



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2016 – 07:01 PM EDT

PDB ID : 1JFF
Title : Refined structure of alpha-beta tubulin from zinc-induced sheets stabilized with taxol
Authors : Lowe, J.; Li, H.; Downing, K.H.; Nogales, E.
Deposited on : 2001-06-20
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

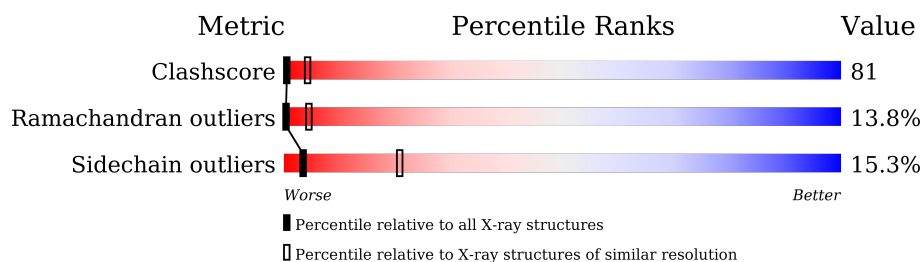
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	
2	B	445	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6702 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 tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3227	2043	551	613	20			

- Molecule 2 is a protein called tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3351	2105	575	646	25			

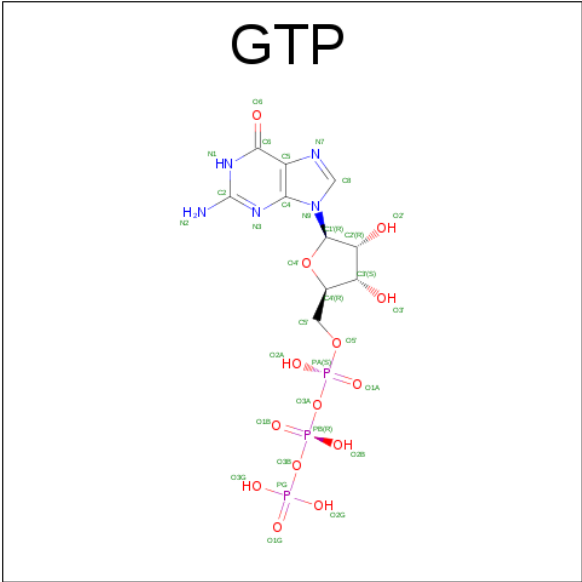
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

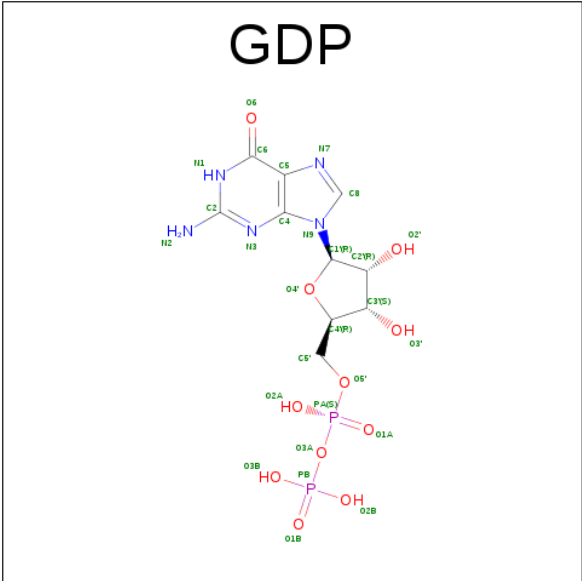
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



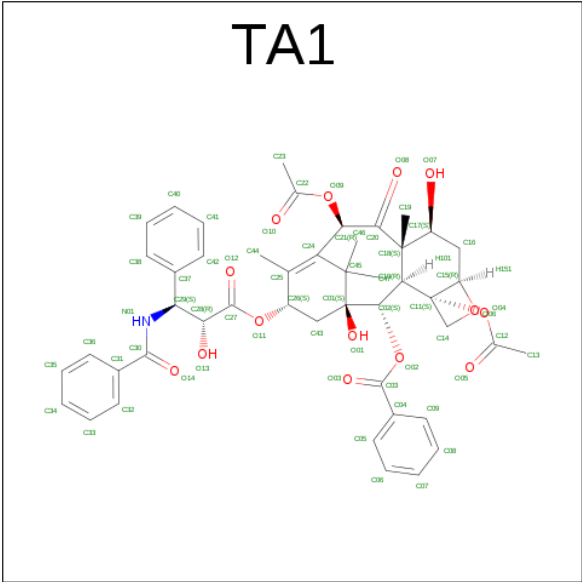
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			62	47	1	14		

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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.20 Å 93.50 Å 90.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.232 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: GDP, GTP, ZN, TA1, 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	0.50	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
All	All	0.51	0/6726	0.75	2/9124 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	235	MET	CG-SD-CE	6.09	109.95	100.20
2	B	217	LEU	N-CA-C	-5.37	96.51	111.00

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	A	3227	0	3143	542	0
2	B	3351	0	3229	553	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	32	0	12	5	0
6	B	28	0	12	1	0
7	B	62	0	51	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6702	0	6447	1068	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 81.

All (1068) 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:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.15
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.12
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.30	1.10
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.37	1.06
2:B:299:LYS:H	2:B:299:LYS:HD3	1.24	1.03
1:A:243:ARG:HH21	1:A:252:LEU:N	1.57	1.01
1:A:109:THR:HG22	1:A:110:ILE:N	1.70	1.01
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.43	1.00
2:B:236:SER:O	2:B:240:THR:HG23	1.61	1.00
2:B:281:GLN:O	2:B:283:TYR:N	2.00	0.95
1:A:251:ASP:N	1:A:254:GLU:HG3	1.82	0.94
2:B:70:LEU:H	2:B:145:THR:HG21	1.33	0.94
1:A:316:CYS:HB3	1:A:378:LEU:HD11	1.48	0.93
1:A:98:ASP:HB2	1:A:105:ARG:HH21	1.31	0.93
1:A:237:SER:HB2	1:A:376:CYS:SG	2.08	0.93
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.48	0.93
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.47	0.92
1:A:151:SER:HB3	1:A:193:THR:HG21	1.50	0.92
1:A:251:ASP:H	1:A:254:GLU:HG3	1.33	0.92
2:B:264:ARG:O	2:B:265:LEU:HB3	1.69	0.92
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.51	0.92
2:B:147:SER:O	2:B:151:THR:HB	1.71	0.91
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.50	0.91
1:A:109:THR:HG22	1:A:110:ILE:H	1.33	0.90
1:A:184:PRO:HG2	1:A:398:MET:HE1	1.54	0.90
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.53	0.89
2:B:101:ASN:HD21	2:B:143:GLY:HA2	1.38	0.89
1:A:343:PHE:CZ	1:A:351:PHE:CE1	2.61	0.89
1:A:122:ILE:HD12	1:A:157:LEU:HD21	1.54	0.88
1:A:407:TRP:HE1	2:B:260:VAL:HG23	1.38	0.88
2:B:8:GLN:OE1	2:B:67:LEU:HD22	1.72	0.88
2:B:93:VAL:HG11	2:B:118:VAL:CG2	2.03	0.88
1:A:147:SER:HB2	1:A:190:THR:OG1	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:HD21	2:B:408:TYR:HA	1.38	0.87
2:B:10:GLY:HA2	2:B:145:THR:HB	1.55	0.87
2:B:264:ARG:HB2	2:B:266:HIS:CD2	2.08	0.87
2:B:311:ARG:HD3	2:B:342:TYR:HA	1.56	0.87
2:B:360:PRO:HG2	2:B:371:LEU:HB3	1.56	0.87
1:A:110:ILE:HG23	1:A:111:GLY:H	1.38	0.86
2:B:153:LEU:O	2:B:157:ILE:HG12	1.75	0.86
2:B:6:HIS:CE1	2:B:8:GLN:HG2	2.10	0.86
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.57	0.85
2:B:276:THR:HB	2:B:281:GLN:HG3	1.56	0.85
2:B:234:THR:HG21	2:B:270:PRO:CB	2.06	0.85
2:B:242:LEU:HD22	2:B:250:ALA:H	1.41	0.85
2:B:209:LEU:HB3	2:B:227:LEU:HD22	1.59	0.85
1:A:316:CYS:HB3	1:A:378:LEU:CD1	2.08	0.84
2:B:20:PHE:CD2	2:B:235:MET:SD	2.71	0.84
2:B:150:GLY:HA2	2:B:153:LEU:HD22	1.59	0.83
1:A:264:ARG:O	1:A:266:HIS:N	2.09	0.83
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.57	0.83
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.60	0.83
1:A:106:GLY:O	1:A:111:GLY:HA3	1.78	0.83
2:B:287:THR:O	2:B:288:VAL:HG23	1.78	0.83
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.61	0.83
2:B:148:GLY:O	2:B:151:THR:HG22	1.79	0.83
2:B:3:GLU:O	2:B:133:GLN:HB3	1.78	0.82
1:A:151:SER:CB	1:A:193:THR:HG21	2.09	0.82
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.13	0.82
2:B:101:ASN:ND2	2:B:143:GLY:HA2	1.94	0.82
2:B:110:GLU:O	2:B:113:GLU:HG2	1.79	0.82
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.59	0.82
2:B:20:PHE:CZ	2:B:24:ILE:HD12	2.15	0.82
2:B:147:SER:HB2	2:B:190:SER:HB3	1.60	0.82
2:B:4:ILE:HD13	2:B:136:GLN:HE21	1.42	0.82
2:B:156:LYS:HE2	2:B:156:LYS:HA	1.61	0.81
2:B:264:ARG:HB2	2:B:266:HIS:HD2	1.45	0.81
1:A:234:ILE:HG13	1:A:270:ALA:HB1	1.59	0.81
2:B:324:SER:HB3	2:B:327:GLU:HG2	1.60	0.81
1:A:234:ILE:HD13	1:A:234:ILE:O	1.81	0.81
1:A:267:PHE:CD1	1:A:267:PHE:N	2.49	0.81
1:A:6:SER:HB3	1:A:136:SER:OG	1.81	0.81
1:A:220:GLU:C	1:A:222:PRO:HD3	2.02	0.80
1:A:248:LEU:HD23	1:A:353:VAL:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.46	0.80
1:A:7:ILE:HG22	1:A:66:VAL:HG22	1.63	0.80
1:A:132:LEU:HD23	1:A:132:LEU:H	1.46	0.80
2:B:236:SER:O	2:B:240:THR:CG2	2.29	0.79
2:B:68:VAL:HG12	2:B:149:MET:SD	2.22	0.79
1:A:241:SER:O	1:A:244:PHE:HB3	1.82	0.79
1:A:313:MET:HB3	1:A:344:VAL:HG21	1.63	0.79
1:A:109:THR:CG2	1:A:110:ILE:N	2.44	0.79
2:B:259:MET:HA	2:B:314:THR:HG21	1.65	0.79
2:B:413:MET:HG3	2:B:414:ASP:H	1.47	0.78
2:B:205:ASP:OD1	2:B:304:ALA:HB2	1.84	0.78
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.66	0.78
1:A:155:GLU:HA	1:A:197:HIS:ND1	1.99	0.78
1:A:11:GLN:HG3	1:A:74:VAL:CG1	2.13	0.78
2:B:265:LEU:HD12	2:B:265:LEU:O	1.83	0.77
1:A:199:ASP:HB3	1:A:256:GLN:NE2	1.98	0.77
1:A:425:MET:HE2	1:A:428:LEU:HD23	1.66	0.77
1:A:69:ASP:HA	1:A:145:THR:HG21	1.66	0.77
2:B:35:SER:HB3	2:B:59:ASN:HA	1.65	0.77
1:A:110:ILE:HG23	1:A:111:GLY:N	1.99	0.77
2:B:192:HIS:ND1	2:B:424:ASN:OD1	2.18	0.77
1:A:221:ARG:HD3	1:A:221:ARG:O	1.85	0.77
2:B:234:THR:CG2	2:B:270:PRO:HB2	2.11	0.77
2:B:198:THR:O	2:B:265:LEU:HD22	1.85	0.77
2:B:396:THR:HG23	2:B:422:GLU:OE2	1.83	0.77
1:A:172:TYR:HD1	1:A:172:TYR:C	1.87	0.76
1:A:225:THR:O	1:A:229:ARG:HG3	1.86	0.76
1:A:231:ILE:HA	1:A:234:ILE:HG22	1.66	0.76
1:A:331:ALA:O	1:A:335:ILE:HG12	1.86	0.76
1:A:362:VAL:HG13	1:A:368:LEU:HD12	1.68	0.76
1:A:223:THR:HB	1:A:225:THR:HG22	1.67	0.76
1:A:163:LYS:O	1:A:164:LYS:HG2	1.86	0.76
2:B:259:MET:HG2	2:B:314:THR:HG21	1.67	0.76
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.21	0.76
1:A:276:ILE:HG23	1:A:369:ALA:CB	2.16	0.75
1:A:205:ASP:CB	1:A:303:VAL:HA	2.17	0.75
2:B:250:ALA:HA	2:B:254:LYS:HE2	1.67	0.75
2:B:19:LYS:HG3	2:B:228:ASN:CB	2.17	0.75
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.87	0.75
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.68	0.75
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HG21	1:A:302:MET:HE3	1.69	0.75
2:B:103:TRP:CZ3	2:B:108:TYR:HE1	2.05	0.75
2:B:176:LYS:HE3	2:B:207:GLU:HG3	1.68	0.74
2:B:242:LEU:HD13	2:B:250:ALA:C	2.08	0.74
2:B:274:PRO:HG2	2:B:371:LEU:HD21	1.70	0.74
2:B:168:THR:HB	2:B:201:THR:HG23	1.68	0.74
2:B:209:LEU:HG	2:B:230:LEU:HD22	1.69	0.74
1:A:101:ASN:ND2	2:B:254:LYS:HD2	2.02	0.74
2:B:8:GLN:CD	2:B:67:LEU:HD22	2.08	0.74
1:A:243:ARG:HH21	1:A:252:LEU:H	0.79	0.73
1:A:306:ASP:O	1:A:308:ARG:N	2.20	0.73
1:A:172:TYR:C	1:A:172:TYR:CD1	2.61	0.73
2:B:217:LEU:C	2:B:219:LEU:H	1.91	0.73
1:A:104:ALA:CB	1:A:413:MET:HG3	2.18	0.73
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.27	0.73
1:A:104:ALA:HB2	1:A:413:MET:HG3	1.71	0.73
1:A:242:LEU:HG	1:A:250:VAL:O	1.88	0.73
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.18	0.73
1:A:264:ARG:C	1:A:266:HIS:H	1.91	0.73
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.19	0.73
2:B:217:LEU:O	2:B:219:LEU:N	2.22	0.72
2:B:6:HIS:HE1	2:B:8:GLN:HG2	1.52	0.72
1:A:242:LEU:HD21	1:A:250:VAL:HB	1.71	0.72
1:A:63:PRO:O	1:A:64:ARG:HG2	1.88	0.72
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.24	0.72
2:B:243:ARG:NH2	2:B:252:LEU:HG	2.05	0.72
1:A:105:ARG:O	1:A:110:ILE:HG22	1.89	0.72
2:B:76:ASP:HA	2:B:79:ARG:HG2	1.71	0.72
2:B:356:CYS:SG	2:B:357:ASP:N	2.62	0.72
1:A:7:ILE:HD11	1:A:137:VAL:HG22	1.71	0.72
2:B:10:GLY:O	2:B:14:ASN:HB2	1.90	0.72
2:B:201:THR:OG1	2:B:265:LEU:HD11	1.90	0.72
2:B:325:MET:HE3	2:B:325:MET:HA	1.72	0.72
1:A:112:LYS:O	1:A:115:ILE:HG22	1.89	0.71
1:A:166:LYS:HE3	1:A:199:ASP:OD1	1.90	0.71
1:A:312:TYR:O	1:A:344:VAL:HG23	1.90	0.71
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.52	0.71
2:B:111:GLY:O	2:B:115:VAL:HG23	1.89	0.71
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.73	0.71
2:B:70:LEU:HG	2:B:145:THR:CG2	2.20	0.71
2:B:175:PRO:HD2	2:B:207:GLU:OE2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:GLU:OE1	2:B:432:TYR:HA	1.91	0.71
1:A:12:ALA:HB3	1:A:140:SER:OG	1.91	0.71
1:A:148:GLY:O	1:A:151:SER:HB2	1.91	0.71
1:A:25:CYS:HB2	1:A:30:ILE:O	1.89	0.71
2:B:237:GLY:O	2:B:241:CYS:HB3	1.90	0.71
1:A:88:HIS:C	1:A:90:GLU:H	1.95	0.70
2:B:48:ARG:HG2	2:B:243:ARG:O	1.90	0.70
1:A:317:LEU:HD12	1:A:351:PHE:HD2	1.56	0.70
2:B:70:LEU:HG	2:B:145:THR:HG23	1.74	0.70
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.20	0.70
1:A:237:SER:CB	1:A:376:CYS:SG	2.80	0.70
2:B:291:LEU:O	2:B:295:MET:HG3	1.91	0.70
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.74	0.70
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.06	0.70
1:A:244:PHE:HD2	1:A:245:ASP:N	1.89	0.70
1:A:133:GLN:HG2	1:A:243:ARG:HH22	1.57	0.69
1:A:371:VAL:HG12	1:A:372:GLN:H	1.57	0.69
2:B:255:LEU:O	2:B:259:MET:HG3	1.91	0.69
1:A:315:CYS:HB3	1:A:377:MET:HE2	1.73	0.69
1:A:199:ASP:HB3	1:A:256:GLN:HE21	1.57	0.69
2:B:180:THR:HG22	2:B:181:VAL:N	2.07	0.69
1:A:243:ARG:NH2	1:A:252:LEU:N	2.28	0.69
2:B:299:LYS:N	2:B:299:LYS:HD3	2.04	0.69
1:A:115:ILE:CD1	1:A:119:LEU:HG	2.23	0.69
2:B:251:ASP:O	2:B:253:ARG:N	2.26	0.69
2:B:257:VAL:O	2:B:257:VAL:HG12	1.93	0.69
1:A:5:ILE:HG22	1:A:6:SER:N	2.07	0.69
1:A:71:GLU:HG3	2:B:2:ARG:HH21	1.58	0.69
1:A:141:PHE:O	1:A:147:SER:HB3	1.94	0.68
1:A:381:THR:C	1:A:383:ALA:H	1.95	0.68
2:B:234:THR:O	2:B:238:VAL:HG23	1.92	0.68
2:B:256:ALA:O	2:B:260:VAL:HG22	1.94	0.68
2:B:24:ILE:HD11	2:B:52:TYR:CE1	2.28	0.68
1:A:217:LEU:HD12	1:A:277:SER:HB3	1.75	0.68
1:A:394:LYS:HG2	2:B:348:PRO:HG3	1.75	0.68
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.68
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.29	0.68
1:A:63:PRO:C	1:A:64:ARG:HG2	2.12	0.68
1:A:221:ARG:N	1:A:222:PRO:HD3	2.09	0.68
2:B:325:MET:CE	2:B:355:VAL:HG21	2.24	0.68
1:A:407:TRP:HE1	2:B:260:VAL:CG2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HD2	2:B:326:LYS:HB3	1.74	0.67
2:B:107:HIS:CD2	2:B:151:THR:CG2	2.77	0.67
2:B:209:LEU:HD23	2:B:227:LEU:HB3	1.75	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.94	0.67
2:B:44:LEU:HD12	2:B:49:ILE:HD13	1.76	0.67
1:A:343:PHE:CZ	1:A:351:PHE:HE1	2.08	0.67
1:A:95:GLY:O	1:A:97:GLU:N	2.27	0.67
2:B:310:GLY:HA3	2:B:436:GLN:HE21	1.59	0.67
2:B:4:ILE:HG21	2:B:136:GLN:HG2	1.76	0.67
2:B:66:ILE:C	2:B:67:LEU:HD23	2.15	0.67
2:B:267:PHE:CD1	2:B:267:PHE:N	2.62	0.67
1:A:259:LEU:HD11	1:A:378:LEU:CD1	2.20	0.67
2:B:182:VAL:HG23	2:B:186:ASN:HD21	1.60	0.67
2:B:242:LEU:CD2	2:B:250:ALA:H	2.06	0.67
2:B:103:TRP:HZ3	2:B:108:TYR:HE1	1.42	0.67
2:B:230:LEU:HD23	2:B:231:VAL:N	2.10	0.67
1:A:251:ASP:O	1:A:254:GLU:HB2	1.94	0.66
2:B:250:ALA:HB1	2:B:254:LYS:HB2	1.76	0.66
1:A:175:PRO:HG3	1:A:304:LYS:HG2	1.76	0.66
1:A:276:ILE:O	1:A:369:ALA:HB2	1.95	0.66
2:B:204:ILE:HD13	2:B:231:VAL:HG22	1.76	0.66
1:A:343:PHE:HZ	1:A:351:PHE:CE1	2.10	0.66
1:A:341:ILE:HG12	1:A:341:ILE:O	1.95	0.66
1:A:7:ILE:HD12	1:A:153:LEU:CD2	2.24	0.66
1:A:100:ALA:CB	1:A:105:ARG:HD3	2.25	0.66
1:A:68:VAL:HG11	1:A:149:PHE:CZ	2.30	0.66
2:B:265:LEU:HD12	2:B:265:LEU:C	2.16	0.66
1:A:313:MET:HB3	1:A:344:VAL:CG2	2.26	0.66
2:B:276:THR:HB	2:B:281:GLN:CG	2.25	0.66
2:B:413:MET:HG2	2:B:418:PHE:HE1	1.61	0.66
2:B:242:LEU:CD1	2:B:255:LEU:HD11	2.25	0.65
1:A:372:GLN:O	1:A:373:ARG:HB3	1.96	0.65
1:A:217:LEU:HD11	1:A:367:ASP:O	1.96	0.65
2:B:242:LEU:HD12	2:B:255:LEU:HD11	1.78	0.65
2:B:243:ARG:HH22	2:B:252:LEU:HG	1.59	0.65
1:A:206:ASN:OD1	1:A:227:LEU:HD13	1.96	0.65
1:A:152:LEU:HA	1:A:155:GLU:HB2	1.77	0.65
1:A:172:TYR:HD1	1:A:173:PRO:N	1.93	0.65
2:B:241:CYS:O	2:B:244:PHE:HB2	1.97	0.65
2:B:281:GLN:O	2:B:283:TYR:HB2	1.96	0.65
1:A:271:THR:HG23	1:A:300:ASN:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HG23	1:A:116:ASP:N	2.12	0.64
1:A:305:CYS:SG	1:A:384:ILE:HD13	2.37	0.64
2:B:66:ILE:CD1	2:B:122:VAL:HG12	2.26	0.64
2:B:299:LYS:O	2:B:300:ASN:HB2	1.97	0.64
2:B:332:MET:HE3	2:B:351:VAL:HG11	1.79	0.64
2:B:35:SER:HB3	2:B:59:ASN:CA	2.26	0.64
2:B:158:ARG:NE	2:B:197:ASN:O	2.30	0.64
2:B:70:LEU:N	2:B:145:THR:HG21	2.11	0.64
2:B:284:ARG:O	2:B:286:LEU:N	2.31	0.64
1:A:344:VAL:HG12	1:A:345:ASP:N	2.12	0.64
2:B:172:VAL:HG11	2:B:387:LEU:CD2	2.22	0.64
1:A:234:ILE:HD13	1:A:234:ILE:C	2.18	0.64
2:B:63:PRO:HD2	2:B:86:ILE:HG12	1.80	0.64
1:A:224:TYR:CD1	2:B:325:MET:HG2	2.33	0.64
1:A:402:ARG:O	1:A:403:ALA:C	2.36	0.64
1:A:317:LEU:HD12	1:A:351:PHE:CD2	2.32	0.64
1:A:386:GLU:O	1:A:389:ALA:N	2.31	0.64
2:B:431:GLU:O	2:B:434:GLN:HG2	1.97	0.64
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.79	0.64
1:A:317:LEU:HD11	1:A:351:PHE:HE2	1.63	0.64
2:B:114:LEU:O	2:B:118:VAL:HG23	1.97	0.64
2:B:422:GLU:O	2:B:426:ASN:HB2	1.97	0.64
2:B:192:HIS:O	2:B:195:VAL:HG12	1.98	0.63
1:A:151:SER:O	1:A:155:GLU:HB2	1.98	0.63
2:B:70:LEU:H	2:B:145:THR:CG2	2.10	0.63
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.33	0.63
1:A:152:LEU:HD12	1:A:153:LEU:N	2.14	0.63
2:B:4:ILE:HA	2:B:134:GLY:O	1.99	0.63
2:B:107:HIS:HD2	2:B:151:THR:CG2	2.12	0.63
2:B:137:LEU:HD22	2:B:154:ILE:CG2	2.28	0.63
1:A:269:LEU:O	1:A:378:LEU:HA	1.99	0.63
2:B:105:LYS:O	2:B:110:GLU:HB2	1.98	0.63
7:B:601:TA1:H261	7:B:601:TA1:H463	1.80	0.63
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.63
2:B:427:ASP:O	2:B:430:SER:HB3	1.97	0.63
1:A:7:ILE:CD1	1:A:137:VAL:HG22	2.29	0.63
1:A:175:PRO:HG2	1:A:207:GLU:OE1	1.98	0.63
2:B:180:THR:CG2	2:B:181:VAL:N	2.61	0.63
1:A:315:CYS:HB3	1:A:377:MET:CE	2.29	0.63
1:A:276:ILE:HG23	1:A:369:ALA:HB2	1.80	0.62
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:H	1:A:199:ASP:CG	2.03	0.62
1:A:236:SER:O	1:A:240:ALA:HB3	1.99	0.62
1:A:278:ALA:HA	1:A:282:TYR:OH	2.00	0.62
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.81	0.62
1:A:288:VAL:O	1:A:290:GLU:N	2.33	0.62
2:B:282:GLN:O	2:B:282:GLN:HG2	1.97	0.62
1:A:102:ASN:OD1	1:A:105:ARG:HB3	1.99	0.62
1:A:119:LEU:CD2	1:A:122:ILE:HD11	2.28	0.62
2:B:133:GLN:HG3	2:B:165:ILE:HD11	1.80	0.62
1:A:407:TRP:NE1	2:B:260:VAL:HG23	2.14	0.62
2:B:70:LEU:CG	2:B:145:THR:HG23	2.30	0.62
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.30	0.62
2:B:253:ARG:O	2:B:256:ALA:N	2.33	0.62
2:B:211:ASP:OD1	2:B:212:ILE:N	2.33	0.62
1:A:267:PHE:H	1:A:267:PHE:HD1	1.47	0.62
2:B:4:ILE:HG23	2:B:134:GLY:O	2.00	0.62
1:A:179:THR:HG21	2:B:248:LEU:CD2	2.30	0.61
2:B:114:LEU:HD23	2:B:149:MET:CE	2.30	0.61
2:B:204:ILE:CD1	2:B:231:VAL:HG13	2.30	0.61
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.82	0.61
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.15	0.61
2:B:205:ASP:OD1	2:B:304:ALA:N	2.32	0.61
2:B:285:ALA:HB1	2:B:290:GLU:HG2	1.82	0.61
2:B:318:VAL:HA	2:B:354:ALA:HB3	1.81	0.61
1:A:7:ILE:HG22	1:A:66:VAL:CG2	2.28	0.61
1:A:88:HIS:O	1:A:90:GLU:N	2.33	0.61
1:A:115:ILE:HG13	1:A:152:LEU:HD13	1.81	0.61
2:B:230:LEU:O	2:B:233:ALA:HB3	2.00	0.61
1:A:345:ASP:C	1:A:347:CYS:H	2.04	0.61
1:A:23:LEU:HD22	1:A:232:GLY:O	1.99	0.61
2:B:243:ARG:HH21	2:B:252:LEU:H	1.45	0.61
1:A:168:GLU:OE1	1:A:198:SER:HB2	2.01	0.61
1:A:248:LEU:CD2	1:A:353:VAL:O	2.49	0.61
2:B:324:SER:CB	2:B:327:GLU:HG2	2.30	0.61
2:B:108:TYR:CD1	2:B:413:MET:HE1	2.36	0.61
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.82	0.61
1:A:179:THR:HG22	2:B:352:LYS:NZ	2.15	0.61
1:A:169:PHE:CE1	1:A:235:VAL:HG22	2.36	0.61
2:B:128:SER:OG	2:B:129:CYS:N	2.34	0.61
1:A:177:VAL:CG1	2:B:329:ASP:HB3	2.31	0.60
1:A:311:LYS:HE3	1:A:342:GLN:CD	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG21	2:B:258:ASN:O	2.01	0.60
2:B:172:VAL:CG1	2:B:387:LEU:HD21	2.24	0.60
1:A:118:VAL:HG11	1:A:149:PHE:HZ	1.65	0.60
1:A:167:LEU:HA	1:A:200:CYS:O	2.01	0.60
1:A:284:GLU:O	1:A:286:LEU:N	2.35	0.60
2:B:115:VAL:HG21	2:B:152:LEU:HD23	1.84	0.60
2:B:324:SER:O	2:B:328:VAL:HG23	2.01	0.60
1:A:344:VAL:HG11	1:A:346:TRP:NE1	2.16	0.60
2:B:93:VAL:CG1	2:B:118:VAL:HG22	2.19	0.60
2:B:279:GLY:O	2:B:282:GLN:HB3	2.01	0.60
1:A:115:ILE:HD13	1:A:115:ILE:O	2.02	0.60
2:B:324:SER:C	2:B:326:LYS:H	2.03	0.60
2:B:332:MET:CE	2:B:351:VAL:HG11	2.32	0.60
2:B:217:LEU:C	2:B:219:LEU:N	2.55	0.60
2:B:49:ILE:O	2:B:51:VAL:N	2.35	0.60
1:A:179:THR:HG21	2:B:248:LEU:HD21	1.81	0.60
1:A:229:ARG:NH1	1:A:363:VAL:HG21	2.16	0.60
1:A:362:VAL:HG13	1:A:368:LEU:HB2	1.83	0.60
1:A:191:THR:HG21	1:A:425:MET:SD	2.41	0.59
1:A:413:MET:O	1:A:414:GLU:HG3	2.02	0.59
2:B:102:ASN:ND2	2:B:407:TRP:O	2.35	0.59
2:B:229:HIS:HD1	2:B:229:HIS:C	2.05	0.59
2:B:161:TYR:C	2:B:163:ASP:H	2.05	0.59
2:B:30:ILE:HD13	2:B:53:TYR:CE2	2.38	0.59
1:A:177:VAL:HG11	2:B:329:ASP:HB3	1.82	0.59
1:A:11:GLN:HE21	1:A:74:VAL:HG22	1.66	0.59
1:A:369:ALA:O	1:A:370:LYS:HB3	2.03	0.59
2:B:204:ILE:HG21	2:B:231:VAL:HG22	1.84	0.59
2:B:408:TYR:CG	2:B:418:PHE:HZ	2.20	0.59
2:B:151:THR:OG1	2:B:193:GLN:HB3	2.03	0.59
2:B:349:ASN:C	2:B:349:ASN:HD22	2.07	0.59
1:A:119:LEU:O	1:A:122:ILE:HG12	2.02	0.59
1:A:317:LEU:HD11	1:A:351:PHE:CE2	2.38	0.59
2:B:141:LEU:N	2:B:141:LEU:CD1	2.65	0.58
2:B:299:LYS:O	2:B:300:ASN:CB	2.51	0.58
1:A:407:TRP:O	1:A:411:GLU:HG2	2.02	0.58
1:A:435:VAL:HG12	1:A:435:VAL:O	2.02	0.58
1:A:6:SER:HA	1:A:136:SER:O	2.02	0.58
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.18	0.58
2:B:299:LYS:CD	2:B:299:LYS:H	2.07	0.58
2:B:89:PRO:HA	2:B:92:PHE:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:OD1	2:B:304:ALA:CB	2.50	0.58
2:B:307:PRO:HB3	2:B:312:TYR:OH	2.04	0.58
2:B:70:LEU:C	2:B:99:ALA:HB2	2.24	0.58
1:A:165:SER:HA	1:A:199:ASP:OD2	2.04	0.58
1:A:371:VAL:HG12	1:A:372:GLN:N	2.17	0.58
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.33	0.58
2:B:270:PRO:HA	2:B:377:PHE:O	2.04	0.58
2:B:19:LYS:CG	2:B:228:ASN:HB3	2.31	0.58
1:A:11:GLN:CG	1:A:74:VAL:HG11	2.28	0.58
2:B:253:ARG:O	2:B:254:LYS:C	2.42	0.58
1:A:2:ARG:N	1:A:131:GLY:O	2.36	0.58
1:A:202:PHE:CE2	1:A:378:LEU:HD22	2.38	0.58
2:B:319:PHE:HA	2:B:375:ALA:HA	1.86	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.03	0.58
1:A:338:LYS:O	1:A:340:THR:N	2.34	0.57
1:A:362:VAL:HG11	1:A:368:LEU:O	2.04	0.57
2:B:198:THR:HG22	2:B:265:LEU:HD22	1.86	0.57
1:A:313:MET:O	1:A:314:ALA:HB2	2.04	0.57
2:B:4:ILE:HD13	2:B:136:GLN:NE2	2.17	0.57
2:B:149:MET:O	2:B:153:LEU:HD13	2.05	0.57
2:B:422:GLU:O	2:B:426:ASN:N	2.37	0.57
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.40	0.57
1:A:166:LYS:HD2	1:A:197:HIS:O	2.04	0.57
1:A:117:LEU:HD11	1:A:121:ARG:HH22	1.69	0.57
1:A:218:ASP:O	1:A:219:ILE:HG23	2.04	0.57
1:A:278:ALA:HB2	1:A:369:ALA:HA	1.85	0.57
1:A:345:ASP:O	1:A:347:CYS:N	2.38	0.57
2:B:30:ILE:HA	2:B:35:SER:O	2.04	0.57
2:B:312:TYR:O	2:B:344:VAL:HB	2.05	0.57
2:B:14:ASN:OD1	2:B:75:MET:HG2	2.05	0.57
1:A:286:LEU:HD12	1:A:290:GLU:HG2	1.87	0.57
2:B:68:VAL:CG1	2:B:149:MET:SD	2.90	0.57
2:B:274:PRO:CG	2:B:371:LEU:HD21	2.34	0.57
2:B:301:MET:CE	2:B:377:PHE:HE2	2.17	0.57
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.35	0.56
2:B:319:PHE:CD2	2:B:375:ALA:HB2	2.40	0.56
1:A:175:PRO:HG3	1:A:304:LYS:CG	2.35	0.56
2:B:283:TYR:C	2:B:284:ARG:HG2	2.24	0.56
2:B:6:HIS:HB3	2:B:65:ALA:HB2	1.87	0.56
1:A:11:GLN:HE22	2:B:249:ASN:ND2	2.03	0.56
1:A:362:VAL:CG1	1:A:368:LEU:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:THR:O	1:A:382:THR:HG22	2.05	0.56
2:B:70:LEU:CD1	2:B:145:THR:HG23	2.35	0.56
2:B:253:ARG:O	2:B:257:VAL:N	2.33	0.56
1:A:436:GLY:C	1:A:438:ASP:H	2.08	0.56
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.18	0.56
2:B:216:THR:O	2:B:217:LEU:HD12	2.05	0.56
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.29	0.56
1:A:210:TYR:CE2	1:A:227:LEU:HD11	2.40	0.56
1:A:231:ILE:HA	1:A:234:ILE:CG2	2.36	0.56
1:A:394:LYS:HG2	2:B:348:PRO:CG	2.35	0.56
2:B:320:ARG:O	2:B:359:PRO:HA	2.04	0.56
1:A:152:LEU:HA	1:A:155:GLU:CB	2.35	0.56
1:A:242:LEU:C	1:A:244:PHE:H	2.09	0.56
1:A:381:THR:C	1:A:383:ALA:N	2.56	0.56
1:A:63:PRO:HD3	1:A:86:LEU:O	2.04	0.56
2:B:182:VAL:HG23	2:B:186:ASN:ND2	2.20	0.56
2:B:19:LYS:O	2:B:23:VAL:HG23	2.06	0.56
2:B:250:ALA:CA	2:B:254:LYS:HE2	2.35	0.56
1:A:110:ILE:CG2	1:A:111:GLY:H	2.15	0.56
1:A:264:ARG:HB2	1:A:266:HIS:HD2	1.67	0.56
2:B:166:MET:HB3	2:B:198:THR:OG1	2.06	0.56
2:B:180:THR:CG2	2:B:181:VAL:H	2.17	0.56
2:B:259:MET:CA	2:B:314:THR:HG21	2.35	0.56
1:A:19:ALA:CB	1:A:228:ASN:HB3	2.35	0.56
1:A:409:VAL:C	1:A:411:GLU:H	2.09	0.56
2:B:50:ASN:O	2:B:64:ARG:NH2	2.38	0.56
1:A:147:SER:CB	1:A:190:THR:OG1	2.52	0.56
1:A:331:ALA:O	1:A:334:THR:HG22	2.05	0.56
1:A:88:HIS:C	1:A:90:GLU:N	2.57	0.56
2:B:132:LEU:CD2	2:B:164:ARG:HG3	2.32	0.56
2:B:210:TYR:HD2	2:B:227:LEU:HD21	1.71	0.56
1:A:172:TYR:OH	1:A:387:ALA:O	2.24	0.55
2:B:311:ARG:HD2	2:B:344:VAL:H	1.71	0.55
1:A:216:ASN:O	1:A:217:LEU:HB2	2.05	0.55
1:A:408:TYR:CD1	1:A:418:PHE:HZ	2.24	0.55
2:B:67:LEU:HD23	2:B:67:LEU:N	2.22	0.55
2:B:151:THR:OG1	2:B:193:GLN:CB	2.54	0.55
2:B:324:SER:C	2:B:326:LYS:N	2.59	0.55
2:B:31:ASP:O	2:B:32:PRO:C	2.44	0.55
1:A:150:THR:O	1:A:153:LEU:N	2.40	0.55
2:B:311:ARG:HG2	2:B:311:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:HIS:HE1	2:B:168:THR:HG23	1.71	0.55
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.41	0.55
2:B:204:ILE:HG21	2:B:231:VAL:CG2	2.36	0.55
2:B:223:THR:HG22	2:B:224:TYR:N	2.21	0.55
2:B:191:VAL:HA	2:B:194:LEU:HD12	1.87	0.55
1:A:6:SER:O	1:A:65:ALA:HB1	2.07	0.55
1:A:381:THR:OG1	1:A:383:ALA:HB3	2.07	0.54
1:A:408:TYR:O	1:A:411:GLU:N	2.39	0.54
2:B:272:PHE:HB3	2:B:275:LEU:HD22	1.88	0.54
1:A:5:ILE:CG2	1:A:6:SER:N	2.70	0.54
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.42	0.54
2:B:20:PHE:CE2	2:B:24:ILE:HD12	2.43	0.54
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.88	0.54
1:A:253:THR:O	1:A:256:GLN:HG2	2.06	0.54
2:B:190:SER:O	2:B:194:LEU:HG	2.06	0.54
2:B:119:LEU:O	2:B:123:ARG:HG3	2.06	0.54
2:B:242:LEU:HD22	2:B:250:ALA:N	2.19	0.54
2:B:310:GLY:CA	2:B:436:GLN:HE21	2.19	0.54
1:A:17:GLY:O	1:A:21:TRP:HB2	2.08	0.54
2:B:213:CYS:SG	2:B:219:LEU:HD23	2.48	0.54
2:B:27:GLU:HG2	2:B:27:GLU:O	2.08	0.54
2:B:325:MET:O	2:B:329:ASP:HB2	2.07	0.54
2:B:424:ASN:HD22	2:B:424:ASN:C	2.09	0.54
2:B:44:LEU:O	2:B:49:ILE:HG12	2.07	0.54
1:A:110:ILE:O	1:A:112:LYS:N	2.41	0.54
1:A:9:VAL:CG1	1:A:139:HIS:HB3	2.38	0.54
1:A:248:LEU:HB3	1:A:355:ILE:H	1.73	0.54
2:B:323:MET:HG3	2:B:328:VAL:HG21	1.90	0.54
2:B:165:ILE:HD13	2:B:165:ILE:H	1.70	0.54
2:B:239:THR:HG22	2:B:240:THR:N	2.22	0.54
2:B:259:MET:CG	2:B:314:THR:HG21	2.36	0.54
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.89	0.54
2:B:343:PHE:O	2:B:344:VAL:O	2.26	0.54
2:B:107:HIS:HD2	2:B:151:THR:HG22	1.72	0.54
2:B:325:MET:CE	2:B:355:VAL:HG11	2.38	0.54
2:B:427:ASP:OD1	2:B:428:LEU:N	2.41	0.54
2:B:239:THR:O	2:B:241:CYS:N	2.41	0.54
2:B:179:ASP:HB2	6:B:600:GDP:H3'	1.90	0.54
1:A:101:ASN:CG	2:B:254:LYS:HD2	2.28	0.53
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.42	0.53
1:A:121:ARG:O	1:A:125:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:CZ	1:A:252:LEU:HG	2.39	0.53
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.89	0.53
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.73	0.53
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.53
2:B:259:MET:HG2	2:B:314:THR:CG2	2.38	0.53
2:B:431:GLU:O	2:B:434:GLN:CG	2.56	0.53
1:A:101:ASN:ND2	5:A:500:GTP:O3G	2.42	0.53
1:A:98:ASP:O	1:A:110:ILE:HD13	2.08	0.53
2:B:194:LEU:C	2:B:196:GLU:H	2.11	0.53
2:B:322:ARG:HH11	2:B:322:ARG:HG3	1.73	0.53
1:A:150:THR:O	1:A:151:SER:C	2.47	0.53
1:A:163:LYS:O	1:A:163:LYS:HG2	2.08	0.53
1:A:182:VAL:O	1:A:184:PRO:N	2.41	0.53
1:A:5:ILE:O	1:A:136:SER:N	2.40	0.53
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.43	0.53
1:A:215:ARG:C	1:A:216:ASN:HD22	2.12	0.53
1:A:5:ILE:O	1:A:135:PHE:HA	2.09	0.53
1:A:115:ILE:C	1:A:115:ILE:HD13	2.28	0.53
2:B:68:VAL:HG12	2:B:149:MET:CE	2.38	0.53
2:B:229:HIS:ND1	2:B:229:HIS:C	2.62	0.53
1:A:196:GLU:C	1:A:197:HIS:CD2	2.82	0.53
2:B:70:LEU:HD12	2:B:145:THR:HG23	1.91	0.53
2:B:147:SER:O	2:B:151:THR:CB	2.52	0.53
1:A:339:ARG:C	1:A:341:ILE:H	2.11	0.53
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.42	0.53
1:A:173:PRO:HB2	1:A:391:LEU:CD1	2.38	0.53
2:B:141:LEU:HA	2:B:147:SER:HB3	1.91	0.53
2:B:226:ASP:O	2:B:227:LEU:C	2.46	0.53
1:A:179:THR:HG22	2:B:352:LYS:HZ1	1.74	0.53
2:B:5:VAL:O	2:B:5:VAL:HG23	2.09	0.53
2:B:210:TYR:CD2	2:B:227:LEU:HD21	2.44	0.52
2:B:226:ASP:O	2:B:229:HIS:N	2.42	0.52
2:B:345:GLU:C	2:B:347:ILE:H	2.13	0.52
1:A:231:ILE:HD13	1:A:231:ILE:N	2.25	0.52
1:A:275:VAL:HG21	1:A:300:ASN:OD1	2.09	0.52
2:B:212:ILE:O	2:B:216:THR:HB	2.09	0.52
2:B:331:GLN:O	2:B:335:VAL:HG23	2.08	0.52
2:B:360:PRO:HB2	7:B:601:TA1:H281	1.91	0.52
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.44	0.52
1:A:206:ASN:OD1	1:A:227:LEU:CD1	2.58	0.52
2:B:273:ALA:CB	2:B:274:PRO:HD3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:O	1:A:240:ALA:C	2.48	0.52
1:A:24:TYR:CE2	1:A:240:ALA:HB2	2.45	0.52
1:A:283:HIS:O	1:A:284:GLU:C	2.47	0.52
1:A:8:HIS:HB3	1:A:13:GLY:O	2.09	0.52
2:B:320:ARG:HA	2:B:356:CYS:HB3	1.92	0.52
1:A:4:CYS:HA	1:A:134:GLY:O	2.10	0.52
1:A:324:VAL:O	1:A:327:ASP:HB2	2.08	0.52
1:A:244:PHE:C	1:A:244:PHE:CD2	2.83	0.52
2:B:188:THR:HA	2:B:425:MET:CE	2.40	0.52
1:A:201:ALA:O	1:A:267:PHE:HA	2.10	0.52
2:B:295:MET:SD	2:B:375:ALA:O	2.68	0.52
2:B:168:THR:CB	2:B:201:THR:HG23	2.38	0.52
2:B:264:ARG:HA	2:B:264:ARG:HE	1.75	0.52
2:B:314:THR:CG2	2:B:315:VAL:N	2.73	0.52
2:B:425:MET:O	2:B:428:LEU:HB3	2.09	0.52
1:A:23:LEU:HD23	1:A:236:SER:CB	2.37	0.52
1:A:362:VAL:HG13	1:A:368:LEU:CD1	2.38	0.52
2:B:4:ILE:CG2	2:B:136:GLN:HG2	2.38	0.52
2:B:200:GLU:N	2:B:265:LEU:HD13	2.25	0.52
2:B:424:ASN:C	2:B:424:ASN:ND2	2.61	0.52
1:A:417:GLU:OE1	1:A:417:GLU:HA	2.10	0.51
2:B:103:TRP:CE2	2:B:189:LEU:HB3	2.45	0.51
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.51
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.40	0.51
1:A:140:SER:O	1:A:142:GLY:N	2.44	0.51
1:A:345:ASP:OD2	1:A:439:SER:HB3	2.10	0.51
2:B:149:MET:O	2:B:153:LEU:HD22	2.10	0.51
2:B:188:THR:HA	2:B:425:MET:HE3	1.91	0.51
2:B:198:THR:HG22	2:B:265:LEU:CD2	2.39	0.51
2:B:277:SER:OG	2:B:281:GLN:HB2	2.10	0.51
2:B:297:ASP:OD1	2:B:298:ALA:N	2.39	0.51
1:A:243:ARG:NH2	1:A:251:ASP:OD1	2.44	0.51
1:A:264:ARG:C	1:A:266:HIS:N	2.60	0.51
2:B:49:ILE:O	2:B:50:ASN:C	2.48	0.51
1:A:251:ASP:OD1	1:A:252:LEU:N	2.43	0.51
2:B:209:LEU:O	2:B:210:TYR:C	2.48	0.51
1:A:231:ILE:CA	1:A:234:ILE:HG22	2.38	0.51
1:A:238:ILE:O	1:A:242:LEU:HB2	2.11	0.51
2:B:431:GLU:OE1	2:B:432:TYR:CA	2.57	0.51
1:A:171:ILE:O	1:A:171:ILE:HG22	2.10	0.51
1:A:402:ARG:O	1:A:403:ALA:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:MET:HG2	2:B:149:MET:O	2.10	0.51
2:B:296:PHE:CZ	2:B:315:VAL:HG11	2.46	0.51
1:A:151:SER:HB3	1:A:193:THR:CG2	2.34	0.51
1:A:196:GLU:O	1:A:197:HIS:CD2	2.64	0.51
1:A:230:LEU:O	1:A:233:GLN:N	2.35	0.51
1:A:173:PRO:HB2	1:A:391:LEU:HD11	1.91	0.51
2:B:21:TRP:HZ2	2:B:65:ALA:HB2	1.76	0.51
1:A:67:PHE:HE1	1:A:87:PHE:CE2	2.29	0.50
2:B:49:ILE:HG13	2:B:50:ASN:H	1.76	0.50
1:A:305:CYS:O	1:A:306:ASP:C	2.49	0.50
2:B:323:MET:HG3	2:B:328:VAL:CG2	2.41	0.50
1:A:191:THR:HG23	1:A:192:HIS:N	2.25	0.50
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.46	0.50
2:B:107:HIS:CD2	2:B:151:THR:HG22	2.45	0.50
2:B:383:ALA:C	2:B:385:GLN:H	2.15	0.50
1:A:9:VAL:HG21	1:A:149:PHE:CD1	2.46	0.50
2:B:369:ARG:C	2:B:369:ARG:HD2	2.32	0.50
1:A:132:LEU:CD2	1:A:164:LYS:HE3	2.41	0.50
1:A:133:GLN:HB3	1:A:243:ARG:HH12	1.76	0.50
2:B:298:ALA:O	2:B:299:LYS:C	2.50	0.50
2:B:173:PRO:HB3	2:B:183:GLU:CG	2.42	0.50
1:A:115:ILE:CG2	1:A:116:ASP:N	2.75	0.50
1:A:119:LEU:HA	1:A:122:ILE:HG12	1.93	0.50
1:A:149:PHE:HE1	1:A:153:LEU:HD22	1.77	0.50
2:B:156:LYS:CE	2:B:156:LYS:HA	2.38	0.50
2:B:260:VAL:HG23	2:B:260:VAL:O	2.10	0.50
2:B:333:LEU:O	2:B:336:GLN:N	2.45	0.50
1:A:11:GLN:O	1:A:14:VAL:HB	2.12	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.50
2:B:113:GLU:HG3	2:B:114:LEU:N	2.26	0.50
2:B:168:THR:O	2:B:201:THR:HA	2.12	0.50
2:B:24:ILE:HG22	2:B:25:SER:N	2.27	0.50
2:B:345:GLU:O	2:B:347:ILE:N	2.45	0.50
2:B:3:GLU:HA	2:B:51:VAL:HA	1.93	0.50
1:A:310:GLY:HA3	1:A:383:ALA:N	2.26	0.50
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.94	0.50
2:B:269:MET:HB3	2:B:303:ALA:HB2	1.94	0.50
2:B:4:ILE:HD12	2:B:239:THR:CG2	2.42	0.50
1:A:115:ILE:HD11	1:A:119:LEU:HG	1.92	0.49
1:A:133:GLN:CB	1:A:243:ARG:HH12	2.24	0.49
2:B:173:PRO:HB3	2:B:183:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:PHE:O	2:B:264:ARG:N	2.45	0.49
2:B:431:GLU:HA	2:B:434:GLN:CG	2.42	0.49
2:B:4:ILE:HG22	2:B:5:VAL:N	2.27	0.49
1:A:227:LEU:O	1:A:231:ILE:HG12	2.12	0.49
1:A:244:PHE:CD2	1:A:245:ASP:N	2.76	0.49
1:A:414:GLU:OE1	1:A:414:GLU:N	2.46	0.49
2:B:265:LEU:O	2:B:266:HIS:O	2.29	0.49
2:B:240:THR:HG23	2:B:241:CYS:H	1.76	0.49
2:B:336:GLN:HE22	2:B:349:ASN:ND2	2.10	0.49
2:B:265:LEU:HD12	2:B:266:HIS:O	2.12	0.49
1:A:16:ILE:HG23	1:A:17:GLY:N	2.26	0.49
1:A:188:ILE:O	1:A:191:THR:HG22	2.13	0.49
1:A:283:HIS:O	1:A:285:GLN:N	2.45	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
1:A:12:ALA:CB	1:A:140:SER:OG	2.59	0.49
1:A:392:ASP:O	1:A:395:PHE:HB3	2.13	0.49
1:A:192:HIS:CD2	1:A:424:ASP:OD2	2.66	0.49
1:A:203:MET:SD	1:A:267:PHE:HB3	2.53	0.49
2:B:142:GLY:HA3	2:B:183:GLU:OE2	2.13	0.49
2:B:199:ASP:O	2:B:200:GLU:HG3	2.13	0.49
2:B:387:LEU:HD23	2:B:388:PHE:CD2	2.47	0.49
2:B:431:GLU:OE1	2:B:432:TYR:N	2.46	0.49
2:B:308:ARG:HG3	2:B:342:TYR:OH	2.13	0.49
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.78	0.49
1:A:118:VAL:HG21	1:A:149:PHE:CE2	2.48	0.49
1:A:242:LEU:C	1:A:244:PHE:N	2.66	0.49
1:A:96:LYS:O	1:A:97:GLU:O	2.31	0.49
2:B:137:LEU:HD22	2:B:154:ILE:HG21	1.95	0.49
2:B:175:PRO:CD	2:B:207:GLU:OE1	2.61	0.49
1:A:172:TYR:CD1	1:A:173:PRO:N	2.80	0.48
2:B:191:VAL:HG13	2:B:192:HIS:N	2.28	0.48
2:B:176:LYS:CE	2:B:207:GLU:HG3	2.39	0.48
2:B:20:PHE:CG	2:B:235:MET:SD	3.07	0.48
2:B:237:GLY:O	2:B:241:CYS:CB	2.61	0.48
2:B:154:ILE:HG22	2:B:166:MET:HE1	1.96	0.48
2:B:176:LYS:HG3	2:B:177:VAL:H	1.78	0.48
2:B:209:LEU:O	2:B:213:CYS:N	2.47	0.48
2:B:8:GLN:HB3	2:B:14:ASN:HA	1.94	0.48
1:A:98:ASP:CB	1:A:105:ARG:HH21	2.14	0.48
1:A:115:ILE:O	1:A:116:ASP:C	2.51	0.48
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:CG1	1:A:270:ALA:HB1	2.38	0.48
1:A:286:LEU:CD1	1:A:290:GLU:HG2	2.44	0.48
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.94	0.48
1:A:158:SER:OG	1:A:197:HIS:HB3	2.13	0.48
1:A:274:PRO:CB	1:A:371:VAL:HG21	2.43	0.48
2:B:307:PRO:HB3	2:B:312:TYR:CZ	2.49	0.48
2:B:49:ILE:HG13	2:B:50:ASN:N	2.28	0.48
1:A:104:ALA:CB	1:A:408:TYR:HD2	2.26	0.48
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.48
1:A:163:LYS:C	1:A:164:LYS:HG2	2.33	0.48
1:A:344:VAL:HG12	1:A:345:ASP:H	1.74	0.48
2:B:154:ILE:HG22	2:B:166:MET:CE	2.44	0.48
2:B:211:ASP:OD1	2:B:212:ILE:HG13	2.13	0.48
1:A:151:SER:OG	1:A:193:THR:HG21	2.13	0.48
1:A:328:VAL:C	1:A:330:ALA:H	2.16	0.48
1:A:386:GLU:O	1:A:388:TRP:N	2.47	0.48
1:A:5:ILE:HG22	1:A:6:SER:H	1.78	0.48
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.28	0.48
2:B:69:ASP:HA	2:B:145:THR:HG21	1.95	0.48
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.48
1:A:317:LEU:CD1	1:A:351:PHE:CD2	2.97	0.48
2:B:2:ARG:NH1	2:B:251:ASP:OD2	2.46	0.48
1:A:110:ILE:CG2	1:A:111:GLY:N	2.71	0.47
1:A:335:ILE:O	1:A:337:THR:N	2.47	0.47
1:A:384:ILE:HG22	1:A:388:TRP:CD1	2.49	0.47
2:B:297:ASP:OD2	2:B:299:LYS:HE2	2.14	0.47
1:A:99:ALA:O	1:A:100:ALA:HB3	2.14	0.47
1:A:147:SER:O	1:A:190:THR:HG23	2.14	0.47
1:A:175:PRO:HD2	1:A:207:GLU:HB3	1.96	0.47
1:A:241:SER:HB3	1:A:320:ARG:NH2	2.29	0.47
1:A:369:ALA:O	1:A:370:LYS:CB	2.62	0.47
2:B:384:ILE:HG23	2:B:384:ILE:O	2.14	0.47
1:A:9:VAL:HG11	1:A:150:THR:OG1	2.13	0.47
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.49	0.47
1:A:210:TYR:CE2	1:A:227:LEU:HD21	2.49	0.47
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.95	0.47
1:A:97:GLU:HB2	1:A:110:ILE:HD11	1.96	0.47
1:A:191:THR:CG2	1:A:192:HIS:N	2.76	0.47
2:B:101:ASN:O	2:B:101:ASN:ND2	2.47	0.47
2:B:243:ARG:HD3	2:B:243:ARG:N	2.26	0.47
2:B:20:PHE:O	2:B:24:ILE:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:CE	1:A:199:ASP:OD1	2.62	0.47
1:A:217:LEU:CD1	1:A:277:SER:HA	2.44	0.47
1:A:339:ARG:C	1:A:341:ILE:N	2.68	0.47
1:A:396:ASP:O	1:A:397:LEU:C	2.53	0.47
1:A:6:SER:OG	1:A:65:ALA:HB2	2.14	0.47
1:A:148:GLY:O	1:A:151:SER:CB	2.61	0.47
1:A:119:LEU:HD11	1:A:156:ARG:HD2	1.97	0.47
1:A:260:VAL:O	1:A:260:VAL:CG2	2.63	0.47
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.79	0.47
2:B:115:VAL:CG2	2:B:152:LEU:HD23	2.44	0.47
1:A:132:LEU:HD21	1:A:164:LYS:HE3	1.96	0.47
1:A:226:ASN:O	1:A:229:ARG:N	2.48	0.47
1:A:253:THR:O	1:A:254:GLU:C	2.52	0.47
1:A:255:PHE:O	1:A:256:GLN:C	2.53	0.47
1:A:25:CYS:SG	1:A:83:TYR:HE2	2.38	0.47
1:A:345:ASP:C	1:A:347:CYS:N	2.68	0.47
1:A:99:ALA:H	2:B:2:ARG:HH22	1.63	0.47
2:B:175:PRO:O	2:B:176:LYS:C	2.52	0.47
2:B:387:LEU:O	2:B:387:LEU:HG	2.15	0.47
2:B:70:LEU:O	2:B:99:ALA:HB2	2.15	0.47
1:A:224:TYR:CG	2:B:325:MET:HG2	2.50	0.47
1:A:404:PHE:CD1	1:A:404:PHE:N	2.83	0.47
2:B:175:PRO:HD2	2:B:207:GLU:CD	2.35	0.47
2:B:287:THR:O	2:B:288:VAL:CG2	2.58	0.47
1:A:191:THR:O	1:A:195:LEU:HB2	2.15	0.47
1:A:407:TRP:O	1:A:411:GLU:CG	2.63	0.47
1:A:436:GLY:O	1:A:438:ASP:N	2.48	0.47
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.47
2:B:24:ILE:CD1	2:B:52:TYR:CE1	2.97	0.47
1:A:145:THR:O	1:A:149:PHE:HB3	2.15	0.47
1:A:278:ALA:HB2	1:A:369:ALA:CA	2.45	0.47
1:A:185:TYR:OH	1:A:399:TYR:HA	2.15	0.47
2:B:226:ASP:O	2:B:229:HIS:HB3	2.14	0.47
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.45	0.47
1:A:224:TYR:HD1	2:B:247:GLN:HB3	1.80	0.47
2:B:272:PHE:CE1	7:B:601:TA1:H391	2.50	0.47
2:B:230:LEU:HD21	2:B:302:MET:HE2	1.97	0.47
1:A:120:ASP:O	1:A:124:LYS:HB2	2.15	0.46
1:A:9:VAL:HG21	1:A:149:PHE:HD1	1.80	0.46
1:A:34:GLY:C	1:A:61:HIS:N	2.68	0.46
2:B:198:THR:HG23	2:B:200:GLU:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:THR:N	2:B:200:GLU:O	2.43	0.46
2:B:209:LEU:CD2	2:B:227:LEU:HD13	2.44	0.46
2:B:243:ARG:HH21	2:B:252:LEU:N	2.12	0.46
2:B:324:SER:OG	2:B:326:LYS:HB3	2.15	0.46
2:B:408:TYR:O	2:B:411:GLU:HB2	2.16	0.46
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.97	0.46
1:A:115:ILE:CG1	1:A:152:LEU:HD13	2.46	0.46
1:A:256:GLN:O	1:A:260:VAL:HG13	2.15	0.46
1:A:384:ILE:HG22	1:A:384:ILE:O	2.15	0.46
2:B:134:GLY:HA3	2:B:165:ILE:HG12	1.97	0.46
1:A:107:HIS:CE1	1:A:152:LEU:HB3	2.49	0.46
1:A:19:ALA:HB2	1:A:228:ASN:HB3	1.96	0.46
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.97	0.46
1:A:286:LEU:HG	1:A:290:GLU:HB2	1.98	0.46
1:A:402:ARG:O	1:A:405:VAL:N	2.49	0.46
2:B:242:LEU:HD11	2:B:250:ALA:HB3	1.97	0.46
1:A:154:MET:HA	1:A:157:LEU:HD12	1.96	0.46
1:A:234:ILE:HB	1:A:302:MET:HE1	1.96	0.46
1:A:317:LEU:CD1	1:A:351:PHE:CE2	2.99	0.46
1:A:95:GLY:C	1:A:97:GLU:N	2.69	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
2:B:250:ALA:HB1	2:B:254:LYS:CB	2.44	0.46
2:B:263:PRO:O	2:B:264:ARG:C	2.52	0.46
2:B:360:PRO:O	2:B:369:ARG:C	2.54	0.46
1:A:241:SER:C	1:A:244:PHE:HB3	2.36	0.46
1:A:381:THR:O	1:A:383:ALA:N	2.49	0.46
2:B:204:ILE:HD13	2:B:231:VAL:CG2	2.45	0.46
2:B:208:ALA:O	2:B:212:ILE:HG13	2.16	0.46
2:B:287:THR:N	2:B:290:GLU:OE1	2.48	0.46
1:A:392:ASP:OD2	1:A:422:ARG:NE	2.48	0.46
1:A:11:GLN:NE2	1:A:74:VAL:HG22	2.30	0.46
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.31	0.46
2:B:103:TRP:HZ3	2:B:108:TYR:CE1	2.27	0.46
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.46
1:A:243:ARG:NH2	1:A:252:LEU:CB	2.78	0.46
1:A:265:GLY:O	1:A:266:HIS:O	2.33	0.46
2:B:296:PHE:HZ	2:B:315:VAL:HG11	1.78	0.46
1:A:408:TYR:CG	1:A:418:PHE:HZ	2.34	0.46
2:B:113:GLU:CG	2:B:114:LEU:N	2.79	0.46
2:B:185:TYR:HD2	2:B:395:PHE:CE1	2.33	0.46
1:A:114:ILE:O	1:A:118:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:HG12	1:A:326:LYS:H	1.81	0.46
2:B:224:TYR:O	2:B:225:GLY:C	2.53	0.46
1:A:243:ARG:NH2	1:A:252:LEU:HB2	2.31	0.46
1:A:286:LEU:O	1:A:287:SER:O	2.34	0.46
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.30	0.45
1:A:210:TYR:CD2	1:A:227:LEU:HD21	2.51	0.45
1:A:276:ILE:HG12	1:A:277:SER:N	2.32	0.45
1:A:274:PRO:HB2	1:A:371:VAL:HG21	1.98	0.45
2:B:209:LEU:HD23	2:B:227:LEU:HD13	1.98	0.45
2:B:313:LEU:O	2:B:347:ILE:HD12	2.16	0.45
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.98	0.45
1:A:334:THR:CG2	1:A:335:ILE:N	2.79	0.45
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.81	0.45
2:B:307:PRO:C	2:B:309:HIS:H	2.18	0.45
1:A:180:ALA:HA	2:B:352:LYS:NZ	2.31	0.45
2:B:6:HIS:HB3	2:B:21:TRP:HZ2	1.81	0.45
1:A:117:LEU:HD12	1:A:121:ARG:HH12	1.80	0.45
1:A:210:TYR:CZ	1:A:227:LEU:HD11	2.51	0.45
1:A:229:ARG:HG2	1:A:229:ARG:NH1	2.31	0.45
1:A:22:GLU:O	1:A:23:LEU:C	2.54	0.45
1:A:5:ILE:CG2	1:A:6:SER:H	2.29	0.45
2:B:11:GLN:O	2:B:14:ASN:HB3	2.16	0.45
2:B:106:GLY:O	2:B:149:MET:HB2	2.16	0.45
2:B:264:ARG:HA	2:B:264:ARG:NE	2.29	0.45
2:B:94:PHE:CD2	2:B:94:PHE:N	2.84	0.45
1:A:203:MET:SD	1:A:267:PHE:CB	3.04	0.45
1:A:392:ASP:OD2	1:A:422:ARG:CZ	2.65	0.45
2:B:257:VAL:O	2:B:257:VAL:CG1	2.64	0.45
2:B:409:THR:HA	2:B:413:MET:HB3	1.99	0.45
1:A:212:ILE:HD11	1:A:302:MET:H	1.82	0.45
1:A:278:ALA:O	1:A:279:GLU:HG2	2.15	0.45
1:A:308:ARG:O	1:A:309:HIS:HB3	2.17	0.45
1:A:413:MET:C	1:A:414:GLU:HG3	2.36	0.45
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.98	0.45
2:B:133:GLN:O	2:B:165:ILE:CD1	2.64	0.45
2:B:210:TYR:CE2	2:B:227:LEU:HD11	2.51	0.45
2:B:194:LEU:O	2:B:265:LEU:HD23	2.16	0.45
2:B:413:MET:HG3	2:B:414:ASP:N	2.22	0.45
2:B:67:LEU:HD12	2:B:92:PHE:CD2	2.51	0.45
1:A:286:LEU:O	1:A:287:SER:C	2.55	0.45
2:B:135:PHE:CD1	2:B:135:PHE:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HD12	2:B:155:SER:N	2.31	0.45
2:B:273:ALA:CB	2:B:274:PRO:CD	2.93	0.45
2:B:324:SER:O	2:B:326:LYS:N	2.50	0.45
2:B:323:MET:CE	2:B:328:VAL:HG22	2.46	0.45
1:A:115:ILE:HG23	1:A:116:ASP:H	1.79	0.45
1:A:434:GLU:C	1:A:436:GLY:H	2.18	0.45
2:B:409:THR:O	2:B:412:GLY:N	2.48	0.45
2:B:35:SER:CB	2:B:59:ASN:HA	2.42	0.45
7:B:601:TA1:C26	7:B:601:TA1:H463	2.46	0.45
1:A:328:VAL:O	1:A:330:ALA:N	2.38	0.45
1:A:423:GLU:O	1:A:426:ALA:HB3	2.16	0.45
1:A:7:ILE:HD11	1:A:137:VAL:CG2	2.44	0.45
2:B:23:VAL:O	2:B:25:SER:N	2.50	0.45
2:B:102:ASN:ND2	2:B:408:TYR:HA	2.20	0.45
2:B:72:PRO:O	2:B:74:THR:N	2.50	0.45
1:A:148:GLY:O	1:A:149:PHE:C	2.55	0.45
1:A:182:VAL:O	1:A:184:PRO:CD	2.65	0.45
1:A:255:PHE:O	1:A:259:LEU:N	2.50	0.45
2:B:137:LEU:HD22	2:B:154:ILE:HG23	1.98	0.45
2:B:14:ASN:O	2:B:17:GLY:N	2.50	0.45
2:B:196:GLU:O	2:B:197:ASN:OD1	2.34	0.45
2:B:242:LEU:HD22	2:B:250:ALA:O	2.17	0.45
2:B:24:ILE:CG2	2:B:25:SER:N	2.80	0.45
2:B:82:PRO:C	2:B:84:GLY:H	2.20	0.45
1:A:278:ALA:CA	1:A:282:TYR:OH	2.65	0.45
1:A:288:VAL:HA	1:A:291:ILE:HG12	1.98	0.45
1:A:303:VAL:CG1	1:A:303:VAL:O	2.65	0.45
1:A:4:CYS:SG	1:A:252:LEU:CD1	3.02	0.45
2:B:167:ASN:HA	2:B:200:GLU:O	2.17	0.45
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.52	0.45
1:A:10:GLY:O	1:A:11:GLN:C	2.53	0.44
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.98	0.44
1:A:196:GLU:C	1:A:197:HIS:HD2	2.19	0.44
1:A:316:CYS:HB3	1:A:378:LEU:HD12	1.95	0.44
2:B:4:ILE:HD12	2:B:239:THR:HG21	1.98	0.44
2:B:8:GLN:CG	2:B:67:LEU:HD22	2.47	0.44
1:A:11:GLN:HE21	1:A:74:VAL:CG2	2.29	0.44
1:A:295:CYS:HB3	1:A:377:MET:HG2	1.99	0.44
2:B:288:VAL:N	2:B:289:PRO:CD	2.80	0.44
1:A:280:LYS:HB3	1:A:281:ALA:H	1.49	0.44
2:B:175:PRO:HG2	2:B:207:GLU:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:TYR:HE1	2:B:240:THR:HB	1.82	0.44
2:B:288:VAL:N	2:B:289:PRO:HD2	2.32	0.44
2:B:295:MET:SD	2:B:375:ALA:HB3	2.57	0.44
2:B:189:LEU:HD23	2:B:421:ALA:CB	2.47	0.44
2:B:194:LEU:C	2:B:196:GLU:N	2.70	0.44
1:A:101:ASN:ND2	2:B:254:LYS:CD	2.75	0.44
1:A:105:ARG:O	1:A:110:ILE:CG2	2.64	0.44
1:A:8:HIS:HA	1:A:138:PHE:HB2	2.00	0.44
1:A:204:VAL:O	1:A:204:VAL:HG12	2.17	0.44
1:A:288:VAL:C	1:A:290:GLU:N	2.71	0.44
1:A:287:SER:N	1:A:290:GLU:OE1	2.51	0.44
2:B:212:ILE:O	2:B:212:ILE:HG22	2.18	0.44
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.83	0.44
1:A:218:ASP:C	1:A:219:ILE:HG12	2.37	0.44
1:A:363:VAL:CG1	1:A:364:PRO:HD2	2.48	0.44
1:A:271:THR:O	1:A:376:CYS:HA	2.17	0.44
2:B:167:ASN:HD21	2:B:252:LEU:HD22	1.82	0.44
2:B:312:TYR:HA	2:B:381:SER:HA	1.99	0.44
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.52	0.44
1:A:12:ALA:HB2	5:A:500:GTP:C8	2.52	0.44
1:A:152:LEU:HD12	1:A:152:LEU:C	2.38	0.44
1:A:23:LEU:CD2	1:A:232:GLY:O	2.64	0.44
1:A:23:LEU:O	1:A:26:LEU:HB3	2.17	0.44
2:B:239:THR:O	2:B:240:THR:C	2.56	0.44
2:B:280:SER:OG	2:B:281:GLN:N	2.49	0.44
1:A:343:PHE:HZ	1:A:351:PHE:CZ	2.36	0.44
1:A:377:MET:O	1:A:377:MET:HG3	2.18	0.44
1:A:72:PRO:HG2	1:A:73:THR:H	1.83	0.44
2:B:102:ASN:OD1	2:B:408:TYR:CZ	2.70	0.44
2:B:161:TYR:O	2:B:163:ASP:N	2.51	0.44
2:B:168:THR:CG2	2:B:201:THR:HG23	2.48	0.44
2:B:242:LEU:C	2:B:244:PHE:H	2.19	0.44
1:A:153:LEU:O	1:A:157:LEU:HG	2.18	0.44
1:A:263:PRO:O	1:A:264:ARG:C	2.56	0.44
1:A:121:ARG:NH1	1:A:121:ARG:HG2	2.33	0.43
1:A:343:PHE:CE1	1:A:351:PHE:HE1	2.36	0.43
1:A:154:MET:CE	1:A:166:LYS:HB3	2.48	0.43
1:A:122:ILE:CD1	1:A:157:LEU:HD21	2.35	0.43
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.47	0.43
1:A:362:VAL:HG13	1:A:368:LEU:CG	2.48	0.43
1:A:268:PRO:CA	1:A:379:SER:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HB1	1:A:413:MET:HG3	1.95	0.43
2:B:240:THR:HG23	2:B:241:CYS:N	2.33	0.43
2:B:307:PRO:C	2:B:309:HIS:N	2.71	0.43
2:B:431:GLU:O	2:B:434:GLN:N	2.48	0.43
1:A:231:ILE:H	1:A:231:ILE:HD13	1.82	0.43
1:A:304:LYS:HG3	1:A:304:LYS:O	2.19	0.43
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.81	0.43
1:A:63:PRO:HG2	1:A:91:GLN:OE1	2.18	0.43
2:B:26:ASP:C	2:B:28:HIS:H	2.21	0.43
2:B:282:GLN:HB3	2:B:282:GLN:HE21	1.51	0.43
1:A:390:ARG:HG3	1:A:390:ARG:HH11	1.83	0.43
2:B:187:ALA:O	2:B:188:THR:C	2.57	0.43
1:A:149:PHE:O	1:A:150:THR:C	2.56	0.43
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.99	0.43
1:A:310:GLY:HA3	1:A:383:ALA:CA	2.49	0.43
1:A:436:GLY:C	1:A:438:ASP:N	2.72	0.43
1:A:63:PRO:C	1:A:64:ARG:CG	2.83	0.43
2:B:7:ILE:N	2:B:136:GLN:O	2.51	0.43
2:B:141:LEU:N	2:B:141:LEU:HD12	2.32	0.43
2:B:310:GLY:HA3	2:B:436:GLN:NE2	2.29	0.43
1:A:21:TRP:HE1	1:A:63:PRO:HB3	1.83	0.43
1:A:252:LEU:O	1:A:253:THR:C	2.56	0.43
1:A:262:TYR:HB3	1:A:263:PRO:HD2	2.00	0.43
1:A:344:VAL:CG1	1:A:345:ASP:N	2.78	0.43
1:A:104:ALA:HB3	1:A:408:TYR:HD2	1.84	0.43
1:A:409:VAL:C	1:A:411:GLU:N	2.71	0.43
2:B:105:LYS:HG2	2:B:110:GLU:CG	2.48	0.43
2:B:288:VAL:C	2:B:290:GLU:N	2.70	0.43
2:B:383:ALA:C	2:B:385:GLN:N	2.72	0.43
1:A:144:GLY:H	5:A:500:GTP:PG	2.41	0.43
1:A:13:GLY:C	1:A:16:ILE:HG22	2.38	0.43
1:A:378:LEU:O	1:A:378:LEU:HD12	2.19	0.43
2:B:153:LEU:HD13	2:B:153:LEU:N	2.34	0.43
1:A:103:TYR:O	1:A:104:ALA:C	2.57	0.43
1:A:230:LEU:O	1:A:231:ILE:C	2.57	0.43
1:A:25:CYS:SG	1:A:26:LEU:N	2.92	0.43
2:B:242:LEU:HA	2:B:242:LEU:HD23	1.76	0.43
2:B:269:MET:HE1	2:B:381:SER:OG	2.19	0.43
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.93	0.43
2:B:192:HIS:NE2	2:B:420:GLU:HG2	2.34	0.43
1:A:238:ILE:O	1:A:242:LEU:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HD11	1:A:378:LEU:HD23	2.01	0.43
1:A:76:ASP:O	1:A:79:ARG:N	2.52	0.43
1:A:8:HIS:CD2	1:A:138:PHE:CD1	3.07	0.43
2:B:210:TYR:O	2:B:211:ASP:C	2.57	0.43
2:B:409:THR:C	2:B:411:GLU:H	2.22	0.43
1:A:209:ILE:CD1	1:A:231:ILE:CD1	2.97	0.42
1:A:283:HIS:ND1	1:A:283:HIS:O	2.49	0.42
2:B:12:CYS:C	2:B:14:ASN:N	2.71	0.42
2:B:48:ARG:HG2	2:B:243:ARG:HB3	2.01	0.42
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.42
2:B:301:MET:O	2:B:303:ALA:N	2.51	0.42
2:B:6:HIS:HB3	2:B:65:ALA:CB	2.48	0.42
1:A:115:ILE:CG2	1:A:116:ASP:H	2.32	0.42
1:A:15:GLN:NE2	5:A:500:GTP:N7	2.67	0.42
1:A:272:TYR:CE2	1:A:274:PRO:HD2	2.53	0.42
2:B:161:TYR:N	2:B:161:TYR:CD1	2.86	0.42
2:B:182:VAL:O	2:B:183:GLU:C	2.56	0.42
2:B:282:GLN:O	2:B:282:GLN:CG	2.65	0.42
2:B:435:TYR:C	2:B:437:ASP:N	2.72	0.42
2:B:70:LEU:HB2	2:B:99:ALA:CB	2.48	0.42
2:B:360:PRO:HG2	2:B:371:LEU:CB	2.38	0.42
2:B:301:MET:HE1	2:B:377:PHE:HE2	1.84	0.42
2:B:114:LEU:HD23	2:B:149:MET:HE2	2.00	0.42
2:B:138:THR:O	2:B:139:HIS:HB3	2.20	0.42
1:A:251:ASP:CA	1:A:254:GLU:HG3	2.49	0.42
1:A:363:VAL:HG13	1:A:364:PRO:HD2	2.02	0.42
2:B:106:GLY:O	2:B:149:MET:CA	2.68	0.42
2:B:98:GLY:O	2:B:100:GLY:N	2.49	0.42
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.42
2:B:333:LEU:O	2:B:334:ASN:C	2.58	0.42
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.50	0.42
1:A:328:VAL:C	1:A:330:ALA:N	2.73	0.42
2:B:250:ALA:CB	2:B:254:LYS:HE2	2.49	0.42
2:B:72:PRO:HG2	2:B:73:GLY:H	1.83	0.42
1:A:166:LYS:HB2	1:A:199:ASP:OD1	2.20	0.42
2:B:103:TRP:HB2	2:B:186:ASN:HA	2.01	0.42
2:B:273:ALA:HB1	2:B:291:LEU:HG	2.01	0.42
1:A:147:SER:HB2	1:A:186:ASN:O	2.19	0.42
1:A:305:CYS:SG	1:A:383:ALA:HB1	2.60	0.42
2:B:171:VAL:O	2:B:171:VAL:HG12	2.20	0.42
2:B:2:ARG:NH1	2:B:251:ASP:CG	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:VAL:HG11	2:B:153:LEU:HD21	2.00	0.42
2:B:72:PRO:O	2:B:73:GLY:C	2.58	0.42
1:A:204:VAL:CG1	1:A:231:ILE:HD12	2.42	0.42
1:A:67:PHE:HB2	1:A:92:LEU:HD23	2.02	0.42
2:B:343:PHE:CD2	2:B:350:ASN:ND2	2.88	0.42
2:B:118:VAL:O	2:B:122:VAL:HG13	2.19	0.41
2:B:199:ASP:C	2:B:265:LEU:HD13	2.40	0.41
2:B:307:PRO:O	2:B:309:HIS:N	2.53	0.41
2:B:409:THR:C	2:B:411:GLU:N	2.73	0.41
1:A:289:ALA:HB3	1:A:290:GLU:OE2	2.21	0.41
2:B:311:ARG:NH1	2:B:311:ARG:HG2	2.34	0.41
2:B:274:PRO:HD3	2:B:374:SER:HA	2.03	0.41
2:B:75:MET:HE1	2:B:94:PHE:HB3	2.02	0.41
1:A:115:ILE:C	1:A:115:ILE:CD1	2.87	0.41
1:A:255:PHE:O	1:A:257:THR:N	2.53	0.41
1:A:398:MET:HB2	1:A:398:MET:HE3	1.91	0.41
1:A:144:GLY:N	5:A:500:GTP:O3G	2.48	0.41
2:B:264:ARG:O	2:B:265:LEU:CB	2.53	0.41
2:B:421:ALA:O	2:B:422:GLU:C	2.58	0.41
1:A:210:TYR:OH	2:B:325:MET:HB3	2.20	0.41
1:A:243:ARG:NH2	1:A:252:LEU:HG	2.35	0.41
2:B:165:ILE:CD1	2:B:165:ILE:H	2.31	0.41
2:B:262:PHE:HA	2:B:263:PRO:HD2	1.65	0.41
2:B:288:VAL:HG22	2:B:323:MET:HE3	2.01	0.41
1:A:76:ASP:O	1:A:80:THR:N	2.53	0.41
2:B:333:LEU:HD11	2:B:337:ASN:HD21	1.85	0.41
1:A:152:LEU:CD1	1:A:152:LEU:C	2.89	0.41
1:A:213:CYS:O	1:A:219:ILE:HG13	2.20	0.41
1:A:273:ALA:HB2	1:A:375:VAL:HB	2.03	0.41
2:B:202:TYR:CE2	2:B:268:PHE:HD1	2.38	0.41
2:B:20:PHE:CD2	2:B:235:MET:CG	3.04	0.41
2:B:276:THR:O	7:B:601:TA1:H192	2.21	0.41
1:A:101:ASN:HD21	2:B:254:LYS:NZ	2.18	0.41
1:A:110:ILE:O	1:A:111:GLY:C	2.57	0.41
1:A:175:PRO:HG3	1:A:304:LYS:CB	2.50	0.41
1:A:179:THR:HG22	2:B:352:LYS:HZ2	1.86	0.41
1:A:204:VAL:CG1	1:A:209:ILE:HD11	2.42	0.41
1:A:231:ILE:C	1:A:233:GLN:N	2.73	0.41
1:A:335:ILE:C	1:A:337:THR:N	2.73	0.41
1:A:414:GLU:C	1:A:416:GLY:N	2.74	0.41
2:B:168:THR:O	2:B:202:TYR:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:PRO:O	2:B:177:VAL:N	2.53	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HD3	2.01	0.41
1:A:434:GLU:C	1:A:436:GLY:N	2.74	0.41
2:B:105:LYS:HG2	2:B:110:GLU:HG3	2.03	0.41
2:B:25:SER:O	2:B:28:HIS:N	2.53	0.41
2:B:399:PHE:O	2:B:401:ARG:N	2.53	0.41
2:B:417:GLU:O	2:B:420:GLU:HB3	2.21	0.41
1:A:130:THR:O	1:A:131:GLY:C	2.59	0.41
1:A:132:LEU:CD2	1:A:132:LEU:H	2.23	0.41
1:A:332:ILE:CD1	1:A:353:VAL:HG22	2.51	0.41
2:B:139:HIS:HE1	2:B:168:THR:CG2	2.34	0.41
2:B:161:TYR:C	2:B:163:ASP:N	2.71	0.41
2:B:168:THR:HB	2:B:198:THR:HG21	2.03	0.41
2:B:242:LEU:HB3	2:B:250:ALA:O	2.20	0.41
2:B:274:PRO:HG2	2:B:371:LEU:CD2	2.43	0.41
1:A:30:ILE:HG22	1:A:30:ILE:O	2.21	0.41
1:A:23:LEU:HD11	1:A:361:THR:O	2.21	0.41
1:A:413:MET:C	1:A:414:GLU:CG	2.90	0.41
2:B:147:SER:HB2	2:B:190:SER:CB	2.41	0.41
2:B:135:PHE:CD1	2:B:166:MET:SD	3.14	0.41
2:B:210:TYR:O	2:B:214:PHE:N	2.52	0.41
1:A:100:ALA:HB2	1:A:105:ARG:HD3	2.02	0.41
1:A:199:ASP:CB	1:A:256:GLN:NE2	2.77	0.41
2:B:238:VAL:HB	2:B:239:THR:H	1.65	0.41
1:A:181:VAL:HG23	2:B:258:ASN:HB3	2.03	0.41
2:B:291:LEU:HD21	2:B:373:MET:HG2	2.03	0.41
2:B:78:VAL:O	2:B:84:GLY:HA3	2.22	0.41
1:A:401:LYS:C	1:A:403:ALA:H	2.24	0.40
1:A:425:MET:O	1:A:428:LEU:N	2.45	0.40
2:B:125:GLU:O	2:B:128:SER:HB3	2.22	0.40
2:B:132:LEU:O	2:B:164:ARG:HD2	2.21	0.40
2:B:380:ASN:C	2:B:380:ASN:HD22	2.24	0.40
2:B:427:ASP:OD1	2:B:427:ASP:C	2.58	0.40
1:A:149:PHE:CD1	1:A:150:THR:N	2.89	0.40
1:A:272:TYR:O	1:A:300:ASN:ND2	2.54	0.40
1:A:95:GLY:C	1:A:97:GLU:H	2.23	0.40
2:B:188:THR:O	2:B:191:VAL:HG12	2.21	0.40
2:B:19:LYS:HG3	2:B:228:ASN:HB2	2.01	0.40
2:B:422:GLU:O	2:B:426:ASN:CB	2.67	0.40
1:A:179:THR:HG21	2:B:248:LEU:HD22	2.04	0.40
1:A:286:LEU:HG	1:A:290:GLU:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:PRO:HB2	2:B:360:PRO:CD	2.49	0.40
1:A:207:GLU:O	1:A:210:TYR:N	2.51	0.40
1:A:234:ILE:C	1:A:234:ILE:CD1	2.86	0.40
1:A:318:LEU:HB2	1:A:376:CYS:SG	2.61	0.40
2:B:118:VAL:O	2:B:121:VAL:N	2.54	0.40
2:B:204:ILE:HG23	2:B:209:LEU:HD11	2.03	0.40
1:A:393:HIS:O	1:A:394:LYS:C	2.60	0.40
2:B:12:CYS:O	2:B:14:ASN:N	2.55	0.40
2:B:268:PHE:HA	2:B:379:GLY:O	2.22	0.40
2:B:405:LEU:O	2:B:405:LEU:HD23	2.21	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	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	4
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	5
All	All	832/896 (93%)	539 (65%)	178 (21%)	115 (14%)	0	4

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	97	GLU
1	A	108	TYR
1	A	109	THR
1	A	141	PHE
1	A	183	GLU
1	A	217	LEU
1	A	240	ALA

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	255	PHE
1	A	266	HIS
1	A	280	LYS
1	A	284	GLU
1	A	285	GLN
1	A	289	ALA
1	A	309	HIS
1	A	346	TRP
1	A	370	LYS
1	A	387	ALA
1	A	403	ALA
1	A	437	VAL
2	B	23	VAL
2	B	24	ILE
2	B	32	PRO
2	B	50	ASN
2	B	82	PRO
2	B	97	SER
2	B	128	SER
2	B	176	LYS
2	B	183	GLU
2	B	218	LYS
2	B	238	VAL
2	B	239	THR
2	B	240	THR
2	B	252	LEU
2	B	263	PRO
2	B	266	HIS
2	B	273	ALA
2	B	278	ARG
2	B	280	SER
2	B	281	GLN
2	B	282	GLN
2	B	288	VAL
2	B	294	GLN
2	B	295	MET
2	B	343	PHE
2	B	344	VAL
2	B	346	TRP
2	B	369	ARG
2	B	403	ALA

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Mol	Chain	Res	Type
1	A	24	TYR
1	A	63	PRO
1	A	103	TYR
1	A	111	GLY
1	A	131	GLY
1	A	218	ASP
1	A	219	ILE
1	A	238	ILE
1	A	265	GLY
1	A	287	SER
1	A	314	ALA
1	A	339	ARG
1	A	342	GLN
1	A	373	ARG
1	A	386	GLU
2	B	38	GLY
2	B	73	GLY
2	B	175	PRO
2	B	265	LEU
2	B	279	GLY
2	B	298	ALA
2	B	300	ASN
2	B	311	ARG
1	A	104	ALA
1	A	148	GLY
1	A	149	PHE
1	A	173	PRO
1	A	239	THR
1	A	245	ASP
1	A	263	PRO
1	A	279	GLU
1	A	288	VAL
1	A	330	ALA
1	A	336	LYS
1	A	369	ALA
2	B	83	PHE
2	B	99	ALA
2	B	100	GLY
2	B	302	MET
2	B	386	GLU
1	A	89	PRO
1	A	129	CYS

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Mol	Chain	Res	Type
1	A	300	ASN
1	A	348	PRO
2	B	34	GLY
2	B	96	GLN
2	B	395	PHE
1	A	256	GLN
1	A	303	VAL
1	A	307	PRO
1	A	382	THR
2	B	57	ALA
2	B	74	THR
2	B	285	ALA
1	A	31	GLN
1	A	273	ALA
2	B	51	VAL
2	B	58	GLY
2	B	145	THR
2	B	162	PRO
2	B	400	ARG
2	B	424	ASN
2	B	195	VAL
1	A	115	ILE
2	B	72	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/377 (92%)	298 (86%)	49 (14%)	4	24
2	B	367/381 (96%)	307 (84%)	60 (16%)	3	17
All	All	714/758 (94%)	605 (85%)	109 (15%)	3	21

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	20	CYS
1	A	21	TRP
1	A	32	PRO
1	A	76	ASP
1	A	82	THR
1	A	98	ASP
1	A	115	ILE
1	A	120	ASP
1	A	125	LEU
1	A	127	ASP
1	A	130	THR
1	A	135	PHE
1	A	141	PHE
1	A	150	THR
1	A	152	LEU
1	A	155	GLU
1	A	169	PHE
1	A	172	TYR
1	A	173	PRO
1	A	183	GLU
1	A	192	HIS
1	A	204	VAL
1	A	219	ILE
1	A	224	TYR
1	A	231	ILE
1	A	234	ILE
1	A	243	ARG
1	A	244	PHE
1	A	253	THR
1	A	260	VAL
1	A	267	PHE
1	A	269	LEU
1	A	276	ILE
1	A	284	GLU
1	A	303	VAL
1	A	325	PRO
1	A	334	THR
1	A	345	ASP
1	A	352	LYS
1	A	368	LEU
1	A	376	CYS
1	A	378	LEU

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Mol	Chain	Res	Type
1	A	380	ASN
1	A	404	PHE
1	A	415	GLU
1	A	417	GLU
1	A	431	ASP
1	A	432	TYR
2	B	14	ASN
2	B	24	ILE
2	B	26	ASP
2	B	32	PRO
2	B	41	ASP
2	B	68	VAL
2	B	76	ASP
2	B	90	ASP
2	B	94	PHE
2	B	101	ASN
2	B	122	VAL
2	B	129	CYS
2	B	135	PHE
2	B	141	LEU
2	B	145	THR
2	B	149	MET
2	B	153	LEU
2	B	161	TYR
2	B	163	ASP
2	B	165	ILE
2	B	174	SER
2	B	198	THR
2	B	201	THR
2	B	203	CYS
2	B	207	GLU
2	B	211	ASP
2	B	214	PHE
2	B	215	ARG
2	B	224	TYR
2	B	227	LEU
2	B	230	LEU
2	B	236	SER
2	B	240	THR
2	B	244	PHE
2	B	265	LEU
2	B	267	PHE

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Mol	Chain	Res	Type
2	B	275	LEU
2	B	282	GLN
2	B	283	TYR
2	B	284	ARG
2	B	289	PRO
2	B	299	LYS
2	B	306	ASP
2	B	309	HIS
2	B	322	ARG
2	B	324	SER
2	B	325	MET
2	B	343	PHE
2	B	344	VAL
2	B	349	ASN
2	B	369	ARG
2	B	380	ASN
2	B	387	LEU
2	B	413	MET
2	B	414	ASP
2	B	424	ASN
2	B	427	ASP
2	B	431	GLU
2	B	432	TYR
2	B	437	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	28	HIS
1	A	128	GLN
1	A	133	GLN
1	A	139	HIS
1	A	197	HIS
1	A	216	ASN
1	A	226	ASN
1	A	256	GLN
1	A	309	HIS
1	A	380	ASN
2	B	14	ASN
2	B	91	ASN

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Mol	Chain	Res	Type
2	B	101	ASN
2	B	102	ASN
2	B	107	HIS
2	B	136	GLN
2	B	139	HIS
2	B	197	ASN
2	B	282	GLN
2	B	331	GLN
2	B	334	ASN
2	B	337	ASN
2	B	349	ASN
2	B	380	ASN
2	B	406	HIS
2	B	436	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
5	GTP	A	500	4	26,34,34	1.35	1 (3%)	29,54,54	2.29	4 (13%)
6	GDP	B	600	-	24,30,30	2.65	8 (33%)	26,47,47	3.29	8 (30%)
7	TA1	B	601	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	500	4	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
7	TA1	B	601	-	-	0/41/127/127	0/5/7/7

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	TA1	C08-C07	-4.95	1.25	1.38
6	B	600	GDP	PB-O2B	-4.19	1.40	1.54
7	B	601	TA1	C04-C03	-2.32	1.44	1.49
7	B	601	TA1	C10-C02	2.03	1.62	1.57
7	B	601	TA1	C41-C42	2.04	1.42	1.38
7	B	601	TA1	C18-C20	2.06	1.62	1.56
6	B	600	GDP	O3'-C3'	2.08	1.47	1.43
7	B	601	TA1	C37-C29	2.13	1.54	1.51
7	B	601	TA1	C01-C45	2.14	1.66	1.56
7	B	601	TA1	C11-C10	2.14	1.61	1.55
7	B	601	TA1	C16-C15	2.19	1.56	1.52
7	B	601	TA1	C26-C25	2.42	1.56	1.51
6	B	600	GDP	C5-C4	2.42	1.46	1.40
7	B	601	TA1	C43-C26	2.43	1.58	1.52
6	B	600	GDP	PB-O3B	2.65	1.63	1.54
7	B	601	TA1	C43-C01	2.85	1.60	1.54
7	B	601	TA1	C46-C45	2.94	1.60	1.53
7	B	601	TA1	C25-C24	3.00	1.39	1.34
6	B	600	GDP	C8-N7	3.31	1.41	1.34
7	B	601	TA1	O02-C03	3.38	1.41	1.34
7	B	601	TA1	C45-C24	3.39	1.61	1.54
7	B	601	TA1	C36-C31	3.53	1.45	1.39
6	B	600	GDP	O6-C6	4.06	1.34	1.24
7	B	601	TA1	C18-C10	4.17	1.69	1.57
7	B	601	TA1	C05-C04	4.55	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	GTP	C6-N1	4.82	1.41	1.33
7	B	601	TA1	C06-C05	5.71	1.50	1.38
6	B	600	GDP	O4'-C1'	5.99	1.49	1.41
6	B	600	GDP	C2-N1	7.31	1.49	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	C6-C5-C4	-9.93	109.52	120.86
5	A	500	GTP	C5-C6-N1	-7.78	113.35	123.52
6	B	600	GDP	N2-C2-N1	-5.70	107.80	117.20
6	B	600	GDP	N3-C2-N1	-5.37	120.25	127.56
7	B	601	TA1	C06-C05-C04	-4.81	114.61	120.35
7	B	601	TA1	C05-C04-C03	-3.96	111.46	120.38
5	A	500	GTP	N3-C2-N1	-3.51	122.78	127.56
6	B	600	GDP	C1'-N9-C4	-2.67	123.83	126.81
7	B	601	TA1	O04-C11-C14	-2.49	101.75	108.08
5	A	500	GTP	C6-C5-C4	-2.12	118.44	120.86
6	B	600	GDP	O2'-C2'-C3'	2.26	119.16	111.86
7	B	601	TA1	O01-C01-C43	2.51	113.39	106.82
7	B	601	TA1	C17-C18-C20	2.56	109.82	102.14
7	B	601	TA1	C45-C01-C02	3.08	115.20	111.64
6	B	600	GDP	C2'-C3'-C4'	3.22	109.23	102.64
7	B	601	TA1	C09-C04-C03	3.55	128.37	120.38
6	B	600	GDP	C4'-O4'-C1'	4.15	114.04	109.64
7	B	601	TA1	C07-C08-C09	5.14	127.35	120.20
5	A	500	GTP	C6-N1-C2	7.51	124.68	115.88
6	B	600	GDP	N2-C2-N3	7.58	131.94	117.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	GTP	5	0
6	B	600	GDP	1	0
7	B	601	TA1	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.