



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:22 am GMT

PDB ID : 3EDL
EMDB ID: : EMD-5027
Title : Kinesin13-Microtubule Ring complex
Authors : Tan, D.; Rice, W.J.; Sosa, H.
Deposited on : 2008-09-03
Resolution : 28.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

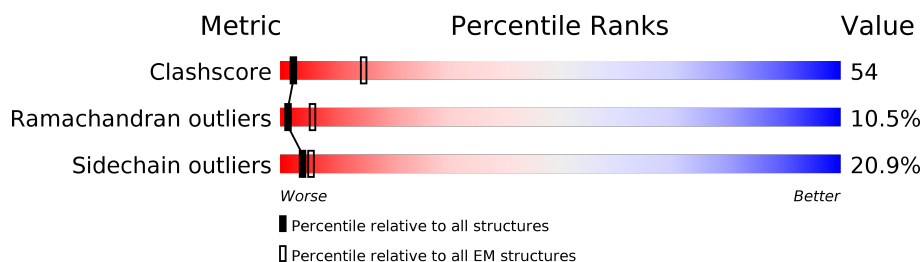
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 28.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	451	
2	B	445	
2	G	445	
3	D	331	
4	F	451	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Alpha-tubulin.

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

- Molecule 2 is a protein called Beta tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
2	G	419	Total	C	N	O	S	0	0
			3237	2037	544	631	25		

- Molecule 3 is a protein called Kinesin13 Motor domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	301	Total	C	N	O	S	0	0
			2368	1496	416	438	18		

- Molecule 4 is a protein called Alpha-tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	421	Total	C	N	O	S	0	0
			3220	2043	544	612	21		

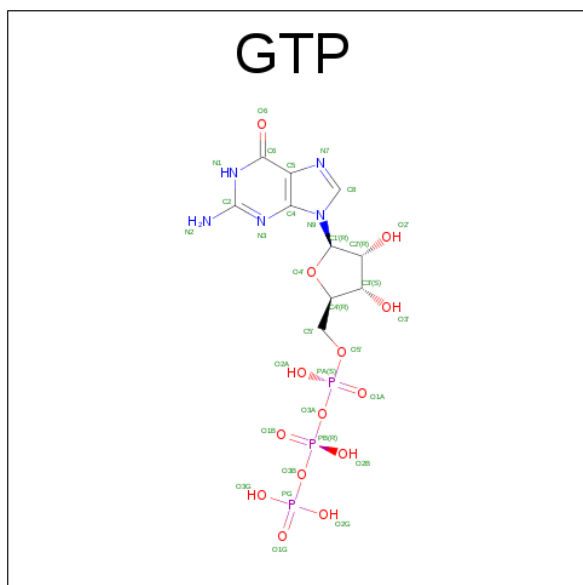
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

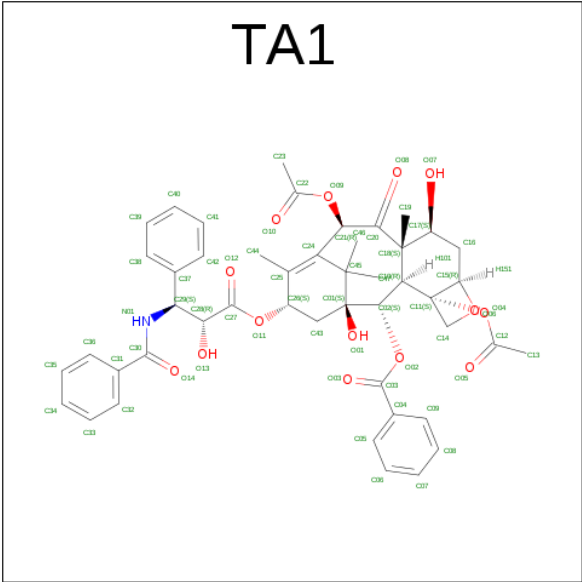
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

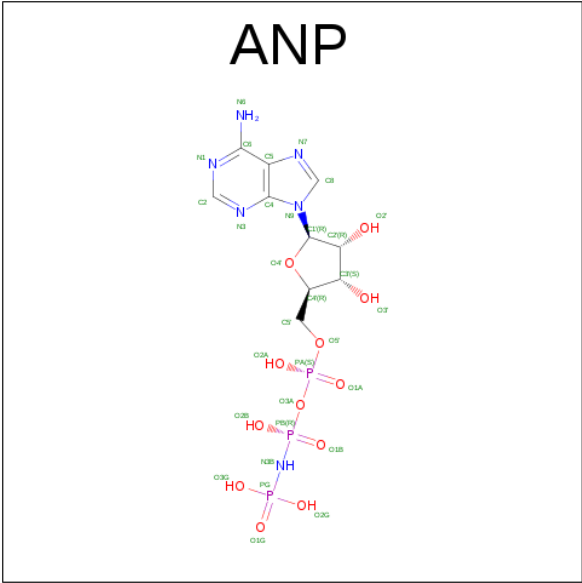
- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP, GDP) (formula: $C_{10}H_{16}N_5O_{14}P_3$, $C_{10}H_{15}N_5O_{11}P_2$).





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

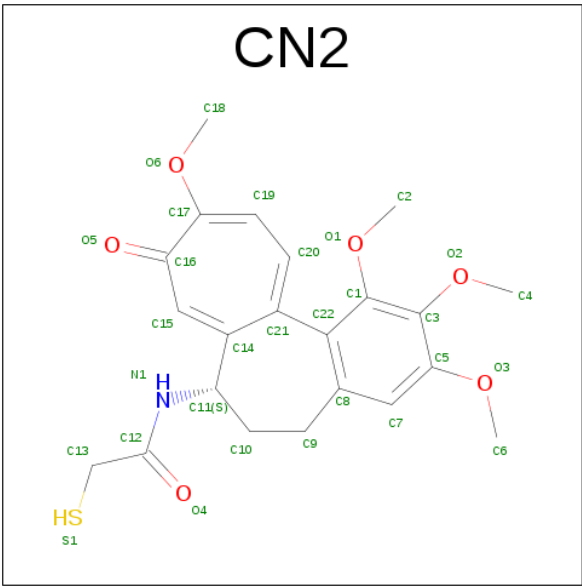
- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 10 is 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRAHYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula:

C₂₂H₂₅NO₆S).



Mol	Chain	Residues	Atoms					AltConf
10	G	1	Total	C	N	O	S	0
			30	22	1	6	1	

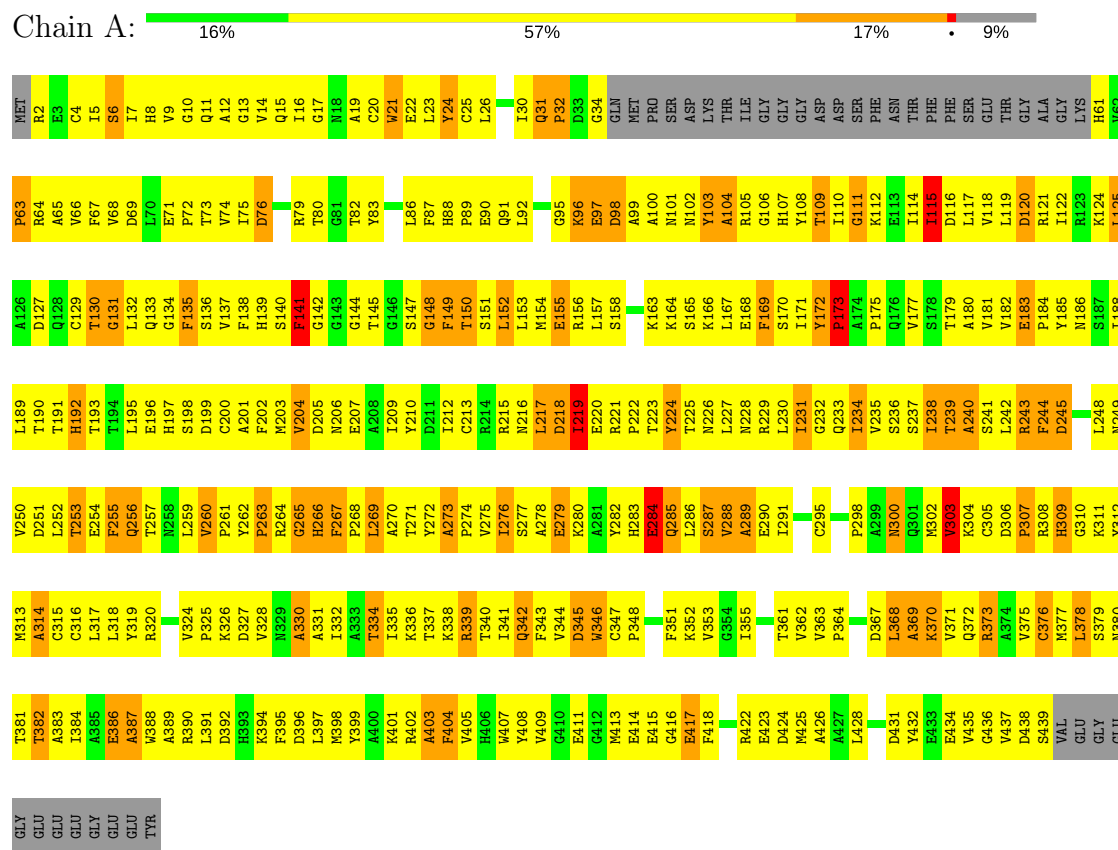
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	D	98	Total	O	0
			98	98	
11	F	9	Total	O	0
			9	9	

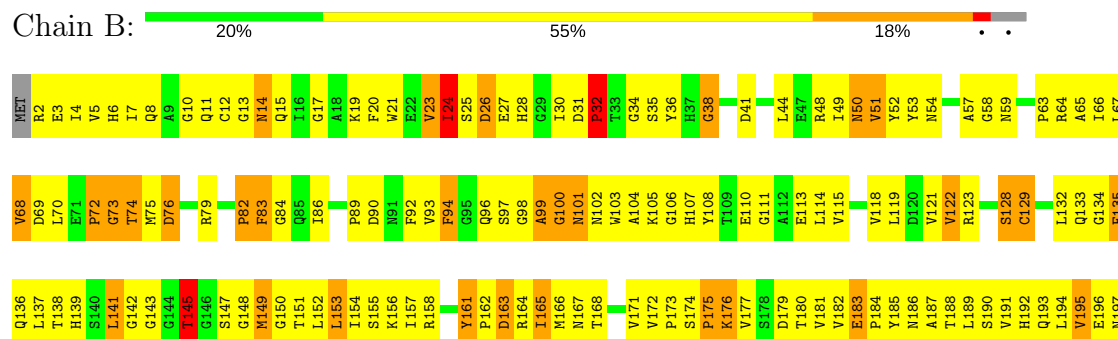
3 Residue-property plots

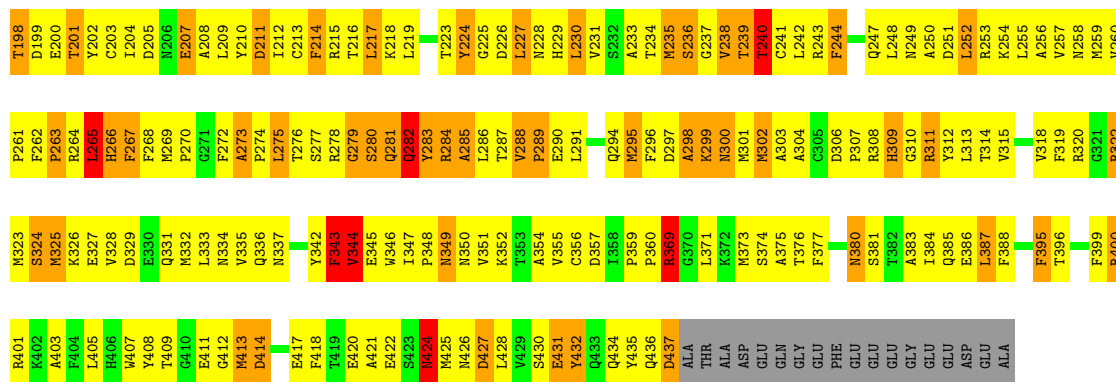
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: Alpha-tubulin

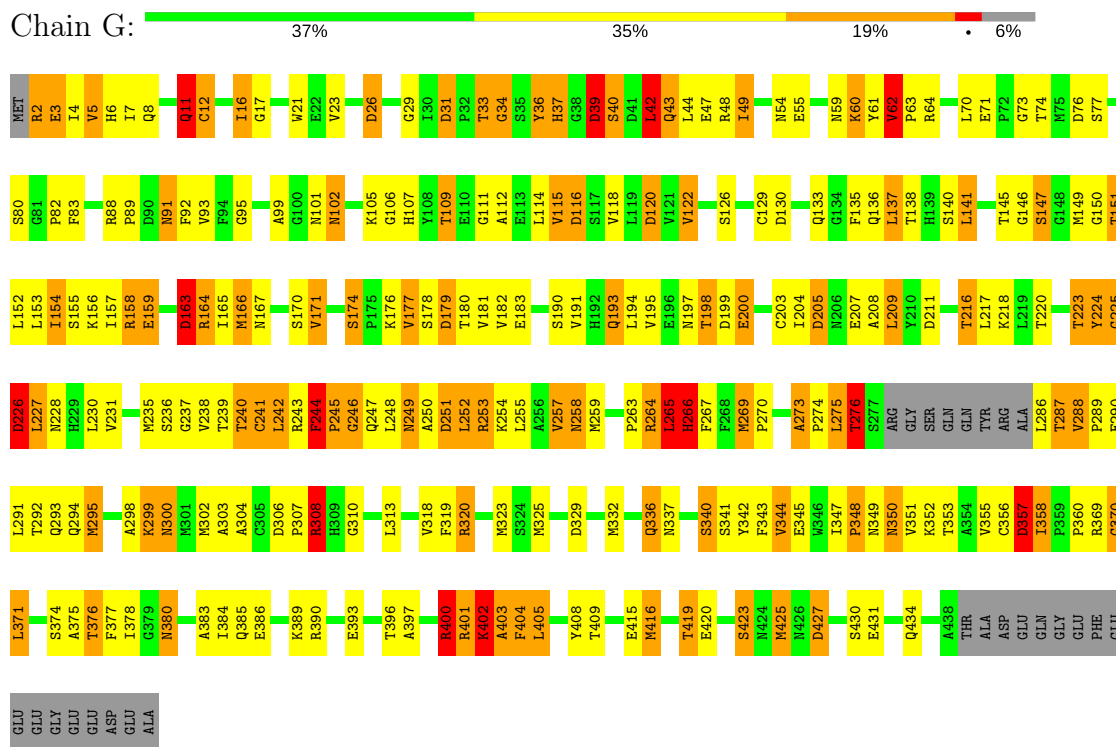


• Molecule 2: Beta tubulin

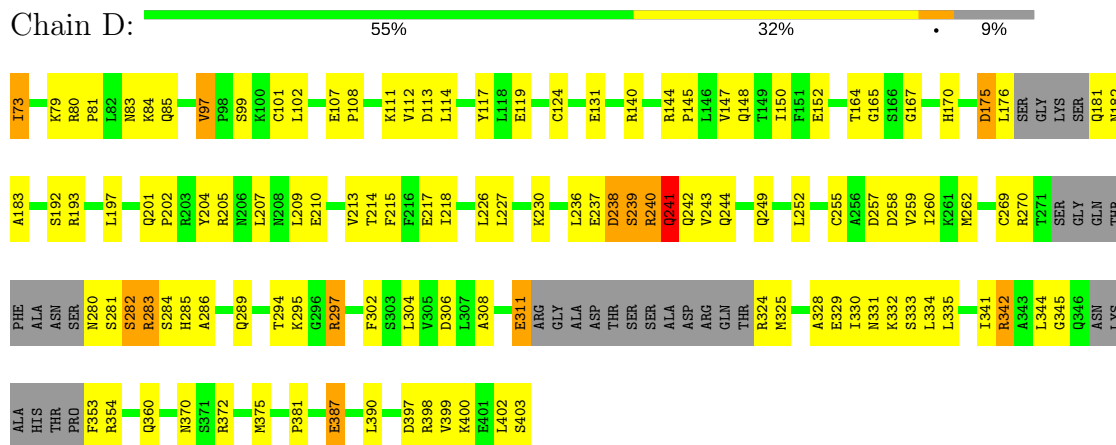




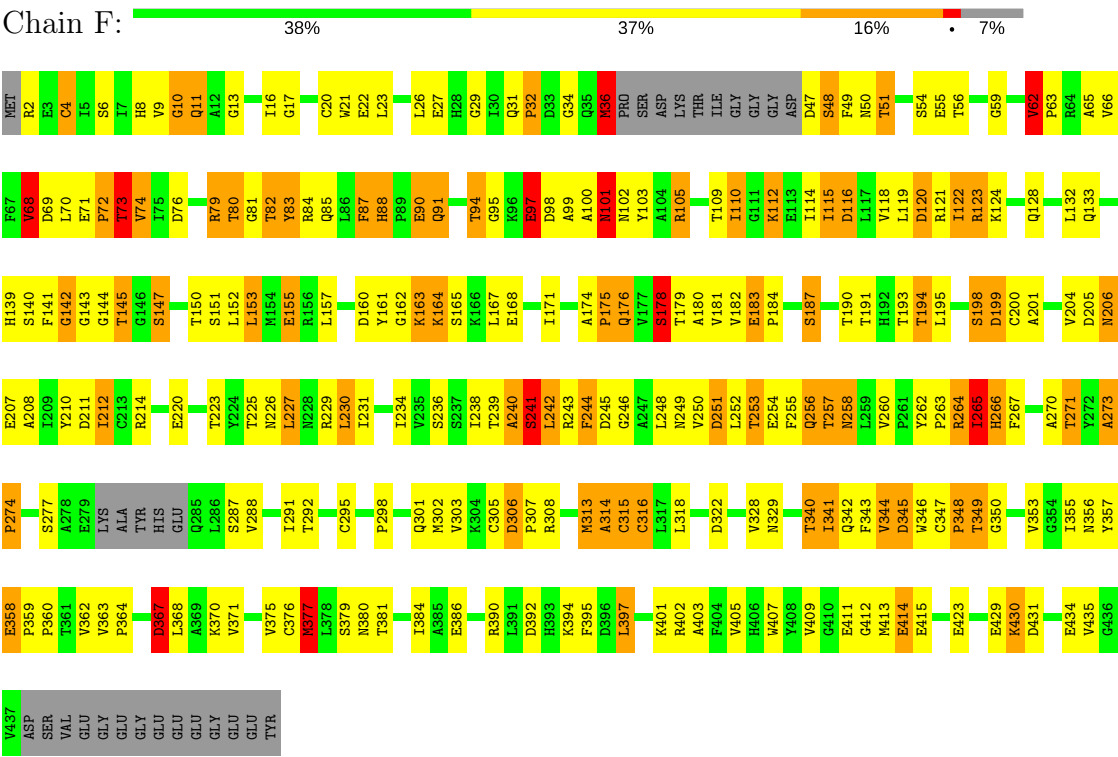
• Molecule 2: Beta tubulin



• Molecule 3: Kinesin13 Motor domain



● Molecule 4: Alpha-tubulin



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Each particle	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Film Kodak SO163	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CN2, TA1, ZN, GTP, ANP

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.51	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
2	G	0.61	0/3309	1.00	20/4494 (0.4%)
3	D	0.46	0/2398	0.71	2/3217 (0.1%)
4	F	0.66	2/3292 (0.1%)	0.95	15/4479 (0.3%)
All	All	0.56	2/15725 (0.0%)	0.84	39/21314 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	97	GLU	CD-OE1	-6.53	1.18	1.25
4	F	97	GLU	CD-OE2	-5.40	1.19	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	160	ASP	CB-CG-OD2	6.88	124.49	118.30
2	G	205	ASP	CB-CG-OD2	6.84	124.45	118.30
2	G	163	ASP	CB-CG-OD2	6.73	124.36	118.30
4	F	244	PHE	N-CA-C	6.73	129.17	111.00
2	G	116	ASP	CB-CG-OD2	6.32	123.99	118.30
2	G	179	ASP	CB-CG-OD2	6.29	123.97	118.30
2	G	244	PHE	N-CA-C	6.19	127.70	111.00
4	F	397	LEU	CA-CB-CG	6.14	129.43	115.30
2	G	242	LEU	CA-CB-CG	6.13	129.40	115.30
2	B	235	MET	CG-SD-CE	6.09	109.95	100.20
2	G	26	ASP	CB-CG-OD2	5.95	123.65	118.30
4	F	116	ASP	CB-CG-OD2	5.93	123.63	118.30
3	D	241	GLN	C-N-CA	-5.91	106.93	121.70
2	G	357	ASP	CB-CG-OD2	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	120	ASP	CB-CG-OD2	5.83	123.54	118.30
2	G	266	HIS	CB-CA-C	5.76	121.91	110.40
4	F	142	GLY	N-CA-C	-5.71	98.84	113.10
4	F	95	GLY	N-CA-C	5.70	127.35	113.10
4	F	76	ASP	CB-CG-OD2	5.62	123.35	118.30
2	G	427	ASP	CB-CG-OD2	5.52	123.27	118.30
3	D	241	GLN	O-C-N	-5.41	114.05	122.70
4	F	97	GLU	OE1-CD-OE2	-5.38	116.84	123.30
4	F	322	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	217	LEU	N-CA-C	-5.36	96.52	111.00
4	F	36	MET	CG-SD-CE	5.34	108.74	100.20
2	G	211	ASP	CB-CG-OD2	5.33	123.10	118.30
2	G	39	ASP	CB-CG-OD2	5.31	123.08	118.30
2	G	226	ASP	CB-CG-OD2	5.30	123.07	118.30
2	G	199	ASP	CB-CG-OD2	5.28	123.05	118.30
2	G	308	ARG	N-CA-C	-5.27	96.78	111.00
4	F	68	VAL	CB-CA-C	-5.25	101.43	111.40
4	F	199	ASP	CB-CG-OD2	5.23	123.00	118.30
4	F	367	ASP	CB-CG-OD2	5.21	122.99	118.30
2	G	306	ASP	CB-CG-OD2	5.13	122.92	118.30
2	G	31	ASP	CB-CG-OD2	5.08	122.87	118.30
2	G	246	GLY	N-CA-C	-5.07	100.43	113.10
4	F	345	ASP	CB-CG-OD2	5.05	122.85	118.30
2	G	163	ASP	N-CA-CB	-5.03	101.54	110.60
2	G	329	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3143	548	0
2	B	3351	0	3229	545	0
2	G	3237	0	3060	269	0
3	D	2368	0	2410	219	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	3220	0	3074	232	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	60	0	24	5	0
7	F	60	0	24	3	0
8	B	62	0	51	6	0
9	D	31	0	13	3	0
10	G	30	0	23	8	0
11	D	98	0	0	4	0
11	F	9	0	0	10	0
All	All	15757	0	15051	1665	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 54.

All (1665) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:ASP:CA	2:G:419:THR:HB	1.24	1.61
3:D:237:GLU:O	2:G:420:GLU:HA	1.30	1.28
3:D:236:LEU:CD2	2:G:416:MET:CE	2.11	1.28
3:D:238:ASP:CB	2:G:419:THR:HB	1.63	1.27
3:D:112:VAL:HG11	4:F:435:VAL:CG2	1.62	1.27
3:D:236:LEU:CD2	2:G:416:MET:SD	2.25	1.24
3:D:238:ASP:HA	2:G:419:THR:CB	1.67	1.24
3:D:113:ASP:HA	4:F:262:TYR:CD2	1.75	1.22
3:D:238:ASP:HB2	2:G:419:THR:CG2	1.70	1.21
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.19
3:D:236:LEU:HD21	2:G:416:MET:CE	1.73	1.18
3:D:236:LEU:HD23	2:G:416:MET:SD	1.87	1.14
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.14
2:G:273:ALA:HB3	2:G:274:PRO:HD3	1.22	1.14
3:D:112:VAL:HB	4:F:431:ASP:HB3	1.19	1.14
3:D:237:GLU:HG2	2:G:423:SER:CB	1.78	1.13
3:D:237:GLU:CG	2:G:423:SER:HB3	1.77	1.13
3:D:113:ASP:HB2	4:F:262:TYR:CE2	1.84	1.13
3:D:238:ASP:CA	2:G:419:THR:CB	2.21	1.12
4:F:198:SER:CB	4:F:265:ILE:HD11	1.78	1.12
3:D:353:PHE:N	2:G:434:GLN:HE22	1.45	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:99:ALA:HB2	4:F:145:THR:HG22	1.21	1.11
3:D:176:LEU:HG	3:D:181:GLN:HG3	1.32	1.10
3:D:238:ASP:CB	2:G:419:THR:CB	2.28	1.10
3:D:236:LEU:HD23	2:G:416:MET:CE	1.76	1.10
3:D:353:PHE:N	2:G:434:GLN:NE2	1.97	1.10
3:D:342:ARG:HG2	3:D:342:ARG:HH11	1.11	1.09
3:D:237:GLU:HG2	2:G:423:SER:HB3	1.30	1.08
3:D:236:LEU:HD21	2:G:416:MET:HE1	1.22	1.08
4:F:79:ARG:NH2	4:F:94:THR:HG21	1.68	1.08
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.30	1.08
4:F:88:HIS:HB2	4:F:91:GLN:HE21	1.15	1.08
4:F:434:GLU:CB	11:F:606:HOH:O	2.01	1.08
4:F:198:SER:HB3	4:F:265:ILE:CD1	1.85	1.06
3:D:114:LEU:HD11	4:F:263:PRO:HG3	1.32	1.06
4:F:273:ALA:CB	4:F:274:PRO:HD3	1.86	1.05
3:D:176:LEU:HG	3:D:181:GLN:CG	1.87	1.03
3:D:112:VAL:HG11	4:F:435:VAL:HG23	1.04	1.03
1:A:243:ARG:HH21	1:A:252:LEU:N	1.57	1.03
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.37	1.02
3:D:237:GLU:CG	2:G:423:SER:CB	2.36	1.02
3:D:238:ASP:HB2	2:G:419:THR:HG21	1.38	1.01
3:D:237:GLU:H	2:G:420:GLU:HG3	1.20	1.01
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.43	1.01
4:F:79:ARG:HH22	4:F:94:THR:CG2	1.74	1.01
3:D:112:VAL:CB	4:F:431:ASP:HB3	1.90	1.01
2:G:48:ARG:HH12	2:G:245:PRO:HD2	1.22	1.01
3:D:239:SER:H	2:G:419:THR:HG22	1.24	1.00
1:A:109:THR:HG22	1:A:110:ILE:N	1.70	1.00
4:F:434:GLU:HB2	11:F:606:HOH:O	1.57	1.00
2:B:236:SER:O	2:B:240:THR:HG23	1.61	1.00
3:D:238:ASP:O	2:G:423:SER:HB2	1.60	1.00
4:F:79:ARG:HH22	4:F:94:THR:HG21	0.84	1.00
2:G:273:ALA:CB	2:G:274:PRO:HD3	1.92	0.99
2:B:299:LYS:H	2:B:299:LYS:HD3	1.24	0.99
3:D:402:LEU:O	3:D:402:LEU:HD13	1.61	0.99
3:D:113:ASP:CB	4:F:262:TYR:CE2	2.45	0.98
4:F:99:ALA:CB	4:F:145:THR:HG22	1.94	0.97
3:D:114:LEU:HD21	4:F:263:PRO:CG	1.95	0.96
1:A:98:ASP:HB2	1:A:105:ARG:HH21	1.31	0.96
3:D:238:ASP:O	2:G:423:SER:CB	2.14	0.95
1:A:316:CYS:HB3	1:A:378:LEU:HD11	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:291:LEU:HD21	2:G:375:ALA:HB2	1.49	0.94
3:D:286:ALA:HB3	3:D:306:ASP:HB3	1.49	0.94
2:B:281:GLN:O	2:B:283:TYR:N	2.00	0.94
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.50	0.94
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.47	0.94
1:A:237:SER:HB2	1:A:376:CYS:SG	2.08	0.94
1:A:251:ASP:N	1:A:254:GLU:HG3	1.82	0.93
2:B:70:LEU:H	2:B:145:THR:HG21	1.33	0.93
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.48	0.93
2:G:291:LEU:HD21	2:G:375:ALA:CB	1.96	0.93
1:A:251:ASP:H	1:A:254:GLU:HG3	1.33	0.93
3:D:114:LEU:HD21	4:F:263:PRO:HG2	1.51	0.93
3:D:237:GLU:O	2:G:420:GLU:CA	2.17	0.93
3:D:241:GLN:HA	2:G:423:SER:OG	1.69	0.92
4:F:273:ALA:CB	4:F:375:VAL:H	1.82	0.92
4:F:431:ASP:N	11:F:706:HOH:O	2.01	0.92
2:B:264:ARG:O	2:B:265:LEU:HB3	1.69	0.92
3:D:112:VAL:CG1	4:F:435:VAL:CG2	2.47	0.91
3:D:113:ASP:HA	4:F:262:TYR:CE2	2.05	0.91
3:D:236:LEU:HD23	2:G:416:MET:HE3	1.52	0.91
1:A:151:SER:HB3	1:A:193:THR:HG21	1.51	0.91
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.51	0.91
2:B:147:SER:O	2:B:151:THR:HB	1.71	0.91
3:D:238:ASP:HB2	2:G:419:THR:CB	1.95	0.90
4:F:273:ALA:HB3	4:F:274:PRO:HD3	1.53	0.90
2:B:101:ASN:HD21	2:B:143:GLY:HA2	1.38	0.89
3:D:237:GLU:H	2:G:420:GLU:CG	1.85	0.89
1:A:110:ILE:HG23	1:A:111:GLY:H	1.38	0.89
2:B:93:VAL:HG11	2:B:118:VAL:CG2	2.03	0.88
2:B:102:ASN:HD21	2:B:408:TYR:HA	1.38	0.88
2:B:8:GLN:OE1	2:B:67:LEU:HD22	1.72	0.88
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.53	0.88
1:A:343:PHE:CZ	1:A:351:PHE:CE1	2.61	0.88
1:A:407:TRP:HE1	2:B:260:VAL:HG23	1.38	0.88
1:A:147:SER:HB2	1:A:190:THR:OG1	1.73	0.88
2:B:276:THR:HB	2:B:281:GLN:HG3	1.56	0.88
2:B:311:ARG:HD3	2:B:342:TYR:HA	1.56	0.88
2:G:247:GLN:HG2	2:G:248:LEU:H	1.37	0.88
3:D:111:LYS:HE2	4:F:434:GLU:OE2	1.72	0.88
2:B:264:ARG:HB2	2:B:266:HIS:CD2	2.08	0.87
2:B:360:PRO:HG2	2:B:371:LEU:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HD12	1:A:157:LEU:HD21	1.54	0.87
2:B:10:GLY:HA2	2:B:145:THR:HB	1.55	0.86
3:D:282:SER:OG	3:D:283:ARG:N	2.07	0.86
3:D:112:VAL:CG1	4:F:435:VAL:HG23	1.98	0.86
4:F:273:ALA:HB2	4:F:375:VAL:H	1.38	0.86
2:B:6:HIS:CE1	2:B:8:GLN:HG2	2.10	0.86
2:G:308:ARG:HH11	2:G:308:ARG:HG3	1.39	0.86
2:B:153:LEU:O	2:B:157:ILE:HG12	1.76	0.86
1:A:109:THR:HG22	1:A:110:ILE:H	1.33	0.85
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.57	0.85
3:D:112:VAL:HB	4:F:431:ASP:CB	2.03	0.85
1:A:184:PRO:HG2	1:A:398:MET:HE1	1.57	0.85
2:B:234:THR:HG21	2:B:270:PRO:CB	2.06	0.85
2:G:332:MET:HG3	2:G:353:THR:HG21	1.55	0.85
3:D:311:GLU:O	4:F:414:GLU:CG	2.25	0.85
2:G:336:GLN:OE1	2:G:351:VAL:HG11	1.75	0.85
2:G:287:THR:HG23	2:G:289:PRO:HD2	1.56	0.85
1:A:264:ARG:O	1:A:266:HIS:N	2.09	0.85
3:D:238:ASP:HA	2:G:419:THR:HB	0.87	0.85
2:B:242:LEU:HD22	2:B:250:ALA:H	1.42	0.85
3:D:353:PHE:CD1	2:G:434:GLN:NE2	2.45	0.85
3:D:342:ARG:HH11	3:D:402:LEU:HB2	1.40	0.85
4:F:178:SER:HB3	10:G:701:CN2:S1	2.17	0.85
3:D:114:LEU:CD1	4:F:263:PRO:HG3	2.07	0.84
1:A:234:ILE:HG13	1:A:270:ALA:HB1	1.59	0.84
4:F:273:ALA:HB1	4:F:274:PRO:HD3	1.57	0.84
4:F:431:ASP:HA	11:F:706:HOH:O	1.77	0.84
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.59	0.84
3:D:113:ASP:CA	4:F:262:TYR:CE2	2.60	0.84
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.57	0.84
2:B:20:PHE:CD2	2:B:235:MET:SD	2.71	0.84
2:B:324:SER:HB3	2:B:327:GLU:HG2	1.60	0.84
3:D:282:SER:C	3:D:283:ARG:HG2	1.98	0.84
4:F:341:ILE:HG12	4:F:342:GLN:H	1.43	0.83
4:F:273:ALA:CB	4:F:274:PRO:CD	2.57	0.83
3:D:353:PHE:N	2:G:434:GLN:CD	2.31	0.83
2:B:101:ASN:ND2	2:B:143:GLY:HA2	1.94	0.83
2:B:156:LYS:HE2	2:B:156:LYS:HA	1.61	0.83
2:B:209:LEU:HB3	2:B:227:LEU:HD22	1.59	0.83
2:B:3:GLU:O	2:B:133:GLN:HB3	1.78	0.83
2:B:148:GLY:O	2:B:151:THR:HG22	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:CYS:HB3	1:A:378:LEU:CD1	2.08	0.83
1:A:106:GLY:O	1:A:111:GLY:HA3	1.78	0.83
2:G:265:LEU:HD12	2:G:265:LEU:O	1.79	0.83
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.13	0.82
2:B:150:GLY:HA2	2:B:153:LEU:HD22	1.59	0.82
2:B:287:THR:O	2:B:288:VAL:HG23	1.78	0.82
2:B:4:ILE:HD13	2:B:136:GLN:HE21	1.42	0.82
4:F:386:GLU:O	4:F:390:ARG:HG3	1.79	0.82
3:D:237:GLU:CD	2:G:423:SER:HB3	1.99	0.82
2:G:48:ARG:NH1	2:G:245:PRO:HD2	1.93	0.82
1:A:151:SER:CB	1:A:193:THR:HG21	2.09	0.82
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.60	0.82
4:F:341:ILE:HG12	4:F:342:GLN:N	1.95	0.82
2:B:147:SER:HB2	2:B:190:SER:HB3	1.60	0.81
4:F:198:SER:HB3	4:F:265:ILE:HD11	0.89	0.81
1:A:248:LEU:HD23	1:A:353:VAL:O	1.80	0.81
4:F:98:ASP:HB3	2:G:251:ASP:OD2	1.81	0.81
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.60	0.81
1:A:313:MET:HB3	1:A:344:VAL:HG21	1.63	0.81
4:F:105:ARG:NH1	2:G:253:ARG:HH21	1.78	0.81
1:A:109:THR:CG2	1:A:110:ILE:N	2.44	0.80
2:B:110:GLU:O	2:B:113:GLU:HG2	1.79	0.80
2:B:20:PHE:CZ	2:B:24:ILE:HD12	2.15	0.80
3:D:342:ARG:HG2	3:D:342:ARG:NH1	1.87	0.80
1:A:220:GLU:C	1:A:222:PRO:HD3	2.02	0.80
3:D:237:GLU:N	2:G:420:GLU:HG3	1.96	0.80
2:G:205:ASP:OD1	2:G:207:GLU:HB3	1.81	0.80
2:B:236:SER:O	2:B:240:THR:CG2	2.29	0.80
3:D:353:PHE:HD1	2:G:434:GLN:NE2	1.80	0.80
4:F:316:CYS:O	4:F:377:MET:HA	1.81	0.80
1:A:7:ILE:HG22	1:A:66:VAL:HG22	1.63	0.80
3:D:164:THR:HG23	9:D:500:ANP:O1G	1.81	0.80
1:A:234:ILE:HD13	1:A:234:ILE:O	1.81	0.79
2:G:70:LEU:HA	2:G:95:GLY:HA3	1.64	0.79
1:A:267:PHE:CD1	1:A:267:PHE:N	2.49	0.79
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.46	0.79
2:B:259:MET:HA	2:B:314:THR:HG21	1.65	0.79
2:B:68:VAL:HG12	2:B:149:MET:SD	2.22	0.79
4:F:229:ARG:HH11	4:F:229:ARG:HG2	1.46	0.79
1:A:6:SER:HB3	1:A:136:SER:OG	1.81	0.79
1:A:132:LEU:HD23	1:A:132:LEU:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ALA:O	4:F:101:ASN:HB2	1.81	0.79
2:B:413:MET:HG3	2:B:414:ASP:H	1.47	0.78
3:D:113:ASP:HB2	4:F:262:TYR:HE2	1.43	0.78
1:A:199:ASP:HB3	1:A:256:GLN:NE2	1.98	0.78
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.66	0.78
2:B:264:ARG:HB2	2:B:266:HIS:HD2	1.45	0.78
2:B:265:LEU:HD12	2:B:265:LEU:O	1.83	0.78
1:A:241:SER:O	1:A:244:PHE:HB3	1.82	0.78
2:B:234:THR:CG2	2:B:270:PRO:HB2	2.11	0.78
3:D:282:SER:O	3:D:283:ARG:CG	2.32	0.78
3:D:84:LYS:HB2	3:D:85:GLN:HE22	1.48	0.78
3:D:84:LYS:HB2	3:D:85:GLN:NE2	1.97	0.78
1:A:69:ASP:HA	1:A:145:THR:HG21	1.66	0.78
1:A:155:GLU:HA	1:A:197:HIS:ND1	1.99	0.78
3:D:239:SER:N	2:G:419:THR:HG22	1.99	0.78
2:G:273:ALA:HB3	2:G:274:PRO:CD	2.07	0.77
1:A:172:TYR:HD1	1:A:172:TYR:C	1.87	0.77
2:B:396:THR:HG23	2:B:422:GLU:OE2	1.83	0.77
1:A:243:ARG:HH21	1:A:252:LEU:H	0.79	0.77
3:D:204:TYR:HA	3:D:207:LEU:HD23	1.64	0.77
1:A:11:GLN:HG3	1:A:74:VAL:CG1	2.13	0.77
2:B:205:ASP:OD1	2:B:304:ALA:HB2	1.84	0.77
2:B:35:SER:HB3	2:B:59:ASN:HA	1.65	0.77
3:D:328:ALA:HA	4:F:409:VAL:HG11	1.65	0.77
1:A:110:ILE:HG23	1:A:111:GLY:N	1.99	0.77
1:A:225:THR:O	1:A:229:ARG:HG3	1.85	0.77
2:B:192:HIS:ND1	2:B:424:ASN:OD1	2.18	0.76
2:G:247:GLN:CG	2:G:248:LEU:H	1.97	0.76
2:B:250:ALA:HA	2:B:254:LYS:HE2	1.67	0.76
2:B:259:MET:HG2	2:B:314:THR:HG21	1.67	0.76
2:B:198:THR:O	2:B:265:LEU:HD22	1.85	0.76
1:A:231:ILE:HA	1:A:234:ILE:HG22	1.66	0.76
3:D:282:SER:O	3:D:283:ARG:HG3	1.85	0.76
4:F:133:GLN:HE21	4:F:252:LEU:HG	1.49	0.76
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.21	0.76
1:A:221:ARG:HD3	1:A:221:ARG:O	1.85	0.76
1:A:163:LYS:O	1:A:164:LYS:HG2	1.86	0.76
1:A:223:THR:HB	1:A:225:THR:HG22	1.67	0.76
3:D:239:SER:H	2:G:419:THR:CG2	1.98	0.76
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.69	0.76
2:B:176:LYS:HE3	2:B:207:GLU:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:335:ILE:HG12	1.86	0.75
4:F:142:GLY:HA3	4:F:183:GLU:HG3	1.68	0.75
3:D:238:ASP:CB	2:G:419:THR:CG2	2.55	0.75
1:A:205:ASP:CB	1:A:303:VAL:HA	2.17	0.75
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.87	0.75
3:D:114:LEU:HD21	4:F:263:PRO:HG3	1.66	0.75
3:D:311:GLU:O	4:F:414:GLU:HG3	1.87	0.75
2:B:209:LEU:HG	2:B:230:LEU:HD22	1.69	0.75
3:D:111:LYS:HG2	4:F:434:GLU:OE2	1.86	0.75
2:G:21:TRP:CZ3	2:G:63:PRO:HB3	2.22	0.75
1:A:101:ASN:ND2	2:B:254:LYS:HD2	2.02	0.75
1:A:306:ASP:O	1:A:308:ARG:N	2.20	0.75
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.27	0.75
2:B:19:LYS:HG3	2:B:228:ASN:CB	2.17	0.75
2:G:36:TYR:OH	2:G:40:SER:O	2.03	0.75
1:A:276:ILE:HG23	1:A:369:ALA:CB	2.16	0.74
3:D:342:ARG:NH1	3:D:402:LEU:HB2	2.03	0.74
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.68	0.74
3:D:342:ARG:HG2	3:D:402:LEU:HB2	1.68	0.74
2:B:168:THR:HB	2:B:201:THR:HG23	1.68	0.74
2:B:217:LEU:C	2:B:219:LEU:H	1.90	0.74
2:B:274:PRO:HG2	2:B:371:LEU:HD21	1.69	0.74
1:A:264:ARG:C	1:A:266:HIS:H	1.91	0.74
3:D:85:GLN:CD	3:D:85:GLN:H	1.90	0.74
3:D:353:PHE:N	2:G:434:GLN:OE1	2.20	0.74
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.52	0.74
4:F:70:LEU:HD23	4:F:110:ILE:HG23	1.69	0.74
1:A:362:VAL:HG13	1:A:368:LEU:HD12	1.68	0.74
2:B:242:LEU:HD13	2:B:250:ALA:C	2.08	0.74
3:D:117:TYR:OH	4:F:430:LYS:HE3	1.88	0.74
2:G:265:LEU:O	2:G:266:HIS:O	2.05	0.74
3:D:345:GLY:O	3:D:402:LEU:HD11	1.87	0.74
4:F:101:ASN:HD22	2:G:254:LYS:HG2	1.53	0.74
2:B:103:TRP:CZ3	2:B:108:TYR:HE1	2.05	0.73
3:D:236:LEU:HD21	2:G:416:MET:SD	2.23	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:104:ALA:HB2	1:A:413:MET:HG3	1.71	0.73
2:B:217:LEU:O	2:B:219:LEU:N	2.22	0.73
2:B:325:MET:HA	2:B:325:MET:HE3	1.70	0.73
3:D:237:GLU:HG2	2:G:423:SER:HB2	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:CB	1:A:413:MET:HG3	2.18	0.73
3:D:176:LEU:HG	3:D:181:GLN:HG2	1.71	0.73
1:A:7:ILE:HD11	1:A:137:VAL:HG22	1.71	0.73
2:B:8:GLN:CD	2:B:67:LEU:HD22	2.08	0.73
2:B:76:ASP:HA	2:B:79:ARG:HG2	1.71	0.73
1:A:112:LYS:O	1:A:115:ILE:HG22	1.89	0.73
1:A:63:PRO:O	1:A:64:ARG:HG2	1.88	0.73
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.24	0.73
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.19	0.72
1:A:172:TYR:C	1:A:172:TYR:CD1	2.61	0.72
2:B:356:CYS:SG	2:B:357:ASP:N	2.62	0.72
2:G:247:GLN:HG3	2:G:248:LEU:HG	1.71	0.72
2:G:273:ALA:CB	2:G:274:PRO:CD	2.67	0.72
1:A:105:ARG:O	1:A:110:ILE:HG22	1.89	0.72
2:B:243:ARG:NH2	2:B:252:LEU:HG	2.05	0.72
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.20	0.72
1:A:312:TYR:O	1:A:344:VAL:HG23	1.90	0.72
2:B:70:LEU:HG	2:B:145:THR:CG2	2.20	0.72
3:D:238:ASP:O	2:G:423:SER:OG	2.07	0.72
3:D:282:SER:C	3:D:283:ARG:CG	2.58	0.72
1:A:425:MET:HE2	1:A:428:LEU:HD23	1.72	0.72
4:F:181:VAL:HB	2:G:258:ASN:ND2	2.05	0.72
4:F:273:ALA:HB3	4:F:274:PRO:CD	2.17	0.72
1:A:166:LYS:HE3	1:A:199:ASP:OD1	1.90	0.72
2:B:237:GLY:O	2:B:241:CYS:HB3	1.90	0.72
2:B:48:ARG:HG2	2:B:243:ARG:O	1.90	0.72
1:A:259:LEU:HD11	1:A:378:LEU:CD1	2.20	0.71
1:A:343:PHE:CZ	1:A:351:PHE:HE1	2.08	0.71
3:D:80:ARG:O	3:D:381:PRO:HG3	1.90	0.71
2:B:111:GLY:O	2:B:115:VAL:HG23	1.89	0.71
2:B:201:THR:OG1	2:B:265:LEU:HD11	1.90	0.71
3:D:238:ASP:C	2:G:419:THR:O	2.28	0.71
3:D:114:LEU:HD11	4:F:263:PRO:CG	2.17	0.71
2:G:251:ASP:C	2:G:253:ARG:H	1.94	0.71
4:F:88:HIS:HB2	4:F:91:GLN:NE2	1.98	0.71
2:G:347:ILE:HG22	2:G:350:ASN:HB3	1.72	0.71
3:D:175:ASP:O	3:D:176:LEU:HB2	1.89	0.71
2:B:431:GLU:OE1	2:B:432:TYR:HA	1.91	0.71
2:G:319:PHE:HB2	2:G:355:VAL:HG12	1.73	0.71
3:D:238:ASP:HA	2:G:419:THR:C	2.11	0.71
3:D:111:LYS:HG2	4:F:434:GLU:CD	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HB3	1:A:140:SER:OG	1.91	0.71
2:B:10:GLY:O	2:B:14:ASN:HB2	1.90	0.71
2:G:12:CYS:SG	2:G:171:VAL:HG21	2.30	0.71
1:A:25:CYS:HB2	1:A:30:ILE:O	1.89	0.70
1:A:317:LEU:HD12	1:A:351:PHE:HD2	1.55	0.70
2:B:70:LEU:HG	2:B:145:THR:HG23	1.74	0.70
1:A:242:LEU:HD21	1:A:250:VAL:HB	1.71	0.70
2:B:175:PRO:HD2	2:B:207:GLU:OE2	1.91	0.70
1:A:63:PRO:C	1:A:64:ARG:HG2	2.12	0.70
3:D:147:VAL:O	3:D:150:ILE:HG12	1.92	0.70
2:G:140:SER:HA	2:G:171:VAL:HG23	1.74	0.70
1:A:88:HIS:C	1:A:90:GLU:H	1.95	0.70
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.06	0.70
2:B:255:LEU:O	2:B:259:MET:HG3	1.91	0.70
2:B:6:HIS:HE1	2:B:8:GLN:HG2	1.52	0.70
2:B:291:LEU:O	2:B:295:MET:HG3	1.91	0.70
1:A:234:ILE:HG21	1:A:302:MET:HE3	1.73	0.69
1:A:5:ILE:HG22	1:A:6:SER:N	2.07	0.69
2:B:24:ILE:HD11	2:B:52:TYR:CE1	2.28	0.69
1:A:244:PHE:HD2	1:A:245:ASP:N	1.89	0.69
2:B:180:THR:HG22	2:B:181:VAL:N	2.07	0.69
2:B:234:THR:O	2:B:238:VAL:HG23	1.92	0.69
2:B:332:MET:HE3	2:B:351:VAL:HG11	1.73	0.69
3:D:113:ASP:CA	4:F:262:TYR:CD2	2.66	0.69
2:G:164:ARG:HE	2:G:164:ARG:HA	1.57	0.69
1:A:148:GLY:O	1:A:151:SER:HB2	1.91	0.69
3:D:342:ARG:HH12	3:D:402:LEU:HD23	1.58	0.69
1:A:222:PRO:HD2	2:B:326:LYS:HB3	1.74	0.69
3:D:236:LEU:CD2	2:G:416:MET:HE3	2.10	0.69
3:D:311:GLU:O	4:F:414:GLU:HG2	1.91	0.69
2:B:251:ASP:O	2:B:253:ARG:N	2.26	0.69
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.69
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.74	0.69
1:A:394:LYS:HG2	2:B:348:PRO:HG3	1.75	0.69
4:F:70:LEU:HD12	4:F:70:LEU:N	2.07	0.69
3:D:236:LEU:CD2	2:G:416:MET:HE1	1.96	0.69
1:A:343:PHE:HZ	1:A:351:PHE:CE1	2.10	0.69
2:G:307:PRO:O	2:G:308:ARG:CD	2.41	0.69
2:G:307:PRO:O	2:G:308:ARG:HD3	1.93	0.68
1:A:237:SER:CB	1:A:376:CYS:SG	2.80	0.68
2:B:209:LEU:HD23	2:B:227:LEU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:VAL:O	2:B:257:VAL:HG12	1.93	0.68
4:F:431:ASP:CA	11:F:706:HOH:O	2.28	0.68
2:G:337:ASN:HA	2:G:340:SER:HB3	1.76	0.68
2:G:54:ASN:HB2	2:G:64:ARG:HD3	1.76	0.68
1:A:141:PHE:O	1:A:147:SER:HB3	1.93	0.68
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.73	0.68
1:A:221:ARG:N	1:A:222:PRO:HD3	2.09	0.68
1:A:217:LEU:HD12	1:A:277:SER:HB3	1.75	0.68
2:B:242:LEU:CD2	2:B:250:ALA:H	2.07	0.68
3:D:111:LYS:CE	4:F:434:GLU:OE2	2.40	0.68
2:G:352:LYS:HG3	10:G:701:CN2:O5	1.94	0.68
2:B:204:ILE:HD13	2:B:231:VAL:HG22	1.76	0.68
1:A:381:THR:C	1:A:383:ALA:H	1.95	0.68
4:F:423:GLU:OE1	11:F:698:HOH:O	2.12	0.68
2:G:241:CYS:CB	2:G:248:LEU:HD12	2.24	0.68
1:A:115:ILE:CD1	1:A:119:LEU:HG	2.23	0.68
1:A:7:ILE:HD12	1:A:153:LEU:CD2	2.24	0.68
1:A:407:TRP:HE1	2:B:260:VAL:CG2	2.07	0.68
3:D:175:ASP:OD1	3:D:175:ASP:N	2.27	0.68
1:A:95:GLY:O	1:A:97:GLU:N	2.27	0.68
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.29	0.67
1:A:71:GLU:HG3	2:B:2:ARG:HH21	1.58	0.67
2:B:44:LEU:HD12	2:B:49:ILE:HD13	1.76	0.67
1:A:133:GLN:HG2	1:A:243:ARG:HH22	1.57	0.67
1:A:371:VAL:HG12	1:A:372:GLN:H	1.57	0.67
2:B:107:HIS:CD2	2:B:151:THR:CG2	2.78	0.67
2:B:108:TYR:CD1	2:B:413:MET:HE1	2.29	0.67
2:B:310:GLY:HA3	2:B:436:GLN:HE21	1.59	0.67
2:B:66:ILE:C	2:B:67:LEU:HD23	2.15	0.67
3:D:111:LYS:HG2	4:F:434:GLU:OE1	1.95	0.67
2:G:133:GLN:HE21	2:G:252:LEU:HB3	1.59	0.67
3:D:236:LEU:HD22	2:G:416:MET:SD	2.31	0.67
2:B:299:LYS:N	2:B:299:LYS:HD3	2.04	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.94	0.67
2:B:325:MET:CE	2:B:355:VAL:HG21	2.24	0.67
2:G:238:VAL:HG13	2:G:378:ILE:HD11	1.76	0.67
1:A:251:ASP:O	1:A:254:GLU:HB2	1.94	0.67
3:D:112:VAL:CA	4:F:431:ASP:HB3	2.25	0.67
3:D:240:ARG:C	3:D:241:GLN:CG	2.62	0.67
2:G:350:ASN:HD22	2:G:350:ASN:H	1.43	0.67
1:A:100:ALA:CB	1:A:105:ARG:HD3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASP:HB3	1:A:256:GLN:HE21	1.57	0.67
2:B:276:THR:HB	2:B:281:GLN:CG	2.25	0.67
2:B:250:ALA:HB1	2:B:254:LYS:HB2	1.75	0.67
2:B:256:ALA:O	2:B:260:VAL:HG22	1.94	0.67
2:G:247:GLN:CG	2:G:248:LEU:N	2.56	0.67
1:A:152:LEU:HA	1:A:155:GLU:HB2	1.77	0.66
2:B:4:ILE:HG21	2:B:136:GLN:HG2	1.76	0.66
2:B:243:ARG:HH22	2:B:252:LEU:HG	1.59	0.66
3:D:113:ASP:HB2	4:F:262:TYR:CZ	2.31	0.66
1:A:276:ILE:O	1:A:369:ALA:HB2	1.95	0.66
3:D:240:ARG:O	3:D:241:GLN:HG3	1.95	0.66
4:F:123:ARG:HD3	4:F:161:TYR:OH	1.94	0.66
2:G:308:ARG:NH1	2:G:308:ARG:HG3	2.11	0.66
2:G:289:PRO:O	2:G:293:GLN:HG3	1.96	0.66
2:G:42:LEU:O	2:G:44:LEU:N	2.29	0.66
1:A:172:TYR:HD1	1:A:173:PRO:N	1.93	0.66
1:A:341:ILE:HG12	1:A:341:ILE:O	1.95	0.66
2:B:230:LEU:HD23	2:B:231:VAL:N	2.10	0.66
4:F:430:LYS:C	11:F:706:HOH:O	2.32	0.66
3:D:176:LEU:CG	3:D:181:GLN:CG	2.68	0.66
3:D:238:ASP:HA	2:G:419:THR:CA	2.26	0.66
2:G:88:ARG:O	2:G:91:ASN:HB2	1.96	0.66
2:B:265:LEU:HD12	2:B:265:LEU:C	2.16	0.66
3:D:238:ASP:C	2:G:419:THR:HB	2.13	0.66
1:A:68:VAL:HG11	1:A:149:PHE:CZ	2.31	0.65
1:A:217:LEU:HD11	1:A:367:ASP:O	1.96	0.65
1:A:372:GLN:O	1:A:373:ARG:HB3	1.96	0.65
4:F:273:ALA:HB2	4:F:375:VAL:N	2.11	0.65
1:A:305:CYS:SG	1:A:384:ILE:HD13	2.37	0.65
4:F:249:ASN:HB3	4:F:255:PHE:CD2	2.32	0.65
2:B:242:LEU:CD1	2:B:255:LEU:HD11	2.26	0.65
1:A:175:PRO:HG3	1:A:304:LYS:HG2	1.76	0.65
3:D:324:ARG:HG3	3:D:324:ARG:O	1.97	0.65
2:B:182:VAL:HG23	2:B:186:ASN:HD21	1.60	0.65
3:D:193:ARG:O	3:D:197:LEU:HD13	1.95	0.65
1:A:313:MET:HB3	1:A:344:VAL:CG2	2.26	0.65
2:B:66:ILE:CD1	2:B:122:VAL:HG12	2.26	0.65
2:B:431:GLU:O	2:B:434:GLN:HG2	1.97	0.65
1:A:115:ILE:HG23	1:A:116:ASP:N	2.12	0.65
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.65
2:B:242:LEU:HD12	2:B:255:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:241:CYS:HB2	2:G:248:LEU:HD12	1.76	0.65
2:B:267:PHE:CD1	2:B:267:PHE:N	2.62	0.65
1:A:271:THR:HG23	1:A:300:ASN:O	1.97	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
2:B:281:GLN:O	2:B:283:TYR:HB2	1.96	0.64
2:B:284:ARG:O	2:B:286:LEU:N	2.31	0.64
2:B:422:GLU:O	2:B:426:ASN:HB2	1.97	0.64
1:A:206:ASN:OD1	1:A:227:LEU:HD13	1.96	0.64
2:B:241:CYS:O	2:B:244:PHE:HB2	1.97	0.64
1:A:224:TYR:CD1	2:B:325:MET:HG2	2.33	0.64
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.79	0.64
1:A:317:LEU:HD12	1:A:351:PHE:CD2	2.32	0.64
2:B:103:TRP:HZ3	2:B:108:TYR:HE1	1.42	0.64
3:D:202:PRO:HA	3:D:205:ARG:HD2	1.80	0.64
1:A:151:SER:O	1:A:155:GLU:HB2	1.98	0.64
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.79	0.64
2:B:35:SER:HB3	2:B:59:ASN:CA	2.26	0.64
2:B:243:ARG:HH21	2:B:252:LEU:H	1.45	0.64
2:B:299:LYS:O	2:B:300:ASN:HB2	1.97	0.64
2:B:413:MET:HG2	2:B:418:PHE:HE1	1.61	0.64
1:A:386:GLU:O	1:A:389:ALA:N	2.31	0.64
4:F:208:ALA:O	4:F:212:ILE:HD12	1.98	0.64
2:B:114:LEU:O	2:B:118:VAL:HG23	1.98	0.64
2:B:158:ARG:NE	2:B:197:ASN:O	2.30	0.64
2:G:369:ARG:O	2:G:370:GLY:C	2.34	0.64
1:A:315:CYS:HB3	1:A:377:MET:HE2	1.78	0.64
2:B:105:LYS:O	2:B:110:GLU:HB2	1.97	0.64
2:B:192:HIS:O	2:B:195:VAL:HG12	1.98	0.64
2:B:427:ASP:O	2:B:430:SER:HB3	1.97	0.64
2:B:180:THR:CG2	2:B:181:VAL:N	2.61	0.64
4:F:133:GLN:NE2	4:F:252:LEU:HG	2.13	0.64
1:A:7:ILE:HG22	1:A:66:VAL:CG2	2.28	0.63
1:A:269:LEU:O	1:A:378:LEU:HA	1.99	0.63
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.81	0.63
1:A:276:ILE:HG23	1:A:369:ALA:HB2	1.80	0.63
3:D:324:ARG:O	3:D:324:ARG:CG	2.46	0.63
4:F:98:ASP:OD1	4:F:99:ALA:N	2.32	0.63
2:G:59:ASN:O	2:G:60:LYS:O	2.16	0.63
1:A:234:ILE:HD13	1:A:234:ILE:C	2.18	0.63
2:B:137:LEU:HD22	2:B:154:ILE:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:HIS:HD2	2:B:151:THR:CG2	2.12	0.63
2:G:401:ARG:HH11	2:G:401:ARG:HG3	1.63	0.63
4:F:100:ALA:O	4:F:101:ASN:CB	2.46	0.63
4:F:434:GLU:HB3	11:F:606:HOH:O	1.79	0.63
2:G:396:THR:HG22	2:G:400:ARG:HH21	1.63	0.63
10:G:701:CN2:H43	10:G:701:CN2:H62	1.80	0.63
2:B:63:PRO:HD2	2:B:86:ILE:HG12	1.80	0.63
3:D:238:ASP:O	2:G:419:THR:O	2.16	0.63
1:A:175:PRO:HG2	1:A:207:GLU:OE1	1.98	0.63
2:B:133:GLN:HG3	2:B:165:ILE:HD11	1.80	0.63
2:B:282:GLN:O	2:B:282:GLN:HG2	1.97	0.63
2:B:205:ASP:OD1	2:B:304:ALA:N	2.32	0.63
1:A:23:LEU:HD22	1:A:232:GLY:O	1.99	0.63
3:D:144:ARG:HB3	3:D:145:PRO:HD3	1.81	0.63
1:A:7:ILE:CD1	1:A:137:VAL:HG22	2.29	0.62
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.34	0.62
1:A:152:LEU:HD12	1:A:153:LEU:N	2.14	0.62
4:F:99:ALA:HB2	4:F:145:THR:CG2	2.14	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
1:A:236:SER:O	1:A:240:ALA:HB3	1.99	0.62
1:A:288:VAL:O	1:A:290:GLU:N	2.33	0.62
2:B:4:ILE:HA	2:B:134:GLY:O	1.99	0.62
4:F:206:ASN:HD21	7:F:601:GTP:HN22	1.47	0.62
1:A:278:ALA:HA	1:A:282:TYR:OH	1.99	0.62
1:A:315:CYS:HB3	1:A:377:MET:CE	2.29	0.62
2:B:318:VAL:HA	2:B:354:ALA:HB3	1.81	0.62
3:D:176:LEU:CG	3:D:181:GLN:HG2	2.28	0.62
2:G:266:HIS:H	2:G:266:HIS:CD2	2.17	0.62
1:A:166:LYS:H	1:A:199:ASP:CG	2.03	0.62
1:A:243:ARG:NH2	1:A:252:LEU:N	2.28	0.62
1:A:402:ARG:O	1:A:403:ALA:C	2.36	0.62
3:D:111:LYS:CD	4:F:434:GLU:OE2	2.47	0.62
1:A:118:VAL:HG11	1:A:149:PHE:HZ	1.65	0.62
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.33	0.62
2:G:158:ARG:O	2:G:159:GLU:HB2	2.00	0.62
2:G:263:PRO:O	2:G:265:LEU:N	2.31	0.62
2:B:204:ILE:CD1	2:B:231:VAL:HG13	2.30	0.62
3:D:148:GLN:O	3:D:152:GLU:HG3	2.00	0.62
1:A:88:HIS:O	1:A:90:GLU:N	2.33	0.62
2:B:230:LEU:O	2:B:233:ALA:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:176:GLN:H	4:F:176:GLN:NE2	1.98	0.62
2:G:237:GLY:HA3	2:G:376:THR:HG21	1.82	0.62
2:G:287:THR:HG22	2:G:290:GLU:HG3	1.82	0.62
2:B:4:ILE:HG23	2:B:134:GLY:O	2.00	0.61
8:B:601:TA1:H261	8:B:601:TA1:H463	1.80	0.61
1:A:168:GLU:OE1	1:A:198:SER:HB2	2.01	0.61
1:A:179:THR:HG21	2:B:248:LEU:HD21	1.82	0.61
2:B:70:LEU:CG	2:B:145:THR:HG23	2.30	0.61
2:B:211:ASP:OD1	2:B:212:ILE:N	2.33	0.61
4:F:229:ARG:HH11	4:F:229:ARG:CG	2.14	0.61
4:F:249:ASN:HB3	4:F:255:PHE:HD2	1.65	0.61
1:A:177:VAL:HG11	2:B:329:ASP:HB3	1.83	0.61
1:A:179:THR:HG22	2:B:352:LYS:NZ	2.15	0.61
2:G:223:THR:HB	2:G:225:GLY:H	1.65	0.61
1:A:179:THR:HG21	2:B:248:LEU:CD2	2.30	0.61
1:A:407:TRP:NE1	2:B:260:VAL:HG23	2.14	0.61
2:B:172:VAL:CG1	2:B:387:LEU:HD21	2.24	0.61
1:A:102:ASN:OD1	1:A:105:ARG:HB3	2.00	0.61
1:A:317:LEU:HD11	1:A:351:PHE:HE2	1.63	0.61
2:B:114:LEU:HD23	2:B:149:MET:CE	2.30	0.61
3:D:210:GLU:HG3	3:D:252:LEU:HD11	1.82	0.61
2:G:403:ALA:C	2:G:405:LEU:H	2.03	0.61
1:A:115:ILE:HG13	1:A:152:LEU:HD13	1.81	0.61
3:D:335:LEU:HD11	4:F:402:ARG:HG3	1.82	0.61
2:G:287:THR:CG2	2:G:290:GLU:HG3	2.30	0.61
1:A:167:LEU:HA	1:A:200:CYS:O	2.01	0.61
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.82	0.61
3:D:230:LYS:HE3	3:D:269:CYS:O	2.01	0.61
1:A:11:GLN:HE21	1:A:74:VAL:HG22	1.66	0.60
1:A:362:VAL:HG13	1:A:368:LEU:HB2	1.83	0.60
3:D:112:VAL:HG11	4:F:435:VAL:HG22	1.78	0.60
3:D:239:SER:HB2	2:G:419:THR:HG22	1.82	0.60
2:G:6:HIS:HE1	2:G:8:GLN:HE21	1.48	0.60
1:A:311:LYS:HE3	1:A:342:GLN:CD	2.22	0.60
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.15	0.60
3:D:112:VAL:CG1	4:F:435:VAL:HG22	2.32	0.60
1:A:345:ASP:C	1:A:347:CYS:H	2.04	0.60
3:D:79:LYS:HE3	3:D:381:PRO:HB3	1.82	0.60
1:A:177:VAL:CG1	2:B:329:ASP:HB3	2.31	0.60
2:B:204:ILE:HG21	2:B:231:VAL:HG22	1.84	0.60
2:B:324:SER:O	2:B:328:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:MET:CE	2:B:351:VAL:HG11	2.31	0.60
1:A:181:VAL:HG21	2:B:258:ASN:O	2.01	0.60
2:G:126:SER:O	2:G:129:CYS:HB2	2.01	0.60
1:A:267:PHE:H	1:A:267:PHE:HD1	1.47	0.60
2:B:324:SER:CB	2:B:327:GLU:HG2	2.30	0.60
3:D:114:LEU:CD2	4:F:263:PRO:HG3	2.31	0.60
2:G:151:THR:HB	2:G:193:GLN:HG2	1.83	0.60
2:G:158:ARG:O	2:G:159:GLU:CB	2.49	0.60
2:G:136:GLN:HA	2:G:167:ASN:O	2.02	0.60
1:A:119:LEU:O	1:A:122:ILE:HG12	2.02	0.60
2:B:49:ILE:O	2:B:51:VAL:N	2.35	0.60
4:F:105:ARG:CZ	2:G:253:ARG:HH21	2.14	0.60
4:F:115:ILE:CD1	4:F:119:LEU:HD13	2.32	0.60
1:A:248:LEU:CD2	1:A:353:VAL:O	2.49	0.60
1:A:229:ARG:NH1	1:A:363:VAL:HG21	2.16	0.60
2:B:324:SER:C	2:B:326:LYS:H	2.03	0.60
2:G:205:ASP:OD2	2:G:390:ARG:NH1	2.34	0.60
1:A:284:GLU:O	1:A:286:LEU:N	2.35	0.60
3:D:207:LEU:HB3	3:D:209:LEU:HG	1.83	0.60
3:D:329:GLU:HA	3:D:332:LYS:HE3	1.83	0.60
1:A:191:THR:HG21	1:A:425:MET:SD	2.41	0.59
1:A:169:PHE:CE1	1:A:235:VAL:HG22	2.36	0.59
2:B:279:GLY:O	2:B:282:GLN:HB3	2.01	0.59
2:B:205:ASP:OD1	2:B:304:ALA:CB	2.50	0.59
2:B:408:TYR:CG	2:B:418:PHE:HZ	2.20	0.59
1:A:435:VAL:HG12	1:A:435:VAL:O	2.01	0.59
2:G:164:ARG:HE	2:G:164:ARG:CA	2.14	0.59
2:G:247:GLN:HG2	2:G:248:LEU:N	2.13	0.59
2:B:70:LEU:N	2:B:145:THR:HG21	2.11	0.59
2:B:285:ALA:HB1	2:B:290:GLU:HG2	1.82	0.59
1:A:344:VAL:HG11	1:A:346:TRP:NE1	2.16	0.59
1:A:6:SER:HA	1:A:136:SER:O	2.03	0.59
2:B:141:LEU:N	2:B:141:LEU:CD1	2.65	0.59
1:A:115:ILE:HD13	1:A:115:ILE:O	2.02	0.59
2:B:102:ASN:ND2	2:B:407:TRP:O	2.35	0.59
1:A:371:VAL:HG12	1:A:372:GLN:N	2.17	0.59
2:B:115:VAL:HG21	2:B:152:LEU:HD23	1.84	0.59
2:B:68:VAL:CG1	2:B:149:MET:SD	2.90	0.59
2:B:30:ILE:HD13	2:B:53:TYR:CE2	2.38	0.59
2:B:299:LYS:O	2:B:300:ASN:CB	2.51	0.59
3:D:97:VAL:HG22	3:D:97:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:275:LEU:O	2:G:276:THR:HB	2.03	0.59
1:A:278:ALA:HB2	1:A:369:ALA:HA	1.85	0.59
2:B:161:TYR:C	2:B:163:ASP:H	2.05	0.59
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
3:D:294:THR:HG23	3:D:295:LYS:H	1.68	0.58
4:F:66:VAL:HG11	4:F:122:ILE:HG22	1.85	0.58
4:F:264:ARG:O	4:F:266:HIS:CD2	2.56	0.58
4:F:70:LEU:CD1	4:F:70:LEU:N	2.65	0.58
1:A:413:MET:O	1:A:414:GLU:HG3	2.03	0.58
2:B:198:THR:HG22	2:B:265:LEU:HD22	1.85	0.58
2:G:348:PRO:O	2:G:350:ASN:N	2.36	0.58
1:A:407:TRP:O	1:A:411:GLU:HG2	2.02	0.58
2:B:349:ASN:C	2:B:349:ASN:HD22	2.06	0.58
4:F:265:ILE:CG2	4:F:267:PHE:CZ	2.86	0.58
2:B:270:PRO:HA	2:B:377:PHE:O	2.04	0.58
2:B:70:LEU:H	2:B:145:THR:CG2	2.10	0.58
1:A:2:ARG:N	1:A:131:GLY:O	2.36	0.58
1:A:381:THR:C	1:A:383:ALA:N	2.56	0.58
2:B:151:THR:OG1	2:B:193:GLN:HB3	2.03	0.58
3:D:304:LEU:N	3:D:304:LEU:HD22	2.18	0.58
4:F:181:VAL:HB	2:G:258:ASN:HD22	1.69	0.58
1:A:166:LYS:HD2	1:A:197:HIS:O	2.04	0.58
2:B:180:THR:CG2	2:B:181:VAL:H	2.17	0.58
4:F:168:GLU:HG2	4:F:201:ALA:HB2	1.85	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.04	0.58
1:A:88:HIS:C	1:A:90:GLU:N	2.57	0.58
2:B:320:ARG:O	2:B:359:PRO:HA	2.04	0.58
3:D:328:ALA:CA	4:F:409:VAL:HG11	2.31	0.58
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.33	0.58
2:B:253:ARG:O	2:B:254:LYS:C	2.42	0.58
2:B:307:PRO:HB3	2:B:312:TYR:OH	2.04	0.58
1:A:119:LEU:CD2	1:A:122:ILE:HD11	2.28	0.58
1:A:218:ASP:O	1:A:219:ILE:HG23	2.04	0.58
2:B:70:LEU:C	2:B:99:ALA:HB2	2.24	0.58
1:A:63:PRO:HD3	1:A:86:LEU:O	2.04	0.58
2:B:93:VAL:CG1	2:B:118:VAL:HG22	2.19	0.58
4:F:298:PRO:HA	4:F:301:GLN:NE2	2.19	0.58
1:A:317:LEU:HD11	1:A:351:PHE:CE2	2.38	0.57
3:D:114:LEU:CD2	4:F:263:PRO:CG	2.79	0.57
1:A:264:ARG:HB2	1:A:266:HIS:HD2	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:313:MET:O	4:F:314:ALA:HB2	2.04	0.57
3:D:111:LYS:CG	4:F:434:GLU:OE2	2.51	0.57
2:B:19:LYS:CG	2:B:228:ASN:HB3	2.31	0.57
3:D:387:GLU:CD	3:D:387:GLU:H	2.07	0.57
4:F:301:GLN:HE22	4:F:307:PRO:HD3	1.70	0.57
1:A:117:LEU:HD11	1:A:121:ARG:HH22	1.69	0.57
1:A:202:PHE:CE2	1:A:378:LEU:HD22	2.38	0.57
1:A:362:VAL:HG11	1:A:368:LEU:O	2.04	0.57
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.18	0.57
4:F:8:HIS:CD2	4:F:17:GLY:HA3	2.39	0.57
2:G:135:PHE:HB2	2:G:166:MET:CE	2.34	0.57
1:A:338:LYS:O	1:A:340:THR:N	2.34	0.57
2:B:132:LEU:CD2	2:B:164:ARG:HG3	2.32	0.57
2:B:217:LEU:C	2:B:219:LEU:N	2.55	0.57
2:B:319:PHE:HA	2:B:375:ALA:HA	1.86	0.57
2:B:301:MET:CE	2:B:377:PHE:HE2	2.17	0.57
7:F:603:GDP:O3B	2:G:145:THR:HG23	2.05	0.57
2:G:357:ASP:OD2	2:G:357:ASP:N	2.38	0.57
3:D:237:GLU:HG3	2:G:423:SER:CB	2.32	0.57
4:F:249:ASN:CB	4:F:255:PHE:CD2	2.87	0.57
4:F:11:GLN:HB3	7:F:601:GTP:O2A	2.04	0.57
4:F:69:ASP:C	4:F:70:LEU:HD12	2.25	0.57
2:G:358:ILE:HG23	2:G:358:ILE:O	2.04	0.57
1:A:152:LEU:HA	1:A:155:GLU:CB	2.35	0.57
1:A:369:ALA:O	1:A:370:LYS:HB3	2.03	0.57
4:F:346:TRP:CE3	4:F:347:CYS:HB2	2.40	0.57
2:G:240:THR:HG21	2:G:320:ARG:CZ	2.34	0.57
2:G:266:HIS:HB3	2:G:380:ASN:HD21	1.70	0.57
1:A:286:LEU:HD12	1:A:290:GLU:HG2	1.87	0.57
1:A:345:ASP:O	1:A:347:CYS:N	2.38	0.57
2:B:274:PRO:CG	2:B:371:LEU:HD21	2.34	0.57
2:B:319:PHE:CD2	2:B:375:ALA:HB2	2.40	0.57
1:A:362:VAL:CG1	1:A:368:LEU:HB2	2.35	0.57
4:F:29:GLY:O	4:F:36:MET:HB3	2.05	0.57
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.35	0.57
1:A:19:ALA:CB	1:A:228:ASN:HB3	2.35	0.57
2:B:50:ASN:O	2:B:64:ARG:NH2	2.38	0.57
4:F:328:VAL:HG11	4:F:353:VAL:HG11	1.85	0.57
3:D:238:ASP:CB	2:G:419:THR:HG21	2.23	0.57
1:A:165:SER:HA	1:A:199:ASP:OD2	2.04	0.56
1:A:313:MET:O	1:A:314:ALA:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ILE:HA	2:B:35:SER:O	2.04	0.56
2:B:259:MET:CA	2:B:314:THR:HG21	2.35	0.56
4:F:265:ILE:HG22	4:F:267:PHE:CZ	2.40	0.56
1:A:331:ALA:O	1:A:334:THR:HG22	2.05	0.56
1:A:409:VAL:C	1:A:411:GLU:H	2.09	0.56
2:B:283:TYR:C	2:B:284:ARG:HG2	2.25	0.56
2:B:6:HIS:HB3	2:B:65:ALA:HB2	1.87	0.56
4:F:187:SER:O	4:F:191:THR:HG22	2.05	0.56
2:B:14:ASN:OD1	2:B:75:MET:HG2	2.05	0.56
4:F:308:ARG:HA	4:F:340:THR:HG21	1.85	0.56
1:A:175:PRO:HG3	1:A:304:LYS:CG	2.35	0.56
2:B:182:VAL:HG23	2:B:186:ASN:ND2	2.20	0.56
2:B:216:THR:O	2:B:217:LEU:HD12	2.05	0.56
2:B:4:ILE:HD13	2:B:136:GLN:NE2	2.18	0.56
3:D:240:ARG:O	3:D:241:GLN:CG	2.54	0.56
4:F:23:LEU:HD23	4:F:236:SER:HB2	1.87	0.56
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.87	0.56
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.41	0.56
2:B:149:MET:O	2:B:153:LEU:HD13	2.05	0.56
3:D:342:ARG:NH1	3:D:342:ARG:CG	2.65	0.56
4:F:180:ALA:O	4:F:183:GLU:HB2	2.05	0.56
2:G:203:CYS:SG	2:G:267:PHE:HB3	2.45	0.56
2:G:287:THR:CG2	2:G:289:PRO:HD2	2.32	0.56
2:G:403:ALA:O	2:G:405:LEU:N	2.38	0.56
1:A:210:TYR:CE2	1:A:227:LEU:HD11	2.40	0.56
2:B:139:HIS:HE1	2:B:168:THR:HG23	1.71	0.56
2:B:312:TYR:O	2:B:344:VAL:HB	2.05	0.56
2:G:135:PHE:HB2	2:G:166:MET:HE1	1.86	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.56
2:B:147:SER:O	2:B:151:THR:CB	2.51	0.56
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.18	0.56
1:A:110:ILE:CG2	1:A:111:GLY:H	2.15	0.56
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.40	0.56
1:A:11:GLN:HE22	2:B:249:ASN:ND2	2.03	0.56
2:B:31:ASP:O	2:B:32:PRO:C	2.44	0.56
3:D:329:GLU:O	3:D:332:LYS:HG2	2.06	0.56
2:G:226:ASP:N	2:G:226:ASP:OD1	2.37	0.56
1:A:242:LEU:C	1:A:244:PHE:H	2.09	0.56
1:A:394:LYS:HG2	2:B:348:PRO:CG	2.35	0.56
2:B:151:THR:OG1	2:B:193:GLN:CB	2.54	0.56
2:B:166:MET:HB3	2:B:198:THR:OG1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:247:GLN:CG	2:G:248:LEU:HG	2.36	0.56
1:A:216:ASN:O	1:A:217:LEU:HB2	2.05	0.56
1:A:231:ILE:HA	1:A:234:ILE:CG2	2.36	0.56
1:A:253:THR:O	1:A:256:GLN:HG2	2.06	0.56
2:B:70:LEU:CD1	2:B:145:THR:HG23	2.35	0.56
2:B:190:SER:O	2:B:194:LEU:HG	2.06	0.56
3:D:165:GLY:H	9:D:500:ANP:HNB1	1.52	0.56
2:B:191:VAL:HA	2:B:194:LEU:HD12	1.87	0.55
2:B:204:ILE:HG21	2:B:231:VAL:CG2	2.36	0.55
2:B:210:TYR:HD2	2:B:227:LEU:HD21	1.71	0.55
2:B:311:ARG:HD2	2:B:344:VAL:H	1.71	0.55
1:A:436:GLY:C	1:A:438:ASP:H	2.08	0.55
2:B:119:LEU:O	2:B:123:ARG:HG3	2.06	0.55
2:B:310:GLY:CA	2:B:436:GLN:HE21	2.19	0.55
2:B:422:GLU:O	2:B:426:ASN:N	2.37	0.55
1:A:408:TYR:CD1	1:A:418:PHE:HZ	2.24	0.55
2:B:239:THR:HG22	2:B:240:THR:N	2.22	0.55
2:G:177:VAL:HG12	2:G:177:VAL:O	2.07	0.55
2:G:191:VAL:HG11	2:G:425:MET:CE	2.37	0.55
2:B:19:LYS:O	2:B:23:VAL:HG23	2.06	0.55
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.87	0.55
3:D:81:PRO:HB3	3:D:131:GLU:HB2	1.89	0.55
3:D:227:LEU:HD22	3:D:262:MET:HE3	1.87	0.55
2:G:209:LEU:HB3	2:G:227:LEU:HD11	1.88	0.55
2:B:223:THR:HG22	2:B:224:TYR:N	2.21	0.55
2:B:272:PHE:HB3	2:B:275:LEU:HD22	1.88	0.55
3:D:240:ARG:C	3:D:241:GLN:HG2	2.27	0.55
4:F:256:GLN:C	4:F:258:ASN:N	2.59	0.55
4:F:265:ILE:O	4:F:266:HIS:O	2.24	0.55
2:G:5:VAL:HG22	2:G:135:PHE:CD2	2.41	0.55
2:G:180:THR:HG21	2:G:182:VAL:HG22	1.89	0.55
1:A:5:ILE:CG2	1:A:6:SER:N	2.70	0.55
1:A:150:THR:O	1:A:153:LEU:N	2.40	0.55
1:A:381:THR:OG1	1:A:383:ALA:HB3	2.07	0.55
2:B:424:ASN:HD22	2:B:424:ASN:C	2.09	0.55
3:D:294:THR:HG23	3:D:295:LYS:N	2.22	0.55
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.42	0.55
2:B:250:ALA:CA	2:B:254:LYS:HE2	2.35	0.55
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.42	0.54
2:B:239:THR:O	2:B:241:CYS:N	2.41	0.54
2:B:44:LEU:O	2:B:49:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:171:VAL:HA	2:G:204:ILE:O	2.07	0.54
4:F:252:LEU:O	4:F:253:THR:C	2.45	0.54
2:B:324:SER:C	2:B:326:LYS:N	2.59	0.54
2:G:2:ARG:HH11	2:G:133:GLN:HA	1.72	0.54
1:A:101:ASN:CG	2:B:254:LYS:HD2	2.27	0.54
1:A:172:TYR:OH	1:A:387:ALA:O	2.24	0.54
2:B:67:LEU:HD23	2:B:67:LEU:N	2.22	0.54
3:D:210:GLU:HG3	3:D:252:LEU:CD1	2.36	0.54
2:G:342:TYR:N	2:G:342:TYR:CD2	2.75	0.54
1:A:115:ILE:C	1:A:115:ILE:HD13	2.28	0.54
1:A:9:VAL:CG1	1:A:139:HIS:HB3	2.38	0.54
2:B:165:ILE:HD13	2:B:165:ILE:H	1.71	0.54
2:G:408:TYR:O	2:G:409:THR:C	2.45	0.54
1:A:6:SER:O	1:A:65:ALA:HB1	2.07	0.54
1:A:98:ASP:CB	1:A:105:ARG:HH21	2.14	0.54
2:B:194:LEU:C	2:B:196:GLU:H	2.11	0.54
2:B:20:PHE:CE2	2:B:24:ILE:HD12	2.43	0.54
2:G:223:THR:HB	2:G:225:GLY:N	2.23	0.54
3:D:237:GLU:HG3	2:G:423:SER:OG	2.08	0.54
1:A:17:GLY:O	1:A:21:TRP:HB2	2.08	0.54
4:F:256:GLN:C	4:F:258:ASN:H	2.11	0.54
2:G:194:LEU:O	2:G:265:LEU:CD2	2.56	0.54
1:A:382:THR:O	1:A:382:THR:HG22	2.05	0.54
2:B:27:GLU:HG2	2:B:27:GLU:O	2.08	0.54
2:B:424:ASN:C	2:B:424:ASN:ND2	2.62	0.54
2:B:427:ASP:OD1	2:B:428:LEU:N	2.41	0.54
2:G:401:ARG:NH1	2:G:401:ARG:HG3	2.23	0.54
1:A:173:PRO:HB2	1:A:391:LEU:CD1	2.38	0.54
1:A:408:TYR:O	1:A:411:GLU:N	2.39	0.54
2:B:323:MET:HG3	2:B:328:VAL:HG21	1.90	0.54
2:B:343:PHE:O	2:B:344:VAL:O	2.26	0.54
1:A:110:ILE:O	1:A:112:LYS:N	2.41	0.53
1:A:339:ARG:C	1:A:341:ILE:H	2.11	0.53
1:A:248:LEU:HB3	1:A:355:ILE:H	1.73	0.53
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.73	0.53
2:B:213:CYS:SG	2:B:219:LEU:HD23	2.48	0.53
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.90	0.53
1:A:163:LYS:O	1:A:163:LYS:HG2	2.08	0.53
1:A:324:VAL:O	1:A:327:ASP:HB2	2.08	0.53
2:B:259:MET:CG	2:B:314:THR:HG21	2.36	0.53
3:D:255:CYS:SG	3:D:257:ASP:HB2	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:331:ASN:O	3:D:335:LEU:HG	2.07	0.53
2:B:325:MET:CE	2:B:355:VAL:HG11	2.38	0.53
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.43	0.53
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.44	0.53
1:A:98:ASP:O	1:A:110:ILE:HD13	2.08	0.53
1:A:179:THR:HG22	2:B:352:LYS:HZ1	1.73	0.53
1:A:243:ARG:CZ	1:A:252:LEU:HG	2.39	0.53
1:A:5:ILE:O	1:A:135:PHE:HA	2.09	0.53
2:B:4:ILE:CG2	2:B:136:GLN:HG2	2.38	0.53
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.89	0.53
2:B:325:MET:O	2:B:329:ASP:HB2	2.07	0.53
2:B:431:GLU:O	2:B:434:GLN:CG	2.56	0.53
2:B:68:VAL:HG12	2:B:149:MET:CE	2.38	0.53
3:D:176:LEU:CG	3:D:181:GLN:HG3	2.22	0.53
4:F:407:TRP:CD2	2:G:257:VAL:HG23	2.43	0.53
2:G:307:PRO:O	2:G:308:ARG:HD2	2.09	0.53
2:B:273:ALA:CB	2:B:274:PRO:HD3	2.31	0.53
4:F:21:TRP:CZ3	4:F:63:PRO:HB3	2.43	0.53
2:B:198:THR:HG22	2:B:265:LEU:CD2	2.39	0.53
2:B:311:ARG:HG2	2:B:311:ARG:HH11	1.71	0.53
2:B:322:ARG:HH11	2:B:322:ARG:HG3	1.73	0.53
2:G:216:THR:HG21	2:G:299:LYS:HD3	1.90	0.53
1:A:150:THR:O	1:A:151:SER:C	2.47	0.53
1:A:5:ILE:O	1:A:136:SER:N	2.40	0.53
1:A:121:ARG:O	1:A:125:LEU:HB2	2.08	0.53
2:B:141:LEU:HA	2:B:147:SER:HB3	1.91	0.53
2:B:345:GLU:C	2:B:347:ILE:H	2.13	0.53
1:A:215:ARG:C	1:A:216:ASN:HD22	2.12	0.53
1:A:275:VAL:HG21	1:A:300:ASN:OD1	2.09	0.53
2:B:107:HIS:HD2	2:B:151:THR:HG22	1.72	0.53
2:B:179:ASP:HB2	7:B:600:GDP:H3'	1.90	0.53
3:D:113:ASP:CB	4:F:262:TYR:CZ	2.91	0.53
2:G:2:ARG:O	2:G:3:GLU:HB2	2.09	0.53
2:G:383:ALA:O	2:G:386:GLU:HB2	2.08	0.53
1:A:283:HIS:O	1:A:284:GLU:C	2.47	0.52
1:A:11:GLN:CG	1:A:74:VAL:HG11	2.28	0.52
2:B:212:ILE:O	2:B:216:THR:HB	2.10	0.52
2:B:210:TYR:CD2	2:B:227:LEU:HD21	2.44	0.52
2:B:229:HIS:ND1	2:B:229:HIS:C	2.62	0.52
3:D:400:LYS:HE2	11:D:629:HOH:O	2.09	0.52
2:G:140:SER:O	2:G:147:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PRO:HB2	1:A:391:LEU:HD11	1.91	0.52
2:B:425:MET:O	2:B:428:LEU:HB3	2.10	0.52
1:A:345:ASP:OD2	1:A:439:SER:HB3	2.10	0.52
1:A:362:VAL:HG13	1:A:368:LEU:CD1	2.38	0.52
2:B:331:GLN:O	2:B:335:VAL:HG23	2.08	0.52
2:B:360:PRO:HB2	8:B:601:TA1:H281	1.91	0.52
1:A:101:ASN:ND2	7:B:500:GTP:O3G	2.42	0.52
3:D:345:GLY:C	3:D:402:LEU:HD11	2.29	0.52
4:F:249:ASN:CB	4:F:255:PHE:HD2	2.21	0.52
2:G:16:ILE:HG22	2:G:17:GLY:N	2.25	0.52
1:A:196:GLU:C	1:A:197:HIS:CD2	2.82	0.52
1:A:231:ILE:HD13	1:A:231:ILE:N	2.24	0.52
1:A:239:THR:O	1:A:240:ALA:C	2.48	0.52
2:B:226:ASP:O	2:B:227:LEU:C	2.46	0.52
2:B:5:VAL:O	2:B:5:VAL:HG23	2.09	0.52
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.42	0.52
2:G:287:THR:O	2:G:288:VAL:HB	2.09	0.52
2:B:70:LEU:HD12	2:B:145:THR:HG23	1.91	0.52
2:G:36:TYR:HD1	2:G:37:HIS:H	1.58	0.52
1:A:182:VAL:O	1:A:184:PRO:N	2.41	0.52
2:B:297:ASP:OD1	2:B:298:ALA:N	2.39	0.52
3:D:85:GLN:CD	3:D:85:GLN:N	2.62	0.52
1:A:206:ASN:OD1	1:A:227:LEU:CD1	2.57	0.52
2:B:128:SER:OG	2:B:129:CYS:N	2.34	0.52
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.52
2:B:200:GLU:N	2:B:265:LEU:HD13	2.25	0.52
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.29	0.52
2:B:277:SER:OG	2:B:281:GLN:HB2	2.10	0.52
4:F:198:SER:CB	4:F:265:ILE:CD1	2.66	0.52
1:A:191:THR:HG23	1:A:192:HIS:N	2.25	0.52
2:B:188:THR:HA	2:B:425:MET:CE	2.40	0.52
2:B:49:ILE:O	2:B:50:ASN:C	2.48	0.52
2:G:241:CYS:HB3	2:G:248:LEU:HD12	1.92	0.52
1:A:4:CYS:HA	1:A:134:GLY:O	2.10	0.52
3:D:402:LEU:O	3:D:402:LEU:CD1	2.48	0.52
4:F:10:GLY:O	4:F:13:GLY:N	2.43	0.52
4:F:270:ALA:HB3	4:F:302:MET:HG3	1.92	0.52
1:A:234:ILE:HB	1:A:302:MET:HE1	1.91	0.52
1:A:8:HIS:HB3	1:A:13:GLY:O	2.09	0.52
2:B:149:MET:O	2:B:153:LEU:HD22	2.10	0.52
2:B:226:ASP:O	2:B:229:HIS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:MET:SD	2:B:375:ALA:O	2.68	0.52
4:F:271:THR:HG23	4:F:301:GLN:HA	1.91	0.52
2:G:11:GLN:HG3	2:G:74:THR:CG2	2.40	0.52
1:A:244:PHE:CD2	1:A:245:ASP:N	2.76	0.51
3:D:214:THR:OG1	3:D:289:GLN:HB2	2.10	0.51
1:A:243:ARG:NH2	1:A:251:ASP:OD1	2.43	0.51
2:B:260:VAL:HG23	2:B:260:VAL:O	2.10	0.51
2:B:314:THR:CG2	2:B:315:VAL:N	2.73	0.51
2:G:205:ASP:OD1	2:G:207:GLU:N	2.43	0.51
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.39	0.51
1:A:344:VAL:HG12	1:A:345:ASP:H	1.74	0.51
3:D:192:SER:OG	3:D:259:VAL:HG11	2.10	0.51
4:F:105:ARG:HD2	4:F:411:GLU:OE1	2.10	0.51
4:F:407:TRP:CG	2:G:257:VAL:HG23	2.45	0.51
2:G:295:MET:HG2	2:G:295:MET:O	2.11	0.51
1:A:151:SER:HB3	1:A:193:THR:CG2	2.34	0.51
1:A:24:TYR:CE2	1:A:240:ALA:HB2	2.45	0.51
1:A:251:ASP:OD1	1:A:252:LEU:N	2.43	0.51
1:A:67:PHE:HE1	1:A:87:PHE:CE2	2.29	0.51
2:B:149:MET:HG2	2:B:149:MET:O	2.10	0.51
2:B:264:ARG:HA	2:B:264:ARG:HE	1.74	0.51
2:G:241:CYS:HB3	2:G:248:LEU:CD1	2.41	0.51
1:A:231:ILE:CA	1:A:234:ILE:HG22	2.38	0.51
1:A:201:ALA:O	1:A:267:PHE:HA	2.10	0.51
2:B:107:HIS:CD2	2:B:151:THR:HG22	2.45	0.51
2:B:296:PHE:CZ	2:B:315:VAL:HG11	2.46	0.51
3:D:238:ASP:CA	2:G:419:THR:C	2.77	0.51
1:A:417:GLU:OE1	1:A:417:GLU:HA	2.10	0.51
2:B:168:THR:CB	2:B:201:THR:HG23	2.38	0.51
4:F:239:THR:O	4:F:241:SER:N	2.44	0.51
4:F:270:ALA:O	4:F:302:MET:CG	2.58	0.51
2:G:3:GLU:HG2	2:G:64:ARG:NH2	2.25	0.51
1:A:264:ARG:C	1:A:266:HIS:N	2.60	0.51
2:B:103:TRP:CE2	2:B:189:LEU:HB3	2.45	0.51
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.94	0.51
2:G:336:GLN:CD	2:G:351:VAL:HG11	2.30	0.51
2:B:253:ARG:O	2:B:257:VAL:N	2.33	0.51
2:B:259:MET:HG2	2:B:314:THR:CG2	2.38	0.51
4:F:252:LEU:O	4:F:254:GLU:N	2.43	0.51
2:G:320:ARG:NH1	2:G:360:PRO:HG3	2.26	0.51
1:A:16:ILE:HG23	1:A:17:GLY:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:O	1:A:197:HIS:CD2	2.64	0.51
1:A:234:ILE:CG1	1:A:270:ALA:HB1	2.38	0.51
2:B:320:ARG:HA	2:B:356:CYS:HB3	1.92	0.51
2:B:413:MET:HG3	2:B:414:ASP:N	2.22	0.51
2:B:431:GLU:OE1	2:B:432:TYR:CA	2.57	0.51
3:D:85:GLN:NE2	11:D:646:HOH:O	2.44	0.51
2:G:298:ALA:C	2:G:300:ASN:H	2.14	0.51
2:G:44:LEU:O	2:G:49:ILE:HG22	2.11	0.51
1:A:119:LEU:HA	1:A:122:ILE:HG12	1.93	0.51
1:A:140:SER:O	1:A:142:GLY:N	2.44	0.51
1:A:171:ILE:HG22	1:A:171:ILE:O	2.10	0.51
1:A:147:SER:CB	1:A:190:THR:OG1	2.52	0.51
2:B:49:ILE:HG13	2:B:50:ASN:H	1.76	0.51
4:F:340:THR:O	4:F:340:THR:HG22	2.11	0.51
4:F:8:HIS:HE1	4:F:21:TRP:HE1	1.59	0.51
2:G:180:THR:CG2	2:G:182:VAL:HG22	2.41	0.51
3:D:328:ALA:CA	4:F:409:VAL:CG1	2.88	0.50
2:G:404:PHE:HD1	2:G:404:PHE:H	1.58	0.50
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.46	0.50
2:B:323:MET:HG3	2:B:328:VAL:CG2	2.41	0.50
4:F:315:CYS:SG	4:F:377:MET:CE	2.99	0.50
2:B:113:GLU:HG3	2:B:114:LEU:N	2.26	0.50
2:G:2:ARG:NH1	2:G:133:GLN:HA	2.27	0.50
2:G:29:GLY:O	2:G:36:TYR:HA	2.11	0.50
2:B:240:THR:HG23	2:B:241:CYS:H	1.76	0.50
2:B:333:LEU:O	2:B:336:GLN:N	2.44	0.50
4:F:270:ALA:O	4:F:302:MET:HG2	2.12	0.50
2:G:163:ASP:OD1	2:G:164:ARG:HD2	2.11	0.50
1:A:310:GLY:HA3	1:A:383:ALA:N	2.26	0.50
1:A:402:ARG:O	1:A:403:ALA:O	2.29	0.50
2:B:265:LEU:O	2:B:266:HIS:O	2.29	0.50
2:B:369:ARG:C	2:B:369:ARG:HD2	2.32	0.50
1:A:115:ILE:CG2	1:A:116:ASP:N	2.75	0.50
1:A:9:VAL:HG21	1:A:149:PHE:CD1	2.46	0.50
1:A:305:CYS:O	1:A:306:ASP:C	2.49	0.50
2:B:173:PRO:HB3	2:B:183:GLU:HG2	1.93	0.50
2:G:7:ILE:O	2:G:137:LEU:HA	2.12	0.50
1:A:133:GLN:HB3	1:A:243:ARG:HH12	1.76	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.50
2:B:176:LYS:CE	2:B:207:GLU:HG3	2.39	0.50
2:B:21:TRP:HZ2	2:B:65:ALA:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:HA	2:B:51:VAL:HA	1.93	0.50
1:A:132:LEU:CD2	1:A:164:LYS:HE3	2.41	0.50
2:B:156:LYS:CE	2:B:156:LYS:HA	2.38	0.50
2:B:209:LEU:O	2:B:210:TYR:C	2.48	0.50
4:F:176:GLN:H	4:F:176:GLN:HE21	1.58	0.50
2:G:236:SER:O	2:G:240:THR:HG23	2.11	0.50
1:A:115:ILE:HD11	1:A:119:LEU:HG	1.92	0.49
1:A:11:GLN:O	1:A:14:VAL:HB	2.12	0.49
2:B:168:THR:O	2:B:201:THR:HA	2.12	0.49
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.77	0.49
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.94	0.49
2:B:336:GLN:HE22	2:B:349:ASN:ND2	2.10	0.49
2:B:345:GLU:O	2:B:347:ILE:N	2.45	0.49
2:G:153:LEU:O	2:G:157:ILE:HG12	2.11	0.49
2:G:165:ILE:HD11	2:G:252:LEU:HG	1.93	0.49
2:G:251:ASP:HB2	2:G:254:LYS:HD2	1.94	0.49
1:A:133:GLN:CB	1:A:243:ARG:HH12	2.24	0.49
1:A:414:GLU:OE1	1:A:414:GLU:N	2.46	0.49
2:B:69:ASP:HA	2:B:145:THR:HG21	1.95	0.49
3:D:101:CYS:O	3:D:124:CYS:HA	2.12	0.49
3:D:217:GLU:HG2	3:D:226:LEU:HD21	1.95	0.49
3:D:345:GLY:HA3	3:D:402:LEU:CD1	2.42	0.49
4:F:48:SER:O	4:F:243:ARG:O	2.29	0.49
3:D:114:LEU:CG	4:F:263:PRO:HG3	2.41	0.49
2:G:135:PHE:N	2:G:135:PHE:CD1	2.80	0.49
1:A:238:ILE:O	1:A:242:LEU:HB2	2.11	0.49
1:A:244:PHE:C	1:A:244:PHE:CD2	2.83	0.49
3:D:112:VAL:N	4:F:431:ASP:OD1	2.45	0.49
1:A:227:LEU:O	1:A:231:ILE:HG12	2.12	0.49
2:B:262:PHE:O	2:B:264:ARG:N	2.45	0.49
2:B:269:MET:HB3	2:B:303:ALA:HB2	1.94	0.49
1:A:149:PHE:HE1	1:A:153:LEU:HD22	1.77	0.49
1:A:283:HIS:O	1:A:285:GLN:N	2.45	0.49
3:D:140:ARG:HH11	3:D:140:ARG:HG3	1.76	0.49
1:A:158:SER:OG	1:A:197:HIS:HB3	2.13	0.49
2:B:24:ILE:HG22	2:B:25:SER:N	2.27	0.49
2:B:431:GLU:OE1	2:B:432:TYR:N	2.46	0.49
3:D:325:MET:HG3	4:F:412:GLY:N	2.28	0.49
2:G:225:GLY:O	2:G:227:LEU:N	2.45	0.49
1:A:23:LEU:HD23	1:A:236:SER:CB	2.37	0.49
1:A:328:VAL:C	1:A:330:ALA:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LYS:HG3	2:B:177:VAL:H	1.78	0.49
2:B:173:PRO:HB3	2:B:183:GLU:CG	2.42	0.49
2:B:199:ASP:O	2:B:200:GLU:HG3	2.13	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
2:B:298:ALA:O	2:B:299:LYS:C	2.50	0.49
2:B:431:GLU:HA	2:B:434:GLN:CG	2.43	0.49
3:D:241:GLN:HA	2:G:423:SER:HG	1.72	0.49
2:B:383:ALA:C	2:B:385:GLN:H	2.15	0.49
2:B:4:ILE:HG22	2:B:5:VAL:N	2.27	0.49
3:D:238:ASP:C	2:G:419:THR:C	2.70	0.49
4:F:267:PHE:N	4:F:267:PHE:CD1	2.79	0.49
4:F:313:MET:O	4:F:314:ALA:CB	2.61	0.49
2:G:11:GLN:HG3	2:G:74:THR:HG22	1.95	0.49
1:A:163:LYS:C	1:A:164:LYS:HG2	2.33	0.49
1:A:192:HIS:CD2	1:A:424:ASP:OD2	2.66	0.49
2:B:8:GLN:HB3	2:B:14:ASN:HA	1.94	0.49
3:D:282:SER:HB2	3:D:308:ALA:HA	1.94	0.49
1:A:392:ASP:O	1:A:395:PHE:HB3	2.13	0.48
2:B:211:ASP:OD1	2:B:212:ILE:HG13	2.13	0.48
2:B:387:LEU:HD23	2:B:388:PHE:CD2	2.47	0.48
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.48
3:D:99:SER:OG	3:D:102:LEU:HB2	2.13	0.48
3:D:201:GLN:O	3:D:205:ARG:HG3	2.12	0.48
3:D:328:ALA:HA	4:F:409:VAL:CG1	2.39	0.48
2:G:393:GLU:O	2:G:397:ALA:HB2	2.12	0.48
1:A:99:ALA:O	1:A:100:ALA:HB3	2.13	0.48
1:A:191:THR:CG2	1:A:192:HIS:N	2.76	0.48
1:A:203:MET:SD	1:A:267:PHE:HB3	2.53	0.48
2:B:4:ILE:HD12	2:B:239:THR:CG2	2.42	0.48
3:D:243:VAL:HG21	3:D:360:GLN:CG	2.44	0.48
2:G:240:THR:HG21	2:G:320:ARG:NE	2.28	0.48
2:G:267:PHE:CD1	2:G:267:PHE:N	2.81	0.48
1:A:118:VAL:HG21	1:A:149:PHE:CE2	2.48	0.48
2:B:209:LEU:O	2:B:213:CYS:N	2.47	0.48
2:B:49:ILE:HG13	2:B:50:ASN:N	2.28	0.48
3:D:270:ARG:CZ	3:D:286:ALA:HB2	2.43	0.48
4:F:90:GLU:HB3	4:F:121:ARG:HD3	1.94	0.48
2:G:177:VAL:O	2:G:177:VAL:CG1	2.61	0.48
2:G:241:CYS:CB	2:G:248:LEU:CD1	2.92	0.48
1:A:151:SER:OG	1:A:193:THR:HG21	2.13	0.48
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:239:THR:O	4:F:240:ALA:C	2.52	0.48
1:A:384:ILE:HG22	1:A:388:TRP:CD1	2.49	0.48
2:B:2:ARG:NH1	2:B:251:ASP:OD2	2.46	0.48
2:B:307:PRO:HB3	2:B:312:TYR:CZ	2.49	0.48
3:D:341:ILE:O	3:D:344:LEU:HB3	2.12	0.48
4:F:163:LYS:HG3	4:F:163:LYS:H	1.48	0.48
1:A:188:ILE:O	1:A:191:THR:HG22	2.13	0.48
1:A:104:ALA:CB	1:A:408:TYR:HD2	2.26	0.48
1:A:96:LYS:O	1:A:97:GLU:O	2.31	0.48
4:F:70:LEU:O	4:F:97:GLU:O	2.31	0.48
1:A:115:ILE:O	1:A:116:ASP:C	2.51	0.48
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.49	0.48
1:A:316:CYS:HB3	1:A:378:LEU:HD12	1.95	0.48
1:A:9:VAL:HG11	1:A:150:THR:OG1	2.13	0.48
2:B:142:GLY:HA3	2:B:183:GLU:OE2	2.13	0.48
2:B:265:LEU:HD12	2:B:266:HIS:O	2.12	0.48
2:G:291:LEU:HD21	2:G:375:ALA:HB3	1.87	0.48
2:G:237:GLY:CA	2:G:376:THR:HG21	2.44	0.48
2:B:175:PRO:CD	2:B:207:GLU:OE1	2.61	0.48
2:B:264:ARG:HA	2:B:264:ARG:NE	2.29	0.48
2:B:24:ILE:CD1	2:B:52:TYR:CE1	2.97	0.48
3:D:294:THR:CG2	3:D:297:ARG:HE	2.26	0.48
4:F:102:ASN:O	4:F:103:TYR:C	2.51	0.48
4:F:204:VAL:HG13	4:F:302:MET:HE3	1.96	0.48
4:F:315:CYS:SG	4:F:377:MET:HE2	2.54	0.48
4:F:431:ASP:HA	11:F:606:HOH:O	2.12	0.48
2:G:205:ASP:HB3	2:G:303:ALA:HA	1.96	0.48
2:G:295:MET:SD	2:G:377:PHE:HB2	2.54	0.48
1:A:132:LEU:HD21	1:A:164:LYS:HE3	1.96	0.48
2:B:296:PHE:HZ	2:B:315:VAL:HG11	1.78	0.48
2:B:20:PHE:CG	2:B:235:MET:SD	3.07	0.48
2:G:385:GLN:HE21	2:G:389:LYS:HD2	1.79	0.48
10:G:701:CN2:H15	10:G:701:CN2:C12	2.43	0.48
1:A:286:LEU:CD1	1:A:290:GLU:HG2	2.44	0.47
2:B:137:LEU:HD22	2:B:154:ILE:HG21	1.94	0.47
2:B:175:PRO:O	2:B:176:LYS:C	2.52	0.47
2:B:191:VAL:HG13	2:B:192:HIS:N	2.28	0.47
2:B:209:LEU:CD2	2:B:227:LEU:HD13	2.44	0.47
2:B:297:ASP:OD2	2:B:299:LYS:HE2	2.14	0.47
2:G:180:THR:HG22	2:G:182:VAL:H	1.79	0.47
2:G:174:SER:HB2	2:G:207:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:HB2	1:A:110:ILE:HD11	1.96	0.47
1:A:242:LEU:C	1:A:244:PHE:N	2.66	0.47
1:A:274:PRO:CB	1:A:371:VAL:HG21	2.43	0.47
1:A:369:ALA:O	1:A:370:LYS:CB	2.62	0.47
4:F:115:ILE:HD13	4:F:119:LEU:HD13	1.95	0.47
4:F:167:LEU:HD11	4:F:256:GLN:NE2	2.27	0.47
4:F:229:ARG:NH1	4:F:229:ARG:CG	2.75	0.47
1:A:339:ARG:C	1:A:341:ILE:N	2.68	0.47
3:D:255:CYS:O	3:D:258:ASP:HB2	2.15	0.47
4:F:98:ASP:CB	2:G:251:ASP:OD2	2.58	0.47
2:G:33:THR:O	2:G:34:GLY:O	2.32	0.47
1:A:107:HIS:CE1	1:A:152:LEU:HB3	2.49	0.47
1:A:210:TYR:CE2	1:A:227:LEU:HD21	2.49	0.47
1:A:253:THR:O	1:A:254:GLU:C	2.52	0.47
1:A:6:SER:OG	1:A:65:ALA:HB2	2.14	0.47
2:B:272:PHE:CE1	8:B:601:TA1:H391	2.50	0.47
3:D:243:VAL:HG21	3:D:360:GLN:HG3	1.96	0.47
3:D:342:ARG:NH1	3:D:402:LEU:HD23	2.28	0.47
2:G:5:VAL:CG2	2:G:135:PHE:CD2	2.97	0.47
2:G:209:LEU:HD21	2:G:231:VAL:HG22	1.96	0.47
2:G:36:TYR:HH	2:G:40:SER:C	2.08	0.47
1:A:148:GLY:O	1:A:151:SER:CB	2.61	0.47
1:A:175:PRO:HD2	1:A:207:GLU:HB3	1.97	0.47
1:A:217:LEU:CD1	1:A:277:SER:HA	2.44	0.47
1:A:226:ASN:O	1:A:229:ARG:N	2.48	0.47
1:A:384:ILE:HG22	1:A:384:ILE:O	2.15	0.47
1:A:396:ASP:O	1:A:397:LEU:C	2.53	0.47
1:A:185:TYR:OH	1:A:399:TYR:HA	2.15	0.47
2:B:20:PHE:O	2:B:24:ILE:HB	2.14	0.47
2:B:387:LEU:O	2:B:387:LEU:HG	2.15	0.47
2:G:200:GLU:OE2	2:G:255:LEU:HD12	2.14	0.47
2:G:248:LEU:HB2	2:G:249:ASN:H	1.46	0.47
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.47
1:A:120:ASP:O	1:A:124:LYS:HB2	2.15	0.47
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.96	0.47
1:A:147:SER:O	1:A:190:THR:HG23	2.14	0.47
1:A:407:TRP:O	1:A:411:GLU:CG	2.63	0.47
1:A:99:ALA:H	2:B:2:ARG:HH22	1.63	0.47
2:B:226:ASP:O	2:B:229:HIS:HB3	2.14	0.47
4:F:71:GLU:HG3	4:F:73:THR:OG1	2.15	0.47
1:A:191:THR:O	1:A:195:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HG22	2:B:166:MET:CE	2.44	0.47
2:B:237:GLY:O	2:B:241:CYS:CB	2.61	0.47
2:B:308:ARG:HG3	2:B:342:TYR:OH	2.13	0.47
3:D:397:ASP:OD2	3:D:400:LYS:NZ	2.46	0.47
4:F:344:VAL:HG13	4:F:344:VAL:O	2.14	0.47
2:G:259:MET:SD	10:G:701:CN2:H182	2.55	0.47
1:A:154:MET:HA	1:A:157:LEU:HD12	1.97	0.47
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.97	0.47
2:B:198:THR:HG23	2:B:200:GLU:H	1.79	0.47
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.45	0.47
2:B:70:LEU:O	2:B:99:ALA:HB2	2.15	0.47
1:A:317:LEU:CD1	1:A:351:PHE:CD2	2.97	0.47
2:B:115:VAL:CG2	2:B:152:LEU:HD23	2.44	0.47
2:B:185:TYR:HD2	2:B:395:PHE:CE1	2.33	0.47
2:B:307:PRO:C	2:B:309:HIS:H	2.18	0.47
1:A:224:TYR:CG	2:B:325:MET:HG2	2.50	0.47
4:F:395:PHE:C	4:F:395:PHE:CD2	2.87	0.47
2:G:107:HIS:ND1	2:G:152:LEU:HB2	2.29	0.47
1:A:241:SER:HB3	1:A:320:ARG:NH2	2.30	0.47
1:A:255:PHE:O	1:A:256:GLN:C	2.53	0.47
4:F:70:LEU:HD23	4:F:110:ILE:CG2	2.40	0.47
4:F:191:THR:HA	4:F:194:THR:HG22	1.96	0.47
1:A:145:THR:O	1:A:149:PHE:HB3	2.15	0.47
1:A:154:MET:HE3	1:A:166:LYS:HB3	1.97	0.47
1:A:243:ARG:NH2	1:A:252:LEU:HB2	2.30	0.47
1:A:386:GLU:O	1:A:388:TRP:N	2.47	0.47
2:B:101:ASN:O	2:B:101:ASN:ND2	2.48	0.47
2:B:287:THR:N	2:B:290:GLU:OE1	2.48	0.47
2:B:360:PRO:O	2:B:369:ARG:C	2.54	0.47
2:G:154:ILE:HD12	2:G:198:THR:HG22	1.97	0.47
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.97	0.46
1:A:22:GLU:O	1:A:23:LEU:C	2.54	0.46
1:A:278:ALA:HB2	1:A:369:ALA:CA	2.45	0.46
1:A:436:GLY:O	1:A:438:ASP:N	2.48	0.46
2:B:134:GLY:HA3	2:B:165:ILE:HG12	1.97	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
2:B:175:PRO:HD2	2:B:207:GLU:CD	2.35	0.46
4:F:346:TRP:CZ3	4:F:347:CYS:HB2	2.50	0.46
2:B:154:ILE:HG22	2:B:166:MET:HE1	1.97	0.46
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.46
4:F:423:GLU:CD	11:F:698:HOH:O	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:82:THR:O	4:F:83:TYR:CB	2.63	0.46
3:D:238:ASP:HB3	2:G:419:THR:CB	2.38	0.46
1:A:10:GLY:O	1:A:11:GLN:C	2.54	0.46
1:A:166:LYS:CE	1:A:199:ASP:OD1	2.62	0.46
1:A:19:ALA:HB2	1:A:228:ASN:HB3	1.96	0.46
1:A:260:VAL:O	1:A:260:VAL:CG2	2.63	0.46
1:A:335:ILE:O	1:A:337:THR:N	2.48	0.46
1:A:34:GLY:C	1:A:61:HIS:N	2.68	0.46
2:B:137:LEU:HD22	2:B:154:ILE:HG23	1.97	0.46
1:A:114:ILE:O	1:A:118:VAL:HG23	2.16	0.46
1:A:324:VAL:HG12	1:A:326:LYS:H	1.81	0.46
1:A:392:ASP:OD2	1:A:422:ARG:NE	2.48	0.46
2:B:384:ILE:HG23	2:B:384:ILE:O	2.14	0.46
3:D:332:LYS:HG3	3:D:333:SER:N	2.31	0.46
2:G:62:VAL:O	2:G:62:VAL:HG22	2.15	0.46
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.30	0.46
1:A:117:LEU:HD12	1:A:121:ARG:HH12	1.80	0.46
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.46
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.79	0.46
1:A:95:GLY:C	1:A:97:GLU:N	2.69	0.46
1:A:224:TYR:HD1	2:B:247:GLN:HB3	1.80	0.46
2:B:408:TYR:O	2:B:411:GLU:HB2	2.15	0.46
4:F:26:LEU:HD21	4:F:364:PRO:HD3	1.96	0.46
2:G:102:ASN:OD1	2:G:105:LYS:HB2	2.15	0.46
2:G:336:GLN:OE1	2:G:351:VAL:CG1	2.58	0.46
1:A:196:GLU:C	1:A:197:HIS:HD2	2.19	0.46
1:A:210:TYR:CZ	1:A:227:LEU:HD11	2.51	0.46
1:A:23:LEU:CD2	1:A:232:GLY:O	2.64	0.46
1:A:25:CYS:SG	1:A:83:TYR:HE2	2.38	0.46
2:B:133:GLN:O	2:B:165:ILE:CD1	2.64	0.46
2:B:224:TYR:O	2:B:225:GLY:C	2.53	0.46
8:B:601:TA1:C26	8:B:601:TA1:H463	2.46	0.46
4:F:87:PHE:N	4:F:87:PHE:CD2	2.82	0.46
2:G:308:ARG:C	2:G:310:GLY:H	2.19	0.46
2:G:320:ARG:HA	2:G:356:CYS:O	2.15	0.46
1:A:241:SER:C	1:A:244:PHE:HB3	2.36	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
1:A:288:VAL:HA	1:A:291:ILE:HG12	1.98	0.46
2:B:196:GLU:O	2:B:197:ASN:OD1	2.34	0.46
4:F:313:MET:HG3	4:F:380:ASN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:112:ALA:HA	2:G:115:VAL:CG2	2.45	0.46
1:A:132:LEU:CD2	1:A:132:LEU:H	2.23	0.46
1:A:345:ASP:C	1:A:347:CYS:N	2.68	0.46
2:G:251:ASP:C	2:G:253:ARG:N	2.64	0.46
1:A:278:ALA:O	1:A:279:GLU:HG2	2.15	0.46
1:A:317:LEU:CD1	1:A:351:PHE:CE2	2.99	0.46
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.31	0.46
2:B:242:LEU:HD11	2:B:250:ALA:HB3	1.97	0.46
2:B:243:ARG:HD3	2:B:243:ARG:HA	1.62	0.46
4:F:263:PRO:O	4:F:265:ILE:N	2.38	0.46
2:G:116:ASP:O	2:G:120:ASP:HB2	2.16	0.46
1:A:256:GLN:O	1:A:260:VAL:HG13	2.15	0.46
1:A:286:LEU:O	1:A:287:SER:O	2.34	0.46
1:A:344:VAL:CG1	1:A:345:ASP:N	2.79	0.46
1:A:5:ILE:CG2	1:A:6:SER:H	2.29	0.46
2:B:274:PRO:HG2	2:B:371:LEU:CD2	2.43	0.46
3:D:375:MET:HE3	3:D:399:VAL:HG21	1.96	0.46
4:F:183:GLU:HB3	4:F:184:PRO:HD3	1.98	0.46
4:F:346:TRP:HZ2	4:F:435:VAL:HG13	1.80	0.46
2:G:5:VAL:CG2	2:G:135:PHE:HD2	2.28	0.46
1:A:115:ILE:CG1	1:A:152:LEU:HD13	2.46	0.45
1:A:308:ARG:O	1:A:309:HIS:HB3	2.17	0.45
1:A:381:THR:O	1:A:383:ALA:N	2.49	0.45
1:A:408:TYR:CG	1:A:418:PHE:HZ	2.34	0.45
1:A:423:GLU:O	1:A:426:ALA:HB3	2.16	0.45
2:B:154:ILE:HD12	2:B:155:SER:N	2.31	0.45
2:B:208:ALA:O	2:B:212:ILE:HG13	2.16	0.45
2:B:210:TYR:CE2	2:B:227:LEU:HD11	2.51	0.45
2:B:263:PRO:O	2:B:264:ARG:C	2.52	0.45
2:B:194:LEU:O	2:B:265:LEU:HD23	2.16	0.45
1:A:180:ALA:HA	2:B:352:LYS:NZ	2.30	0.45
4:F:87:PHE:N	4:F:87:PHE:HD2	2.13	0.45
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.98	0.45
1:A:148:GLY:O	1:A:149:PHE:C	2.54	0.45
1:A:203:MET:SD	1:A:267:PHE:CB	3.04	0.45
1:A:286:LEU:HG	1:A:290:GLU:HB2	1.97	0.45
1:A:404:PHE:CD1	1:A:404:PHE:N	2.83	0.45
1:A:413:MET:C	1:A:414:GLU:HG3	2.37	0.45
2:B:6:HIS:HB3	2:B:21:TRP:HZ2	1.81	0.45
2:B:243:ARG:HD3	2:B:243:ARG:N	2.26	0.45
4:F:122:ILE:HD11	4:F:157:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:CB	1:A:140:SER:OG	2.60	0.45
1:A:122:ILE:CD1	1:A:157:LEU:HD21	2.35	0.45
1:A:229:ARG:HG2	1:A:229:ARG:NH1	2.31	0.45
1:A:276:ILE:HG12	1:A:277:SER:N	2.31	0.45
1:A:392:ASP:OD2	1:A:422:ARG:CZ	2.65	0.45
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.98	0.45
2:B:313:LEU:O	2:B:347:ILE:HD12	2.16	0.45
3:D:342:ARG:NH1	3:D:402:LEU:CB	2.76	0.45
3:D:111:LYS:C	4:F:431:ASP:OD1	2.54	0.45
1:A:212:ILE:HD11	1:A:302:MET:H	1.82	0.45
1:A:334:THR:CG2	1:A:335:ILE:N	2.79	0.45
3:D:204:TYR:CA	3:D:207:LEU:HD23	2.40	0.45
2:G:287:THR:HG22	2:G:290:GLU:H	1.81	0.45
2:G:431:GLU:O	2:G:434:GLN:HB2	2.17	0.45
2:B:324:SER:OG	2:B:326:LYS:HB3	2.15	0.45
2:B:324:SER:O	2:B:326:LYS:N	2.50	0.45
4:F:190:THR:CG2	4:F:191:THR:N	2.79	0.45
2:G:342:TYR:N	2:G:342:TYR:HD2	2.15	0.45
2:G:273:ALA:HB2	2:G:375:ALA:HB3	1.99	0.45
1:A:434:GLU:C	1:A:436:GLY:H	2.18	0.45
1:A:9:VAL:HG21	1:A:149:PHE:HD1	1.80	0.45
2:B:113:GLU:CG	2:B:114:LEU:N	2.79	0.45
2:B:209:LEU:HD23	2:B:227:LEU:HD13	1.98	0.45
2:B:409:THR:HA	2:B:413:MET:HB3	1.99	0.45
2:G:265:LEU:O	2:G:266:HIS:C	2.55	0.45
1:A:115:ILE:HG23	1:A:116:ASP:H	1.79	0.45
1:A:182:VAL:O	1:A:184:PRO:CD	2.65	0.45
1:A:204:VAL:O	1:A:204:VAL:HG12	2.17	0.45
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.99	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:CD2	2.51	0.45
4:F:132:LEU:HG	4:F:133:GLN:N	2.31	0.45
4:F:174:ALA:HA	4:F:175:PRO:HD2	1.66	0.45
4:F:82:THR:O	4:F:83:TYR:HB2	2.17	0.45
2:G:150:GLY:O	2:G:154:ILE:HG23	2.17	0.45
1:A:231:ILE:HD13	1:A:231:ILE:H	1.82	0.45
1:A:271:THR:O	1:A:376:CYS:HA	2.17	0.45
1:A:104:ALA:HB1	1:A:413:MET:HG3	1.95	0.45
2:B:11:GLN:O	2:B:14:ASN:HB3	2.16	0.45
2:B:194:LEU:C	2:B:196:GLU:N	2.70	0.45
2:B:23:VAL:O	2:B:25:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:HD22	2:B:250:ALA:O	2.17	0.45
2:B:230:LEU:HD21	2:B:302:MET:HE2	1.98	0.45
2:B:102:ASN:OD1	2:B:408:TYR:CZ	2.70	0.45
3:D:397:ASP:HA	3:D:400:LYS:NZ	2.32	0.45
4:F:298:PRO:HA	4:F:301:GLN:HE21	1.82	0.45
1:A:110:ILE:CG2	1:A:111:GLY:N	2.71	0.45
1:A:152:LEU:HD12	1:A:152:LEU:C	2.38	0.45
1:A:278:ALA:CA	1:A:282:TYR:OH	2.65	0.45
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.82	0.45
3:D:204:TYR:O	3:D:207:LEU:HB2	2.16	0.45
4:F:244:PHE:N	4:F:245:ASP:HA	2.32	0.45
3:D:328:ALA:N	4:F:409:VAL:CG1	2.80	0.45
2:G:178:SER:HB2	2:G:183:GLU:OE1	2.16	0.45
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.47	0.45
1:A:303:VAL:CG1	1:A:303:VAL:O	2.65	0.45
1:A:274:PRO:HB2	1:A:371:VAL:HG21	1.99	0.45
1:A:295:CYS:HB3	1:A:377:MET:HG2	1.99	0.45
2:B:4:ILE:HD12	2:B:239:THR:HG21	1.99	0.45
2:B:250:ALA:HB1	2:B:254:LYS:CB	2.44	0.45
2:B:288:VAL:N	2:B:289:PRO:HD2	2.32	0.45
2:B:307:PRO:C	2:B:309:HIS:N	2.71	0.45
2:B:323:MET:CE	2:B:328:VAL:HG22	2.46	0.45
4:F:174:ALA:CB	4:F:207:GLU:HB2	2.47	0.45
4:F:51:THR:HG21	4:F:242:LEU:O	2.17	0.45
2:G:250:ALA:CB	10:G:701:CN2:H7	2.46	0.45
1:A:119:LEU:HD11	1:A:156:ARG:HD2	1.97	0.44
1:A:288:VAL:C	1:A:290:GLU:N	2.71	0.44
2:B:135:PHE:CD1	2:B:135:PHE:N	2.84	0.44
2:B:167:ASN:HD21	2:B:252:LEU:HD22	1.82	0.44
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.98	0.44
4:F:292:THR:O	4:F:295:CYS:HB2	2.17	0.44
4:F:318:LEU:HB2	4:F:376:CYS:HB3	1.99	0.44
2:G:269:MET:HA	2:G:270:PRO:HD3	1.75	0.44
2:G:401:ARG:O	2:G:402:LYS:C	2.55	0.44
1:A:11:GLN:HE21	1:A:74:VAL:CG2	2.29	0.44
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.52	0.44
1:A:210:TYR:CD2	1:A:227:LEU:HD21	2.51	0.44
1:A:23:LEU:O	1:A:26:LEU:HB3	2.17	0.44
1:A:4:CYS:SG	1:A:252:LEU:CD1	3.02	0.44
2:B:242:LEU:C	2:B:244:PHE:H	2.19	0.44
2:B:242:LEU:HD22	2:B:250:ALA:N	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.52	0.44
3:D:330:ILE:O	3:D:334:LEU:HG	2.17	0.44
4:F:315:CYS:SG	4:F:377:MET:HE1	2.57	0.44
1:A:153:LEU:O	1:A:157:LEU:HG	2.18	0.44
1:A:283:HIS:ND1	1:A:283:HIS:O	2.49	0.44
1:A:362:VAL:HG13	1:A:368:LEU:CG	2.48	0.44
2:B:175:PRO:HG2	2:B:207:GLU:OE1	2.16	0.44
2:B:189:LEU:HD23	2:B:421:ALA:CB	2.47	0.44
2:B:239:THR:O	2:B:240:THR:C	2.56	0.44
2:B:288:VAL:N	2:B:289:PRO:CD	2.80	0.44
2:B:72:PRO:O	2:B:74:THR:N	2.50	0.44
3:D:295:LYS:C	3:D:297:ARG:H	2.19	0.44
4:F:97:GLU:OE2	2:G:164:ARG:NH1	2.50	0.44
1:A:286:LEU:O	1:A:287:SER:C	2.55	0.44
2:B:295:MET:SD	2:B:375:ALA:HB3	2.57	0.44
4:F:151:SER:O	4:F:155:GLU:HG2	2.17	0.44
4:F:251:ASP:OD1	4:F:251:ASP:O	2.36	0.44
2:G:308:ARG:NH1	2:G:342:TYR:HE1	2.15	0.44
1:A:12:ALA:HB2	7:B:500:GTP:C8	2.52	0.44
1:A:268:PRO:CA	1:A:379:SER:O	2.65	0.44
2:B:106:GLY:O	2:B:149:MET:HB2	2.16	0.44
2:B:182:VAL:O	2:B:183:GLU:C	2.56	0.44
2:B:8:GLN:CG	2:B:67:LEU:HD22	2.47	0.44
4:F:256:GLN:O	4:F:258:ASN:N	2.51	0.44
1:A:5:ILE:HG22	1:A:6:SER:H	1.78	0.44
2:B:108:TYR:CE1	2:B:413:MET:HE1	2.52	0.44
2:B:14:ASN:O	2:B:17:GLY:N	2.50	0.44
2:B:161:TYR:O	2:B:163:ASP:N	2.51	0.44
4:F:266:HIS:H	4:F:266:HIS:CD2	2.35	0.44
2:G:343:PHE:O	2:G:344:VAL:C	2.55	0.44
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.83	0.44
1:A:121:ARG:NH1	1:A:121:ARG:HG2	2.33	0.44
1:A:144:GLY:H	7:B:500:GTP:PG	2.41	0.44
3:D:218:ILE:HB	3:D:285:HIS:HB2	1.99	0.44
4:F:164:LYS:H	4:F:164:LYS:HG2	1.68	0.44
2:G:6:HIS:HD2	2:G:136:GLN:HG3	1.83	0.44
1:A:377:MET:O	1:A:377:MET:HG3	2.18	0.44
2:B:26:ASP:C	2:B:28:HIS:H	2.21	0.44
2:B:52:TYR:HE1	2:B:240:THR:HB	1.82	0.44
4:F:80:THR:HG22	4:F:81:GLY:N	2.33	0.44
1:A:287:SER:N	1:A:290:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ARG:HH21	2:B:252:LEU:N	2.12	0.44
2:B:312:TYR:HA	2:B:381:SER:HA	1.99	0.44
2:B:360:PRO:HG2	2:B:371:LEU:CB	2.38	0.44
2:B:82:PRO:C	2:B:84:GLY:H	2.20	0.44
4:F:260:VAL:O	4:F:260:VAL:HG23	2.18	0.44
1:A:218:ASP:C	1:A:219:ILE:HG12	2.37	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:63:PRO:HG2	1:A:91:GLN:OE1	2.17	0.43
1:A:72:PRO:HG2	1:A:73:THR:H	1.83	0.43
2:B:103:TRP:HZ3	2:B:108:TYR:CE1	2.27	0.43
2:B:141:LEU:N	2:B:141:LEU:HD12	2.33	0.43
2:B:12:CYS:C	2:B:14:ASN:N	2.71	0.43
2:B:161:TYR:CD1	2:B:161:TYR:N	2.86	0.43
2:B:310:GLY:HA3	2:B:436:GLN:NE2	2.29	0.43
2:B:229:HIS:HE2	8:B:601:TA1:H361	1.83	0.43
3:D:170:HIS:CD2	3:D:175:ASP:HA	2.52	0.43
3:D:83:ASN:HB2	11:D:630:HOH:O	2.18	0.43
4:F:31:GLN:O	4:F:32:PRO:C	2.56	0.43
1:A:149:PHE:O	1:A:150:THR:C	2.56	0.43
1:A:272:TYR:CE2	1:A:274:PRO:HD2	2.53	0.43
1:A:363:VAL:CG1	1:A:364:PRO:HD2	2.48	0.43
1:A:7:ILE:HD11	1:A:137:VAL:CG2	2.44	0.43
2:B:168:THR:CG2	2:B:201:THR:HG23	2.48	0.43
2:B:301:MET:O	2:B:303:ALA:N	2.51	0.43
4:F:273:ALA:HB1	4:F:274:PRO:CD	2.35	0.43
2:G:251:ASP:O	2:G:253:ARG:N	2.50	0.43
2:G:240:THR:CG2	2:G:320:ARG:CZ	2.95	0.43
3:D:239:SER:N	2:G:419:THR:CG2	2.71	0.43
1:A:230:LEU:O	1:A:231:ILE:C	2.57	0.43
1:A:310:GLY:HA3	1:A:383:ALA:CA	2.49	0.43
2:B:212:ILE:O	2:B:212:ILE:HG22	2.18	0.43
2:B:72:PRO:HG2	2:B:73:GLY:H	1.83	0.43
2:G:378:ILE:HD12	10:G:701:CN2:C4	2.48	0.43
1:A:11:GLN:NE2	1:A:74:VAL:HG22	2.30	0.43
2:B:7:ILE:N	2:B:136:GLN:O	2.51	0.43
2:B:68:VAL:HG11	2:B:153:LEU:HD21	2.00	0.43
2:B:288:VAL:C	2:B:290:GLU:N	2.70	0.43
3:D:283:ARG:HD2	3:D:283:ARG:HH11	1.60	0.43
3:D:328:ALA:N	4:F:409:VAL:HG12	2.33	0.43
1:A:132:LEU:HD23	1:A:132:LEU:N	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:C	1:A:16:ILE:HG22	2.38	0.43
1:A:172:TYR:CD1	1:A:173:PRO:N	2.80	0.43
1:A:343:PHE:CE1	1:A:351:PHE:HE1	2.36	0.43
2:B:24:ILE:CG2	2:B:25:SER:N	2.80	0.43
4:F:6:SER:O	4:F:65:ALA:HA	2.19	0.43
2:G:111:GLY:HA2	2:G:149:MET:CE	2.49	0.43
1:A:238:ILE:HD11	1:A:378:LEU:HD23	2.01	0.43
1:A:238:ILE:O	1:A:242:LEU:CB	2.67	0.43
1:A:304:LYS:HG3	1:A:304:LYS:O	2.18	0.43
2:B:187:ALA:O	2:B:188:THR:C	2.57	0.43
2:B:422:GLU:O	2:B:426:ASN:CB	2.67	0.43
4:F:359:PRO:HA	4:F:360:PRO:HD3	1.84	0.43
1:A:101:ASN:ND2	2:B:254:LYS:CD	2.76	0.43
1:A:263:PRO:O	1:A:264:ARG:C	2.56	0.43
1:A:425:MET:O	1:A:428:LEU:N	2.45	0.43
2:B:114:LEU:HD23	2:B:149:MET:HE1	2.01	0.43
2:B:161:TYR:C	2:B:163:ASP:N	2.71	0.43
2:B:383:ALA:C	2:B:385:GLN:N	2.72	0.43
3:D:176:LEU:HB2	3:D:181:GLN:HB2	2.00	0.43
4:F:143:GLY:O	4:F:147:SER:OG	2.33	0.43
4:F:358:GLU:HA	4:F:359:PRO:HD3	1.84	0.43
1:A:154:MET:CE	1:A:166:LYS:HB3	2.48	0.43
1:A:21:TRP:HE1	1:A:63:PRO:HB3	1.83	0.43
1:A:209:ILE:CD1	1:A:231:ILE:CD1	2.97	0.43
1:A:63:PRO:C	1:A:64:ARG:CG	2.83	0.43
1:A:76:ASP:O	1:A:79:ARG:N	2.52	0.43
2:B:210:TYR:O	2:B:214:PHE:N	2.52	0.43
4:F:152:LEU:HA	4:F:155:GLU:HG3	2.01	0.43
4:F:205:ASP:HB2	4:F:303:VAL:HA	2.00	0.43
2:G:118:VAL:O	2:G:122:VAL:HG13	2.19	0.43
2:G:298:ALA:O	2:G:300:ASN:N	2.52	0.43
2:G:400:ARG:HE	2:G:400:ARG:HB2	1.56	0.43
1:A:378:LEU:O	1:A:378:LEU:HD12	2.19	0.43
2:B:105:LYS:HG2	2:B:110:GLU:CG	2.48	0.43
2:B:311:ARG:NH1	2:B:311:ARG:HG2	2.34	0.43
2:B:192:HIS:NE2	2:B:420:GLU:HG2	2.34	0.43
3:D:167:GLY:HA2	9:D:500:ANP:H8	2.00	0.43
3:D:239:SER:N	2:G:419:THR:CB	2.82	0.43
2:G:209:LEU:HD21	2:G:231:VAL:CG2	2.48	0.43
2:B:118:VAL:O	2:B:122:VAL:HG13	2.19	0.43
2:B:333:LEU:O	2:B:334:ASN:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:PHE:CD2	2:B:94:PHE:N	2.83	0.43
4:F:68:VAL:HG11	4:F:118:VAL:HG21	2.01	0.43
1:A:230:LEU:O	1:A:233:GLN:N	2.35	0.42
1:A:25:CYS:SG	1:A:26:LEU:N	2.92	0.42
1:A:409:VAL:C	1:A:411:GLU:N	2.71	0.42
2:B:359:PRO:CB	2:B:360:PRO:HD2	2.45	0.42
1:A:15:GLN:NE2	7:B:500:GTP:N7	2.67	0.42
2:B:82:PRO:HB2	2:B:83:PHE:H	1.56	0.42
4:F:210:TYR:CE1	4:F:214:ARG:HD2	2.54	0.42
4:F:71:GLU:HG2	4:F:71:GLU:O	2.17	0.42
2:G:141:LEU:HD12	2:G:141:LEU:HA	1.81	0.42
1:A:363:VAL:HG13	1:A:364:PRO:HD2	2.01	0.42
2:B:421:ALA:O	2:B:422:GLU:C	2.58	0.42
2:B:48:ARG:HG2	2:B:243:ARG:HB3	2.01	0.42
2:B:35:SER:CB	2:B:59:ASN:HA	2.42	0.42
2:B:72:PRO:O	2:B:73:GLY:C	2.58	0.42
3:D:85:GLN:NE2	3:D:85:GLN:H	2.16	0.42
4:F:54:SER:O	4:F:56:THR:N	2.52	0.42
1:A:103:TYR:O	1:A:104:ALA:C	2.57	0.42
1:A:8:HIS:CD2	1:A:138:PHE:CD1	3.07	0.42
1:A:231:ILE:C	1:A:233:GLN:N	2.73	0.42
1:A:402:ARG:O	1:A:405:VAL:N	2.49	0.42
2:B:11:GLN:O	2:B:15:GLN:N	2.41	0.42
2:B:280:SER:OG	2:B:281:GLN:N	2.49	0.42
2:G:106:GLY:O	2:G:111:GLY:HA3	2.19	0.42
1:A:105:ARG:O	1:A:110:ILE:CG2	2.64	0.42
1:A:8:HIS:HA	1:A:138:PHE:HB2	2.00	0.42
1:A:436:GLY:C	1:A:438:ASP:N	2.72	0.42
2:B:409:THR:C	2:B:411:GLU:H	2.22	0.42
3:D:237:GLU:OE2	2:G:423:SER:HB3	2.18	0.42
1:A:119:LEU:HD11	1:A:156:ARG:HD3	2.01	0.42
1:A:147:SER:HB2	1:A:186:ASN:O	2.19	0.42
1:A:67:PHE:HB2	1:A:92:LEU:HD23	2.02	0.42
2:B:427:ASP:OD1	2:B:427:ASP:C	2.58	0.42
2:B:70:LEU:HB2	2:B:99:ALA:CB	2.49	0.42
4:F:277:SER:HA	4:F:367:ASP:O	2.19	0.42
4:F:306:ASP:HA	4:F:307:PRO:HD3	1.57	0.42
1:A:328:VAL:C	1:A:330:ALA:N	2.73	0.42
1:A:390:ARG:HG3	1:A:390:ARG:HH11	1.83	0.42
2:B:103:TRP:HB2	2:B:186:ASN:HA	2.01	0.42
2:B:106:GLY:O	2:B:149:MET:CA	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:TYR:O	2:B:211:ASP:C	2.57	0.42
2:B:250:ALA:CB	2:B:254:LYS:HE2	2.50	0.42
3:D:112:VAL:HB	4:F:431:ASP:C	2.39	0.42
4:F:84:ARG:HE	4:F:84:ARG:HB3	1.65	0.42
2:G:264:ARG:O	2:G:266:HIS:N	2.51	0.42
2:G:319:PHE:CD1	2:G:319:PHE:N	2.87	0.42
1:A:213:CYS:O	1:A:219:ILE:HG13	2.20	0.42
2:B:150:GLY:HA2	2:B:153:LEU:CD2	2.41	0.42
2:B:204:ILE:HD13	2:B:231:VAL:CG2	2.45	0.42
2:B:333:LEU:HD11	2:B:337:ASN:HD21	1.85	0.42
2:B:343:PHE:CD2	2:B:350:ASN:ND2	2.88	0.42
2:B:435:TYR:C	2:B:437:ASP:N	2.72	0.42
2:B:6:HIS:HB3	2:B:65:ALA:CB	2.48	0.42
3:D:112:VAL:HB	4:F:431:ASP:CA	2.47	0.42
4:F:179:THR:HB	4:F:180:ALA:H	1.73	0.42
4:F:21:TRP:CH2	4:F:63:PRO:HB3	2.55	0.42
4:F:62:VAL:HA	4:F:63:PRO:HD3	1.85	0.42
1:A:207:GLU:O	1:A:210:TYR:N	2.51	0.42
1:A:199:ASP:CB	1:A:256:GLN:NE2	2.77	0.42
1:A:175:PRO:HG3	1:A:304:LYS:CB	2.50	0.42
1:A:95:GLY:C	1:A:97:GLU:H	2.24	0.42
2:B:2:ARG:NH1	2:B:251:ASP:CG	2.73	0.42
2:B:273:ALA:HB1	2:B:291:LEU:HG	2.01	0.42
3:D:113:ASP:O	3:D:114:LEU:HB2	2.19	0.42
4:F:153:LEU:HD22	4:F:157:LEU:HG	2.01	0.42
4:F:407:TRP:CE2	2:G:257:VAL:HA	2.54	0.42
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.42
1:A:384:ILE:C	1:A:386:GLU:N	2.72	0.42
2:B:138:THR:O	2:B:139:HIS:HB3	2.19	0.42
2:B:153:LEU:HD13	2:B:153:LEU:N	2.34	0.42
2:B:171:VAL:O	2:B:171:VAL:HG12	2.20	0.42
2:B:242:LEU:HB3	2:B:250:ALA:O	2.20	0.42
2:B:273:ALA:CB	2:B:274:PRO:CD	2.93	0.42
2:B:399:PHE:O	2:B:401:ARG:N	2.53	0.42
3:D:304:LEU:N	3:D:304:LEU:CD2	2.82	0.42
1:A:210:TYR:OH	2:B:325:MET:HB3	2.20	0.42
1:A:242:LEU:HD11	1:A:250:VAL:HG23	2.02	0.42
1:A:255:PHE:O	1:A:257:THR:N	2.53	0.42
1:A:388:TRP:CE3	1:A:425:MET:HE3	2.55	0.42
2:B:188:THR:HA	2:B:425:MET:HE3	2.00	0.42
2:B:240:THR:HG23	2:B:241:CYS:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:335:LEU:CD1	4:F:402:ARG:HG3	2.47	0.42
2:G:231:VAL:HG12	2:G:235:MET:HE2	2.02	0.42
2:G:255:LEU:HD23	10:G:701:CN2:C22	2.50	0.42
1:A:204:VAL:CG1	1:A:209:ILE:HD11	2.42	0.41
1:A:343:PHE:HZ	1:A:351:PHE:CZ	2.36	0.41
4:F:274:PRO:HG3	4:F:291:ILE:HG21	2.02	0.41
4:F:47:ASP:O	4:F:49:PHE:N	2.53	0.41
1:A:243:ARG:NH2	1:A:252:LEU:HG	2.35	0.41
1:A:175:PRO:CG	1:A:304:LYS:HG2	2.47	0.41
2:B:192:HIS:HD1	2:B:424:ASN:CG	2.20	0.41
2:B:242:LEU:HA	2:B:242:LEU:HD23	1.76	0.41
2:B:274:PRO:HD3	2:B:374:SER:HA	2.03	0.41
2:B:413:MET:CG	2:B:414:ASP:H	2.26	0.41
2:B:417:GLU:O	2:B:420:GLU:HB3	2.21	0.41
4:F:230:LEU:O	4:F:230:LEU:HD12	2.20	0.41
2:G:403:ALA:C	2:G:405:LEU:N	2.71	0.41
1:A:152:LEU:CD1	1:A:152:LEU:C	2.89	0.41
1:A:332:ILE:CD1	1:A:353:VAL:HG22	2.51	0.41
1:A:428:LEU:HA	1:A:428:LEU:HD12	1.79	0.41
2:B:175:PRO:O	2:B:177:VAL:N	2.53	0.41
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.41
2:B:307:PRO:O	2:B:309:HIS:N	2.53	0.41
2:G:133:GLN:HE21	2:G:252:LEU:CB	2.31	0.41
1:A:104:ALA:HB3	1:A:408:TYR:HD2	1.84	0.41
1:A:110:ILE:O	1:A:111:GLY:C	2.57	0.41
1:A:130:THR:O	1:A:131:GLY:C	2.59	0.41
1:A:305:CYS:SG	1:A:383:ALA:HB1	2.60	0.41
4:F:139:HIS:CD2	4:F:150:THR:HG21	2.55	0.41
4:F:291:ILE:HD12	4:F:375:VAL:HG23	2.03	0.41
2:G:332:MET:CG	2:G:353:THR:HG21	2.38	0.41
1:A:101:ASN:HD21	2:B:254:LYS:NZ	2.19	0.41
1:A:115:ILE:C	1:A:115:ILE:CD1	2.87	0.41
1:A:115:ILE:CG2	1:A:116:ASP:H	2.32	0.41
1:A:166:LYS:HB2	1:A:199:ASP:OD1	2.20	0.41
1:A:23:LEU:HD11	1:A:361:THR:O	2.21	0.41
2:B:119:LEU:O	2:B:122:VAL:HG22	2.21	0.41
2:B:259:MET:HE3	2:B:268:PHE:CE1	2.56	0.41
3:D:183:ALA:HB3	3:D:260:ILE:HG23	2.03	0.41
3:D:73:ILE:HG23	3:D:403:SER:HB3	2.03	0.41
4:F:171:ILE:HG23	4:F:206:ASN:ND2	2.35	0.41
2:G:416:MET:HG3	2:G:416:MET:H	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:427:ASP:O	2:G:431:GLU:HG3	2.20	0.41
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.93	0.41
1:A:288:VAL:O	1:A:289:ALA:C	2.59	0.41
2:B:12:CYS:O	2:B:13:GLY:C	2.59	0.41
2:B:202:TYR:CE2	2:B:268:PHE:HD1	2.38	0.41
2:B:409:THR:C	2:B:411:GLU:N	2.73	0.41
3:D:107:GLU:HA	3:D:108:PRO:HD3	1.79	0.41
2:G:198:THR:OG1	2:G:265:LEU:HD22	2.20	0.41
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.50	0.41
1:A:221:ARG:N	1:A:222:PRO:CD	2.83	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
1:A:67:PHE:CE1	1:A:87:PHE:CE2	3.08	0.41
2:B:132:LEU:O	2:B:164:ARG:HD2	2.21	0.41
2:B:135:PHE:CD1	2:B:166:MET:SD	3.14	0.41
2:B:168:THR:HB	2:B:198:THR:HG21	2.03	0.41
2:B:182:VAL:O	2:B:184:PRO:N	2.54	0.41
2:B:147:SER:CB	2:B:190:SER:HB3	2.42	0.41
2:B:380:ASN:C	2:B:380:ASN:HD22	2.24	0.41
2:G:239:THR:O	2:G:240:THR:C	2.59	0.41
2:G:208:ALA:HB2	2:G:304:ALA:N	2.35	0.41
2:G:404:PHE:CD1	2:G:404:PHE:N	2.89	0.41
2:B:98:GLY:C	2:B:100:GLY:H	2.24	0.41
2:B:199:ASP:C	2:B:265:LEU:HD13	2.41	0.41
2:G:54:ASN:O	2:G:62:VAL:O	2.39	0.41
2:G:93:VAL:HG12	2:G:114:LEU:HD11	2.01	0.41
1:A:289:ALA:HB3	1:A:290:GLU:OE2	2.20	0.41
1:A:434:GLU:C	1:A:436:GLY:N	2.74	0.41
1:A:76:ASP:O	1:A:80:THR:N	2.53	0.41
2:B:133:GLN:CG	2:B:165:ILE:HD11	2.49	0.41
2:B:276:THR:O	8:B:601:TA1:H192	2.21	0.41
3:D:237:GLU:O	2:G:423:SER:HB2	2.21	0.41
4:F:115:ILE:HG13	4:F:152:LEU:CD2	2.51	0.41
4:F:190:THR:O	4:F:194:THR:HB	2.20	0.41
4:F:392:ASP:OD1	4:F:429:GLU:OE1	2.38	0.41
2:G:164:ARG:NH2	2:G:253:ARG:HH22	2.18	0.41
1:A:149:PHE:CD1	1:A:150:THR:N	2.89	0.41
1:A:273:ALA:O	1:A:275:VAL:N	2.54	0.41
2:B:239:THR:CG2	2:B:240:THR:N	2.80	0.41
2:B:282:GLN:O	2:B:282:GLN:CG	2.65	0.41
2:B:291:LEU:HD21	2:B:373:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:217:GLU:HA	3:D:285:HIS:O	2.21	0.41
2:G:270:PRO:HA	2:G:377:PHE:O	2.21	0.41
1:A:204:VAL:CG1	1:A:231:ILE:HD12	2.42	0.41
1:A:318:LEU:HB2	1:A:376:CYS:SG	2.61	0.41
2:B:11:GLN:HA	2:B:74:THR:HG21	2.03	0.41
2:B:176:LYS:HD2	2:B:207:GLU:HB2	2.03	0.41
2:B:409:THR:O	2:B:412:GLY:N	2.48	0.41
3:D:269:CYS:SG	3:D:269:CYS:O	2.79	0.41
3:D:372:ARG:NH2	11:D:659:HOH:O	2.47	0.41
4:F:227:LEU:O	4:F:231:ILE:HG13	2.20	0.41
2:G:264:ARG:O	2:G:266:HIS:CD2	2.74	0.41
2:G:347:ILE:O	2:G:348:PRO:O	2.39	0.41
1:A:209:ILE:HD13	1:A:231:ILE:HD11	2.03	0.40
2:B:118:VAL:O	2:B:121:VAL:N	2.54	0.40
2:B:23:VAL:O	2:B:24:ILE:C	2.59	0.40
2:B:70:LEU:HB2	2:B:99:ALA:HB2	2.03	0.40
3:D:285:HIS:CD2	3:D:308:ALA:H	2.39	0.40
4:F:205:ASP:CB	4:F:303:VAL:HA	2.51	0.40
4:F:347:CYS:HA	4:F:348:PRO:HD2	1.88	0.40
2:G:224:TYR:O	2:G:228:ASN:ND2	2.54	0.40
2:G:62:VAL:HA	2:G:63:PRO:HD2	1.88	0.40
1:A:362:VAL:HG13	1:A:368:LEU:CB	2.50	0.40
1:A:320:ARG:O	1:A:373:ARG:HA	2.21	0.40
1:A:273:ALA:HB2	1:A:375:VAL:HB	2.03	0.40
2:B:25:SER:O	2:B:28:HIS:N	2.53	0.40
4:F:72:PRO:O	4:F:74:VAL:N	2.55	0.40
2:G:358:ILE:O	2:G:358:ILE:CG2	2.68	0.40
1:A:100:ALA:HB2	1:A:105:ARG:HD3	2.02	0.40
1:A:425:MET:O	1:A:426:ALA:C	2.60	0.40
2:B:20:PHE:CD2	2:B:235:MET:CG	3.04	0.40
4:F:238:ILE:HG23	4:F:255:PHE:HZ	1.86	0.40
2:G:89:PRO:O	2:G:92:PHE:HD1	2.03	0.40
1:A:217:LEU:HD12	1:A:277:SER:CB	2.49	0.40
1:A:286:LEU:HG	1:A:290:GLU:CB	2.52	0.40
1:A:401:LYS:O	1:A:402:ARG:HB2	2.21	0.40
1:A:413:MET:C	1:A:414:GLU:CG	2.90	0.40
1:A:14:VAL:HG11	1:A:75:ILE:HD13	2.04	0.40
1:A:98:ASP:N	1:A:98:ASP:OD1	2.55	0.40
2:B:99:ALA:O	2:B:100:GLY:C	2.60	0.40
3:D:284:SER:O	3:D:308:ALA:HB2	2.22	0.40
3:D:241:GLN:CA	2:G:423:SER:OG	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:HD2	1:A:284:GLU:HG3	1.86	0.40
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.81	0.40
2:B:274:PRO:CB	2:B:371:LEU:HD21	2.52	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	5
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	6
2	G	415/445 (93%)	310 (75%)	57 (14%)	48 (12%)	0	8
3	D	291/331 (88%)	275 (94%)	13 (4%)	3 (1%)	18	61
4	F	415/451 (92%)	316 (76%)	59 (14%)	40 (10%)	1	13
All	All	1953/2123 (92%)	1440 (74%)	307 (16%)	206 (10%)	1	10

All (206) 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
1	A	249	ASN
1	A	255	PHE

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Mol	Chain	Res	Type
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
3	D	238	ASP
3	D	282	SER

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Mol	Chain	Res	Type
4	F	11	GLN
4	F	55	GLU
4	F	62	VAL
4	F	73	THR
4	F	178	SER
4	F	240	ALA
4	F	253	THR
4	F	265	ILE
4	F	266	HIS
4	F	273	ALA
4	F	314	ALA
4	F	345	ASP
4	F	348	PRO
4	F	377	MET
2	G	3	GLU
2	G	11	GLN
2	G	42	LEU
2	G	43	GLN
2	G	60	LYS
2	G	62	VAL
2	G	115	VAL
2	G	159	GLU
2	G	217	LEU
2	G	218	LYS
2	G	220	THR
2	G	264	ARG
2	G	265	LEU
2	G	266	HIS
2	G	273	ALA
2	G	276	THR
2	G	288	VAL
2	G	348	PRO
2	G	371	LEU
2	G	404	PHE
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

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Mol	Chain	Res	Type
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
4	F	72	PRO
4	F	83	TYR
4	F	144	GLY
4	F	164	LYS
4	F	246	GLY
4	F	305	CYS
4	F	350	GLY
4	F	357	TYR
4	F	403	ALA
2	G	34	GLY
2	G	73	GLY
2	G	82	PRO
2	G	109	THR
2	G	163	ASP
2	G	225	GLY
2	G	227	LEU
2	G	245	PRO
2	G	249	ASN
2	G	299	LYS
2	G	308	ARG
2	G	349	ASN
2	G	370	GLY
2	G	400	ARG
2	G	402	LYS
2	G	403	ALA
1	A	104	ALA
1	A	148	GLY

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Mol	Chain	Res	Type
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	34	GLY
2	B	83	PHE
2	B	99	ALA
2	B	100	GLY
2	B	302	MET
2	B	386	GLU
4	F	59	GLY
4	F	112	LYS
4	F	175	PRO
4	F	257	THR
4	F	264	ARG
4	F	349	THR
2	G	226	ASP
2	G	244	PHE
2	G	340	SER
1	A	89	PRO
1	A	129	CYS
1	A	256	GLN
1	A	300	ASN
1	A	348	PRO
2	B	96	GLN
2	B	395	PHE
4	F	32	PRO
4	F	48	SER
4	F	101	ASN
4	F	109	THR
4	F	248	LEU
2	G	47	GLU
2	G	99	ALA
2	G	246	GLY
2	G	252	LEU
2	G	344	VAL

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Mol	Chain	Res	Type
1	A	303	VAL
1	A	382	THR
2	B	57	ALA
2	B	74	THR
2	B	285	ALA
2	B	424	ASN
4	F	34	GLY
4	F	241	SER
2	G	37	HIS
2	G	39	ASP
2	G	146	GLY
1	A	31	GLN
1	A	273	ALA
1	A	307	PRO
2	B	51	VAL
2	B	58	GLY
2	B	145	THR
2	B	162	PRO
2	B	400	ARG
3	D	354	ARG
4	F	4	CYS
2	G	240	THR
2	B	195	VAL
4	F	162	GLY
1	A	115	ILE
4	F	274	PRO
2	B	72	PRO
4	F	10	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/377 (92%)	298 (86%)	49 (14%)	4	22
2	B	367/381 (96%)	307 (84%)	60 (16%)	3	17
2	G	348/381 (91%)	241 (69%)	107 (31%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	261/286 (91%)	237 (91%)	24 (9%)	11	37
4	F	336/378 (89%)	229 (68%)	107 (32%)	0	2
All	All	1659/1803 (92%)	1312 (79%)	347 (21%)	4	8

All (347) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
3	D	73	ILE
3	D	97	VAL
3	D	119	GLU
3	D	175	ASP
3	D	182	ASN
3	D	213	VAL
3	D	215	PHE
3	D	239	SER
3	D	240	ARG

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Mol	Chain	Res	Type
3	D	241	GLN
3	D	242	GLN
3	D	244	GLN
3	D	249	GLN
3	D	280	ASN
3	D	281	SER
3	D	283	ARG
3	D	297	ARG
3	D	302	PHE
3	D	311	GLU
3	D	342	ARG
3	D	370	ASN
3	D	387	GLU
3	D	390	LEU
3	D	398	ARG
4	F	2	ARG
4	F	4	CYS
4	F	9	VAL
4	F	16	ILE
4	F	20	CYS
4	F	22	GLU
4	F	27	GLU
4	F	36	MET
4	F	50	ASN
4	F	51	THR
4	F	62	VAL
4	F	68	VAL
4	F	73	THR
4	F	74	VAL
4	F	79	ARG
4	F	80	THR
4	F	82	THR
4	F	85	GLN
4	F	87	PHE
4	F	88	HIS
4	F	90	GLU
4	F	91	GLN
4	F	94	THR
4	F	97	GLU
4	F	101	ASN
4	F	105	ARG
4	F	110	ILE

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Mol	Chain	Res	Type
4	F	112	LYS
4	F	114	ILE
4	F	115	ILE
4	F	116	ASP
4	F	120	ASP
4	F	122	ILE
4	F	123	ARG
4	F	124	LYS
4	F	128	GLN
4	F	140	SER
4	F	141	PHE
4	F	145	THR
4	F	147	SER
4	F	153	LEU
4	F	155	GLU
4	F	163	LYS
4	F	165	SER
4	F	176	GLN
4	F	178	SER
4	F	182	VAL
4	F	183	GLU
4	F	187	SER
4	F	193	THR
4	F	194	THR
4	F	195	LEU
4	F	198	SER
4	F	199	ASP
4	F	200	CYS
4	F	206	ASN
4	F	211	ASP
4	F	212	ILE
4	F	220	GLU
4	F	223	THR
4	F	225	THR
4	F	226	ASN
4	F	227	LEU
4	F	230	LEU
4	F	234	ILE
4	F	241	SER
4	F	242	LEU
4	F	250	VAL
4	F	251	ASP

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Mol	Chain	Res	Type
4	F	256	GLN
4	F	257	THR
4	F	258	ASN
4	F	265	ILE
4	F	271	THR
4	F	287	SER
4	F	288	VAL
4	F	306	ASP
4	F	313	MET
4	F	315	CYS
4	F	316	CYS
4	F	329	ASN
4	F	340	THR
4	F	341	ILE
4	F	343	PHE
4	F	344	VAL
4	F	349	THR
4	F	355	ILE
4	F	356	ASN
4	F	358	GLU
4	F	362	VAL
4	F	363	VAL
4	F	367	ASP
4	F	368	LEU
4	F	370	LYS
4	F	371	VAL
4	F	377	MET
4	F	379	SER
4	F	381	THR
4	F	384	ILE
4	F	394	LYS
4	F	397	LEU
4	F	401	LYS
4	F	405	VAL
4	F	413	MET
4	F	414	GLU
4	F	415	GLU
4	F	430	LYS
2	G	2	ARG
2	G	4	ILE
2	G	5	VAL
2	G	11	GLN

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Mol	Chain	Res	Type
2	G	12	CYS
2	G	16	ILE
2	G	23	VAL
2	G	26	ASP
2	G	31	ASP
2	G	33	THR
2	G	36	TYR
2	G	39	ASP
2	G	40	SER
2	G	42	LEU
2	G	43	GLN
2	G	49	ILE
2	G	55	GLU
2	G	61	TYR
2	G	62	VAL
2	G	71	GLU
2	G	76	ASP
2	G	77	SER
2	G	80	SER
2	G	83	PHE
2	G	91	ASN
2	G	101	ASN
2	G	102	ASN
2	G	109	THR
2	G	120	ASP
2	G	122	VAL
2	G	130	ASP
2	G	137	LEU
2	G	138	THR
2	G	141	LEU
2	G	147	SER
2	G	151	THR
2	G	154	ILE
2	G	155	SER
2	G	156	LYS
2	G	158	ARG
2	G	164	ARG
2	G	166	MET
2	G	170	SER
2	G	171	VAL
2	G	174	SER
2	G	176	LYS

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Mol	Chain	Res	Type
2	G	177	VAL
2	G	179	ASP
2	G	181	VAL
2	G	190	SER
2	G	193	GLN
2	G	195	VAL
2	G	197	ASN
2	G	198	THR
2	G	200	GLU
2	G	209	LEU
2	G	216	THR
2	G	223	THR
2	G	224	TYR
2	G	226	ASP
2	G	230	LEU
2	G	241	CYS
2	G	242	LEU
2	G	243	ARG
2	G	244	PHE
2	G	251	ASP
2	G	253	ARG
2	G	257	VAL
2	G	258	ASN
2	G	265	LEU
2	G	269	MET
2	G	275	LEU
2	G	276	THR
2	G	286	LEU
2	G	287	THR
2	G	292	THR
2	G	294	GLN
2	G	295	MET
2	G	300	ASN
2	G	302	MET
2	G	308	ARG
2	G	313	LEU
2	G	318	VAL
2	G	320	ARG
2	G	323	MET
2	G	325	MET
2	G	336	GLN
2	G	341	SER

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Mol	Chain	Res	Type
2	G	345	GLU
2	G	350	ASN
2	G	357	ASP
2	G	358	ILE
2	G	371	LEU
2	G	374	SER
2	G	376	THR
2	G	380	ASN
2	G	384	ILE
2	G	400	ARG
2	G	401	ARG
2	G	402	LYS
2	G	405	LEU
2	G	415	GLU
2	G	416	MET
2	G	419	THR
2	G	423	SER
2	G	425	MET
2	G	430	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) 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
2	B	101	ASN
2	B	102	ASN
2	B	107	HIS
2	B	136	GLN
2	B	139	HIS

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Mol	Chain	Res	Type
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
3	D	85	GLN
3	D	182	ASN
3	D	208	ASN
3	D	244	GLN
3	D	285	HIS
3	D	370	ASN
3	D	391	ASN
4	F	8	HIS
4	F	88	HIS
4	F	91	GLN
4	F	101	ASN
4	F	107	HIS
4	F	133	GLN
4	F	139	HIS
4	F	176	GLN
4	F	206	ASN
4	F	256	GLN
4	F	258	ASN
4	F	266	HIS
4	F	301	GLN
4	F	329	ASN
4	F	372	GLN
2	G	6	HIS
2	G	43	GLN
2	G	54	ASN
2	G	136	GLN
2	G	139	HIS
2	G	294	GLN
2	G	300	ASN
2	G	339	ASN
2	G	350	ASN
2	G	380	ASN
2	G	385	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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
7	GTP	B	500	6	27,34,34	1.52	3 (11%)	27,54,54	2.15	5 (18%)
7	GDP	B	600	-	25,30,30	2.61	8 (32%)	26,47,47	3.63	9 (34%)
8	TA1	B	601	-	68,68,68	1.97	21 (30%)	105,105,105	1.33	8 (7%)
9	ANP	D	500	6	29,33,33	1.75	4 (13%)	28,52,52	3.36	11 (39%)
7	GTP	F	601	6	27,34,34	1.20	3 (11%)	27,54,54	2.02	9 (33%)
7	GDP	F	603	-	25,30,30	1.04	1 (4%)	26,47,47	2.02	6 (23%)
10	CN2	G	701	-	31,32,32	3.12	7 (22%)	28,45,45	3.04	10 (35%)

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
7	GTP	B	500	6	-	0/18/38/38	0/3/3/3
7	GDP	B	600	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TA1	B	601	-	-	0/41/127/127	0/5/7/7
9	ANP	D	500	6	-	0/13/38/38	0/3/3/3
7	GTP	F	601	6	-	0/18/38/38	0/3/3/3
7	GDP	F	603	-	-	0/12/32/32	0/3/3/3
10	CN2	G	701	-	-	0/10/27/27	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	701	CN2	C20-C21	-9.91	1.24	1.40
10	G	701	CN2	C19-C17	-7.84	1.25	1.39
10	G	701	CN2	C19-C20	-5.44	1.24	1.40
8	B	601	TA1	C08-C07	-5.15	1.25	1.38
9	D	500	ANP	PB-O2B	-3.81	1.46	1.56
7	B	600	GDP	PB-O2B	-3.54	1.40	1.54
8	B	601	TA1	C04-C03	-2.35	1.44	1.49
7	F	601	GTP	O4'-C4'	-2.31	1.39	1.45
10	G	701	CN2	C11-N1	-2.28	1.43	1.46
7	B	500	GTP	C8-N7	-2.02	1.30	1.34
8	B	601	TA1	C08-C09	2.00	1.42	1.38
8	B	601	TA1	C10-C02	2.05	1.62	1.57
8	B	601	TA1	C41-C42	2.09	1.42	1.38
7	B	600	GDP	O3'-C3'	2.10	1.47	1.43
8	B	601	TA1	C16-C15	2.14	1.56	1.52
8	B	601	TA1	C37-C29	2.18	1.54	1.51
7	F	601	GTP	PG-O3B	2.18	1.63	1.60
8	B	601	TA1	C18-C20	2.19	1.62	1.56
7	B	600	GDP	PB-O3B	2.22	1.63	1.54
8	B	601	TA1	C01-C45	2.22	1.66	1.56
8	B	601	TA1	C11-C10	2.30	1.61	1.55
7	B	600	GDP	C5-C4	2.39	1.45	1.40
8	B	601	TA1	C26-C25	2.46	1.56	1.51
8	B	601	TA1	C43-C26	2.51	1.58	1.52
7	F	603	GDP	C6-N1	2.81	1.38	1.33
10	G	701	CN2	C22-C8	2.83	1.45	1.40
8	B	601	TA1	C43-C01	2.92	1.60	1.54
8	B	601	TA1	C46-C45	3.03	1.59	1.53
8	B	601	TA1	C25-C24	3.06	1.39	1.34
9	D	500	ANP	C2-N1	3.39	1.40	1.33
7	B	600	GDP	C8-N7	3.41	1.41	1.34
8	B	601	TA1	C36-C31	3.42	1.45	1.39
8	B	601	TA1	C45-C24	3.44	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	601	TA1	O02-C03	3.47	1.42	1.34
7	F	601	GTP	C6-N1	3.78	1.39	1.33
7	B	500	GTP	PG-O3B	3.93	1.66	1.60
9	D	500	ANP	PG-O1G	3.99	1.50	1.46
7	B	600	GDP	O6-C6	4.12	1.34	1.24
8	B	601	TA1	C18-C10	4.24	1.68	1.57
9	D	500	ANP	PB-O3A	4.35	1.64	1.59
8	B	601	TA1	C05-C04	4.45	1.46	1.39
7	B	500	GTP	C6-N1	4.83	1.41	1.33
10	G	701	CN2	O6-C17	5.56	1.45	1.37
8	B	601	TA1	C06-C05	5.79	1.50	1.38
7	B	600	GDP	O4'-C1'	6.12	1.49	1.41
10	G	701	CN2	C15-C16	7.35	1.54	1.39
7	B	600	GDP	C2-N1	7.60	1.49	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	GDP	C6-C5-C4	-11.34	109.57	120.84
10	G	701	CN2	C10-C11-N1	-8.63	93.97	110.05
9	D	500	ANP	O5'-PA-O1A	-7.47	79.12	109.25
7	B	500	GTP	C5-C6-N1	-7.12	113.34	123.48
10	G	701	CN2	C13-C12-N1	-6.61	104.90	115.51
9	D	500	ANP	N3-C2-N1	-6.49	123.20	128.86
9	D	500	ANP	O3A-PB-N3B	-6.46	88.66	106.59
7	B	600	GDP	N2-C2-N1	-5.87	107.86	117.24
9	D	500	ANP	O2A-PA-O5'	-5.78	80.84	108.14
7	F	603	GDP	N3-C2-N1	-5.55	119.36	127.46
7	F	601	GTP	N3-C2-N1	-5.47	119.47	127.46
7	B	600	GDP	C4-C5-N7	-5.03	104.55	109.41
7	B	600	GDP	N3-C2-N1	-4.94	120.24	127.46
8	B	601	TA1	C06-C05-C04	-4.87	114.63	120.35
10	G	701	CN2	O3-C5-C7	-4.60	116.42	124.17
10	G	701	CN2	C10-C9-C8	-4.59	103.36	113.62
8	B	601	TA1	C05-C04-C03	-3.96	111.48	120.39
7	F	601	GTP	O3'-C3'-C4'	-3.41	101.12	111.09
7	B	500	GTP	N3-C2-N1	-3.19	122.79	127.46
7	F	603	GDP	C5-C6-N1	-2.83	119.45	123.48
8	B	601	TA1	O04-C11-C14	-2.76	101.75	108.14
9	D	500	ANP	O1G-PG-N3B	-2.74	107.70	111.79
10	G	701	CN2	C21-C22-C8	-2.73	117.47	120.48
7	F	601	GTP	C1'-N9-C4	-2.69	121.99	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	500	ANP	O4'-C4'-C3'	-2.46	100.28	105.17
7	F	601	GTP	C5-C6-N1	-2.45	120.00	123.48
7	F	603	GDP	C4-C5-N7	-2.44	107.05	109.41
9	D	500	ANP	C5-C6-N1	-2.41	112.40	119.70
7	F	601	GTP	C6-C5-C4	-2.40	118.45	120.84
7	B	500	GTP	C6-C5-C4	-2.34	118.51	120.84
7	B	500	GTP	O5'-C5'-C4'	2.02	116.15	109.00
7	B	600	GDP	O2'-C2'-C3'	2.27	119.11	111.83
7	F	601	GTP	C4'-O4'-C1'	2.33	112.25	109.77
8	B	601	TA1	O01-C01-C43	2.48	113.40	106.86
8	B	601	TA1	C45-C01-C02	2.67	115.20	111.85
10	G	701	CN2	O4-C12-N1	2.67	127.59	122.97
7	F	601	GTP	N2-C2-N1	2.69	121.54	117.24
7	F	603	GDP	C6-N1-C2	2.81	120.10	116.06
8	B	601	TA1	C17-C18-C20	2.84	109.82	102.33
7	F	601	GTP	C6-N1-C2	2.87	120.19	116.06
9	D	500	ANP	C2-N1-C6	3.04	124.08	118.77
10	G	701	CN2	C4-O2-C3	3.26	123.74	114.81
10	G	701	CN2	O4-C12-C13	3.33	127.50	121.63
7	B	600	GDP	C2'-C3'-C4'	3.35	109.15	102.62
10	G	701	CN2	O3-C5-C3	3.45	121.29	115.22
7	F	603	GDP	C4'-O4'-C1'	3.48	113.47	109.77
9	D	500	ANP	C5-C6-N6	3.48	127.57	120.47
8	B	601	TA1	C09-C04-C03	3.53	128.34	120.39
7	B	600	GDP	C2-N3-C4	3.54	119.30	115.16
9	D	500	ANP	C4'-O4'-C1'	3.57	113.57	109.77
7	B	600	GDP	C4'-O4'-C1'	4.04	114.07	109.77
7	F	601	GTP	C2-N3-C4	4.40	120.30	115.16
8	B	601	TA1	C07-C08-C09	5.20	127.35	120.21
7	F	603	GDP	C2-N3-C4	5.25	121.29	115.16
10	G	701	CN2	C20-C19-C17	5.34	142.56	129.76
7	B	500	GTP	C6-N1-C2	5.98	124.66	116.06
7	B	600	GDP	N2-C2-N3	7.66	131.89	117.75
9	D	500	ANP	O2B-PB-O1B	8.68	127.91	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	500	GTP	4	0
7	B	600	GDP	1	0
8	B	601	TA1	6	0
9	D	500	ANP	3	0
7	F	601	GTP	2	0
7	F	603	GDP	1	0
10	G	701	CN2	8	0

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.