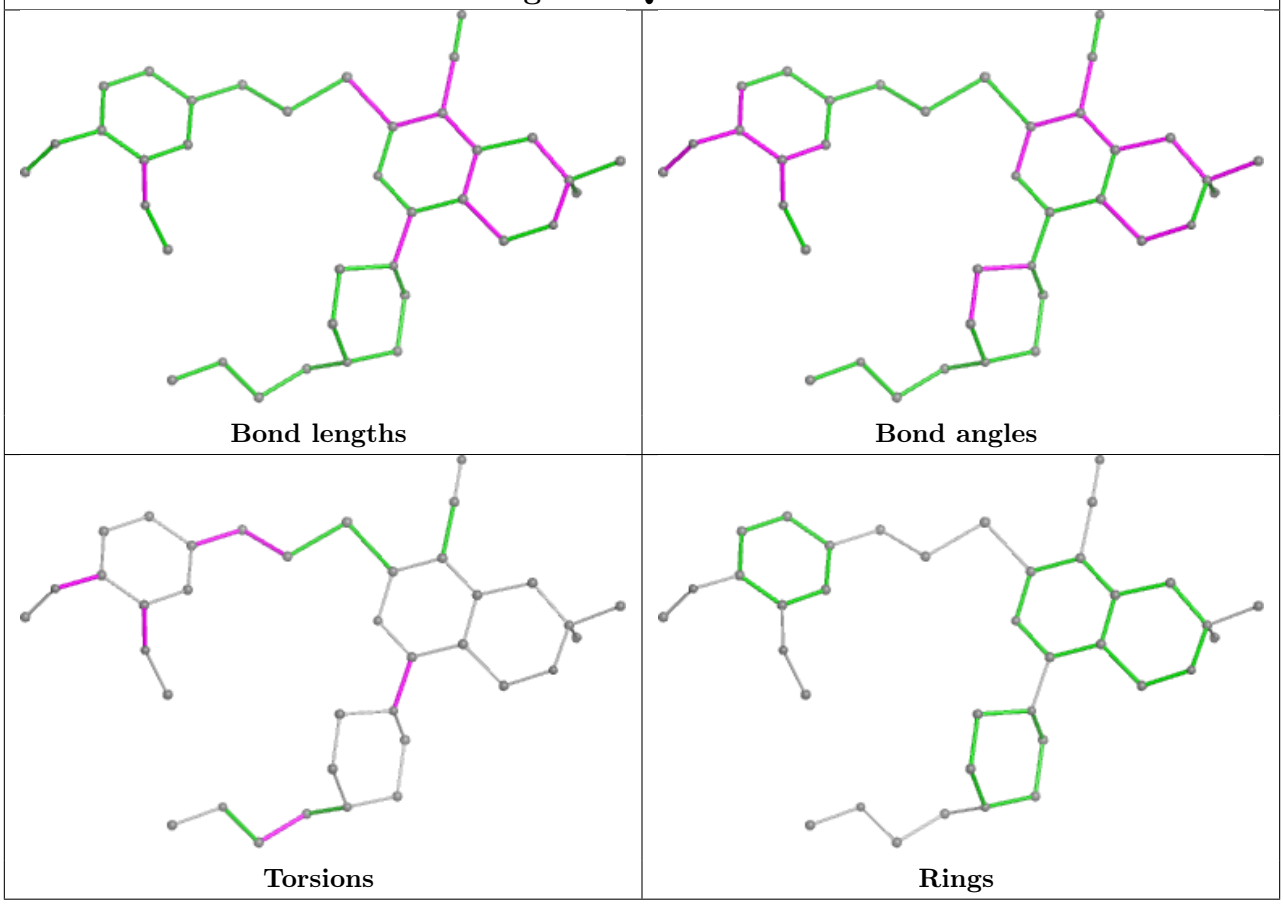


Torsions



Rings

Ligand 5QF J 1101



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	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	68:VAL	C	69:ARG	N	1.16

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3636. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.