Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 11:01 PM EDT

PDB ID	:	3EUK
Title	:	Crystal structure of MukE-MukF(residues 292-443)-MukB(head domain)-ATPgammaS complex, asymmetric dimer
Authors	:	Woo, J.S.; Lim, J.H.; Shin, H.C.; Oh, B.H.
Deposited on	:	2008-10-10
Resolution	:	4.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

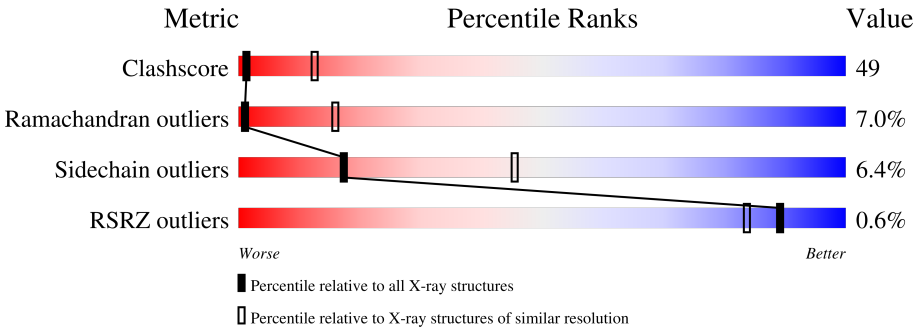
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	483	31% 54% 5% • 8%
1	C	483	33% 53% 8% 6%
1	F	483	31% 53% 7% 7%
1	H	483	32% 55% 8% • 5%
2	E	152	27% 33% 6% • 34%
2	J	152	25% 45% 11% 18%

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Mol	Chain	Length	Quality of chain
3	L	238	2% 21% 47% 5% 27%
3	M	238	3% 16% 24% 55%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18401 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chromosome partition protein mukB, Linker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3502	2212	616	659	15			
1	C	455	Total	C	N	O	S	0	0	0
			3594	2268	636	676	14			
1	F	447	Total	C	N	O	S	0	0	0
			3524	2226	622	662	14			
1	H	459	Total	C	N	O	S	0	0	0
			3620	2284	641	679	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP Q7VL96
A	31	HIS	-	expression tag	UNP Q7VL96
A	32	MET	-	expression tag	UNP Q7VL96
A	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
A	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96
A	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
A	1435	GLN	GLU	engineered mutation	UNP Q7VL96
A	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96
C	30	GLY	-	expression tag	UNP Q7VL96
C	31	HIS	-	expression tag	UNP Q7VL96
C	32	MET	-	expression tag	UNP Q7VL96
C	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
C	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96
C	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
C	1435	GLN	GLU	engineered mutation	UNP Q7VL96
C	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96
F	30	GLY	-	expression tag	UNP Q7VL96
F	31	HIS	-	expression tag	UNP Q7VL96
F	32	MET	-	expression tag	UNP Q7VL96
F	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
F	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
F	1435	GLN	GLU	engineered mutation	UNP Q7VL96
F	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96
H	30	GLY	-	expression tag	UNP Q7VL96
H	31	HIS	-	expression tag	UNP Q7VL96
H	32	MET	-	expression tag	UNP Q7VL96
H	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
H	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96
H	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
H	1435	GLN	GLU	engineered mutation	UNP Q7VL96
H	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96

- Molecule 2 is a protein called Chromosome partition protein mukF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	101	Total	C	N	O	S	0	0	0
			803	509	139	153	2			
2	J	124	Total	C	N	O	S	0	0	0
			978	618	166	192	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	372	ASN	ASP	SEE REMARK 999	UNP Q7VL94
E	384	GLN	ARG	SEE REMARK 999	UNP Q7VL94
J	372	ASN	ASP	SEE REMARK 999	UNP Q7VL94
J	384	GLN	ARG	SEE REMARK 999	UNP Q7VL94

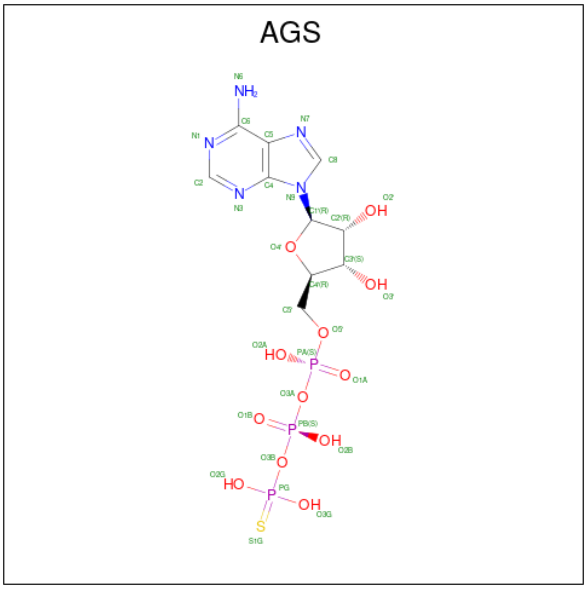
- Molecule 3 is a protein called Chromosome partition protein mukE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	173	Total	C	N	O	S	0	0	0
			1392	892	248	246	6			
3	M	107	Total	C	N	O	S	0	0	0
			860	554	143	157	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	219	ALA	GLU	SEE REMARK 999	UNP Q7VL95
M	219	ALA	GLU	SEE REMARK 999	UNP Q7VL95

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

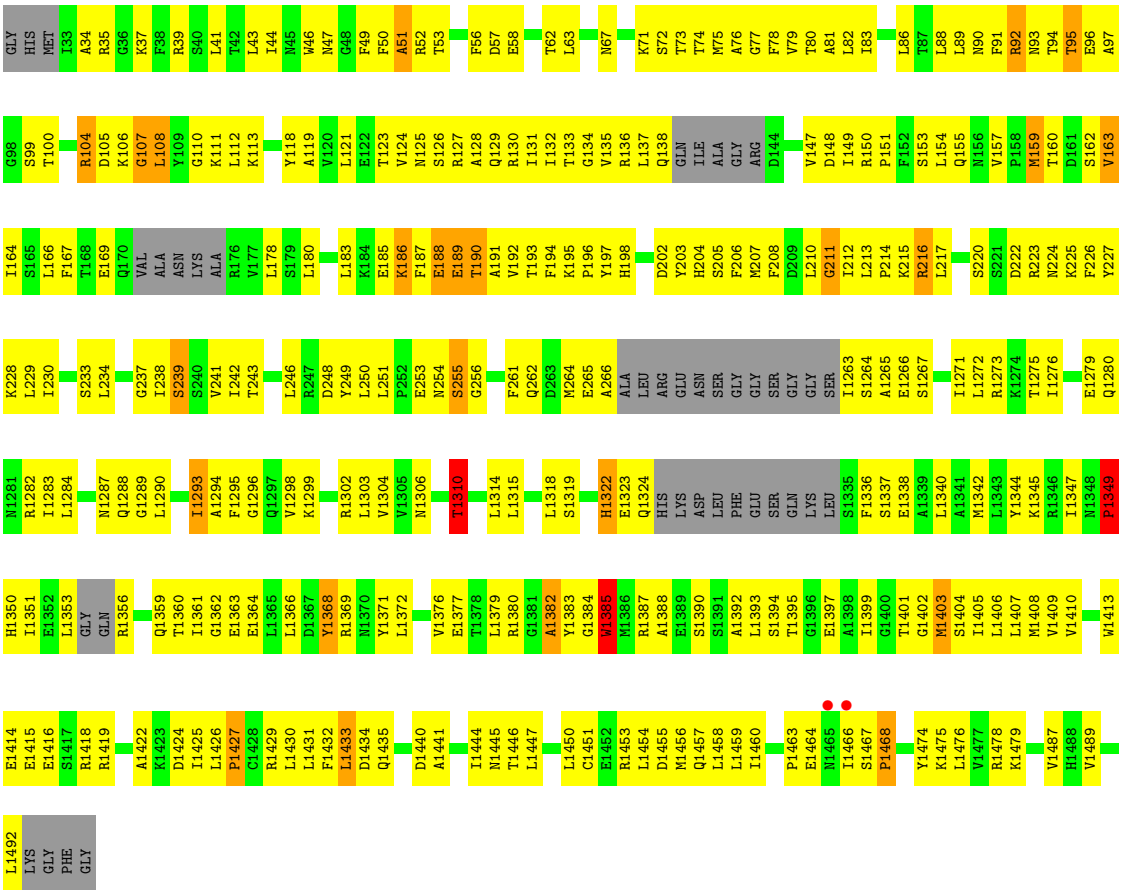
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	F	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		

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

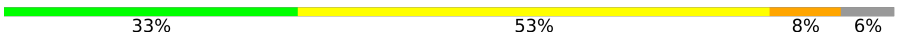
• Molecule 1: Chromosome partition protein mukB, Linker

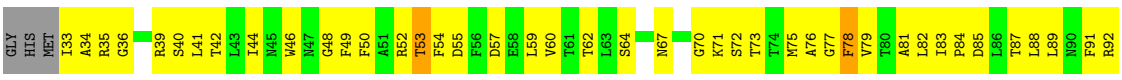
Chain A:

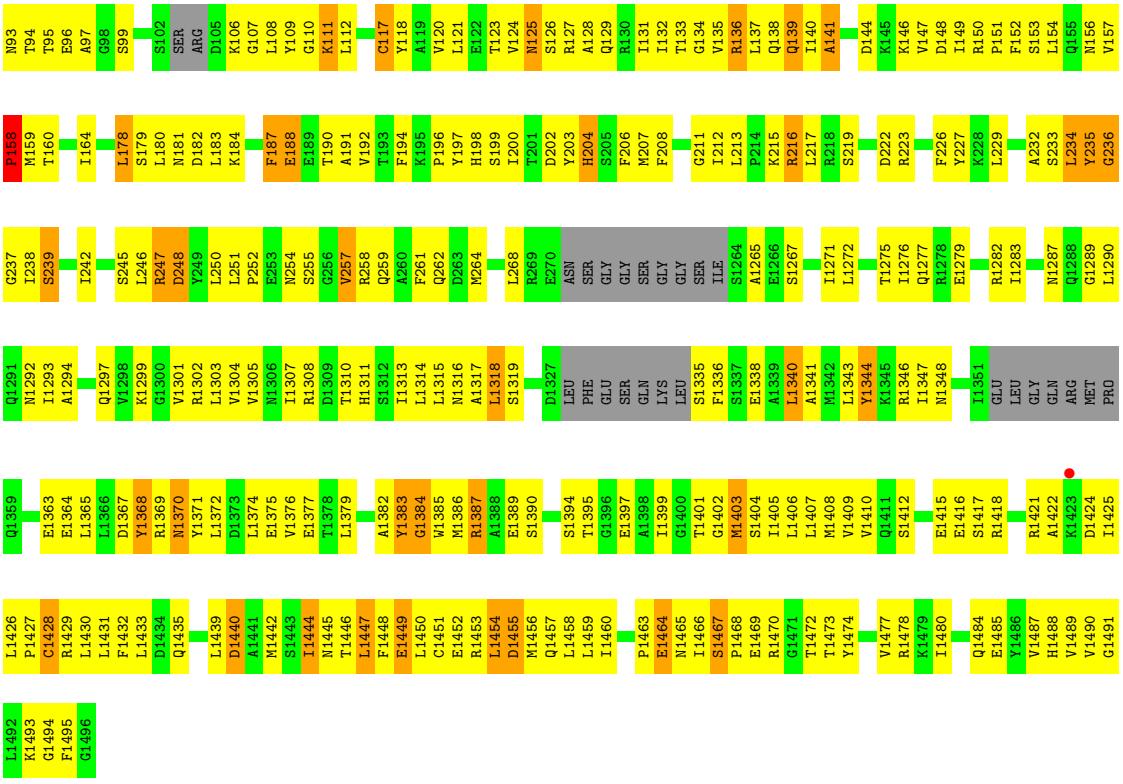


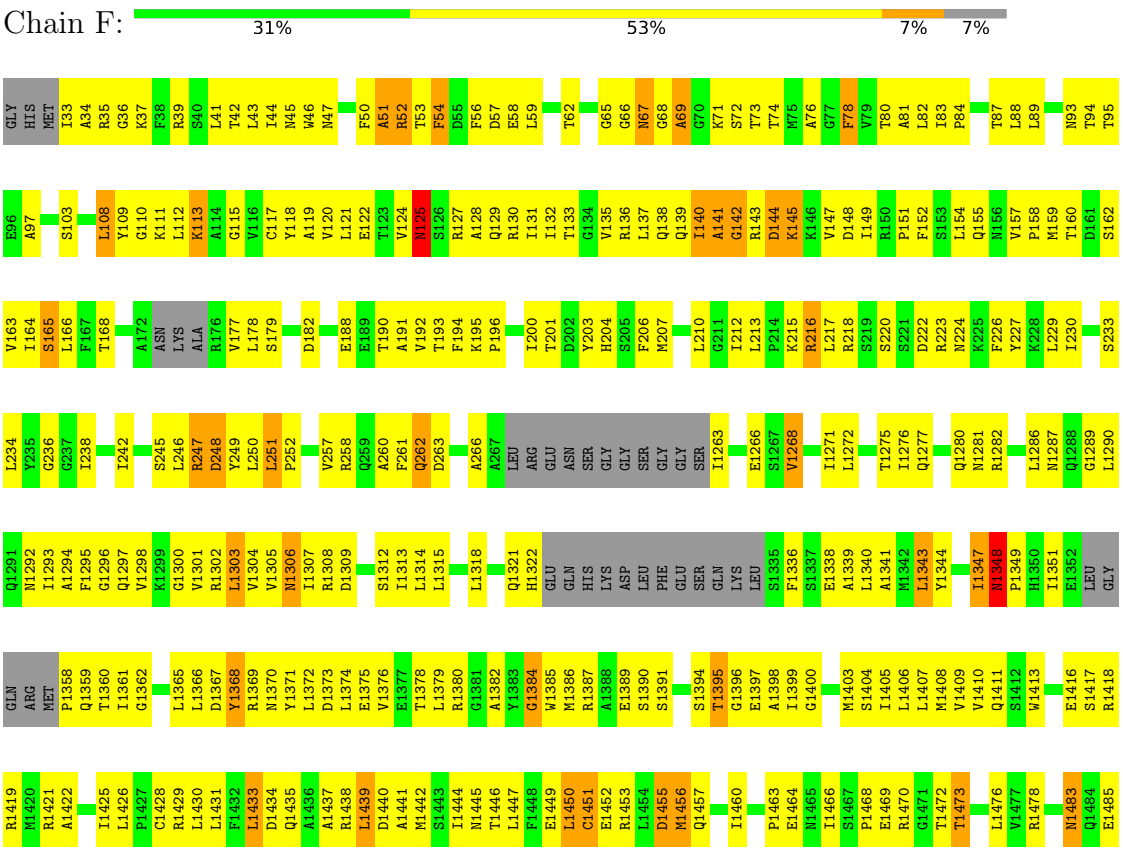
• Molecule 1: Chromosome partition protein mukB, Linker

Chain C:



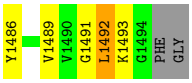






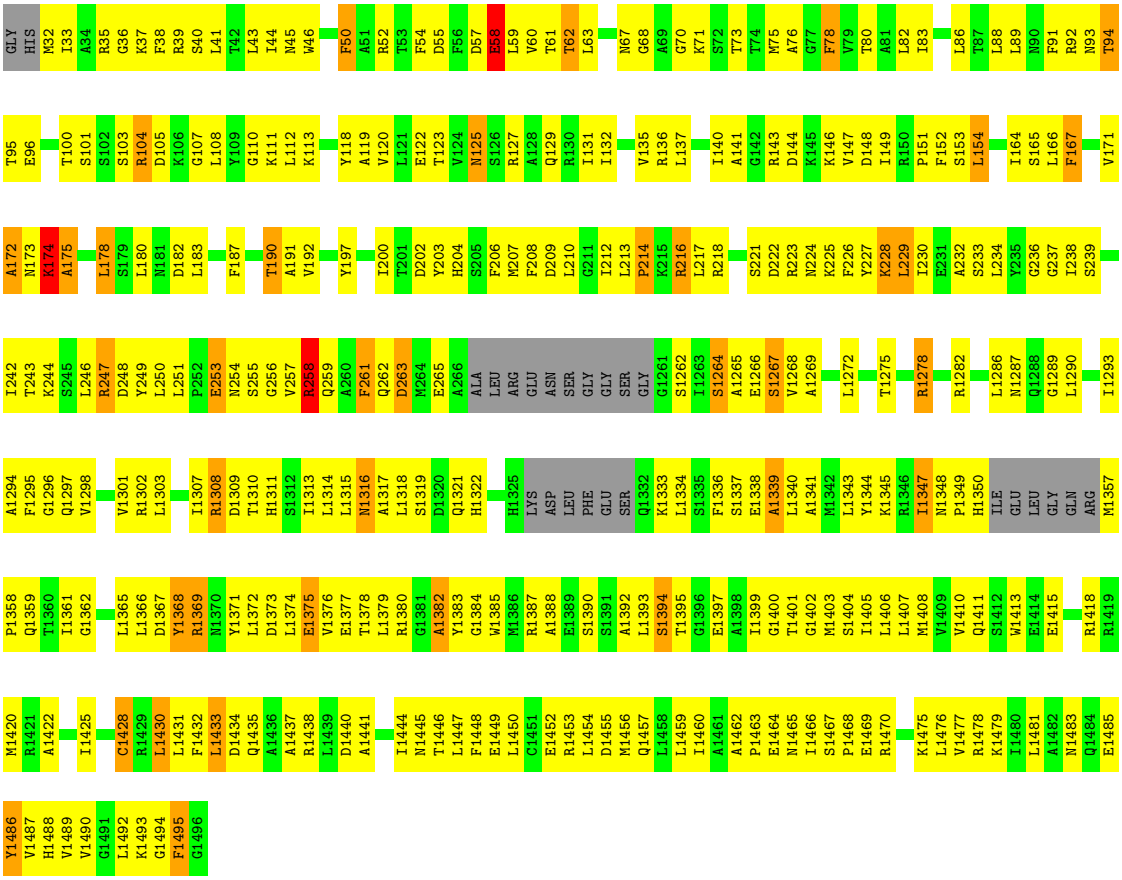
• Molecule 1: Chromosome partition protein mukB, Linker

Chain F:



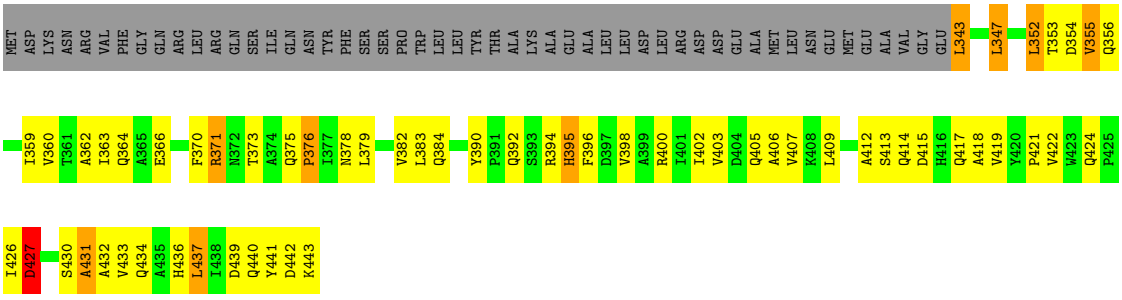
• Molecule 1: Chromosome partition protein mukB, Linker

Chain H:



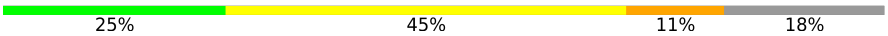
• Molecule 2: Chromosome partition protein mukF

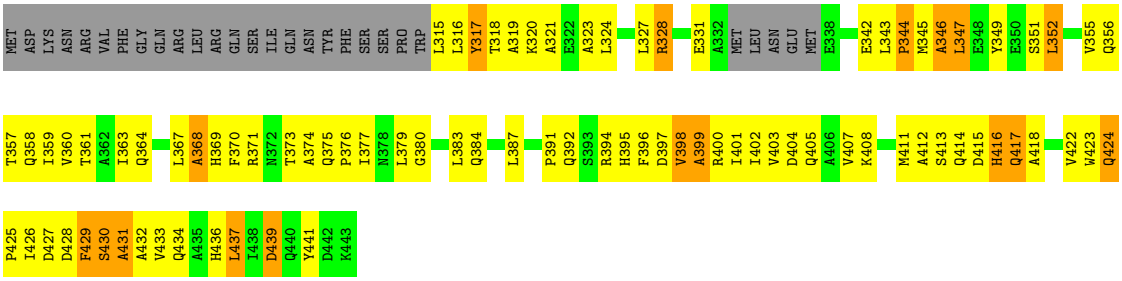
Chain E:



• Molecule 2: Chromosome partition protein mukF

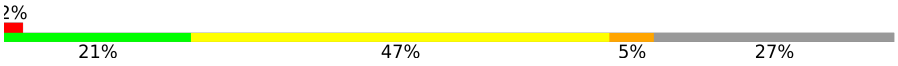
Chain J:

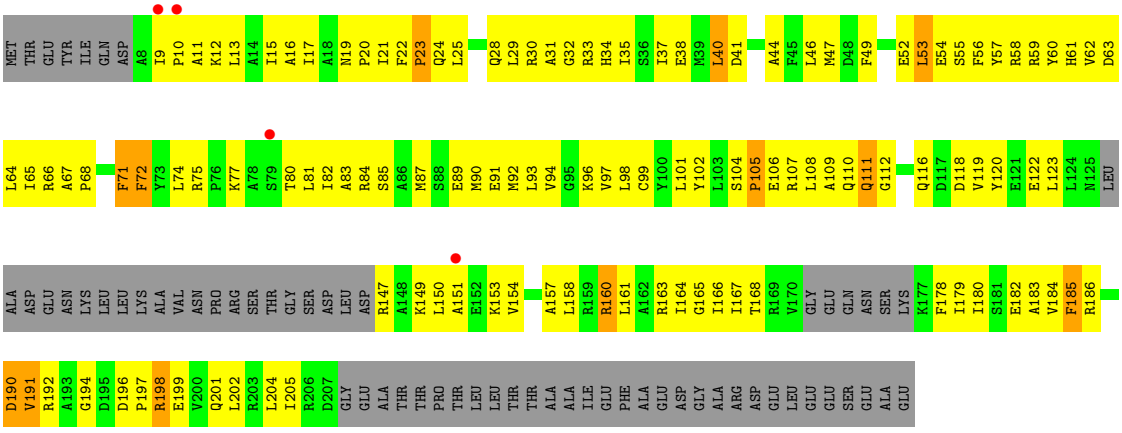




• Molecule 3: Chromosome partition protein mukE

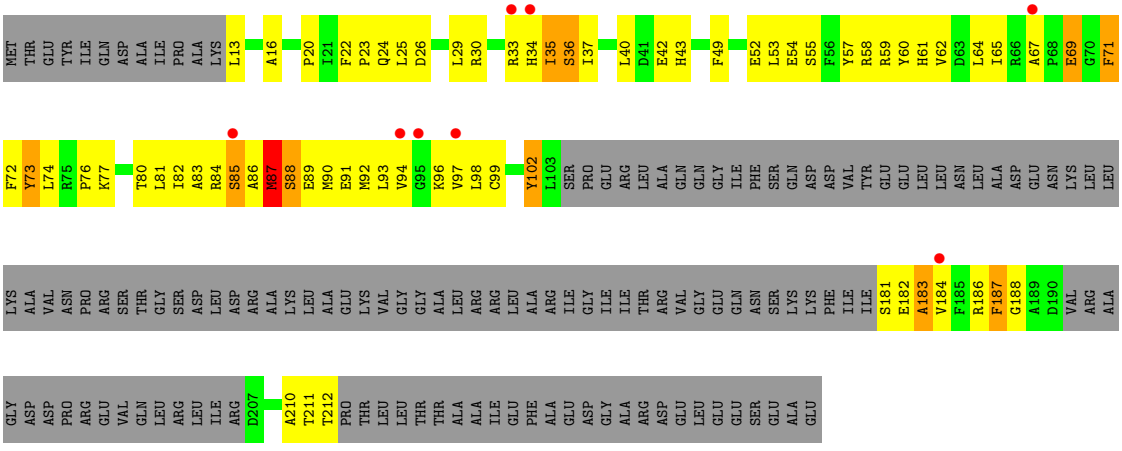
Chain L:





• Molecule 3: Chromosome partition protein mukE

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	172.41Å 172.41Å 491.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 29.92 – 3.99	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-4.00) 92.7 (29.92-3.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.324 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	113.0	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	18401	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.35	1/3551 (0.0%)	0.59	0/4784
1	C	0.35	0/3645	0.59	0/4908
1	F	0.36	0/3574	0.60	1/4816 (0.0%)
1	H	0.38	0/3673	0.61	1/4946 (0.0%)
2	E	0.34	0/820	0.58	0/1118
2	J	0.43	0/995	0.60	0/1354
3	L	0.36	1/1415 (0.1%)	0.55	0/1902
3	M	0.41	0/877	0.61	0/1180
All	All	0.36	2/18550 (0.0%)	0.60	2/25008 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	11	ALA	CA-CB	5.20	1.63	1.52
1	A	189	GLU	CD-OE1	5.17	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1348	ASN	N-CA-C	5.71	126.42	111.00
1	H	58	GLU	N-CA-C	-5.63	95.79	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3557	343	0
1	C	3594	0	3648	371	0
1	F	3524	0	3587	366	0
1	H	3620	0	3680	369	0
2	E	803	0	784	68	0
2	J	978	0	953	149	0
3	L	1392	0	1424	147	0
3	M	860	0	845	130	0
4	A	31	0	12	6	0
4	C	31	0	12	1	0
4	F	31	0	12	6	0
4	H	31	0	12	8	0
5	A	2	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
All	All	18401	0	18526	1821	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 49.

All (1821) 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)
2:J:321:ALA:HA	3:M:83:ALA:HB3	1.26	1.14
1:C:247:ARG:HD3	1:C:1369:ARG:HD3	1.12	1.11
1:A:190:THR:HG22	1:A:191:ALA:H	1.11	1.11
1:H:44:ILE:HB	1:H:118:TYR:HB2	1.29	1.06
1:C:1405:ILE:HA	1:C:1408:MET:HE2	1.38	1.06
2:E:426:ILE:HG22	2:E:427:ASP:H	1.16	1.05
1:C:73:THR:HG22	1:C:111:LYS:HD3	1.40	1.03
2:E:437:LEU:H	2:E:437:LEU:HD12	1.22	1.00
3:M:76:PRO:HB2	3:M:84:ARG:HB2	1.44	0.99
1:F:47:ASN:HA	1:F:113:LYS:HG2	1.45	0.98
1:H:178:LEU:HD23	1:H:178:LEU:H	1.30	0.95
1:C:1287:ASN:HD21	1:C:1303:LEU:H	1.09	0.95
1:F:73:THR:HG22	1:F:111:LYS:HD3	1.47	0.94
1:F:162:SER:HB3	1:F:165:SER:HB2	1.49	0.94
2:J:426:ILE:HG22	2:J:427:ASP:H	1.33	0.94
1:F:140:ILE:HG22	1:F:141:ALA:H	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:55:SER:HA	3:M:58:ARG:HE	1.32	0.93
1:H:171:VAL:HG12	1:H:172:ALA:H	1.34	0.93
1:C:247:ARG:CD	1:C:1369:ARG:HD3	1.98	0.92
1:F:83:ILE:HD11	1:F:230:ILE:HD12	1.50	0.92
1:C:254:ASN:HB2	1:C:257:VAL:HG23	1.50	0.91
2:J:321:ALA:CA	3:M:83:ALA:HB3	2.01	0.91
1:H:190:THR:HG22	1:H:191:ALA:H	1.35	0.91
2:J:437:LEU:H	2:J:437:LEU:HD12	1.36	0.91
1:H:229:LEU:HG	1:H:1406:LEU:HD11	1.50	0.91
1:C:1467:SER:HB2	1:C:1468:PRO:HD2	1.52	0.90
2:J:320:LYS:HB3	3:M:85:SER:HB2	1.53	0.90
3:L:191:VAL:HG12	3:L:194:GLY:H	1.34	0.90
1:H:250:LEU:HD13	1:H:1303:LEU:CD1	2.02	0.90
2:J:394:ARG:O	2:J:398:VAL:HG23	1.73	0.89
1:A:1287:ASN:HD21	1:A:1303:LEU:H	1.17	0.89
1:F:190:THR:HG22	1:F:191:ALA:H	1.38	0.89
1:F:1266:GLU:HG2	1:F:1321:GLN:HE22	1.36	0.88
1:C:180:LEU:HD23	1:C:183:LEU:HD12	1.56	0.88
3:L:19:ASN:OD1	3:L:21:ILE:HG12	1.75	0.87
3:L:102:TYR:HB2	3:L:180:ILE:HG21	1.57	0.87
1:C:252:PRO:HG3	1:C:1416:GLU:OE1	1.72	0.87
1:C:251:LEU:HD11	1:C:1374:LEU:HD11	1.57	0.86
1:H:41:LEU:HD22	1:H:78:PHE:HB2	1.56	0.86
1:A:127:ARG:HG3	1:A:1425:ILE:HD11	1.58	0.85
1:C:112:LEU:HD21	1:C:137:LEU:HD22	1.59	0.85
3:L:30:ARG:HH11	3:M:30:ARG:HH12	1.22	0.85
1:H:253:GLU:HG2	1:H:1369:ARG:NH1	1.91	0.84
1:H:171:VAL:HG12	1:H:172:ALA:N	1.89	0.84
3:L:180:ILE:HG23	3:L:184:VAL:HG21	1.59	0.84
1:F:251:LEU:HD11	1:F:1374:LEU:CD1	2.07	0.84
1:H:1338:GLU:HG3	1:H:1358:PRO:HB2	1.59	0.84
1:C:204:HIS:CE1	1:C:217:LEU:HD23	2.12	0.84
1:H:250:LEU:HD13	1:H:1303:LEU:HD13	1.60	0.84
3:M:76:PRO:O	3:M:84:ARG:HD3	1.78	0.84
3:L:9:ILE:HG23	3:L:52:GLU:HB3	1.59	0.83
3:L:160:ARG:O	3:L:164:ILE:HG13	1.78	0.83
1:C:1430:LEU:O	1:C:1431:LEU:HD12	1.78	0.83
1:A:190:THR:HG22	1:A:191:ALA:N	1.91	0.82
1:F:112:LEU:HD21	1:F:137:LEU:HD23	1.59	0.82
1:F:251:LEU:N	1:F:251:LEU:HD12	1.93	0.82
1:F:130:ARG:HH11	1:F:159:MET:HA	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:HH21	1:C:1425:ILE:HD11	1.45	0.82
3:M:87:MET:HA	3:M:87:MET:CE	2.09	0.82
2:J:321:ALA:HA	3:M:83:ALA:CB	2.09	0.82
1:A:187:PHE:CE2	1:A:192:VAL:HG21	2.14	0.82
1:C:35:ARG:HD2	1:C:1455:ASP:OD2	1.80	0.82
1:C:247:ARG:HD3	1:C:1369:ARG:CD	2.02	0.81
1:H:58:GLU:O	1:H:1457:GLN:HG2	1.80	0.81
1:F:1304:VAL:HG12	1:F:1306:ASN:ND2	1.95	0.81
1:F:1348:ASN:HB2	1:F:1349:PRO:CD	2.10	0.81
3:M:91:GLU:O	3:M:94:VAL:HB	1.79	0.81
1:C:107:GLY:O	1:C:111:LYS:HE3	1.79	0.81
1:H:1379:LEU:HA	1:H:1384:GLY:O	1.81	0.81
1:A:126:SER:HB2	1:A:1425:ILE:HD13	1.61	0.81
2:J:359:ILE:O	2:J:363:ILE:HG13	1.79	0.81
1:C:264:MET:O	1:C:268:LEU:HG	1.81	0.81
1:H:1448:PHE:CZ	1:H:1468:PRO:HG2	2.16	0.81
1:C:42:THR:HG21	1:C:164:ILE:HG12	1.61	0.81
1:C:41:LEU:HD22	1:C:78:PHE:HB2	1.64	0.80
1:A:155:GLN:O	1:A:192:VAL:HG13	1.80	0.80
1:F:142:GLY:O	3:L:190:ASP:HB2	1.82	0.80
1:F:80:THR:HG21	1:F:137:LEU:HD21	1.64	0.80
1:A:135:VAL:HG22	1:A:151:PRO:HA	1.63	0.80
3:M:60:TYR:HD2	3:M:82:ILE:HD11	1.47	0.80
1:C:1310:THR:HG23	1:C:1348:ASN:HD21	1.46	0.79
2:E:426:ILE:HG22	2:E:427:ASP:N	1.95	0.79
1:H:1295:PHE:HB2	1:H:1298:VAL:HB	1.64	0.79
2:J:429:PHE:N	2:J:429:PHE:HD1	1.81	0.79
1:A:1456:MET:HG2	1:A:1457:GLN:N	1.95	0.79
1:F:1438:ARG:NH1	1:H:95:THR:HG22	1.96	0.79
1:A:112:LEU:HD21	1:A:137:LEU:HD22	1.63	0.79
1:C:1376:VAL:HG11	1:C:1405:ILE:HD11	1.64	0.79
1:C:1290:LEU:HD22	1:C:1293:ILE:HD11	1.64	0.79
1:C:1422:ALA:HB3	1:C:1425:ILE:HD13	1.63	0.79
1:F:1290:LEU:HD22	1:F:1293:ILE:HD11	1.65	0.78
1:H:1349:PRO:HD2	3:L:38:GLU:OE1	1.83	0.78
3:L:158:LEU:HA	3:L:161:LEU:HD12	1.63	0.78
3:M:25:LEU:O	3:M:29:LEU:HG	1.84	0.78
3:L:90:MET:O	3:L:94:VAL:HG23	1.83	0.78
2:E:405:GLN:O	2:E:409:LEU:HD13	1.83	0.78
1:F:251:LEU:HD11	1:F:1374:LEU:HD11	1.64	0.78
3:M:90:MET:O	3:M:94:VAL:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:O	1:A:192:VAL:CG2	2.31	0.77
1:H:131:ILE:HD13	1:H:210:LEU:HD13	1.63	0.77
1:A:228:LYS:HD3	1:A:241:VAL:HG11	1.66	0.77
1:H:1334:LEU:HD21	1:H:1339:ALA:HA	1.64	0.77
1:A:104:ARG:NH2	1:C:1390:SER:HB2	2.00	0.77
1:C:1493:LYS:O	2:E:431:ALA:HA	1.85	0.77
1:F:42:THR:HB	1:F:120:VAL:HB	1.66	0.77
1:A:187:PHE:CD2	1:A:192:VAL:HB	2.20	0.77
1:C:84:PRO:HB2	1:C:149:ILE:HG21	1.67	0.77
2:E:383:LEU:HD13	2:E:433:VAL:HG21	1.67	0.77
1:A:229:LEU:HD12	1:A:1409:VAL:HG11	1.67	0.77
1:C:1403:MET:CE	1:C:1431:LEU:HD23	2.14	0.77
1:A:191:ALA:O	1:A:192:VAL:HG22	1.85	0.76
1:A:261:PHE:CZ	1:A:1336:PHE:HB3	2.20	0.76
1:C:1405:ILE:O	1:C:1409:VAL:HG23	1.86	0.76
2:E:383:LEU:CD1	2:E:433:VAL:HG21	2.16	0.76
2:E:437:LEU:H	2:E:437:LEU:CD1	1.99	0.76
3:L:30:ARG:HH11	3:M:30:ARG:NH1	1.83	0.76
1:F:140:ILE:HG22	1:F:141:ALA:N	2.01	0.76
1:F:215:LYS:O	1:F:217:LEU:HD12	1.86	0.76
1:F:1348:ASN:HB2	1:F:1349:PRO:HD3	1.66	0.76
3:M:36:SER:HB3	3:M:182:GLU:OE1	1.86	0.76
2:E:414:GLN:HG3	2:E:417:GLN:HG3	1.67	0.75
1:C:132:ILE:HD12	1:C:157:VAL:HG21	1.68	0.75
1:F:251:LEU:HD12	1:F:251:LEU:H	1.51	0.75
3:L:16:ALA:O	3:L:22:PHE:HB2	1.85	0.75
1:H:89:LEU:HD23	1:H:227:TYR:CE2	2.21	0.75
3:M:60:TYR:CD2	3:M:82:ILE:HD11	2.21	0.75
1:C:1318:LEU:HD21	1:C:1343:LEU:HD11	1.67	0.75
1:H:89:LEU:HD23	1:H:227:TYR:HE2	1.52	0.75
3:M:93:LEU:O	3:M:93:LEU:HD23	1.85	0.75
1:F:131:ILE:HD13	1:F:210:LEU:HD13	1.68	0.75
2:E:421:PRO:HB3	2:E:436:HIS:CD2	2.22	0.75
1:F:250:LEU:HD13	1:F:1303:LEU:HD11	1.69	0.75
1:F:1298:VAL:HA	1:F:1379:LEU:O	1.87	0.74
1:A:1322:HIS:O	1:A:1323:GLU:HG3	1.86	0.74
1:A:1451:CYS:SG	1:A:1458:LEU:HG	2.28	0.74
1:A:1433:LEU:HB3	1:A:1460:ILE:HG22	1.68	0.74
1:F:1293:ILE:HA	1:F:1446:THR:HG21	1.69	0.74
1:H:1380:ARG:HH22	1:H:1392:ALA:HB1	1.52	0.74
1:F:83:ILE:CD1	1:F:230:ILE:HD12	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HH12	1:A:37:LYS:HE3	1.53	0.74
1:A:37:LYS:O	1:A:123:THR:HG23	1.87	0.74
1:A:1310:THR:HG22	1:A:1344:TYR:HE1	1.53	0.74
1:F:1491:GLY:HA3	2:J:349:TYR:HD2	1.53	0.74
1:H:1407:LEU:HD22	1:H:1456:MET:CE	2.18	0.74
1:C:1403:MET:CE	1:C:1403:MET:HA	2.17	0.73
1:H:1269:ALA:HB2	1:H:1318:LEU:HD12	1.69	0.73
1:H:171:VAL:CG1	1:H:172:ALA:H	2.01	0.73
2:J:360:VAL:HG22	2:J:401:ILE:HG21	1.68	0.73
1:F:207:MET:CB	1:F:213:LEU:HD23	2.17	0.73
1:H:1286:LEU:HD22	1:H:1411:GLN:NE2	2.03	0.73
1:F:1302:ARG:HG3	1:F:1385:TRP:CH2	2.22	0.73
1:H:1337:SER:O	1:H:1362:GLY:HA3	1.88	0.73
1:H:1435:GLN:HE22	1:H:1463:PRO:HG3	1.54	0.73
1:F:1421:ARG:HG2	1:F:1422:ALA:H	1.50	0.73
2:J:426:ILE:HG22	2:J:427:ASP:N	2.03	0.73
3:L:15:ILE:O	3:L:19:ASN:HB2	1.87	0.73
3:L:166:ILE:HG23	3:L:184:VAL:HG22	1.68	0.73
3:M:73:TYR:CE2	3:M:186:ARG:HD2	2.22	0.73
1:F:143:ARG:HG3	1:F:144:ASP:N	2.04	0.73
1:A:253:GLU:HG3	1:A:1369:ARG:NH1	2.02	0.73
1:F:1306:ASN:HB2	1:F:1373:ASP:O	1.88	0.73
1:F:35:ARG:HA	1:F:1426:LEU:HB2	1.70	0.72
1:H:178:LEU:HD23	1:H:178:LEU:N	2.04	0.72
2:J:429:PHE:N	2:J:429:PHE:CD1	2.52	0.72
1:A:1263:ILE:HG22	1:A:1264:SER:H	1.53	0.72
3:M:29:LEU:O	3:M:74:LEU:HD12	1.89	0.72
1:H:167:PHE:HA	1:H:178:LEU:HD21	1.71	0.72
1:H:140:ILE:HG22	1:H:141:ALA:N	2.04	0.72
3:L:30:ARG:NH1	3:M:30:ARG:HH12	1.87	0.72
3:L:46:LEU:HA	3:L:53:LEU:CD1	2.20	0.72
1:A:95:THR:O	1:C:97:ALA:HB3	1.90	0.72
1:A:163:VAL:HA	1:A:166:LEU:HD12	1.70	0.72
1:H:178:LEU:H	1:H:178:LEU:CD2	2.02	0.72
3:M:71:PHE:CE2	3:M:186:ARG:HG3	2.24	0.72
1:C:1310:THR:CG2	1:C:1348:ASN:HD21	2.01	0.72
1:H:1486:TYR:OH	2:J:415:ASP:HB3	1.90	0.72
1:F:1379:LEU:HB2	1:F:1385:TRP:CZ3	2.25	0.71
3:L:106:GLU:HB3	3:L:110:GLN:NE2	2.05	0.71
1:A:261:PHE:HZ	1:A:1336:PHE:HB3	1.53	0.71
1:C:111:LYS:C	1:C:112:LEU:HD12	2.10	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:421:PRO:HB3	2:E:436:HIS:NE2	2.06	0.71
1:C:135:VAL:HG13	1:C:149:ILE:HG23	1.71	0.71
1:C:1276:ILE:HA	1:C:1368:TYR:CE2	2.26	0.71
1:F:33:ILE:HG22	1:F:34:ALA:H	1.55	0.71
1:F:190:THR:HG22	1:F:191:ALA:N	2.04	0.71
2:J:392:GLN:HA	2:J:395:HIS:ND1	2.05	0.71
1:F:246:LEU:HD11	1:F:1376:VAL:HG23	1.73	0.71
1:H:136:ARG:HD3	1:H:180:LEU:HG	1.73	0.71
1:H:257:VAL:O	1:H:261:PHE:HB2	1.91	0.71
3:L:17:ILE:HA	3:L:22:PHE:CB	2.21	0.71
1:H:1435:GLN:HB3	1:H:1438:ARG:NH2	2.05	0.70
1:C:151:PRO:HB3	1:C:203:TYR:CD1	2.26	0.70
1:A:1376:VAL:HG11	1:A:1405:ILE:HD11	1.73	0.70
3:M:87:MET:O	3:M:88:SER:HB2	1.90	0.70
1:F:1429:ARG:HD2	1:F:1456:MET:HE3	1.72	0.70
1:C:250:LEU:HD13	1:C:1303:LEU:HD11	1.73	0.70
3:L:178:PHE:C	3:L:179:ILE:HD12	2.12	0.70
1:A:97:ALA:HB3	1:C:96:GLU:HA	1.74	0.70
1:H:1405:ILE:HA	1:H:1408:MET:CE	2.21	0.70
1:C:1495:PHE:CE2	2:E:396:PHE:HA	2.27	0.69
1:F:1295:PHE:CD2	1:F:1400:GLY:HA3	2.27	0.69
1:H:253:GLU:HG2	1:H:1369:ARG:HH12	1.56	0.69
1:A:1456:MET:HG2	1:A:1457:GLN:H	1.54	0.69
1:H:153:SER:O	1:H:154:LEU:HG	1.92	0.69
2:J:379:LEU:H	2:J:379:LEU:HD12	1.57	0.69
1:C:180:LEU:HB2	2:J:428:ASP:OD2	1.92	0.69
1:A:220:SER:HA	1:A:223:ARG:HH21	1.58	0.69
1:C:71:LYS:HE3	1:C:1463:PRO:HA	1.73	0.69
3:M:62:VAL:HG22	3:M:76:PRO:HA	1.73	0.69
1:A:253:GLU:CG	1:A:1369:ARG:HH11	2.05	0.69
1:F:1441:ALA:HA	1:F:1444:ILE:HD12	1.73	0.69
1:A:90:ASN:OD1	1:A:92:ARG:HG3	1.92	0.69
1:C:36:GLY:HA2	1:C:124:VAL:O	1.92	0.69
1:C:1294:ALA:H	1:C:1446:THR:HG21	1.57	0.69
1:H:212:ILE:HG22	1:H:213:LEU:HD12	1.73	0.69
1:H:229:LEU:HD23	1:H:230:ILE:N	2.07	0.69
1:H:1303:LEU:CD2	1:H:1376:VAL:HG22	2.22	0.69
1:H:1407:LEU:HD22	1:H:1456:MET:HE1	1.74	0.69
1:F:62:THR:HB	1:F:1473:THR:HG23	1.75	0.69
1:H:1449:GLU:O	1:H:1453:ARG:HG3	1.93	0.69
1:C:1318:LEU:HD21	1:C:1343:LEU:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:HD21	1:C:137:LEU:CD2	2.23	0.68
3:L:32:GLY:O	3:L:164:ILE:HG23	1.93	0.68
1:A:130:ARG:HD3	1:A:159:MET:HG2	1.73	0.68
1:A:135:VAL:HG13	1:A:150:ARG:C	2.14	0.68
1:F:1491:GLY:HA3	2:J:349:TYR:CD2	2.27	0.68
1:A:1351:ILE:H	1:A:1351:ILE:HD12	1.57	0.68
1:C:1469:GLU:HA	2:E:396:PHE:CE1	2.28	0.68
3:M:29:LEU:HD12	3:M:57:TYR:OH	1.93	0.68
1:A:190:THR:CG2	1:A:191:ALA:H	1.96	0.68
1:F:1306:ASN:H	1:F:1306:ASN:HD22	1.41	0.68
2:J:346:ALA:O	2:J:347:LEU:HB2	1.93	0.68
3:L:93:LEU:O	3:L:97:VAL:HG23	1.94	0.68
1:C:1424:ASP:C	1:C:1425:ILE:HD12	2.15	0.68
1:H:39:ARG:HB3	1:H:122:GLU:OE1	1.94	0.68
3:M:54:GLU:O	3:M:58:ARG:HG3	1.93	0.68
3:M:87:MET:HA	3:M:87:MET:HE3	1.76	0.68
1:F:1437:ALA:HB1	1:H:1437:ALA:HB1	1.75	0.68
1:H:1303:LEU:HD21	1:H:1376:VAL:HG22	1.76	0.68
1:F:87:THR:C	1:F:88:LEU:HD12	2.15	0.67
1:H:1387:ARG:HG2	1:H:1388:ALA:N	2.09	0.67
1:A:262:GLN:NE2	1:A:1359:GLN:OE1	2.27	0.67
1:C:207:MET:HB3	1:C:212:ILE:HB	1.76	0.67
1:F:1390:SER:O	1:H:93:ASN:HB2	1.95	0.67
1:A:130:ARG:NH2	1:A:163:VAL:HG13	2.10	0.67
1:H:174:LYS:O	1:H:175:ALA:HB2	1.93	0.67
3:M:61:HIS:HB2	3:M:80:THR:HA	1.76	0.67
1:A:51:ALA:HB3	2:E:343:LEU:HD11	1.77	0.67
1:A:187:PHE:CD2	1:A:192:VAL:HG21	2.29	0.67
1:C:1403:MET:HE2	1:C:1431:LEU:HD23	1.77	0.67
1:F:73:THR:HG22	1:F:111:LYS:CD	2.21	0.67
3:M:35:ILE:H	3:M:35:ILE:HD12	1.60	0.67
3:M:36:SER:HA	3:M:71:PHE:HA	1.76	0.67
1:A:1380:ARG:H	1:A:1384:GLY:HA2	1.59	0.67
1:A:1441:ALA:O	1:A:1444:ILE:HG22	1.93	0.67
1:C:123:THR:HB	1:C:131:ILE:HB	1.77	0.67
3:L:191:VAL:HG12	3:L:194:GLY:N	2.09	0.67
1:C:1279:GLU:HB3	1:C:1368:TYR:OH	1.94	0.67
1:F:1358:PRO:HG2	1:F:1359:GLN:H	1.57	0.67
1:F:234:LEU:HD23	1:F:1434:ASP:HB2	1.76	0.67
1:H:1466:ILE:HA	2:J:400:ARG:HH22	1.60	0.67
1:A:73:THR:HG22	1:A:111:LYS:NZ	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1405:ILE:O	1:F:1409:VAL:HG23	1.93	0.67
1:H:39:ARG:HH11	1:H:39:ARG:HG3	1.60	0.67
1:H:88:LEU:HD21	1:H:224:ASN:HA	1.76	0.67
1:H:250:LEU:HD13	1:H:1303:LEU:HD11	1.76	0.67
1:A:1403:MET:HE2	1:A:1403:MET:HA	1.76	0.66
1:C:1451:CYS:SG	1:C:1458:LEU:HG	2.35	0.66
1:H:1287:ASN:HD21	1:H:1303:LEU:H	1.43	0.66
1:H:1387:ARG:HG2	1:H:1388:ALA:H	1.60	0.66
1:A:136:ARG:HD3	1:A:180:LEU:CD1	2.26	0.66
1:F:82:LEU:HD23	1:F:82:LEU:O	1.95	0.66
1:F:1406:LEU:O	1:F:1410:VAL:HG23	1.94	0.66
1:A:67:ASN:HA	4:A:2001:AGS:S1G	2.35	0.66
1:A:89:LEU:HD23	1:A:227:TYR:HE2	1.58	0.66
1:F:215:LYS:HD2	1:F:1413:TRP:NE1	2.11	0.66
1:H:1315:LEU:HD11	1:H:1371:TYR:CD2	2.30	0.66
1:C:108:LEU:HD22	1:C:147:VAL:HG21	1.77	0.66
1:H:83:ILE:HD11	1:H:226:PHE:CD2	2.30	0.66
1:C:250:LEU:HD13	1:C:1303:LEU:CD1	2.25	0.66
1:F:81:ALA:HB2	1:F:119:ALA:HB1	1.77	0.66
1:H:89:LEU:HA	1:H:227:TYR:CE2	2.31	0.66
3:M:22:PHE:HB3	3:M:23:PRO:HD3	1.78	0.66
1:A:104:ARG:HH22	1:C:1390:SER:HB2	1.61	0.66
1:A:135:VAL:HG11	1:A:149:ILE:CG2	2.26	0.66
1:C:120:VAL:HG13	1:C:134:GLY:HA3	1.78	0.66
1:H:1435:GLN:HB3	1:H:1438:ARG:HH21	1.61	0.66
1:H:1488:HIS:CD2	2:J:407:VAL:HG13	2.30	0.66
1:C:1494:GLY:HA3	2:E:431:ALA:HA	1.77	0.66
1:A:1315:LEU:O	1:A:1319:SER:HB2	1.94	0.66
1:C:1490:VAL:HG11	2:E:403:VAL:HG13	1.78	0.66
1:F:258:ARG:O	1:F:262:GLN:HB2	1.96	0.66
1:F:1301:VAL:HG22	1:F:1378:THR:HG22	1.78	0.66
1:H:62:THR:HG23	1:H:1460:ILE:HG13	1.78	0.66
2:J:377:ILE:HG13	2:J:441:TYR:OH	1.95	0.66
3:M:25:LEU:HD13	3:M:42:GLU:OE1	1.96	0.66
1:A:1362:GLY:O	1:A:1366:LEU:HG	1.96	0.65
1:C:41:LEU:CD2	1:C:78:PHE:HB2	2.26	0.65
1:F:1294:ALA:H	1:F:1446:THR:HG21	1.61	0.65
1:H:1287:ASN:ND2	1:H:1302:ARG:HB3	2.12	0.65
1:F:110:GLY:HA3	4:F:2003:AGS:N1	2.11	0.65
1:C:73:THR:HG22	1:C:111:LYS:CD	2.23	0.65
1:F:41:LEU:HD11	1:F:78:PHE:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:LYS:C	1:F:112:LEU:HD12	2.17	0.65
1:C:1307:ILE:HG23	1:C:1371:TYR:O	1.97	0.65
2:E:354:ASP:C	2:E:356:GLN:H	1.99	0.65
1:H:112:LEU:HD21	1:H:137:LEU:CD2	2.27	0.65
1:C:1402:GLY:O	1:C:1406:LEU:HD13	1.96	0.65
1:H:1278:ARG:CG	1:H:1282:ARG:HH21	2.09	0.65
2:J:343:LEU:HD23	2:J:344:PRO:HD2	1.79	0.65
3:L:24:GLN:HG2	3:M:81:LEU:HD22	1.79	0.65
1:C:39:ARG:CZ	1:C:124:VAL:HG21	2.26	0.65
1:C:1289:GLY:O	1:C:1290:LEU:HD23	1.97	0.65
1:F:1290:LEU:HB3	1:F:1293:ILE:HD11	1.79	0.65
1:H:1290:LEU:HB3	1:H:1293:ILE:HD11	1.79	0.65
3:L:167:ILE:HG21	3:L:178:PHE:HB2	1.79	0.65
1:A:1393:LEU:HB3	1:A:1397:GLU:HB2	1.78	0.65
1:C:254:ASN:CB	1:C:257:VAL:HG23	2.27	0.65
1:C:1293:ILE:HD11	1:C:1450:LEU:HD21	1.78	0.64
1:C:1371:TYR:O	1:C:1372:LEU:HD12	1.98	0.64
1:F:207:MET:HB3	1:F:213:LEU:HD23	1.78	0.64
1:H:1478:ARG:HH21	1:H:1487:VAL:CG2	2.10	0.64
2:E:398:VAL:O	2:E:402:ILE:HG13	1.97	0.64
1:H:93:ASN:O	1:H:95:THR:N	2.31	0.64
2:J:368:ALA:O	2:J:371:ARG:HB3	1.98	0.64
2:E:384:GLN:HB2	2:E:426:ILE:HD12	1.80	0.64
1:H:207:MET:HB3	1:H:212:ILE:HB	1.78	0.64
1:A:187:PHE:CD2	1:A:192:VAL:CG2	2.81	0.64
1:C:1299:LYS:O	1:C:1379:LEU:HD23	1.96	0.64
1:F:207:MET:HB2	1:F:213:LEU:HD23	1.79	0.64
3:M:71:PHE:HE2	3:M:186:ARG:HG3	1.59	0.64
1:A:154:LEU:HD22	1:A:187:PHE:CE1	2.33	0.64
1:A:136:ARG:HD3	1:A:180:LEU:HD11	1.80	0.64
1:A:211:GLY:O	1:A:212:ILE:HD13	1.98	0.64
1:F:1361:ILE:O	1:F:1365:LEU:HG	1.98	0.64
2:J:379:LEU:HD12	2:J:379:LEU:N	2.12	0.64
3:L:116:GLN:HE21	3:L:158:LEU:HD23	1.63	0.64
2:E:356:GLN:HA	2:E:359:ILE:HD12	1.79	0.64
1:F:1433:LEU:HD21	1:F:1439:LEU:HD11	1.78	0.64
3:L:98:LEU:HD13	3:L:167:ILE:HD11	1.80	0.64
1:A:1290:LEU:HD13	1:A:1404:SER:HB3	1.79	0.64
1:A:1387:ARG:HB3	1:A:1387:ARG:HH11	1.63	0.63
1:C:138:GLN:HB3	2:J:429:PHE:CE2	2.32	0.63
1:C:1410:VAL:HG11	1:C:1429:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1439:LEU:HD12	1:F:1439:LEU:H	1.63	0.63
1:F:1379:LEU:HD12	1:F:1384:GLY:O	1.98	0.63
1:C:33:ILE:HD12	1:C:33:ILE:N	2.14	0.63
1:H:1435:GLN:NE2	1:H:1463:PRO:HG3	2.13	0.63
1:H:1488:HIS:HD2	2:J:407:VAL:HG13	1.64	0.63
2:J:320:LYS:HD2	3:M:85:SER:CB	2.28	0.63
3:M:61:HIS:CB	3:M:80:THR:HA	2.27	0.63
3:M:102:TYR:HH	3:M:181:SER:N	1.97	0.63
1:F:125:ASN:HB2	1:F:129:GLN:HB2	1.80	0.63
1:F:1338:GLU:O	1:F:1341:ALA:HB3	1.99	0.63
1:A:229:LEU:C	1:A:229:LEU:HD23	2.18	0.63
1:C:52:ARG:HG3	1:C:54:PHE:CE1	2.33	0.63
1:C:1335:SER:HB2	1:C:1338:GLU:HB3	1.81	0.63
1:H:187:PHE:HD2	1:H:192:VAL:HG21	1.63	0.63
1:A:215:LYS:HD2	1:A:1413:TRP:CE2	2.34	0.63
1:C:1297:GLN:HB2	1:C:1397:GLU:OE2	1.99	0.63
3:L:182:GLU:CD	3:L:182:GLU:H	2.01	0.63
3:M:55:SER:HA	3:M:58:ARG:NE	2.10	0.63
1:A:135:VAL:HG12	1:A:136:ARG:N	2.13	0.63
1:A:1293:ILE:HG23	1:A:1295:PHE:CD1	2.33	0.63
1:H:1478:ARG:HH21	1:H:1487:VAL:HG21	1.63	0.63
2:J:315:LEU:CD2	3:M:89:GLU:HG2	2.29	0.63
3:M:94:VAL:O	3:M:94:VAL:HG12	1.99	0.63
3:L:184:VAL:C	3:L:186:ARG:H	2.02	0.62
1:C:211:GLY:O	1:C:1427:PRO:HA	1.98	0.62
1:F:1306:ASN:HD22	1:F:1306:ASN:N	1.97	0.62
1:A:136:ARG:C	1:A:137:LEU:HD12	2.19	0.62
1:F:250:LEU:CD1	1:F:1303:LEU:HD11	2.28	0.62
1:H:44:ILE:CB	1:H:118:TYR:HB2	2.19	0.62
1:H:1466:ILE:CA	2:J:400:ARG:HH22	2.12	0.62
2:J:398:VAL:HG12	2:J:402:ILE:HD11	1.81	0.62
1:A:178:LEU:HG	1:A:183:LEU:HG	1.80	0.62
1:A:217:LEU:HD12	1:A:217:LEU:N	2.14	0.62
1:A:1379:LEU:HB2	1:A:1385:TRP:CZ3	2.33	0.62
1:C:57:ASP:HB2	1:C:1472:THR:OG1	1.98	0.62
2:E:356:GLN:O	2:E:360:VAL:HG23	1.99	0.62
2:E:384:GLN:HA	2:E:426:ILE:CG2	2.29	0.62
2:J:437:LEU:H	2:J:437:LEU:CD1	2.10	0.62
1:F:67:ASN:HB2	1:H:1440:ASP:OD2	1.99	0.62
1:A:52:ARG:CZ	1:A:1489:VAL:HB	2.29	0.62
1:A:225:LYS:NZ	1:A:248:ASP:HB3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1440:ASP:O	1:F:1444:ILE:HG13	1.99	0.62
3:M:34:HIS:ND1	3:M:73:TYR:HB3	2.15	0.62
1:A:225:LYS:HB3	1:A:249:TYR:CE2	2.35	0.62
1:C:1450:LEU:O	1:C:1453:ARG:HB2	2.00	0.62
1:F:52:ARG:HE	1:F:1489:VAL:CG2	2.13	0.62
1:F:1430:LEU:HG	1:F:1457:GLN:O	2.00	0.62
3:L:63:ASP:OD1	3:L:77:LYS:HE3	2.00	0.62
1:H:40:SER:HB3	1:H:55:ASP:HA	1.80	0.62
3:M:88:SER:CB	3:M:91:GLU:OE1	2.47	0.62
1:A:95:THR:HG21	1:C:237:GLY:HA3	1.81	0.62
3:M:73:TYR:CZ	3:M:186:ARG:HD2	2.34	0.62
1:A:1368:TYR:O	1:A:1371:TYR:HB2	2.00	0.61
1:F:78:PHE:O	1:F:82:LEU:HB2	2.00	0.61
2:J:315:LEU:HD21	3:M:89:GLU:HG2	1.82	0.61
3:L:17:ILE:HG23	3:L:22:PHE:CD2	2.35	0.61
1:C:112:LEU:HD12	1:C:112:LEU:N	2.14	0.61
1:C:135:VAL:CG1	1:C:149:ILE:HG23	2.30	0.61
1:F:1390:SER:HB2	1:H:104:ARG:HH22	1.65	0.61
1:A:187:PHE:CD2	1:A:192:VAL:CB	2.83	0.61
1:C:247:ARG:HG2	1:C:247:ARG:HH11	1.66	0.61
3:M:60:TYR:HD2	3:M:82:ILE:CD1	2.12	0.61
1:F:135:VAL:CG1	1:F:149:ILE:HG23	2.30	0.61
3:L:49:PHE:O	3:L:53:LEU:HG	1.99	0.61
1:C:83:ILE:HD11	1:C:226:PHE:CE2	2.35	0.61
1:H:39:ARG:HB2	1:H:122:GLU:O	1.99	0.61
1:F:155:GLN:O	1:F:192:VAL:HG13	2.00	0.61
1:F:160:THR:HG22	1:F:160:THR:O	2.00	0.61
1:F:1396:GLY:HA2	1:F:1399:ILE:HD12	1.82	0.61
1:A:191:ALA:C	1:A:192:VAL:HG23	2.21	0.61
1:F:1263:ILE:HD12	1:F:1263:ILE:N	2.15	0.61
1:H:1481:LEU:HD22	2:J:411:MET:CE	2.31	0.61
1:C:76:ALA:HA	1:C:91:PHE:CE2	2.36	0.61
1:H:40:SER:HB2	1:H:54:PHE:O	2.01	0.61
1:H:1367:ASP:OD2	1:H:1369:ARG:CD	2.48	0.61
1:F:140:ILE:CG2	1:F:141:ALA:H	2.11	0.61
1:F:1349:PRO:O	1:F:1351:ILE:HG13	2.01	0.61
1:H:190:THR:HG22	1:H:191:ALA:N	2.13	0.61
3:L:63:ASP:HB2	3:L:75:ARG:HB3	1.82	0.61
3:M:29:LEU:CD2	3:M:35:ILE:HD11	2.30	0.61
1:A:51:ALA:HB3	2:E:343:LEU:CD1	2.30	0.61
1:A:1435:GLN:HA	1:A:1435:GLN:NE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:25:LEU:HD23	3:L:25:LEU:C	2.22	0.61
3:L:167:ILE:HG22	3:L:168:THR:H	1.65	0.61
1:A:226:PHE:CE2	1:A:230:ILE:HD11	2.35	0.60
1:C:1403:MET:HE1	1:C:1431:LEU:HD23	1.80	0.60
1:H:127:ARG:O	1:H:129:GLN:HG3	2.01	0.60
1:H:1287:ASN:HD21	1:H:1302:ARG:HB3	1.65	0.60
3:L:71:PHE:CE2	3:L:183:ALA:HA	2.36	0.60
3:M:59:ARG:O	3:M:81:LEU:HD12	2.00	0.60
1:C:1430:LEU:HD23	1:C:1431:LEU:N	2.15	0.60
1:C:1491:GLY:HA3	2:E:434:GLN:HB3	1.82	0.60
1:A:251:LEU:HD12	1:A:251:LEU:N	2.16	0.60
1:C:73:THR:CG2	1:C:111:LYS:HD3	2.25	0.60
1:C:190:THR:HG22	1:C:191:ALA:N	2.16	0.60
1:F:81:ALA:HB2	1:F:119:ALA:CB	2.31	0.60
1:F:157:VAL:HG11	1:F:166:LEU:HD11	1.83	0.60
1:F:246:LEU:HD22	1:F:1374:LEU:HB2	1.83	0.60
1:H:208:PHE:CE2	1:H:216:ARG:HG2	2.36	0.60
1:C:229:LEU:HD12	1:C:1409:VAL:HG11	1.82	0.60
1:C:76:ALA:HA	1:C:91:PHE:HE2	1.66	0.60
1:F:52:ARG:HE	1:F:1489:VAL:HG23	1.65	0.60
1:F:1347:ILE:HG22	1:F:1348:ASN:N	2.15	0.60
1:F:1395:THR:HG22	1:F:1399:ILE:HD11	1.82	0.60
1:A:237:GLY:N	1:A:1399:ILE:HD13	2.16	0.60
1:C:1275:THR:HG22	1:C:1368:TYR:HD2	1.67	0.60
1:C:1456:MET:HG2	1:C:1457:GLN:N	2.16	0.60
1:H:73:THR:O	1:H:76:ALA:HB3	2.02	0.60
1:H:1357:MET:O	1:H:1361:ILE:HG13	2.02	0.60
1:H:1406:LEU:O	1:H:1410:VAL:HG23	2.00	0.60
2:J:373:THR:C	2:J:375:GLN:H	2.04	0.60
1:C:52:ARG:HG3	1:C:54:PHE:HE1	1.66	0.60
1:C:93:ASN:ND2	1:C:95:THR:OG1	2.35	0.60
1:F:229:LEU:HD23	1:F:229:LEU:C	2.22	0.60
1:H:140:ILE:CG2	1:H:141:ALA:N	2.64	0.60
1:H:1403:MET:O	1:H:1407:LEU:HG	2.02	0.60
1:A:178:LEU:HD21	1:A:183:LEU:HD21	1.82	0.60
1:C:1403:MET:HA	1:C:1403:MET:HE2	1.84	0.60
2:E:384:GLN:HA	2:E:426:ILE:HG23	1.82	0.60
1:H:120:VAL:HG12	1:H:132:ILE:HG22	1.83	0.60
1:H:108:LEU:HD23	1:H:108:LEU:O	2.02	0.60
3:M:88:SER:HB2	3:M:91:GLU:OE1	2.02	0.60
1:H:1405:ILE:HA	1:H:1408:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:HA	1:A:205:SER:HB3	1.84	0.59
1:H:123:THR:HG21	1:H:212:ILE:HG12	1.83	0.59
2:J:317:TYR:CD1	3:M:84:ARG:HD2	2.37	0.59
2:J:320:LYS:O	3:M:83:ALA:HB3	2.01	0.59
2:J:383:LEU:HD12	2:J:433:VAL:CG2	2.32	0.59
1:C:1304:VAL:HG21	1:C:1377:GLU:OE2	2.01	0.59
2:J:320:LYS:O	3:M:83:ALA:CB	2.49	0.59
1:A:132:ILE:HD12	1:A:132:ILE:N	2.18	0.59
1:A:153:SER:O	1:A:194:PHE:HA	2.03	0.59
1:C:60:VAL:HG21	1:C:1448:PHE:CZ	2.38	0.59
1:C:110:GLY:O	1:C:112:LEU:N	2.36	0.59
1:C:254:ASN:HB2	1:C:257:VAL:CG2	2.28	0.59
1:C:1480:ILE:N	1:C:1480:ILE:HD12	2.18	0.59
1:F:215:LYS:HD2	1:F:1413:TRP:CE2	2.37	0.59
1:A:1399:ILE:HG21	1:A:1433:LEU:HD11	1.85	0.59
1:H:101:SER:HB3	1:H:104:ARG:HG3	1.83	0.59
1:H:1405:ILE:HA	1:H:1408:MET:HE2	1.83	0.59
1:H:1415:GLU:HA	1:H:1418:ARG:HG3	1.84	0.59
1:F:35:ARG:HD2	1:F:1455:ASP:HB3	1.83	0.59
1:F:1451:CYS:SG	1:F:1456:MET:HB3	2.42	0.59
1:H:207:MET:HB2	1:H:213:LEU:HD13	1.85	0.59
1:A:1478:ARG:HE	1:A:1487:VAL:CG2	2.16	0.59
1:C:132:ILE:HB	1:C:154:LEU:HB2	1.85	0.59
1:F:1314:LEU:O	1:F:1318:LEU:HG	2.02	0.59
1:F:1349:PRO:HG2	1:F:1351:ILE:HD11	1.83	0.59
1:F:1433:LEU:HD21	1:F:1439:LEU:CD1	2.32	0.59
1:A:1385:TRP:HA	1:A:1385:TRP:CE3	2.38	0.59
1:A:1407:LEU:HD13	1:A:1454:LEU:HD22	1.85	0.59
1:C:158:PRO:C	1:C:160:THR:H	2.06	0.59
1:C:1367:ASP:HB2	1:C:1370:ASN:ND2	2.17	0.59
2:E:398:VAL:HG12	2:E:402:ILE:HD11	1.84	0.59
1:H:253:GLU:HG2	1:H:1369:ARG:CZ	2.33	0.59
1:H:1430:LEU:C	1:H:1431:LEU:HD12	2.23	0.59
1:C:1287:ASN:HD21	1:C:1303:LEU:N	1.92	0.59
1:F:1430:LEU:O	1:F:1431:LEU:HD12	2.02	0.59
1:H:135:VAL:HG11	1:H:149:ILE:HG23	1.83	0.59
1:H:1485:GLU:O	1:H:1486:TYR:HB2	2.02	0.59
2:J:380:GLY:HA3	2:J:424:GLN:HG2	1.84	0.59
1:A:1380:ARG:HH21	1:A:1393:LEU:HD23	1.66	0.59
1:C:96:GLU:HB3	1:C:99:SER:OG	2.01	0.59
1:C:1444:ILE:HD13	1:C:1444:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:LEU:HD21	1:F:224:ASN:HA	1.85	0.59
1:A:57:ASP:O	1:A:1457:GLN:NE2	2.36	0.59
1:A:132:ILE:HB	1:A:154:LEU:HB2	1.84	0.58
1:F:1478:ARG:HH12	4:F:2003:AGS:H4'	1.67	0.58
1:H:76:ALA:HA	1:H:91:PHE:HE2	1.67	0.58
2:J:373:THR:O	2:J:375:GLN:N	2.36	0.58
3:M:186:ARG:C	3:M:188:GLY:H	2.04	0.58
1:A:1422:ALA:HB1	1:A:1424:ASP:OD1	2.02	0.58
1:C:127:ARG:NH2	1:C:1425:ILE:HD11	2.16	0.58
3:M:35:ILE:HD12	3:M:35:ILE:N	2.17	0.58
1:A:261:PHE:CE1	1:A:1336:PHE:HD2	2.21	0.58
1:F:229:LEU:HD23	1:F:229:LEU:O	2.04	0.58
1:H:127:ARG:NH2	1:H:1425:ILE:HD11	2.19	0.58
1:H:171:VAL:O	1:H:172:ALA:C	2.41	0.58
3:M:60:TYR:HB3	3:M:82:ILE:HG12	1.85	0.58
1:F:1286:LEU:HD22	1:F:1411:GLN:NE2	2.19	0.58
1:F:1309:ASP:O	1:F:1313:ILE:HG13	2.04	0.58
1:F:1430:LEU:HD23	1:F:1431:LEU:N	2.19	0.58
3:M:36:SER:O	3:M:43:HIS:HB2	2.03	0.58
1:H:218:ARG:HG2	1:H:218:ARG:HH11	1.68	0.58
3:L:166:ILE:CG2	3:L:184:VAL:HG22	2.33	0.58
1:C:1444:ILE:HD13	1:C:1444:ILE:C	2.24	0.58
1:C:1430:LEU:C	1:C:1431:LEU:HD12	2.24	0.58
1:H:38:PHE:HZ	1:H:212:ILE:HG23	1.69	0.58
3:M:90:MET:O	3:M:94:VAL:CG2	2.51	0.58
1:A:76:ALA:HA	1:A:91:PHE:CE2	2.39	0.58
1:A:160:THR:HG22	1:A:160:THR:O	2.03	0.58
1:A:207:MET:CB	1:A:213:LEU:HD23	2.34	0.58
1:A:1372:LEU:HD12	1:A:1372:LEU:N	2.19	0.58
1:C:1346:ARG:HG2	1:C:1347:ILE:HD13	1.84	0.58
2:E:360:VAL:O	2:E:364:GLN:HG3	2.04	0.58
2:E:442:ASP:O	2:E:443:LYS:HB2	2.04	0.58
1:F:141:ALA:O	1:F:143:ARG:N	2.37	0.58
1:F:1389:GLU:C	1:F:1391:SER:H	2.07	0.58
3:L:98:LEU:HD11	3:L:161:LEU:HD13	1.85	0.58
1:C:1439:LEU:HD12	1:C:1439:LEU:N	2.19	0.58
1:H:83:ILE:HD11	1:H:226:PHE:CE2	2.38	0.58
2:J:320:LYS:HD2	3:M:85:SER:HB3	1.86	0.57
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.69	0.57
1:C:246:LEU:HD11	1:C:1376:VAL:HG23	1.86	0.57
1:F:190:THR:CG2	1:F:191:ALA:H	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:LEU:O	1:H:112:LEU:HD13	2.04	0.57
1:H:1272:LEU:HD13	1:H:1371:TYR:CE2	2.39	0.57
2:J:320:LYS:CB	3:M:85:SER:HB2	2.32	0.57
1:C:251:LEU:CD1	1:C:1374:LEU:HD11	2.33	0.57
1:C:1467:SER:HB2	1:C:1468:PRO:CD	2.31	0.57
2:E:413:SER:HB3	2:E:439:ASP:HB2	1.87	0.57
1:H:35:ARG:HD2	1:H:1455:ASP:OD1	2.04	0.57
1:A:86:LEU:HD11	1:A:147:VAL:O	2.03	0.57
1:A:135:VAL:HG11	1:A:149:ILE:HG23	1.86	0.57
1:A:191:ALA:C	1:A:192:VAL:CG2	2.72	0.57
1:A:233:SER:HB2	1:A:1432:PHE:H	1.70	0.57
1:A:1347:ILE:HD13	1:F:1483:ASN:HD21	1.69	0.57
1:H:120:VAL:CG1	1:H:132:ILE:HG22	2.35	0.57
1:H:1467:SER:H	2:J:400:ARG:HH12	1.52	0.57
1:H:1492:LEU:CD2	2:J:433:VAL:HG13	2.34	0.57
2:J:426:ILE:CG2	2:J:427:ASP:H	2.14	0.57
3:M:29:LEU:HD22	3:M:35:ILE:HD11	1.86	0.57
1:A:251:LEU:HB3	1:A:1368:TYR:OH	2.05	0.57
1:A:253:GLU:HG3	1:A:1369:ARG:HH11	1.65	0.57
1:C:46:TRP:CH2	1:C:77:GLY:HA2	2.40	0.57
1:H:1264:SER:HB3	1:H:1267:SER:CB	2.34	0.57
1:H:1490:VAL:HG11	2:J:403:VAL:HG13	1.87	0.57
1:F:247:ARG:NH2	1:F:1370:ASN:HA	2.20	0.57
3:L:167:ILE:CG2	3:L:178:PHE:HB2	2.33	0.57
1:C:53:THR:HB	1:C:164:ILE:HD11	1.87	0.57
1:F:178:LEU:HD23	1:F:178:LEU:H	1.69	0.57
1:H:164:ILE:O	1:H:166:LEU:N	2.37	0.57
1:H:1479:LYS:O	1:H:1486:TYR:HB3	2.04	0.57
1:H:1488:HIS:HD2	2:J:407:VAL:CG1	2.17	0.57
1:A:207:MET:HB2	1:A:213:LEU:HD23	1.86	0.57
1:A:1347:ILE:CD1	1:F:1483:ASN:HD21	2.17	0.57
1:F:52:ARG:HH11	1:F:52:ARG:HG3	1.69	0.57
1:F:204:HIS:ND1	1:F:217:LEU:HD22	2.19	0.57
1:F:251:LEU:HD11	1:F:1374:LEU:HD12	1.83	0.57
1:H:38:PHE:CZ	1:H:212:ILE:HG23	2.40	0.57
3:L:123:LEU:HD23	3:L:123:LEU:O	2.05	0.57
1:A:243:THR:HA	1:A:246:LEU:HD21	1.87	0.57
1:A:253:GLU:HG2	1:A:1369:ARG:HH11	1.69	0.56
1:A:1385:TRP:HA	1:A:1385:TRP:HE3	1.70	0.56
1:A:1403:MET:HA	1:A:1403:MET:CE	2.35	0.56
1:C:40:SER:HA	1:C:54:PHE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1371:TYR:C	1:C:1372:LEU:HD12	2.25	0.56
1:C:1403:MET:HG2	1:C:1447:LEU:HD21	1.87	0.56
1:F:93:ASN:HD21	1:H:1395:THR:HA	1.70	0.56
1:F:138:GLN:O	1:F:147:VAL:HG13	2.04	0.56
1:F:157:VAL:HG11	1:F:166:LEU:CD1	2.35	0.56
1:F:1297:GLN:O	1:F:1380:ARG:HA	2.05	0.56
1:A:1359:GLN:O	1:A:1363:GLU:HB2	2.06	0.56
1:C:1290:LEU:HD22	1:C:1293:ILE:CD1	2.34	0.56
1:C:1379:LEU:HB2	1:C:1385:TRP:CZ3	2.40	0.56
3:L:81:LEU:N	3:L:81:LEU:HD12	2.20	0.56
1:A:83:ILE:N	1:A:83:ILE:HD12	2.19	0.56
1:A:108:LEU:O	1:A:108:LEU:HD23	2.05	0.56
1:A:1435:GLN:HA	1:A:1435:GLN:HE21	1.69	0.56
1:F:43:LEU:O	1:F:44:ILE:HD13	2.05	0.56
1:F:140:ILE:O	1:F:142:GLY:N	2.38	0.56
1:F:204:HIS:CE1	1:F:217:LEU:HD22	2.40	0.56
2:J:394:ARG:HG3	2:J:394:ARG:HH11	1.70	0.56
3:L:56:PHE:C	3:L:58:ARG:H	2.09	0.56
1:H:207:MET:CE	1:H:212:ILE:HG21	2.34	0.56
1:H:233:SER:HB2	1:H:1432:PHE:H	1.70	0.56
3:L:80:THR:HG22	3:L:82:ILE:H	1.71	0.56
3:M:13:LEU:HG	3:M:52:GLU:HG3	1.87	0.56
1:A:46:TRP:CD2	1:A:112:LEU:HG	2.40	0.56
1:F:67:ASN:HA	4:F:2003:AGS:S1G	2.45	0.56
1:F:1371:TYR:C	1:F:1372:LEU:HD12	2.26	0.56
1:H:250:LEU:CD1	1:H:1303:LEU:HD11	2.35	0.56
1:A:73:THR:HG23	4:A:2001:AGS:PA	2.45	0.56
1:F:136:ARG:NH2	1:F:148:ASP:OD2	2.38	0.56
1:H:1493:LYS:HE2	2:J:423:TRP:CD2	2.41	0.56
2:J:397:ASP:O	2:J:401:ILE:HG13	2.06	0.56
1:C:1310:THR:HG23	1:C:1348:ASN:ND2	2.17	0.56
1:C:1338:GLU:O	1:C:1341:ALA:HB3	2.04	0.56
1:F:1293:ILE:HA	1:F:1446:THR:CG2	2.36	0.56
1:H:1387:ARG:HB3	1:H:1387:ARG:HH11	1.71	0.56
3:M:184:VAL:O	3:M:184:VAL:HG22	2.06	0.56
1:H:1481:LEU:HD22	2:J:411:MET:HE2	1.88	0.56
1:C:216:ARG:HH11	1:C:216:ARG:HG3	1.71	0.56
1:F:212:ILE:N	1:F:212:ILE:HD12	2.21	0.56
1:F:1439:LEU:HA	1:H:67:ASN:OD1	2.06	0.56
1:H:1264:SER:HB3	1:H:1267:SER:HB2	1.88	0.56
1:C:212:ILE:HD12	1:C:212:ILE:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ARG:HH21	1:F:163:VAL:HG22	1.70	0.56
1:H:88:LEU:CD2	1:H:224:ASN:HA	2.36	0.56
1:H:1372:LEU:HD12	1:H:1372:LEU:N	2.21	0.56
1:F:247:ARG:HA	1:F:251:LEU:HD13	1.88	0.55
1:F:1446:THR:O	1:F:1450:LEU:HB2	2.06	0.55
1:A:137:LEU:HD12	1:A:137:LEU:N	2.21	0.55
3:L:106:GLU:HB3	3:L:110:GLN:HE21	1.69	0.55
1:A:35:ARG:HH12	1:A:37:LYS:CE	2.19	0.55
1:F:78:PHE:CE2	1:F:82:LEU:HD12	2.42	0.55
1:A:220:SER:CA	1:A:223:ARG:HH21	2.19	0.55
1:C:184:LYS:O	1:C:188:GLU:N	2.37	0.55
1:C:1308:ARG:HD2	1:C:1311:HIS:CE1	2.41	0.55
2:J:343:LEU:CD2	2:J:344:PRO:HD2	2.36	0.55
3:L:96:LYS:O	3:L:99:CYS:HB3	2.05	0.55
3:L:160:ARG:HA	3:L:163:ARG:NH1	2.22	0.55
1:F:41:LEU:O	1:F:53:THR:HG23	2.07	0.55
1:H:1368:TYR:CG	1:H:1369:ARG:N	2.75	0.55
1:H:1448:PHE:HD1	1:H:1448:PHE:H	1.55	0.55
2:J:327:LEU:N	2:J:327:LEU:HD12	2.22	0.55
2:J:416:HIS:CD2	2:J:416:HIS:N	2.74	0.55
1:C:73:THR:O	1:C:76:ALA:HB3	2.05	0.55
1:C:1454:LEU:O	1:C:1455:ASP:CB	2.55	0.55
1:F:251:LEU:H	1:F:251:LEU:CD1	2.19	0.55
1:H:1345:LYS:C	1:H:1347:ILE:H	2.10	0.55
1:F:93:ASN:C	1:F:95:THR:H	2.09	0.55
1:H:217:LEU:N	1:H:217:LEU:HD12	2.20	0.55
1:H:1302:ARG:O	1:H:1376:VAL:HG13	2.07	0.55
1:A:1430:LEU:C	1:A:1431:LEU:HD12	2.27	0.55
1:F:108:LEU:HD23	1:F:108:LEU:C	2.28	0.55
1:F:125:ASN:ND2	1:F:210:LEU:O	2.40	0.55
1:H:164:ILE:C	1:H:166:LEU:H	2.10	0.55
1:A:1492:LEU:HD11	2:E:352:LEU:HD13	1.89	0.55
3:L:10:PRO:O	3:L:13:LEU:HB3	2.07	0.55
1:A:1430:LEU:C	1:A:1430:LEU:HD23	2.28	0.54
1:C:131:ILE:HG22	1:C:133:THR:HG23	1.89	0.54
1:F:54:PHE:N	1:F:54:PHE:CD1	2.75	0.54
1:F:246:LEU:HD23	1:F:246:LEU:C	2.28	0.54
3:L:87:MET:HE2	3:L:92:MET:SD	2.47	0.54
3:M:98:LEU:HB3	3:M:184:VAL:HG21	1.88	0.54
1:A:191:ALA:O	1:A:192:VAL:HG23	2.08	0.54
1:F:41:LEU:HB2	1:F:56:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:ARG:HH21	3:L:163:ARG:HA	1.72	0.54
1:A:1351:ILE:HD12	1:A:1351:ILE:N	2.21	0.54
1:C:41:LEU:HG	1:C:41:LEU:O	2.07	0.54
1:C:59:LEU:HD11	1:C:1452:GLU:HG2	1.89	0.54
1:F:39:ARG:HB2	1:F:122:GLU:HG2	1.89	0.54
3:M:91:GLU:C	3:M:94:VAL:HB	2.27	0.54
3:M:96:LYS:HG2	3:M:187:PHE:O	2.08	0.54
1:A:215:LYS:O	1:A:217:LEU:HD12	2.07	0.54
1:A:1435:GLN:HE21	1:A:1435:GLN:CA	2.19	0.54
2:J:360:VAL:O	2:J:364:GLN:N	2.38	0.54
3:L:29:LEU:HB3	3:L:74:LEU:HG	1.88	0.54
3:L:56:PHE:O	3:L:58:ARG:N	2.40	0.54
1:A:86:LEU:HD21	1:A:149:ILE:HD12	1.88	0.54
4:A:2001:AGS:H3'	1:C:1397:GLU:OE1	2.08	0.54
3:M:88:SER:HB3	3:M:91:GLU:HB2	1.88	0.54
1:A:1478:ARG:HB2	1:A:1487:VAL:HG22	1.89	0.54
1:C:136:ARG:HE	1:C:136:ARG:C	2.10	0.54
1:C:229:LEU:HD23	1:C:229:LEU:C	2.28	0.54
1:C:1340:LEU:O	1:C:1343:LEU:HB2	2.08	0.54
1:C:1440:ASP:OD1	1:C:1442:MET:N	2.40	0.54
1:F:1387:ARG:NH1	1:F:1387:ARG:HB2	2.22	0.54
1:H:112:LEU:HD21	1:H:137:LEU:HD23	1.90	0.54
3:M:60:TYR:HA	3:M:81:LEU:HB2	1.89	0.54
1:A:41:LEU:HB2	1:A:56:PHE:CZ	2.42	0.54
1:A:225:LYS:HZ1	1:A:248:ASP:HB3	1.72	0.54
1:C:33:ILE:HG22	1:C:1426:LEU:HD11	1.88	0.54
2:E:371:ARG:HG2	2:E:441:TYR:CE2	2.43	0.54
1:H:178:LEU:HB2	1:H:182:ASP:HB2	1.89	0.54
3:L:33:ARG:HG3	3:L:165:GLY:HA3	1.90	0.54
1:A:119:ALA:O	1:A:134:GLY:HA3	2.08	0.54
1:A:1478:ARG:HE	1:A:1487:VAL:HG22	1.72	0.54
1:F:1387:ARG:NH1	1:F:1387:ARG:CB	2.71	0.54
3:L:179:ILE:HD12	3:L:179:ILE:N	2.23	0.54
3:M:40:LEU:HD23	3:M:40:LEU:O	2.08	0.54
1:A:130:ARG:HH22	1:A:163:VAL:HG13	1.72	0.54
1:C:150:ARG:HH22	1:C:198:HIS:CD2	2.26	0.54
1:C:1395:THR:O	1:C:1399:ILE:HG13	2.07	0.54
1:H:174:LYS:O	1:H:175:ALA:CB	2.56	0.54
1:H:1289:GLY:O	1:H:1290:LEU:HD23	2.08	0.54
2:J:315:LEU:O	3:M:210:ALA:HA	2.07	0.54
1:A:1476:LEU:HD12	1:A:1476:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1421:ARG:HG2	1:C:1422:ALA:H	1.73	0.54
1:C:1488:HIS:CD2	2:E:407:VAL:HG13	2.43	0.54
1:F:57:ASP:HB2	1:F:1472:THR:CB	2.38	0.54
1:H:39:ARG:HG3	1:H:39:ARG:NH1	2.22	0.54
1:H:46:TRP:HZ2	1:H:119:ALA:HB2	1.72	0.54
1:H:60:VAL:HG21	1:H:1448:PHE:CD2	2.43	0.54
1:H:238:ILE:HD11	1:H:1401:THR:HG21	1.90	0.54
2:J:324:LEU:HD23	2:J:324:LEU:C	2.29	0.54
2:J:422:VAL:HG12	2:J:423:TRP:N	2.23	0.54
3:L:119:VAL:O	3:L:123:LEU:HB2	2.08	0.54
1:A:1379:LEU:HD12	1:A:1384:GLY:CA	2.38	0.53
1:C:246:LEU:O	1:C:246:LEU:HD23	2.07	0.53
1:F:154:LEU:HD23	1:F:194:PHE:HA	1.90	0.53
1:F:1340:LEU:HA	1:F:1343:LEU:HB2	1.90	0.53
1:H:261:PHE:HE2	1:H:1336:PHE:CE2	2.25	0.53
1:H:1278:ARG:HG2	1:H:1282:ARG:HH21	1.72	0.53
1:H:1379:LEU:HD12	1:H:1384:GLY:O	2.08	0.53
3:L:164:ILE:HB	3:L:166:ILE:HG13	1.89	0.53
3:M:98:LEU:CB	3:M:184:VAL:HG21	2.37	0.53
1:A:249:TYR:O	1:A:250:LEU:HD23	2.08	0.53
4:A:2001:AGS:O3B	1:C:1394:SER:HB2	2.07	0.53
1:F:84:PRO:HG2	1:F:200:ILE:CD1	2.38	0.53
1:F:1430:LEU:C	1:F:1431:LEU:HD12	2.29	0.53
1:H:135:VAL:CG1	1:H:149:ILE:HG23	2.38	0.53
1:H:1266:GLU:HG2	1:H:1318:LEU:O	2.08	0.53
1:A:135:VAL:HG13	1:A:150:ARG:O	2.07	0.53
1:A:1492:LEU:HD23	1:A:1492:LEU:O	2.07	0.53
1:C:1430:LEU:HD23	1:C:1430:LEU:C	2.29	0.53
1:C:1435:GLN:HE22	1:C:1463:PRO:HB3	1.73	0.53
1:F:117:CYS:HB2	1:F:137:LEU:O	2.09	0.53
1:F:1304:VAL:CG1	1:F:1306:ASN:ND2	2.70	0.53
1:H:1430:LEU:C	1:H:1430:LEU:HD23	2.29	0.53
3:L:65:ILE:N	3:L:65:ILE:HD12	2.23	0.53
1:F:1305:VAL:O	1:F:1305:VAL:HG12	2.07	0.53
1:F:1343:LEU:O	1:F:1347:ILE:HD13	2.08	0.53
3:L:87:MET:HB3	3:L:91:GLU:CD	2.28	0.53
1:A:50:PHE:HD1	2:E:343:LEU:HD13	1.73	0.53
1:A:127:ARG:HG3	1:A:1425:ILE:CD1	2.34	0.53
1:C:83:ILE:HD11	1:C:226:PHE:HE2	1.74	0.53
1:C:89:LEU:HD23	1:C:227:TYR:HE2	1.72	0.53
1:C:213:LEU:HD13	1:C:217:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1287:ASN:ND2	1:C:1303:LEU:H	1.91	0.53
1:F:71:LYS:O	1:F:74:THR:HB	2.09	0.53
1:H:206:PHE:CE1	1:H:210:LEU:HD11	2.44	0.53
2:J:355:VAL:O	2:J:355:VAL:HG12	2.08	0.53
3:M:60:TYR:HA	3:M:81:LEU:HD12	1.89	0.53
1:A:96:GLU:HB3	1:A:99:SER:OG	2.09	0.53
2:E:392:GLN:HA	2:E:395:HIS:ND1	2.24	0.53
1:F:1438:ARG:HA	1:H:1435:GLN:NE2	2.24	0.53
1:H:110:GLY:HA3	4:H:2004:AGS:N1	2.24	0.53
1:H:125:ASN:OD1	1:H:210:LEU:HB3	2.09	0.53
1:H:1272:LEU:HD13	1:H:1371:TYR:HE2	1.73	0.53
1:H:1402:GLY:O	1:H:1406:LEU:HB2	2.09	0.53
2:J:320:LYS:NZ	3:M:86:ALA:O	2.39	0.53
3:L:64:LEU:C	3:L:65:ILE:HD12	2.29	0.53
3:L:87:MET:HB3	3:L:91:GLU:OE1	2.09	0.53
1:A:1302:ARG:HD3	1:A:1385:TRP:CZ2	2.44	0.53
1:C:53:THR:CB	1:C:164:ILE:HD11	2.39	0.53
1:C:1383:TYR:O	1:C:1384:GLY:C	2.47	0.53
1:F:1394:SER:OG	1:F:1397:GLU:HG3	2.08	0.53
1:H:208:PHE:C	1:H:210:LEU:H	2.12	0.53
2:J:367:LEU:O	2:J:370:PHE:N	2.42	0.53
3:M:89:GLU:O	3:M:93:LEU:N	2.41	0.53
1:A:1475:LYS:C	1:A:1476:LEU:HD12	2.29	0.53
2:E:384:GLN:HB2	2:E:426:ILE:CD1	2.38	0.53
1:F:81:ALA:HA	1:F:135:VAL:HG21	1.91	0.53
1:F:87:THR:HB	1:F:88:LEU:HD12	1.91	0.53
1:H:1357:MET:N	1:H:1358:PRO:HD2	2.24	0.53
2:J:392:GLN:NE2	2:J:427:ASP:OD2	2.41	0.53
3:M:98:LEU:C	3:M:184:VAL:HG21	2.29	0.53
1:A:1283:ILE:O	1:A:1284:LEU:C	2.47	0.53
1:A:1360:THR:O	1:A:1364:GLU:HG3	2.08	0.53
1:H:1456:MET:HG2	1:H:1457:GLN:N	2.23	0.53
1:H:1481:LEU:C	1:H:1483:ASN:H	2.11	0.53
1:A:127:ARG:O	1:A:128:ALA:HB3	2.09	0.53
1:A:1492:LEU:HD11	2:E:352:LEU:CD1	2.39	0.53
1:F:151:PRO:HB3	1:F:203:TYR:CD1	2.44	0.53
1:H:151:PRO:HB3	1:H:203:TYR:CD1	2.44	0.53
1:H:263:ASP:C	1:H:265:GLU:H	2.12	0.53
1:H:1269:ALA:HB2	1:H:1318:LEU:CD1	2.39	0.53
1:A:89:LEU:HD23	1:A:227:TYR:CE2	2.42	0.52
1:C:81:ALA:HA	1:C:135:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:407:VAL:C	2:E:409:LEU:H	2.13	0.52
1:F:52:ARG:NH1	2:J:345:MET:HG2	2.23	0.52
1:F:65:GLY:O	1:F:1463:PRO:HA	2.10	0.52
1:F:229:LEU:HG	1:F:1406:LEU:HG	1.91	0.52
1:F:1347:ILE:HG22	1:F:1348:ASN:CG	2.29	0.52
1:F:57:ASP:HB2	1:F:1472:THR:HB	1.91	0.52
1:F:109:TYR:HB2	1:F:145:LYS:O	2.10	0.52
1:F:1268:VAL:O	1:F:1272:LEU:HG	2.08	0.52
1:H:187:PHE:CD2	1:H:192:VAL:HG21	2.43	0.52
1:A:113:LYS:HE2	1:A:113:LYS:HA	1.91	0.52
1:A:251:LEU:N	1:A:251:LEU:CD1	2.72	0.52
1:C:250:LEU:CD1	1:C:1303:LEU:HD11	2.37	0.52
1:F:1302:ARG:HD3	1:F:1385:TRP:CZ2	2.44	0.52
1:F:1468:PRO:O	1:F:1470:ARG:N	2.43	0.52
1:H:226:PHE:CE2	1:H:230:ILE:HD11	2.44	0.52
3:M:69:GLU:CG	3:M:71:PHE:HE1	2.23	0.52
1:A:92:ARG:HD2	1:A:99:SER:HB2	1.90	0.52
1:A:203:TYR:O	1:A:206:PHE:HB3	2.10	0.52
1:C:1416:GLU:O	1:C:1416:GLU:HG2	2.09	0.52
1:F:88:LEU:CD2	1:F:224:ASN:HA	2.39	0.52
1:F:1394:SER:HB3	4:H:2004:AGS:H5'1	1.91	0.52
1:F:1476:LEU:HD12	1:F:1476:LEU:N	2.25	0.52
1:F:1492:LEU:HD21	2:J:352:LEU:HD13	1.91	0.52
1:H:1307:ILE:O	1:H:1308:ARG:C	2.48	0.52
1:H:1481:LEU:C	1:H:1483:ASN:N	2.63	0.52
3:L:56:PHE:HE1	3:L:59:ARG:HH22	1.57	0.52
3:L:97:VAL:O	3:L:101:LEU:HD13	2.10	0.52
1:A:1273:ARG:NH1	1:A:1315:LEU:HB3	2.25	0.52
1:A:1405:ILE:O	1:A:1409:VAL:HG23	2.08	0.52
1:C:132:ILE:O	1:C:153:SER:HA	2.09	0.52
1:C:227:TYR:C	1:C:227:TYR:CD1	2.82	0.52
2:E:414:GLN:HG3	2:E:417:GLN:CG	2.38	0.52
1:F:216:ARG:HH11	1:F:218:ARG:HD2	1.74	0.52
1:H:1393:LEU:HA	1:H:1397:GLU:OE1	2.09	0.52
1:A:1434:ASP:O	1:A:1435:GLN:HB2	2.10	0.52
1:C:219:SER:HB3	1:C:222:ASP:OD1	2.09	0.52
1:C:261:PHE:HZ	1:C:1336:PHE:CD2	2.26	0.52
1:C:1464:GLU:HG2	1:C:1465:ASN:H	1.75	0.52
1:F:178:LEU:HD12	1:F:182:ASP:HB3	1.92	0.52
1:F:1437:ALA:CB	1:H:1437:ALA:HB1	2.40	0.52
3:L:25:LEU:HD11	3:L:46:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:116:GLN:HE21	3:L:158:LEU:CD2	2.22	0.52
3:M:88:SER:HB3	3:M:91:GLU:OE1	2.09	0.52
1:C:1456:MET:CG	1:C:1457:GLN:N	2.73	0.52
2:J:316:LEU:HD12	3:M:187:PHE:CD1	2.45	0.52
2:J:373:THR:CG2	2:J:375:GLN:HG3	2.40	0.52
3:L:52:GLU:O	3:L:54:GLU:N	2.43	0.52
1:A:73:THR:HG22	1:A:111:LYS:HZ3	1.75	0.52
1:C:35:ARG:NH1	1:C:1427:PRO:O	2.42	0.52
1:C:1313:ILE:N	1:C:1313:ILE:HD12	2.25	0.52
1:C:1429:ARG:O	1:C:1456:MET:HG3	2.10	0.52
1:F:83:ILE:HD11	1:F:230:ILE:CD1	2.32	0.52
1:F:1390:SER:HB2	1:H:104:ARG:NH2	2.24	0.52
1:H:229:LEU:O	1:H:232:ALA:HB3	2.10	0.52
1:H:1294:ALA:HB3	1:H:1446:THR:OG1	2.09	0.52
3:L:44:ALA:O	3:L:47:MET:HB3	2.09	0.52
1:C:1276:ILE:HA	1:C:1368:TYR:HE2	1.72	0.52
1:H:41:LEU:HD12	1:H:120:VAL:O	2.09	0.52
1:A:217:LEU:HD12	1:A:217:LEU:H	1.73	0.52
1:H:1481:LEU:HD23	2:J:416:HIS:HE1	1.75	0.52
1:A:92:ARG:NH1	1:A:99:SER:H	2.08	0.51
1:A:253:GLU:CG	1:A:1369:ARG:NH1	2.67	0.51
1:C:252:PRO:HG3	1:C:1416:GLU:CD	2.31	0.51
2:E:379:LEU:HD11	2:E:406:ALA:HB1	1.92	0.51
1:F:1493:LYS:O	2:J:351:SER:HA	2.11	0.51
1:H:140:ILE:HD12	1:H:146:LYS:HG2	1.92	0.51
1:H:1347:ILE:HG12	3:L:111:GLN:NE2	2.25	0.51
3:L:80:THR:HG22	3:L:82:ILE:N	2.25	0.51
3:L:120:TYR:OH	3:L:151:ALA:HB2	2.10	0.51
1:A:1402:GLY:O	1:A:1406:LEU:HD13	2.10	0.51
1:C:1467:SER:CB	1:C:1468:PRO:HD2	2.34	0.51
1:H:1467:SER:HB2	1:H:1468:PRO:CD	2.39	0.51
1:A:131:ILE:C	1:A:132:ILE:HD12	2.29	0.51
1:A:1304:VAL:HG21	1:A:1377:GLU:OE2	2.10	0.51
1:C:110:GLY:C	1:C:112:LEU:H	2.14	0.51
1:C:1389:GLU:HA	1:C:1389:GLU:OE2	2.09	0.51
2:J:318:THR:HG23	2:J:318:THR:O	2.10	0.51
2:J:387:LEU:HD22	2:J:395:HIS:CD2	2.45	0.51
1:A:237:GLY:H	1:A:1399:ILE:HD13	1.73	0.51
1:C:247:ARG:HG2	1:C:247:ARG:NH1	2.25	0.51
1:F:245:SER:HB3	1:F:248:ASP:CG	2.31	0.51
1:F:1410:VAL:HG11	1:F:1456:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:367:LEU:O	2:J:369:HIS:N	2.44	0.51
1:H:1432:PHE:O	1:H:1433:LEU:HB2	2.10	0.51
1:A:192:VAL:HG12	1:A:193:THR:N	2.25	0.51
1:A:1447:LEU:O	1:A:1450:LEU:HB2	2.11	0.51
3:L:33:ARG:HB2	3:L:163:ARG:O	2.11	0.51
1:A:132:ILE:HD13	1:A:154:LEU:O	2.11	0.51
1:A:1440:ASP:OD2	1:C:67:ASN:HB2	2.10	0.51
1:A:1467:SER:O	1:A:1468:PRO:O	2.29	0.51
1:F:131:ILE:CD1	1:F:210:LEU:HB3	2.41	0.51
1:F:1295:PHE:CE2	1:F:1400:GLY:HA3	2.45	0.51
1:H:1407:LEU:HD22	1:H:1456:MET:HE2	1.90	0.51
2:J:387:LEU:HD12	2:J:426:ILE:HG21	1.92	0.51
3:L:17:ILE:HA	3:L:22:PHE:HB3	1.92	0.51
3:L:158:LEU:HD12	3:L:161:LEU:HD12	1.92	0.51
3:M:71:PHE:CD2	3:M:183:ALA:HA	2.46	0.51
1:A:1342:MET:HA	1:A:1345:LYS:HB2	1.93	0.51
1:C:1305:VAL:HG13	1:C:1372:LEU:HD23	1.93	0.51
1:F:143:ARG:HG3	1:F:144:ASP:H	1.76	0.51
1:H:52:ARG:CZ	1:H:1489:VAL:HB	2.40	0.51
1:H:59:LEU:HD11	1:H:1452:GLU:CG	2.40	0.51
1:H:1362:GLY:O	1:H:1366:LEU:HG	2.11	0.51
1:H:1441:ALA:O	1:H:1444:ILE:HG22	2.11	0.51
1:A:206:PHE:CZ	1:A:210:LEU:HD11	2.46	0.51
1:H:147:VAL:HG12	1:H:148:ASP:N	2.26	0.51
1:H:227:TYR:C	1:H:227:TYR:CD1	2.84	0.51
1:H:1337:SER:HB3	1:H:1359:GLN:HG3	1.93	0.51
1:H:1444:ILE:HG23	1:H:1445:ASN:N	2.26	0.51
1:A:43:LEU:O	1:A:44:ILE:HD13	2.10	0.50
1:A:208:PHE:HE2	1:A:216:ARG:NH1	2.09	0.50
1:A:1377:GLU:HG2	1:A:1387:ARG:HA	1.92	0.50
1:F:1429:ARG:HB3	1:F:1456:MET:HG3	1.92	0.50
1:F:1440:ASP:OD1	1:F:1442:MET:N	2.44	0.50
1:H:62:THR:HG22	1:H:63:LEU:H	1.76	0.50
1:H:173:ASN:O	2:J:417:GLN:OE1	2.27	0.50
1:H:1430:LEU:HA	1:H:1457:GLN:O	2.12	0.50
2:J:416:HIS:O	2:J:418:ALA:N	2.43	0.50
2:J:430:SER:O	2:J:431:ALA:O	2.29	0.50
3:L:34:HIS:O	3:L:35:ILE:HD13	2.12	0.50
1:A:195:LYS:HE3	1:A:197:TYR:OH	2.11	0.50
1:C:1401:THR:O	1:C:1405:ILE:HG12	2.11	0.50
1:H:1466:ILE:HA	2:J:400:ARG:NH2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:C	1:A:83:ILE:HD12	2.32	0.50
1:A:135:VAL:HG22	1:A:151:PRO:CA	2.38	0.50
1:C:49:PHE:CE2	1:C:1487:VAL:HG21	2.46	0.50
1:F:73:THR:O	1:F:76:ALA:HB3	2.12	0.50
1:F:132:ILE:HD12	1:F:157:VAL:HG21	1.94	0.50
1:F:192:VAL:HG12	1:F:193:THR:N	2.26	0.50
1:F:1368:TYR:CD1	1:F:1369:ARG:N	2.79	0.50
1:H:1309:ASP:O	1:H:1313:ILE:HG12	2.11	0.50
1:H:1367:ASP:OD2	1:H:1369:ARG:HD3	2.10	0.50
3:L:157:ALA:HA	3:L:160:ARG:HE	1.75	0.50
1:A:124:VAL:CG1	1:A:128:ALA:HA	2.42	0.50
1:C:1302:ARG:HD3	1:C:1385:TRP:CH2	2.46	0.50
1:C:1387:ARG:CB	1:C:1387:ARG:HH11	2.24	0.50
1:F:45:ASN:ND2	1:F:117:CYS:SG	2.83	0.50
1:H:140:ILE:CG2	1:H:141:ALA:H	2.23	0.50
2:J:413:SER:HB3	2:J:439:ASP:HB2	1.93	0.50
3:L:59:ARG:HH11	3:L:59:ARG:HG3	1.76	0.50
3:L:89:GLU:O	3:L:93:LEU:HG	2.11	0.50
3:M:211:THR:HG22	3:M:212:THR:N	2.26	0.50
1:A:110:GLY:HA3	4:A:2001:AGS:N1	2.25	0.50
1:A:183:LEU:O	1:A:186:LYS:HB2	2.12	0.50
1:A:1347:ILE:O	1:A:1349:PRO:HD3	2.11	0.50
1:C:204:HIS:ND1	1:C:217:LEU:HD23	2.25	0.50
1:F:1303:LEU:HD23	1:F:1375:GLU:O	2.10	0.50
1:F:1387:ARG:HB2	1:F:1387:ARG:CZ	2.41	0.50
1:H:1440:ASP:O	1:H:1444:ILE:HG22	2.10	0.50
1:A:77:GLY:O	1:A:81:ALA:N	2.45	0.50
1:C:72:SER:HA	1:C:75:MET:CE	2.41	0.50
1:C:125:ASN:O	1:C:128:ALA:N	2.44	0.50
1:F:1287:ASN:HD21	1:F:1303:LEU:N	2.09	0.50
1:H:250:LEU:CD1	1:H:1303:LEU:CD1	2.84	0.50
3:L:9:ILE:HB	3:L:10:PRO:HD3	1.92	0.50
1:A:204:HIS:C	1:A:206:PHE:H	2.14	0.50
1:A:1454:LEU:HD12	1:A:1454:LEU:N	2.27	0.50
1:C:1495:PHE:HE2	2:E:396:PHE:HA	1.75	0.50
1:F:84:PRO:HG2	1:F:200:ILE:HD11	1.92	0.50
1:F:130:ARG:NH1	1:F:159:MET:HA	2.20	0.50
1:F:226:PHE:O	1:F:230:ILE:HG13	2.10	0.50
3:L:15:ILE:O	3:L:15:ILE:HG22	2.12	0.50
3:M:35:ILE:HD13	3:M:72:PHE:HB2	1.92	0.50
3:M:49:PHE:O	3:M:53:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:CE1	1:A:1487:VAL:HB	2.46	0.50
1:A:112:LEU:HD12	1:A:112:LEU:N	2.27	0.50
1:A:135:VAL:CG1	1:A:136:ARG:N	2.75	0.50
1:A:163:VAL:HG12	1:A:166:LEU:HD12	1.93	0.50
1:C:52:ARG:HG2	1:C:1489:VAL:HG21	1.93	0.50
1:C:81:ALA:HA	1:C:135:VAL:CG2	2.42	0.50
1:F:59:LEU:HD22	1:F:1452:GLU:CG	2.42	0.50
1:F:1362:GLY:O	1:F:1366:LEU:HD13	2.12	0.50
1:A:124:VAL:HG13	1:A:128:ALA:HA	1.94	0.50
1:C:1415:GLU:HA	1:C:1418:ARG:HG3	1.94	0.50
1:C:1490:VAL:HG11	2:E:403:VAL:CG1	2.41	0.50
2:E:354:ASP:C	2:E:356:GLN:N	2.64	0.50
1:F:249:TYR:HB3	1:F:1409:VAL:HG13	1.92	0.50
3:L:9:ILE:O	3:L:13:LEU:HB2	2.11	0.50
1:A:72:SER:OG	1:A:1434:ASP:OD1	2.30	0.49
1:C:89:LEU:HD22	1:C:91:PHE:CE1	2.46	0.49
1:C:140:ILE:O	1:C:141:ALA:C	2.51	0.49
1:C:181:ASN:ND2	2:J:384:GLN:NE2	2.60	0.49
1:F:1292:ASN:HD22	1:F:1292:ASN:N	2.10	0.49
1:H:73:THR:HG23	4:H:2004:AGS:O2A	2.12	0.49
3:L:72:PHE:N	3:L:72:PHE:CD1	2.79	0.49
3:L:196:ASP:OD1	3:L:198:ARG:N	2.45	0.49
1:A:261:PHE:HE1	1:A:1336:PHE:HD2	1.60	0.49
1:C:1444:ILE:HG23	1:C:1445:ASN:N	2.27	0.49
1:F:140:ILE:HG23	2:J:331:GLU:HB3	1.94	0.49
1:H:1434:ASP:OD2	1:H:1435:GLN:N	2.45	0.49
1:H:1494:GLY:O	1:H:1495:PHE:O	2.30	0.49
1:C:1344:TYR:O	1:C:1348:ASN:HB2	2.12	0.49
1:C:1464:GLU:HG2	1:C:1465:ASN:N	2.27	0.49
1:F:178:LEU:HD23	1:F:178:LEU:N	2.26	0.49
1:H:1286:LEU:HD22	1:H:1411:GLN:CD	2.32	0.49
3:M:69:GLU:O	3:M:182:GLU:HG2	2.13	0.49
1:C:158:PRO:O	1:C:160:THR:N	2.46	0.49
1:C:179:SER:O	1:C:182:ASP:HB2	2.13	0.49
1:C:1456:MET:HG2	1:C:1457:GLN:H	1.77	0.49
1:F:229:LEU:HD13	1:F:1413:TRP:HZ3	1.77	0.49
1:F:246:LEU:HD23	1:F:246:LEU:O	2.13	0.49
1:F:1438:ARG:HH12	1:H:95:THR:HG22	1.75	0.49
1:A:47:ASN:H	1:A:112:LEU:HA	1.76	0.49
1:A:88:LEU:HD21	1:A:224:ASN:HA	1.95	0.49
1:A:1430:LEU:HD23	1:A:1431:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ILE:O	1:C:117:CYS:HB3	2.11	0.49
1:C:148:ASP:HB3	2:J:429:PHE:CD2	2.48	0.49
1:F:44:ILE:C	1:F:46:TRP:H	2.16	0.49
1:H:178:LEU:CD1	1:H:183:LEU:HD23	2.43	0.49
1:H:222:ASP:O	1:H:223:ARG:C	2.51	0.49
1:H:1350:HIS:ND1	1:H:1350:HIS:O	2.45	0.49
1:C:138:GLN:HB3	2:J:429:PHE:HE2	1.73	0.49
2:E:353:THR:HG23	2:E:353:THR:O	2.11	0.49
1:F:1294:ALA:HB3	1:F:1446:THR:OG1	2.13	0.49
1:H:180:LEU:HA	1:H:183:LEU:HD12	1.95	0.49
1:H:247:ARG:HH11	1:H:247:ARG:HG3	1.78	0.49
3:L:201:GLN:HE22	3:L:204:LEU:HD23	1.77	0.49
3:M:69:GLU:HG2	3:M:71:PHE:HE1	1.78	0.49
1:C:203:TYR:O	1:C:206:PHE:HB3	2.13	0.49
1:C:1377:GLU:HG2	1:C:1387:ARG:HA	1.94	0.49
3:L:199:GLU:HG3	3:L:202:LEU:HD12	1.92	0.49
1:C:1313:ILE:O	1:C:1317:ALA:N	2.46	0.49
2:E:370:PHE:O	2:E:373:THR:O	2.30	0.49
1:F:247:ARG:CA	1:F:251:LEU:HD13	2.43	0.49
1:F:1266:GLU:HG2	1:F:1321:GLN:NE2	2.17	0.49
1:H:229:LEU:HD23	1:H:229:LEU:C	2.33	0.49
3:L:167:ILE:HG22	3:L:168:THR:N	2.27	0.49
1:C:72:SER:HA	1:C:75:MET:HE2	1.93	0.49
1:C:93:ASN:C	1:C:95:THR:H	2.14	0.49
1:F:250:LEU:O	1:F:252:PRO:HD3	2.12	0.49
1:A:100:THR:O	1:A:100:THR:HG22	2.13	0.49
1:A:163:VAL:O	1:A:166:LEU:HB2	2.13	0.49
1:A:208:PHE:CD2	1:A:216:ARG:HD3	2.47	0.49
1:A:1287:ASN:O	1:A:1289:GLY:N	2.46	0.49
1:A:1394:SER:HB3	4:C:2002:AGS:H5'1	1.95	0.49
1:C:233:SER:HB2	1:C:1432:PHE:H	1.77	0.49
1:C:234:LEU:O	1:C:236:GLY:N	2.46	0.49
1:F:50:PHE:O	1:F:51:ALA:HB2	2.12	0.49
1:F:93:ASN:O	1:F:95:THR:N	2.46	0.49
1:F:164:ILE:HG21	2:J:345:MET:CE	2.43	0.49
1:F:1275:THR:HG22	1:F:1368:TYR:CD2	2.48	0.49
2:J:373:THR:C	2:J:375:GLN:N	2.66	0.49
1:A:1413:TRP:O	1:A:1416:GLU:HB3	2.12	0.48
1:C:197:TYR:HD1	1:C:202:ASP:HB3	1.78	0.48
1:F:57:ASP:HB2	1:F:1472:THR:OG1	2.13	0.48
1:F:1304:VAL:CG1	1:F:1306:ASN:HD21	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:PHE:CA	1:H:178:LEU:HD21	2.41	0.48
1:A:1287:ASN:HD21	1:A:1303:LEU:N	1.98	0.48
1:A:1293:ILE:HG23	1:A:1295:PHE:HD1	1.77	0.48
1:A:1415:GLU:HA	1:A:1418:ARG:HG3	1.94	0.48
1:C:33:ILE:CG2	1:C:1426:LEU:HD11	2.43	0.48
1:F:1314:LEU:O	1:F:1314:LEU:HD23	2.14	0.48
1:H:112:LEU:HD21	1:H:137:LEU:HD22	1.96	0.48
3:L:22:PHE:HB3	3:L:23:PRO:HD3	1.94	0.48
1:A:1299:LYS:CB	1:A:1379:LEU:HD23	2.43	0.48
1:C:33:ILE:HG22	1:C:1426:LEU:CD1	2.43	0.48
1:C:1277:GLN:HA	1:C:1277:GLN:HE21	1.78	0.48
1:C:1435:GLN:HA	1:C:1435:GLN:NE2	2.29	0.48
1:A:216:ARG:HH11	1:A:216:ARG:CG	2.27	0.48
1:A:1351:ILE:H	1:A:1351:ILE:CD1	2.23	0.48
1:A:1405:ILE:HA	1:A:1408:MET:HG2	1.95	0.48
1:C:151:PRO:HB3	1:C:203:TYR:CG	2.48	0.48
1:A:1304:VAL:HG12	1:A:1306:ASN:ND2	2.28	0.48
1:A:1380:ARG:O	1:A:1384:GLY:HA2	2.14	0.48
1:A:1429:ARG:O	1:A:1456:MET:HG3	2.13	0.48
1:C:46:TRP:NE1	1:C:118:TYR:O	2.42	0.48
1:C:84:PRO:CG	1:C:200:ILE:HD13	2.43	0.48
2:E:362:ALA:O	2:E:366:GLU:HB2	2.13	0.48
1:F:62:THR:HG23	1:F:1460:ILE:HG13	1.96	0.48
1:F:136:ARG:C	1:F:137:LEU:HD12	2.34	0.48
1:F:238:ILE:HG13	1:F:1398:ALA:HB1	1.96	0.48
1:H:82:LEU:C	1:H:83:ILE:HD13	2.34	0.48
1:H:1367:ASP:OD2	1:H:1369:ARG:HD2	2.13	0.48
1:H:1463:PRO:HB3	4:H:2004:AGS:S1G	2.54	0.48
3:L:62:VAL:HG12	3:L:63:ASP:N	2.29	0.48
1:A:1314:LEU:HD23	1:A:1314:LEU:O	2.14	0.48
1:C:84:PRO:HG2	1:C:200:ILE:HD13	1.96	0.48
1:C:1470:ARG:HH11	1:C:1470:ARG:HG3	1.78	0.48
1:C:1478:ARG:NH1	1:C:1485:GLU:OE2	2.47	0.48
2:E:392:GLN:O	2:E:392:GLN:HG2	2.13	0.48
1:F:59:LEU:HD22	1:F:1452:GLU:CD	2.34	0.48
3:L:29:LEU:HB3	3:L:74:LEU:CD1	2.44	0.48
3:L:87:MET:CE	3:L:92:MET:SD	3.02	0.48
1:A:82:LEU:CB	1:A:83:ILE:HD12	2.43	0.48
1:C:254:ASN:ND2	1:C:254:ASN:H	2.12	0.48
1:C:1433:LEU:HG	1:C:1433:LEU:O	2.12	0.48
1:F:1358:PRO:HG2	1:F:1359:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:PHE:CD1	1:H:50:PHE:C	2.87	0.48
3:L:12:LYS:O	3:L:16:ALA:HB2	2.12	0.48
3:L:150:LEU:O	3:L:154:VAL:HG23	2.14	0.48
3:M:67:ALA:HB1	3:M:69:GLU:OE2	2.13	0.48
1:A:52:ARG:HG3	1:A:53:THR:N	2.29	0.48
1:A:229:LEU:HD12	1:A:1409:VAL:CG1	2.42	0.48
1:A:243:THR:O	1:A:246:LEU:HG	2.14	0.48
1:F:44:ILE:HB	1:F:118:TYR:HB2	1.95	0.48
1:H:178:LEU:HD11	1:H:183:LEU:HD23	1.96	0.48
3:L:9:ILE:N	3:L:9:ILE:HD12	2.28	0.48
3:L:37:ILE:HG22	3:L:37:ILE:O	2.13	0.48
3:L:59:ARG:HB3	3:M:23:PRO:HG2	1.95	0.48
3:L:116:GLN:NE2	3:L:158:LEU:HD23	2.29	0.48
1:A:111:LYS:C	1:A:112:LEU:HD12	2.34	0.48
1:A:1407:LEU:HD13	1:A:1454:LEU:CD2	2.44	0.48
1:C:125:ASN:C	1:C:127:ARG:H	2.16	0.48
1:F:1276:ILE:HD12	1:F:1372:LEU:CD1	2.44	0.48
1:F:1318:LEU:HD21	1:F:1343:LEU:HD13	1.96	0.48
1:C:1456:MET:CG	1:C:1457:GLN:H	2.26	0.48
1:F:1290:LEU:HB3	1:F:1293:ILE:CD1	2.44	0.48
1:H:36:GLY:O	1:H:37:LYS:HG2	2.14	0.48
3:M:69:GLU:HG2	3:M:71:PHE:CE1	2.48	0.48
1:A:112:LEU:CD2	1:A:137:LEU:HD22	2.41	0.47
1:C:1368:TYR:HD1	1:C:1369:ARG:N	2.12	0.47
1:F:127:ARG:NE	1:F:1425:ILE:HD11	2.29	0.47
1:H:1314:LEU:O	1:H:1314:LEU:HD23	2.14	0.47
1:H:1433:LEU:HB3	1:H:1460:ILE:HG22	1.96	0.47
2:J:367:LEU:C	2:J:369:HIS:N	2.66	0.47
1:A:1287:ASN:ND2	1:A:1303:LEU:H	1.97	0.47
2:E:359:ILE:O	2:E:363:ILE:HG13	2.15	0.47
2:E:383:LEU:HD12	2:E:433:VAL:HG21	1.93	0.47
1:H:243:THR:HA	1:H:246:LEU:HD21	1.95	0.47
1:H:1314:LEU:HD23	1:H:1314:LEU:C	2.35	0.47
2:J:357:THR:HG23	2:J:358:GLN:N	2.29	0.47
1:A:1350:HIS:HB2	1:A:1351:ILE:HD12	1.95	0.47
1:C:181:ASN:HD21	2:J:384:GLN:NE2	2.12	0.47
1:C:1459:LEU:O	1:C:1459:LEU:HG	2.14	0.47
1:F:68:GLY:O	1:F:69:ALA:C	2.52	0.47
1:H:89:LEU:HA	1:H:227:TYR:HE2	1.78	0.47
3:L:167:ILE:HG23	3:L:179:ILE:O	2.14	0.47
1:F:247:ARG:HA	1:F:251:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:387:LEU:HD12	2:J:426:ILE:CG2	2.43	0.47
2:J:437:LEU:HD12	2:J:437:LEU:N	2.18	0.47
1:A:208:PHE:HE2	1:A:216:ARG:HH11	1.62	0.47
1:C:1275:THR:HG22	1:C:1368:TYR:CD2	2.49	0.47
1:F:1277:GLN:HA	1:F:1277:GLN:HE21	1.79	0.47
1:H:1372:LEU:N	1:H:1372:LEU:CD1	2.77	0.47
1:H:1476:LEU:N	1:H:1476:LEU:HD12	2.29	0.47
3:L:30:ARG:NH1	3:M:30:ARG:NH1	2.55	0.47
1:A:57:ASP:OD1	1:A:58:GLU:N	2.47	0.47
1:C:1335:SER:HB2	1:C:1338:GLU:CB	2.45	0.47
1:F:44:ILE:CG1	1:F:118:TYR:HB2	2.44	0.47
1:F:57:ASP:OD1	1:F:58:GLU:N	2.47	0.47
1:F:84:PRO:HB2	1:F:149:ILE:HG21	1.97	0.47
1:F:1403:MET:O	1:F:1407:LEU:HG	2.13	0.47
1:H:137:LEU:N	1:H:137:LEU:HD12	2.30	0.47
1:H:207:MET:HE1	1:H:212:ILE:HG21	1.97	0.47
1:A:157:VAL:HG22	1:A:192:VAL:CG1	2.44	0.47
1:A:1454:LEU:O	1:A:1455:ASP:C	2.52	0.47
1:C:237:GLY:HA2	1:C:1399:ILE:HA	1.97	0.47
1:F:1287:ASN:HD21	1:F:1303:LEU:H	1.63	0.47
1:F:1340:LEU:HD23	1:F:1343:LEU:HD12	1.96	0.47
1:F:1435:GLN:O	1:F:1438:ARG:HG3	2.14	0.47
1:H:1345:LYS:C	1:H:1347:ILE:N	2.67	0.47
1:A:1356:ARG:HB3	1:A:1361:ILE:HD11	1.96	0.47
1:C:1313:ILE:HA	1:C:1316:ASN:HB3	1.97	0.47
1:F:103:SER:OG	3:L:65:ILE:HG23	2.15	0.47
3:L:49:PHE:HB2	3:L:53:LEU:HD11	1.95	0.47
1:A:79:VAL:HG21	1:A:234:LEU:HD11	1.96	0.47
1:A:1273:ARG:HH11	1:A:1315:LEU:HB3	1.80	0.47
1:A:1303:LEU:HG	1:A:1408:MET:HE2	1.97	0.47
1:F:1276:ILE:HD12	1:F:1372:LEU:HD11	1.96	0.47
1:H:1295:PHE:O	1:H:1297:GLN:N	2.47	0.47
1:H:1377:GLU:HG2	1:H:1387:ARG:HA	1.97	0.47
3:L:19:ASN:O	3:L:21:ILE:N	2.47	0.47
3:M:72:PHE:O	3:M:73:TYR:HB3	2.15	0.47
1:C:109:TYR:CZ	1:C:139:GLN:NE2	2.83	0.47
1:F:127:ARG:O	1:F:128:ALA:HB3	2.15	0.47
1:F:1308:ARG:HG2	1:F:1308:ARG:NH1	2.29	0.47
1:F:1468:PRO:C	1:F:1470:ARG:N	2.68	0.47
3:L:186:ARG:HG2	3:L:186:ARG:HH11	1.80	0.47
1:A:130:ARG:CD	1:A:159:MET:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1275:THR:HG22	1:A:1368:TYR:CD2	2.50	0.46
1:C:152:PHE:HB2	1:C:194:PHE:HE1	1.80	0.46
1:C:1494:GLY:HA3	2:E:431:ALA:CA	2.43	0.46
1:F:52:ARG:HH12	2:J:345:MET:HG2	1.79	0.46
1:F:66:GLY:O	1:F:67:ASN:C	2.53	0.46
1:F:1395:THR:HG22	1:F:1399:ILE:CD1	2.46	0.46
3:L:29:LEU:HB3	3:L:74:LEU:CG	2.44	0.46
1:C:1403:MET:HA	1:C:1403:MET:HE3	1.93	0.46
1:F:140:ILE:HD11	1:F:148:ASP:N	2.31	0.46
1:F:261:PHE:CZ	1:F:1268:VAL:HG22	2.50	0.46
1:H:242:ILE:N	1:H:242:ILE:HD12	2.31	0.46
1:H:263:ASP:C	1:H:265:GLU:N	2.68	0.46
1:H:1444:ILE:HG12	1:H:1448:PHE:CE1	2.50	0.46
3:M:98:LEU:HB3	3:M:184:VAL:CG2	2.45	0.46
1:A:1299:LYS:HB2	1:A:1379:LEU:HD23	1.97	0.46
1:C:112:LEU:N	1:C:112:LEU:CD1	2.78	0.46
2:E:355:VAL:HG12	2:E:355:VAL:O	2.14	0.46
1:F:233:SER:HB3	1:F:1406:LEU:CD2	2.45	0.46
1:F:1308:ARG:HG2	1:F:1308:ARG:HH11	1.80	0.46
1:F:1368:TYR:CG	1:F:1369:ARG:N	2.83	0.46
1:H:78:PHE:C	1:H:78:PHE:CD2	2.89	0.46
1:H:1431:LEU:HD12	1:H:1431:LEU:N	2.30	0.46
3:L:29:LEU:C	3:L:74:LEU:HD12	2.35	0.46
3:L:182:GLU:OE2	3:L:182:GLU:N	2.41	0.46
3:M:34:HIS:CD2	3:M:183:ALA:HB1	2.51	0.46
3:M:89:GLU:O	3:M:92:MET:N	2.48	0.46
1:A:1453:ARG:C	1:A:1454:LEU:HD12	2.36	0.46
1:C:1401:THR:O	1:C:1404:SER:HB2	2.16	0.46
1:F:120:VAL:HG12	1:F:121:LEU:N	2.28	0.46
1:H:152:PHE:HA	1:H:197:TYR:HD2	1.81	0.46
1:H:1266:GLU:O	1:H:1267:SER:C	2.54	0.46
1:H:1481:LEU:HD22	2:J:411:MET:HE1	1.97	0.46
2:J:319:ALA:HB2	3:M:74:LEU:HB2	1.98	0.46
3:L:13:LEU:O	3:L:17:ILE:HG13	2.15	0.46
3:L:17:ILE:HA	3:L:22:PHE:CG	2.49	0.46
3:L:17:ILE:HG12	3:L:22:PHE:CD1	2.50	0.46
3:L:28:GLN:HA	3:L:31:ALA:HB3	1.96	0.46
1:A:1393:LEU:HB3	1:A:1397:GLU:CB	2.46	0.46
1:C:62:THR:OG1	1:C:1460:ILE:HD11	2.15	0.46
1:C:1267:SER:O	1:C:1271:ILE:HG12	2.15	0.46
1:C:1429:ARG:HB3	1:C:1456:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:LEU:HB2	1:F:251:LEU:HD12	1.96	0.46
1:F:1290:LEU:CD2	1:F:1293:ILE:HD11	2.40	0.46
1:F:1362:GLY:O	1:F:1366:LEU:CD1	2.64	0.46
1:H:140:ILE:HG13	1:H:147:VAL:HA	1.98	0.46
1:H:224:ASN:O	1:H:228:LYS:HB2	2.15	0.46
1:H:1347:ILE:HG22	1:H:1348:ASN:N	2.31	0.46
1:H:1390:SER:C	1:H:1392:ALA:H	2.18	0.46
2:J:383:LEU:HD12	2:J:433:VAL:HG21	1.98	0.46
2:J:412:ALA:HB1	2:J:436:HIS:HB3	1.97	0.46
3:L:13:LEU:HD11	3:L:56:PHE:HB2	1.97	0.46
3:M:33:ARG:HH11	3:M:33:ARG:HG3	1.81	0.46
1:A:34:ALA:O	1:A:1426:LEU:HD12	2.16	0.46
1:A:169:GLU:OE1	1:A:178:LEU:HB3	2.15	0.46
1:A:1444:ILE:HG23	1:A:1445:ASN:N	2.31	0.46
1:C:136:ARG:NH2	1:C:148:ASP:O	2.49	0.46
1:C:1410:VAL:C	1:C:1412:SER:H	2.18	0.46
1:C:1450:LEU:O	1:C:1453:ARG:N	2.49	0.46
1:F:177:VAL:HG12	1:F:178:LEU:N	2.31	0.46
1:F:178:LEU:HD12	1:F:182:ASP:CB	2.45	0.46
1:F:1276:ILE:HD13	1:F:1368:TYR:HD2	1.80	0.46
1:H:216:ARG:HH12	1:H:1420:MET:CE	2.28	0.46
1:H:237:GLY:N	1:H:1399:ILE:HA	2.30	0.46
1:H:253:GLU:O	1:H:255:SER:N	2.49	0.46
3:L:24:GLN:HG2	3:M:81:LEU:CD2	2.44	0.46
3:M:37:ILE:O	3:M:37:ILE:HG22	2.15	0.46
1:A:136:ARG:HG2	1:A:137:LEU:N	2.31	0.46
1:C:1375:GLU:HG2	1:C:1376:VAL:N	2.31	0.46
1:C:1447:LEU:HD22	1:C:1458:LEU:HD11	1.98	0.46
1:F:47:ASN:HA	1:F:113:LYS:CG	2.30	0.46
1:H:93:ASN:O	1:H:94:THR:C	2.54	0.46
1:H:187:PHE:HD2	1:H:192:VAL:CG2	2.28	0.46
1:H:1343:LEU:HD23	1:H:1343:LEU:C	2.36	0.46
1:H:1447:LEU:O	1:H:1450:LEU:HB2	2.16	0.46
3:M:64:LEU:HA	3:M:74:LEU:HD23	1.96	0.46
1:A:1387:ARG:HB3	1:A:1387:ARG:NH1	2.30	0.46
1:F:113:LYS:HE2	1:F:113:LYS:HA	1.98	0.46
3:L:108:LEU:C	3:L:110:GLN:H	2.18	0.46
1:A:77:GLY:HA2	1:A:80:THR:HB	1.98	0.46
1:A:187:PHE:O	1:A:188:GLU:C	2.55	0.46
1:C:1343:LEU:O	1:C:1346:ARG:HB3	2.15	0.46
1:F:1389:GLU:C	1:F:1391:SER:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:PHE:HE1	1:H:1428:CYS:HG	1.60	0.46
1:H:1303:LEU:HD23	1:H:1303:LEU:HA	1.80	0.46
1:H:1378:THR:O	1:H:1385:TRP:HE3	1.98	0.46
1:A:1464:GLU:HG2	1:A:1466:ILE:H	1.81	0.46
1:C:1406:LEU:HA	1:C:1409:VAL:HG23	1.97	0.46
1:F:66:GLY:O	1:F:69:ALA:HB2	2.16	0.46
1:F:247:ARG:H	1:F:247:ARG:HG3	1.47	0.46
1:F:1314:LEU:HD23	1:F:1314:LEU:C	2.37	0.46
1:H:57:ASP:OD1	1:H:59:LEU:N	2.40	0.46
3:L:60:TYR:O	3:L:81:LEU:HD13	2.16	0.46
3:M:71:PHE:CZ	3:M:186:ARG:HG3	2.51	0.46
1:A:216:ARG:HH11	1:A:216:ARG:HG2	1.81	0.45
1:A:1276:ILE:HG12	1:A:1372:LEU:HD11	1.97	0.45
1:C:1283:ILE:O	1:C:1287:ASN:OD1	2.34	0.45
2:E:412:ALA:HB3	2:E:415:ASP:HB2	1.98	0.45
1:H:225:LYS:HA	1:H:249:TYR:OH	2.15	0.45
1:H:1339:ALA:O	1:H:1340:LEU:C	2.53	0.45
1:H:1475:LYS:HE3	2:J:404:ASP:HB2	1.96	0.45
2:J:398:VAL:O	2:J:399:ALA:C	2.55	0.45
1:A:44:ILE:HB	1:A:118:TYR:HB2	1.98	0.45
1:A:1267:SER:O	1:A:1271:ILE:HG12	2.16	0.45
1:C:190:THR:HG22	1:C:191:ALA:H	1.80	0.45
1:C:1477:VAL:HB	1:C:1488:HIS:HB3	1.97	0.45
1:F:1314:LEU:HD12	1:F:1344:TYR:CD1	2.51	0.45
1:H:1382:ALA:O	1:H:1383:TYR:C	2.55	0.45
1:H:1466:ILE:HA	2:J:400:ARG:HH12	1.81	0.45
3:L:28:GLN:O	3:L:31:ALA:HB3	2.16	0.45
3:L:196:ASP:OD1	3:L:198:ARG:HB2	2.16	0.45
3:M:54:GLU:HG3	3:M:64:LEU:H	1.82	0.45
3:M:87:MET:CE	3:M:87:MET:CA	2.89	0.45
3:M:211:THR:CG2	3:M:212:THR:N	2.79	0.45
1:A:187:PHE:HE2	1:A:192:VAL:HG21	1.73	0.45
1:A:1276:ILE:O	1:A:1280:GLN:HB2	2.16	0.45
1:C:41:LEU:HD22	1:C:78:PHE:CB	2.41	0.45
1:C:194:PHE:CZ	1:C:196:PRO:HG3	2.52	0.45
1:C:1493:LYS:O	2:E:432:ALA:N	2.50	0.45
2:E:394:ARG:HG2	2:E:394:ARG:HH11	1.82	0.45
1:F:33:ILE:HG22	1:F:34:ALA:N	2.25	0.45
1:F:39:ARG:CZ	1:F:124:VAL:HG21	2.47	0.45
1:F:89:LEU:HD23	1:F:227:TYR:HE2	1.81	0.45
1:F:1367:ASP:HB3	1:F:1370:ASN:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1416:GLU:O	1:F:1416:GLU:HG2	2.16	0.45
1:F:1421:ARG:HG2	1:F:1422:ALA:N	2.25	0.45
2:J:394:ARG:HG3	2:J:394:ARG:NH1	2.31	0.45
1:A:73:THR:HG22	1:A:111:LYS:HZ2	1.79	0.45
1:A:1314:LEU:HD13	1:A:1371:TYR:OH	2.16	0.45
1:A:1337:SER:HB3	1:A:1362:GLY:HA3	1.98	0.45
1:C:55:ASP:HB2	1:C:1474:TYR:OH	2.16	0.45
1:C:78:PHE:O	1:C:79:VAL:C	2.52	0.45
1:C:199:SER:O	1:C:200:ILE:C	2.55	0.45
1:C:217:LEU:N	1:C:217:LEU:HD12	2.31	0.45
1:C:234:LEU:C	1:C:236:GLY:H	2.18	0.45
1:H:216:ARG:HH11	1:H:216:ARG:HG3	1.80	0.45
1:H:1311:HIS:O	1:H:1315:LEU:HD12	2.16	0.45
2:J:399:ALA:O	2:J:400:ARG:C	2.54	0.45
3:L:67:ALA:HB1	3:L:68:PRO:HD2	1.98	0.45
1:A:229:LEU:HD13	1:A:1413:TRP:HZ3	1.82	0.45
1:A:1314:LEU:HD23	1:A:1314:LEU:C	2.36	0.45
1:C:91:PHE:HB2	1:C:107:GLY:HA3	1.99	0.45
1:F:46:TRP:O	1:F:47:ASN:C	2.55	0.45
1:F:130:ARG:NH1	1:F:158:PRO:O	2.50	0.45
1:H:103:SER:O	1:H:104:ARG:C	2.55	0.45
1:H:230:ILE:HG23	1:H:1432:PHE:CE2	2.50	0.45
1:H:1430:LEU:HD23	1:H:1430:LEU:O	2.16	0.45
2:J:425:PRO:HA	2:J:432:ALA:HB2	1.97	0.45
3:L:71:PHE:CD1	3:L:71:PHE:N	2.84	0.45
1:C:41:LEU:HA	1:C:120:VAL:O	2.16	0.45
1:F:1266:GLU:CG	1:F:1321:GLN:HE22	2.18	0.45
1:F:1492:LEU:HD11	2:J:352:LEU:HD13	1.99	0.45
1:H:86:LEU:HD11	1:H:147:VAL:O	2.17	0.45
3:L:28:GLN:OE1	3:L:33:ARG:HD2	2.17	0.45
3:L:61:HIS:ND1	3:L:81:LEU:HD11	2.32	0.45
3:M:94:VAL:O	3:M:94:VAL:CG1	2.65	0.45
1:A:1279:GLU:O	1:A:1282:ARG:HB3	2.17	0.45
1:C:1368:TYR:CD1	1:C:1368:TYR:C	2.90	0.45
1:F:88:LEU:HD12	1:F:88:LEU:N	2.32	0.45
1:F:220:SER:HA	1:F:223:ARG:NH1	2.31	0.45
1:H:262:GLN:O	1:H:265:GLU:HB3	2.17	0.45
1:H:1490:VAL:HG11	2:J:403:VAL:CG1	2.46	0.45
3:L:201:GLN:O	3:L:205:ILE:HG13	2.17	0.45
1:A:208:PHE:CE2	1:A:216:ARG:NH1	2.85	0.45
1:A:265:GLU:OE2	1:A:1263:ILE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:LEU:O	1:A:1276:ILE:HG13	2.17	0.45
1:A:1379:LEU:HD12	1:A:1380:ARG:H	1.80	0.45
1:C:1363:GLU:O	1:C:1364:GLU:C	2.55	0.45
2:E:396:PHE:CE1	2:E:400:ARG:NH2	2.85	0.45
1:F:39:ARG:N	1:F:122:GLU:O	2.39	0.45
1:H:43:LEU:C	1:H:44:ILE:HD12	2.37	0.45
1:H:78:PHE:O	1:H:78:PHE:HD2	2.00	0.45
1:H:206:PHE:CZ	1:H:210:LEU:HD11	2.52	0.45
1:H:1268:VAL:HG21	1:H:1336:PHE:HZ	1.82	0.45
1:H:1341:ALA:HB2	1:H:1361:ILE:HB	1.99	0.45
1:H:1448:PHE:HZ	1:H:1468:PRO:HG2	1.72	0.45
2:J:346:ALA:O	2:J:347:LEU:CB	2.63	0.45
1:A:1263:ILE:HG22	1:A:1264:SER:N	2.26	0.45
1:A:1379:LEU:HG	1:A:1380:ARG:N	2.31	0.45
1:C:1376:VAL:HG21	1:C:1405:ILE:HD12	1.98	0.45
1:C:1450:LEU:HA	1:C:1453:ARG:HB2	1.98	0.45
2:E:426:ILE:CG2	2:E:427:ASP:H	2.01	0.45
1:F:179:SER:O	1:F:182:ASP:HB2	2.17	0.45
1:F:206:PHE:CZ	1:F:210:LEU:HD11	2.52	0.45
1:F:1348:ASN:CB	1:F:1349:PRO:CD	2.86	0.45
3:M:186:ARG:C	3:M:188:GLY:N	2.69	0.45
1:C:125:ASN:C	1:C:127:ARG:N	2.69	0.45
1:F:140:ILE:HG23	2:J:331:GLU:CB	2.47	0.45
1:F:1277:GLN:HA	1:F:1277:GLN:NE2	2.32	0.45
1:H:251:LEU:N	1:H:251:LEU:HD12	2.32	0.45
1:H:1333:LYS:O	1:H:1333:LYS:HG2	2.17	0.45
1:A:35:ARG:HH11	1:A:35:ARG:HG3	1.82	0.44
1:A:93:ASN:O	1:A:94:THR:C	2.55	0.44
1:A:133:THR:HG21	1:A:207:MET:HE2	1.99	0.44
1:A:178:LEU:HD11	1:A:183:LEU:HD23	1.99	0.44
1:C:120:VAL:HG13	1:C:134:GLY:CA	2.46	0.44
1:F:1407:LEU:HD22	1:F:1456:MET:SD	2.57	0.44
1:H:32:MET:C	1:H:33:ILE:HG13	2.36	0.44
2:J:315:LEU:HD22	3:M:89:GLU:HG2	1.99	0.44
3:M:37:ILE:HG13	3:M:182:GLU:OE2	2.17	0.44
1:A:1310:THR:HG22	1:A:1344:TYR:CE1	2.43	0.44
2:E:394:ARG:O	2:E:398:VAL:HG23	2.17	0.44
1:F:1271:ILE:O	1:F:1272:LEU:C	2.55	0.44
1:F:1394:SER:HB2	4:H:2004:AGS:O3B	2.17	0.44
1:F:1404:SER:O	1:F:1407:LEU:N	2.50	0.44
4:F:2003:AGS:N7	1:H:1392:ALA:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:ILE:HD12	1:H:44:ILE:N	2.31	0.44
3:M:182:GLU:C	3:M:184:VAL:H	2.20	0.44
1:C:127:ARG:HE	1:C:1425:ILE:HD11	1.82	0.44
1:C:158:PRO:C	1:C:160:THR:N	2.69	0.44
1:C:234:LEU:C	1:C:236:GLY:N	2.71	0.44
1:H:125:ASN:HD22	1:H:125:ASN:HA	1.53	0.44
1:H:208:PHE:CZ	1:H:216:ARG:HG2	2.52	0.44
1:H:258:ARG:O	1:H:259:GLN:C	2.55	0.44
1:A:1266:GLU:HG2	1:A:1318:LEU:O	2.17	0.44
1:C:137:LEU:HD12	1:C:137:LEU:N	2.33	0.44
1:C:207:MET:HB2	1:C:213:LEU:CD1	2.47	0.44
2:E:417:GLN:O	2:E:419:VAL:HG23	2.17	0.44
1:F:78:PHE:O	1:F:78:PHE:HD2	1.99	0.44
1:F:1268:VAL:HG21	1:F:1336:PHE:CE2	2.52	0.44
1:F:1293:ILE:HD12	1:F:1300:GLY:HA2	2.00	0.44
1:H:229:LEU:HD13	1:H:1413:TRP:CZ3	2.52	0.44
3:L:160:ARG:HA	3:L:163:ARG:HH11	1.81	0.44
1:A:62:THR:OG1	1:A:1460:ILE:HD11	2.16	0.44
2:J:426:ILE:CG2	2:J:427:ASP:N	2.75	0.44
3:M:60:TYR:CA	3:M:81:LEU:HB2	2.48	0.44
1:A:91:PHE:C	1:A:92:ARG:O	2.55	0.44
1:C:106:LYS:HG2	1:C:107:GLY:H	1.83	0.44
1:C:246:LEU:HD22	1:C:1374:LEU:CB	2.47	0.44
1:C:1302:ARG:HG3	1:C:1385:TRP:CZ3	2.53	0.44
1:C:1368:TYR:CD1	1:C:1369:ARG:N	2.86	0.44
2:E:354:ASP:O	2:E:356:GLN:N	2.51	0.44
1:F:215:LYS:HG2	1:F:216:ARG:N	2.33	0.44
2:J:356:GLN:O	2:J:359:ILE:HB	2.17	0.44
2:J:379:LEU:H	2:J:379:LEU:CD1	2.26	0.44
3:L:60:TYR:HA	3:L:81:LEU:HD22	2.00	0.44
3:L:112:GLY:O	3:L:179:ILE:HG23	2.18	0.44
1:C:1287:ASN:ND2	1:C:1302:ARG:HA	2.33	0.44
1:F:1429:ARG:HB3	1:F:1456:MET:CE	2.47	0.44
1:H:111:LYS:C	1:H:112:LEU:HD12	2.38	0.44
2:J:320:LYS:C	3:M:83:ALA:HB3	2.38	0.44
3:L:56:PHE:C	3:L:58:ARG:N	2.71	0.44
1:F:1286:LEU:HD23	1:F:1286:LEU:HA	1.88	0.44
1:F:1362:GLY:O	1:F:1365:LEU:HB2	2.17	0.44
1:F:1464:GLU:HG3	1:H:1464:GLU:OE2	2.18	0.44
1:H:61:THR:O	1:H:1459:LEU:HD12	2.17	0.44
1:H:254:ASN:C	1:H:256:GLY:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1444:ILE:HG12	1:H:1448:PHE:HE1	1.83	0.44
2:J:425:PRO:HA	2:J:432:ALA:CB	2.48	0.44
3:L:150:LEU:HA	3:L:153:LYS:HB2	1.99	0.44
1:A:178:LEU:HG	1:A:178:LEU:O	2.18	0.44
1:C:85:ASP:OD1	1:C:87:THR:HB	2.17	0.44
1:C:1494:GLY:HA3	2:E:431:ALA:N	2.33	0.44
1:F:52:ARG:NE	1:F:1489:VAL:CG2	2.79	0.44
1:F:131:ILE:HD13	1:F:210:LEU:HB3	1.98	0.44
1:F:135:VAL:HG13	1:F:149:ILE:HG23	1.99	0.44
1:F:140:ILE:HD11	1:F:148:ASP:HB2	1.99	0.44
1:F:154:LEU:HD21	1:F:194:PHE:HD1	1.83	0.44
1:F:227:TYR:CD1	1:F:227:TYR:C	2.91	0.44
1:F:1387:ARG:CB	1:F:1387:ARG:HH11	2.30	0.44
1:A:208:PHE:HD1	1:A:213:LEU:O	2.01	0.43
1:A:265:GLU:O	1:A:266:ALA:C	2.56	0.43
1:A:1353:LEU:HD12	1:A:1353:LEU:N	2.33	0.43
1:A:1382:ALA:C	1:A:1384:GLY:H	2.21	0.43
1:C:150:ARG:NH2	1:C:198:HIS:CD2	2.86	0.43
1:C:255:SER:O	1:C:259:GLN:NE2	2.50	0.43
1:C:1272:LEU:HD12	1:C:1315:LEU:CD2	2.47	0.43
1:F:54:PHE:N	1:F:54:PHE:HD1	2.16	0.43
1:F:1296:GLY:HA2	1:H:67:ASN:O	2.18	0.43
1:F:1449:GLU:C	1:F:1451:CYS:H	2.20	0.43
2:J:407:VAL:O	2:J:407:VAL:HG12	2.17	0.43
3:L:98:LEU:CD1	3:L:161:LEU:HD13	2.48	0.43
1:A:207:MET:HB3	1:A:213:LEU:HD23	2.00	0.43
1:A:1387:ARG:NH1	1:A:1387:ARG:CB	2.81	0.43
1:C:187:PHE:N	1:C:187:PHE:CD1	2.87	0.43
1:C:1386:MET:O	1:C:1387:ARG:C	2.55	0.43
1:H:1286:LEU:HD22	1:H:1411:GLN:HE22	1.82	0.43
2:J:316:LEU:HD11	3:M:186:ARG:O	2.17	0.43
3:L:29:LEU:HB3	3:L:74:LEU:HD11	2.00	0.43
3:L:147:ARG:O	3:L:147:ARG:HG2	2.18	0.43
1:A:254:ASN:O	1:A:256:GLY:N	2.51	0.43
1:A:1395:THR:O	1:A:1399:ILE:HG12	2.18	0.43
1:C:82:LEU:O	1:C:84:PRO:HD3	2.18	0.43
1:C:88:LEU:HD12	1:C:88:LEU:N	2.33	0.43
1:C:131:ILE:CG2	1:C:133:THR:HG23	2.47	0.43
1:F:1290:LEU:CD2	1:F:1450:LEU:HD21	2.47	0.43
1:A:1294:ALA:H	1:A:1446:THR:HG21	1.82	0.43
1:C:48:GLY:O	1:C:1487:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:C	1:C:136:ARG:NE	2.72	0.43
1:C:217:LEU:N	1:C:217:LEU:CD1	2.81	0.43
1:H:237:GLY:H	1:H:1399:ILE:HA	1.83	0.43
1:H:1336:PHE:O	1:H:1339:ALA:HB3	2.17	0.43
1:H:1365:LEU:O	1:H:1366:LEU:HD23	2.19	0.43
3:L:184:VAL:O	3:L:186:ARG:N	2.52	0.43
3:M:91:GLU:O	3:M:94:VAL:CB	2.60	0.43
1:A:237:GLY:H	1:A:1399:ILE:HA	1.82	0.43
1:C:136:ARG:NH1	2:J:429:PHE:CE1	2.86	0.43
1:C:1369:ARG:O	1:C:1371:TYR:N	2.51	0.43
1:F:103:SER:HB2	3:L:54:GLU:OE1	2.19	0.43
1:F:213:LEU:HD12	1:F:217:LEU:HD11	2.00	0.43
1:F:1375:GLU:OE2	1:F:1387:ARG:NH2	2.49	0.43
1:H:1313:ILE:HG22	1:H:1347:ILE:HD13	2.00	0.43
1:A:39:ARG:HG3	1:A:39:ARG:NH1	2.33	0.43
1:A:113:LYS:HA	1:A:113:LYS:CE	2.49	0.43
1:A:163:VAL:HA	1:A:166:LEU:CD1	2.46	0.43
1:A:1463:PRO:HB3	4:A:2001:AGS:S1G	2.59	0.43
1:C:187:PHE:O	1:C:188:GLU:C	2.57	0.43
1:C:237:GLY:O	1:C:1402:GLY:HA3	2.18	0.43
1:C:1317:ALA:C	1:C:1319:SER:H	2.22	0.43
1:C:1415:GLU:C	1:C:1417:SER:H	2.21	0.43
1:F:41:LEU:HB2	1:F:56:PHE:CE2	2.54	0.43
1:F:109:TYR:CE1	1:F:139:GLN:NE2	2.86	0.43
1:F:164:ILE:HG21	2:J:345:MET:HE2	2.00	0.43
1:F:1298:VAL:HG12	1:F:1300:GLY:H	1.83	0.43
1:F:1396:GLY:HA2	1:F:1399:ILE:HB	2.01	0.43
1:H:62:THR:HG22	1:H:63:LEU:N	2.33	0.43
1:H:105:ASP:CG	1:H:107:GLY:H	2.22	0.43
1:H:204:HIS:ND1	1:H:217:LEU:HD22	2.33	0.43
1:H:1350:HIS:ND1	1:H:1350:HIS:C	2.72	0.43
2:J:403:VAL:O	2:J:404:ASP:C	2.57	0.43
3:L:17:ILE:HG12	3:L:22:PHE:CG	2.53	0.43
3:L:205:ILE:O	3:L:205:ILE:HG22	2.19	0.43
1:A:75:MET:HG2	1:A:1459:LEU:HD21	2.00	0.43
1:A:123:THR:HG21	1:A:212:ILE:HD12	2.00	0.43
1:A:1414:GLU:HG3	1:A:1427:PRO:HG2	2.00	0.43
1:C:52:ARG:HD2	1:C:1489:VAL:HG21	2.01	0.43
1:C:156:ASN:O	1:C:192:VAL:HG22	2.18	0.43
1:C:1488:HIS:HD2	2:E:407:VAL:HG13	1.84	0.43
2:E:390:TYR:CD1	2:E:390:TYR:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:430:SER:O	2:E:431:ALA:C	2.57	0.43
1:F:1468:PRO:C	1:F:1470:ARG:H	2.21	0.43
1:H:190:THR:CG2	1:H:191:ALA:H	2.16	0.43
1:H:217:LEU:N	1:H:217:LEU:CD1	2.82	0.43
1:H:1268:VAL:HG21	1:H:1336:PHE:CZ	2.54	0.43
3:L:66:ARG:HG2	3:L:66:ARG:HH11	1.82	0.43
1:A:204:HIS:C	1:A:206:PHE:N	2.72	0.43
1:A:1409:VAL:HG12	1:A:1413:TRP:CE3	2.52	0.43
1:C:83:ILE:N	1:C:83:ILE:HD12	2.33	0.43
1:H:91:PHE:N	1:H:91:PHE:CD1	2.87	0.43
2:J:320:LYS:O	3:M:83:ALA:HB1	2.17	0.43
2:J:396:PHE:O	2:J:397:ASP:C	2.57	0.43
3:L:102:TYR:CE1	3:L:107:ARG:CZ	3.02	0.43
1:A:41:LEU:HB2	1:A:56:PHE:CE2	2.54	0.43
1:A:71:LYS:O	1:A:74:THR:HB	2.19	0.43
1:A:105:ASP:C	1:A:107:GLY:N	2.73	0.43
1:A:189:GLU:O	1:A:190:THR:O	2.36	0.43
1:A:1380:ARG:N	1:A:1384:GLY:HA2	2.30	0.43
1:F:58:GLU:HA	1:F:1457:GLN:HE21	1.84	0.43
1:F:133:THR:HG21	1:F:207:MET:HE2	2.00	0.43
1:F:140:ILE:CD1	1:F:148:ASP:HB2	2.48	0.43
1:F:1302:ARG:HB3	1:F:1303:LEU:H	1.68	0.43
1:F:1303:LEU:HD12	1:F:1408:MET:SD	2.59	0.43
1:H:38:PHE:CD1	1:H:123:THR:HG23	2.54	0.43
1:H:207:MET:HE2	1:H:212:ILE:HG21	2.00	0.43
1:H:1465:ASN:O	2:J:400:ARG:NH2	2.52	0.43
3:L:60:TYR:C	3:L:81:LEU:HD13	2.39	0.43
1:A:94:THR:O	1:A:96:GLU:N	2.52	0.43
1:A:1298:VAL:HA	1:A:1379:LEU:O	2.19	0.43
1:C:34:ALA:O	1:C:1426:LEU:HD12	2.19	0.43
1:C:89:LEU:HD13	1:C:108:LEU:CD1	2.49	0.43
1:C:120:VAL:O	1:C:121:LEU:HD23	2.19	0.43
1:C:197:TYR:CD1	1:C:202:ASP:HB3	2.54	0.43
1:C:200:ILE:HG21	1:C:223:ARG:CZ	2.49	0.43
1:C:238:ILE:HG22	1:C:238:ILE:O	2.18	0.43
1:C:1314:LEU:O	1:C:1314:LEU:HD23	2.19	0.43
1:F:1290:LEU:CB	1:F:1293:ILE:HD11	2.47	0.43
1:H:40:SER:CB	1:H:55:ASP:HA	2.47	0.43
1:H:70:GLY:HA2	4:H:2004:AGS:O2A	2.19	0.43
1:A:43:LEU:HD22	1:A:46:TRP:CE2	2.53	0.42
1:A:105:ASP:C	1:A:107:GLY:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG13	1:A:151:PRO:N	2.34	0.42
1:A:162:SER:O	1:A:164:ILE:N	2.52	0.42
1:A:226:PHE:CZ	1:A:230:ILE:HD11	2.53	0.42
1:A:1419:ARG:HD3	1:A:1419:ARG:HA	1.89	0.42
1:C:1301:VAL:HA	1:C:1377:GLU:O	2.18	0.42
1:C:1445:ASN:O	1:C:1448:PHE:HB2	2.19	0.42
1:F:1281:ASN:O	1:F:1282:ARG:C	2.58	0.42
1:H:71:LYS:HE3	1:H:1463:PRO:HA	2.01	0.42
1:H:1316:ASN:O	1:H:1319:SER:HB2	2.18	0.42
1:H:1444:ILE:CG2	1:H:1445:ASN:N	2.82	0.42
2:J:315:LEU:HD21	3:M:89:GLU:CG	2.48	0.42
2:J:318:THR:O	2:J:319:ALA:C	2.57	0.42
3:M:22:PHE:CB	3:M:23:PRO:HD3	2.47	0.42
3:M:53:LEU:O	3:M:64:LEU:HD12	2.19	0.42
3:M:92:MET:HG3	3:M:187:PHE:CD1	2.54	0.42
1:C:245:SER:O	1:C:248:ASP:HB2	2.19	0.42
2:E:407:VAL:C	2:E:409:LEU:N	2.72	0.42
1:H:88:LEU:N	1:H:88:LEU:HD12	2.34	0.42
1:H:108:LEU:HD21	1:H:137:LEU:HD23	2.01	0.42
1:H:164:ILE:C	1:H:166:LEU:N	2.72	0.42
1:H:167:PHE:C	1:H:178:LEU:HD21	2.40	0.42
1:H:254:ASN:C	1:H:256:GLY:N	2.72	0.42
1:H:1301:VAL:HG12	1:H:1302:ARG:N	2.34	0.42
2:J:383:LEU:HB2	2:J:426:ILE:HD12	2.01	0.42
2:J:430:SER:O	2:J:431:ALA:C	2.57	0.42
3:M:33:ARG:HG3	3:M:33:ARG:NH1	2.34	0.42
1:A:67:ASN:HA	1:A:67:ASN:HD22	1.65	0.42
1:A:72:SER:O	1:A:75:MET:N	2.52	0.42
1:A:129:GLN:O	1:A:131:ILE:HG12	2.18	0.42
1:C:88:LEU:HD23	1:C:227:TYR:HB3	2.01	0.42
1:C:1489:VAL:HG12	1:C:1490:VAL:N	2.33	0.42
1:F:36:GLY:O	1:F:1428:CYS:HB3	2.19	0.42
1:F:87:THR:HG22	1:F:87:THR:O	2.19	0.42
1:H:68:GLY:HA2	4:H:2004:AGS:O3A	2.19	0.42
1:H:1387:ARG:NH1	1:H:1387:ARG:CB	2.82	0.42
2:J:383:LEU:HD22	2:J:402:ILE:HD12	2.01	0.42
2:J:401:ILE:O	2:J:405:GLN:HB2	2.19	0.42
1:A:105:ASP:O	1:A:107:GLY:N	2.52	0.42
1:C:123:THR:HG22	1:C:124:VAL:N	2.35	0.42
1:C:136:ARG:HE	1:C:137:LEU:N	2.18	0.42
1:C:1404:SER:O	1:C:1407:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1447:LEU:HD22	1:C:1458:LEU:CD1	2.49	0.42
1:C:1450:LEU:HD23	1:C:1453:ARG:HD2	2.01	0.42
1:F:195:LYS:HA	1:F:196:PRO:HD2	1.93	0.42
1:F:1449:GLU:C	1:F:1451:CYS:N	2.72	0.42
1:H:68:GLY:HA2	4:H:2004:AGS:PB	2.60	0.42
1:H:1374:LEU:O	1:H:1375:GLU:HB2	2.20	0.42
1:H:1441:ALA:C	1:H:1444:ILE:HG22	2.40	0.42
2:J:373:THR:HG22	2:J:375:GLN:HG3	2.02	0.42
3:L:184:VAL:C	3:L:186:ARG:N	2.69	0.42
3:M:16:ALA:O	3:M:22:PHE:HB2	2.19	0.42
3:M:33:ARG:HG2	3:M:34:HIS:N	2.35	0.42
3:M:40:LEU:HD23	3:M:40:LEU:C	2.39	0.42
1:C:108:LEU:O	1:C:112:LEU:HD13	2.19	0.42
1:C:157:VAL:O	1:C:158:PRO:C	2.58	0.42
1:C:178:LEU:HB2	1:C:182:ASP:CB	2.50	0.42
1:C:250:LEU:C	1:C:251:LEU:HD12	2.40	0.42
1:F:143:ARG:HH11	1:F:144:ASP:HB2	1.85	0.42
1:H:1448:PHE:CD1	1:H:1448:PHE:N	2.87	0.42
1:A:135:VAL:HG12	1:A:136:ARG:O	2.20	0.42
1:A:1387:ARG:HG2	1:A:1388:ALA:O	2.20	0.42
1:C:1425:ILE:HD12	1:C:1425:ILE:N	2.33	0.42
1:H:1378:THR:O	1:H:1385:TRP:CE3	2.73	0.42
2:J:391:PRO:O	2:J:395:HIS:ND1	2.52	0.42
1:A:1290:LEU:CD1	1:A:1404:SER:HB3	2.49	0.42
1:C:246:LEU:HD22	1:C:1374:LEU:HB3	2.01	0.42
1:H:59:LEU:HD11	1:H:1452:GLU:HG2	2.02	0.42
1:H:108:LEU:HD23	1:H:108:LEU:C	2.39	0.42
1:H:112:LEU:HB3	1:H:113:LYS:H	1.74	0.42
1:H:218:ARG:HG2	1:H:218:ARG:NH1	2.32	0.42
1:H:1454:LEU:O	1:H:1455:ASP:C	2.58	0.42
1:H:1464:GLU:C	1:H:1466:ILE:H	2.23	0.42
1:H:1481:LEU:O	1:H:1483:ASN:N	2.52	0.42
2:J:413:SER:CB	2:J:439:ASP:HB2	2.50	0.42
1:A:95:THR:O	1:C:97:ALA:CB	2.62	0.42
1:A:1390:SER:C	1:A:1392:ALA:H	2.23	0.42
1:A:1413:TRP:O	1:A:1414:GLU:C	2.57	0.42
1:C:1449:GLU:O	1:C:1453:ARG:HG3	2.20	0.42
2:E:394:ARG:HG2	2:E:394:ARG:NH1	2.35	0.42
1:F:1387:ARG:HH11	1:F:1387:ARG:HB3	1.83	0.42
1:H:140:ILE:HB	1:H:146:LYS:O	2.20	0.42
1:H:210:LEU:O	1:H:1425:ILE:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1266:GLU:O	1:H:1268:VAL:N	2.52	0.42
1:H:1310:THR:HG22	1:H:1344:TYR:CE1	2.54	0.42
2:J:318:THR:HG21	3:M:87:MET:SD	2.60	0.42
1:A:194:PHE:CZ	1:A:196:PRO:HG3	2.54	0.42
1:A:1456:MET:CG	1:A:1457:GLN:N	2.74	0.42
1:C:64:SER:OG	1:C:1473:THR:HG23	2.19	0.42
1:C:1415:GLU:C	1:C:1417:SER:N	2.74	0.42
1:C:1466:ILE:HG22	1:C:1467:SER:N	2.35	0.42
1:F:44:ILE:HG13	1:F:118:TYR:HB2	2.00	0.42
1:H:83:ILE:HD11	1:H:226:PHE:HD2	1.83	0.42
1:H:110:GLY:C	1:H:112:LEU:H	2.23	0.42
1:H:127:ARG:HH21	1:H:1425:ILE:HD11	1.85	0.42
1:H:239:SER:OG	1:H:242:ILE:HD13	2.20	0.42
2:J:416:HIS:C	2:J:418:ALA:H	2.23	0.42
3:L:98:LEU:O	3:L:101:LEU:HB2	2.20	0.42
3:M:13:LEU:N	3:M:52:GLU:HG2	2.35	0.42
3:M:57:TYR:CD1	3:M:74:LEU:HD21	2.54	0.42
3:M:76:PRO:HB3	3:M:80:THR:HG21	2.01	0.42
1:A:39:ARG:O	1:A:56:PHE:N	2.52	0.42
1:A:135:VAL:CG1	1:A:149:ILE:HG23	2.48	0.42
1:A:162:SER:C	1:A:164:ILE:N	2.73	0.42
1:A:178:LEU:HD23	1:A:178:LEU:H	1.85	0.42
1:C:82:LEU:HB2	1:C:83:ILE:HD12	2.01	0.42
1:F:1306:ASN:ND2	1:F:1306:ASN:N	2.66	0.42
1:H:75:MET:O	1:H:76:ALA:C	2.58	0.42
1:H:200:ILE:HD11	1:H:223:ARG:HD2	2.01	0.42
3:L:33:ARG:HG3	3:L:165:GLY:CA	2.50	0.42
3:M:36:SER:OG	3:M:71:PHE:HB3	2.19	0.42
1:A:1451:CYS:C	1:A:1453:ARG:H	2.22	0.41
1:C:1379:LEU:HD22	1:C:1385:TRP:CH2	2.54	0.41
1:C:1404:SER:O	1:C:1408:MET:HG3	2.20	0.41
2:E:343:LEU:O	2:E:343:LEU:HG	2.19	0.41
1:F:226:PHE:CZ	1:F:230:ILE:HD11	2.54	0.41
1:F:1429:ARG:CB	1:F:1456:MET:HG3	2.50	0.41
1:H:54:PHE:N	1:H:54:PHE:CD1	2.88	0.41
1:H:221:SER:O	1:H:225:LYS:HG3	2.19	0.41
1:H:1317:ALA:C	1:H:1319:SER:H	2.23	0.41
1:H:1343:LEU:HD23	1:H:1343:LEU:O	2.20	0.41
3:L:84:ARG:HG2	3:L:85:SER:N	2.35	0.41
3:M:58:ARG:C	3:M:60:TYR:H	2.22	0.41
1:A:148:ASP:C	1:A:149:ILE:HG13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HA	1:A:214:PRO:HD3	1.91	0.41
1:F:1272:LEU:HD13	1:F:1371:TYR:CZ	2.55	0.41
1:H:95:THR:O	1:H:96:GLU:HG3	2.20	0.41
1:H:140:ILE:HG22	1:H:141:ALA:H	1.79	0.41
1:H:1264:SER:HB3	1:H:1267:SER:HB3	1.99	0.41
1:H:1453:ARG:C	1:H:1454:LEU:HD12	2.40	0.41
3:L:118:ASP:O	3:L:122:GLU:HB2	2.20	0.41
3:L:190:ASP:O	3:L:192:ARG:N	2.53	0.41
1:A:178:LEU:HG	1:A:183:LEU:CG	2.47	0.41
1:C:52:ARG:CG	1:C:1489:VAL:HG21	2.50	0.41
1:C:67:ASN:HD22	1:C:67:ASN:HA	1.60	0.41
1:C:1406:LEU:HB3	1:C:1431:LEU:HD21	2.01	0.41
1:C:1439:LEU:N	1:C:1439:LEU:CD1	2.82	0.41
1:F:242:ILE:HD13	1:F:249:TYR:CZ	2.55	0.41
1:F:1314:LEU:HD21	1:F:1318:LEU:HD11	2.01	0.41
1:H:190:THR:CG2	1:H:192:VAL:HG22	2.50	0.41
1:H:213:LEU:HA	1:H:214:PRO:HD3	1.72	0.41
1:H:1387:ARG:HH11	1:H:1387:ARG:CB	2.33	0.41
2:J:316:LEU:HD11	3:M:186:ARG:C	2.40	0.41
2:J:422:VAL:HG12	2:J:423:TRP:H	1.85	0.41
3:L:104:SER:HA	3:L:105:PRO:HD3	1.85	0.41
3:M:29:LEU:HD21	3:M:35:ILE:HD11	1.99	0.41
3:M:99:CYS:O	3:M:99:CYS:SG	2.76	0.41
1:A:1368:TYR:CD1	1:A:1369:ARG:N	2.88	0.41
1:A:1377:GLU:CG	1:A:1387:ARG:HA	2.51	0.41
1:C:39:ARG:O	1:C:55:ASP:HA	2.21	0.41
1:C:41:LEU:HD13	1:C:121:LEU:HD21	2.02	0.41
1:C:88:LEU:N	1:C:88:LEU:CD1	2.83	0.41
1:C:190:THR:CG2	1:C:191:ALA:N	2.81	0.41
1:C:232:ALA:HB1	1:C:239:SER:HB2	2.03	0.41
1:F:1435:GLN:OE1	4:F:2003:AGS:O2G	2.37	0.41
1:H:78:PHE:HE1	1:H:1430:LEU:HD11	1.84	0.41
2:J:399:ALA:O	2:J:402:ILE:N	2.54	0.41
3:L:40:LEU:HD23	3:L:40:LEU:C	2.40	0.41
1:A:1450:LEU:O	1:A:1453:ARG:HB2	2.20	0.41
1:C:93:ASN:C	1:C:95:THR:N	2.74	0.41
1:C:208:PHE:HD1	1:C:213:LEU:O	2.03	0.41
1:C:1310:THR:CG2	1:C:1348:ASN:ND2	2.79	0.41
1:F:88:LEU:O	1:F:227:TYR:CZ	2.73	0.41
1:F:1276:ILE:HG22	1:F:1280:GLN:NE2	2.35	0.41
1:H:88:LEU:HD23	1:H:227:TYR:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:THR:HG22	1:H:100:THR:O	2.20	0.41
1:H:1278:ARG:HD3	1:H:1282:ARG:HH21	1.84	0.41
2:J:315:LEU:N	3:M:210:ALA:HB1	2.35	0.41
2:J:357:THR:HG23	2:J:358:GLN:H	1.86	0.41
2:J:404:ASP:O	2:J:408:LYS:HG3	2.20	0.41
3:L:149:LYS:HE2	3:L:153:LYS:NZ	2.36	0.41
3:M:22:PHE:O	3:M:26:ASP:N	2.54	0.41
3:M:97:VAL:C	3:M:99:CYS:H	2.24	0.41
1:A:1372:LEU:N	1:A:1372:LEU:CD1	2.83	0.41
1:A:1406:LEU:O	1:A:1410:VAL:HG23	2.20	0.41
1:C:49:PHE:CZ	1:C:1487:VAL:HG11	2.55	0.41
1:C:127:ARG:HD2	1:C:129:GLN:OE1	2.20	0.41
1:C:250:LEU:HD13	1:C:1303:LEU:HD13	2.02	0.41
1:F:42:THR:HG23	1:F:53:THR:OG1	2.21	0.41
1:F:112:LEU:HD12	1:F:112:LEU:N	2.35	0.41
1:F:195:LYS:HE3	1:F:195:LYS:HB2	1.92	0.41
1:F:1315:LEU:HG	1:F:1371:TYR:CE2	2.56	0.41
1:H:1462:ALA:C	1:H:1464:GLU:N	2.73	0.41
2:J:375:GLN:HA	2:J:376:PRO:HD3	1.80	0.41
1:C:1379:LEU:HD13	1:C:1385:TRP:CD2	2.56	0.41
1:F:78:PHE:CE2	1:F:121:LEU:HD11	2.56	0.41
1:F:152:PHE:CD1	1:F:152:PHE:C	2.94	0.41
1:F:1289:GLY:O	1:F:1290:LEU:HD23	2.20	0.41
1:F:1294:ALA:N	1:F:1446:THR:HG21	2.32	0.41
1:H:1477:VAL:O	1:H:1487:VAL:HG13	2.20	0.41
2:J:395:HIS:O	2:J:396:PHE:C	2.58	0.41
2:J:412:ALA:HB1	2:J:436:HIS:CB	2.50	0.41
2:J:416:HIS:CD2	2:J:416:HIS:H	2.38	0.41
2:J:423:TRP:CE3	2:J:434:GLN:HB2	2.56	0.41
2:J:423:TRP:NE1	2:J:434:GLN:NE2	2.68	0.41
3:M:61:HIS:HB2	3:M:80:THR:CA	2.47	0.41
1:A:41:LEU:HA	1:A:121:LEU:HD23	2.02	0.41
1:C:52:ARG:CD	1:C:1489:VAL:HG21	2.51	0.41
1:C:82:LEU:CB	1:C:83:ILE:HD12	2.51	0.41
1:C:120:VAL:HG11	1:C:132:ILE:HG23	2.02	0.41
1:F:115:GLY:O	1:F:138:GLN:HG3	2.20	0.41
1:F:165:SER:HA	1:F:168:THR:OG1	2.21	0.41
1:F:178:LEU:HB2	1:F:182:ASP:CB	2.51	0.41
1:F:200:ILE:HG23	1:F:201:THR:N	2.34	0.41
1:F:263:ASP:O	1:F:266:ALA:HB3	2.21	0.41
1:H:1275:THR:O	1:H:1278:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD23	1:A:1474:TYR:HB2	2.03	0.41
1:A:202:ASP:O	1:A:206:PHE:N	2.54	0.41
1:C:144:ASP:O	1:C:146:LYS:N	2.53	0.41
1:C:212:ILE:HA	1:C:1428:CYS:SG	2.61	0.41
1:C:216:ARG:HG3	1:C:216:ARG:NH1	2.33	0.41
1:C:1299:LYS:C	1:C:1379:LEU:HB3	2.42	0.41
1:C:1466:ILE:O	1:C:1467:SER:HB3	2.21	0.41
2:E:375:GLN:HA	2:E:376:PRO:HD3	1.88	0.41
1:F:35:ARG:O	1:F:37:LYS:HG2	2.20	0.41
1:F:229:LEU:HD13	1:F:1413:TRP:CZ3	2.55	0.41
1:F:246:LEU:CD2	1:F:250:LEU:HD12	2.50	0.41
1:F:247:ARG:HH22	1:F:1370:ASN:HA	1.84	0.41
1:F:1358:PRO:HG2	1:F:1359:GLN:HG3	2.02	0.41
1:H:1400:GLY:O	1:H:1403:MET:HB3	2.20	0.41
1:H:1493:LYS:HG2	2:J:423:TRP:CZ3	2.55	0.41
2:J:323:ALA:HB1	3:L:85:SER:OG	2.20	0.41
2:J:400:ARG:O	2:J:403:VAL:HB	2.21	0.41
2:J:414:GLN:O	2:J:436:HIS:ND1	2.54	0.41
1:A:225:LYS:HZ3	1:A:248:ASP:HB3	1.86	0.41
1:A:238:ILE:HD11	1:A:1401:THR:HB	2.03	0.41
1:A:1430:LEU:HA	1:A:1457:GLN:O	2.21	0.41
1:C:93:ASN:ND2	1:C:95:THR:HG23	2.36	0.41
1:C:239:SER:OG	1:C:242:ILE:HG13	2.21	0.41
1:C:1464:GLU:OE1	1:C:1466:ILE:N	2.54	0.41
2:E:378:ASN:O	2:E:382:VAL:HG23	2.21	0.41
1:F:72:SER:HB2	4:F:2003:AGS:O1A	2.21	0.41
1:F:93:ASN:C	1:F:95:THR:N	2.73	0.41
1:F:93:ASN:OD1	1:H:1393:LEU:O	2.38	0.41
1:H:1308:ARG:O	1:H:1309:ASP:C	2.60	0.41
3:L:33:ARG:HA	3:L:164:ILE:HA	2.01	0.41
1:C:75:MET:O	1:C:79:VAL:HG23	2.21	0.40
1:C:138:GLN:HB3	2:J:429:PHE:CZ	2.57	0.40
1:C:152:PHE:CD1	1:C:152:PHE:C	2.95	0.40
1:F:143:ARG:NH1	1:F:144:ASP:HB2	2.36	0.40
1:F:1390:SER:HB3	1:H:96:GLU:OE2	2.22	0.40
1:F:1442:MET:O	1:F:1445:ASN:HB3	2.21	0.40
2:J:345:MET:HE3	2:J:345:MET:HB2	1.86	0.40
2:J:360:VAL:O	2:J:363:ILE:HB	2.21	0.40
3:M:20:PRO:O	3:M:24:GLN:NE2	2.48	0.40
1:A:123:THR:HG21	1:A:212:ILE:CD1	2.52	0.40
1:A:123:THR:HG22	1:A:124:VAL:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:SER:CB	1:A:223:ARG:HH21	2.35	0.40
1:C:1495:PHE:CE1	2:E:431:ALA:HB1	2.56	0.40
1:F:207:MET:HB3	1:F:212:ILE:HB	2.04	0.40
1:F:1307:ILE:HG22	1:F:1312:SER:HB3	2.03	0.40
1:H:216:ARG:HG3	1:H:216:ARG:NH1	2.36	0.40
1:H:1266:GLU:OE1	1:H:1319:SER:HA	2.21	0.40
1:H:1278:ARG:CD	1:H:1282:ARG:HH21	2.34	0.40
1:H:1477:VAL:O	1:H:1487:VAL:HA	2.21	0.40
3:L:33:ARG:HG2	3:L:34:HIS:O	2.21	0.40
1:A:83:ILE:HD11	1:A:230:ILE:CD1	2.51	0.40
1:A:138:GLN:O	1:A:147:VAL:HG13	2.21	0.40
1:A:1318:LEU:HD11	1:A:1340:LEU:HD21	2.03	0.40
1:C:125:ASN:O	1:C:127:ARG:N	2.55	0.40
1:C:125:ASN:HD22	1:C:126:SER:H	1.69	0.40
1:C:190:THR:HG22	1:C:192:VAL:H	1.87	0.40
1:C:215:LYS:HG2	1:C:216:ARG:N	2.36	0.40
1:C:235:TYR:H	1:C:235:TYR:HD1	1.65	0.40
1:C:1466:ILE:O	1:C:1467:SER:CB	2.70	0.40
1:F:50:PHE:CE1	2:J:343:LEU:HD12	2.56	0.40
1:H:1394:SER:O	1:H:1395:THR:C	2.59	0.40
1:A:50:PHE:O	1:A:51:ALA:HB2	2.21	0.40
1:A:95:THR:CG2	1:C:237:GLY:HA3	2.49	0.40
1:A:254:ASN:O	1:A:255:SER:C	2.60	0.40
1:C:93:ASN:O	1:C:95:THR:N	2.54	0.40
1:C:258:ARG:O	1:C:262:GLN:HG3	2.22	0.40
1:C:1279:GLU:OE2	1:C:1282:ARG:HG2	2.22	0.40
1:C:1292:ASN:HB2	1:C:1453:ARG:NH2	2.36	0.40
1:F:1321:GLN:HE21	1:F:1321:GLN:HB2	1.63	0.40
1:H:200:ILE:HD13	1:H:223:ARG:NE	2.36	0.40
1:H:1278:ARG:CG	1:H:1282:ARG:NH2	2.80	0.40
1:H:1302:ARG:HD3	1:H:1385:TRP:CH2	2.57	0.40
3:L:55:SER:O	3:L:58:ARG:HB2	2.21	0.40
1:A:239:SER:OG	1:A:242:ILE:HG12	2.21	0.40
1:A:1287:ASN:C	1:A:1289:GLY:H	2.25	0.40
1:A:1353:LEU:HD12	1:A:1353:LEU:H	1.87	0.40
1:C:136:ARG:C	1:C:137:LEU:HD12	2.41	0.40
1:C:140:ILE:CG2	1:C:141:ALA:N	2.84	0.40
1:C:247:ARG:H	1:C:247:ARG:HG3	1.68	0.40
1:F:1417:SER:O	1:F:1419:ARG:N	2.55	0.40
1:H:50:PHE:C	1:H:50:PHE:HD1	2.24	0.40
3:L:40:LEU:O	3:L:41:ASP:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:46:LEU:HA	3:L:53:LEU:HD12	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	430/483 (89%)	328 (76%)	75 (17%)	27 (6%)	1 18
1	C	445/483 (92%)	338 (76%)	82 (18%)	25 (6%)	2 20
1	F	437/483 (90%)	334 (76%)	73 (17%)	30 (7%)	1 16
1	H	451/483 (93%)	314 (70%)	102 (23%)	35 (8%)	1 14
2	E	99/152 (65%)	69 (70%)	23 (23%)	7 (7%)	1 16
2	J	120/152 (79%)	88 (73%)	20 (17%)	12 (10%)	0 9
3	L	167/238 (70%)	127 (76%)	27 (16%)	13 (8%)	1 14
3	M	101/238 (42%)	74 (73%)	18 (18%)	9 (9%)	1 12
All	All	2250/2712 (83%)	1672 (74%)	420 (19%)	158 (7%)	1 16

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	A	190	THR
1	A	1382	ALA
1	A	1468	PRO
1	C	111	LYS
1	C	234	LEU
1	C	1265	ALA
1	C	1440	ASP
2	E	376	PRO

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Mol	Chain	Res	Type
2	E	440	GLN
1	F	69	ALA
1	F	142	GLY
1	F	1339	ALA
1	F	1348	ASN
1	F	1382	ALA
1	F	1418	ARG
1	H	94	THR
1	H	165	SER
1	H	174	LYS
1	H	175	ALA
1	H	1368	TYR
1	H	1382	ALA
1	H	1433	LEU
1	H	1469	GLU
1	H	1495	PHE
2	J	347	LEU
2	J	417	GLN
2	J	431	ALA
2	J	439	ASP
3	L	53	LEU
3	L	57	TYR
3	L	83	ALA
3	L	198	ARG
3	M	77	LYS
3	M	88	SER
1	A	104	ARG
1	A	107	GLY
1	A	211	GLY
1	A	255	SER
1	A	264	MET
1	A	1265	ALA
1	A	1288	GLN
1	A	1296	GLY
1	A	1349	PRO
1	C	92	ARG
1	C	159	MET
1	C	236	GLY
1	C	257	VAL
1	C	1370	ASN
1	C	1384	GLY
2	E	427	ASP

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Mol	Chain	Res	Type
2	E	431	ALA
1	F	51	ALA
1	F	67	ASN
1	F	94	THR
1	F	140	ILE
1	F	141	ALA
1	F	1395	THR
1	F	1469	GLU
1	F	1483	ASN
1	F	1485	GLU
1	H	92	ARG
1	H	104	ARG
1	H	154	LEU
1	H	190	THR
1	H	236	GLY
1	H	253	GLU
1	H	1321	GLN
1	H	1422	ALA
1	H	1486	TYR
2	J	374	ALA
2	J	398	VAL
3	L	40	LEU
3	L	111	GLN
3	L	191	VAL
3	M	36	SER
1	A	51	ALA
1	A	92	ARG
1	A	239	SER
1	A	1310	THR
1	A	1427	PRO
1	A	1433	LEU
1	C	70	GLY
1	C	94	THR
1	C	141	ALA
1	C	235	TYR
1	C	1455	ASP
1	F	113	LYS
1	F	260	ALA
1	F	1433	LEU
1	H	143	ARG
1	H	209	ASP
1	H	244	LYS

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Mol	Chain	Res	Type
1	H	258	ARG
1	H	1369	ARG
1	H	1375	GLU
1	H	1470	ARG
2	J	328	ARG
2	J	368	ALA
2	J	399	ALA
3	L	23	PRO
3	L	185	PHE
1	A	95	THR
1	A	108	LEU
1	A	125	ASN
1	C	1365	LEU
1	C	1382	ALA
1	F	125	ASN
1	F	1486	TYR
1	H	45	ASN
1	H	172	ALA
1	H	1265	ALA
1	H	1278	ARG
1	H	1308	ARG
2	J	346	ALA
3	M	73	TYR
3	M	183	ALA
3	M	187	PHE
1	A	106	LYS
1	A	167	PHE
1	A	1385	TRP
1	C	239	SER
1	C	1318	LEU
1	C	1449	GLU
2	E	347	LEU
2	E	355	VAL
2	E	418	ALA
1	F	97	ALA
1	F	108	LEU
1	F	144	ASP
1	F	236	GLY
1	H	1267	SER
2	J	430	SER
3	L	109	ALA
3	L	197	PRO

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Mol	Chain	Res	Type
3	M	71	PHE
3	M	87	MET
1	A	198	HIS
1	C	139	GLN
1	C	158	PRO
1	C	188	GLU
1	C	204	HIS
1	C	1467	SER
1	F	145	LYS
1	F	188	GLU
1	H	214	PRO
1	H	1296	GLY
1	H	1339	ALA
2	J	344	PRO
1	F	1347	ILE
1	F	1384	GLY
3	L	20	PRO
3	L	105	PRO
3	M	65	ILE
1	A	163	VAL
1	H	1347	ILE
1	F	257	VAL
1	F	1466	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	385/413 (93%)	368 (96%)	17 (4%)	28 55
1	C	391/413 (95%)	367 (94%)	24 (6%)	18 47
1	F	385/413 (93%)	357 (93%)	28 (7%)	14 42
1	H	395/413 (96%)	366 (93%)	29 (7%)	14 42
2	E	85/129 (66%)	76 (89%)	9 (11%)	6 27
2	J	102/129 (79%)	93 (91%)	9 (9%)	10 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	145/198 (73%)	140 (97%)	5 (3%)	37 61
3	M	90/198 (46%)	85 (94%)	5 (6%)	21 49
All	All	1978/2306 (86%)	1852 (94%)	126 (6%)	17 45

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	PHE
1	A	159	MET
1	A	185	GLU
1	A	186	LYS
1	A	216	ARG
1	A	222	ASP
1	A	1293	ILE
1	A	1310	THR
1	A	1322	HIS
1	A	1324	GLN
1	A	1338	GLU
1	A	1349	PRO
1	A	1368	TYR
1	A	1383	TYR
1	A	1385	TRP
1	A	1403	MET
1	A	1479	LYS
1	C	50	PHE
1	C	53	THR
1	C	78	PHE
1	C	117	CYS
1	C	125	ASN
1	C	136	ARG
1	C	158	PRO
1	C	178	LEU
1	C	187	PHE
1	C	216	ARG
1	C	247	ARG
1	C	248	ASP
1	C	1340	LEU
1	C	1344	TYR
1	C	1368	TYR
1	C	1383	TYR
1	C	1387	ARG

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Mol	Chain	Res	Type
1	C	1403	MET
1	C	1428	CYS
1	C	1444	ILE
1	C	1447	LEU
1	C	1454	LEU
1	C	1464	GLU
1	C	1484	GLN
2	E	343	LEU
2	E	347	LEU
2	E	352	LEU
2	E	371	ARG
2	E	395	HIS
2	E	422	VAL
2	E	424	GLN
2	E	427	ASP
2	E	437	LEU
1	F	52	ARG
1	F	54	PHE
1	F	78	PHE
1	F	125	ASN
1	F	165	SER
1	F	216	ARG
1	F	222	ASP
1	F	247	ARG
1	F	248	ASP
1	F	251	LEU
1	F	262	GLN
1	F	1268	VAL
1	F	1303	LEU
1	F	1306	ASN
1	F	1322	HIS
1	F	1343	LEU
1	F	1360	THR
1	F	1368	TYR
1	F	1386	MET
1	F	1439	LEU
1	F	1447	LEU
1	F	1450	LEU
1	F	1451	CYS
1	F	1453	ARG
1	F	1455	ASP
1	F	1456	MET

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Mol	Chain	Res	Type
1	F	1473	THR
1	F	1492	LEU
1	H	50	PHE
1	H	58	GLU
1	H	62	THR
1	H	78	PHE
1	H	80	THR
1	H	125	ASN
1	H	144	ASP
1	H	167	PHE
1	H	174	LYS
1	H	178	LEU
1	H	202	ASP
1	H	216	ARG
1	H	228	LYS
1	H	229	LEU
1	H	234	LEU
1	H	247	ARG
1	H	248	ASP
1	H	258	ARG
1	H	261	PHE
1	H	263	ASP
1	H	1262	SER
1	H	1264	SER
1	H	1316	ASN
1	H	1322	HIS
1	H	1373	ASP
1	H	1394	SER
1	H	1404	SER
1	H	1428	CYS
1	H	1430	LEU
2	J	317	TYR
2	J	328	ARG
2	J	342	GLU
2	J	352	LEU
2	J	361	THR
2	J	416	HIS
2	J	424	GLN
2	J	429	PHE
2	J	437	LEU
3	L	71	PHE
3	L	72	PHE

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Mol	Chain	Res	Type
3	L	160	ARG
3	L	185	PHE
3	L	190	ASP
3	M	35	ILE
3	M	69	GLU
3	M	85	SER
3	M	87	MET
3	M	102	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	90	ASN
1	A	125	ASN
1	A	155	GLN
1	A	1277	GLN
1	A	1280	GLN
1	A	1287	ASN
1	A	1291	GLN
1	A	1306	ASN
1	A	1435	GLN
1	C	47	ASN
1	C	93	ASN
1	C	125	ASN
1	C	155	GLN
1	C	181	ASN
1	C	198	HIS
1	C	254	ASN
1	C	259	GLN
1	C	1277	GLN
1	C	1280	GLN
1	C	1287	ASN
1	C	1291	GLN
1	C	1324	GLN
1	C	1348	ASN
1	C	1370	ASN
1	C	1435	GLN
1	C	1484	GLN
1	C	1488	HIS
2	E	364	GLN
2	E	405	GLN

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Mol	Chain	Res	Type
2	E	424	GLN
2	E	440	GLN
1	F	125	ASN
1	F	155	GLN
1	F	1277	GLN
1	F	1280	GLN
1	F	1285	GLN
1	F	1287	ASN
1	F	1292	ASN
1	F	1306	ASN
1	F	1321	GLN
1	F	1370	ASN
1	F	1411	GLN
1	F	1435	GLN
1	F	1483	ASN
1	H	93	ASN
1	H	1277	GLN
1	H	1280	GLN
1	H	1287	ASN
1	H	1291	GLN
1	H	1311	HIS
1	H	1316	ASN
1	H	1411	GLN
1	H	1435	GLN
1	H	1488	HIS
2	J	384	GLN
2	J	405	GLN
2	J	416	HIS
2	J	424	GLN
2	J	434	GLN
3	L	50	GLN
3	L	110	GLN
3	L	111	GLN
3	L	116	GLN
3	L	201	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AGS	H	2004	-	26,33,33	2.15	7 (26%)	26,52,52	1.34	4 (15%)
4	AGS	A	2001	-	26,33,33	2.09	7 (26%)	26,52,52	1.31	3 (11%)
4	AGS	F	2003	-	26,33,33	2.13	7 (26%)	26,52,52	1.38	3 (11%)
4	AGS	C	2002	-	26,33,33	2.07	8 (30%)	26,52,52	1.31	3 (11%)

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
4	AGS	H	2004	-	-	1/17/38/38	0/3/3/3
4	AGS	A	2001	-	-	1/17/38/38	0/3/3/3
4	AGS	F	2003	-	-	3/17/38/38	0/3/3/3
4	AGS	C	2002	-	-	1/17/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2004	AGS	PG-S1G	-5.32	1.79	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2004	AGS	C4-N3	5.25	1.42	1.35
4	C	2002	AGS	C4-N3	5.18	1.42	1.35
4	A	2001	AGS	C4-N3	5.18	1.42	1.35
4	F	2003	AGS	PG-S1G	-5.06	1.79	1.90
4	F	2003	AGS	C4-N3	4.98	1.42	1.35
4	A	2001	AGS	PG-S1G	-4.76	1.80	1.90
4	C	2002	AGS	PG-S1G	-4.53	1.80	1.90
4	F	2003	AGS	C2-N1	3.57	1.40	1.33
4	A	2001	AGS	C2-N1	3.52	1.40	1.33
4	H	2004	AGS	C2-N1	3.41	1.40	1.33
4	F	2003	AGS	C6-N6	3.38	1.46	1.34
4	A	2001	AGS	C6-N6	3.35	1.46	1.34
4	C	2002	AGS	C2-N1	3.30	1.40	1.33
4	C	2002	AGS	C6-N6	3.29	1.46	1.34
4	F	2003	AGS	C2-N3	3.29	1.37	1.32
4	C	2002	AGS	C2-N3	3.28	1.37	1.32
4	H	2004	AGS	C2-N3	3.27	1.37	1.32
4	A	2001	AGS	C2-N3	3.26	1.37	1.32
4	H	2004	AGS	C6-N6	3.25	1.45	1.34
4	F	2003	AGS	PG-O3G	-2.66	1.46	1.54
4	A	2001	AGS	PG-O3G	-2.54	1.46	1.54
4	H	2004	AGS	PG-O3G	-2.47	1.46	1.54
4	C	2002	AGS	O4'-C4'	-2.41	1.39	1.45
4	C	2002	AGS	PG-O3G	-2.29	1.47	1.54
4	H	2004	AGS	O4'-C4'	-2.24	1.40	1.45
4	F	2003	AGS	O4'-C4'	-2.21	1.40	1.45
4	A	2001	AGS	O4'-C4'	-2.15	1.40	1.45
4	C	2002	AGS	O4'-C1'	-2.03	1.38	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2004	AGS	C4-C5-N7	3.37	112.91	109.40
4	C	2002	AGS	C4-C5-N7	3.24	112.78	109.40
4	A	2001	AGS	C4-C5-N7	3.02	112.54	109.40
4	F	2003	AGS	C4-C5-N7	2.77	112.28	109.40
4	H	2004	AGS	N3-C2-N1	-2.31	125.07	128.68
4	F	2003	AGS	N3-C2-N1	-2.25	125.16	128.68
4	C	2002	AGS	N3-C2-N1	-2.21	125.22	128.68
4	A	2001	AGS	N3-C2-N1	-2.17	125.28	128.68
4	A	2001	AGS	O3G-PG-O3B	-2.13	97.54	104.64
4	C	2002	AGS	O2A-PA-O1A	2.09	122.56	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2003	AGS	O3G-PG-O3B	-2.06	97.76	104.64
4	H	2004	AGS	C2'-C3'-C4'	2.03	106.60	102.64
4	H	2004	AGS	O3G-PG-O3B	-2.03	97.88	104.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2003	AGS	PB-O3B-PG-O2G
4	F	2003	AGS	PB-O3B-PG-O3G
4	A	2001	AGS	PA-O3A-PB-O1B
4	C	2002	AGS	PA-O3A-PB-O1B
4	F	2003	AGS	PA-O3A-PB-O1B
4	H	2004	AGS	PA-O3A-PB-O1B

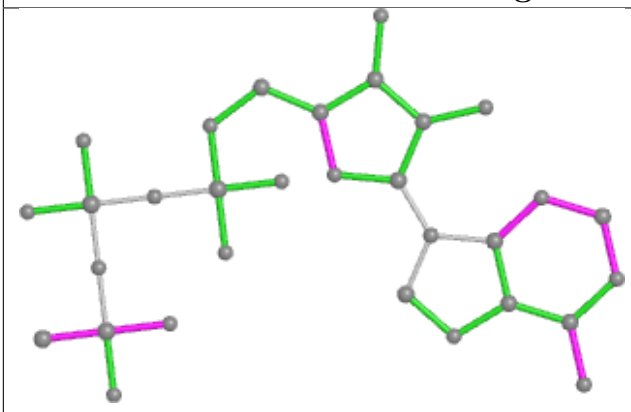
There are no ring outliers.

4 monomers are involved in 21 short contacts:

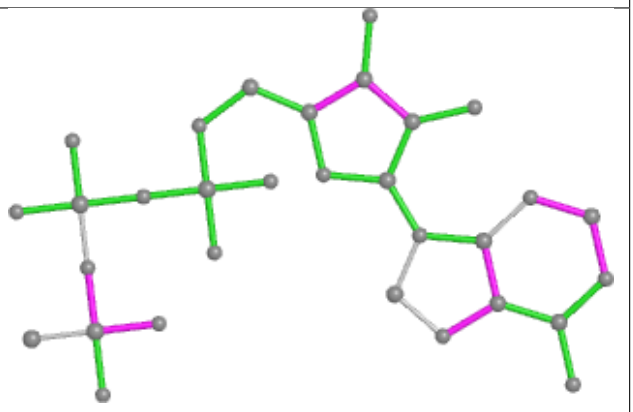
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2004	AGS	8	0
4	A	2001	AGS	6	0
4	F	2003	AGS	6	0
4	C	2002	AGS	1	0

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.

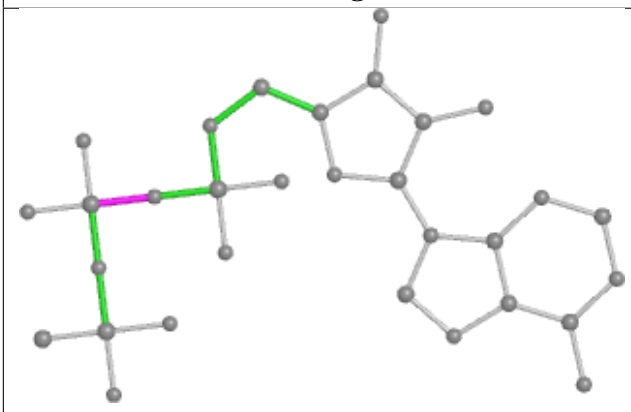
Ligand AGS H 2004



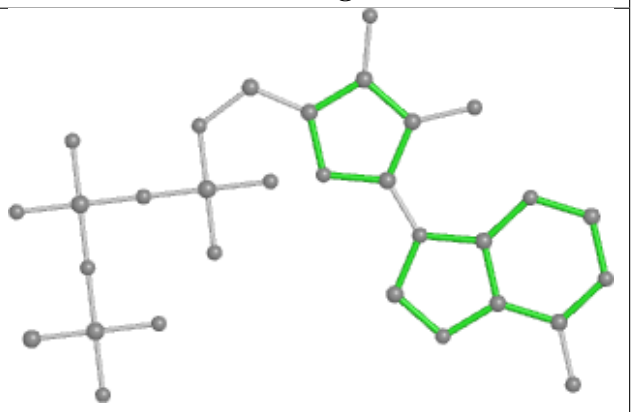
Bond lengths



Bond angles

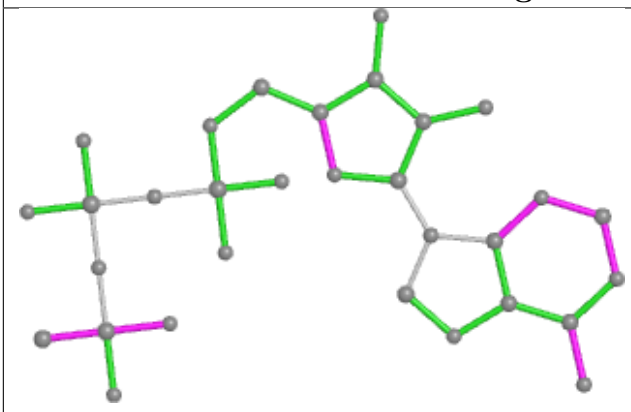


Torsions

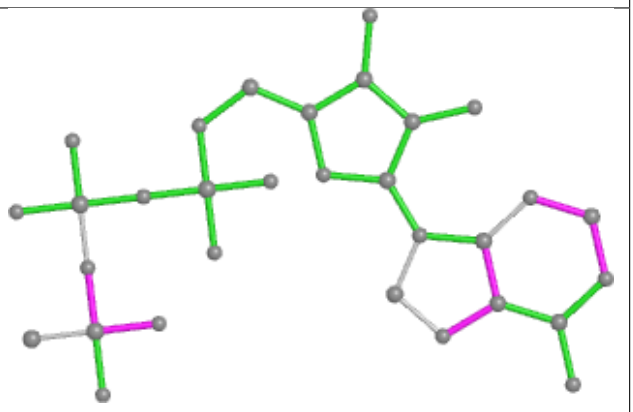


Rings

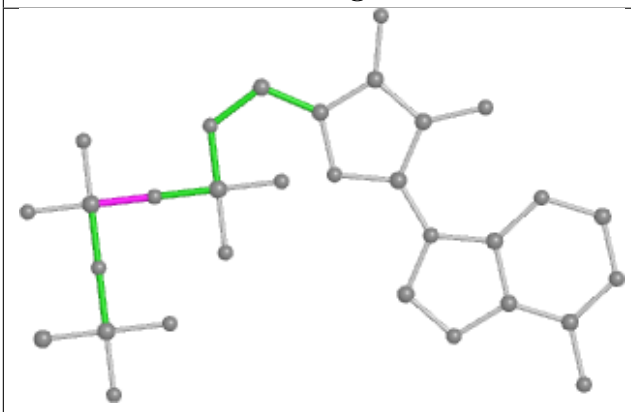
Ligand AGS A 2001



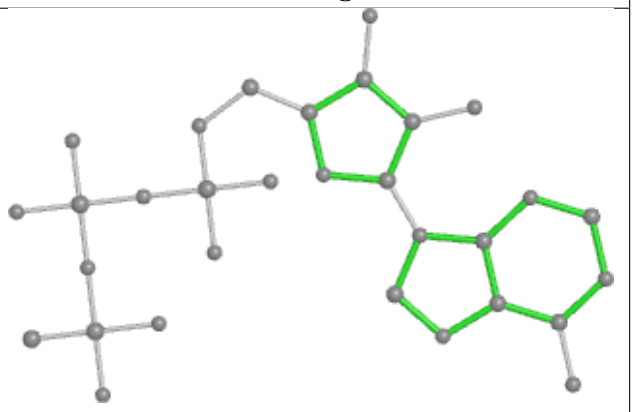
Bond lengths



Bond angles

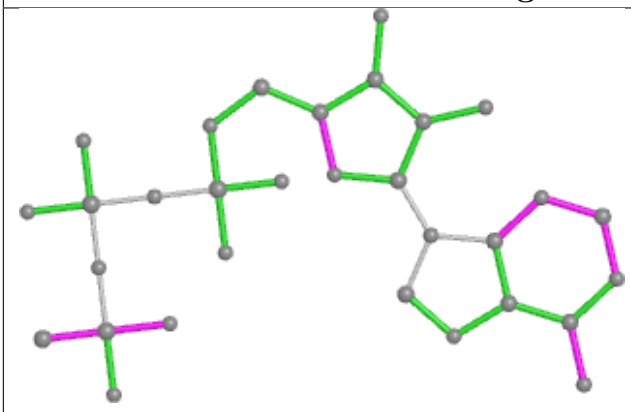


Torsions

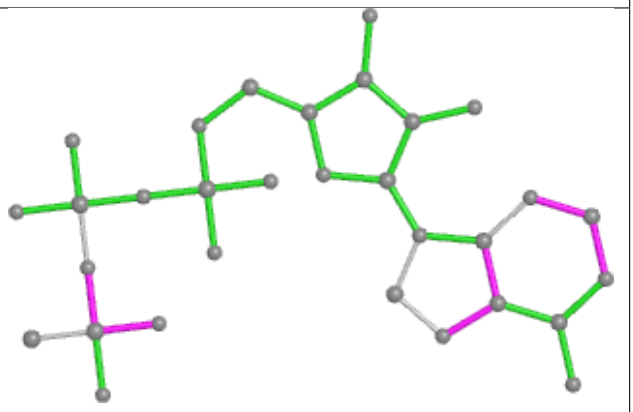


Rings

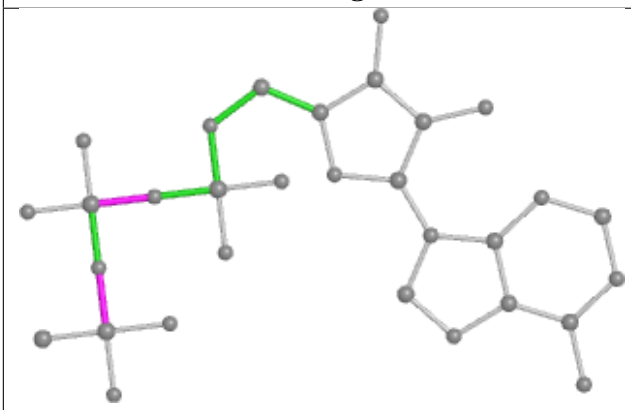
Ligand AGS F 2003



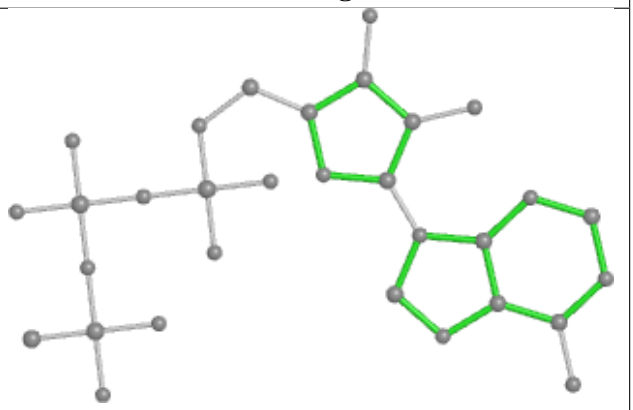
Bond lengths



Bond angles

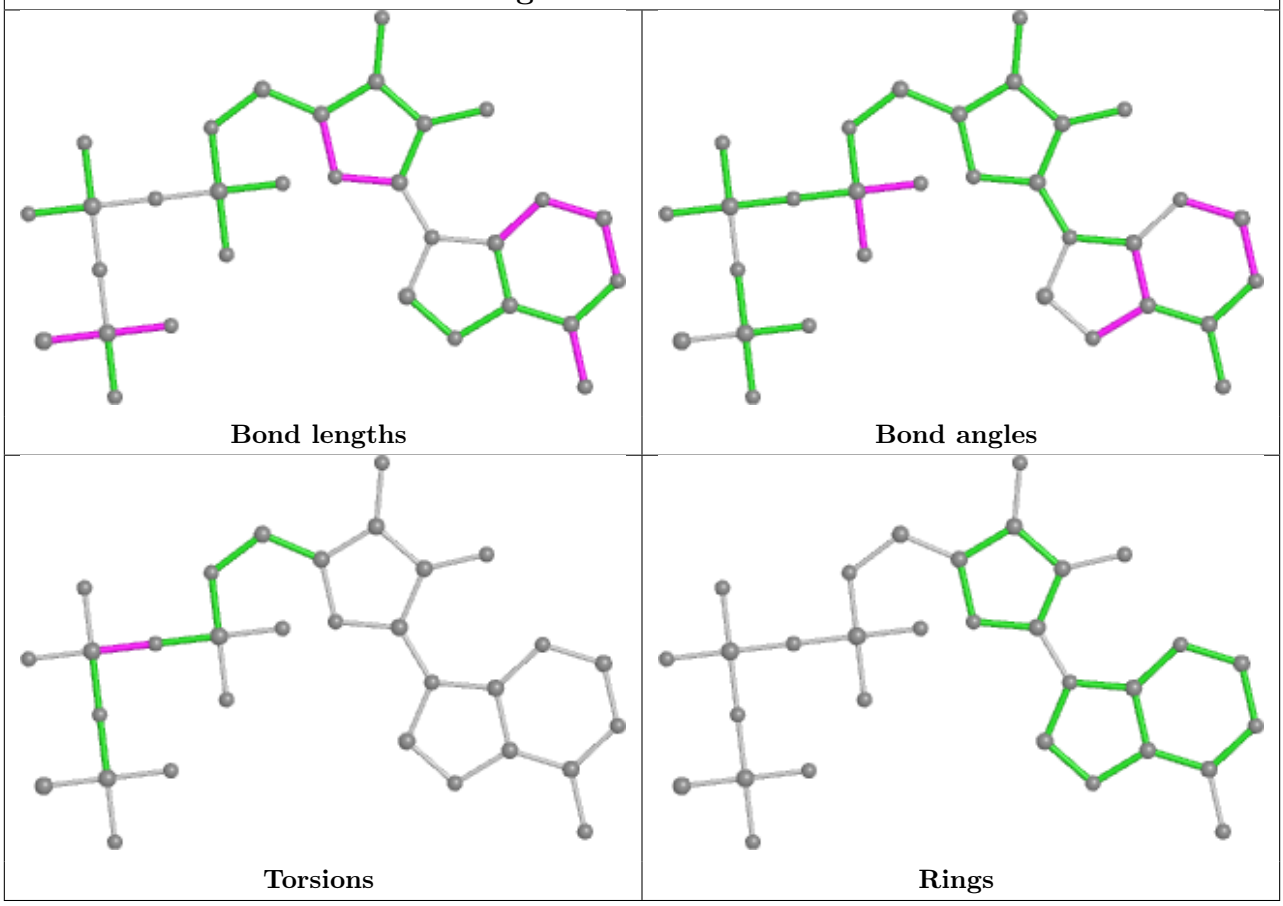


Torsions



Rings

Ligand AGS C 2002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	442/483 (91%)	-0.47	2 (0%) 91 85	66, 137, 179, 199	0
1	C	455/483 (94%)	-0.56	1 (0%) 95 93	75, 121, 160, 182	0
1	F	447/483 (92%)	-0.52	0 100 100	67, 120, 157, 176	0
1	H	459/483 (95%)	-0.67	0 100 100	51, 106, 143, 158	0
2	E	101/152 (66%)	-0.52	0 100 100	95, 130, 178, 193	0
2	J	124/152 (81%)	-0.51	0 100 100	88, 124, 188, 194	0
3	L	173/238 (72%)	-0.23	4 (2%) 60 51	93, 168, 195, 198	0
3	M	107/238 (44%)	0.41	8 (7%) 14 12	102, 199, 200, 200	0
All	All	2308/2712 (85%)	-0.48	15 (0%) 89 84	51, 126, 192, 200	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	79	SER	2.9
3	M	34	HIS	2.7
3	M	33	ARG	2.6
1	A	1465	ASN	2.6
3	L	10	PRO	2.5
3	M	184	VAL	2.5
3	M	97	VAL	2.5
3	L	151	ALA	2.5
1	C	1423	LYS	2.4
3	L	9	ILE	2.3
3	M	95	GLY	2.2
1	A	1466	ILE	2.1
3	M	85	SER	2.1
3	M	67	ALA	2.1
3	M	94	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

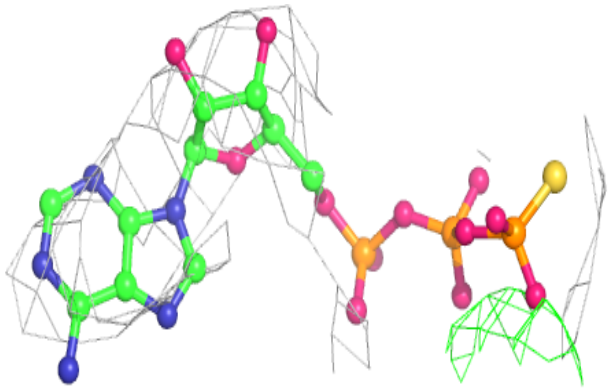
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

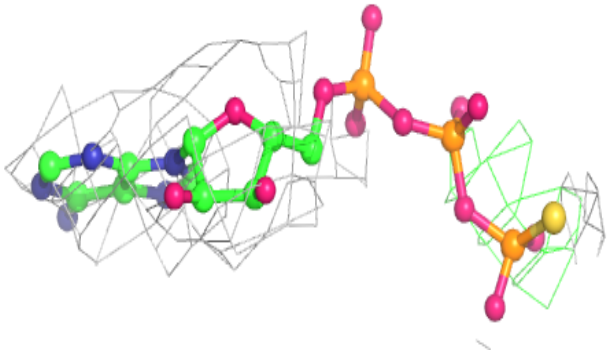
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AGS	A	2001	31/31	0.92	0.32	115,144,156,157	0
4	AGS	H	2004	31/31	0.93	0.27	98,101,105,105	0
4	AGS	F	2003	31/31	0.96	0.17	87,93,101,103	0
4	AGS	C	2002	31/31	0.96	0.24	85,91,99,99	0
5	MG	H	2014	1/1	0.98	0.42	107,107,107,107	0
5	MG	A	2012	1/1	0.99	0.42	77,77,77,77	0
5	MG	F	2013	1/1	0.99	0.27	29,29,29,29	0
5	MG	A	2011	1/1	0.99	0.56	56,56,56,56	0

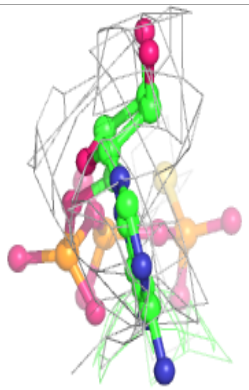
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS A 2001:

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

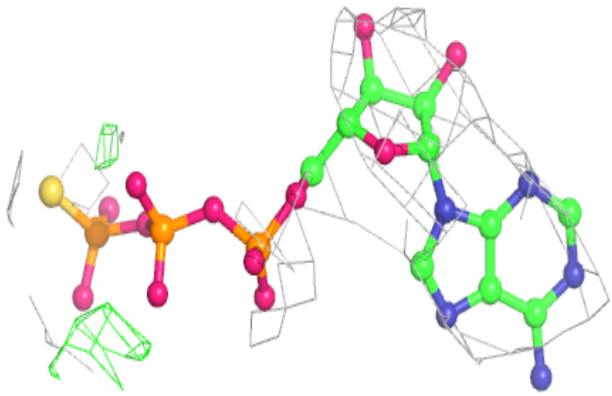


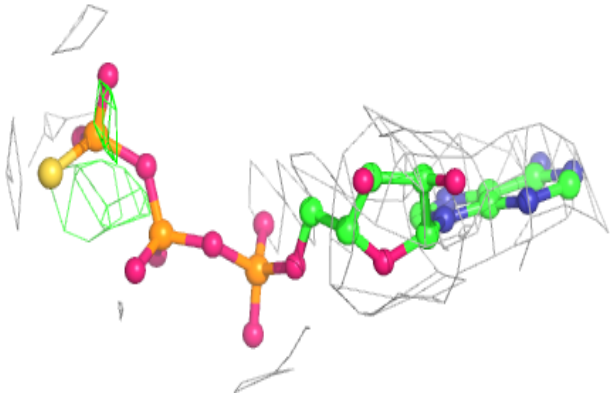


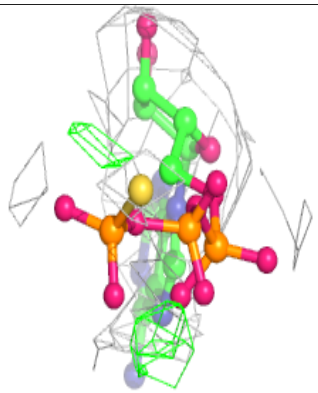


Electron density around AGS H 2004:

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

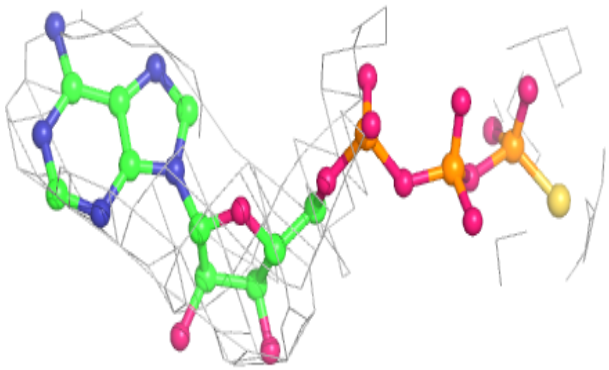


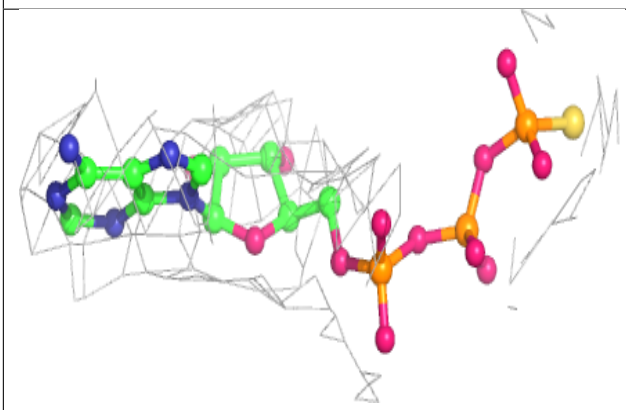


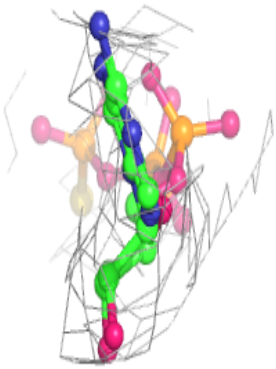


Electron density around AGS F 2003:

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

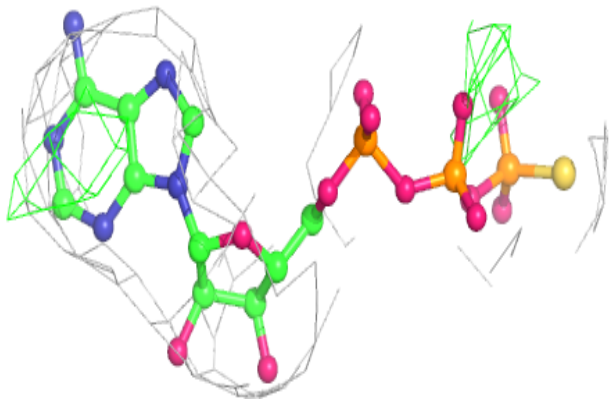


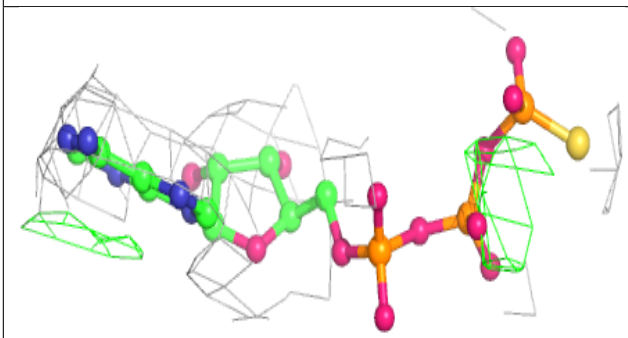


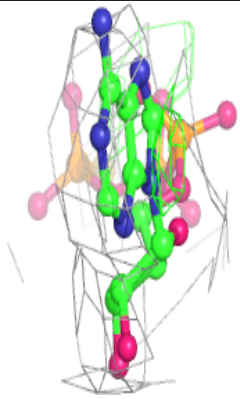


Electron density around AGS C 2002:

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







6.5 Other polymers (i)

There are no such residues in this entry.