Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 10:08 AM EST

PDB ID	:	1QBK
Title	:	STRUCTURE OF THE KARYOPHERIN BETA2-RAN GPPNHP NUCLEAR TRANSPORT COMPLEX
Authors	:	Chook, Y.M.; Blobel, G.
Deposited on	:	1999-04-23
Resolution	:	3.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

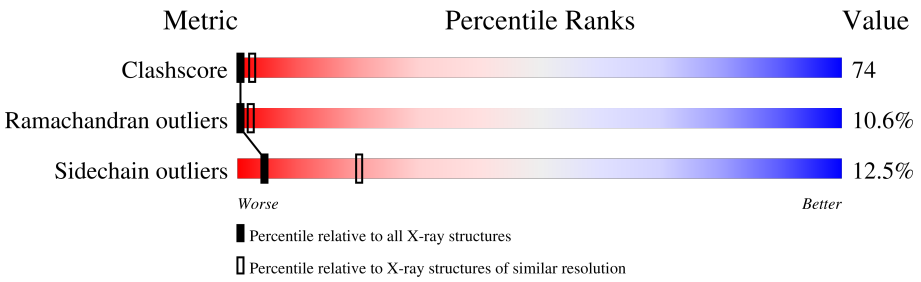
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	890	32% 51% 15% ··
2	C	216	24% 43% 19% · 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8572 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 KARYOPHERIN BETA2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	B	880	7011	4471	1170	1320	26	24	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	THR	ILE	conflict	UNP Q92973
B	175	MSE	MET	modified residue	UNP Q92973
B	210	MSE	MET	modified residue	UNP Q92973
B	237	ARG	MET	modified residue	UNP Q92973
B	247	MET	MET	modified residue	UNP Q92973
B	254	MSE	MET	modified residue	UNP Q92973
B	261	MSE	MET	modified residue	UNP Q92973
B	308	MSE	MET	modified residue	UNP Q92973
B	429	MSE	MET	modified residue	UNP Q92973
B	432	MSE	MET	modified residue	UNP Q92973
B	482	MSE	MET	modified residue	UNP Q92973
B	564	MSE	MET	modified residue	UNP Q92973
B	566	MSE	MET	modified residue	UNP Q92973
B	575	MSE	MET	modified residue	UNP Q92973
B	624	MSE	MET	modified residue	UNP Q92973
B	641	MSE	MET	modified residue	UNP Q92973
B	672	MSE	MET	modified residue	UNP Q92973
B	680	MSE	MET	modified residue	UNP Q92973
B	710	MSE	MET	modified residue	UNP Q92973
B	739	MSE	MET	modified residue	UNP Q92973
B	743	MSE	MET	modified residue	UNP Q92973
B	749	MSE	MET	modified residue	UNP Q92973
B	789	MSE	MET	modified residue	UNP Q92973
B	820	MSE	MET	modified residue	UNP Q92973
B	852	MSE	MET	modified residue	UNP Q92973

- Molecule 2 is a protein called RAN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	C	190	1528	993	265	264	3	3	0	0	0

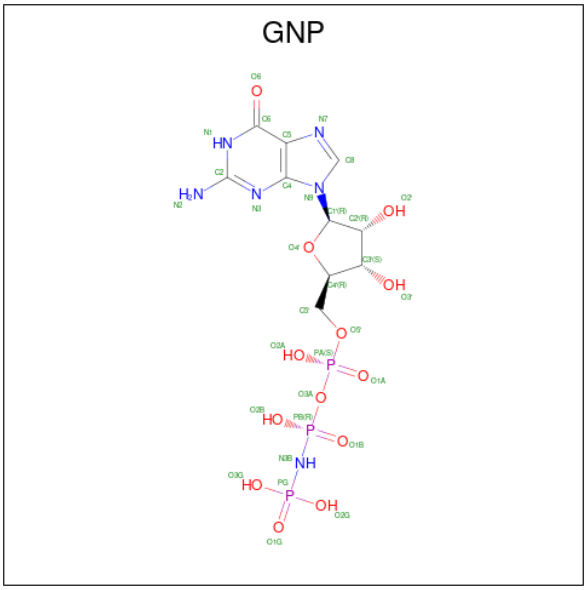
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ARG	SER	conflict	UNP P62826
C	89	MSE	MET	modified residue	UNP P62826
C	179	MSE	MET	modified residue	UNP P62826
C	189	MSE	MET	modified residue	UNP P62826

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	C	1	1	1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	C	1	32	10	6	13	3	0	0

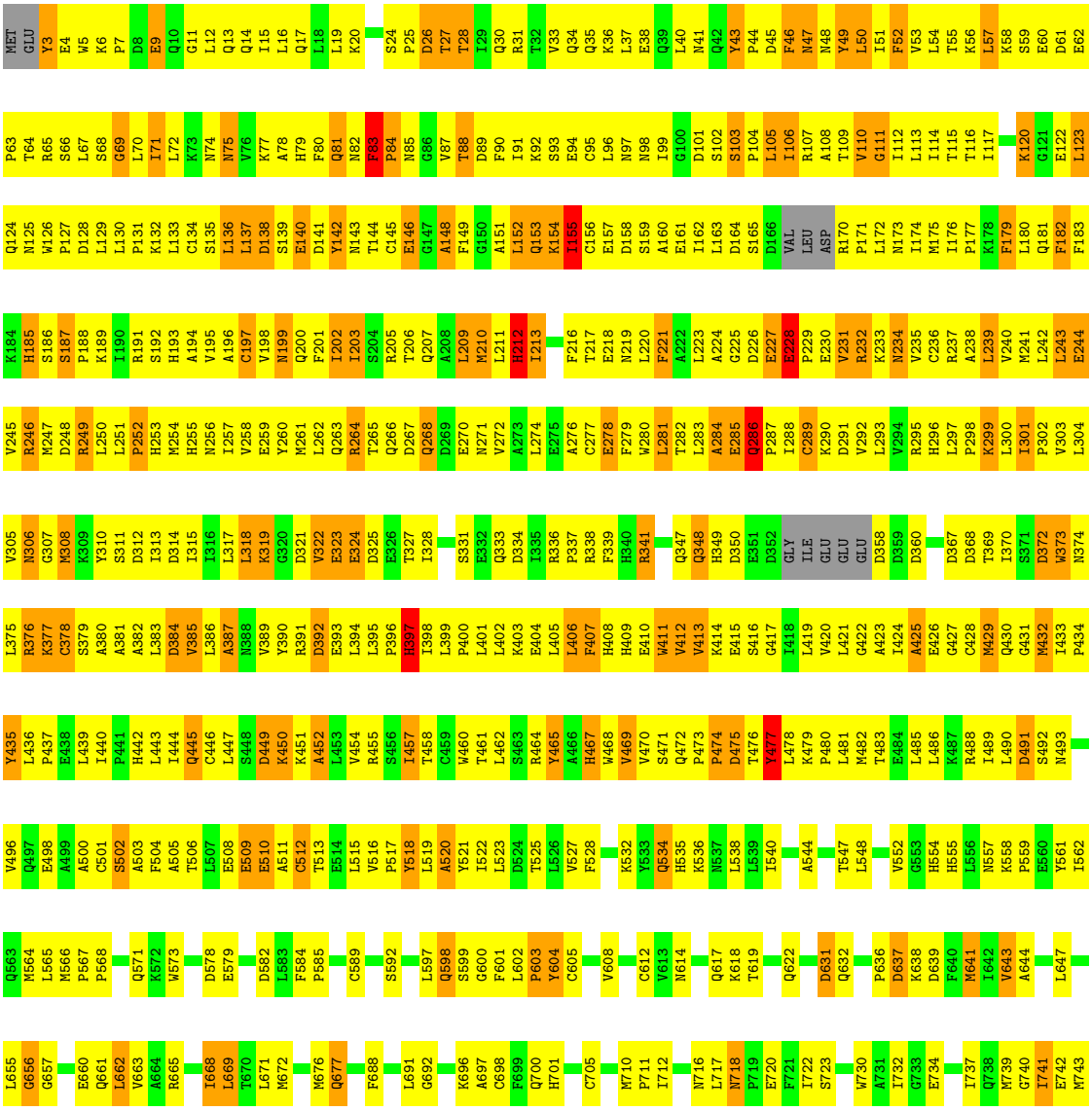
3 Residue-property plots (i)

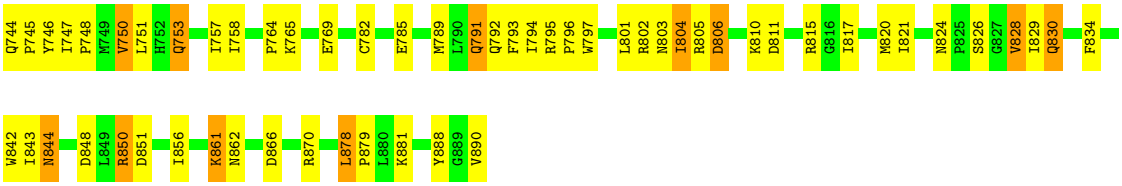
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: KARYOPHERIN BETA2

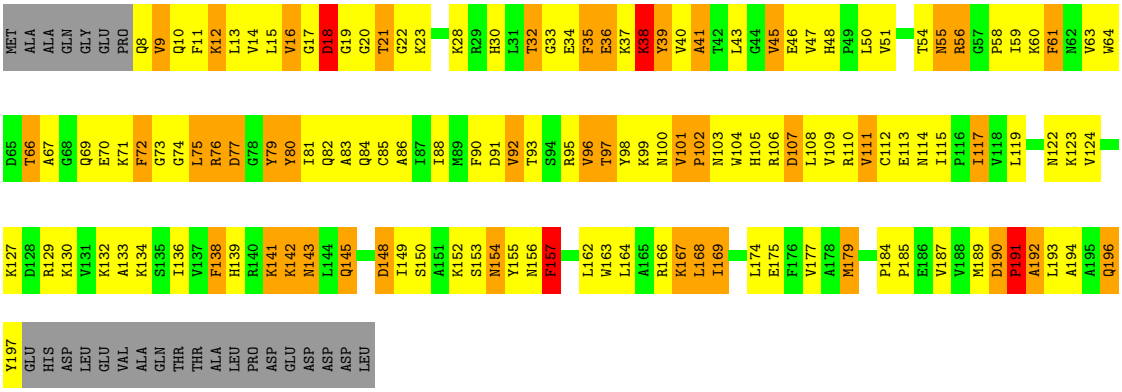
Chain B: 32% 51% 15% ••





- Molecule 2: RAN

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.11Å 133.11Å 138.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	500.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.3 (500.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 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	B	0.56	2/7134 (0.0%)	0.71	0/9651
2	C	0.49	0/1564	0.69	0/2113
All	All	0.55	2/8698 (0.0%)	0.71	0/11764

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	605	CYS	CB-SG	-5.15	1.73	1.81
1	B	641	MSE	CG-SE	-5.03	1.78	1.95

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7011	0	6991	1059	0
2	C	1528	0	1553	228	0
3	C	1	0	0	0	0
4	C	32	0	13	4	0
All	All	8572	0	8557	1265	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 74.

All (1265) 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:C:83:ALA:HB3	2:C:112:CYS:SG	1.55	1.46
1:B:143:ASN:HA	1:B:148:ALA:O	1.42	1.17
1:B:196:ALA:HB2	1:B:233:LYS:HB3	1.31	1.12
2:C:12:LYS:HG2	2:C:83:ALA:HA	1.15	1.11
1:B:301:ILE:H	1:B:302:PRO:HD2	1.17	1.09
2:C:95:ARG:HA	2:C:95:ARG:HH11	1.07	1.09
1:B:99:ILE:HD13	1:B:133:LEU:HD11	1.28	1.09
1:B:512:CYS:O	1:B:513:THR:OG1	1.68	1.09
1:B:341:ARG:H	1:B:341:ARG:HD3	1.17	1.08
1:B:378:CYS:HA	1:B:381:ALA:HB3	1.33	1.05
2:C:83:ALA:CB	2:C:112:CYS:SG	2.45	1.05
1:B:145:CYS:HB3	1:B:151:ALA:HB3	1.34	1.01
1:B:310:TYR:OH	1:B:375:LEU:HB2	1.58	1.01
1:B:59:SER:HB2	1:B:63:PRO:HD3	1.42	1.01
1:B:213:ILE:HD12	1:B:213:ILE:H	1.25	1.00
1:B:242:LEU:HG	1:B:280:TRP:HA	1.42	1.00
1:B:117:ILE:HG12	1:B:162:ILE:HG12	1.41	1.00
1:B:386:LEU:HB3	1:B:394:LEU:HD11	1.43	1.00
1:B:103:SER:H	1:B:104:PRO:HD2	1.26	0.99
1:B:177:PRO:HG3	1:B:209:LEU:HD11	1.43	0.99
1:B:191:ARG:HE	1:B:192:SER:H	1.02	0.98
1:B:511:ALA:HB3	1:B:515:LEU:HD11	1.46	0.97
2:C:174:LEU:HD12	2:C:175:GLU:N	1.78	0.97
1:B:866:ASP:O	1:B:870:ARG:HG2	1.63	0.96
2:C:43:LEU:HD23	2:C:71:LYS:HB3	1.43	0.96
2:C:50:LEU:HD12	2:C:63:VAL:HG21	1.47	0.94
1:B:51:ILE:HG23	1:B:67:LEU:HD13	1.48	0.93
1:B:387:ALA:HB1	1:B:427:GLY:HA3	1.47	0.93
1:B:93:SER:HA	1:B:96:LEU:HB2	1.51	0.92
2:C:106:ARG:HG3	2:C:107:ASP:H	1.32	0.92
1:B:668:ILE:HD12	1:B:669:LEU:H	1.32	0.92
1:B:348:GLN:HB2	1:B:805:ARG:HD2	1.52	0.92
1:B:372:ASP:HB3	1:B:377:LYS:NZ	1.85	0.91
1:B:404:GLU:HG2	1:B:408:HIS:HB2	1.52	0.91
2:C:12:LYS:CG	2:C:83:ALA:HA	2.00	0.91
1:B:373:TRP:HE3	1:B:373:TRP:H	0.98	0.91
1:B:203:ILE:CG1	1:B:240:VAL:HG11	2.00	0.91
1:B:449:ASP:HB3	1:B:451:LYS:HG2	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:ARG:HA	2:C:95:ARG:NH1	1.86	0.90
2:C:153:SER:O	2:C:154:ASN:HB2	1.67	0.90
1:B:149:PHE:O	1:B:153:GLN:HB3	1.69	0.90
1:B:523:LEU:HB3	1:B:564:MSE:HE2	1.53	0.90
1:B:285:GLU:HG2	1:B:287:PRO:HD2	1.54	0.89
1:B:245:VAL:HG12	1:B:246:ARG:HH11	1.37	0.89
1:B:99:ILE:HD13	1:B:133:LEU:CD1	2.01	0.89
1:B:220:LEU:HD21	1:B:253:HIS:HB2	1.55	0.89
1:B:283:LEU:HD12	1:B:385:VAL:HG11	1.52	0.89
2:C:96:VAL:HG13	2:C:97:THR:H	1.37	0.89
1:B:99:ILE:HG21	1:B:133:LEU:HD22	1.55	0.88
1:B:20:LYS:HA	1:B:65:ARG:HE	1.38	0.88
1:B:264:ARG:HH21	1:B:267:ASP:HB3	1.39	0.88
1:B:51:ILE:HG13	1:B:67:LEU:HB2	1.54	0.88
1:B:850:ARG:HG3	1:B:850:ARG:HH11	1.35	0.87
1:B:65:ARG:NH1	2:C:81:ILE:HB	1.89	0.86
1:B:297:LEU:HD11	1:B:301:ILE:HD11	1.54	0.86
1:B:245:VAL:HG12	1:B:246:ARG:NH1	1.90	0.86
1:B:53:VAL:O	1:B:57:LEU:HB2	1.75	0.86
1:B:409:HIS:HB3	1:B:413:VAL:HG21	1.58	0.86
1:B:230:GLU:HG3	1:B:233:LYS:HE3	1.56	0.86
1:B:203:ILE:HG13	1:B:240:VAL:HG11	1.56	0.86
1:B:64:THR:O	1:B:68:SER:HB2	1.76	0.85
1:B:65:ARG:HG2	2:C:81:ILE:HG21	1.57	0.85
1:B:191:ARG:HB3	1:B:194:ALA:HB3	1.58	0.85
2:C:43:LEU:O	2:C:72:PHE:HB2	1.74	0.85
2:C:106:ARG:HG3	2:C:107:ASP:N	1.89	0.85
1:B:235:VAL:HG22	1:B:272:VAL:HG22	1.59	0.85
1:B:242:LEU:HB3	1:B:279:PHE:O	1.76	0.85
1:B:274:LEU:HD12	1:B:375:LEU:HD23	1.59	0.85
1:B:515:LEU:C	1:B:517:PRO:HD2	1.98	0.84
1:B:676:MSE:HE3	1:B:688:PHE:HE2	1.42	0.84
2:C:12:LYS:HE3	2:C:12:LYS:HA	1.59	0.84
1:B:27:THR:O	1:B:31:ARG:HG2	1.78	0.84
1:B:584:PHE:HB2	1:B:585:PRO:HD3	1.59	0.84
1:B:171:PRO:HD2	1:B:173:ASN:ND2	1.92	0.84
1:B:145:CYS:SG	1:B:151:ALA:HB1	2.17	0.83
1:B:843:ILE:HG13	1:B:844:ASN:H	1.40	0.83
2:C:54:THR:HB	2:C:174:LEU:HD11	1.58	0.83
2:C:86:ALA:HB3	2:C:117:ILE:HG23	1.60	0.83
1:B:64:THR:HA	1:B:67:LEU:HG	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLU:HB3	1:B:152:LEU:HD11	1.60	0.83
1:B:470:VAL:HA	1:B:478:LEU:HD22	1.61	0.83
1:B:306:ASN:HD21	1:B:375:LEU:HB3	1.44	0.83
1:B:50:LEU:HA	1:B:53:VAL:HB	1.59	0.83
1:B:300:LEU:HD21	1:B:394:LEU:HD22	1.58	0.83
1:B:425:ALA:HB2	1:B:465:TYR:HD2	1.44	0.83
1:B:249:ARG:H	1:B:249:ARG:HD2	1.42	0.83
2:C:45:VAL:H	2:C:72:PHE:HD1	1.24	0.83
1:B:43:TYR:H	1:B:44:PRO:HD2	1.41	0.82
1:B:103:SER:H	1:B:104:PRO:CD	1.91	0.82
1:B:454:VAL:O	1:B:457:ILE:HD12	1.79	0.82
1:B:637:ASP:OD1	1:B:639:ASP:HB2	1.79	0.82
1:B:203:ILE:HG21	1:B:240:VAL:HG21	1.60	0.82
1:B:223:LEU:HA	1:B:226:ASP:HB2	1.60	0.82
1:B:341:ARG:H	1:B:341:ARG:CD	1.91	0.82
1:B:141:ASP:HA	1:B:152:LEU:HB3	1.60	0.82
1:B:145:CYS:CB	1:B:151:ALA:HB3	2.09	0.81
1:B:300:LEU:HD23	1:B:398:ILE:HD11	1.63	0.81
1:B:213:ILE:H	1:B:213:ILE:CD1	1.93	0.81
1:B:145:CYS:SG	1:B:151:ALA:CB	2.69	0.81
1:B:181:GLN:HE21	1:B:212:HIS:HB3	1.45	0.81
1:B:135:SER:HA	1:B:138:ASP:HB2	1.62	0.80
1:B:449:ASP:CG	1:B:450:LYS:H	1.82	0.80
1:B:228:GLU:HA	1:B:234:ASN:HB3	1.63	0.80
1:B:241:MSE:HG2	1:B:242:LEU:HD22	1.64	0.80
1:B:50:LEU:HB3	1:B:54:LEU:HG	1.64	0.80
1:B:386:LEU:CB	1:B:394:LEU:HD11	2.11	0.80
1:B:449:ASP:CG	1:B:451:LYS:HE3	2.02	0.80
1:B:34:GLN:HG3	1:B:35:GLN:HG3	1.64	0.80
1:B:130:LEU:HB3	1:B:131:PRO:HD3	1.61	0.79
1:B:210:MSE:HE3	1:B:246:ARG:HE	1.47	0.79
1:B:411:TRP:HD1	1:B:412:VAL:N	1.79	0.79
1:B:235:VAL:HG13	1:B:272:VAL:HA	1.63	0.79
1:B:301:ILE:H	1:B:302:PRO:CD	1.96	0.79
1:B:373:TRP:HE3	1:B:373:TRP:N	1.80	0.79
2:C:91:ASP:OD2	2:C:123:LYS:HD2	1.82	0.79
2:C:190:ASP:HB3	2:C:194:ALA:HB3	1.64	0.79
1:B:191:ARG:O	1:B:195:VAL:HG23	1.82	0.79
1:B:402:LEU:HD21	1:B:421:LEU:HD13	1.64	0.79
1:B:12:LEU:HD11	1:B:47:ASN:HB3	1.64	0.78
1:B:339:PHE:HB3	2:C:127:LYS:HD2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:C	1:B:298:PRO:HD2	2.04	0.78
1:B:213:ILE:HD12	1:B:213:ILE:N	1.99	0.78
1:B:286:GLN:HG3	1:B:287:PRO:HD3	1.65	0.78
1:B:409:HIS:CG	1:B:410:GLU:H	2.00	0.78
1:B:451:LYS:HB2	1:B:454:VAL:CG2	2.13	0.78
1:B:198:VAL:O	1:B:202:ILE:HG13	1.84	0.77
1:B:264:ARG:CZ	1:B:264:ARG:HA	2.13	0.77
1:B:383:LEU:O	1:B:383:LEU:HD23	1.83	0.77
2:C:47:VAL:HG22	2:C:64:TRP:CD1	2.19	0.77
1:B:163:LEU:HD23	1:B:201:PHE:HZ	1.49	0.77
1:B:191:ARG:HE	1:B:192:SER:N	1.80	0.77
2:C:191:PRO:HD2	2:C:194:ALA:HB3	1.65	0.77
1:B:603:PRO:O	1:B:604:TYR:CG	2.36	0.77
1:B:163:LEU:HD23	1:B:201:PHE:CZ	2.19	0.77
1:B:117:ILE:HG23	1:B:162:ILE:HA	1.67	0.77
1:B:323:GLU:HG3	1:B:492:SER:C	2.06	0.76
1:B:454:VAL:HA	1:B:457:ILE:HD11	1.68	0.76
1:B:411:TRP:CD1	1:B:412:VAL:N	2.53	0.76
1:B:99:ILE:CD1	1:B:133:LEU:HD11	2.13	0.76
1:B:602:LEU:HB2	1:B:603:PRO:HD3	1.67	0.76
1:B:203:ILE:HG21	1:B:240:VAL:CG2	2.14	0.76
1:B:331:SER:HB3	1:B:334:ASP:OD2	1.85	0.76
1:B:751:LEU:HD23	1:B:789:MSE:HE1	1.67	0.76
2:C:12:LYS:HG2	2:C:83:ALA:CA	2.08	0.76
2:C:54:THR:HB	2:C:174:LEU:CD1	2.16	0.75
2:C:132:LYS:HD3	2:C:133:ALA:N	2.01	0.75
2:C:38:LYS:HG2	2:C:40:VAL:HG23	1.69	0.75
2:C:16:VAL:HG23	2:C:17:GLY:N	2.01	0.75
1:B:143:ASN:CA	1:B:148:ALA:O	2.30	0.75
1:B:90:PHE:O	1:B:94:GLU:HG3	1.87	0.75
1:B:221:PHE:HA	1:B:224:ALA:HB3	1.69	0.75
1:B:183:PHE:HB3	1:B:202:ILE:HG12	1.66	0.75
1:B:639:ASP:OD2	2:C:127:LYS:HE2	1.86	0.75
1:B:61:ASP:O	1:B:65:ARG:HG3	1.86	0.74
1:B:96:LEU:O	1:B:99:ILE:HD12	1.87	0.74
1:B:238:ALA:HA	1:B:241:MSE:HE1	1.69	0.74
1:B:149:PHE:CE1	1:B:191:ARG:HD2	2.22	0.74
1:B:283:LEU:HA	1:B:288:ILE:HG21	1.68	0.74
1:B:718:ASN:ND2	1:B:720:GLU:H	1.84	0.74
1:B:789:MSE:HG2	1:B:792:GLN:NE2	2.02	0.74
1:B:33:VAL:HA	1:B:36:LYS:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ALA:CB	1:B:515:LEU:HD11	2.17	0.74
1:B:562:ILE:HD11	1:B:597:LEU:HG	1.69	0.74
2:C:96:VAL:HG13	2:C:97:THR:N	2.03	0.74
1:B:51:ILE:HG21	1:B:112:ILE:HD11	1.70	0.74
2:C:75:LEU:HB3	2:C:79:TYR:OH	1.86	0.74
1:B:20:LYS:HA	1:B:65:ARG:NE	2.01	0.74
1:B:372:ASP:HB3	1:B:377:LYS:HZ1	1.51	0.74
1:B:394:LEU:HB3	1:B:398:ILE:HD11	1.67	0.74
1:B:888:TYR:HE2	1:B:890:VAL:HG22	1.52	0.74
1:B:193:HIS:O	1:B:197:CYS:HB2	1.88	0.73
1:B:230:GLU:O	1:B:231:VAL:HG23	1.88	0.73
2:C:141:LYS:HA	2:C:141:LYS:NZ	2.02	0.73
1:B:249:ARG:H	1:B:249:ARG:CD	2.00	0.73
1:B:96:LEU:HD22	1:B:130:LEU:HG	1.68	0.73
2:C:95:ARG:HH11	2:C:95:ARG:CA	1.95	0.73
1:B:126:TRP:HE1	1:B:129:LEU:HD13	1.53	0.73
1:B:668:ILE:CD1	1:B:669:LEU:H	2.02	0.73
2:C:191:PRO:HD2	2:C:194:ALA:CB	2.18	0.73
1:B:211:LEU:N	1:B:213:ILE:HD13	2.03	0.73
1:B:425:ALA:CB	1:B:465:TYR:HD2	2.01	0.73
1:B:228:GLU:HB3	1:B:234:ASN:ND2	2.04	0.72
1:B:156:CYS:SG	1:B:198:VAL:HG22	2.29	0.72
2:C:45:VAL:HG23	2:C:72:PHE:CD1	2.23	0.72
1:B:223:LEU:HA	1:B:226:ASP:CB	2.18	0.72
1:B:491:ASP:H	1:B:532:LYS:NZ	1.86	0.72
1:B:283:LEU:CD1	1:B:385:VAL:HG11	2.20	0.72
1:B:370:ILE:HD13	2:C:133:ALA:HB1	1.70	0.72
2:C:37:LYS:O	2:C:38:LYS:HB3	1.88	0.72
2:C:64:TRP:CE3	2:C:79:TYR:HB3	2.25	0.72
1:B:75:ASN:HD22	1:B:75:ASN:N	1.88	0.71
1:B:451:LYS:CG	1:B:454:VAL:HB	2.19	0.71
1:B:511:ALA:HB3	1:B:515:LEU:CD1	2.20	0.71
2:C:145:GLN:HG3	2:C:163:TRP:CE2	2.24	0.71
1:B:33:VAL:O	1:B:37:LEU:HG	1.90	0.71
1:B:110:VAL:HG13	1:B:158:ASP:OD1	1.90	0.71
1:B:323:GLU:HA	1:B:493:ASN:HB3	1.72	0.71
1:B:850:ARG:HG3	1:B:850:ARG:NH1	2.00	0.71
1:B:96:LEU:CD2	1:B:130:LEU:HG	2.19	0.71
1:B:378:CYS:CA	1:B:381:ALA:HB3	2.18	0.71
1:B:582:ASP:O	1:B:585:PRO:HD2	1.91	0.71
1:B:106:ILE:HA	1:B:109:THR:OG1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:ILE:HD13	1:B:805:ARG:N	2.06	0.71
1:B:227:GLU:HG3	1:B:228:GLU:H	1.53	0.70
1:B:515:LEU:H	1:B:515:LEU:HD12	1.56	0.70
1:B:248:ASP:HB2	1:B:249:ARG:CZ	2.20	0.70
2:C:76:ARG:HG3	2:C:77:ASP:H	1.54	0.70
1:B:196:ALA:CB	1:B:233:LYS:HB3	2.17	0.70
1:B:257:ILE:O	1:B:261:MSE:HB2	1.91	0.70
1:B:451:LYS:HG3	1:B:454:VAL:HB	1.70	0.70
2:C:174:LEU:HD12	2:C:175:GLU:H	1.55	0.70
1:B:552:VAL:HG12	1:B:555:HIS:HB2	1.74	0.70
2:C:8:GLN:OE1	2:C:60:LYS:HE3	1.91	0.70
1:B:26:ASP:O	1:B:30:GLN:HB3	1.92	0.70
1:B:251:LEU:HB2	1:B:252:PRO:HD3	1.72	0.70
1:B:283:LEU:HD12	1:B:385:VAL:HG21	1.72	0.70
1:B:126:TRP:CH2	1:B:130:LEU:HB2	2.27	0.70
1:B:372:ASP:HB3	1:B:377:LYS:HZ2	1.53	0.69
1:B:126:TRP:CE2	1:B:129:LEU:HB3	2.28	0.69
2:C:38:LYS:CG	2:C:40:VAL:HG23	2.22	0.69
1:B:136:LEU:O	1:B:137:LEU:HG	1.93	0.69
1:B:137:LEU:HA	1:B:140:GLU:HB2	1.74	0.69
1:B:82:ASN:C	1:B:84:PRO:HD3	2.13	0.69
1:B:143:ASN:HB3	1:B:148:ALA:HB1	1.75	0.68
1:B:160:ALA:HA	1:B:201:PHE:CE1	2.28	0.68
2:C:96:VAL:O	2:C:98:TYR:N	2.25	0.68
1:B:297:LEU:N	1:B:298:PRO:CD	2.56	0.68
1:B:299:LYS:HB2	1:B:299:LYS:HZ3	1.59	0.68
1:B:231:VAL:HA	1:B:234:ASN:ND2	2.09	0.68
1:B:491:ASP:H	1:B:532:LYS:HZ1	1.40	0.68
1:B:744:GLN:HB3	1:B:745:PRO:HD3	1.75	0.68
2:C:45:VAL:HG23	2:C:72:PHE:HD1	1.57	0.68
1:B:72:LEU:HB3	2:C:76:ARG:CZ	2.23	0.68
1:B:95:CYS:C	1:B:97:ASN:H	1.97	0.68
1:B:152:LEU:O	1:B:155:ILE:HG13	1.92	0.68
1:B:198:VAL:HG12	1:B:202:ILE:HD11	1.75	0.68
1:B:232:ARG:HE	1:B:233:LYS:HZ1	1.42	0.68
1:B:417:GLY:O	1:B:420:VAL:HG22	1.93	0.68
1:B:428:CYS:O	1:B:432:MSE:HB2	1.94	0.68
1:B:185:HIS:O	1:B:187:SER:N	2.27	0.68
1:B:220:LEU:HD11	1:B:257:ILE:HD11	1.74	0.67
2:C:177:VAL:O	2:C:177:VAL:HG23	1.94	0.67
1:B:292:VAL:HA	1:B:295:ARG:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:LYS:HB3	2:C:84:GLN:H	1.60	0.67
1:B:57:LEU:O	1:B:58:LYS:HD2	1.94	0.67
1:B:317:LEU:O	1:B:319:LYS:N	2.26	0.67
2:C:132:LYS:CD	2:C:134:LYS:H	2.07	0.67
1:B:843:ILE:HG13	1:B:844:ASN:N	2.08	0.67
1:B:508:GLU:HA	1:B:515:LEU:HD21	1.75	0.67
1:B:429:MSE:HE2	1:B:433:ILE:HG12	1.75	0.67
1:B:451:LYS:HD3	1:B:454:VAL:HG11	1.75	0.67
1:B:619:THR:HG22	1:B:641:MSE:HE2	1.76	0.67
1:B:668:ILE:HD13	1:B:669:LEU:HD23	1.76	0.67
1:B:113:LEU:HD13	1:B:158:ASP:OD2	1.95	0.67
1:B:196:ALA:HB2	1:B:233:LYS:CB	2.18	0.67
1:B:281:LEU:HB2	1:B:382:ALA:HB1	1.74	0.67
1:B:491:ASP:H	1:B:532:LYS:CE	2.08	0.67
1:B:35:GLN:HA	1:B:38:GLU:OE2	1.95	0.67
1:B:99:ILE:HG21	1:B:133:LEU:CD2	2.25	0.67
1:B:311:SER:O	1:B:315:ILE:HG13	1.95	0.67
1:B:323:GLU:HG3	1:B:492:SER:HA	1.75	0.67
1:B:486:LEU:HD21	1:B:504:PHE:CE1	2.30	0.67
2:C:11:PHE:CE1	2:C:168:LEU:HD13	2.29	0.67
2:C:16:VAL:HA	2:C:66:THR:HG21	1.77	0.67
1:B:72:LEU:HB3	2:C:76:ARG:NH2	2.10	0.66
1:B:210:MSE:HG3	1:B:210:MSE:O	1.95	0.66
1:B:663:VAL:HG13	1:B:668:ILE:HD11	1.77	0.66
1:B:89:ASP:HA	1:B:92:LYS:HB3	1.77	0.66
1:B:304:LEU:HD21	1:B:405:LEU:HD11	1.77	0.66
1:B:718:ASN:HD21	1:B:720:GLU:HB2	1.61	0.66
1:B:376:ARG:NH2	1:B:415:GLU:OE2	2.28	0.66
2:C:38:LYS:HG2	2:C:39:TYR:N	2.10	0.66
1:B:141:ASP:C	1:B:143:ASN:H	1.98	0.66
1:B:235:VAL:CG2	1:B:272:VAL:HG22	2.26	0.66
1:B:284:ALA:N	1:B:288:ILE:HD12	2.10	0.66
1:B:62:GLU:HB3	1:B:63:PRO:HD3	1.77	0.66
1:B:313:ILE:O	1:B:317:LEU:HD13	1.95	0.66
1:B:722:ILE:HG13	1:B:723:SER:N	2.10	0.66
1:B:247:MET:O	1:B:251:LEU:HG	1.96	0.66
1:B:602:LEU:O	1:B:604:TYR:N	2.23	0.65
2:C:193:LEU:HA	2:C:196:GLN:NE2	2.11	0.65
1:B:40:LEU:H	1:B:40:LEU:HD23	1.59	0.65
1:B:206:THR:O	1:B:210:MSE:HE2	1.96	0.65
1:B:323:GLU:HG3	1:B:492:SER:CA	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:MSE:HE2	1:B:742:GLU:HG2	1.78	0.65
1:B:301:ILE:N	1:B:302:PRO:HD2	1.98	0.65
1:B:638:LYS:HD2	1:B:641:MSE:HE3	1.77	0.65
2:C:28:LYS:O	2:C:32:THR:HG23	1.96	0.65
1:B:390:TYR:HB3	1:B:393:GLU:CD	2.16	0.65
1:B:794:ILE:HG12	1:B:828:VAL:HG22	1.78	0.65
1:B:829:ILE:HG23	1:B:830:GLN:N	2.11	0.65
1:B:171:PRO:HD2	1:B:173:ASN:HD22	1.56	0.65
1:B:240:VAL:HA	1:B:243:LEU:HD23	1.79	0.65
1:B:349:HIS:HE1	1:B:769:GLU:OE2	1.80	0.65
1:B:888:TYR:CE2	1:B:890:VAL:HG22	2.30	0.65
1:B:126:TRP:HZ2	1:B:129:LEU:HD22	1.61	0.65
1:B:722:ILE:CD1	1:B:764:PRO:HG2	2.27	0.65
1:B:477:TYR:HA	1:B:480:PRO:CG	2.27	0.64
1:B:557:ASN:O	1:B:558:LYS:HG2	1.97	0.64
1:B:669:LEU:HD12	1:B:705:CYS:SG	2.37	0.64
2:C:11:PHE:HA	2:C:84:GLN:OE1	1.96	0.64
1:B:454:VAL:HA	1:B:457:ILE:CD1	2.27	0.64
1:B:261:MSE:HE2	1:B:276:ALA:HB1	1.80	0.64
1:B:312:ASP:OD2	1:B:312:ASP:N	2.27	0.64
1:B:425:ALA:HB2	1:B:465:TYR:CD2	2.30	0.64
1:B:506:THR:HA	1:B:509:GLU:OE2	1.97	0.64
2:C:106:ARG:C	2:C:108:LEU:H	1.98	0.64
1:B:51:ILE:HG12	1:B:112:ILE:HD13	1.77	0.64
1:B:254:MSE:HE3	1:B:257:ILE:HB	1.79	0.64
1:B:442:HIS:O	1:B:445:GLN:HB2	1.97	0.64
1:B:50:LEU:HD13	1:B:54:LEU:HD11	1.78	0.64
1:B:65:ARG:O	1:B:69:GLY:HA3	1.96	0.64
1:B:203:ILE:HG12	1:B:240:VAL:HG11	1.79	0.64
1:B:668:ILE:HD12	1:B:669:LEU:N	2.10	0.64
2:C:193:LEU:HA	2:C:196:GLN:HE22	1.61	0.64
1:B:16:LEU:HD21	1:B:66:SER:OG	1.97	0.64
1:B:91:ILE:HA	1:B:94:GLU:OE1	1.97	0.64
2:C:50:LEU:HD12	2:C:63:VAL:CG2	2.23	0.64
1:B:65:ARG:NH1	2:C:82:GLN:HE21	1.96	0.64
1:B:177:PRO:O	1:B:181:GLN:HG3	1.97	0.64
1:B:263:GLN:NE2	1:B:264:ARG:N	2.45	0.64
1:B:57:LEU:HD12	1:B:58:LYS:HG2	1.78	0.64
1:B:676:MSE:HE3	1:B:688:PHE:CE2	2.27	0.64
1:B:171:PRO:C	1:B:172:LEU:HD12	2.19	0.64
1:B:830:GLN:HA	1:B:830:GLN:HE21	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:LYS:HD2	1:B:641:MSE:CE	2.28	0.64
1:B:20:LYS:CA	1:B:65:ARG:HE	2.11	0.63
1:B:498:GLU:HG3	1:B:540:ILE:CD1	2.28	0.63
1:B:43:TYR:H	1:B:44:PRO:CD	2.11	0.63
1:B:160:ALA:HA	1:B:201:PHE:CZ	2.33	0.63
1:B:177:PRO:HG3	1:B:209:LEU:CD1	2.24	0.63
1:B:43:TYR:N	1:B:44:PRO:HD2	2.12	0.63
1:B:296:HIS:HE1	1:B:396:PRO:HG2	1.63	0.63
1:B:491:ASP:H	1:B:532:LYS:HE3	1.63	0.63
1:B:16:LEU:HB3	1:B:62:GLU:HG2	1.79	0.63
1:B:130:LEU:C	1:B:132:LYS:H	2.02	0.63
2:C:190:ASP:O	2:C:191:PRO:C	2.35	0.63
1:B:870:ARG:HH11	1:B:870:ARG:HG3	1.64	0.63
2:C:55:ASN:HD22	2:C:56:ARG:N	1.97	0.63
1:B:117:ILE:HA	1:B:162:ILE:HG23	1.79	0.63
1:B:126:TRP:HE1	1:B:129:LEU:CD1	2.11	0.63
1:B:171:PRO:HB2	1:B:172:LEU:HD12	1.80	0.63
2:C:98:TYR:OH	2:C:136:ILE:HA	1.98	0.63
2:C:132:LYS:HD2	2:C:134:LYS:H	1.62	0.63
1:B:791:GLN:H	1:B:791:GLN:HE21	1.44	0.63
1:B:861:LYS:HE3	1:B:866:ASP:OD2	1.99	0.63
1:B:6:LYS:N	1:B:7:PRO:HD2	2.14	0.63
1:B:50:LEU:HB3	1:B:54:LEU:CG	2.28	0.63
1:B:145:CYS:HB2	1:B:152:LEU:HD23	1.81	0.63
1:B:264:ARG:NH2	1:B:267:ASP:HB3	2.11	0.62
1:B:64:THR:HA	1:B:67:LEU:CG	2.28	0.62
1:B:416:SER:O	1:B:420:VAL:HG13	1.99	0.62
1:B:265:THR:CG2	1:B:277:CYS:HB2	2.28	0.62
2:C:55:ASN:HD22	2:C:55:ASN:C	2.02	0.62
1:B:88:THR:HG23	1:B:91:ILE:CG2	2.29	0.62
1:B:126:TRP:N	1:B:127:PRO:CD	2.63	0.62
1:B:60:GLU:C	1:B:63:PRO:HD2	2.19	0.62
1:B:237:ARG:C	1:B:239:LEU:H	2.03	0.62
2:C:88:ILE:O	2:C:119:LEU:HD12	1.99	0.62
1:B:9:GLU:HA	1:B:47:ASN:ND2	2.15	0.62
1:B:71:ILE:HG23	1:B:72:LEU:H	1.65	0.62
1:B:263:GLN:NE2	1:B:264:ARG:H	1.97	0.62
1:B:65:ARG:HH12	2:C:82:GLN:HE21	1.48	0.62
1:B:117:ILE:CG1	1:B:162:ILE:HG12	2.23	0.62
1:B:134:CYS:HB3	1:B:179:PHE:CE2	2.35	0.62
1:B:249:ARG:C	1:B:252:PRO:HD2	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:CYS:HB2	1:B:458:THR:HG21	1.82	0.62
1:B:508:GLU:OE2	1:B:548:LEU:HB2	1.99	0.62
1:B:9:GLU:HA	1:B:47:ASN:HD21	1.65	0.62
1:B:283:LEU:HD12	1:B:385:VAL:CG1	2.29	0.62
1:B:490:LEU:HD13	1:B:528:PHE:HD2	1.64	0.62
2:C:59:ILE:HD11	2:C:169:ILE:HD11	1.82	0.62
1:B:310:TYR:OH	1:B:375:LEU:CB	2.44	0.61
1:B:430:GLN:HA	1:B:433:ILE:CD1	2.30	0.61
1:B:232:ARG:HG3	1:B:233:LYS:CE	2.29	0.61
1:B:430:GLN:O	1:B:434:PRO:HD3	2.00	0.61
1:B:451:LYS:O	1:B:454:VAL:N	2.24	0.61
1:B:125:ASN:O	1:B:126:TRP:HB3	1.99	0.61
2:C:19:GLY:HA2	4:C:218:GNP:O3G	2.00	0.61
1:B:12:LEU:CD1	1:B:47:ASN:HB3	2.29	0.61
1:B:172:LEU:HB3	1:B:175:MSE:SE	2.50	0.61
1:B:183:PHE:HB3	1:B:202:ILE:CG1	2.31	0.61
2:C:43:LEU:HD23	2:C:71:LYS:CB	2.25	0.61
1:B:117:ILE:HG12	1:B:162:ILE:CG1	2.23	0.61
1:B:449:ASP:CG	1:B:450:LYS:N	2.53	0.61
1:B:96:LEU:HD11	1:B:126:TRP:HH2	1.65	0.61
1:B:312:ASP:HA	1:B:315:ILE:HG13	1.83	0.61
1:B:431:GLY:O	1:B:434:PRO:HD2	2.00	0.61
1:B:722:ILE:HD13	1:B:764:PRO:HG2	1.81	0.61
1:B:59:SER:HB2	1:B:63:PRO:CD	2.27	0.61
1:B:170:ARG:HA	1:B:173:ASN:HD22	1.66	0.61
1:B:216:PHE:HD2	1:B:219:ASN:HB3	1.66	0.61
1:B:387:ALA:CB	1:B:427:GLY:HA3	2.28	0.61
1:B:447:LEU:HD11	1:B:462:LEU:CD1	2.31	0.60
2:C:105:HIS:HE1	2:C:142:LYS:HB3	1.66	0.60
1:B:48:ASN:C	1:B:50:LEU:H	2.04	0.60
1:B:93:SER:O	1:B:97:ASN:HB2	2.00	0.60
1:B:249:ARG:O	1:B:252:PRO:HD2	2.02	0.60
1:B:390:TYR:CD2	1:B:393:GLU:HB3	2.36	0.60
1:B:56:LYS:HE2	1:B:56:LYS:HA	1.82	0.60
1:B:189:LYS:HG2	1:B:194:ALA:CB	2.32	0.60
2:C:66:THR:HG23	2:C:67:ALA:N	2.15	0.60
2:C:141:LYS:C	2:C:143:ASN:H	2.04	0.60
1:B:135:SER:HA	1:B:138:ASP:CB	2.30	0.60
1:B:696:LYS:HG3	1:B:734:GLU:HG2	1.83	0.60
2:C:96:VAL:HG22	2:C:97:THR:N	2.16	0.60
1:B:59:SER:CB	1:B:63:PRO:HD3	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:O	1:B:84:PRO:HD2	2.01	0.60
1:B:24:SER:HB2	1:B:25:PRO:HD3	1.84	0.60
1:B:286:GLN:CG	1:B:287:PRO:HD3	2.32	0.60
1:B:451:LYS:HD3	1:B:454:VAL:CG1	2.32	0.60
1:B:811:ASP:OD1	1:B:815:ARG:NH1	2.35	0.60
1:B:227:GLU:O	1:B:229:PRO:HD3	2.02	0.60
1:B:474:PRO:O	1:B:476:THR:N	2.35	0.60
2:C:47:VAL:HG13	2:C:64:TRP:CD1	2.37	0.60
2:C:72:PHE:C	2:C:74:GLY:H	2.04	0.60
1:B:143:ASN:HA	1:B:148:ALA:C	2.22	0.60
1:B:409:HIS:CG	1:B:410:GLU:N	2.70	0.60
2:C:105:HIS:CE1	2:C:142:LYS:HB3	2.37	0.60
1:B:65:ARG:C	1:B:69:GLY:HA3	2.23	0.60
1:B:88:THR:HG23	1:B:91:ILE:HG21	1.83	0.60
1:B:179:PHE:O	1:B:182:PHE:HB3	2.02	0.60
1:B:373:TRP:N	1:B:373:TRP:CE3	2.59	0.60
1:B:516:VAL:N	1:B:517:PRO:HD2	2.17	0.60
1:B:109:THR:HG22	1:B:109:THR:O	2.02	0.59
1:B:82:ASN:O	1:B:84:PRO:HD3	2.02	0.59
1:B:751:LEU:CD2	1:B:789:MSE:HE1	2.31	0.59
1:B:261:MSE:N	1:B:263:GLN:HE21	2.00	0.59
1:B:261:MSE:C	1:B:263:GLN:H	2.06	0.59
1:B:113:LEU:HD13	1:B:158:ASP:CG	2.23	0.59
1:B:140:GLU:HB3	1:B:152:LEU:CD1	2.30	0.59
1:B:392:ASP:HA	1:B:395:LEU:HG	1.85	0.59
1:B:597:LEU:O	1:B:598:GLN:C	2.41	0.59
1:B:72:LEU:HB3	2:C:76:ARG:NE	2.17	0.59
1:B:81:GLN:HG2	1:B:85:ASN:HB3	1.85	0.59
1:B:232:ARG:NE	1:B:233:LYS:NZ	2.51	0.59
1:B:447:LEU:O	1:B:488:ARG:HD2	2.03	0.59
1:B:793:PHE:O	1:B:796:PRO:HD2	2.02	0.59
2:C:14:VAL:HG21	2:C:108:LEU:HD11	1.85	0.59
1:B:65:ARG:HH12	2:C:81:ILE:HB	1.68	0.59
1:B:238:ALA:HA	1:B:241:MSE:CE	2.32	0.59
1:B:672:MSE:HE1	1:B:691:LEU:CA	2.33	0.59
1:B:447:LEU:HD21	1:B:462:LEU:HD12	1.84	0.59
1:B:92:LYS:HB2	1:B:92:LYS:NZ	2.18	0.58
1:B:141:ASP:O	1:B:143:ASN:N	2.25	0.58
1:B:451:LYS:HB2	1:B:454:VAL:HG21	1.83	0.58
1:B:40:LEU:HD12	1:B:43:TYR:CE1	2.38	0.58
1:B:299:LYS:C	1:B:302:PRO:HD2	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASP:O	1:B:536:LYS:HE3	2.03	0.58
1:B:409:HIS:HB3	1:B:413:VAL:CG2	2.32	0.58
1:B:192:SER:HA	1:B:230:GLU:CD	2.23	0.58
1:B:265:THR:HG23	1:B:277:CYS:HB2	1.84	0.58
2:C:80:TYR:O	2:C:112:CYS:SG	2.51	0.58
1:B:117:ILE:HD11	1:B:161:GLU:OE2	2.03	0.58
1:B:198:VAL:O	1:B:201:PHE:HB3	2.03	0.58
1:B:280:TRP:CH2	1:B:299:LYS:NZ	2.67	0.58
1:B:385:VAL:HG22	1:B:389:VAL:HB	1.86	0.58
1:B:143:ASN:OD1	1:B:149:PHE:HD2	1.86	0.58
1:B:238:ALA:HA	1:B:241:MSE:SE	2.54	0.58
1:B:479:LYS:H	1:B:480:PRO:HD2	1.68	0.58
2:C:81:ILE:HG22	2:C:82:GLN:HG3	1.83	0.58
1:B:817:ILE:HD13	1:B:820:MSE:HE3	1.85	0.58
1:B:189:LYS:HG2	1:B:194:ALA:HB3	1.86	0.58
1:B:806:ASP:HA	1:B:810:LYS:HD3	1.85	0.58
2:C:191:PRO:O	2:C:192:ALA:HB2	2.04	0.58
1:B:137:LEU:CA	1:B:140:GLU:HB2	2.33	0.58
1:B:449:ASP:CB	1:B:451:LYS:HG2	2.31	0.58
1:B:597:LEU:O	1:B:600:GLY:N	2.36	0.58
1:B:109:THR:HG21	1:B:154:LYS:HB3	1.86	0.58
1:B:449:ASP:CB	1:B:451:LYS:HE3	2.32	0.58
2:C:80:TYR:HD1	2:C:108:LEU:HA	1.68	0.58
2:C:81:ILE:HD13	2:C:111:VAL:CG1	2.34	0.58
1:B:603:PRO:O	1:B:604:TYR:CD1	2.56	0.57
1:B:16:LEU:HD21	1:B:66:SER:CB	2.35	0.57
1:B:390:TYR:HB3	1:B:393:GLU:OE1	2.04	0.57
1:B:98:ASN:HA	1:B:101:ASP:OD2	2.04	0.57
1:B:461:THR:O	1:B:464:ARG:HB3	2.05	0.57
1:B:515:LEU:HD12	1:B:515:LEU:N	2.19	0.57
1:B:149:PHE:C	1:B:151:ALA:H	2.07	0.57
1:B:240:VAL:HA	1:B:243:LEU:HB3	1.86	0.57
1:B:498:GLU:HG3	1:B:540:ILE:HD12	1.86	0.57
2:C:21:THR:HG21	2:C:90:PHE:HA	1.85	0.57
2:C:47:VAL:HG22	2:C:64:TRP:NE1	2.19	0.57
1:B:439:LEU:O	1:B:442:HIS:HB3	2.04	0.57
2:C:12:LYS:HB3	2:C:84:GLN:N	2.19	0.57
1:B:139:SER:HB2	1:B:142:TYR:CD2	2.39	0.57
1:B:391:ARG:O	1:B:393:GLU:N	2.37	0.57
1:B:421:LEU:HD11	1:B:439:LEU:HD13	1.86	0.57
1:B:518:TYR:O	1:B:522:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:VAL:O	2:C:41:ALA:O	2.22	0.57
1:B:280:TRP:HH2	1:B:299:LYS:HZ2	1.47	0.57
1:B:261:MSE:CE	1:B:264:ARG:HB3	2.35	0.57
1:B:106:ILE:HG13	1:B:154:LYS:HD3	1.85	0.56
1:B:116:THR:CG2	1:B:162:ILE:HD13	2.35	0.56
1:B:392:ASP:HB3	1:B:395:LEU:CD1	2.35	0.56
2:C:80:TYR:CD1	2:C:108:LEU:HD12	2.39	0.56
2:C:95:ARG:NH1	2:C:95:ARG:CA	2.62	0.56
2:C:141:LYS:HA	2:C:141:LYS:HZ1	1.70	0.56
1:B:109:THR:HG21	1:B:154:LYS:CG	2.35	0.56
1:B:144:THR:OG1	1:B:152:LEU:HG	2.05	0.56
1:B:392:ASP:HB3	1:B:395:LEU:HD11	1.85	0.56
1:B:516:VAL:N	1:B:517:PRO:CD	2.68	0.56
1:B:117:ILE:CG2	1:B:162:ILE:HA	2.35	0.56
1:B:185:HIS:O	1:B:188:PRO:HD2	2.04	0.56
1:B:232:ARG:NE	1:B:233:LYS:HZ1	2.03	0.56
2:C:10:GLN:HA	2:C:60:LYS:HB2	1.87	0.56
1:B:48:ASN:OD1	1:B:49:TYR:N	2.39	0.56
1:B:48:ASN:C	1:B:50:LEU:N	2.58	0.56
1:B:83:PHE:C	1:B:85:ASN:H	2.08	0.56
1:B:158:ASP:HA	1:B:161:GLU:HG2	1.88	0.56
2:C:97:THR:O	2:C:101:VAL:HG23	2.05	0.56
2:C:152:LYS:HB2	4:C:218:GNP:N1	2.20	0.56
1:B:126:TRP:CZ2	1:B:129:LEU:HD22	2.39	0.56
1:B:511:ALA:O	1:B:512:CYS:C	2.43	0.56
1:B:643:VAL:CG1	1:B:644:ALA:N	2.68	0.56
1:B:199:ASN:O	1:B:202:ILE:N	2.38	0.56
1:B:279:PHE:HZ	2:C:141:LYS:CE	2.17	0.56
1:B:467:HIS:ND1	1:B:467:HIS:C	2.59	0.56
2:C:80:TYR:HD2	2:C:80:TYR:N	2.04	0.56
1:B:153:GLN:NE2	1:B:191:ARG:HD3	2.21	0.56
1:B:446:CYS:HB2	1:B:458:THR:CG2	2.35	0.56
1:B:810:LYS:HE2	1:B:842:TRP:CE2	2.41	0.56
1:B:486:LEU:HD22	1:B:525:THR:HG21	1.87	0.56
1:B:844:ASN:O	1:B:844:ASN:ND2	2.39	0.56
1:B:420:VAL:HA	1:B:423:ALA:HB3	1.88	0.56
1:B:741:ILE:C	1:B:743:MSE:H	2.09	0.56
2:C:16:VAL:O	2:C:23:LYS:HD3	2.06	0.56
1:B:114:ILE:N	1:B:114:ILE:HD12	2.21	0.55
1:B:399:LEU:O	1:B:403:LYS:N	2.39	0.55
1:B:447:LEU:HD23	1:B:458:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ALA:HA	1:B:455:ARG:NE	2.21	0.55
1:B:250:LEU:O	1:B:254:MSE:HB2	2.06	0.55
1:B:341:ARG:HD3	1:B:341:ARG:N	2.01	0.55
1:B:395:LEU:HD11	1:B:431:GLY:HA3	1.88	0.55
1:B:132:LYS:HB3	1:B:136:LEU:HD12	1.87	0.55
1:B:425:ALA:O	1:B:429:MSE:HB2	2.07	0.55
1:B:677:GLN:HE22	1:B:712:ILE:CD1	2.19	0.55
2:C:18:ASP:CG	2:C:100:ASN:HD22	2.09	0.55
2:C:75:LEU:HD22	2:C:79:TYR:CE1	2.41	0.55
1:B:75:ASN:HB3	1:B:79:HIS:NE2	2.22	0.55
1:B:402:LEU:HA	1:B:405:LEU:HD12	1.88	0.55
2:C:76:ARG:CG	2:C:77:ASP:H	2.20	0.55
1:B:105:LEU:O	1:B:107:ARG:N	2.39	0.55
1:B:176:ILE:HG22	1:B:180:LEU:HG	1.88	0.55
1:B:153:GLN:C	1:B:155:ILE:H	2.10	0.55
1:B:102:SER:O	1:B:103:SER:HB2	2.06	0.55
1:B:758:ILE:HG13	1:B:796:PRO:HB2	1.89	0.55
2:C:90:PHE:HB2	2:C:97:THR:HB	1.88	0.55
1:B:48:ASN:O	1:B:50:LEU:N	2.39	0.55
1:B:287:PRO:HA	1:B:290:LYS:HG2	1.88	0.55
1:B:419:LEU:C	1:B:419:LEU:HD23	2.27	0.55
1:B:602:LEU:CB	1:B:603:PRO:HD3	2.35	0.55
2:C:38:LYS:CG	2:C:39:TYR:N	2.69	0.55
1:B:153:GLN:O	1:B:153:GLN:HG2	2.07	0.54
1:B:241:MSE:HG2	1:B:242:LEU:CD2	2.35	0.54
1:B:382:ALA:C	1:B:384:ASP:H	2.10	0.54
1:B:511:ALA:CB	1:B:515:LEU:CD1	2.82	0.54
1:B:523:LEU:O	1:B:527:VAL:HG23	2.06	0.54
2:C:9:VAL:O	2:C:60:LYS:HB2	2.06	0.54
1:B:192:SER:HA	1:B:230:GLU:HG3	1.88	0.54
1:B:261:MSE:HE3	1:B:264:ARG:HB3	1.88	0.54
1:B:263:GLN:O	1:B:266:GLN:HB3	2.07	0.54
1:B:602:LEU:HB2	1:B:603:PRO:CD	2.38	0.54
2:C:80:TYR:N	2:C:80:TYR:CD2	2.74	0.54
1:B:16:LEU:HB3	1:B:62:GLU:CG	2.37	0.54
1:B:200:GLN:NE2	1:B:236:CYS:HB2	2.23	0.54
1:B:192:SER:HA	1:B:230:GLU:CG	2.37	0.54
1:B:404:GLU:OE1	1:B:408:HIS:HD2	1.91	0.54
1:B:747:ILE:HB	1:B:748:PRO:HD3	1.88	0.54
1:B:109:THR:O	1:B:113:LEU:HD12	2.07	0.54
1:B:126:TRP:NE1	1:B:129:LEU:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:O	1:B:383:LEU:HB2	2.07	0.54
1:B:83:PHE:O	1:B:85:ASN:N	2.39	0.54
2:C:106:ARG:O	2:C:108:LEU:N	2.39	0.54
2:C:167:LYS:CE	2:C:167:LYS:HA	2.36	0.54
2:C:13:LEU:HA	2:C:85:CYS:O	2.08	0.54
2:C:101:VAL:HG12	2:C:102:PRO:N	2.22	0.54
1:B:52:PHE:HZ	1:B:98:ASN:ND2	2.06	0.54
1:B:123:LEU:HD12	1:B:126:TRP:CE3	2.43	0.54
1:B:170:ARG:CZ	1:B:174:ILE:HD12	2.38	0.54
1:B:710:MSE:HE1	1:B:732:ILE:HG23	1.90	0.54
2:C:81:ILE:HD13	2:C:111:VAL:HG13	1.90	0.54
1:B:420:VAL:O	1:B:424:ILE:HG12	2.07	0.54
2:C:95:ARG:O	2:C:99:LYS:HD3	2.08	0.54
1:B:157:GLU:C	1:B:159:SER:H	2.10	0.54
1:B:158:ASP:O	1:B:162:ILE:HG13	2.08	0.54
1:B:210:MSE:CE	1:B:246:ARG:HE	2.20	0.54
1:B:280:TRP:O	1:B:282:THR:N	2.39	0.54
1:B:336:ARG:CZ	1:B:367:ASP:HB3	2.37	0.54
1:B:402:LEU:O	1:B:406:LEU:HG	2.07	0.54
1:B:668:ILE:CD1	1:B:669:LEU:N	2.69	0.54
2:C:10:GLN:NE2	2:C:60:LYS:HG3	2.23	0.54
2:C:46:GLU:CD	2:C:47:VAL:H	2.11	0.54
1:B:241:MSE:HG2	1:B:242:LEU:N	2.23	0.53
1:B:274:LEU:O	1:B:278:GLU:HB3	2.08	0.53
1:B:394:LEU:O	1:B:398:ILE:HG13	2.08	0.53
2:C:101:VAL:O	2:C:103:ASN:N	2.42	0.53
2:C:123:LYS:HG2	4:C:218:GNP:C6	2.38	0.53
1:B:430:GLN:HA	1:B:433:ILE:HD12	1.91	0.53
1:B:491:ASP:N	1:B:532:LYS:HZ1	2.05	0.53
1:B:804:ILE:HD13	1:B:805:ARG:H	1.72	0.53
1:B:98:ASN:O	1:B:101:ASP:HB2	2.08	0.53
1:B:489:ILE:HD12	1:B:501:CYS:SG	2.48	0.53
1:B:598:GLN:C	1:B:600:GLY:H	2.12	0.53
1:B:12:LEU:CD1	1:B:47:ASN:HD22	2.22	0.53
1:B:129:LEU:HD23	1:B:129:LEU:C	2.29	0.53
1:B:192:SER:HB2	1:B:233:LYS:HE3	1.90	0.53
1:B:200:GLN:HB2	1:B:236:CYS:SG	2.48	0.53
1:B:306:ASN:C	1:B:308:MSE:H	2.12	0.53
1:B:722:ILE:HG13	1:B:723:SER:H	1.73	0.53
1:B:40:LEU:HG	1:B:40:LEU:O	2.09	0.53
1:B:45:ASP:CB	1:B:91:ILE:HD11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:CYS:C	1:B:97:ASN:N	2.62	0.53
1:B:106:ILE:HG13	1:B:154:LYS:HG2	1.91	0.53
1:B:552:VAL:CG1	1:B:555:HIS:HB2	2.39	0.53
1:B:24:SER:O	1:B:27:THR:HB	2.09	0.53
1:B:51:ILE:HA	1:B:67:LEU:HD22	1.89	0.53
1:B:411:TRP:O	1:B:413:VAL:N	2.41	0.53
1:B:519:LEU:HD11	1:B:552:VAL:HG21	1.90	0.53
1:B:554:HIS:CE1	1:B:598:GLN:OE1	2.62	0.53
2:C:91:ASP:OD1	2:C:93:THR:N	2.40	0.53
1:B:106:ILE:H	1:B:106:ILE:CD1	2.21	0.53
1:B:49:TYR:CD2	1:B:53:VAL:HG21	2.44	0.53
1:B:260:TYR:C	1:B:263:GLN:NE2	2.63	0.53
1:B:420:VAL:O	1:B:423:ALA:HB3	2.09	0.53
2:C:95:ARG:HD2	2:C:130:LYS:HB3	1.91	0.53
1:B:103:SER:N	1:B:104:PRO:CD	2.65	0.52
1:B:144:THR:N	1:B:148:ALA:O	2.42	0.52
1:B:221:PHE:HA	1:B:224:ALA:CB	2.38	0.52
1:B:297:LEU:HD13	1:B:397:HIS:HD2	1.73	0.52
2:C:145:GLN:HG3	2:C:163:TRP:NE1	2.24	0.52
1:B:216:PHE:HB3	1:B:219:ASN:OD1	2.09	0.52
1:B:322:VAL:O	1:B:324:GLU:N	2.43	0.52
1:B:110:VAL:C	1:B:112:ILE:H	2.13	0.52
1:B:231:VAL:O	1:B:235:VAL:HG23	2.08	0.52
1:B:612:CYS:SG	1:B:647:LEU:HD23	2.49	0.52
1:B:861:LYS:HG3	1:B:862:ASN:N	2.25	0.52
2:C:98:TYR:CZ	2:C:136:ILE:HA	2.44	0.52
1:B:137:LEU:C	1:B:140:GLU:HB2	2.30	0.52
1:B:619:THR:CG2	1:B:641:MSE:HE2	2.38	0.52
2:C:16:VAL:O	2:C:23:LYS:CD	2.57	0.52
1:B:196:ALA:CB	1:B:233:LYS:HD2	2.39	0.52
1:B:297:LEU:CD1	1:B:301:ILE:HD11	2.36	0.52
1:B:296:HIS:CE1	1:B:396:PRO:HG2	2.43	0.52
1:B:603:PRO:O	1:B:604:TYR:CD2	2.63	0.52
1:B:718:ASN:ND2	1:B:718:ASN:C	2.61	0.52
1:B:65:ARG:NH1	2:C:82:GLN:NE2	2.57	0.52
1:B:143:ASN:CB	1:B:148:ALA:HB1	2.40	0.52
1:B:171:PRO:HG2	1:B:172:LEU:H	1.74	0.52
1:B:402:LEU:HD12	1:B:406:LEU:HG	1.91	0.52
1:B:676:MSE:CE	1:B:688:PHE:HE2	2.17	0.52
2:C:70:GLU:OE1	2:C:73:GLY:HA3	2.10	0.52
1:B:78:ALA:HB3	1:B:122:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:PHE:O	1:B:202:ILE:HD13	2.10	0.52
1:B:504:PHE:O	1:B:508:GLU:HG3	2.10	0.52
2:C:51:VAL:HG22	2:C:60:LYS:HD3	1.92	0.52
2:C:98:TYR:CE1	2:C:136:ILE:HG23	2.45	0.52
1:B:105:LEU:CD2	1:B:107:ARG:HB2	2.40	0.52
1:B:310:TYR:CD1	1:B:313:ILE:HG13	2.45	0.52
1:B:370:ILE:O	2:C:139:HIS:NE2	2.43	0.52
1:B:657:GLY:H	1:B:697:ALA:HB1	1.74	0.52
1:B:27:THR:HG22	1:B:28:THR:N	2.25	0.52
1:B:200:GLN:O	1:B:203:ILE:HG22	2.10	0.52
1:B:263:GLN:HE22	1:B:264:ARG:HB2	1.75	0.52
2:C:45:VAL:HG13	2:C:66:THR:HA	1.90	0.52
2:C:72:PHE:CE2	2:C:75:LEU:HB2	2.45	0.52
1:B:135:SER:C	1:B:137:LEU:H	2.13	0.51
1:B:386:LEU:HD13	1:B:394:LEU:CD1	2.40	0.51
1:B:452:ALA:HA	1:B:455:ARG:HE	1.75	0.51
2:C:193:LEU:HD13	2:C:197:TYR:OH	2.11	0.51
1:B:12:LEU:O	1:B:16:LEU:HD13	2.10	0.51
1:B:64:THR:HG22	1:B:108:ALA:HB2	1.92	0.51
1:B:176:ILE:N	1:B:177:PRO:CD	2.72	0.51
1:B:566:MSE:HB2	1:B:567:PRO:HD3	1.93	0.51
1:B:429:MSE:O	1:B:432:MSE:N	2.43	0.51
1:B:472:GLN:HB3	1:B:473:PRO:CD	2.40	0.51
1:B:515:LEU:C	1:B:517:PRO:CD	2.76	0.51
1:B:106:ILE:H	1:B:106:ILE:HD12	1.75	0.51
1:B:126:TRP:N	1:B:127:PRO:HD3	2.24	0.51
1:B:183:PHE:HB3	1:B:202:ILE:CD1	2.40	0.51
1:B:6:LYS:N	1:B:7:PRO:CD	2.73	0.51
1:B:51:ILE:HA	1:B:67:LEU:HB2	1.93	0.51
1:B:90:PHE:O	1:B:94:GLU:N	2.42	0.51
1:B:137:LEU:HA	1:B:140:GLU:CB	2.39	0.51
1:B:312:ASP:C	1:B:314:ASP:N	2.61	0.51
1:B:209:LEU:O	1:B:211:LEU:N	2.39	0.51
1:B:227:GLU:OE1	1:B:227:GLU:HA	2.11	0.51
1:B:264:ARG:O	1:B:264:ARG:HG3	2.10	0.51
1:B:449:ASP:OD2	1:B:451:LYS:N	2.44	0.51
1:B:795:ARG:HG2	1:B:834:PHE:CZ	2.45	0.51
1:B:6:LYS:H	1:B:7:PRO:HD2	1.75	0.51
1:B:129:LEU:HD23	1:B:129:LEU:O	2.11	0.51
1:B:195:VAL:HG11	1:B:229:PRO:CB	2.41	0.51
1:B:249:ARG:CD	1:B:249:ARG:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ARG:CD	1:B:341:ARG:N	2.65	0.51
1:B:310:TYR:HD1	1:B:313:ILE:HG13	1.76	0.51
1:B:420:VAL:HG23	1:B:421:LEU:N	2.25	0.51
1:B:815:ARG:NH2	1:B:848:ASP:HB3	2.25	0.51
2:C:157:PHE:C	2:C:157:PHE:CD2	2.83	0.51
1:B:174:ILE:O	1:B:174:ILE:HG22	2.09	0.51
1:B:317:LEU:C	1:B:319:LYS:N	2.62	0.51
1:B:479:LYS:N	1:B:480:PRO:HD2	2.25	0.51
1:B:482:MSE:O	1:B:482:MSE:HG2	2.11	0.51
1:B:829:ILE:CG2	1:B:830:GLN:N	2.73	0.51
2:C:37:LYS:HG2	2:C:38:LYS:N	2.26	0.51
2:C:72:PHE:C	2:C:74:GLY:N	2.64	0.51
1:B:31:ARG:HA	1:B:34:GLN:CD	2.31	0.51
1:B:68:SER:OG	1:B:111:GLY:HA3	2.11	0.51
1:B:126:TRP:NE1	1:B:129:LEU:HD13	2.24	0.51
1:B:817:ILE:O	1:B:821:ILE:HG13	2.10	0.51
2:C:76:ARG:HG3	2:C:77:ASP:N	2.25	0.51
1:B:220:LEU:O	1:B:224:ALA:N	2.44	0.50
1:B:303:VAL:O	1:B:306:ASN:HB3	2.10	0.50
1:B:491:ASP:CG	1:B:492:SER:H	2.14	0.50
1:B:830:GLN:HE21	1:B:830:GLN:CA	2.20	0.50
2:C:35:PHE:O	2:C:36:GLU:HB2	2.09	0.50
1:B:120:LYS:O	1:B:124:GLN:HA	2.11	0.50
1:B:139:SER:HB2	1:B:142:TYR:HD2	1.76	0.50
1:B:191:ARG:NE	1:B:192:SER:H	1.87	0.50
1:B:221:PHE:C	1:B:223:LEU:H	2.14	0.50
1:B:189:LYS:HG3	1:B:191:ARG:H	1.76	0.50
1:B:338:ARG:CZ	1:B:585:PRO:HG3	2.41	0.50
1:B:436:LEU:N	1:B:437:PRO:HD2	2.25	0.50
2:C:105:HIS:O	2:C:109:VAL:HG23	2.12	0.50
1:B:281:LEU:HD22	1:B:281:LEU:H	1.76	0.50
1:B:668:ILE:HD12	1:B:668:ILE:N	2.27	0.50
2:C:162:LEU:HD21	2:C:166:ARG:NH2	2.26	0.50
1:B:51:ILE:HD12	1:B:51:ILE:N	2.26	0.50
1:B:318:LEU:HA	1:B:321:ASP:CB	2.42	0.50
1:B:141:ASP:C	1:B:143:ASN:N	2.64	0.50
1:B:143:ASN:OD1	1:B:149:PHE:CD2	2.64	0.50
1:B:211:LEU:O	1:B:213:ILE:N	2.45	0.50
1:B:306:ASN:OD1	1:B:379:SER:HB3	2.12	0.50
1:B:368:ASP:O	1:B:370:ILE:N	2.45	0.50
1:B:601:PHE:HZ	1:B:608:VAL:HG21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LYS:C	1:B:235:VAL:N	2.65	0.50
1:B:323:GLU:CG	1:B:492:SER:HA	2.42	0.50
1:B:401:LEU:O	1:B:405:LEU:HG	2.11	0.50
1:B:192:SER:OG	1:B:193:HIS:N	2.45	0.49
1:B:288:ILE:O	1:B:288:ILE:HG22	2.12	0.49
1:B:516:VAL:HB	1:B:517:PRO:HD3	1.93	0.49
1:B:523:LEU:HB3	1:B:564:MSE:CE	2.34	0.49
1:B:672:MSE:HE1	1:B:691:LEU:HA	1.94	0.49
1:B:753:GLN:O	1:B:757:ILE:HG13	2.12	0.49
1:B:110:VAL:HG12	1:B:114:ILE:HD11	1.94	0.49
1:B:254:MSE:O	1:B:258:VAL:HG12	2.11	0.49
2:C:64:TRP:CZ3	2:C:79:TYR:HB3	2.47	0.49
2:C:106:ARG:O	2:C:110:ARG:HG2	2.11	0.49
1:B:16:LEU:HD21	1:B:66:SER:HB3	1.93	0.49
1:B:75:ASN:HD22	1:B:75:ASN:H	1.54	0.49
1:B:149:PHE:HB2	1:B:153:GLN:HB2	1.94	0.49
1:B:261:MSE:C	1:B:263:GLN:N	2.66	0.49
1:B:399:LEU:N	1:B:400:PRO:HD2	2.27	0.49
1:B:243:LEU:HG	1:B:243:LEU:O	2.13	0.49
1:B:256:ASN:HA	1:B:259:GLU:OE1	2.11	0.49
1:B:284:ALA:CA	1:B:288:ILE:HD12	2.42	0.49
1:B:285:GLU:O	1:B:288:ILE:HG13	2.12	0.49
1:B:325:ASP:HA	1:B:328:ILE:HG13	1.94	0.49
1:B:392:ASP:CA	1:B:395:LEU:HG	2.41	0.49
1:B:492:SER:HB3	1:B:496:VAL:HB	1.95	0.49
1:B:597:LEU:O	1:B:598:GLN:O	2.30	0.49
1:B:133:LEU:HA	1:B:136:LEU:HB2	1.94	0.49
2:C:132:LYS:HD3	2:C:133:ALA:H	1.76	0.49
1:B:159:SER:O	1:B:163:LEU:HB3	2.12	0.49
1:B:219:ASN:O	1:B:223:LEU:HD12	2.13	0.49
1:B:429:MSE:HE1	1:B:436:LEU:HD22	1.95	0.49
1:B:106:ILE:HG23	1:B:154:LYS:HZ2	1.77	0.49
1:B:297:LEU:N	1:B:298:PRO:HD3	2.26	0.49
2:C:92:VAL:HG22	2:C:122:ASN:O	2.13	0.49
2:C:106:ARG:C	2:C:108:LEU:N	2.66	0.49
2:C:112:CYS:HB3	2:C:115:ILE:HG23	1.95	0.49
2:C:124:VAL:HG22	2:C:149:ILE:O	2.12	0.49
2:C:155:TYR:O	2:C:156:ASN:HB2	2.13	0.49
1:B:192:SER:HB2	1:B:233:LYS:NZ	2.28	0.49
1:B:199:ASN:HA	1:B:202:ILE:HD12	1.95	0.49
1:B:205:ARG:NH2	1:B:244:GLU:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:H	1:B:298:PRO:HD3	1.78	0.49
1:B:310:TYR:O	1:B:314:ASP:HB2	2.12	0.49
1:B:261:MSE:CE	1:B:276:ALA:HB1	2.42	0.49
1:B:300:LEU:CD2	1:B:394:LEU:HB3	2.42	0.49
1:B:196:ALA:O	1:B:198:VAL:N	2.46	0.48
1:B:409:HIS:ND1	1:B:410:GLU:N	2.49	0.48
1:B:242:LEU:CG	1:B:280:TRP:HA	2.29	0.48
1:B:75:ASN:N	1:B:75:ASN:ND2	2.60	0.48
1:B:106:ILE:HG23	1:B:154:LYS:NZ	2.28	0.48
1:B:139:SER:O	1:B:142:TYR:HD2	1.96	0.48
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.94	0.48
1:B:379:SER:OG	1:B:380:ALA:N	2.45	0.48
1:B:516:VAL:HA	1:B:519:LEU:HD13	1.95	0.48
1:B:519:LEU:O	1:B:521:TYR:N	2.46	0.48
1:B:661:GLN:O	1:B:665:ARG:HG3	2.14	0.48
1:B:15:ILE:HD12	1:B:33:VAL:HG12	1.96	0.48
1:B:228:GLU:HB3	1:B:234:ASN:HD22	1.76	0.48
1:B:233:LYS:O	1:B:235:VAL:N	2.47	0.48
1:B:398:ILE:HA	1:B:401:LEU:HD12	1.95	0.48
2:C:81:ILE:O	2:C:82:GLN:NE2	2.45	0.48
1:B:55:THR:HG23	1:B:60:GLU:OE1	2.14	0.48
1:B:67:LEU:O	1:B:71:ILE:HG21	2.14	0.48
1:B:92:LYS:O	1:B:96:LEU:HG	2.12	0.48
1:B:302:PRO:HG2	1:B:303:VAL:H	1.79	0.48
1:B:602:LEU:CB	1:B:603:PRO:CD	2.91	0.48
2:C:46:GLU:CD	2:C:47:VAL:N	2.67	0.48
1:B:161:GLU:O	1:B:165:SER:HB2	2.14	0.48
1:B:180:LEU:HA	1:B:183:PHE:CD1	2.49	0.48
1:B:295:ARG:CA	1:B:298:PRO:HD2	2.44	0.48
1:B:419:LEU:HD23	1:B:423:ALA:HB2	1.96	0.48
1:B:433:ILE:HG23	1:B:468:TRP:NE1	2.29	0.48
1:B:492:SER:OG	1:B:496:VAL:HG11	2.13	0.48
2:C:162:LEU:HD21	2:C:166:ARG:CZ	2.43	0.48
1:B:43:TYR:N	1:B:44:PRO:CD	2.75	0.48
1:B:718:ASN:C	1:B:718:ASN:HD22	2.16	0.48
1:B:223:LEU:C	1:B:225:GLY:H	2.17	0.48
1:B:385:VAL:O	1:B:389:VAL:HG12	2.13	0.48
1:B:512:CYS:C	1:B:513:THR:OG1	2.45	0.48
1:B:562:ILE:CD1	1:B:597:LEU:HG	2.40	0.48
1:B:253:HIS:O	1:B:257:ILE:HD13	2.14	0.48
1:B:385:VAL:HG22	1:B:389:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ARG:C	1:B:393:GLU:H	2.16	0.48
1:B:504:PHE:C	1:B:504:PHE:CD2	2.87	0.48
2:C:55:ASN:HD21	2:C:174:LEU:HA	1.79	0.48
2:C:81:ILE:HA	2:C:111:VAL:CG1	2.44	0.48
2:C:46:GLU:OE2	2:C:47:VAL:N	2.47	0.48
2:C:177:VAL:HB	2:C:179:MSE:HE2	1.96	0.48
1:B:103:SER:O	1:B:105:LEU:N	2.46	0.47
1:B:116:THR:HB	1:B:162:ILE:CD1	2.44	0.47
1:B:347:GLN:HB3	1:B:804:ILE:HD11	1.96	0.47
1:B:386:LEU:HD13	1:B:394:LEU:HD11	1.94	0.47
1:B:447:LEU:HD11	1:B:462:LEU:HD11	1.95	0.47
1:B:502:SER:O	1:B:505:ALA:HB3	2.14	0.47
1:B:710:MSE:HG2	1:B:746:TYR:CG	2.49	0.47
1:B:870:ARG:HG3	1:B:870:ARG:NH1	2.29	0.47
2:C:45:VAL:HG22	2:C:66:THR:HA	1.96	0.47
1:B:163:LEU:C	1:B:163:LEU:HD12	2.33	0.47
1:B:231:VAL:HA	1:B:234:ASN:HD21	1.75	0.47
1:B:232:ARG:HG3	1:B:233:LYS:HE2	1.96	0.47
1:B:284:ALA:HB3	1:B:288:ILE:CD1	2.44	0.47
1:B:508:GLU:O	1:B:510:GLU:N	2.47	0.47
1:B:59:SER:HB2	1:B:62:GLU:HB3	1.96	0.47
1:B:149:PHE:HB2	1:B:153:GLN:CB	2.45	0.47
1:B:109:THR:HG21	1:B:154:LYS:HG2	1.96	0.47
1:B:491:ASP:O	1:B:492:SER:HB2	2.14	0.47
2:C:35:PHE:CG	2:C:36:GLU:N	2.75	0.47
2:C:61:PHE:HE1	2:C:85:CYS:SG	2.37	0.47
1:B:82:ASN:C	1:B:84:PRO:CD	2.82	0.47
1:B:305:VAL:O	1:B:305:VAL:HG12	2.15	0.47
1:B:395:LEU:N	1:B:396:PRO:HD2	2.30	0.47
1:B:411:TRP:HD1	1:B:412:VAL:H	1.45	0.47
1:B:440:ILE:O	1:B:444:ILE:HG13	2.13	0.47
1:B:716:ASN:C	1:B:718:ASN:H	2.17	0.47
2:C:141:LYS:HE3	2:C:141:LYS:O	2.13	0.47
1:B:51:ILE:HG12	1:B:112:ILE:CD1	2.44	0.47
1:B:117:ILE:HG12	1:B:162:ILE:HA	1.97	0.47
1:B:235:VAL:CG1	1:B:272:VAL:HA	2.39	0.47
1:B:255:HIS:O	1:B:259:GLU:CD	2.52	0.47
1:B:281:LEU:CB	1:B:382:ALA:HB1	2.42	0.47
1:B:402:LEU:HA	1:B:405:LEU:HB2	1.95	0.47
1:B:478:LEU:HD12	1:B:478:LEU:O	2.15	0.47
1:B:622:GLN:CG	1:B:636:PRO:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:ILE:HD11	2:C:169:ILE:CD1	2.44	0.47
2:C:69:GLN:OE1	2:C:69:GLN:HA	2.15	0.47
1:B:57:LEU:CD1	1:B:58:LYS:HG2	2.44	0.47
1:B:74:ASN:HA	1:B:77:LYS:HD2	1.97	0.47
1:B:96:LEU:HD21	1:B:130:LEU:HG	1.95	0.47
1:B:177:PRO:HA	1:B:212:HIS:CE1	2.49	0.47
1:B:187:SER:HB3	1:B:188:PRO:CD	2.45	0.47
1:B:193:HIS:C	1:B:197:CYS:HB2	2.35	0.47
1:B:200:GLN:CD	1:B:236:CYS:HB2	2.35	0.47
1:B:323:GLU:O	1:B:324:GLU:HB2	2.14	0.47
1:B:383:LEU:HG	1:B:386:LEU:HD12	1.96	0.47
1:B:451:LYS:HB2	1:B:454:VAL:HG23	1.93	0.47
1:B:519:LEU:HD23	1:B:561:TYR:CE2	2.48	0.47
2:C:8:GLN:N	2:C:58:PRO:HG2	2.30	0.47
1:B:109:THR:HG21	1:B:154:LYS:CB	2.45	0.47
1:B:161:GLU:HG3	1:B:162:ILE:N	2.30	0.47
1:B:382:ALA:C	1:B:384:ASP:N	2.67	0.47
1:B:419:LEU:HD23	1:B:420:VAL:N	2.30	0.47
1:B:433:ILE:O	1:B:436:LEU:HB3	2.14	0.47
1:B:452:ALA:CA	1:B:455:ARG:HH21	2.28	0.47
2:C:69:GLN:C	2:C:71:LYS:H	2.18	0.47
2:C:106:ARG:CG	2:C:107:ASP:N	2.70	0.47
1:B:218:GLU:C	1:B:220:LEU:H	2.17	0.47
1:B:280:TRP:HH2	1:B:299:LYS:NZ	2.11	0.47
1:B:301:ILE:N	1:B:302:PRO:CD	2.64	0.47
1:B:411:TRP:O	1:B:412:VAL:C	2.53	0.47
1:B:655:LEU:O	1:B:656:GLY:C	2.52	0.47
1:B:806:ASP:OD1	1:B:806:ASP:N	2.48	0.47
1:B:14:GLN:HA	1:B:17:GLN:OE1	2.15	0.47
1:B:106:ILE:CG1	1:B:154:LYS:HD3	2.45	0.47
1:B:133:LEU:HB3	1:B:137:LEU:HD12	1.97	0.47
1:B:139:SER:O	1:B:142:TYR:HB2	2.15	0.47
1:B:145:CYS:SG	1:B:151:ALA:HB3	2.50	0.47
1:B:191:ARG:O	1:B:195:VAL:CG2	2.60	0.47
1:B:65:ARG:CG	2:C:81:ILE:HG21	2.36	0.46
1:B:134:CYS:O	1:B:138:ASP:HB2	2.15	0.46
1:B:519:LEU:HB3	1:B:561:TYR:CE1	2.49	0.46
1:B:791:GLN:H	1:B:791:GLN:NE2	2.12	0.46
1:B:116:THR:HG22	1:B:162:ILE:HD13	1.97	0.46
1:B:133:LEU:O	1:B:137:LEU:HB2	2.15	0.46
1:B:196:ALA:HB3	1:B:233:LYS:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:O	1:B:130:LEU:HD23	2.15	0.46
1:B:175:MSE:HG3	1:B:176:ILE:HG13	1.96	0.46
1:B:227:GLU:OE2	1:B:264:ARG:NH1	2.48	0.46
1:B:312:ASP:HA	1:B:315:ILE:CG1	2.46	0.46
1:B:452:ALA:HB2	1:B:455:ARG:HH21	1.80	0.46
1:B:631:ASP:OD2	1:B:632:GLN:HG2	2.14	0.46
1:B:698:CYS:HB2	1:B:701:HIS:HD2	1.80	0.46
2:C:80:TYR:CE1	2:C:107:ASP:O	2.68	0.46
2:C:101:VAL:C	2:C:103:ASN:H	2.18	0.46
2:C:189:MSE:O	2:C:190:ASP:O	2.33	0.46
1:B:232:ARG:HG3	1:B:233:LYS:NZ	2.30	0.46
1:B:295:ARG:HA	1:B:298:PRO:HD2	1.97	0.46
1:B:395:LEU:HB2	1:B:396:PRO:CD	2.45	0.46
1:B:534:GLN:OE1	1:B:534:GLN:HA	2.15	0.46
2:C:132:LYS:HD2	2:C:134:LYS:CB	2.46	0.46
1:B:31:ARG:HA	1:B:34:GLN:HG2	1.97	0.46
1:B:163:LEU:HD12	1:B:163:LEU:O	2.15	0.46
1:B:172:LEU:HD23	1:B:175:MSE:SE	2.65	0.46
1:B:280:TRP:CZ3	1:B:299:LYS:HD3	2.50	0.46
1:B:389:VAL:CG1	1:B:390:TYR:N	2.78	0.46
1:B:395:LEU:HB2	1:B:396:PRO:HD3	1.98	0.46
1:B:447:LEU:HD21	1:B:462:LEU:CD1	2.44	0.46
1:B:603:PRO:C	1:B:604:TYR:CG	2.88	0.46
1:B:4:GLU:O	1:B:7:PRO:HD2	2.16	0.46
1:B:49:TYR:CE1	1:B:52:PHE:CE1	3.04	0.46
1:B:81:GLN:O	1:B:82:ASN:HB3	2.16	0.46
1:B:231:VAL:C	1:B:233:LYS:H	2.18	0.46
1:B:265:THR:HG21	1:B:277:CYS:HB2	1.96	0.46
1:B:300:LEU:HD21	1:B:394:LEU:HB3	1.97	0.46
1:B:457:ILE:HD12	1:B:457:ILE:H	1.81	0.46
1:B:83:PHE:C	1:B:85:ASN:N	2.68	0.46
1:B:126:TRP:CZ2	1:B:129:LEU:HB3	2.51	0.46
1:B:192:SER:HB2	1:B:233:LYS:CE	2.45	0.46
1:B:243:LEU:O	1:B:243:LEU:CG	2.63	0.46
1:B:397:HIS:CE1	1:B:398:ILE:HG12	2.50	0.46
2:C:92:VAL:HG11	2:C:129:ARG:NE	2.30	0.46
2:C:96:VAL:HG22	2:C:97:THR:H	1.78	0.46
1:B:61:ASP:OD1	2:C:82:GLN:HG2	2.16	0.46
1:B:105:LEU:HD23	1:B:108:ALA:H	1.81	0.46
1:B:447:LEU:HD23	1:B:458:THR:CG2	2.46	0.46
1:B:508:GLU:C	1:B:510:GLU:N	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:GLY:O	2:C:22:GLY:N	2.49	0.46
2:C:138:PHE:CE1	2:C:142:LYS:HG3	2.50	0.46
1:B:5:TRP:HB3	1:B:43:TYR:HD2	1.81	0.46
1:B:233:LYS:C	1:B:235:VAL:H	2.18	0.46
1:B:317:LEU:O	1:B:318:LEU:C	2.55	0.46
1:B:421:LEU:O	1:B:424:ILE:HG13	2.16	0.46
1:B:431:GLY:C	1:B:434:PRO:HD2	2.36	0.46
1:B:637:ASP:OD1	1:B:639:ASP:N	2.49	0.46
2:C:16:VAL:CG2	2:C:17:GLY:N	2.69	0.46
2:C:51:VAL:HA	2:C:59:ILE:O	2.15	0.46
1:B:489:ILE:HG22	1:B:490:LEU:HD23	1.98	0.45
2:C:11:PHE:CD1	2:C:168:LEU:HD13	2.50	0.45
2:C:99:LYS:C	2:C:101:VAL:H	2.20	0.45
1:B:264:ARG:HH21	1:B:267:ASP:CB	2.17	0.45
1:B:465:TYR:HD1	1:B:465:TYR:O	1.99	0.45
1:B:232:ARG:C	1:B:233:LYS:HD3	2.36	0.45
1:B:451:LYS:CD	1:B:454:VAL:HB	2.46	0.45
1:B:477:TYR:C	1:B:480:PRO:HD2	2.37	0.45
1:B:878:LEU:HB3	1:B:879:PRO:CD	2.45	0.45
2:C:113:GLU:O	2:C:113:GLU:HG2	2.16	0.45
1:B:46:PHE:C	1:B:48:ASN:H	2.19	0.45
1:B:153:GLN:HE21	1:B:191:ARG:HG2	1.82	0.45
1:B:237:ARG:C	1:B:239:LEU:N	2.68	0.45
1:B:339:PHE:CB	2:C:127:LYS:HD2	2.42	0.45
2:C:38:LYS:HG3	2:C:40:VAL:HG23	1.97	0.45
1:B:187:SER:H	1:B:188:PRO:HD2	1.82	0.45
1:B:390:TYR:HD2	1:B:393:GLU:HB3	1.77	0.45
1:B:614:ASN:O	1:B:618:LYS:HG3	2.17	0.45
2:C:101:VAL:C	2:C:103:ASN:N	2.70	0.45
1:B:59:SER:CB	1:B:62:GLU:HB3	2.47	0.45
1:B:106:ILE:HA	1:B:109:THR:CB	2.46	0.45
1:B:227:GLU:HG3	1:B:228:GLU:HG3	1.98	0.45
1:B:266:GLN:O	1:B:266:GLN:NE2	2.50	0.45
2:C:124:VAL:HG11	2:C:148:ASP:OD1	2.17	0.45
1:B:13:GLN:O	1:B:17:GLN:HG3	2.16	0.45
1:B:64:THR:CA	1:B:67:LEU:HG	2.38	0.45
1:B:92:LYS:HG2	1:B:96:LEU:HD12	1.99	0.45
1:B:102:SER:O	1:B:151:ALA:HA	2.17	0.45
1:B:175:MSE:HG3	1:B:176:ILE:N	2.32	0.45
1:B:339:PHE:N	1:B:339:PHE:CD1	2.84	0.45
1:B:492:SER:CB	1:B:496:VAL:HG11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:LYS:CG	2:C:39:TYR:H	2.29	0.45
1:B:68:SER:HA	1:B:111:GLY:O	2.17	0.45
1:B:106:ILE:HD12	1:B:106:ILE:N	2.32	0.45
1:B:172:LEU:HD12	1:B:172:LEU:N	2.32	0.45
1:B:211:LEU:CD2	1:B:212:HIS:N	2.80	0.45
1:B:239:LEU:C	1:B:239:LEU:HD23	2.36	0.45
1:B:297:LEU:HD13	1:B:397:HIS:CD2	2.51	0.45
1:B:391:ARG:C	1:B:393:GLU:N	2.70	0.45
2:C:17:GLY:O	2:C:18:ASP:O	2.34	0.45
2:C:83:ALA:CA	2:C:112:CYS:SG	3.03	0.45
1:B:296:HIS:HD2	1:B:300:LEU:HD22	1.82	0.45
1:B:433:ILE:N	1:B:434:PRO:CD	2.80	0.45
1:B:81:GLN:CD	1:B:85:ASN:HB2	2.38	0.45
1:B:189:LYS:HG3	1:B:191:ARG:N	2.31	0.45
1:B:299:LYS:HB2	1:B:299:LYS:NZ	2.28	0.45
1:B:436:LEU:CD1	1:B:440:ILE:HD11	2.46	0.45
1:B:565:LEU:O	1:B:568:PRO:HG2	2.16	0.45
1:B:717:LEU:HD11	1:B:750:VAL:HG22	1.99	0.45
2:C:167:LYS:HA	2:C:167:LYS:HE2	1.99	0.45
1:B:105:LEU:HD21	1:B:107:ARG:HB2	1.98	0.44
1:B:130:LEU:C	1:B:132:LYS:N	2.70	0.44
1:B:154:LYS:HE2	1:B:154:LYS:HA	1.99	0.44
1:B:160:ALA:HA	1:B:201:PHE:CD1	2.52	0.44
1:B:196:ALA:O	1:B:199:ASN:N	2.49	0.44
1:B:386:LEU:HD22	1:B:394:LEU:HD21	1.99	0.44
1:B:741:ILE:C	1:B:743:MSE:N	2.70	0.44
2:C:48:HIS:O	2:C:63:VAL:N	2.49	0.44
2:C:141:LYS:HA	2:C:141:LYS:HZ2	1.78	0.44
1:B:92:LYS:HB2	1:B:92:LYS:HZ2	1.81	0.44
1:B:189:LYS:HG2	1:B:194:ALA:HB1	1.99	0.44
1:B:303:VAL:O	1:B:304:LEU:C	2.55	0.44
1:B:482:MSE:O	1:B:486:LEU:HD12	2.18	0.44
2:C:96:VAL:CG1	2:C:97:THR:H	2.10	0.44
1:B:33:VAL:HA	1:B:36:LYS:CE	2.44	0.44
1:B:306:ASN:ND2	1:B:375:LEU:HB3	2.24	0.44
1:B:390:TYR:O	1:B:391:ARG:HG3	2.17	0.44
1:B:33:VAL:HA	1:B:36:LYS:HG2	2.00	0.44
1:B:69:GLY:O	1:B:71:ILE:N	2.50	0.44
1:B:182:PHE:O	1:B:185:HIS:HB2	2.18	0.44
1:B:192:SER:HB3	1:B:230:GLU:OE1	2.18	0.44
1:B:318:LEU:HA	1:B:321:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:VAL:HG13	1:B:390:TYR:N	2.33	0.44
1:B:440:ILE:HD13	1:B:469:VAL:HG22	1.99	0.44
1:B:554:HIS:CE1	1:B:598:GLN:CD	2.91	0.44
2:C:138:PHE:O	2:C:141:LYS:N	2.48	0.44
1:B:9:GLU:CA	1:B:47:ASN:HD21	2.30	0.44
1:B:296:HIS:CE1	1:B:396:PRO:O	2.71	0.44
1:B:390:TYR:C	1:B:391:ARG:HG3	2.38	0.44
1:B:802:ARG:NH1	1:B:803:ASN:OD1	2.50	0.44
1:B:479:LYS:CE	1:B:518:TYR:HE2	2.30	0.44
2:C:47:VAL:CG2	2:C:64:TRP:NE1	2.80	0.44
2:C:79:TYR:CD1	2:C:79:TYR:N	2.86	0.44
1:B:50:LEU:O	1:B:67:LEU:HB3	2.17	0.44
1:B:283:LEU:HD12	1:B:385:VAL:CG2	2.43	0.44
1:B:676:MSE:HE2	1:B:712:ILE:HG21	2.00	0.44
2:C:92:VAL:HB	2:C:129:ARG:HG3	1.99	0.44
2:C:122:ASN:O	2:C:123:LYS:HB2	2.18	0.44
1:B:9:GLU:C	1:B:11:GLY:H	2.21	0.44
1:B:27:THR:HA	1:B:31:ARG:CZ	2.47	0.44
1:B:45:ASP:HB3	1:B:91:ILE:HD11	1.98	0.44
1:B:51:ILE:HA	1:B:67:LEU:CB	2.47	0.44
1:B:232:ARG:HE	1:B:233:LYS:NZ	2.10	0.44
1:B:395:LEU:CD1	1:B:431:GLY:HA3	2.47	0.44
1:B:573:TRP:CH2	1:B:608:VAL:HA	2.52	0.44
1:B:810:LYS:HE2	1:B:842:TRP:NE1	2.32	0.44
2:C:54:THR:CB	2:C:174:LEU:HD11	2.41	0.44
1:B:239:LEU:HA	1:B:279:PHE:HD1	1.83	0.44
1:B:422:GLY:CA	1:B:464:ARG:HG2	2.48	0.44
1:B:468:TRP:O	1:B:471:SER:N	2.51	0.44
1:B:479:LYS:HE3	1:B:518:TYR:HE2	1.83	0.44
2:C:96:VAL:CG1	2:C:97:THR:N	2.72	0.44
2:C:189:MSE:O	2:C:190:ASP:C	2.55	0.44
1:B:130:LEU:O	1:B:132:LYS:N	2.48	0.43
1:B:141:ASP:N	1:B:152:LEU:HD12	2.33	0.43
1:B:220:LEU:O	1:B:224:ALA:HB2	2.18	0.43
1:B:490:LEU:HD13	1:B:528:PHE:CD2	2.50	0.43
2:C:30:HIS:NE2	2:C:157:PHE:O	2.51	0.43
1:B:211:LEU:HD23	1:B:212:HIS:N	2.33	0.43
1:B:306:ASN:ND2	1:B:375:LEU:HD13	2.33	0.43
1:B:436:LEU:HD11	1:B:440:ILE:HD11	2.00	0.43
1:B:72:LEU:CA	2:C:76:ARG:HH21	2.31	0.43
1:B:582:ASP:C	1:B:585:PRO:HD2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD11	1:B:66:SER:HB3	2.01	0.43
1:B:41:ASN:HA	1:B:44:PRO:CD	2.48	0.43
1:B:126:TRP:NE1	1:B:129:LEU:CB	2.82	0.43
1:B:205:ARG:HD2	1:B:213:ILE:HG21	2.00	0.43
1:B:262:LEU:HD12	1:B:262:LEU:C	2.38	0.43
1:B:404:GLU:HG2	1:B:408:HIS:CB	2.35	0.43
1:B:710:MSE:HG2	1:B:746:TYR:CD2	2.52	0.43
1:B:82:ASN:O	1:B:83:PHE:HB2	2.19	0.43
1:B:535:HIS:CD2	1:B:535:HIS:C	2.90	0.43
1:B:660:GLU:C	1:B:660:GLU:CD	2.77	0.43
2:C:55:ASN:C	2:C:55:ASN:ND2	2.68	0.43
1:B:239:LEU:HD23	1:B:240:VAL:HG22	1.99	0.43
1:B:447:LEU:CD2	1:B:458:THR:HG22	2.49	0.43
1:B:737:ILE:HD13	1:B:737:ILE:HA	1.85	0.43
1:B:810:LYS:HG2	1:B:842:TRP:CZ2	2.54	0.43
2:C:80:TYR:CD1	2:C:108:LEU:HA	2.50	0.43
1:B:75:ASN:OD1	2:C:76:ARG:NH2	2.52	0.43
1:B:504:PHE:O	1:B:504:PHE:CD2	2.71	0.43
1:B:133:LEU:O	1:B:134:CYS:C	2.57	0.43
1:B:198:VAL:CG1	1:B:202:ILE:HD11	2.47	0.43
1:B:248:ASP:HB2	1:B:249:ARG:NH1	2.34	0.43
1:B:145:CYS:SG	1:B:146:GLU:N	2.89	0.43
1:B:211:LEU:H	1:B:213:ILE:HD13	1.83	0.43
1:B:223:LEU:HA	1:B:226:ASP:HB3	1.98	0.43
1:B:308:MSE:HB2	1:B:412:VAL:HG12	2.01	0.43
1:B:312:ASP:O	1:B:315:ILE:N	2.52	0.43
1:B:451:LYS:O	1:B:452:ALA:C	2.58	0.43
1:B:460:TRP:O	1:B:464:ARG:HB2	2.19	0.43
1:B:782:CYS:HB3	1:B:785:GLU:HB2	2.00	0.43
1:B:821:ILE:HD12	1:B:856:ILE:HD13	2.01	0.43
2:C:101:VAL:O	2:C:104:TRP:HD1	2.00	0.43
2:C:150:SER:OG	2:C:152:LYS:HB3	2.19	0.43
1:B:212:HIS:O	1:B:216:PHE:CD1	2.72	0.43
1:B:468:TRP:O	1:B:472:GLN:HG2	2.18	0.43
1:B:696:LYS:CG	1:B:734:GLU:HG2	2.48	0.43
1:B:700:GLN:HG3	1:B:701:HIS:CD2	2.53	0.43
1:B:205:ARG:HH11	1:B:205:ARG:HG2	1.83	0.42
1:B:284:ALA:H	1:B:288:ILE:CD1	2.32	0.42
1:B:406:LEU:O	1:B:407:PHE:HB2	2.19	0.42
1:B:434:PRO:O	1:B:437:PRO:HD2	2.19	0.42
1:B:451:LYS:HD3	1:B:454:VAL:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLU:C	1:B:510:GLU:H	2.23	0.42
1:B:602:LEU:CD2	1:B:655:LEU:HD22	2.49	0.42
1:B:692:GLY:HA3	1:B:730:TRP:CZ3	2.54	0.42
1:B:741:ILE:O	1:B:744:GLN:HB2	2.18	0.42
1:B:878:LEU:O	1:B:881:LYS:HB3	2.19	0.42
1:B:5:TRP:HB3	1:B:43:TYR:CD2	2.55	0.42
1:B:189:LYS:HZ3	1:B:194:ALA:CB	2.31	0.42
1:B:201:PHE:C	1:B:203:ILE:H	2.23	0.42
1:B:52:PHE:O	1:B:56:LYS:HB2	2.19	0.42
1:B:115:THR:C	1:B:117:ILE:H	2.21	0.42
1:B:221:PHE:C	1:B:223:LEU:N	2.72	0.42
1:B:405:LEU:O	1:B:414:LYS:HA	2.19	0.42
1:B:33:VAL:HG13	1:B:36:LYS:HE2	2.00	0.42
1:B:83:PHE:O	1:B:87:VAL:HG23	2.19	0.42
1:B:544:ALA:O	1:B:547:THR:HB	2.19	0.42
2:C:86:ALA:O	2:C:117:ILE:HA	2.20	0.42
1:B:177:PRO:HA	1:B:212:HIS:HE1	1.84	0.42
1:B:283:LEU:HD22	1:B:288:ILE:HG22	2.00	0.42
1:B:561:TYR:O	1:B:564:MSE:HG2	2.20	0.42
2:C:39:TYR:HE1	2:C:41:ALA:HB2	1.84	0.42
1:B:110:VAL:HG12	1:B:114:ILE:CD1	2.49	0.42
1:B:116:THR:HG22	1:B:116:THR:O	2.19	0.42
1:B:157:GLU:HB3	1:B:197:CYS:SG	2.60	0.42
1:B:286:GLN:O	1:B:289:CYS:N	2.51	0.42
1:B:660:GLU:OE2	1:B:701:HIS:NE2	2.51	0.42
1:B:751:LEU:CD2	1:B:789:MSE:CE	2.97	0.42
1:B:210:MSE:O	1:B:210:MSE:CG	2.66	0.42
1:B:210:MSE:C	1:B:213:ILE:HD13	2.40	0.42
1:B:230:GLU:HB2	1:B:231:VAL:H	1.67	0.42
1:B:246:ARG:H	1:B:246:ARG:HG2	1.49	0.42
1:B:435:TYR:C	1:B:437:PRO:HD2	2.39	0.42
1:B:739:MSE:HE2	1:B:742:GLU:CG	2.47	0.42
1:B:797:TRP:CZ2	1:B:817:ILE:HG13	2.55	0.42
2:C:80:TYR:CD1	2:C:107:ASP:O	2.73	0.42
2:C:141:LYS:C	2:C:143:ASN:N	2.72	0.42
1:B:72:LEU:HD22	2:C:76:ARG:NH2	2.35	0.42
1:B:198:VAL:C	1:B:202:ILE:HG13	2.40	0.42
1:B:318:LEU:O	1:B:319:LYS:C	2.58	0.42
1:B:445:GLN:OE1	1:B:445:GLN:HA	2.19	0.42
1:B:508:GLU:OE1	1:B:547:THR:HG22	2.19	0.42
1:B:519:LEU:O	1:B:520:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:THR:HA	1:B:31:ARG:NH1	2.34	0.42
1:B:92:LYS:HD3	1:B:126:TRP:CZ2	2.55	0.42
1:B:196:ALA:HA	1:B:199:ASN:HB3	2.02	0.42
1:B:402:LEU:HD11	1:B:406:LEU:HD21	2.00	0.42
1:B:421:LEU:HG	1:B:465:TYR:OH	2.20	0.42
2:C:43:LEU:HA	2:C:71:LYS:HB3	2.02	0.42
1:B:179:PHE:CD1	1:B:179:PHE:C	2.93	0.42
1:B:393:GLU:HG3	1:B:394:LEU:HG	2.02	0.42
1:B:433:ILE:HB	1:B:434:PRO:HD3	2.01	0.42
2:C:38:LYS:HD3	2:C:39:TYR:H	1.84	0.42
2:C:101:VAL:HG12	2:C:102:PRO:CD	2.50	0.42
2:C:184:PRO:HB2	2:C:187:VAL:HG22	2.02	0.42
2:C:191:PRO:O	2:C:192:ALA:CB	2.68	0.42
1:B:3:TYR:HD1	1:B:4:GLU:HG3	1.85	0.41
1:B:232:ARG:HG3	1:B:233:LYS:HZ3	1.85	0.41
1:B:477:TYR:HA	1:B:480:PRO:CD	2.50	0.41
1:B:538:LEU:HD12	1:B:538:LEU:O	2.19	0.41
1:B:584:PHE:HB2	1:B:585:PRO:CD	2.42	0.41
2:C:12:LYS:HD3	2:C:64:TRP:CZ3	2.55	0.41
2:C:16:VAL:CG2	2:C:88:ILE:HA	2.50	0.41
2:C:92:VAL:HG21	2:C:124:VAL:HG12	2.01	0.41
2:C:132:LYS:HD3	2:C:134:LYS:H	1.82	0.41
1:B:55:THR:HG22	1:B:56:LYS:HE3	2.02	0.41
1:B:140:GLU:O	1:B:152:LEU:HG	2.20	0.41
1:B:158:ASP:O	1:B:162:ILE:CD1	2.67	0.41
1:B:223:LEU:C	1:B:225:GLY:N	2.74	0.41
1:B:254:MSE:HE3	1:B:254:MSE:HA	2.01	0.41
1:B:268:GLN:HA	1:B:268:GLN:OE1	2.19	0.41
1:B:304:LEU:HD21	1:B:405:LEU:CD1	2.48	0.41
1:B:304:LEU:O	1:B:304:LEU:HD23	2.20	0.41
1:B:310:TYR:O	1:B:314:ASP:CB	2.68	0.41
1:B:396:PRO:O	1:B:397:HIS:CB	2.68	0.41
1:B:850:ARG:HH11	1:B:850:ARG:CG	2.16	0.41
2:C:81:ILE:HD13	2:C:111:VAL:HG11	2.01	0.41
1:B:72:LEU:HD13	2:C:77:ASP:OD2	2.20	0.41
1:B:141:ASP:HA	1:B:152:LEU:CB	2.40	0.41
1:B:149:PHE:O	1:B:153:GLN:N	2.42	0.41
1:B:283:LEU:HB2	1:B:385:VAL:HG21	2.01	0.41
1:B:296:HIS:N	1:B:298:PRO:HD2	2.36	0.41
1:B:325:ASP:C	1:B:327:THR:H	2.22	0.41
1:B:348:GLN:OE1	1:B:348:GLN:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ALA:HA	1:B:455:ARG:CZ	2.51	0.41
1:B:60:GLU:OE2	1:B:105:LEU:HD22	2.19	0.41
1:B:60:GLU:CA	1:B:63:PRO:HD2	2.50	0.41
1:B:80:PHE:O	1:B:81:GLN:HB2	2.20	0.41
1:B:196:ALA:O	1:B:197:CYS:C	2.59	0.41
1:B:217:THR:O	1:B:220:LEU:HB3	2.20	0.41
1:B:395:LEU:HD21	1:B:428:CYS:HB3	2.02	0.41
1:B:500:ALA:O	1:B:503:ALA:HB3	2.19	0.41
1:B:109:THR:CG2	1:B:154:LYS:HB3	2.50	0.41
1:B:180:LEU:HD23	1:B:183:PHE:CE1	2.55	0.41
1:B:295:ARG:HA	1:B:298:PRO:CG	2.50	0.41
1:B:383:LEU:CD2	1:B:386:LEU:HD12	2.50	0.41
1:B:765:LYS:O	1:B:769:GLU:HG3	2.20	0.41
2:C:72:PHE:O	2:C:74:GLY:N	2.53	0.41
1:B:52:PHE:CD1	1:B:52:PHE:N	2.77	0.41
1:B:130:LEU:HB3	1:B:131:PRO:CD	2.42	0.41
1:B:435:TYR:CD1	1:B:435:TYR:N	2.89	0.41
1:B:444:ILE:O	1:B:444:ILE:HG22	2.20	0.41
1:B:479:LYS:HE3	1:B:518:TYR:CE2	2.55	0.41
1:B:515:LEU:CD1	1:B:515:LEU:H	2.30	0.41
1:B:71:ILE:HG12	1:B:72:LEU:N	2.36	0.41
1:B:83:PHE:N	1:B:84:PRO:CD	2.83	0.41
1:B:189:LYS:NZ	1:B:194:ALA:HB1	2.35	0.41
1:B:306:ASN:C	1:B:308:MSE:N	2.73	0.41
1:B:461:THR:O	1:B:462:LEU:C	2.59	0.41
1:B:88:THR:O	1:B:91:ILE:HG22	2.20	0.41
1:B:396:PRO:O	1:B:397:HIS:HB3	2.20	0.41
1:B:481:LEU:O	1:B:485:LEU:HB2	2.20	0.41
1:B:751:LEU:HA	1:B:751:LEU:HD12	1.88	0.41
2:C:71:LYS:HA	2:C:71:LYS:HD3	1.95	0.41
1:B:110:VAL:O	1:B:112:ILE:N	2.54	0.41
1:B:206:THR:HG22	1:B:207:GLN:N	2.35	0.41
1:B:239:LEU:HD23	1:B:243:LEU:HD23	2.03	0.41
1:B:397:HIS:CE1	1:B:398:ILE:CG1	3.04	0.41
1:B:426:GLU:O	1:B:426:GLU:HG2	2.20	0.41
1:B:469:VAL:O	1:B:478:LEU:HB2	2.21	0.41
1:B:741:ILE:H	1:B:741:ILE:HG12	1.44	0.41
1:B:829:ILE:HG23	1:B:830:GLN:H	1.85	0.41
2:C:174:LEU:HD12	2:C:174:LEU:C	2.32	0.41
1:B:110:VAL:C	1:B:112:ILE:N	2.75	0.41
1:B:173:ASN:O	1:B:209:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ARG:C	1:B:378:CYS:H	2.25	0.41
1:B:655:LEU:O	1:B:656:GLY:O	2.39	0.41
1:B:830:GLN:HA	1:B:830:GLN:NE2	2.32	0.41
2:C:132:LYS:HD2	2:C:134:LYS:HB3	2.03	0.41
2:C:184:PRO:HA	2:C:185:PRO:HD2	1.95	0.41
1:B:243:LEU:HD12	1:B:243:LEU:C	2.41	0.40
1:B:394:LEU:CB	1:B:398:ILE:HD11	2.46	0.40
1:B:481:LEU:C	1:B:483:THR:H	2.23	0.40
1:B:829:ILE:CG2	1:B:830:GLN:H	2.34	0.40
2:C:100:ASN:O	2:C:104:TRP:NE1	2.53	0.40
1:B:3:TYR:N	1:B:6:LYS:HB2	2.36	0.40
1:B:19:LEU:O	1:B:20:LYS:C	2.60	0.40
1:B:31:ARG:HA	1:B:34:GLN:CG	2.50	0.40
1:B:432:MSE:C	1:B:434:PRO:HD2	2.42	0.40
1:B:637:ASP:OD1	1:B:637:ASP:C	2.59	0.40
1:B:710:MSE:HB3	1:B:711:PRO:CD	2.51	0.40
1:B:26:ASP:O	1:B:30:GLN:CB	2.66	0.40
1:B:385:VAL:HG22	1:B:389:VAL:CB	2.52	0.40
1:B:473:PRO:HB2	1:B:476:THR:OG1	2.21	0.40
2:C:37:LYS:HA	4:C:218:GNP:O2'	2.21	0.40
1:B:41:ASN:C	1:B:44:PRO:HD2	2.41	0.40
1:B:103:SER:N	1:B:104:PRO:HD2	2.10	0.40
1:B:158:ASP:O	1:B:162:ILE:CG1	2.69	0.40
1:B:245:VAL:CG1	1:B:246:ARG:N	2.84	0.40
1:B:286:GLN:O	1:B:288:ILE:N	2.54	0.40
1:B:286:GLN:C	1:B:288:ILE:N	2.75	0.40
1:B:299:LYS:HA	1:B:302:PRO:HG3	2.04	0.40
1:B:319:LYS:HD2	2:C:175:GLU:OE1	2.22	0.40
1:B:603:PRO:C	1:B:604:TYR:CD1	2.95	0.40
1:B:662:LEU:HA	1:B:662:LEU:HD12	1.78	0.40
2:C:164:LEU:HD23	2:C:164:LEU:HA	1.89	0.40
2:C:169:ILE:HD12	2:C:174:LEU:CD2	2.51	0.40
1:B:31:ARG:HD3	1:B:34:GLN:OE1	2.21	0.40
1:B:97:ASN:C	1:B:99:ILE:N	2.73	0.40
1:B:317:LEU:C	1:B:319:LYS:H	2.25	0.40
1:B:443:LEU:C	1:B:445:GLN:N	2.75	0.40
1:B:589:CYS:O	1:B:592:SER:HB2	2.22	0.40
1:B:608:VAL:HG13	1:B:647:LEU:HD21	2.03	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	B	874/890 (98%)	604 (69%)	185 (21%)	85 (10%)	0 2
2	C	188/216 (87%)	130 (69%)	30 (16%)	28 (15%)	0 1
All	All	1062/1106 (96%)	734 (69%)	215 (20%)	113 (11%)	0 2

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	27	THR
1	B	50	LEU
1	B	81	GLN
1	B	83	PHE
1	B	103	SER
1	B	106	ILE
1	B	138	ASP
1	B	148	ALA
1	B	186	SER
1	B	209	LEU
1	B	210	MSE
1	B	213	ILE
1	B	231	VAL
1	B	252	PRO
1	B	284	ALA
1	B	318	LEU
1	B	323	GLU
1	B	324	GLU
1	B	387	ALA
1	B	392	ASP
1	B	407	PHE
1	B	452	ALA
1	B	474	PRO
1	B	475	ASP
1	B	598	GLN

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Mol	Chain	Res	Type
1	B	656	GLY
1	B	878	LEU
2	C	16	VAL
2	C	18	ASP
2	C	21	THR
2	C	38	LYS
2	C	41	ALA
2	C	45	VAL
2	C	96	VAL
2	C	97	THR
2	C	111	VAL
1	B	70	LEU
1	B	120	LYS
1	B	137	LEU
1	B	142	TYR
1	B	146	GLU
1	B	185	HIS
1	B	197	CYS
1	B	212	HIS
1	B	268	GLN
1	B	299	LYS
1	B	319	LYS
1	B	322	VAL
1	B	369	THR
1	B	412	VAL
1	B	425	ALA
1	B	449	ASP
1	B	509	GLU
1	B	512	CYS
1	B	604	TYR
2	C	36	GLU
2	C	76	ARG
2	C	77	ASP
2	C	107	ASP
2	C	192	ALA
1	B	49	TYR
1	B	179	PHE
1	B	187	SER
1	B	199	ASN
1	B	227	GLU
1	B	228	GLU
1	B	278	GLU

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Mol	Chain	Res	Type
1	B	281	LEU
1	B	306	ASN
1	B	378	CYS
1	B	477	TYR
1	B	491	ASP
1	B	520	ALA
1	B	740	GLY
2	C	32	THR
2	C	154	ASN
2	C	168	LEU
1	B	28	THR
1	B	47	ASN
1	B	69	GLY
1	B	84	PRO
1	B	111	GLY
1	B	123	LEU
1	B	128	ASP
1	B	406	LEU
1	B	429	MSE
2	C	33	GLY
2	C	35	PHE
2	C	114	ASN
2	C	138	PHE
2	C	142	LYS
2	C	190	ASP
1	B	43	TYR
1	B	136	LEU
1	B	232	ARG
1	B	234	ASN
1	B	301	ILE
2	C	102	PRO
2	C	191	PRO
1	B	286	GLN
1	B	374	ASN
1	B	385	VAL
1	B	397	HIS
2	C	157	PHE
1	B	155	ILE
1	B	469	VAL
1	B	603	PRO
2	C	101	VAL
1	B	110	VAL

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Mol	Chain	Res	Type
1	B	307	GLY
2	C	169	ILE
1	B	202	ILE
1	B	750	VAL

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	B	790/778 (102%)	697 (88%)	93 (12%)	5 22
2	C	164/182 (90%)	138 (84%)	26 (16%)	2 12
All	All	954/960 (99%)	835 (88%)	119 (12%)	4 20

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	TYR
1	B	9	GLU
1	B	26	ASP
1	B	46	PHE
1	B	52	PHE
1	B	57	LEU
1	B	71	ILE
1	B	75	ASN
1	B	83	PHE
1	B	88	THR
1	B	105	LEU
1	B	140	GLU
1	B	152	LEU
1	B	153	GLN
1	B	154	LYS
1	B	155	ILE
1	B	164	ASP
1	B	182	PHE
1	B	203	ILE

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Mol	Chain	Res	Type
1	B	212	HIS
1	B	221	PHE
1	B	228	GLU
1	B	239	LEU
1	B	243	LEU
1	B	244	GLU
1	B	246	ARG
1	B	249	ARG
1	B	264	ARG
1	B	270	GLU
1	B	271	ASN
1	B	285	GLU
1	B	286	GLN
1	B	289	CYS
1	B	291	ASP
1	B	293	LEU
1	B	308	MSE
1	B	333	GLN
1	B	337	PRO
1	B	341	ARG
1	B	348	GLN
1	B	350	ASP
1	B	358	ASP
1	B	360	ASP
1	B	372	ASP
1	B	373	TRP
1	B	376	ARG
1	B	377	LYS
1	B	384	ASP
1	B	397	HIS
1	B	411	TRP
1	B	413	VAL
1	B	432	MSE
1	B	435	TYR
1	B	445	GLN
1	B	450	LYS
1	B	457	ILE
1	B	465	TYR
1	B	467	HIS
1	B	475	ASP
1	B	477	TYR
1	B	502	SER

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Mol	Chain	Res	Type
1	B	510	GLU
1	B	518	TYR
1	B	534	GLN
1	B	559	PRO
1	B	571	GLN
1	B	578	ASP
1	B	579	GLU
1	B	599	SER
1	B	617	GLN
1	B	631	ASP
1	B	637	ASP
1	B	643	VAL
1	B	662	LEU
1	B	668	ILE
1	B	669	LEU
1	B	671	LEU
1	B	677	GLN
1	B	718	ASN
1	B	741	ILE
1	B	753	GLN
1	B	791	GLN
1	B	801	LEU
1	B	804	ILE
1	B	806	ASP
1	B	824	ASN
1	B	826	SER
1	B	828	VAL
1	B	830	GLN
1	B	844	ASN
1	B	850	ARG
1	B	851	ASP
1	B	861	LYS
2	C	9	VAL
2	C	12	LYS
2	C	15	LEU
2	C	18	ASP
2	C	34	GLU
2	C	38	LYS
2	C	39	TYR
2	C	55	ASN
2	C	56	ARG
2	C	61	PHE

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Mol	Chain	Res	Type
2	C	66	THR
2	C	72	PHE
2	C	75	LEU
2	C	79	TYR
2	C	80	TYR
2	C	92	VAL
2	C	117	ILE
2	C	141	LYS
2	C	143	ASN
2	C	145	GLN
2	C	148	ASP
2	C	157	PHE
2	C	167	LYS
2	C	179	MSE
2	C	191	PRO
2	C	196	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	14	GLN
1	B	47	ASN
1	B	98	ASN
1	B	173	ASN
1	B	181	GLN
1	B	200	GLN
1	B	234	ASN
1	B	253	HIS
1	B	263	GLN
1	B	266	GLN
1	B	286	GLN
1	B	333	GLN
1	B	349	HIS
1	B	535	HIS
1	B	537	ASN
1	B	554	HIS
1	B	610	GLN
1	B	614	ASN
1	B	632	GLN
1	B	677	GLN
1	B	718	ASN
1	B	753	GLN

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Mol	Chain	Res	Type
1	B	791	GLN
1	B	792	GLN
1	B	824	ASN
1	B	830	GLN
1	B	844	ASN
2	C	55	ASN
2	C	82	GLN
2	C	100	ASN
2	C	103	ASN
2	C	105	HIS
2	C	196	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GNP	C	218	3	29,34,34	1.90	5 (17%)	33,54,54	2.26	6 (18%)

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	GNP	C	218	3	-	2/14/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	218	GNP	C6-N1	5.26	1.42	1.33
4	C	218	GNP	PG-O2G	-4.37	1.45	1.56
4	C	218	GNP	C8-N7	-4.12	1.27	1.34
4	C	218	GNP	PB-O2B	-3.51	1.47	1.56
4	C	218	GNP	O4'-C1'	2.55	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	218	GNP	C5-C6-N1	-8.29	112.10	123.43
4	C	218	GNP	C2-N1-C6	6.08	125.59	115.93
4	C	218	GNP	N3-C2-N1	-4.28	121.52	127.22
4	C	218	GNP	O2G-PG-O3G	-2.64	100.60	107.64
4	C	218	GNP	O3G-PG-O1G	-2.25	107.80	113.45
4	C	218	GNP	N2-C2-N3	2.13	121.26	117.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	218	GNP	PG-N3B-PB-O1B
4	C	218	GNP	PG-N3B-PB-O3A

There are no ring outliers.

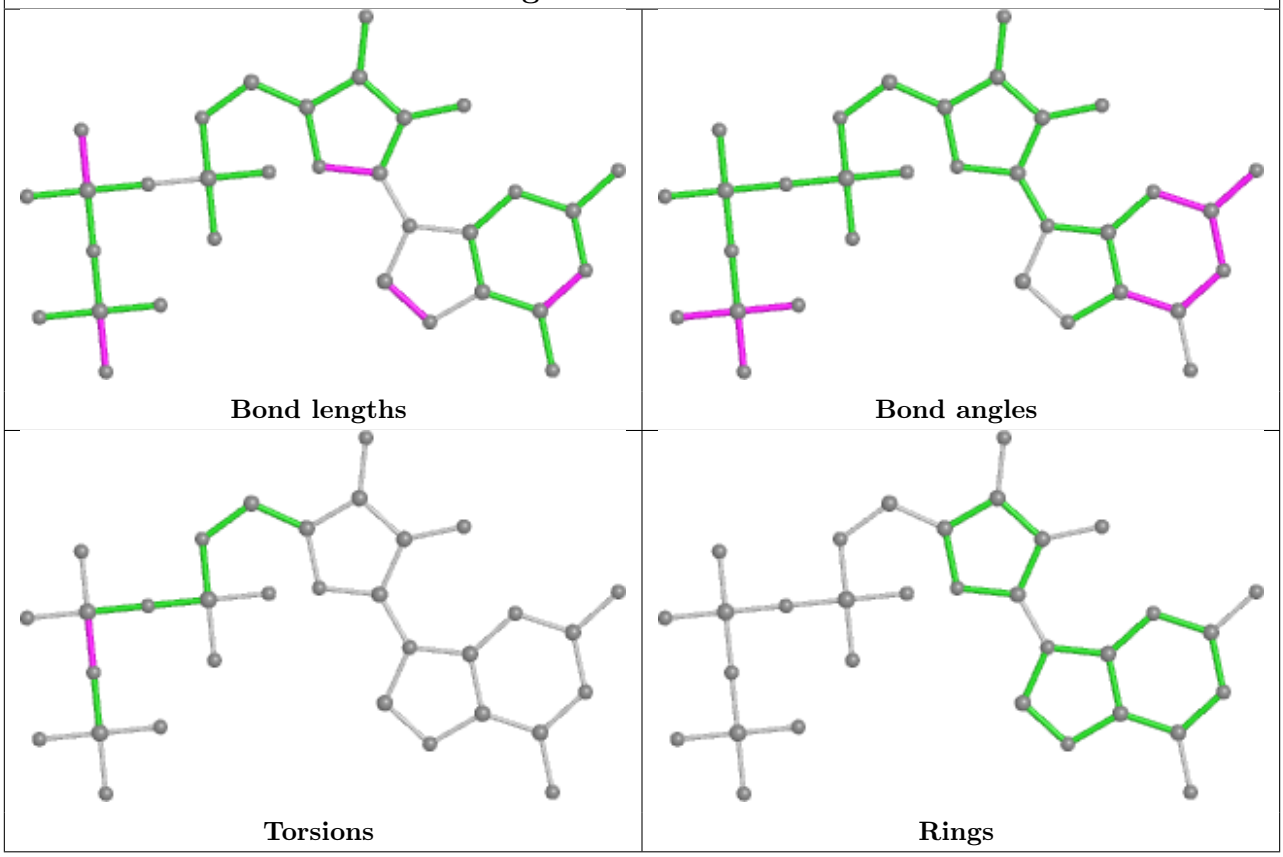
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	218	GNP	4	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 GNP C 218



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.