



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:51 PM UTC

PDB ID : 7K1W / pdb_00007k1w
EMDB ID : EMD-22631
Title : PIKfyve/Fig4/Vac14 complex centered on Fig4 - map3
Authors : Lees, J.A.; Reinisch, K.M.; Li, P.
Deposited on : 2020-09-08
Resolution : 5.10 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

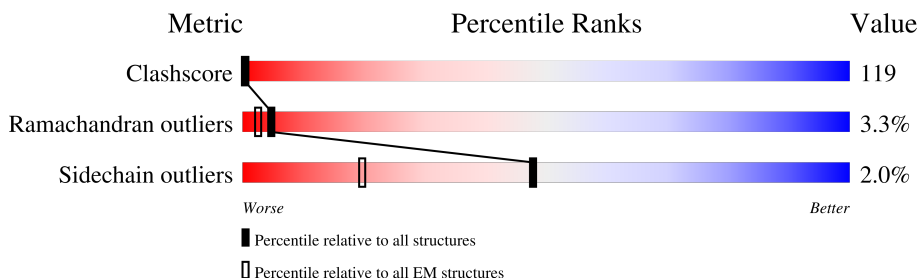
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	F	918	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3721 atoms, of which 0 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.

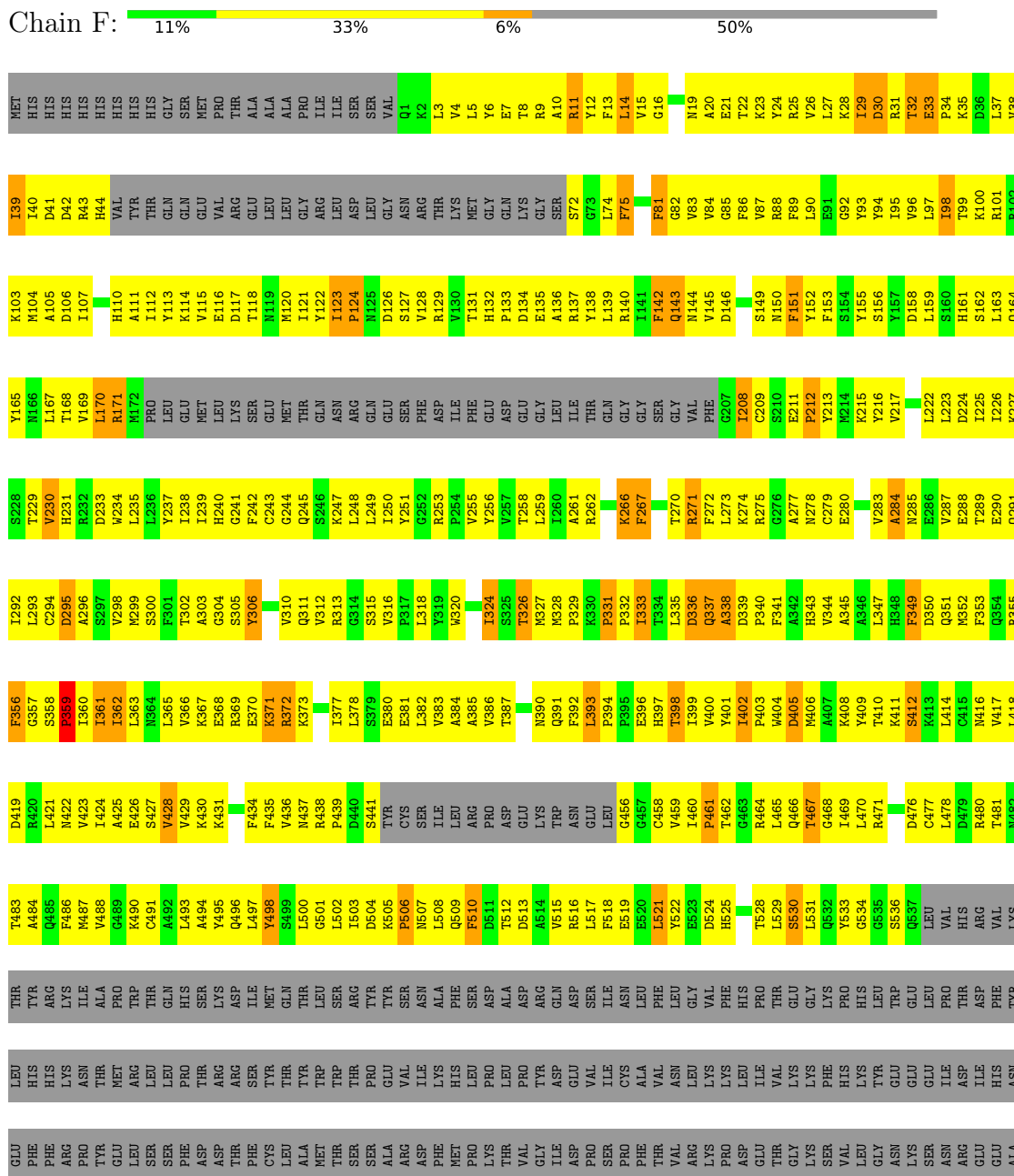
- Molecule 1 is a protein called Fig4 Sac homology model.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	462	3721	2386	636	680	19	0	0

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. 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: Fig4 Sac homology model



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19998	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.4	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](#)

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	F	1.34	0/3804	1.75	56/5152 (1.1%)

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	F	0	1

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	GLN	CG-CD-OE1	-38.20	44.41	120.80
1	F	143	GLN	CG-CD-NE2	-15.35	93.38	116.40
1	F	143	GLN	OE1-CD-NE2	15.18	137.78	122.60
1	F	124	PRO	N-CA-C	11.36	128.05	113.86
1	F	356	PHE	CA-CB-CG	-9.82	103.98	113.80
1	F	338	ALA	CA-C-N	-9.75	111.97	122.89
1	F	338	ALA	C-N-CA	-9.75	111.97	122.89
1	F	337	GLN	N-CA-C	-9.60	100.90	111.36
1	F	142	PHE	CA-CB-CG	-8.21	105.59	113.80
1	F	467	THR	CA-C-N	-7.69	115.36	121.82
1	F	467	THR	C-N-CA	-7.69	115.36	121.82
1	F	456	GLY	N-CA-C	-7.66	105.39	113.58
1	F	510	PHE	CA-CB-CG	-7.50	106.30	113.80
1	F	498	TYR	CB-CA-C	-7.34	98.61	110.79
1	F	371	LYS	N-CA-C	-7.32	103.38	111.36
1	F	349	PHE	CA-CB-CG	-7.02	106.78	113.80
1	F	506	PRO	N-CA-C	6.98	121.00	111.22
1	F	151	PHE	CA-CB-CG	-6.87	106.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	372	ARG	N-CA-C	-6.74	104.31	112.54
1	F	29	ILE	N-CA-C	-6.67	98.82	108.36
1	F	81	PHE	CA-CB-CG	-6.63	107.17	113.80
1	F	427	SER	N-CA-C	-6.58	104.02	111.07
1	F	359	PRO	N-CA-C	6.53	125.91	112.47
1	F	216	TYR	CA-CB-CG	-6.38	102.42	113.90
1	F	126	ASP	CA-CB-CG	-6.32	106.28	112.60
1	F	39	ILE	CB-CA-C	-6.21	101.57	110.83
1	F	441	SER	N-CA-C	-6.21	101.08	110.28
1	F	306	TYR	CA-CB-CG	-5.92	103.24	113.90
1	F	42	ASP	CA-CB-CG	-5.90	106.70	112.60
1	F	513	ASP	CA-CB-CG	-5.83	106.77	112.60
1	F	536	SER	N-CA-C	-5.79	101.83	108.49
1	F	530	SER	CA-C-N	5.74	129.79	120.60
1	F	530	SER	C-N-CA	5.74	129.79	120.60
1	F	240	HIS	N-CA-C	5.73	118.73	111.69
1	F	326	THR	N-CA-C	-5.67	105.24	111.82
1	F	430	LYS	CA-C-N	5.62	128.85	120.31
1	F	430	LYS	C-N-CA	5.62	128.85	120.31
1	F	428	VAL	N-CA-C	5.61	117.11	111.00
1	F	476	ASP	CA-CB-CG	-5.55	107.05	112.60
1	F	30	ASP	CA-C-N	5.55	128.75	120.31
1	F	30	ASP	C-N-CA	5.55	128.75	120.31
1	F	284	ALA	CA-C-N	-5.50	115.30	123.11
1	F	284	ALA	C-N-CA	-5.50	115.30	123.11
1	F	267	PHE	CA-CB-CG	-5.44	108.36	113.80
1	F	33	GLU	N-CA-C	-5.42	105.92	113.45
1	F	212	PRO	N-CA-CB	5.39	108.04	103.35
1	F	331	PRO	N-CA-C	5.37	117.25	110.70
1	F	144	ASN	CA-CB-CG	-5.32	107.28	112.60
1	F	233	ASP	CA-CB-CG	-5.25	107.34	112.60
1	F	416	ASN	CA-CB-CG	-5.25	107.35	112.60
1	F	501	GLY	N-CA-C	-5.22	108.07	115.43
1	F	405	ASP	CA-CB-CG	-5.13	107.47	112.60
1	F	241	GLY	N-CA-C	5.12	125.30	113.18
1	F	402	ILE	CB-CA-C	-5.09	105.02	110.16
1	F	295	ASP	CA-CB-CG	-5.06	107.54	112.60
1	F	30	ASP	CA-CB-CG	-5.04	107.56	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	266	LYS	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	F	3721	0	3717	882	0
All	All	3721	0	3717	882	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 119.

All (882) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ILE:HD11	1:F:306:TYR:CE1	1.17	1.67
1:F:107:ILE:CD1	1:F:306:TYR:CE1	2.02	1.42
1:F:107:ILE:CD1	1:F:306:TYR:HE1	1.44	1.24
1:F:151:PHE:CD1	1:F:238:ILE:CG2	2.19	1.24
1:F:105:ALA:HB1	1:F:245:GLN:NE2	1.57	1.20
1:F:163:LEU:HD23	1:F:435:PHE:CD2	1.77	1.20
1:F:151:PHE:CG	1:F:238:ILE:HG21	1.58	1.16
1:F:123:ILE:HG23	1:F:124:PRO:HD3	1.24	1.15
1:F:151:PHE:CD1	1:F:238:ILE:HG23	1.79	1.14
1:F:151:PHE:CG	1:F:238:ILE:CG2	2.26	1.13
1:F:152:TYR:O	1:F:238:ILE:HA	1.49	1.13
1:F:31:ARG:HA	1:F:123:ILE:HG12	1.31	1.12
1:F:404:TRP:HH2	1:F:418:LEU:HD23	1.08	1.12
1:F:151:PHE:CD1	1:F:238:ILE:HG21	1.83	1.11
1:F:152:TYR:HD2	1:F:239:ILE:HG13	1.16	1.08
1:F:3:LEU:HD21	1:F:14:LEU:HB3	1.29	1.07
1:F:151:PHE:HD1	1:F:238:ILE:HG23	1.12	1.06
1:F:11:ARG:HA	1:F:123:ILE:HD13	1.33	1.05
1:F:5:LEU:HD22	1:F:14:LEU:HG	1.34	1.04
1:F:11:ARG:HD2	1:F:29:ILE:HB	1.40	1.04
1:F:163:LEU:HD21	1:F:435:PHE:CE2	1.92	1.03
1:F:163:LEU:CD2	1:F:435:PHE:CD2	2.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:LEU:CD2	1:F:435:PHE:CE2	2.43	1.01
1:F:11:ARG:HG2	1:F:123:ILE:HB	1.41	1.00
1:F:213:TYR:HE2	1:F:355:ARG:NE	1.59	1.00
1:F:105:ALA:HB1	1:F:245:GLN:HE21	0.83	1.00
1:F:341:PHE:CE2	1:F:385:ALA:HB2	1.97	0.99
1:F:84:VAL:HG23	1:F:96:VAL:HG23	1.43	0.98
1:F:40:ILE:HD11	1:F:43:ARG:HE	1.22	0.98
1:F:11:ARG:HD3	1:F:12:TYR:HD1	1.29	0.98
1:F:152:TYR:HB2	1:F:239:ILE:HG12	1.43	0.97
1:F:377:ILE:HG23	1:F:378:LEU:HD12	1.46	0.97
1:F:259:LEU:HB3	1:F:521:LEU:HD11	1.44	0.97
1:F:250:ILE:HG23	1:F:502:LEU:HD21	1.47	0.96
1:F:105:ALA:CB	1:F:245:GLN:HE21	1.78	0.96
1:F:404:TRP:CH2	1:F:418:LEU:HD23	2.00	0.96
1:F:152:TYR:H	1:F:239:ILE:N	1.61	0.96
1:F:213:TYR:CD2	1:F:355:ARG:NH2	2.33	0.96
1:F:90:LEU:HD12	1:F:135:GLU:HB3	1.43	0.95
1:F:152:TYR:H	1:F:239:ILE:H	0.99	0.95
1:F:507:ASN:HB2	1:F:510:PHE:CE1	2.02	0.95
1:F:223:LEU:HD21	1:F:227:LYS:HB3	1.48	0.95
1:F:393:LEU:HG	1:F:394:PRO:HD3	1.49	0.95
1:F:253:ARG:HD2	1:F:502:LEU:HD12	1.47	0.95
1:F:152:TYR:CD2	1:F:239:ILE:HG13	2.01	0.94
1:F:333:ILE:HG21	1:F:381:GLU:HG2	1.47	0.93
1:F:497:LEU:CD1	1:F:502:LEU:HD13	1.98	0.93
1:F:213:TYR:HD2	1:F:355:ARG:HH21	1.17	0.93
1:F:406:MET:HG2	1:F:414:LEU:CD1	1.99	0.92
1:F:460:ILE:HG12	1:F:461:PRO:HD3	1.50	0.92
1:F:404:TRP:CZ2	1:F:417:VAL:HG13	2.05	0.92
1:F:361:ILE:HG12	1:F:470:LEU:HD22	1.52	0.91
1:F:8:THR:HG23	1:F:10:ALA:H	1.33	0.91
1:F:6:TYR:CE2	1:F:75:PHE:HB2	2.05	0.90
1:F:333:ILE:HG21	1:F:381:GLU:CG	2.01	0.90
1:F:212:PRO:HG2	1:F:237:TYR:HD2	1.35	0.90
1:F:258:THR:HB	1:F:292:ILE:CG1	2.02	0.90
1:F:31:ARG:CA	1:F:123:ILE:HG12	2.01	0.90
1:F:26:VAL:HB	1:F:40:ILE:CG2	2.02	0.89
1:F:81:PHE:CD1	1:F:100:LYS:HA	2.08	0.89
1:F:356:PHE:CD1	1:F:469:ILE:HG21	2.06	0.89
1:F:3:LEU:HD23	1:F:5:LEU:HD21	1.53	0.89
1:F:15:VAL:HG12	1:F:26:VAL:HG22	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:TYR:HD2	1:F:239:ILE:CG1	1.85	0.89
1:F:242:PHE:HD1	1:F:528:THR:HG21	1.38	0.88
1:F:35:LYS:HB2	1:F:93:TYR:CD1	2.07	0.88
1:F:215:LYS:HA	1:F:267:PHE:CE1	2.07	0.88
1:F:242:PHE:CD1	1:F:528:THR:HG21	2.07	0.88
1:F:406:MET:HE3	1:F:414:LEU:HD11	1.55	0.88
1:F:213:TYR:CE1	1:F:215:LYS:HE2	2.09	0.88
1:F:358:SER:HB2	1:F:467:THR:HB	1.54	0.87
1:F:35:LYS:CD	1:F:92:GLY:HA2	2.04	0.87
1:F:107:ILE:HG12	1:F:306:TYR:CZ	2.10	0.87
1:F:11:ARG:CG	1:F:123:ILE:HB	2.05	0.87
1:F:226:ILE:HD11	1:F:234:TRP:HB2	1.56	0.87
1:F:318:LEU:HD12	1:F:341:PHE:CD1	2.09	0.87
1:F:35:LYS:HD2	1:F:92:GLY:HA2	1.57	0.86
1:F:101:ARG:HH22	1:F:152:TYR:HA	1.40	0.86
1:F:123:ILE:CG2	1:F:124:PRO:HD3	2.06	0.86
1:F:84:VAL:HG23	1:F:96:VAL:CG2	2.05	0.86
1:F:507:ASN:HB2	1:F:510:PHE:HE1	1.35	0.86
1:F:401:TYR:CE2	1:F:403:PRO:HD3	2.11	0.86
1:F:295:ASP:HB2	1:F:500:LEU:CD2	2.06	0.86
1:F:404:TRP:CG	1:F:421:LEU:HD23	2.11	0.86
1:F:358:SER:CB	1:F:467:THR:HB	2.06	0.85
1:F:11:ARG:CA	1:F:123:ILE:HD13	2.07	0.85
1:F:107:ILE:CD1	1:F:306:TYR:CZ	2.59	0.85
1:F:11:ARG:HG2	1:F:123:ILE:HD13	1.59	0.85
1:F:223:LEU:HD11	1:F:235:LEU:HD13	1.59	0.84
1:F:37:LEU:HD23	1:F:225:ILE:HG22	1.57	0.84
1:F:213:TYR:CE2	1:F:355:ARG:NH2	2.43	0.84
1:F:15:VAL:CG1	1:F:26:VAL:HG22	2.06	0.84
1:F:377:ILE:CG2	1:F:378:LEU:HD12	2.08	0.84
1:F:165:TYR:O	1:F:168:THR:HG22	1.78	0.84
1:F:28:LYS:HB3	1:F:38:VAL:CG2	2.07	0.84
1:F:87:VAL:HG21	1:F:89:PHE:CZ	2.13	0.83
1:F:391:GLN:NE2	1:F:399:ILE:HD12	1.93	0.83
1:F:414:LEU:O	1:F:417:VAL:HG12	1.77	0.83
1:F:152:TYR:N	1:F:239:ILE:H	1.77	0.83
1:F:101:ARG:HH21	1:F:115:VAL:HG23	1.41	0.83
1:F:11:ARG:HD3	1:F:12:TYR:CD1	2.14	0.83
1:F:223:LEU:HG	1:F:235:LEU:HD22	1.61	0.83
1:F:406:MET:HG2	1:F:414:LEU:HD11	1.59	0.83
1:F:418:LEU:O	1:F:487:MET:HE1	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:CYS:HB2	1:F:306:TYR:CE1	2.14	0.82
1:F:100:LYS:HG3	1:F:116:GLU:HB2	1.59	0.82
1:F:223:LEU:HD13	1:F:237:TYR:CE1	2.14	0.82
1:F:336:ASP:HB2	1:F:339:ASP:HA	1.61	0.82
1:F:107:ILE:CG1	1:F:306:TYR:CE1	2.63	0.82
1:F:4:VAL:O	1:F:5:LEU:HD23	1.80	0.82
1:F:224:ASP:HA	1:F:227:LYS:HE2	1.62	0.82
1:F:508:LEU:HD12	1:F:509:GLN:N	1.95	0.82
1:F:497:LEU:HD12	1:F:502:LEU:HD13	1.59	0.82
1:F:248:LEU:CD1	1:F:255:VAL:HB	2.09	0.82
1:F:363:LEU:HG	1:F:470:LEU:HD21	1.61	0.81
1:F:11:ARG:HA	1:F:123:ILE:CD1	2.10	0.81
1:F:105:ALA:HB3	1:F:112:ILE:HG12	1.63	0.81
1:F:209:CYS:C	1:F:212:PRO:HD2	2.05	0.81
1:F:122:TYR:CG	1:F:124:PRO:HD2	2.15	0.81
1:F:150:ASN:O	1:F:239:ILE:O	1.98	0.81
1:F:215:LYS:HA	1:F:267:PHE:HE1	1.43	0.81
1:F:245:GLN:HG2	1:F:258:THR:HG23	1.61	0.81
1:F:341:PHE:CZ	1:F:385:ALA:HB2	2.14	0.81
1:F:115:VAL:CG2	1:F:238:ILE:HD12	2.11	0.81
1:F:152:TYR:C	1:F:238:ILE:HA	2.06	0.80
1:F:253:ARG:NH1	1:F:500:LEU:HB3	1.96	0.80
1:F:213:TYR:CE2	1:F:355:ARG:CZ	2.65	0.80
1:F:152:TYR:O	1:F:238:ILE:CA	2.28	0.80
1:F:209:CYS:HB2	1:F:237:TYR:CE2	2.17	0.80
1:F:11:ARG:HD2	1:F:29:ILE:CB	2.11	0.80
1:F:139:LEU:HD23	1:F:143:GLN:HG3	1.63	0.80
1:F:335:LEU:HD21	1:F:381:GLU:HG2	1.64	0.80
1:F:223:LEU:CD2	1:F:227:LYS:HB3	2.12	0.80
1:F:163:LEU:HD21	1:F:435:PHE:HE2	1.44	0.79
1:F:81:PHE:CE1	1:F:100:LYS:HA	2.16	0.79
1:F:213:TYR:HE1	1:F:215:LYS:HG3	1.45	0.79
1:F:11:ARG:HB3	1:F:29:ILE:O	1.82	0.79
1:F:40:ILE:HD11	1:F:43:ARG:NE	1.96	0.79
1:F:101:ARG:HD2	1:F:153:PHE:CZ	2.18	0.79
1:F:226:ILE:CG2	1:F:235:LEU:HD21	2.12	0.79
1:F:285:ASN:HD21	1:F:315:SER:HB2	1.48	0.79
1:F:253:ARG:HH12	1:F:500:LEU:HB3	1.45	0.79
1:F:285:ASN:ND2	1:F:315:SER:HB2	1.96	0.79
1:F:31:ARG:HB2	1:F:123:ILE:HD11	1.64	0.79
1:F:122:TYR:CD2	1:F:124:PRO:HD2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:TYR:CD2	1:F:239:ILE:CG1	2.64	0.78
1:F:95:ILE:CG2	1:F:121:ILE:HB	2.13	0.78
1:F:99:THR:HG22	1:F:117:ASP:O	1.84	0.78
1:F:422:ASN:O	1:F:426:GLU:HG2	1.83	0.78
1:F:261:ALA:HB2	1:F:525:HIS:CE1	2.18	0.78
1:F:529:LEU:O	1:F:529:LEU:HD23	1.83	0.78
1:F:96:VAL:HG21	1:F:222:LEU:HD13	1.66	0.78
1:F:213:TYR:CE2	1:F:355:ARG:NE	2.50	0.77
1:F:27:LEU:HD23	1:F:234:TRP:CE2	2.19	0.77
1:F:133:PRO:O	1:F:137:ARG:HG3	1.85	0.77
1:F:360:ILE:HD12	1:F:469:ILE:HD11	1.65	0.77
1:F:408:LYS:HB2	1:F:409:TYR:HA	1.66	0.76
1:F:105:ALA:HB3	1:F:112:ILE:CD1	2.15	0.76
1:F:124:PRO:HB3	1:F:127:SER:HB3	1.67	0.76
1:F:255:VAL:CG1	1:F:293:LEU:HD11	2.15	0.76
1:F:360:ILE:HG23	1:F:469:ILE:HD11	1.67	0.76
1:F:496:GLN:O	1:F:500:LEU:HD13	1.86	0.76
1:F:35:LYS:HB2	1:F:93:TYR:HD1	1.48	0.76
1:F:131:THR:HA	1:F:135:GLU:OE2	1.86	0.76
1:F:350:ASP:HA	1:F:353:PHE:CD2	2.20	0.76
1:F:4:VAL:C	1:F:5:LEU:HD23	2.11	0.75
1:F:8:THR:HG23	1:F:10:ALA:N	2.00	0.75
1:F:90:LEU:HD13	1:F:132:HIS:NE2	2.02	0.75
1:F:163:LEU:HD23	1:F:435:PHE:HD2	1.45	0.75
1:F:213:TYR:HE2	1:F:355:ARG:HE	1.33	0.75
1:F:82:GLY:HA3	1:F:98:ILE:HD11	1.68	0.75
1:F:498:TYR:CE2	1:F:505:LYS:HA	2.21	0.75
1:F:5:LEU:CD2	1:F:14:LEU:HG	2.16	0.75
1:F:11:ARG:HG2	1:F:123:ILE:CB	2.15	0.75
1:F:316:VAL:HG13	1:F:382:LEU:HD13	1.69	0.75
1:F:26:VAL:HB	1:F:40:ILE:HG23	1.69	0.75
1:F:87:VAL:CG1	1:F:222:LEU:HD22	2.16	0.75
1:F:107:ILE:CG1	1:F:306:TYR:CZ	2.70	0.74
1:F:250:ILE:CG2	1:F:502:LEU:HD11	2.16	0.74
1:F:438:ARG:HB3	1:F:461:PRO:HD2	1.69	0.74
1:F:14:LEU:HD21	1:F:95:ILE:HD11	1.68	0.74
1:F:37:LEU:HB3	1:F:225:ILE:HG21	1.67	0.74
1:F:32:THR:HG23	1:F:34:PRO:CD	2.18	0.74
1:F:245:GLN:HG2	1:F:258:THR:CG2	2.16	0.74
1:F:208:ILE:HG13	1:F:209:CYS:H	1.50	0.74
1:F:377:ILE:O	1:F:381:GLU:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ILE:CG2	1:F:502:LEU:HD21	2.18	0.74
1:F:393:LEU:CG	1:F:394:PRO:HD3	2.16	0.74
1:F:261:ALA:HB2	1:F:525:HIS:HE1	1.51	0.74
1:F:258:THR:HB	1:F:292:ILE:HG12	1.68	0.73
1:F:295:ASP:HB2	1:F:500:LEU:HD23	1.70	0.73
1:F:361:ILE:HG12	1:F:470:LEU:CD2	2.18	0.73
1:F:418:LEU:HD11	1:F:483:THR:CG2	2.18	0.73
1:F:122:TYR:CE2	1:F:124:PRO:HG2	2.24	0.73
1:F:361:ILE:HD13	1:F:361:ILE:H	1.53	0.73
1:F:362:ILE:HD13	1:F:363:LEU:N	2.02	0.73
1:F:512:THR:O	1:F:515:VAL:HG12	1.89	0.73
1:F:253:ARG:HD2	1:F:502:LEU:CD1	2.18	0.73
1:F:258:THR:HB	1:F:292:ILE:HG13	1.68	0.73
1:F:139:LEU:CD2	1:F:143:GLN:HG3	2.19	0.72
1:F:143:GLN:HA	1:F:146:ASP:OD2	1.89	0.72
1:F:231:HIS:HB3	1:F:234:TRP:CE3	2.23	0.72
1:F:349:PHE:HB3	1:F:391:GLN:HE22	1.54	0.72
1:F:361:ILE:HD13	1:F:469:ILE:O	1.89	0.72
1:F:29:ILE:HD11	1:F:86:PHE:CZ	2.24	0.72
1:F:259:LEU:HB3	1:F:521:LEU:CD1	2.19	0.72
1:F:404:TRP:HE1	1:F:417:VAL:HG22	1.54	0.72
1:F:95:ILE:CG2	1:F:97:LEU:HD11	2.19	0.72
1:F:502:LEU:HD23	1:F:502:LEU:O	1.89	0.72
1:F:95:ILE:HG23	1:F:97:LEU:HD11	1.70	0.72
1:F:356:PHE:HB2	1:F:360:ILE:HD11	1.71	0.72
1:F:358:SER:O	1:F:468:GLY:HA2	1.89	0.72
1:F:31:ARG:HB2	1:F:123:ILE:CD1	2.20	0.72
1:F:213:TYR:HE2	1:F:355:ARG:CZ	2.00	0.71
1:F:27:LEU:HD23	1:F:234:TRP:NE1	2.05	0.71
1:F:248:LEU:HD12	1:F:255:VAL:HB	1.71	0.71
1:F:5:LEU:HD22	1:F:14:LEU:CG	2.15	0.71
1:F:105:ALA:HB3	1:F:112:ILE:CG1	2.21	0.71
1:F:11:ARG:CD	1:F:29:ILE:HB	2.18	0.71
1:F:95:ILE:HG23	1:F:97:LEU:CD1	2.21	0.71
1:F:101:ARG:HH12	1:F:153:PHE:H	1.39	0.71
1:F:6:TYR:CZ	1:F:8:THR:HB	2.26	0.70
1:F:406:MET:HG2	1:F:414:LEU:HD12	1.73	0.70
1:F:13:PHE:CE2	1:F:28:LYS:HD3	2.26	0.70
1:F:142:PHE:O	1:F:145:VAL:HG22	1.90	0.70
1:F:336:ASP:HB2	1:F:338:ALA:O	1.90	0.70
1:F:356:PHE:HD1	1:F:469:ILE:HG21	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:460:ILE:HG23	1:F:461:PRO:HD2	1.71	0.70
1:F:270:THR:CG2	1:F:271:ARG:HD3	2.22	0.70
1:F:356:PHE:CG	1:F:469:ILE:HG12	2.27	0.70
1:F:531:LEU:HD13	1:F:531:LEU:O	1.91	0.70
1:F:90:LEU:HD12	1:F:135:GLU:CB	2.20	0.70
1:F:11:ARG:CB	1:F:123:ILE:HD13	2.22	0.70
1:F:404:TRP:NE1	1:F:417:VAL:HG22	2.06	0.69
1:F:418:LEU:HD11	1:F:483:THR:HG22	1.73	0.69
1:F:223:LEU:CG	1:F:235:LEU:HD22	2.22	0.69
1:F:391:GLN:HE22	1:F:399:ILE:HD12	1.56	0.69
1:F:14:LEU:HD21	1:F:95:ILE:CD1	2.22	0.69
1:F:316:VAL:CG1	1:F:382:LEU:HD13	2.21	0.69
1:F:421:LEU:HD22	1:F:424:ILE:HD11	1.73	0.69
1:F:363:LEU:CG	1:F:470:LEU:HD21	2.22	0.69
1:F:6:TYR:CD2	1:F:75:PHE:HB2	2.27	0.69
1:F:101:ARG:HH22	1:F:152:TYR:CA	2.05	0.69
1:F:213:TYR:HE1	1:F:215:LYS:CG	2.05	0.69
1:F:139:LEU:HD23	1:F:139:LEU:O	1.93	0.69
1:F:169:VAL:HG13	1:F:211:GLU:OE2	1.93	0.69
1:F:223:LEU:HG	1:F:235:LEU:CD2	2.21	0.69
1:F:366:VAL:CG1	1:F:368:GLU:HG2	2.23	0.69
1:F:10:ALA:O	1:F:11:ARG:HB2	1.92	0.69
1:F:115:VAL:HG23	1:F:238:ILE:HD12	1.73	0.69
1:F:363:LEU:HD12	1:F:470:LEU:HD11	1.74	0.69
1:F:469:ILE:O	1:F:469:ILE:HD12	1.92	0.69
1:F:503:ILE:HG22	1:F:504:ASP:O	1.93	0.69
1:F:223:LEU:O	1:F:223:LEU:HD23	1.93	0.69
1:F:383:VAL:O	1:F:387:THR:HG23	1.93	0.68
1:F:404:TRP:HZ2	1:F:417:VAL:C	2.02	0.68
1:F:11:ARG:CG	1:F:123:ILE:HD13	2.23	0.68
1:F:217:VAL:HG13	1:F:237:TYR:CD1	2.29	0.68
1:F:294:CYS:HB2	1:F:306:TYR:HE1	1.58	0.68
1:F:266:LYS:HD2	1:F:284:ALA:HB1	1.76	0.68
1:F:11:ARG:CD	1:F:12:TYR:HD1	2.04	0.68
1:F:223:LEU:CD1	1:F:235:LEU:HD22	2.24	0.68
1:F:404:TRP:CE2	1:F:421:LEU:HB2	2.29	0.68
1:F:95:ILE:HG22	1:F:121:ILE:HB	1.74	0.68
1:F:99:THR:CG2	1:F:117:ASP:HB2	2.24	0.68
1:F:312:VAL:HG11	1:F:356:PHE:CZ	2.29	0.68
1:F:9:ARG:O	1:F:31:ARG:HD3	1.94	0.67
1:F:37:LEU:HD23	1:F:225:ILE:CG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:PRO:HG2	1:F:237:TYR:CD2	2.25	0.67
1:F:418:LEU:C	1:F:487:MET:HE1	2.19	0.67
1:F:101:ARG:NH1	1:F:113:TYR:HB2	2.08	0.67
1:F:226:ILE:HG23	1:F:235:LEU:HD21	1.76	0.67
1:F:371:LYS:HG3	1:F:372:ARG:N	2.10	0.67
1:F:270:THR:HG23	1:F:271:ARG:HD3	1.75	0.67
1:F:11:ARG:HG2	1:F:123:ILE:CD1	2.23	0.67
1:F:401:TYR:CD2	1:F:403:PRO:HD3	2.29	0.67
1:F:96:VAL:C	1:F:97:LEU:HD12	2.20	0.67
1:F:245:GLN:HG2	1:F:258:THR:OG1	1.95	0.67
1:F:3:LEU:CD2	1:F:5:LEU:HD21	2.25	0.67
1:F:484:ALA:O	1:F:488:VAL:HG23	1.95	0.67
1:F:223:LEU:HD13	1:F:237:TYR:HE1	1.60	0.66
1:F:262:ARG:O	1:F:287:VAL:HG13	1.95	0.66
1:F:16:GLY:H	1:F:24:TYR:HE2	1.43	0.66
1:F:82:GLY:O	1:F:98:ILE:HD13	1.95	0.66
1:F:101:ARG:HH11	1:F:113:TYR:HB2	1.61	0.66
1:F:402:ILE:HG21	1:F:424:ILE:HD11	1.77	0.66
1:F:460:ILE:HG23	1:F:461:PRO:CD	2.25	0.66
1:F:332:PRO:O	1:F:333:ILE:HG22	1.96	0.66
1:F:209:CYS:O	1:F:212:PRO:HD2	1.96	0.66
1:F:383:VAL:O	1:F:386:VAL:HG12	1.96	0.65
1:F:101:ARG:NH2	1:F:115:VAL:HG23	2.11	0.65
1:F:418:LEU:CD1	1:F:483:THR:HG22	2.26	0.65
1:F:92:GLY:HA3	1:F:122:TYR:OH	1.96	0.65
1:F:306:TYR:HB3	1:F:437:ASN:HD21	1.61	0.65
1:F:278:ASN:O	1:F:344:VAL:HG23	1.96	0.65
1:F:370:GLU:C	1:F:373:LYS:H	2.04	0.65
1:F:215:LYS:HD3	1:F:351:GLN:HE22	1.62	0.65
1:F:226:ILE:HD13	1:F:235:LEU:HD23	1.77	0.65
1:F:266:LYS:HA	1:F:267:PHE:CD2	2.32	0.65
1:F:328:MET:HB3	1:F:329:PRO:HD2	1.78	0.65
1:F:360:ILE:HG23	1:F:469:ILE:CD1	2.27	0.65
1:F:431:LYS:HD3	1:F:495:TYR:CE1	2.32	0.65
1:F:498:TYR:HE2	1:F:505:LYS:HA	1.60	0.65
1:F:6:TYR:HE2	1:F:75:PHE:HB2	1.59	0.65
1:F:22:THR:HG23	1:F:23:LYS:CD	2.27	0.65
1:F:312:VAL:HG23	1:F:471:ARG:HG3	1.76	0.65
1:F:460:ILE:CG1	1:F:461:PRO:HD3	2.25	0.65
1:F:95:ILE:HG12	1:F:97:LEU:HD11	1.77	0.65
1:F:318:LEU:HD22	1:F:381:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:LEU:HA	1:F:381:GLU:CD	2.22	0.64
1:F:22:THR:HG23	1:F:23:LYS:HG2	1.80	0.64
1:F:25:ARG:NH2	1:F:41:ASP:HA	2.12	0.64
1:F:95:ILE:HG12	1:F:97:LEU:CD1	2.27	0.64
1:F:245:GLN:CG	1:F:258:THR:HG23	2.27	0.64
1:F:285:ASN:CG	1:F:315:SER:HB2	2.23	0.64
1:F:332:PRO:O	1:F:377:ILE:HD11	1.97	0.64
1:F:380:GLU:O	1:F:383:VAL:HG12	1.97	0.64
1:F:255:VAL:HG13	1:F:293:LEU:HD11	1.78	0.63
1:F:404:TRP:HZ2	1:F:417:VAL:HG13	1.61	0.63
1:F:266:LYS:HG2	1:F:267:PHE:H	1.62	0.63
1:F:101:ARG:HE	1:F:115:VAL:HG22	1.63	0.63
1:F:7:GLU:HB2	1:F:12:TYR:CE2	2.34	0.63
1:F:6:TYR:HE2	1:F:74:LEU:O	1.82	0.63
1:F:82:GLY:CA	1:F:98:ILE:HD11	2.29	0.63
1:F:360:ILE:HD12	1:F:469:ILE:CD1	2.29	0.63
1:F:11:ARG:HD3	1:F:12:TYR:N	2.13	0.63
1:F:410:THR:HA	1:F:414:LEU:HB2	1.80	0.63
1:F:213:TYR:HD1	1:F:215:LYS:H	1.47	0.63
1:F:224:ASP:HA	1:F:227:LYS:CE	2.29	0.62
1:F:293:LEU:HD21	1:F:295:ASP:OD2	1.99	0.62
1:F:213:TYR:CZ	1:F:215:LYS:HE2	2.34	0.62
1:F:296:ALA:HB1	1:F:302:THR:OG1	2.00	0.62
1:F:493:LEU:O	1:F:497:LEU:HD23	1.99	0.62
1:F:361:ILE:HG22	1:F:400:VAL:HB	1.80	0.62
1:F:406:MET:SD	1:F:418:LEU:HD21	2.38	0.62
1:F:493:LEU:HA	1:F:496:GLN:HG2	1.81	0.62
1:F:11:ARG:HB2	1:F:31:ARG:N	2.15	0.62
1:F:404:TRP:CH2	1:F:418:LEU:HA	2.35	0.62
1:F:31:ARG:HG3	1:F:123:ILE:CG1	2.30	0.62
1:F:32:THR:HG23	1:F:34:PRO:HD2	1.81	0.62
1:F:161:HIS:HE1	1:F:355:ARG:NH2	1.98	0.62
1:F:350:ASP:HA	1:F:353:PHE:CE2	2.34	0.62
1:F:13:PHE:C	1:F:14:LEU:HD12	2.25	0.62
1:F:209:CYS:O	1:F:237:TYR:HE2	1.82	0.62
1:F:5:LEU:CD1	1:F:97:LEU:HD21	2.30	0.61
1:F:29:ILE:HD11	1:F:86:PHE:CE1	2.35	0.61
1:F:104:MET:SD	1:F:152:TYR:HE1	2.23	0.61
1:F:360:ILE:CD1	1:F:469:ILE:HG13	2.30	0.61
1:F:132:HIS:CE1	1:F:134:ASP:HB3	2.35	0.61
1:F:349:PHE:CB	1:F:391:GLN:HE22	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:TYR:HA	1:F:498:TYR:HD1	1.64	0.61
1:F:6:TYR:HD1	1:F:13:PHE:HD1	1.48	0.61
1:F:7:GLU:HG3	1:F:12:TYR:CZ	2.34	0.61
1:F:226:ILE:O	1:F:229:THR:HG22	2.00	0.61
1:F:438:ARG:HB3	1:F:461:PRO:CD	2.30	0.61
1:F:11:ARG:CD	1:F:12:TYR:H	2.14	0.61
1:F:28:LYS:HB3	1:F:38:VAL:HG22	1.82	0.61
1:F:253:ARG:HH21	1:F:298:VAL:HG22	1.64	0.61
1:F:438:ARG:HB3	1:F:461:PRO:CG	2.30	0.61
1:F:437:ASN:OD1	1:F:439:PRO:HD3	2.01	0.61
1:F:14:LEU:HD12	1:F:14:LEU:N	2.15	0.61
1:F:406:MET:CE	1:F:480:ARG:HB3	2.30	0.61
1:F:505:LYS:HB2	1:F:506:PRO:HD3	1.83	0.61
1:F:6:TYR:HD1	1:F:13:PHE:CD1	2.18	0.61
1:F:250:ILE:HG23	1:F:502:LEU:HD11	1.83	0.61
1:F:404:TRP:CD2	1:F:421:LEU:HD23	2.36	0.61
1:F:40:ILE:CD1	1:F:43:ARG:HE	2.06	0.60
1:F:88:ARG:HB3	1:F:93:TYR:CE2	2.36	0.60
1:F:208:ILE:HG13	1:F:209:CYS:N	2.15	0.60
1:F:11:ARG:CZ	1:F:29:ILE:HG21	2.32	0.60
1:F:39:ILE:HG12	1:F:231:HIS:NE2	2.16	0.60
1:F:35:LYS:HE2	1:F:122:TYR:OH	2.01	0.60
1:F:255:VAL:HG22	1:F:295:ASP:OD1	2.01	0.60
1:F:31:ARG:CB	1:F:123:ILE:HG12	2.30	0.60
1:F:84:VAL:HG22	1:F:96:VAL:O	2.02	0.60
1:F:226:ILE:HD11	1:F:234:TRP:CB	2.29	0.60
1:F:255:VAL:HG13	1:F:295:ASP:OD1	2.01	0.60
1:F:11:ARG:HD3	1:F:12:TYR:H	1.64	0.60
1:F:208:ILE:HG23	1:F:209:CYS:N	2.16	0.60
1:F:406:MET:CE	1:F:414:LEU:HD11	2.29	0.60
1:F:215:LYS:HA	1:F:267:PHE:CZ	2.36	0.60
1:F:248:LEU:HD12	1:F:248:LEU:C	2.27	0.60
1:F:253:ARG:NH2	1:F:298:VAL:HG22	2.16	0.60
1:F:406:MET:HE2	1:F:480:ARG:HE	1.65	0.60
1:F:250:ILE:HG23	1:F:502:LEU:CD2	2.27	0.59
1:F:99:THR:HG22	1:F:117:ASP:C	2.27	0.59
1:F:270:THR:HG23	1:F:271:ARG:CD	2.32	0.59
1:F:128:VAL:HG23	1:F:129:ARG:N	2.18	0.59
1:F:366:VAL:HG12	1:F:368:GLU:HG2	1.84	0.59
1:F:400:VAL:HG21	1:F:428:VAL:HG11	1.83	0.59
1:F:324:ILE:HG23	1:F:324:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:GLN:OE1	1:F:466:GLN:N	2.35	0.59
1:F:253:ARG:NH2	1:F:298:VAL:H	2.01	0.59
1:F:11:ARG:HE	1:F:123:ILE:HB	1.67	0.59
1:F:25:ARG:HB2	1:F:234:TRP:CH2	2.36	0.59
1:F:250:ILE:CG1	1:F:503:ILE:HD11	2.33	0.59
1:F:349:PHE:CD1	1:F:399:ILE:HD13	2.37	0.59
1:F:6:TYR:CE1	1:F:8:THR:HB	2.38	0.59
1:F:30:ASP:O	1:F:35:LYS:HA	2.03	0.59
1:F:101:ARG:NH2	1:F:152:TYR:HA	2.12	0.58
1:F:167:LEU:HD13	1:F:167:LEU:C	2.28	0.58
1:F:26:VAL:HB	1:F:40:ILE:HG22	1.81	0.58
1:F:81:PHE:HD1	1:F:99:THR:O	1.86	0.58
1:F:298:VAL:HG23	1:F:299:MET:N	2.18	0.58
1:F:402:ILE:HG21	1:F:424:ILE:CD1	2.33	0.58
1:F:98:ILE:HG12	1:F:98:ILE:O	2.03	0.58
1:F:421:LEU:HD13	1:F:421:LEU:O	2.04	0.58
1:F:212:PRO:CG	1:F:237:TYR:HD2	2.14	0.58
1:F:98:ILE:HG22	1:F:115:VAL:HG11	1.85	0.58
1:F:274:LYS:HD3	1:F:274:LYS:C	2.28	0.58
1:F:438:ARG:O	1:F:461:PRO:HD2	2.03	0.58
1:F:33:GLU:HB2	1:F:34:PRO:CD	2.34	0.58
1:F:344:VAL:HG13	1:F:345:ALA:N	2.18	0.58
1:F:495:TYR:HA	1:F:498:TYR:CD1	2.39	0.58
1:F:99:THR:HG23	1:F:100:LYS:N	2.18	0.57
1:F:362:ILE:HG22	1:F:401:TYR:HA	1.85	0.57
1:F:370:GLU:HA	1:F:373:LYS:HA	1.86	0.57
1:F:486:PHE:HD1	1:F:522:TYR:CG	2.22	0.57
1:F:340:PRO:O	1:F:344:VAL:HG12	2.04	0.57
1:F:521:LEU:HD13	1:F:521:LEU:O	2.03	0.57
1:F:434:PHE:HE1	1:F:436:VAL:HG11	1.69	0.57
1:F:31:ARG:O	1:F:31:ARG:HG2	2.05	0.57
1:F:11:ARG:HB2	1:F:31:ARG:H	1.69	0.57
1:F:266:LYS:HG3	1:F:284:ALA:CB	2.34	0.57
1:F:406:MET:HE1	1:F:480:ARG:HB3	1.85	0.57
1:F:438:ARG:HB3	1:F:461:PRO:HG2	1.87	0.57
1:F:469:ILE:HD12	1:F:469:ILE:C	2.29	0.57
1:F:229:THR:HG23	1:F:230:VAL:N	2.20	0.57
1:F:31:ARG:HG3	1:F:123:ILE:HG13	1.87	0.57
1:F:39:ILE:HD11	1:F:229:THR:OG1	2.05	0.57
1:F:304:GLY:O	1:F:439:PRO:HD2	2.05	0.57
1:F:94:TYR:CE2	1:F:122:TYR:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:529:LEU:HD23	1:F:529:LEU:C	2.30	0.57
1:F:7:GLU:HG3	1:F:12:TYR:CE2	2.40	0.57
1:F:97:LEU:HD12	1:F:97:LEU:N	2.20	0.57
1:F:245:GLN:HG2	1:F:258:THR:CB	2.35	0.57
1:F:406:MET:HE2	1:F:480:ARG:NE	2.20	0.57
1:F:515:VAL:O	1:F:519:GLU:HG3	2.05	0.57
1:F:493:LEU:HG	1:F:497:LEU:HD23	1.85	0.56
1:F:502:LEU:HD23	1:F:502:LEU:C	2.29	0.56
1:F:3:LEU:HD21	1:F:14:LEU:CB	2.19	0.56
1:F:167:LEU:HD13	1:F:167:LEU:O	2.05	0.56
1:F:106:ASP:OD1	1:F:111:ALA:HA	2.06	0.56
1:F:248:LEU:HD11	1:F:255:VAL:HB	1.86	0.56
1:F:372:ARG:O	1:F:373:LYS:HG2	2.04	0.56
1:F:406:MET:HE1	1:F:480:ARG:CB	2.35	0.56
1:F:459:VAL:HG13	1:F:459:VAL:O	2.05	0.56
1:F:29:ILE:HG13	1:F:86:PHE:CE1	2.41	0.56
1:F:213:TYR:O	1:F:217:VAL:HG23	2.06	0.56
1:F:226:ILE:HD13	1:F:235:LEU:CD2	2.36	0.56
1:F:280:GLU:C	1:F:347:LEU:HD23	2.30	0.56
1:F:25:ARG:HG3	1:F:231:HIS:HD1	1.71	0.56
1:F:383:VAL:HG13	1:F:384:ALA:N	2.21	0.56
1:F:3:LEU:CD2	1:F:14:LEU:HD23	2.36	0.56
1:F:95:ILE:CG1	1:F:97:LEU:HD11	2.36	0.56
1:F:258:THR:HG22	1:F:259:LEU:N	2.21	0.56
1:F:266:LYS:HZ1	1:F:273:LEU:C	2.14	0.56
1:F:226:ILE:CG1	1:F:235:LEU:HD21	2.37	0.55
1:F:255:VAL:HA	1:F:295:ASP:OD1	2.06	0.55
1:F:406:MET:HG3	1:F:417:VAL:CG1	2.36	0.55
1:F:6:TYR:OH	1:F:8:THR:HB	2.06	0.55
1:F:22:THR:HG23	1:F:23:LYS:CG	2.35	0.55
1:F:149:SER:HB2	1:F:151:PHE:CZ	2.41	0.55
1:F:404:TRP:CZ2	1:F:418:LEU:HA	2.41	0.55
1:F:89:PHE:CE1	1:F:138:TYR:CD1	2.94	0.55
1:F:89:PHE:CD2	1:F:94:TYR:CD1	2.94	0.55
1:F:89:PHE:CD1	1:F:138:TYR:CD1	2.95	0.55
1:F:94:TYR:CE2	1:F:122:TYR:CG	2.95	0.55
1:F:89:PHE:CE1	1:F:138:TYR:CE1	2.95	0.55
1:F:303:ALA:HB1	1:F:438:ARG:HD3	1.89	0.55
1:F:25:ARG:HG3	1:F:231:HIS:ND1	2.22	0.55
1:F:270:THR:HG23	1:F:271:ARG:N	2.22	0.55
1:F:285:ASN:OD1	1:F:315:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:PHE:CE1	1:F:518:PHE:CD2	2.95	0.55
1:F:291:GLN:NE2	1:F:518:PHE:HE1	2.06	0.54
1:F:518:PHE:CZ	1:F:522:TYR:CE1	2.95	0.54
1:F:83:VAL:O	1:F:83:VAL:HG13	2.06	0.54
1:F:373:LYS:O	1:F:373:LYS:HG3	2.06	0.54
1:F:167:LEU:HD21	1:F:462:THR:HG21	1.90	0.54
1:F:421:LEU:HD13	1:F:421:LEU:C	2.31	0.54
1:F:421:LEU:O	1:F:424:ILE:HG12	2.08	0.54
1:F:6:TYR:CD1	1:F:13:PHE:CD1	2.95	0.54
1:F:28:LYS:HE3	1:F:30:ASP:OD2	2.07	0.54
1:F:292:ILE:HD12	1:F:306:TYR:OH	2.08	0.54
1:F:494:ALA:HA	1:F:508:LEU:HD23	1.90	0.54
1:F:25:ARG:HH22	1:F:41:ASP:HA	1.71	0.54
1:F:226:ILE:HG12	1:F:235:LEU:HD21	1.90	0.54
1:F:248:LEU:O	1:F:249:LEU:HD23	2.08	0.54
1:F:350:ASP:HA	1:F:353:PHE:HD2	1.72	0.54
1:F:98:ILE:HD13	1:F:98:ILE:H	1.72	0.54
1:F:529:LEU:C	1:F:531:LEU:H	2.16	0.54
1:F:33:GLU:HB2	1:F:34:PRO:HD3	1.89	0.54
1:F:250:ILE:HG22	1:F:255:VAL:HG21	1.89	0.54
1:F:313:ARG:HD3	1:F:481:THR:HG21	1.88	0.54
1:F:365:LEU:CD2	1:F:404:TRP:HE3	2.21	0.54
1:F:507:ASN:HB2	1:F:510:PHE:CD1	2.41	0.54
1:F:114:LYS:HE2	1:F:150:ASN:HB3	1.90	0.54
1:F:158:ASP:OD2	1:F:212:PRO:HG3	2.08	0.54
1:F:324:ILE:C	1:F:324:ILE:HD13	2.33	0.54
1:F:11:ARG:HG2	1:F:123:ILE:CG1	2.38	0.53
1:F:101:ARG:HD2	1:F:153:PHE:CE2	2.44	0.53
1:F:151:PHE:HA	1:F:239:ILE:O	2.07	0.53
1:F:105:ALA:CB	1:F:112:ILE:HG12	2.37	0.53
1:F:40:ILE:HD11	1:F:43:ARG:CG	2.38	0.53
1:F:107:ILE:HG23	1:F:107:ILE:O	2.08	0.53
1:F:266:LYS:HG3	1:F:284:ALA:HB1	1.89	0.53
1:F:101:ARG:HH12	1:F:153:PHE:N	2.05	0.53
1:F:292:ILE:HB	1:F:306:TYR:CE2	2.43	0.53
1:F:370:GLU:O	1:F:370:GLU:HG2	2.09	0.53
1:F:328:MET:HB3	1:F:329:PRO:CD	2.38	0.53
1:F:21:GLU:HG3	1:F:22:THR:N	2.24	0.53
1:F:101:ARG:NE	1:F:115:VAL:HG22	2.23	0.53
1:F:255:VAL:HG12	1:F:256:TYR:N	2.23	0.53
1:F:470:LEU:HD13	1:F:471:ARG:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:502:LEU:HD22	1:F:503:ILE:HG12	1.91	0.53
1:F:503:ILE:HG22	1:F:504:ASP:N	2.23	0.53
1:F:5:LEU:HD11	1:F:97:LEU:HD21	1.90	0.53
1:F:28:LYS:HE3	1:F:30:ASP:OD1	2.09	0.53
1:F:424:ILE:HG13	1:F:425:ALA:N	2.24	0.53
1:F:431:LYS:HG2	1:F:491:CYS:SG	2.49	0.53
1:F:28:LYS:HE3	1:F:30:ASP:CG	2.34	0.53
1:F:360:ILE:HD12	1:F:469:ILE:CG1	2.39	0.53
1:F:85:GLY:O	1:F:96:VAL:HG22	2.09	0.52
1:F:101:ARG:HE	1:F:115:VAL:CG2	2.21	0.52
1:F:124:PRO:CB	1:F:127:SER:HB3	2.35	0.52
1:F:362:ILE:CG2	1:F:401:TYR:HD1	2.23	0.52
1:F:15:VAL:HG11	1:F:26:VAL:HG22	1.90	0.52
1:F:29:ILE:CD1	1:F:37:LEU:HD13	2.39	0.52
1:F:266:LYS:CG	1:F:284:ALA:HB1	2.38	0.52
1:F:414:LEU:HD13	1:F:480:ARG:HH21	1.74	0.52
1:F:32:THR:CG2	1:F:34:PRO:HG2	2.39	0.52
1:F:266:LYS:CD	1:F:284:ALA:HB1	2.38	0.52
1:F:302:THR:O	1:F:302:THR:HG23	2.10	0.52
1:F:362:ILE:HG21	1:F:401:TYR:HD1	1.75	0.52
1:F:408:LYS:HB2	1:F:409:TYR:CA	2.37	0.52
1:F:470:LEU:HD13	1:F:470:LEU:C	2.34	0.52
1:F:28:LYS:HE2	1:F:38:VAL:HG21	1.92	0.52
1:F:87:VAL:HG13	1:F:222:LEU:HD22	1.91	0.52
1:F:152:TYR:N	1:F:238:ILE:CA	2.73	0.52
1:F:250:ILE:HG13	1:F:503:ILE:HD11	1.92	0.52
1:F:152:TYR:N	1:F:238:ILE:HA	2.25	0.52
1:F:333:ILE:HG21	1:F:381:GLU:CD	2.34	0.52
1:F:418:LEU:HD11	1:F:483:THR:HG21	1.90	0.52
1:F:318:LEU:HD12	1:F:341:PHE:CE1	2.44	0.51
1:F:335:LEU:HD22	1:F:341:PHE:CE2	2.45	0.51
1:F:360:ILE:HD13	1:F:469:ILE:HG13	1.90	0.51
1:F:386:VAL:HG13	1:F:387:THR:N	2.24	0.51
1:F:98:ILE:HG21	1:F:115:VAL:HG21	1.93	0.51
1:F:115:VAL:HG21	1:F:238:ILE:HD12	1.91	0.51
1:F:123:ILE:HD12	1:F:123:ILE:O	2.10	0.51
1:F:223:LEU:HD23	1:F:223:LEU:C	2.35	0.51
1:F:369:ARG:H	1:F:369:ARG:HE	1.57	0.51
1:F:531:LEU:HD13	1:F:531:LEU:C	2.35	0.51
1:F:90:LEU:HD11	1:F:134:ASP:HB3	1.93	0.51
1:F:152:TYR:CB	1:F:239:ILE:HG12	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:LEU:HD12	1:F:15:VAL:C	2.35	0.51
1:F:112:ILE:HD12	1:F:243:CYS:SG	2.51	0.51
1:F:139:LEU:HD23	1:F:139:LEU:C	2.35	0.51
1:F:294:CYS:HB2	1:F:306:TYR:CD1	2.45	0.51
1:F:434:PHE:CD1	1:F:436:VAL:HG13	2.46	0.51
1:F:35:LYS:CE	1:F:92:GLY:HA2	2.41	0.51
1:F:92:GLY:HA3	1:F:122:TYR:CE1	2.46	0.51
1:F:149:SER:HB2	1:F:151:PHE:CE2	2.45	0.51
1:F:95:ILE:HG23	1:F:95:ILE:O	2.11	0.51
1:F:105:ALA:HB3	1:F:112:ILE:HD11	1.92	0.51
1:F:329:PRO:O	1:F:331:PRO:HD3	2.10	0.51
1:F:363:LEU:CD1	1:F:470:LEU:HD21	2.40	0.51
1:F:217:VAL:CG1	1:F:237:TYR:CD1	2.94	0.51
1:F:84:VAL:HG13	1:F:98:ILE:HD12	1.93	0.51
1:F:229:THR:HG21	1:F:231:HIS:HD2	1.75	0.51
1:F:103:LYS:CG	1:F:113:TYR:CE1	2.94	0.50
1:F:333:ILE:HG22	1:F:377:ILE:HG13	1.94	0.50
1:F:335:LEU:HD21	1:F:381:GLU:CG	2.39	0.50
1:F:6:TYR:CZ	1:F:72:SER:CB	2.94	0.50
1:F:507:ASN:HB3	1:F:509:GLN:HG2	1.92	0.50
1:F:7:GLU:CG	1:F:12:TYR:CE2	2.95	0.50
1:F:349:PHE:CD1	1:F:399:ILE:CD1	2.95	0.50
1:F:411:LYS:O	1:F:412:SER:HB2	2.11	0.50
1:F:504:ASP:HB2	1:F:506:PRO:HD2	1.94	0.50
1:F:434:PHE:CE1	1:F:436:VAL:CG1	2.94	0.50
1:F:362:ILE:HD13	1:F:362:ILE:C	2.36	0.50
1:F:28:LYS:HB3	1:F:38:VAL:HG23	1.89	0.50
1:F:208:ILE:CG1	1:F:209:CYS:H	2.20	0.50
1:F:362:ILE:CG2	1:F:401:TYR:CD1	2.95	0.50
1:F:367:LYS:O	1:F:367:LYS:HG3	2.11	0.50
1:F:12:TYR:CZ	1:F:121:ILE:CG2	2.94	0.50
1:F:13:PHE:HE2	1:F:28:LYS:HD3	1.77	0.50
1:F:29:ILE:CG1	1:F:86:PHE:CE1	2.95	0.50
1:F:89:PHE:HD2	1:F:94:TYR:CE1	2.30	0.50
1:F:120:MET:HE2	1:F:142:PHE:HD2	1.77	0.50
1:F:167:LEU:HG	1:F:465:LEU:HD21	1.94	0.50
1:F:215:LYS:HB3	1:F:267:PHE:HZ	1.77	0.50
1:F:7:GLU:HG2	1:F:8:THR:N	2.26	0.49
1:F:89:PHE:HD2	1:F:94:TYR:CD1	2.30	0.49
1:F:244:GLY:O	1:F:258:THR:HG23	2.12	0.49
1:F:353:PHE:O	1:F:357:GLY:HA2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ARG:HD2	1:F:29:ILE:C	2.37	0.49
1:F:107:ILE:HD11	1:F:294:CYS:HB2	1.93	0.49
1:F:335:LEU:HB3	1:F:341:PHE:CD2	2.47	0.49
1:F:358:SER:OG	1:F:359:PRO:HD2	2.13	0.49
1:F:493:LEU:HG	1:F:497:LEU:CD2	2.42	0.49
1:F:40:ILE:HG23	1:F:41:ASP:O	2.11	0.49
1:F:87:VAL:HG23	1:F:87:VAL:O	2.12	0.49
1:F:105:ALA:CB	1:F:112:ILE:HD11	2.42	0.49
1:F:358:SER:HB3	1:F:467:THR:HB	1.90	0.49
1:F:406:MET:HE3	1:F:414:LEU:HD21	1.94	0.49
1:F:6:TYR:CE2	1:F:72:SER:HB2	2.46	0.49
1:F:74:LEU:O	1:F:75:PHE:HD1	1.96	0.49
1:F:266:LYS:HG2	1:F:267:PHE:N	2.27	0.49
1:F:277:ALA:HB3	1:F:344:VAL:CG2	2.42	0.49
1:F:310:VAL:HG12	1:F:311:GLN:N	2.27	0.49
1:F:101:ARG:HB3	1:F:113:TYR:HB3	1.95	0.49
1:F:290:GLU:HG3	1:F:310:VAL:HG22	1.94	0.49
1:F:500:LEU:HD12	1:F:500:LEU:N	2.27	0.49
1:F:3:LEU:HD12	1:F:15:VAL:O	2.13	0.49
1:F:19:ASN:OD1	1:F:24:TYR:HB2	2.13	0.49
1:F:25:ARG:HG3	1:F:231:HIS:CE1	2.48	0.49
1:F:287:VAL:HG12	1:F:288:GLU:N	2.26	0.49
1:F:333:ILE:HG22	1:F:377:ILE:CG1	2.43	0.49
1:F:13:PHE:CE2	1:F:28:LYS:CD	2.94	0.49
1:F:377:ILE:HG23	1:F:378:LEU:N	2.26	0.49
1:F:408:LYS:H	1:F:408:LYS:HD2	1.78	0.49
1:F:419:ASP:O	1:F:423:VAL:HG23	2.11	0.49
1:F:275:ARG:NH1	1:F:378:LEU:HD22	2.26	0.49
1:F:365:LEU:CD2	1:F:404:TRP:CE3	2.96	0.49
1:F:404:TRP:CZ2	1:F:421:LEU:HB2	2.48	0.49
1:F:209:CYS:CB	1:F:237:TYR:CE2	2.94	0.48
1:F:295:ASP:CB	1:F:500:LEU:HD23	2.41	0.48
1:F:21:GLU:HG3	1:F:22:THR:H	1.78	0.48
1:F:224:ASP:OD1	1:F:227:LYS:HE3	2.13	0.48
1:F:283:VAL:O	1:F:284:ALA:HB3	2.13	0.48
1:F:120:MET:HE1	1:F:146:ASP:OD2	2.14	0.48
1:F:335:LEU:HD22	1:F:341:PHE:CD2	2.48	0.48
1:F:11:ARG:NE	1:F:123:ILE:HB	2.28	0.48
1:F:145:VAL:HG23	1:F:146:ASP:N	2.28	0.48
1:F:392:PHE:O	1:F:393:LEU:HB2	2.13	0.48
1:F:274:LYS:HE2	1:F:285:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:GLY:HA3	1:F:122:TYR:CZ	2.49	0.48
1:F:209:CYS:HB2	1:F:237:TYR:CZ	2.49	0.48
1:F:515:VAL:HG13	1:F:516:ARG:N	2.28	0.48
1:F:215:LYS:CA	1:F:267:PHE:CZ	2.97	0.48
1:F:285:ASN:HD21	1:F:315:SER:CB	2.23	0.48
1:F:152:TYR:H	1:F:238:ILE:CA	2.27	0.48
1:F:215:LYS:CB	1:F:267:PHE:HZ	2.27	0.48
1:F:259:LEU:HD12	1:F:290:GLU:O	2.14	0.48
1:F:256:TYR:O	1:F:293:LEU:HD12	2.14	0.47
1:F:88:ARG:O	1:F:88:ARG:HG3	2.13	0.47
1:F:165:TYR:CE1	1:F:355:ARG:HA	2.50	0.47
1:F:211:GLU:HA	1:F:211:GLU:OE1	2.13	0.47
1:F:229:THR:O	1:F:230:VAL:HB	2.14	0.47
1:F:29:ILE:CD1	1:F:86:PHE:CE1	2.97	0.47
1:F:29:ILE:HD13	1:F:37:LEU:CD1	2.44	0.47
1:F:22:THR:HG23	1:F:23:LYS:N	2.29	0.47
1:F:247:LYS:HG2	1:F:256:TYR:CE2	2.48	0.47
1:F:335:LEU:O	1:F:336:ASP:HB3	2.15	0.47
1:F:363:LEU:CD1	1:F:470:LEU:HD11	2.44	0.47
1:F:365:LEU:HD21	1:F:404:TRP:HE3	1.78	0.47
1:F:103:LYS:HG3	1:F:113:TYR:CE1	2.49	0.47
1:F:153:PHE:HA	1:F:159:LEU:HD12	1.97	0.47
1:F:162:SER:HG	1:F:165:TYR:HD2	1.61	0.47
1:F:408:LYS:CB	1:F:409:TYR:HA	2.39	0.47
1:F:460:ILE:CB	1:F:461:PRO:HD3	2.45	0.47
1:F:486:PHE:CE2	1:F:490:LYS:HD2	2.49	0.47
1:F:224:ASP:HA	1:F:227:LYS:HG2	1.97	0.47
1:F:404:TRP:HZ2	1:F:417:VAL:O	1.98	0.47
1:F:434:PHE:CE1	1:F:436:VAL:HG11	2.49	0.47
1:F:22:THR:HG23	1:F:23:LYS:HD3	1.96	0.47
1:F:32:THR:HG23	1:F:34:PRO:N	2.30	0.47
1:F:390:ASN:OD1	1:F:392:PHE:HE1	1.98	0.47
1:F:5:LEU:HD11	1:F:97:LEU:CD2	2.44	0.47
1:F:11:ARG:HD2	1:F:29:ILE:O	2.14	0.47
1:F:120:MET:HE2	1:F:142:PHE:CD2	2.50	0.47
1:F:508:LEU:HD12	1:F:509:GLN:H	1.74	0.47
1:F:40:ILE:HD11	1:F:43:ARG:HG3	1.96	0.46
1:F:112:ILE:O	1:F:112:ILE:HG13	2.15	0.46
1:F:363:LEU:HG	1:F:470:LEU:CD2	2.39	0.46
1:F:434:PHE:HD1	1:F:436:VAL:HG13	1.80	0.46
1:F:11:ARG:NH1	1:F:29:ILE:HB	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:VAL:CG2	1:F:96:VAL:HG23	2.31	0.46
1:F:152:TYR:H	1:F:238:ILE:C	2.21	0.46
1:F:152:TYR:CD2	1:F:239:ILE:HG12	2.48	0.46
1:F:161:HIS:CE1	1:F:213:TYR:HB2	2.50	0.46
1:F:215:LYS:HD3	1:F:351:GLN:NE2	2.30	0.46
1:F:368:GLU:O	1:F:368:GLU:HG3	2.14	0.46
1:F:28:LYS:O	1:F:38:VAL:HG22	2.16	0.46
1:F:163:LEU:CG	1:F:435:PHE:CE2	2.99	0.46
1:F:223:LEU:HG	1:F:226:ILE:HG23	1.96	0.46
1:F:103:LYS:HG2	1:F:113:TYR:CE1	2.49	0.46
1:F:6:TYR:HB2	1:F:44:HIS:NE2	2.31	0.46
1:F:353:PHE:CD1	1:F:353:PHE:C	2.94	0.46
1:F:362:ILE:HG23	1:F:362:ILE:O	2.14	0.46
1:F:518:PHE:CE2	1:F:522:TYR:CE1	3.04	0.46
1:F:107:ILE:CD1	1:F:306:TYR:OH	2.63	0.46
1:F:230:VAL:O	1:F:230:VAL:HG12	2.15	0.46
1:F:356:PHE:HB2	1:F:360:ILE:CD1	2.43	0.46
1:F:165:TYR:HE1	1:F:355:ARG:HA	1.81	0.46
1:F:171:ARG:O	1:F:171:ARG:HG2	2.15	0.46
1:F:335:LEU:HB3	1:F:341:PHE:HD2	1.81	0.46
1:F:226:ILE:CD1	1:F:234:TRP:CB	2.93	0.46
1:F:326:THR:HG23	1:F:327:MET:N	2.31	0.46
1:F:29:ILE:HD11	1:F:37:LEU:HD13	1.98	0.46
1:F:223:LEU:O	1:F:226:ILE:HG23	2.16	0.46
1:F:31:ARG:CB	1:F:123:ILE:CG1	2.93	0.45
1:F:87:VAL:CG2	1:F:89:PHE:CZ	2.93	0.45
1:F:213:TYR:CE1	1:F:215:LYS:CG	2.95	0.45
1:F:296:ALA:HB1	1:F:302:THR:HG1	1.79	0.45
1:F:337:GLN:HG3	1:F:338:ALA:N	2.31	0.45
1:F:524:ASP:O	1:F:528:THR:HG23	2.15	0.45
1:F:28:LYS:HG2	1:F:30:ASP:OD1	2.16	0.45
1:F:98:ILE:HB	1:F:115:VAL:HG13	1.97	0.45
1:F:352:MET:HE1	1:F:471:ARG:HD2	1.98	0.45
1:F:213:TYR:HD1	1:F:215:LYS:N	2.11	0.45
1:F:279:CYS:O	1:F:347:LEU:HD23	2.17	0.45
1:F:292:ILE:HB	1:F:306:TYR:HE2	1.82	0.45
1:F:341:PHE:CZ	1:F:385:ALA:CB	2.95	0.45
1:F:404:TRP:CB	1:F:421:LEU:HD23	2.47	0.45
1:F:333:ILE:CG2	1:F:377:ILE:HG13	2.46	0.45
1:F:27:LEU:CD2	1:F:234:TRP:CE2	2.94	0.45
1:F:90:LEU:HD12	1:F:135:GLU:CA	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:MET:SD	1:F:152:TYR:CE1	3.07	0.45
1:F:153:PHE:CD1	1:F:153:PHE:C	2.95	0.45
1:F:100:LYS:HG2	1:F:117:ASP:HB2	1.99	0.45
1:F:259:LEU:CB	1:F:521:LEU:CD1	2.93	0.45
1:F:6:TYR:CD2	1:F:72:SER:HB2	2.52	0.44
1:F:101:ARG:CD	1:F:153:PHE:CZ	2.94	0.44
1:F:229:THR:CG2	1:F:231:HIS:HD2	2.30	0.44
1:F:21:GLU:HA	1:F:21:GLU:OE1	2.18	0.44
1:F:250:ILE:HG12	1:F:503:ILE:HD11	1.99	0.44
1:F:369:ARG:O	1:F:370:GLU:HB3	2.18	0.44
1:F:32:THR:HG23	1:F:34:PRO:CG	2.47	0.44
1:F:332:PRO:C	1:F:377:ILE:HG12	2.42	0.44
1:F:6:TYR:CD1	1:F:6:TYR:C	2.95	0.44
1:F:107:ILE:HG12	1:F:306:TYR:OH	2.17	0.44
1:F:393:LEU:CB	1:F:394:PRO:HD3	2.48	0.44
1:F:418:LEU:HB3	1:F:487:MET:SD	2.57	0.44
1:F:253:ARG:HD3	1:F:296:ALA:O	2.18	0.44
1:F:318:LEU:CD1	1:F:341:PHE:CE1	3.01	0.44
1:F:360:ILE:CD1	1:F:469:ILE:CG1	2.95	0.44
1:F:136:ALA:O	1:F:140:ARG:HG2	2.17	0.44
1:F:4:VAL:CG1	1:F:15:VAL:CG2	2.96	0.44
1:F:208:ILE:O	1:F:212:PRO:HD3	2.18	0.44
1:F:223:LEU:HD12	1:F:235:LEU:HD22	1.99	0.44
1:F:331:PRO:HA	1:F:332:PRO:HD3	1.72	0.44
1:F:312:VAL:HG23	1:F:471:ARG:HA	2.00	0.44
1:F:408:LYS:CB	1:F:409:TYR:CA	2.96	0.44
1:F:101:ARG:NH1	1:F:153:PHE:CD2	2.86	0.43
1:F:159:LEU:O	1:F:262:ARG:HD3	2.17	0.43
1:F:161:HIS:CE1	1:F:213:TYR:HD2	2.36	0.43
1:F:404:TRP:CE2	1:F:417:VAL:HG22	2.53	0.43
1:F:5:LEU:CD1	1:F:97:LEU:CD2	2.95	0.43
1:F:521:LEU:HD13	1:F:521:LEU:C	2.42	0.43
1:F:151:PHE:H	1:F:238:ILE:HD11	1.51	0.43
1:F:231:HIS:HB3	1:F:234:TRP:CZ3	2.52	0.43
1:F:493:LEU:HD23	1:F:508:LEU:HD22	1.99	0.43
1:F:87:VAL:HG12	1:F:222:LEU:HD22	1.97	0.43
1:F:250:ILE:CG2	1:F:502:LEU:CD1	2.94	0.43
1:F:274:LYS:HE2	1:F:285:ASN:CB	2.48	0.43
1:F:305:SER:OG	1:F:500:LEU:HD21	2.18	0.43
1:F:361:ILE:HD13	1:F:361:ILE:N	2.27	0.43
1:F:169:VAL:O	1:F:170:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:PRO:HB3	1:F:398:THR:O	2.18	0.43
1:F:405:ASP:O	1:F:417:VAL:HG21	2.19	0.43
1:F:434:PHE:CD1	1:F:436:VAL:CG1	3.02	0.43
1:F:19:ASN:CG	1:F:24:TYR:HB2	2.43	0.43
1:F:132:HIS:HB2	1:F:133:PRO:HD2	1.99	0.43
1:F:258:THR:CB	1:F:292:ILE:HG13	2.45	0.43
1:F:299:MET:O	1:F:300:SER:HB3	2.18	0.43
1:F:406:MET:HA	1:F:417:VAL:HG11	2.01	0.43
1:F:5:LEU:HD22	1:F:14:LEU:CB	2.49	0.43
1:F:11:ARG:NH1	1:F:29:ILE:HG13	2.34	0.43
1:F:31:ARG:CB	1:F:123:ILE:HD11	2.41	0.43
1:F:215:LYS:CB	1:F:267:PHE:CZ	3.01	0.43
1:F:259:LEU:CB	1:F:521:LEU:HD11	2.32	0.43
1:F:400:VAL:HG12	1:F:401:TYR:N	2.32	0.43
1:F:12:TYR:CE2	1:F:121:ILE:HG21	2.54	0.43
1:F:29:ILE:HD13	1:F:37:LEU:HD13	2.01	0.42
1:F:99:THR:CG2	1:F:117:ASP:CB	2.95	0.42
1:F:250:ILE:HG23	1:F:250:ILE:O	2.18	0.42
1:F:259:LEU:HD11	1:F:289:THR:CG2	2.49	0.42
1:F:503:ILE:CG2	1:F:504:ASP:N	2.82	0.42
1:F:223:LEU:HD13	1:F:237:TYR:CZ	2.51	0.42
1:F:362:ILE:HG23	1:F:401:TYR:CD1	2.54	0.42
1:F:298:VAL:CG2	1:F:299:MET:N	2.83	0.42
1:F:486:PHE:CE1	1:F:518:PHE:HD2	2.37	0.42
1:F:223:LEU:CD1	1:F:237:TYR:CE1	2.95	0.42
1:F:418:LEU:CB	1:F:487:MET:SD	3.07	0.42
1:F:436:VAL:O	1:F:436:VAL:HG23	2.18	0.42
1:F:94:TYR:CD2	1:F:122:TYR:HB2	2.55	0.42
1:F:270:THR:CG2	1:F:271:ARG:N	2.83	0.42
1:F:312:VAL:HG23	1:F:471:ARG:CG	2.45	0.42
1:F:333:ILE:O	1:F:333:ILE:HG23	2.17	0.42
1:F:439:PRO:HA	1:F:458:CYS:O	2.18	0.42
1:F:6:TYR:CB	1:F:44:HIS:NE2	2.83	0.42
1:F:89:PHE:HE1	1:F:138:TYR:CE1	2.36	0.42
1:F:110:HIS:ND1	1:F:156:SER:HB2	2.33	0.42
1:F:478:LEU:HD23	1:F:530:SER:OG	2.20	0.42
1:F:266:LYS:CG	1:F:267:PHE:N	2.83	0.42
1:F:377:ILE:CG2	1:F:378:LEU:N	2.83	0.42
1:F:486:PHE:CE1	1:F:518:PHE:CE2	3.07	0.42
1:F:500:LEU:N	1:F:500:LEU:CD1	2.83	0.42
1:F:12:TYR:HE1	1:F:123:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ASN:ND2	1:F:24:TYR:HB2	2.35	0.42
1:F:132:HIS:H	1:F:135:GLU:HG2	1.84	0.42
1:F:267:PHE:O	1:F:272:PHE:HE1	2.03	0.42
1:F:436:VAL:CG2	1:F:464:ARG:N	2.83	0.42
1:F:127:SER:O	1:F:131:THR:HG23	2.19	0.42
1:F:128:VAL:CG2	1:F:129:ARG:N	2.82	0.42
1:F:168:THR:CG2	1:F:169:VAL:N	2.83	0.42
1:F:229:THR:CG2	1:F:230:VAL:N	2.82	0.42
1:F:313:ARG:HH11	1:F:481:THR:CG2	2.33	0.42
1:F:25:ARG:O	1:F:234:TRP:HZ2	2.03	0.41
1:F:74:LEU:O	1:F:75:PHE:CD1	2.73	0.41
1:F:273:LEU:HD23	1:F:320:TRP:HB2	2.02	0.41
1:F:425:ALA:C	1:F:429:VAL:HG22	2.45	0.41
1:F:11:ARG:HH11	1:F:29:ILE:HB	1.86	0.41
1:F:99:THR:CG2	1:F:100:LYS:N	2.82	0.41
1:F:344:VAL:CG1	1:F:345:ALA:N	2.82	0.41
1:F:370:GLU:CA	1:F:373:LYS:HA	2.50	0.41
1:F:248:LEU:HB3	1:F:517:LEU:HD12	2.01	0.41
1:F:312:VAL:CG1	1:F:356:PHE:CZ	3.01	0.41
1:F:365:LEU:HD21	1:F:404:TRP:CE3	2.55	0.41
1:F:378:LEU:HD12	1:F:378:LEU:N	2.35	0.41
1:F:391:GLN:O	1:F:397:HIS:HA	2.21	0.41
1:F:521:LEU:CD1	1:F:521:LEU:C	2.93	0.41
1:F:139:LEU:CD2	1:F:139:LEU:C	2.93	0.41
1:F:255:VAL:CG1	1:F:256:TYR:N	2.83	0.41
1:F:255:VAL:HG11	1:F:293:LEU:HD11	1.96	0.41
1:F:326:THR:CG2	1:F:327:MET:N	2.83	0.41
1:F:350:ASP:O	1:F:353:PHE:CD2	2.74	0.41
1:F:153:PHE:HE1	1:F:155:TYR:CZ	2.38	0.41
1:F:217:VAL:O	1:F:217:VAL:HG12	2.21	0.41
1:F:386:VAL:CG1	1:F:387:THR:N	2.83	0.41
1:F:84:VAL:HG22	1:F:96:VAL:C	2.45	0.41
1:F:434:PHE:HE1	1:F:436:VAL:CG1	2.31	0.41
1:F:470:LEU:C	1:F:470:LEU:CD1	2.94	0.41
1:F:4:VAL:HG13	1:F:15:VAL:HG22	2.03	0.41
1:F:29:ILE:HD11	1:F:86:PHE:CE2	2.55	0.41
1:F:106:ASP:H	1:F:245:GLN:NE2	2.18	0.41
1:F:167:LEU:C	1:F:167:LEU:CD1	2.94	0.41
1:F:267:PHE:O	1:F:272:PHE:CE1	2.74	0.41
1:F:393:LEU:CB	1:F:394:PRO:CD	2.98	0.41
1:F:406:MET:CE	1:F:480:ARG:HE	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:MET:HG3	1:F:417:VAL:HG11	2.00	0.41
1:F:408:LYS:HA	1:F:409:TYR:C	2.46	0.41
1:F:477:CYS:HB2	1:F:480:ARG:HG3	2.02	0.41
1:F:494:ALA:O	1:F:498:TYR:CD1	2.73	0.41
1:F:40:ILE:HG12	1:F:41:ASP:N	2.36	0.41
1:F:161:HIS:HB3	1:F:165:TYR:HB2	2.03	0.41
1:F:312:VAL:CG2	1:F:469:ILE:HD13	2.50	0.41
1:F:486:PHE:CD2	1:F:486:PHE:C	2.99	0.41
1:F:87:VAL:CG1	1:F:222:LEU:CD2	2.95	0.41
1:F:115:VAL:HG11	1:F:118:THR:HG22	2.03	0.41
1:F:251:TYR:O	1:F:251:TYR:CD2	2.74	0.41
1:F:310:VAL:CG1	1:F:311:GLN:N	2.82	0.41
1:F:339:ASP:CG	1:F:343:HIS:HD1	2.28	0.41
1:F:345:ALA:O	1:F:349:PHE:CD2	2.74	0.41
1:F:358:SER:CB	1:F:359:PRO:HD2	2.51	0.41
1:F:390:ASN:OD1	1:F:392:PHE:CE1	2.74	0.41
1:F:404:TRP:CZ2	1:F:417:VAL:O	2.74	0.41
1:F:533:TYR:CD2	1:F:534:GLY:N	2.89	0.41
1:F:4:VAL:HG12	1:F:15:VAL:HG23	2.02	0.41
1:F:168:THR:HG23	1:F:169:VAL:N	2.35	0.41
1:F:494:ALA:O	1:F:498:TYR:HD1	2.03	0.41
1:F:318:LEU:CD1	1:F:341:PHE:CD1	2.94	0.40
1:F:20:ALA:O	1:F:21:GLU:HB3	2.20	0.40
1:F:101:ARG:CZ	1:F:153:PHE:CD2	3.05	0.40
1:F:248:LEU:CD1	1:F:248:LEU:C	2.94	0.40
1:F:397:HIS:CD2	1:F:397:HIS:H	2.38	0.40
1:F:361:ILE:CG1	1:F:470:LEU:CD2	2.94	0.40
1:F:37:LEU:CD2	1:F:225:ILE:CG2	2.96	0.40
1:F:209:CYS:HA	1:F:212:PRO:HG2	2.03	0.40
1:F:363:LEU:HD11	1:F:470:LEU:HD21	2.03	0.40
1:F:406:MET:HE2	1:F:480:ARG:CD	2.51	0.40
1:F:502:LEU:CD2	1:F:502:LEU:C	2.94	0.40
1:F:3:LEU:CD1	1:F:15:VAL:C	2.94	0.40
1:F:113:TYR:CE2	1:F:155:TYR:HE2	2.40	0.40
1:F:139:LEU:CD2	1:F:143:GLN:CG	2.95	0.40
1:F:163:LEU:HG	1:F:435:PHE:CE2	2.56	0.40
1:F:312:VAL:HG23	1:F:471:ARG:CB	2.52	0.40
1:F:406:MET:SD	1:F:418:LEU:CD2	3.07	0.40
1:F:421:LEU:C	1:F:421:LEU:CD1	2.94	0.40
1:F:515:VAL:CG1	1:F:516:ARG:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	F	458/918 (50%)	410 (90%)	33 (7%)	15 (3%)	3	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	11	ARG
1	F	75	PHE
1	F	170	LEU
1	F	393	LEU
1	F	412	SER
1	F	32	THR
1	F	333	ILE
1	F	398	THR
1	F	336	ASP
1	F	359	PRO
1	F	396	GLU
1	F	171	ARG
1	F	230	VAL
1	F	461	PRO
1	F	208	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 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	F	409/823 (50%)	401 (98%)	8 (2%)	48	66

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	14	LEU
1	F	98	ILE
1	F	123	ILE
1	F	271	ARG
1	F	324	ILE
1	F	361	ILE
1	F	362	ILE
1	F	521	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	161	HIS
1	F	245	GLN
1	F	311	GLN
1	F	322	GLN
1	F	391	GLN
1	F	397	HIS
1	F	416	ASN
1	F	485	GLN
1	F	507	ASN
1	F	525	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	237:TYR	C	238:ILE	N	3.73

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22631. 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.