



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 02:14 AM UTC

PDB ID : 1JFF / pdb_00001jff
Title : Refined structure of alpha-beta tubulin from zinc-induced sheets stabilized with taxol
Authors : Lowe, J.; Li, H.; Downing, K.H.; Nogales, E.
Deposited on : 2001-06-20
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

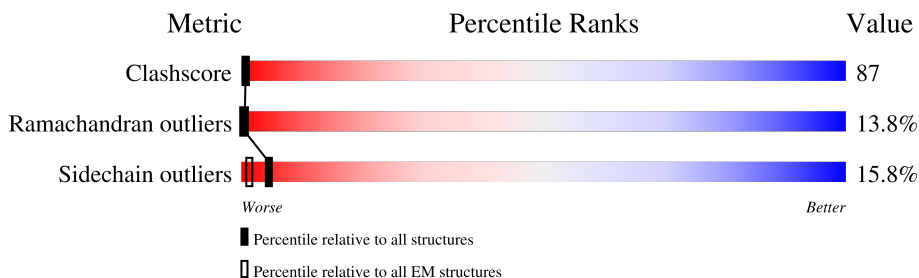
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called tubulin alpha chain.

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

- Molecule 2 is a protein called tubulin beta chain.

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

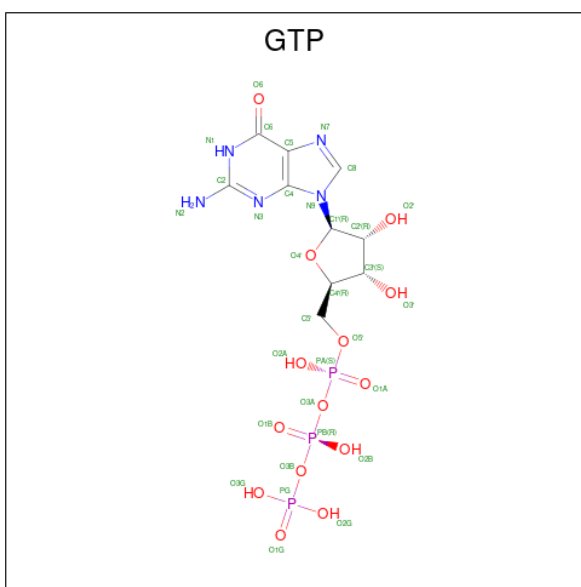
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

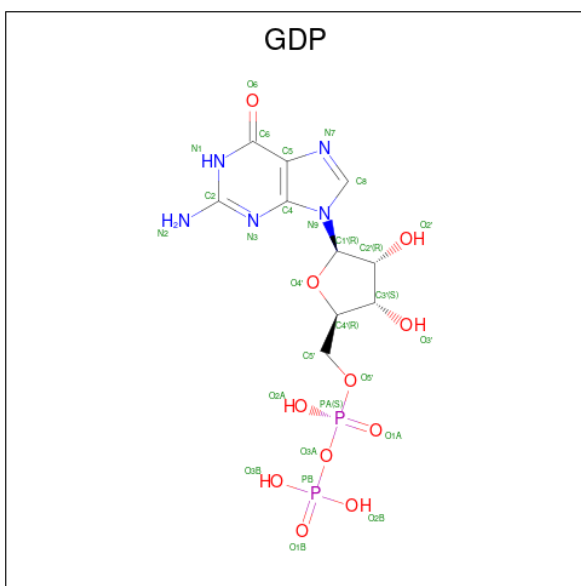
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



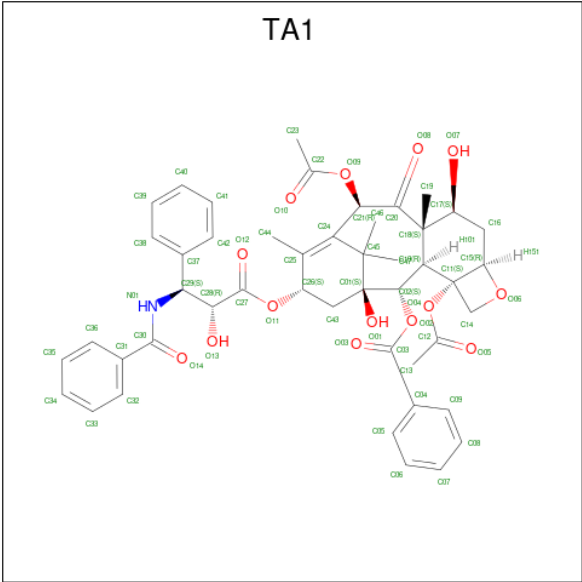
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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

- Molecule 7 is TAXOL (CCD ID: TA1) (formula: $\text{C}_{47}\text{H}_{51}\text{NO}_{14}$).

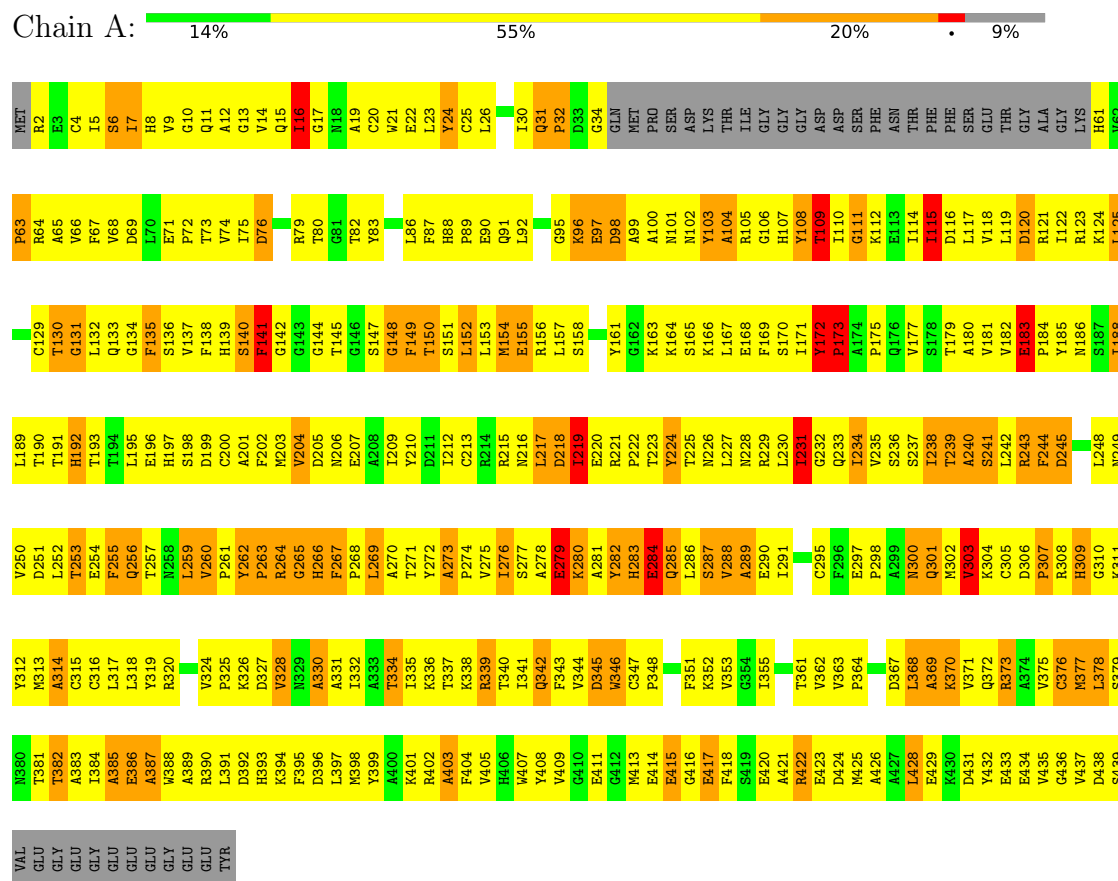


Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			62	47	1	14	

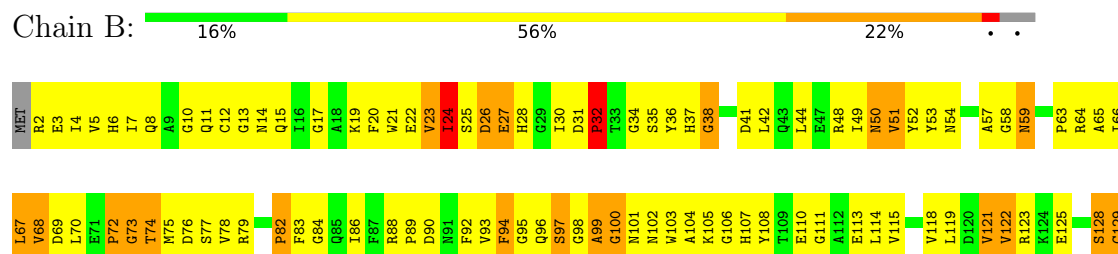
3 Residue-property plots

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

- Molecule 1: tubulin alpha chain



- Molecule 2: tubulin beta chain



GLU	L387	V315	L255	H192	L132
GLU	F388	V318	A256	Q193	Q133
ASP	K389	F319	V257	L194	G134
GLU	R390	R320	N258	V195	F135
ALA	I391	G321	M259	E196	Q136
		R322	V260	N197	F137
	F395	T396	P261	T198	L137
	T396	N323	F262	D199	T138
	F399	S324	P263	E200	H139
	R400	N325	R264	T201	S140
	R401	K326	L265	Y202	L141
	K402	E327	H266	C203	G142
	A403	V328	F267	L204	G143
	F404	D329	F268	D205	G144
	L405	E330	M269	N206	T145
	H406	Q331	P270	E207	G146
	W407	N332	G271	A208	S147
	Y408	L333	F272	L209	G148
	T409	N334	A273	Y210	M149
	G410	V335	P274	D211	G150
	E411	Q336	L275	L212	T151
	G412	N337	T276	C213	L152
	M413	Y342	S277	F214	L153
	D414	F343	R278	T215	I154
		V344	G279	T216	S155
	E417	E345	S280	L217	K156
	F418	W346	Q281	K218	I157
	T419	I347	Y283	L219	R158
	E420	P348	R284	T223	E159
	A421	N349	A285	Y224	E160
	E422	N350	L286	G225	Y161
	S423	V351	T287	D226	P162
	K424	K352	V288	L227	D163
	N425	T353	P289	N228	R164
	N426	A354	E290	H229	I165
	D427	V355	L291	L230	M166
	L428	C356	T292	V231	M167
	Y429	D357	Q293	S232	T168
	S430	T358	Q294	A233	V171
	E431	P359	M295	T234	V172
	Y432	P360	F296	M235	P173
	Q433	K369	D297	S236	S174
	Q434	G370	A298	G237	P175
	Y435	L371	K299	V238	K176
	Q436	N373	N300	T239	V177
	D437	S374	M302	C241	S178
ALA	ALA	A375	A303	L242	D179
THR	ALA	T376	A304	R243	T180
ASP	ASP	F377	G365	F244	V181
GLU	GLU	I378	D306	Q247	V182
GLN	GLN	G379	P307	P184	E183
GLY	GLY	N380	R308	L248	Y185
GLU	GLU	S381	H309	N249	N186
PHE	PHE	T382	G310	A250	A187
GLU	GLU	A383	R311	D251	T188
GLU	GLU	I384	Y312	L252	L189
GLU	GLU	Q385	L313	R253	S190
GLY	GLY	E386	T314	K254	V191

4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.20Å 93.50Å 90.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.232 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	1/3300 (0.0%)	1.09	22/4482 (0.5%)
2	B	0.63	0/3426	1.11	22/4642 (0.5%)
All	All	0.62	1/6726 (0.0%)	1.10	44/9124 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	TYR	CA-C	-5.50	1.48	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	CA-C-N	10.67	133.18	119.84
1	A	172	TYR	C-N-CA	10.67	133.18	119.84
2	B	262	PHE	CA-C-N	9.98	132.32	119.84
2	B	262	PHE	C-N-CA	9.98	132.32	119.84
1	A	283	HIS	N-CA-C	-8.23	101.27	113.61
2	B	77	SER	N-CA-C	-7.90	104.24	114.04
2	B	159	GLU	N-CA-C	-7.79	104.26	114.31
2	B	313	LEU	N-CA-C	-7.70	103.85	113.55
1	A	428	LEU	N-CA-C	-7.52	104.34	113.97
2	B	208	ALA	N-CA-C	-7.50	102.78	112.23
2	B	293	GLN	N-CA-C	-7.36	102.94	110.97
2	B	385	GLN	N-CA-C	-7.08	103.49	111.14
1	A	301	GLN	N-CA-C	7.00	121.51	112.41
2	B	399	PHE	N-CA-C	-7.00	103.58	111.07
2	B	388	PHE	N-CA-C	-6.99	104.01	112.54
2	B	22	GLU	N-CA-C	-6.98	103.36	110.97
1	A	422	ARG	N-CA-C	-6.83	103.07	111.40
2	B	389	LYS	N-CA-C	-6.82	103.54	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ALA	N-CA-C	-6.80	103.11	111.33
1	A	188	ILE	N-CA-C	-6.69	103.19	113.16
1	A	123	ARG	N-CA-C	-6.45	105.98	114.31
2	B	217	LEU	N-CA-C	-6.42	96.51	107.23
2	B	27	GLU	N-CA-C	-6.27	105.99	113.21
2	B	181	VAL	N-CA-C	6.02	116.77	111.90
2	B	88	ARG	N-CA-C	-5.99	102.22	109.83
2	B	243	ARG	N-CA-C	-5.96	106.65	112.97
1	A	264	ARG	N-CA-C	-5.91	101.56	110.24
1	A	231	ILE	N-CA-C	-5.86	103.95	110.62
2	B	296	PHE	N-CA-C	5.80	119.98	113.02
2	B	247	GLN	N-CA-C	-5.75	105.01	111.28
1	A	415	GLU	N-CA-C	-5.59	105.56	112.38
1	A	75	ILE	N-CA-C	-5.54	104.16	111.09
1	A	262	TYR	CA-C-N	5.54	126.76	119.84
1	A	262	TYR	C-N-CA	5.54	126.76	119.84
1	A	297	GLU	N-CA-C	-5.47	101.45	109.50
2	B	59	ASN	N-CA-C	-5.46	105.63	114.09
1	A	259	LEU	N-CA-C	5.43	120.92	113.97
2	B	436	GLN	N-CA-C	-5.35	106.45	112.87
1	A	429	GLU	N-CA-C	-5.28	105.99	112.90
2	B	289	PRO	N-CA-C	-5.17	107.11	113.84
1	A	421	ALA	N-CA-C	-5.08	107.12	113.72
1	A	241	SER	N-CA-C	5.07	116.81	111.28
1	A	140	SER	N-CA-C	5.06	116.30	109.11
1	A	16	ILE	N-CA-C	-5.01	105.51	110.62

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	578	0
2	B	3351	0	3229	595	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	32	0	12	5	0
6	B	28	0	12	1	0
7	B	62	0	51	5	0
All	All	6702	0	6447	1146	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 87.

All (1146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.15
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.12
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.30	1.10
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.37	1.06
2:B:299:LYS:H	2:B:299:LYS:HD3	1.24	1.03
1:A:243:ARG:HH21	1:A:252:LEU:N	1.57	1.01
1:A:109:THR:HG22	1:A:110:ILE:N	1.70	1.01
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.43	1.00
2:B:236:SER:O	2:B:240:THR:HG23	1.61	1.00
2:B:281:GLN:O	2:B:283:TYR:N	2.00	0.95
1:A:251:ASP:N	1:A:254:GLU:HG3	1.82	0.94
2:B:332:MET:HE3	2:B:351:VAL:HG11	1.45	0.94
2:B:70:LEU:H	2:B:145:THR:HG21	1.33	0.94
1:A:316:CYS:HB3	1:A:378:LEU:HD11	1.48	0.93
1:A:98:ASP:HB2	1:A:105:ARG:HH21	1.31	0.93
1:A:237:SER:HB2	1:A:376:CYS:SG	2.08	0.93
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.48	0.93
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.47	0.92
1:A:151:SER:HB3	1:A:193:THR:HG21	1.50	0.92
1:A:251:ASP:H	1:A:254:GLU:HG3	1.33	0.92
2:B:264:ARG:O	2:B:265:LEU:HB3	1.69	0.92
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.51	0.92
2:B:147:SER:O	2:B:151:THR:HB	1.71	0.91
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.50	0.91
1:A:109:THR:HG22	1:A:110:ILE:H	1.33	0.90
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.53	0.89
2:B:101:ASN:HD21	2:B:143:GLY:HA2	1.38	0.89
1:A:343:PHE:CZ	1:A:351:PHE:CE1	2.61	0.89
1:A:122:ILE:HD12	1:A:157:LEU:HD21	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TRP:HE1	2:B:260:VAL:HG23	1.38	0.88
2:B:8:GLN:OE1	2:B:67:LEU:HD22	1.72	0.88
2:B:93:VAL:HG11	2:B:118:VAL:CG2	2.03	0.88
1:A:147:SER:HB2	1:A:190:THR:OG1	1.73	0.88
2:B:102:ASN:HD21	2:B:408:TYR:HA	1.38	0.87
2:B:323:MET:HE2	2:B:328:VAL:HG22	1.54	0.87
2:B:10:GLY:HA2	2:B:145:THR:HB	1.55	0.87
2:B:264:ARG:HB2	2:B:266:HIS:CD2	2.08	0.87
2:B:311:ARG:HD3	2:B:342:TYR:HA	1.56	0.87
2:B:360:PRO:HG2	2:B:371:LEU:HB3	1.56	0.87
1:A:110:ILE:HG23	1:A:111:GLY:H	1.38	0.86
2:B:6:HIS:CE1	2:B:8:GLN:HG2	2.10	0.86
2:B:153:LEU:O	2:B:157:ILE:HG12	1.75	0.86
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.57	0.85
2:B:276:THR:HB	2:B:281:GLN:HG3	1.56	0.85
1:A:220:GLU:C	1:A:222:PRO:HD3	2.02	0.85
2:B:234:THR:HG21	2:B:270:PRO:CB	2.06	0.85
2:B:242:LEU:HD22	2:B:250:ALA:H	1.41	0.85
2:B:209:LEU:HB3	2:B:227:LEU:HD22	1.59	0.85
1:A:316:CYS:HB3	1:A:378:LEU:CD1	2.08	0.84
2:B:20:PHE:CD2	2:B:235:MET:SD	2.71	0.84
2:B:150:GLY:HA2	2:B:153:LEU:HD22	1.59	0.83
1:A:264:ARG:O	1:A:266:HIS:N	2.09	0.83
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.60	0.83
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.57	0.83
1:A:106:GLY:O	1:A:111:GLY:HA3	1.78	0.83
2:B:287:THR:O	2:B:288:VAL:HG23	1.78	0.83
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.61	0.83
2:B:148:GLY:O	2:B:151:THR:HG22	1.79	0.83
2:B:3:GLU:O	2:B:133:GLN:HB3	1.78	0.82
1:A:151:SER:CB	1:A:193:THR:HG21	2.09	0.82
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.13	0.82
2:B:101:ASN:ND2	2:B:143:GLY:HA2	1.94	0.82
2:B:110:GLU:O	2:B:113:GLU:HG2	1.79	0.82
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.59	0.82
2:B:20:PHE:CZ	2:B:24:ILE:HD12	2.15	0.82
2:B:147:SER:HB2	2:B:190:SER:HB3	1.60	0.82
2:B:4:ILE:HD13	2:B:136:GLN:HE21	1.42	0.82
1:A:172:TYR:C	1:A:172:TYR:HD1	1.87	0.81
2:B:156:LYS:HE2	2:B:156:LYS:HA	1.61	0.81
2:B:264:ARG:HB2	2:B:266:HIS:HD2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HG13	1:A:270:ALA:HB1	1.59	0.81
2:B:324:SER:HB3	2:B:327:GLU:HG2	1.60	0.81
1:A:234:ILE:HD13	1:A:234:ILE:O	1.81	0.81
1:A:6:SER:HB3	1:A:136:SER:OG	1.81	0.81
1:A:267:PHE:N	1:A:267:PHE:CD1	2.49	0.81
1:A:248:LEU:HD23	1:A:353:VAL:O	1.80	0.80
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.46	0.80
1:A:7:ILE:HG22	1:A:66:VAL:HG22	1.63	0.80
1:A:132:LEU:HD23	1:A:132:LEU:H	1.46	0.80
2:B:236:SER:O	2:B:240:THR:CG2	2.29	0.79
2:B:68:VAL:HG12	2:B:149:MET:SD	2.22	0.79
1:A:184:PRO:HG2	1:A:398:MET:HE1	1.64	0.79
1:A:241:SER:O	1:A:244:PHE:HB3	1.82	0.79
1:A:313:MET:HB3	1:A:344:VAL:HG21	1.63	0.79
1:A:109:THR:CG2	1:A:110:ILE:N	2.44	0.79
2:B:259:MET:HA	2:B:314:THR:HG21	1.65	0.79
2:B:8:GLN:CD	2:B:67:LEU:HD22	2.08	0.78
1:A:172:TYR:C	1:A:172:TYR:CD1	2.61	0.78
2:B:413:MET:HG3	2:B:414:ASP:H	1.47	0.78
2:B:205:ASP:OD1	2:B:304:ALA:HB2	1.84	0.78
2:B:217:LEU:C	2:B:219:LEU:H	1.91	0.78
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.66	0.78
1:A:11:GLN:HG3	1:A:74:VAL:CG1	2.13	0.78
1:A:155:GLU:HA	1:A:197:HIS:ND1	1.99	0.78
2:B:242:LEU:HD13	2:B:250:ALA:C	2.08	0.78
1:A:264:ARG:C	1:A:266:HIS:H	1.91	0.77
2:B:265:LEU:HD12	2:B:265:LEU:O	1.83	0.77
1:A:199:ASP:HB3	1:A:256:GLN:NE2	1.98	0.77
1:A:69:ASP:HA	1:A:145:THR:HG21	1.66	0.77
2:B:35:SER:HB3	2:B:59:ASN:HA	1.65	0.77
2:B:192:HIS:ND1	2:B:424:ASN:OD1	2.18	0.77
1:A:221:ARG:O	1:A:221:ARG:HD3	1.85	0.77
2:B:234:THR:CG2	2:B:270:PRO:HB2	2.11	0.77
2:B:198:THR:O	2:B:265:LEU:HD22	1.85	0.77
2:B:396:THR:HG23	2:B:422:GLU:OE2	1.83	0.77
1:A:225:THR:O	1:A:229:ARG:HG3	1.86	0.76
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.67	0.76
1:A:231:ILE:HA	1:A:234:ILE:HG22	1.66	0.76
1:A:331:ALA:O	1:A:335:ILE:HG12	1.86	0.76
1:A:362:VAL:HG13	1:A:368:LEU:HD12	1.68	0.76
1:A:223:THR:HB	1:A:225:THR:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:O	1:A:164:LYS:HG2	1.86	0.76
2:B:259:MET:HG2	2:B:314:THR:HG21	1.67	0.76
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.21	0.76
1:A:276:ILE:HG23	1:A:369:ALA:CB	2.16	0.75
1:A:88:HIS:C	1:A:90:GLU:H	1.95	0.75
1:A:205:ASP:CB	1:A:303:VAL:HA	2.17	0.75
2:B:250:ALA:HA	2:B:254:LYS:HE2	1.67	0.75
2:B:19:LYS:HG3	2:B:228:ASN:CB	2.17	0.75
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.87	0.75
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.68	0.75
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.68	0.75
1:A:110:ILE:HG23	1:A:111:GLY:N	1.99	0.75
2:B:103:TRP:CZ3	2:B:108:TYR:HE1	2.05	0.75
2:B:176:LYS:HE3	2:B:207:GLU:HG3	1.68	0.74
2:B:274:PRO:HG2	2:B:371:LEU:HD21	1.70	0.74
2:B:168:THR:HB	2:B:201:THR:HG23	1.68	0.74
2:B:209:LEU:HG	2:B:230:LEU:HD22	1.69	0.74
1:A:101:ASN:ND2	2:B:254:LYS:HD2	2.02	0.74
1:A:243:ARG:HH21	1:A:252:LEU:H	0.79	0.73
1:A:306:ASP:O	1:A:308:ARG:N	2.20	0.73
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.27	0.73
1:A:104:ALA:CB	1:A:413:MET:HG3	2.18	0.73
1:A:381:THR:C	1:A:383:ALA:H	1.95	0.73
1:A:104:ALA:HB2	1:A:413:MET:HG3	1.71	0.73
1:A:242:LEU:HG	1:A:250:VAL:O	1.88	0.73
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.18	0.73
1:A:63:PRO:C	1:A:64:ARG:HG2	2.12	0.73
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.19	0.73
2:B:6:HIS:HE1	2:B:8:GLN:HG2	1.52	0.72
2:B:217:LEU:O	2:B:219:LEU:N	2.22	0.72
1:A:63:PRO:O	1:A:64:ARG:HG2	1.88	0.72
1:A:242:LEU:HD21	1:A:250:VAL:HB	1.71	0.72
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.24	0.72
2:B:108:TYR:CD1	2:B:413:MET:HE1	2.24	0.72
2:B:243:ARG:NH2	2:B:252:LEU:HG	2.05	0.72
1:A:105:ARG:O	1:A:110:ILE:HG22	1.89	0.72
2:B:76:ASP:HA	2:B:79:ARG:HG2	1.71	0.72
2:B:66:ILE:C	2:B:67:LEU:HD23	2.15	0.72
2:B:356:CYS:SG	2:B:357:ASP:N	2.62	0.72
1:A:7:ILE:HD11	1:A:137:VAL:HG22	1.71	0.72
1:A:154:MET:HE1	1:A:166:LYS:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLY:O	2:B:14:ASN:HB2	1.90	0.72
2:B:201:THR:OG1	2:B:265:LEU:HD11	1.90	0.72
1:A:112:LYS:O	1:A:115:ILE:HG22	1.89	0.71
1:A:166:LYS:HE3	1:A:199:ASP:OD1	1.90	0.71
1:A:312:TYR:O	1:A:344:VAL:HG23	1.90	0.71
1:A:234:ILE:HG21	1:A:302:MET:HE1	1.72	0.71
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.52	0.71
2:B:111:GLY:O	2:B:115:VAL:HG23	1.89	0.71
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.73	0.71
2:B:70:LEU:HG	2:B:145:THR:CG2	2.20	0.71
2:B:175:PRO:HD2	2:B:207:GLU:OE2	1.91	0.71
2:B:431:GLU:OE1	2:B:432:TYR:HA	1.91	0.71
1:A:12:ALA:HB3	1:A:140:SER:OG	1.91	0.71
1:A:148:GLY:O	1:A:151:SER:HB2	1.91	0.71
2:B:269:MET:HE2	2:B:381:SER:OG	1.91	0.71
1:A:25:CYS:HB2	1:A:30:ILE:O	1.89	0.71
2:B:237:GLY:O	2:B:241:CYS:HB3	1.90	0.71
2:B:48:ARG:HG2	2:B:243:ARG:O	1.90	0.70
2:B:265:LEU:HD12	2:B:265:LEU:C	2.16	0.70
1:A:317:LEU:HD12	1:A:351:PHE:HD2	1.56	0.70
2:B:70:LEU:HG	2:B:145:THR:HG23	1.74	0.70
2:B:325:MET:HE3	2:B:325:MET:HA	1.72	0.70
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.20	0.70
2:B:230:LEU:HD21	2:B:302:MET:HE2	1.74	0.70
1:A:237:SER:CB	1:A:376:CYS:SG	2.80	0.70
2:B:291:LEU:O	2:B:295:MET:HG3	1.91	0.70
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.74	0.70
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.06	0.70
1:A:244:PHE:HD2	1:A:245:ASP:N	1.89	0.70
1:A:133:GLN:HG2	1:A:243:ARG:HH22	1.57	0.69
1:A:371:VAL:HG12	1:A:372:GLN:H	1.57	0.69
2:B:255:LEU:O	2:B:259:MET:HG3	1.91	0.69
2:B:301:MET:HE1	2:B:377:PHE:HE2	1.58	0.69
1:A:199:ASP:HB3	1:A:256:GLN:HE21	1.57	0.69
1:A:234:ILE:HD13	1:A:234:ILE:C	2.18	0.69
1:A:243:ARG:NH2	1:A:252:LEU:N	2.28	0.69
2:B:180:THR:HG22	2:B:181:VAL:N	2.07	0.69
2:B:299:LYS:HD3	2:B:299:LYS:N	2.04	0.69
1:A:115:ILE:CD1	1:A:119:LEU:HG	2.23	0.69
2:B:251:ASP:O	2:B:253:ARG:N	2.26	0.69
2:B:257:VAL:O	2:B:257:VAL:HG12	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG22	1:A:6:SER:N	2.07	0.69
1:A:71:GLU:HG3	2:B:2:ARG:HH21	1.58	0.69
1:A:402:ARG:O	1:A:403:ALA:C	2.36	0.69
1:A:141:PHE:O	1:A:147:SER:HB3	1.94	0.68
2:B:24:ILE:HD11	2:B:52:TYR:CE1	2.28	0.68
2:B:234:THR:O	2:B:238:VAL:HG23	1.92	0.68
2:B:256:ALA:O	2:B:260:VAL:HG22	1.94	0.68
1:A:217:LEU:HD12	1:A:277:SER:HB3	1.75	0.68
1:A:394:LYS:HG2	2:B:348:PRO:HG3	1.75	0.68
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.68
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.29	0.68
1:A:221:ARG:N	1:A:222:PRO:HD3	2.09	0.68
1:A:234:ILE:CB	1:A:302:MET:HE1	2.24	0.68
2:B:325:MET:CE	2:B:355:VAL:HG21	2.24	0.68
1:A:407:TRP:HE1	2:B:260:VAL:CG2	2.07	0.68
1:A:222:PRO:HD2	2:B:326:LYS:HB3	1.74	0.67
2:B:44:LEU:HD12	2:B:49:ILE:HD13	1.76	0.67
2:B:107:HIS:CD2	2:B:151:THR:CG2	2.77	0.67
2:B:209:LEU:HD23	2:B:227:LEU:HB3	1.75	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.94	0.67
1:A:95:GLY:O	1:A:97:GLU:N	2.27	0.67
1:A:166:LYS:H	1:A:199:ASP:CG	2.03	0.67
1:A:343:PHE:CZ	1:A:351:PHE:HE1	2.08	0.67
2:B:4:ILE:HG21	2:B:136:GLN:HG2	1.76	0.67
2:B:310:GLY:HA3	2:B:436:GLN:HE21	1.59	0.67
2:B:267:PHE:N	2:B:267:PHE:CD1	2.62	0.67
1:A:259:LEU:HD11	1:A:378:LEU:CD1	2.20	0.67
2:B:182:VAL:HG23	2:B:186:ASN:HD21	1.60	0.67
2:B:242:LEU:CD2	2:B:250:ALA:H	2.06	0.67
2:B:103:TRP:HZ3	2:B:108:TYR:HE1	1.42	0.67
2:B:230:LEU:HD23	2:B:231:VAL:N	2.10	0.67
1:A:251:ASP:O	1:A:254:GLU:HB2	1.94	0.66
2:B:250:ALA:HB1	2:B:254:LYS:HB2	1.76	0.66
1:A:175:PRO:HG3	1:A:304:LYS:HG2	1.76	0.66
1:A:276:ILE:O	1:A:369:ALA:HB2	1.95	0.66
2:B:204:ILE:HD13	2:B:231:VAL:HG22	1.76	0.66
1:A:343:PHE:HZ	1:A:351:PHE:CE1	2.10	0.66
1:A:7:ILE:HD12	1:A:153:LEU:CD2	2.24	0.66
1:A:341:ILE:HG12	1:A:341:ILE:O	1.95	0.66
1:A:68:VAL:HG11	1:A:149:PHE:CZ	2.30	0.66
1:A:100:ALA:CB	1:A:105:ARG:HD3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:C	1:A:347:CYS:H	2.04	0.66
1:A:315:CYS:HB3	1:A:377:MET:HE1	1.78	0.66
1:A:313:MET:HB3	1:A:344:VAL:CG2	2.26	0.66
2:B:276:THR:HB	2:B:281:GLN:CG	2.25	0.66
2:B:413:MET:HG2	2:B:418:PHE:HE1	1.61	0.66
2:B:242:LEU:CD1	2:B:255:LEU:HD11	2.25	0.65
1:A:372:GLN:O	1:A:373:ARG:HB3	1.96	0.65
1:A:217:LEU:HD11	1:A:367:ASP:O	1.96	0.65
2:B:242:LEU:HD12	2:B:255:LEU:HD11	1.78	0.65
2:B:243:ARG:HH22	2:B:252:LEU:HG	1.59	0.65
1:A:311:LYS:HE3	1:A:342:GLN:CD	2.22	0.65
1:A:206:ASN:OD1	1:A:227:LEU:HD13	1.96	0.65
1:A:152:LEU:HA	1:A:155:GLU:HB2	1.77	0.65
1:A:172:TYR:HD1	1:A:173:PRO:N	1.93	0.65
2:B:241:CYS:O	2:B:244:PHE:HB2	1.97	0.65
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.32	0.65
2:B:281:GLN:O	2:B:283:TYR:HB2	1.96	0.65
1:A:271:THR:HG23	1:A:300:ASN:O	1.97	0.65
1:A:115:ILE:HG23	1:A:116:ASP:N	2.12	0.64
1:A:234:ILE:CG2	1:A:302:MET:HE1	2.27	0.64
1:A:305:CYS:SG	1:A:384:ILE:HD13	2.37	0.64
2:B:35:SER:HB3	2:B:59:ASN:CA	2.26	0.64
2:B:66:ILE:CD1	2:B:122:VAL:HG12	2.26	0.64
2:B:299:LYS:O	2:B:300:ASN:HB2	1.97	0.64
2:B:158:ARG:NE	2:B:197:ASN:O	2.30	0.64
2:B:324:SER:C	2:B:326:LYS:H	2.03	0.64
2:B:70:LEU:N	2:B:145:THR:HG21	2.11	0.64
2:B:229:HIS:HD1	2:B:229:HIS:C	2.05	0.64
2:B:284:ARG:O	2:B:286:LEU:N	2.31	0.64
1:A:344:VAL:HG12	1:A:345:ASP:N	2.12	0.64
2:B:172:VAL:HG11	2:B:387:LEU:CD2	2.22	0.64
2:B:63:PRO:HD2	2:B:86:ILE:HG12	1.80	0.64
1:A:224:TYR:CD1	2:B:325:MET:HG2	2.33	0.64
2:B:161:TYR:C	2:B:163:ASP:H	2.05	0.64
1:A:317:LEU:HD12	1:A:351:PHE:CD2	2.32	0.64
1:A:386:GLU:O	1:A:389:ALA:N	2.31	0.64
2:B:431:GLU:O	2:B:434:GLN:HG2	1.97	0.64
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.79	0.64
1:A:317:LEU:HD11	1:A:351:PHE:HE2	1.63	0.64
2:B:114:LEU:O	2:B:118:VAL:HG23	1.97	0.64
2:B:349:ASN:C	2:B:349:ASN:HD22	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:GLU:O	2:B:426:ASN:HB2	1.97	0.64
2:B:192:HIS:O	2:B:195:VAL:HG12	1.98	0.63
1:A:151:SER:O	1:A:155:GLU:HB2	1.98	0.63
2:B:70:LEU:H	2:B:145:THR:CG2	2.10	0.63
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.33	0.63
1:A:152:LEU:HD12	1:A:153:LEU:N	2.14	0.63
2:B:4:ILE:HA	2:B:134:GLY:O	1.99	0.63
2:B:107:HIS:HD2	2:B:151:THR:CG2	2.12	0.63
2:B:137:LEU:HD22	2:B:154:ILE:CG2	2.28	0.63
1:A:269:LEU:O	1:A:378:LEU:HA	1.99	0.63
2:B:105:LYS:O	2:B:110:GLU:HB2	1.98	0.63
7:B:601:TA1:H463	7:B:601:TA1:H261	1.80	0.63
1:A:155:GLU:HA	1:A:197:HIS:HD1	1.63	0.63
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.63
2:B:70:LEU:C	2:B:99:ALA:HB2	2.24	0.63
2:B:154:ILE:HG22	2:B:166:MET:HE2	1.81	0.63
2:B:427:ASP:O	2:B:430:SER:HB3	1.97	0.63
1:A:7:ILE:CD1	1:A:137:VAL:HG22	2.29	0.63
1:A:175:PRO:HG2	1:A:207:GLU:OE1	1.98	0.63
2:B:180:THR:CG2	2:B:181:VAL:N	2.61	0.63
1:A:315:CYS:HB3	1:A:377:MET:CE	2.29	0.63
1:A:6:SER:HB3	1:A:136:SER:HG	1.62	0.62
2:B:253:ARG:O	2:B:254:LYS:C	2.42	0.62
1:A:276:ILE:HG23	1:A:369:ALA:HB2	1.80	0.62
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.34	0.62
1:A:236:SER:O	1:A:240:ALA:HB3	1.99	0.62
1:A:278:ALA:HA	1:A:282:TYR:OH	2.00	0.62
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.81	0.62
1:A:288:VAL:O	1:A:290:GLU:N	2.33	0.62
2:B:282:GLN:O	2:B:282:GLN:HG2	1.97	0.62
1:A:102:ASN:OD1	1:A:105:ARG:HB3	1.99	0.62
1:A:119:LEU:CD2	1:A:122:ILE:HD11	2.28	0.62
1:A:407:TRP:NE1	2:B:260:VAL:HG23	2.14	0.62
2:B:133:GLN:HG3	2:B:165:ILE:HD11	1.80	0.62
2:B:70:LEU:CG	2:B:145:THR:HG23	2.30	0.62
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.30	0.62
2:B:253:ARG:O	2:B:256:ALA:N	2.33	0.62
2:B:211:ASP:OD1	2:B:212:ILE:N	2.33	0.62
1:A:267:PHE:HD1	1:A:267:PHE:H	1.47	0.62
2:B:4:ILE:HG23	2:B:134:GLY:O	2.00	0.62
1:A:179:THR:HG21	2:B:248:LEU:CD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.15	0.61
2:B:114:LEU:HD23	2:B:149:MET:CE	2.30	0.61
2:B:204:ILE:CD1	2:B:231:VAL:HG13	2.30	0.61
2:B:205:ASP:OD1	2:B:304:ALA:N	2.32	0.61
2:B:285:ALA:HB1	2:B:290:GLU:HG2	1.82	0.61
2:B:318:VAL:HA	2:B:354:ALA:HB3	1.81	0.61
1:A:7:ILE:HG22	1:A:66:VAL:CG2	2.28	0.61
1:A:88:HIS:O	1:A:90:GLU:N	2.33	0.61
1:A:115:ILE:HG13	1:A:152:LEU:HD13	1.81	0.61
2:B:230:LEU:O	2:B:233:ALA:HB3	2.00	0.61
1:A:23:LEU:HD22	1:A:232:GLY:O	1.99	0.61
2:B:243:ARG:HH21	2:B:252:LEU:H	1.45	0.61
2:B:283:TYR:C	2:B:284:ARG:HG2	2.24	0.61
1:A:168:GLU:OE1	1:A:198:SER:HB2	2.01	0.61
1:A:248:LEU:CD2	1:A:353:VAL:O	2.49	0.61
1:A:436:GLY:C	1:A:438:ASP:H	2.08	0.61
2:B:324:SER:CB	2:B:327:GLU:HG2	2.30	0.61
1:A:179:THR:HG22	2:B:352:LYS:NZ	2.15	0.61
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.82	0.61
1:A:169:PHE:CE1	1:A:235:VAL:HG22	2.36	0.61
2:B:128:SER:OG	2:B:129:CYS:N	2.34	0.61
1:A:242:LEU:C	1:A:244:PHE:H	2.09	0.60
1:A:177:VAL:CG1	2:B:329:ASP:HB3	2.31	0.60
1:A:181:VAL:HG21	2:B:258:ASN:O	2.01	0.60
2:B:172:VAL:CG1	2:B:387:LEU:HD21	2.24	0.60
2:B:188:THR:HA	2:B:425:MET:HE2	1.83	0.60
1:A:118:VAL:HG11	1:A:149:PHE:HZ	1.65	0.60
1:A:167:LEU:HA	1:A:200:CYS:O	2.01	0.60
1:A:284:GLU:O	1:A:286:LEU:N	2.35	0.60
1:A:409:VAL:C	1:A:411:GLU:H	2.09	0.60
2:B:115:VAL:HG21	2:B:152:LEU:HD23	1.84	0.60
2:B:230:LEU:CD2	2:B:302:MET:HE2	2.31	0.60
2:B:324:SER:O	2:B:328:VAL:HG23	2.01	0.60
1:A:344:VAL:HG11	1:A:346:TRP:NE1	2.16	0.60
2:B:93:VAL:CG1	2:B:118:VAL:HG22	2.19	0.60
2:B:279:GLY:O	2:B:282:GLN:HB3	2.01	0.60
1:A:115:ILE:HD13	1:A:115:ILE:O	2.02	0.60
2:B:31:ASP:O	2:B:32:PRO:C	2.44	0.60
2:B:49:ILE:O	2:B:51:VAL:N	2.35	0.60
2:B:324:SER:C	2:B:326:LYS:N	2.59	0.60
1:A:179:THR:HG21	2:B:248:LEU:HD21	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:NH1	1:A:363:VAL:HG21	2.16	0.60
1:A:362:VAL:HG13	1:A:368:LEU:HB2	1.83	0.60
1:A:191:THR:HG21	1:A:425:MET:SD	2.41	0.59
1:A:413:MET:O	1:A:414:GLU:HG3	2.02	0.59
2:B:102:ASN:ND2	2:B:407:TRP:O	2.35	0.59
2:B:30:ILE:HD13	2:B:53:TYR:CE2	2.38	0.59
1:A:177:VAL:HG11	2:B:329:ASP:HB3	1.82	0.59
1:A:11:GLN:HE21	1:A:74:VAL:HG22	1.66	0.59
1:A:369:ALA:O	1:A:370:LYS:HB3	2.03	0.59
1:A:381:THR:C	1:A:383:ALA:N	2.56	0.59
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.85	0.59
2:B:204:ILE:HG21	2:B:231:VAL:HG22	1.84	0.59
2:B:408:TYR:CG	2:B:418:PHE:HZ	2.20	0.59
2:B:151:THR:OG1	2:B:193:GLN:HB3	2.03	0.59
1:A:119:LEU:O	1:A:122:ILE:HG12	2.02	0.59
1:A:317:LEU:HD11	1:A:351:PHE:CE2	2.38	0.59
2:B:141:LEU:CD1	2:B:141:LEU:N	2.65	0.58
2:B:194:LEU:C	2:B:196:GLU:H	2.11	0.58
2:B:299:LYS:O	2:B:300:ASN:CB	2.51	0.58
2:B:424:ASN:C	2:B:424:ASN:HD22	2.09	0.58
1:A:6:SER:HA	1:A:136:SER:O	2.02	0.58
1:A:407:TRP:O	1:A:411:GLU:HG2	2.02	0.58
1:A:435:VAL:HG12	1:A:435:VAL:O	2.02	0.58
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.18	0.58
2:B:89:PRO:HA	2:B:92:PHE:CD1	2.38	0.58
2:B:299:LYS:H	2:B:299:LYS:CD	2.07	0.58
2:B:205:ASP:OD1	2:B:304:ALA:CB	2.50	0.58
2:B:307:PRO:HB3	2:B:312:TYR:OH	2.04	0.58
1:A:101:ASN:CG	2:B:254:LYS:HD2	2.28	0.58
1:A:165:SER:HA	1:A:199:ASP:OD2	2.04	0.58
1:A:371:VAL:HG12	1:A:372:GLN:N	2.17	0.58
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.33	0.58
2:B:270:PRO:HA	2:B:377:PHE:O	2.04	0.58
2:B:19:LYS:CG	2:B:228:ASN:HB3	2.31	0.58
1:A:11:GLN:CG	1:A:74:VAL:HG11	2.28	0.58
1:A:150:THR:O	1:A:151:SER:C	2.47	0.58
1:A:2:ARG:N	1:A:131:GLY:O	2.36	0.58
1:A:202:PHE:CE2	1:A:378:LEU:HD22	2.38	0.58
1:A:234:ILE:HB	1:A:302:MET:HE1	1.85	0.58
1:A:264:ARG:C	1:A:266:HIS:N	2.60	0.58
2:B:319:PHE:HA	2:B:375:ALA:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:C	1:A:216:ASN:HD22	2.12	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.03	0.58
2:B:229:HIS:C	2:B:229:HIS:ND1	2.62	0.58
1:A:338:LYS:O	1:A:340:THR:N	2.34	0.57
1:A:362:VAL:HG11	1:A:368:LEU:O	2.04	0.57
2:B:198:THR:HG22	2:B:265:LEU:HD22	1.86	0.57
1:A:313:MET:O	1:A:314:ALA:HB2	2.04	0.57
1:A:401:LYS:HZ2	2:B:346:TRP:CD1	2.20	0.57
2:B:4:ILE:HD13	2:B:136:GLN:NE2	2.17	0.57
1:A:115:ILE:HD13	1:A:115:ILE:C	2.28	0.57
2:B:149:MET:O	2:B:153:LEU:HD13	2.05	0.57
2:B:226:ASP:O	2:B:227:LEU:C	2.46	0.57
2:B:422:GLU:O	2:B:426:ASN:N	2.37	0.57
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.40	0.57
1:A:166:LYS:HD2	1:A:197:HIS:O	2.04	0.57
1:A:339:ARG:C	1:A:341:ILE:H	2.11	0.57
1:A:117:LEU:HD11	1:A:121:ARG:HH22	1.69	0.57
1:A:218:ASP:O	1:A:219:ILE:HG23	2.04	0.57
1:A:278:ALA:HB2	1:A:369:ALA:HA	1.85	0.57
1:A:345:ASP:O	1:A:347:CYS:N	2.38	0.57
2:B:30:ILE:HA	2:B:35:SER:O	2.04	0.57
2:B:345:GLU:C	2:B:347:ILE:H	2.13	0.57
1:A:196:GLU:C	1:A:197:HIS:CD2	2.82	0.57
1:A:239:THR:O	1:A:240:ALA:C	2.48	0.57
1:A:283:HIS:O	1:A:284:GLU:C	2.47	0.57
2:B:14:ASN:OD1	2:B:75:MET:HG2	2.05	0.57
2:B:312:TYR:O	2:B:344:VAL:HB	2.05	0.57
1:A:244:PHE:C	1:A:244:PHE:CD2	2.83	0.57
1:A:286:LEU:HD12	1:A:290:GLU:HG2	1.87	0.57
2:B:68:VAL:CG1	2:B:149:MET:SD	2.90	0.57
2:B:274:PRO:CG	2:B:371:LEU:HD21	2.34	0.57
2:B:301:MET:CE	2:B:377:PHE:HE2	2.17	0.57
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.35	0.56
2:B:319:PHE:CD2	2:B:375:ALA:HB2	2.40	0.56
1:A:175:PRO:HG3	1:A:304:LYS:CG	2.35	0.56
2:B:6:HIS:HB3	2:B:65:ALA:HB2	1.87	0.56
1:A:11:GLN:HE22	2:B:249:ASN:ND2	2.03	0.56
1:A:362:VAL:CG1	1:A:368:LEU:HB2	2.35	0.56
1:A:382:THR:O	1:A:382:THR:HG22	2.05	0.56
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.18	0.56
2:B:70:LEU:CD1	2:B:145:THR:HG23	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:THR:O	2:B:217:LEU:HD12	2.05	0.56
2:B:253:ARG:O	2:B:257:VAL:N	2.33	0.56
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.29	0.56
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.56
1:A:210:TYR:CE2	1:A:227:LEU:HD11	2.40	0.56
1:A:231:ILE:HA	1:A:234:ILE:CG2	2.36	0.56
1:A:394:LYS:HG2	2:B:348:PRO:CG	2.35	0.56
2:B:320:ARG:O	2:B:359:PRO:HA	2.04	0.56
1:A:63:PRO:HD3	1:A:86:LEU:O	2.04	0.56
1:A:152:LEU:HA	1:A:155:GLU:CB	2.35	0.56
1:A:179:THR:HG22	2:B:352:LYS:HZ1	1.71	0.56
2:B:19:LYS:O	2:B:23:VAL:HG23	2.06	0.56
2:B:49:ILE:O	2:B:50:ASN:C	2.48	0.56
2:B:182:VAL:HG23	2:B:186:ASN:ND2	2.20	0.56
2:B:250:ALA:CA	2:B:254:LYS:HE2	2.35	0.56
1:A:110:ILE:CG2	1:A:111:GLY:H	2.15	0.56
1:A:264:ARG:HB2	1:A:266:HIS:HD2	1.67	0.56
2:B:166:MET:HB3	2:B:198:THR:OG1	2.06	0.56
2:B:180:THR:CG2	2:B:181:VAL:H	2.17	0.56
2:B:209:LEU:O	2:B:210:TYR:C	2.48	0.56
2:B:259:MET:CA	2:B:314:THR:HG21	2.35	0.56
1:A:19:ALA:CB	1:A:228:ASN:HB3	2.35	0.56
2:B:50:ASN:O	2:B:64:ARG:NH2	2.38	0.56
1:A:147:SER:CB	1:A:190:THR:OG1	2.52	0.56
1:A:331:ALA:O	1:A:334:THR:HG22	2.05	0.56
2:B:132:LEU:CD2	2:B:164:ARG:HG3	2.32	0.56
2:B:210:TYR:HD2	2:B:227:LEU:HD21	1.71	0.56
1:A:172:TYR:OH	1:A:387:ALA:O	2.24	0.55
2:B:311:ARG:HD2	2:B:344:VAL:H	1.71	0.55
2:B:424:ASN:C	2:B:424:ASN:ND2	2.61	0.55
1:A:216:ASN:O	1:A:217:LEU:HB2	2.05	0.55
1:A:408:TYR:CD1	1:A:418:PHE:HZ	2.24	0.55
2:B:67:LEU:HD23	2:B:67:LEU:N	2.22	0.55
2:B:108:TYR:CE1	2:B:413:MET:HE1	2.40	0.55
2:B:151:THR:OG1	2:B:193:GLN:CB	2.54	0.55
1:A:150:THR:O	1:A:153:LEU:N	2.40	0.55
1:A:305:CYS:O	1:A:306:ASP:C	2.49	0.55
2:B:311:ARG:HG2	2:B:311:ARG:HH11	1.71	0.55
2:B:139:HIS:HE1	2:B:168:THR:HG23	1.71	0.55
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.41	0.55
2:B:204:ILE:HG21	2:B:231:VAL:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:THR:HG22	2:B:224:TYR:N	2.21	0.55
2:B:369:ARG:C	2:B:369:ARG:HD2	2.32	0.55
2:B:191:VAL:HA	2:B:194:LEU:HD12	1.87	0.55
2:B:298:ALA:O	2:B:299:LYS:C	2.50	0.55
2:B:191:VAL:HG11	2:B:425:MET:HE2	1.89	0.55
1:A:6:SER:O	1:A:65:ALA:HB1	2.07	0.55
1:A:381:THR:OG1	1:A:383:ALA:HB3	2.07	0.54
1:A:408:TYR:O	1:A:411:GLU:N	2.39	0.54
2:B:272:PHE:HB3	2:B:275:LEU:HD22	1.88	0.54
1:A:5:ILE:CG2	1:A:6:SER:N	2.70	0.54
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.42	0.54
2:B:20:PHE:CE2	2:B:24:ILE:HD12	2.43	0.54
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.88	0.54
1:A:253:THR:O	1:A:256:GLN:HG2	2.06	0.54
2:B:190:SER:O	2:B:194:LEU:HG	2.06	0.54
2:B:119:LEU:O	2:B:123:ARG:HG3	2.06	0.54
2:B:242:LEU:HD22	2:B:250:ALA:N	2.19	0.54
2:B:310:GLY:CA	2:B:436:GLN:HE21	2.19	0.54
1:A:17:GLY:O	1:A:21:TRP:HB2	2.08	0.54
2:B:27:GLU:O	2:B:27:GLU:HG2	2.08	0.54
2:B:44:LEU:O	2:B:49:ILE:HG12	2.07	0.54
2:B:213:CYS:SG	2:B:219:LEU:HD23	2.48	0.54
2:B:325:MET:O	2:B:329:ASP:HB2	2.07	0.54
1:A:9:VAL:CG1	1:A:139:HIS:HB3	2.38	0.54
1:A:110:ILE:O	1:A:112:LYS:N	2.41	0.54
1:A:248:LEU:HB3	1:A:355:ILE:H	1.73	0.54
2:B:323:MET:HG3	2:B:328:VAL:HG21	1.90	0.54
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.89	0.54
2:B:165:ILE:HD13	2:B:165:ILE:H	1.70	0.54
2:B:239:THR:HG22	2:B:240:THR:N	2.22	0.54
2:B:259:MET:CG	2:B:314:THR:HG21	2.36	0.54
2:B:343:PHE:O	2:B:344:VAL:O	2.26	0.54
2:B:107:HIS:HD2	2:B:151:THR:HG22	1.72	0.54
2:B:383:ALA:C	2:B:385:GLN:H	2.15	0.54
2:B:427:ASP:OD1	2:B:428:LEU:N	2.41	0.54
2:B:239:THR:O	2:B:241:CYS:N	2.41	0.54
2:B:179:ASP:HB2	6:B:600:GDP:H3'	1.90	0.54
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.42	0.53
1:A:121:ARG:O	1:A:125:LEU:HB2	2.08	0.53
1:A:243:ARG:CZ	1:A:252:LEU:HG	2.39	0.53
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.89	0.53
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.53
2:B:259:MET:HG2	2:B:314:THR:CG2	2.38	0.53
2:B:431:GLU:O	2:B:434:GLN:CG	2.56	0.53
1:A:98:ASP:O	1:A:110:ILE:HD13	2.08	0.53
1:A:101:ASN:ND2	5:A:500:GTP:O3G	2.42	0.53
2:B:322:ARG:HG3	2:B:322:ARG:HH11	1.73	0.53
1:A:5:ILE:O	1:A:136:SER:N	2.40	0.53
1:A:182:VAL:O	1:A:184:PRO:N	2.41	0.53
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.43	0.53
1:A:5:ILE:O	1:A:135:PHE:HA	2.09	0.53
2:B:68:VAL:HG12	2:B:149:MET:CE	2.38	0.53
1:A:115:ILE:O	1:A:116:ASP:C	2.51	0.53
2:B:70:LEU:HD12	2:B:145:THR:HG23	1.91	0.53
2:B:147:SER:O	2:B:151:THR:CB	2.52	0.53
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.42	0.53
1:A:163:LYS:O	1:A:163:LYS:HG2	2.08	0.53
1:A:173:PRO:HB2	1:A:391:LEU:CD1	2.38	0.53
2:B:141:LEU:HA	2:B:147:SER:HB3	1.91	0.53
2:B:346:TRP:CD1	2:B:346:TRP:H	2.27	0.53
1:A:163:LYS:C	1:A:164:LYS:HG2	2.33	0.53
2:B:5:VAL:HG23	2:B:5:VAL:O	2.09	0.53
1:A:328:VAL:C	1:A:330:ALA:H	2.16	0.52
2:B:210:TYR:CD2	2:B:227:LEU:HD21	2.44	0.52
2:B:226:ASP:O	2:B:229:HIS:N	2.42	0.52
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.52
1:A:231:ILE:HD13	1:A:231:ILE:N	2.25	0.52
1:A:275:VAL:HG21	1:A:300:ASN:OD1	2.09	0.52
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.44	0.52
2:B:212:ILE:O	2:B:216:THR:HB	2.09	0.52
2:B:331:GLN:O	2:B:335:VAL:HG23	2.08	0.52
2:B:360:PRO:HB2	7:B:601:TA1:H281	1.91	0.52
1:A:206:ASN:OD1	1:A:227:LEU:CD1	2.58	0.52
2:B:273:ALA:CB	2:B:274:PRO:HD3	2.30	0.52
1:A:8:HIS:HB3	1:A:13:GLY:O	2.09	0.52
1:A:24:TYR:CE2	1:A:240:ALA:HB2	2.45	0.52
1:A:242:LEU:C	1:A:244:PHE:N	2.66	0.52
2:B:320:ARG:HA	2:B:356:CYS:HB3	1.92	0.52
1:A:4:CYS:HA	1:A:134:GLY:O	2.10	0.52
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.90	0.52
1:A:324:VAL:O	1:A:327:ASP:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:O	1:A:397:LEU:C	2.53	0.52
2:B:188:THR:HA	2:B:425:MET:CE	2.40	0.52
2:B:288:VAL:CG2	2:B:323:MET:HE3	2.40	0.52
1:A:201:ALA:O	1:A:267:PHE:HA	2.10	0.52
1:A:255:PHE:O	1:A:256:GLN:C	2.53	0.52
2:B:295:MET:SD	2:B:375:ALA:O	2.68	0.52
1:A:253:THR:O	1:A:254:GLU:C	2.52	0.52
2:B:168:THR:CB	2:B:201:THR:HG23	2.38	0.52
2:B:175:PRO:O	2:B:176:LYS:C	2.52	0.52
2:B:264:ARG:HE	2:B:264:ARG:HA	1.75	0.52
2:B:314:THR:CG2	2:B:315:VAL:N	2.73	0.52
2:B:425:MET:O	2:B:428:LEU:HB3	2.09	0.52
1:A:23:LEU:HD23	1:A:236:SER:CB	2.37	0.52
1:A:345:ASP:C	1:A:347:CYS:N	2.68	0.52
1:A:362:VAL:HG13	1:A:368:LEU:CD1	2.38	0.52
2:B:4:ILE:CG2	2:B:136:GLN:HG2	2.38	0.52
2:B:175:PRO:HD2	2:B:207:GLU:CD	2.35	0.52
2:B:200:GLU:N	2:B:265:LEU:HD13	2.25	0.52
2:B:325:MET:CE	2:B:355:VAL:HG11	2.38	0.52
1:A:417:GLU:HA	1:A:417:GLU:OE1	2.10	0.51
2:B:103:TRP:CE2	2:B:189:LEU:HB3	2.45	0.51
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.92	0.51
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.40	0.51
1:A:140:SER:O	1:A:142:GLY:N	2.44	0.51
1:A:345:ASP:OD2	1:A:439:SER:HB3	2.10	0.51
2:B:149:MET:O	2:B:153:LEU:HD22	2.10	0.51
2:B:198:THR:HG22	2:B:265:LEU:CD2	2.39	0.51
2:B:277:SER:OG	2:B:281:GLN:HB2	2.10	0.51
2:B:297:ASP:OD1	2:B:298:ALA:N	2.39	0.51
1:A:243:ARG:NH2	1:A:251:ASP:OD1	2.44	0.51
1:A:34:GLY:C	1:A:61:HIS:N	2.68	0.51
1:A:251:ASP:OD1	1:A:252:LEU:N	2.43	0.51
1:A:95:GLY:C	1:A:97:GLU:N	2.69	0.51
1:A:231:ILE:CA	1:A:234:ILE:HG22	2.38	0.51
1:A:238:ILE:O	1:A:242:LEU:HB2	2.11	0.51
2:B:360:PRO:O	2:B:369:ARG:C	2.54	0.51
2:B:431:GLU:OE1	2:B:432:TYR:CA	2.57	0.51
1:A:171:ILE:O	1:A:171:ILE:HG22	2.10	0.51
1:A:241:SER:C	1:A:244:PHE:HB3	2.36	0.51
1:A:402:ARG:O	1:A:403:ALA:O	2.29	0.51
2:B:149:MET:O	2:B:149:MET:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:PHE:CZ	2:B:315:VAL:HG11	2.46	0.51
1:A:151:SER:HB3	1:A:193:THR:CG2	2.34	0.51
1:A:173:PRO:HB2	1:A:391:LEU:HD11	1.91	0.51
1:A:196:GLU:O	1:A:197:HIS:CD2	2.64	0.51
1:A:230:LEU:O	1:A:233:GLN:N	2.35	0.51
2:B:21:TRP:HZ2	2:B:65:ALA:HB2	1.76	0.51
1:A:67:PHE:HE1	1:A:87:PHE:CE2	2.29	0.50
2:B:49:ILE:HG13	2:B:50:ASN:H	1.76	0.50
1:A:434:GLU:C	1:A:436:GLY:H	2.18	0.50
2:B:224:TYR:O	2:B:225:GLY:C	2.53	0.50
2:B:323:MET:HG3	2:B:328:VAL:CG2	2.41	0.50
1:A:191:THR:HG23	1:A:192:HIS:N	2.25	0.50
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.46	0.50
2:B:107:HIS:CD2	2:B:151:THR:HG22	2.45	0.50
1:A:9:VAL:HG21	1:A:149:PHE:CD1	2.46	0.50
1:A:339:ARG:C	1:A:341:ILE:N	2.68	0.50
1:A:132:LEU:CD2	1:A:164:LYS:HE3	2.41	0.50
1:A:133:GLN:HB3	1:A:243:ARG:HH12	1.76	0.50
1:A:22:GLU:O	1:A:23:LEU:C	2.54	0.50
1:A:196:GLU:C	1:A:197:HIS:HD2	2.19	0.50
2:B:173:PRO:HB3	2:B:183:GLU:CG	2.42	0.50
1:A:115:ILE:CG2	1:A:116:ASP:N	2.75	0.50
1:A:119:LEU:HA	1:A:122:ILE:HG12	1.93	0.50
1:A:149:PHE:HE1	1:A:153:LEU:HD22	1.77	0.50
2:B:156:LYS:HA	2:B:156:LYS:CE	2.38	0.50
2:B:307:PRO:C	2:B:309:HIS:H	2.18	0.50
2:B:333:LEU:O	2:B:336:GLN:N	2.45	0.50
1:A:11:GLN:O	1:A:14:VAL:HB	2.12	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.50
2:B:3:GLU:HA	2:B:51:VAL:HA	1.93	0.50
2:B:24:ILE:HG22	2:B:25:SER:N	2.27	0.50
2:B:113:GLU:HG3	2:B:114:LEU:N	2.26	0.50
2:B:168:THR:O	2:B:201:THR:HA	2.12	0.50
2:B:345:GLU:O	2:B:347:ILE:N	2.45	0.50
1:A:286:LEU:O	1:A:287:SER:C	2.55	0.50
1:A:310:GLY:HA3	1:A:383:ALA:N	2.26	0.50
2:B:4:ILE:HD12	2:B:239:THR:CG2	2.42	0.50
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.94	0.50
2:B:260:VAL:HG23	2:B:260:VAL:O	2.10	0.50
2:B:269:MET:HB3	2:B:303:ALA:HB2	1.94	0.50
2:B:332:MET:CE	2:B:351:VAL:HG11	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HD11	1:A:119:LEU:HG	1.92	0.49
1:A:133:GLN:CB	1:A:243:ARG:HH12	2.24	0.49
2:B:4:ILE:HG22	2:B:5:VAL:N	2.27	0.49
2:B:173:PRO:HB3	2:B:183:GLU:HG2	1.93	0.49
2:B:262:PHE:O	2:B:264:ARG:N	2.45	0.49
2:B:431:GLU:HA	2:B:434:GLN:CG	2.42	0.49
1:A:227:LEU:O	1:A:231:ILE:HG12	2.12	0.49
1:A:244:PHE:CD2	1:A:245:ASP:N	2.76	0.49
1:A:414:GLU:OE1	1:A:414:GLU:N	2.46	0.49
2:B:265:LEU:O	2:B:266:HIS:O	2.29	0.49
1:A:148:GLY:O	1:A:149:PHE:C	2.55	0.49
2:B:240:THR:HG23	2:B:241:CYS:H	1.76	0.49
2:B:336:GLN:HE22	2:B:349:ASN:ND2	2.10	0.49
2:B:265:LEU:HD12	2:B:266:HIS:O	2.12	0.49
1:A:10:GLY:O	1:A:11:GLN:C	2.53	0.49
2:B:194:LEU:C	2:B:196:GLU:N	2.70	0.49
1:A:16:ILE:HG23	1:A:17:GLY:N	2.26	0.49
1:A:188:ILE:O	1:A:191:THR:HG22	2.13	0.49
1:A:283:HIS:O	1:A:285:GLN:N	2.45	0.49
2:B:82:PRO:C	2:B:84:GLY:H	2.20	0.49
2:B:263:PRO:O	2:B:264:ARG:C	2.52	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
1:A:12:ALA:CB	1:A:140:SER:OG	2.59	0.49
1:A:392:ASP:O	1:A:395:PHE:HB3	2.13	0.49
1:A:192:HIS:CD2	1:A:424:ASP:OD2	2.66	0.49
1:A:203:MET:SD	1:A:267:PHE:HB3	2.53	0.49
2:B:142:GLY:HA3	2:B:183:GLU:OE2	2.13	0.49
2:B:199:ASP:O	2:B:200:GLU:HG3	2.13	0.49
2:B:387:LEU:HD23	2:B:388:PHE:CD2	2.47	0.49
2:B:431:GLU:OE1	2:B:432:TYR:N	2.46	0.49
1:A:413:MET:C	1:A:414:GLU:HG3	2.36	0.49
2:B:308:ARG:HG3	2:B:342:TYR:OH	2.13	0.49
1:A:96:LYS:O	1:A:97:GLU:O	2.31	0.49
1:A:105:ARG:HH11	1:A:105:ARG:HG3	1.78	0.49
1:A:118:VAL:HG21	1:A:149:PHE:CE2	2.48	0.49
2:B:137:LEU:HD22	2:B:154:ILE:HG21	1.95	0.49
2:B:175:PRO:CD	2:B:207:GLU:OE1	2.61	0.49
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.43	0.49
1:A:88:HIS:C	1:A:90:GLU:N	2.57	0.48
1:A:152:LEU:HD12	1:A:152:LEU:C	2.38	0.48
1:A:218:ASP:C	1:A:219:ILE:HG12	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:THR:O	2:B:240:THR:C	2.56	0.48
1:A:172:TYR:CD1	1:A:173:PRO:N	2.80	0.48
2:B:20:PHE:CG	2:B:235:MET:SD	3.07	0.48
2:B:176:LYS:CE	2:B:207:GLU:HG3	2.39	0.48
2:B:191:VAL:HG13	2:B:192:HIS:N	2.28	0.48
2:B:237:GLY:O	2:B:241:CYS:CB	2.61	0.48
1:A:263:PRO:O	1:A:264:ARG:C	2.56	0.48
2:B:176:LYS:HG3	2:B:177:VAL:H	1.78	0.48
2:B:209:LEU:O	2:B:213:CYS:N	2.47	0.48
2:B:8:GLN:HB3	2:B:14:ASN:HA	1.94	0.48
2:B:242:LEU:C	2:B:244:PHE:H	2.19	0.48
1:A:98:ASP:CB	1:A:105:ARG:HH21	2.14	0.48
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.96	0.48
1:A:234:ILE:CG1	1:A:270:ALA:HB1	2.38	0.48
1:A:286:LEU:CD1	1:A:290:GLU:HG2	2.44	0.48
1:A:158:SER:OG	1:A:197:HIS:HB3	2.13	0.48
1:A:274:PRO:CB	1:A:371:VAL:HG21	2.43	0.48
2:B:49:ILE:HG13	2:B:50:ASN:N	2.28	0.48
2:B:307:PRO:HB3	2:B:312:TYR:CZ	2.49	0.48
1:A:104:ALA:CB	1:A:408:TYR:HD2	2.26	0.48
2:B:187:ALA:O	2:B:188:THR:C	2.57	0.48
1:A:13:GLY:C	1:A:16:ILE:HG22	2.38	0.48
1:A:149:PHE:O	1:A:150:THR:C	2.56	0.48
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.48
1:A:344:VAL:HG12	1:A:345:ASP:H	1.74	0.48
1:A:436:GLY:C	1:A:438:ASP:N	2.72	0.48
2:B:154:ILE:HG22	2:B:166:MET:CE	2.44	0.48
2:B:211:ASP:OD1	2:B:212:ILE:HG13	2.13	0.48
2:B:288:VAL:C	2:B:290:GLU:N	2.70	0.48
1:A:5:ILE:HG22	1:A:6:SER:H	1.78	0.48
1:A:63:PRO:C	1:A:64:ARG:CG	2.83	0.48
1:A:151:SER:OG	1:A:193:THR:HG21	2.13	0.48
1:A:252:LEU:O	1:A:253:THR:C	2.56	0.48
1:A:288:VAL:C	1:A:290:GLU:N	2.71	0.48
1:A:386:GLU:O	1:A:388:TRP:N	2.47	0.48
1:A:409:VAL:C	1:A:411:GLU:N	2.71	0.48
2:B:69:ASP:HA	2:B:145:THR:HG21	1.95	0.48
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.28	0.48
2:B:383:ALA:C	2:B:385:GLN:N	2.72	0.48
1:A:317:LEU:CD1	1:A:351:PHE:CD2	2.97	0.48
2:B:2:ARG:NH1	2:B:251:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:PRO:C	2:B:309:HIS:N	2.71	0.48
1:A:110:ILE:CG2	1:A:111:GLY:N	2.71	0.47
1:A:230:LEU:O	1:A:231:ILE:C	2.57	0.47
1:A:335:ILE:O	1:A:337:THR:N	2.47	0.47
1:A:384:ILE:HG22	1:A:388:TRP:CD1	2.49	0.47
2:B:297:ASP:OD2	2:B:299:LYS:HE2	2.14	0.47
1:A:99:ALA:O	1:A:100:ALA:HB3	2.14	0.47
1:A:147:SER:O	1:A:190:THR:HG23	2.14	0.47
1:A:175:PRO:HD2	1:A:207:GLU:HB3	1.96	0.47
1:A:241:SER:HB3	1:A:320:ARG:NH2	2.29	0.47
1:A:369:ALA:O	1:A:370:LYS:CB	2.62	0.47
2:B:384:ILE:O	2:B:384:ILE:HG23	2.14	0.47
1:A:9:VAL:HG11	1:A:150:THR:OG1	2.13	0.47
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.49	0.47
1:A:210:TYR:CE2	1:A:227:LEU:HD21	2.49	0.47
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.95	0.47
2:B:210:TYR:O	2:B:211:ASP:C	2.57	0.47
2:B:409:THR:C	2:B:411:GLU:H	2.22	0.47
1:A:97:GLU:HB2	1:A:110:ILE:HD11	1.96	0.47
1:A:191:THR:CG2	1:A:192:HIS:N	2.76	0.47
2:B:20:PHE:O	2:B:24:ILE:HB	2.14	0.47
2:B:101:ASN:ND2	2:B:101:ASN:O	2.47	0.47
2:B:243:ARG:N	2:B:243:ARG:HD3	2.26	0.47
1:A:6:SER:OG	1:A:65:ALA:HB2	2.14	0.47
1:A:166:LYS:CE	1:A:199:ASP:OD1	2.62	0.47
1:A:217:LEU:CD1	1:A:277:SER:HA	2.44	0.47
2:B:12:CYS:C	2:B:14:ASN:N	2.71	0.47
2:B:182:VAL:O	2:B:183:GLU:C	2.56	0.47
1:A:119:LEU:HD11	1:A:156:ARG:HD2	1.97	0.47
1:A:148:GLY:O	1:A:151:SER:CB	2.61	0.47
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.79	0.47
2:B:26:ASP:C	2:B:28:HIS:H	2.21	0.47
2:B:115:VAL:CG2	2:B:152:LEU:HD23	2.44	0.47
2:B:435:TYR:C	2:B:437:ASP:N	2.72	0.47
1:A:25:CYS:SG	1:A:83:TYR:HE2	2.38	0.47
1:A:99:ALA:H	2:B:2:ARG:HH22	1.63	0.47
1:A:103:TYR:O	1:A:104:ALA:C	2.57	0.47
1:A:132:LEU:HD21	1:A:164:LYS:HE3	1.96	0.47
1:A:224:TYR:CG	2:B:325:MET:HG2	2.50	0.47
1:A:226:ASN:O	1:A:229:ARG:N	2.48	0.47
1:A:404:PHE:CD1	1:A:404:PHE:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:O	2:B:99:ALA:HB2	2.15	0.47
2:B:259:MET:HE1	2:B:378:ILE:CG2	2.45	0.47
2:B:287:THR:O	2:B:288:VAL:CG2	2.58	0.47
2:B:333:LEU:O	2:B:334:ASN:C	2.58	0.47
2:B:387:LEU:O	2:B:387:LEU:HG	2.15	0.47
1:A:191:THR:O	1:A:195:LEU:HB2	2.15	0.47
1:A:328:VAL:C	1:A:330:ALA:N	2.73	0.47
1:A:407:TRP:O	1:A:411:GLU:CG	2.63	0.47
1:A:436:GLY:O	1:A:438:ASP:N	2.48	0.47
2:B:24:ILE:CD1	2:B:52:TYR:CE1	2.97	0.47
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.47
1:A:145:THR:O	1:A:149:PHE:HB3	2.15	0.47
1:A:185:TYR:OH	1:A:399:TYR:HA	2.15	0.47
1:A:224:TYR:HD1	2:B:247:GLN:HB3	1.80	0.47
1:A:278:ALA:HB2	1:A:369:ALA:CA	2.45	0.47
2:B:72:PRO:O	2:B:73:GLY:C	2.58	0.47
2:B:226:ASP:O	2:B:229:HIS:HB3	2.14	0.47
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.45	0.47
2:B:272:PHE:CE1	7:B:601:TA1:H391	2.50	0.47
1:A:9:VAL:HG21	1:A:149:PHE:HD1	1.80	0.46
1:A:120:ASP:O	1:A:124:LYS:HB2	2.15	0.46
2:B:2:ARG:NH1	2:B:251:ASP:CG	2.73	0.46
2:B:168:THR:N	2:B:200:GLU:O	2.43	0.46
2:B:198:THR:HG23	2:B:200:GLU:H	1.79	0.46
2:B:209:LEU:CD2	2:B:227:LEU:HD13	2.44	0.46
2:B:243:ARG:HH21	2:B:252:LEU:N	2.12	0.46
2:B:324:SER:OG	2:B:326:LYS:HB3	2.15	0.46
2:B:408:TYR:O	2:B:411:GLU:HB2	2.16	0.46
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.97	0.46
1:A:115:ILE:CG1	1:A:152:LEU:HD13	2.46	0.46
1:A:256:GLN:O	1:A:260:VAL:HG13	2.15	0.46
1:A:384:ILE:HG22	1:A:384:ILE:O	2.15	0.46
2:B:134:GLY:HA3	2:B:165:ILE:HG12	1.97	0.46
2:B:259:MET:HE1	2:B:378:ILE:HG21	1.98	0.46
1:A:19:ALA:HB2	1:A:228:ASN:HB3	1.96	0.46
1:A:107:HIS:CE1	1:A:152:LEU:HB3	2.49	0.46
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.97	0.46
1:A:286:LEU:HG	1:A:290:GLU:HB2	1.98	0.46
1:A:402:ARG:O	1:A:405:VAL:N	2.49	0.46
2:B:199:ASP:C	2:B:265:LEU:HD13	2.40	0.46
2:B:242:LEU:HD11	2:B:250:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:THR:C	2:B:411:GLU:N	2.73	0.46
1:A:154:MET:HA	1:A:157:LEU:HD12	1.96	0.46
1:A:317:LEU:CD1	1:A:351:PHE:CE2	2.99	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
2:B:250:ALA:HB1	2:B:254:LYS:CB	2.44	0.46
1:A:115:ILE:CD1	1:A:115:ILE:C	2.87	0.46
1:A:381:THR:O	1:A:383:ALA:N	2.49	0.46
2:B:204:ILE:HD13	2:B:231:VAL:CG2	2.45	0.46
2:B:208:ALA:O	2:B:212:ILE:HG13	2.16	0.46
2:B:287:THR:N	2:B:290:GLU:OE1	2.48	0.46
2:B:421:ALA:O	2:B:422:GLU:C	2.58	0.46
1:A:11:GLN:NE2	1:A:74:VAL:HG22	2.30	0.46
1:A:152:LEU:C	1:A:152:LEU:CD1	2.89	0.46
1:A:392:ASP:OD2	1:A:422:ARG:NE	2.48	0.46
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.31	0.46
2:B:103:TRP:HZ3	2:B:108:TYR:CE1	2.27	0.46
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.46
1:A:243:ARG:NH2	1:A:252:LEU:CB	2.78	0.46
1:A:265:GLY:O	1:A:266:HIS:O	2.33	0.46
2:B:296:PHE:HZ	2:B:315:VAL:HG11	1.78	0.46
1:A:100:ALA:C	1:A:102:ASN:H	2.24	0.46
1:A:408:TYR:CG	1:A:418:PHE:HZ	2.34	0.46
2:B:185:TYR:HD2	2:B:395:PHE:CE1	2.33	0.46
2:B:230:LEU:CG	2:B:302:MET:HE2	2.46	0.46
1:A:110:ILE:O	1:A:111:GLY:C	2.57	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:335:ILE:C	1:A:337:THR:N	2.73	0.46
1:A:231:ILE:C	1:A:233:GLN:N	2.73	0.46
1:A:243:ARG:NH2	1:A:252:LEU:HB2	2.31	0.46
1:A:286:LEU:O	1:A:287:SER:O	2.34	0.46
2:B:380:ASN:C	2:B:380:ASN:HD22	2.24	0.46
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.30	0.45
1:A:130:THR:O	1:A:131:GLY:C	2.59	0.45
1:A:210:TYR:CD2	1:A:227:LEU:HD21	2.51	0.45
1:A:274:PRO:HB2	1:A:371:VAL:HG21	1.98	0.45
1:A:276:ILE:HG12	1:A:277:SER:N	2.32	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:313:LEU:O	2:B:347:ILE:HD12	2.16	0.45
1:A:180:ALA:HA	2:B:352:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.98	0.45
1:A:334:THR:CG2	1:A:335:ILE:N	2.79	0.45
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.81	0.45
2:B:6:HIS:HB3	2:B:21:TRP:HZ2	1.81	0.45
1:A:5:ILE:CG2	1:A:6:SER:H	2.29	0.45
1:A:117:LEU:HD12	1:A:121:ARG:HH12	1.80	0.45
1:A:210:TYR:CZ	1:A:227:LEU:HD11	2.51	0.45
1:A:229:ARG:NH1	1:A:229:ARG:HG2	2.31	0.45
1:A:413:MET:C	1:A:414:GLU:CG	2.90	0.45
2:B:11:GLN:O	2:B:14:ASN:HB3	2.16	0.45
2:B:94:PHE:N	2:B:94:PHE:CD2	2.84	0.45
2:B:106:GLY:O	2:B:149:MET:HB2	2.16	0.45
2:B:188:THR:HG23	2:B:425:MET:HE3	1.98	0.45
2:B:264:ARG:HA	2:B:264:ARG:NE	2.29	0.45
1:A:203:MET:SD	1:A:267:PHE:CB	3.04	0.45
1:A:392:ASP:OD2	1:A:422:ARG:CZ	2.65	0.45
2:B:257:VAL:O	2:B:257:VAL:CG1	2.64	0.45
2:B:319:PHE:CD2	2:B:323:MET:HE1	2.52	0.45
2:B:409:THR:HA	2:B:413:MET:HB3	1.99	0.45
2:B:427:ASP:OD1	2:B:427:ASP:C	2.58	0.45
1:A:212:ILE:HD11	1:A:302:MET:H	1.82	0.45
1:A:278:ALA:O	1:A:279:GLU:HG2	2.15	0.45
1:A:308:ARG:O	1:A:309:HIS:HB3	2.17	0.45
1:A:401:LYS:C	1:A:403:ALA:H	2.24	0.45
1:A:434:GLU:C	1:A:436:GLY:N	2.74	0.45
2:B:67:LEU:HD12	2:B:92:PHE:CD2	2.51	0.45
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.98	0.45
2:B:133:GLN:O	2:B:165:ILE:CD1	2.64	0.45
2:B:194:LEU:O	2:B:265:LEU:HD23	2.16	0.45
2:B:210:TYR:CE2	2:B:227:LEU:HD11	2.51	0.45
2:B:413:MET:HG3	2:B:414:ASP:N	2.22	0.45
1:A:95:GLY:C	1:A:97:GLU:H	2.23	0.45
1:A:234:ILE:C	1:A:234:ILE:CD1	2.86	0.45
2:B:135:PHE:CD1	2:B:135:PHE:N	2.84	0.45
2:B:154:ILE:HD12	2:B:155:SER:N	2.31	0.45
2:B:273:ALA:CB	2:B:274:PRO:CD	2.93	0.45
2:B:324:SER:O	2:B:326:LYS:N	2.50	0.45
1:A:115:ILE:HG23	1:A:116:ASP:H	1.79	0.45
2:B:35:SER:CB	2:B:59:ASN:HA	2.42	0.45
2:B:409:THR:O	2:B:412:GLY:N	2.48	0.45
7:B:601:TA1:H463	7:B:601:TA1:C26	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HD11	1:A:137:VAL:CG2	2.44	0.45
1:A:393:HIS:O	1:A:394:LYS:C	2.60	0.45
1:A:423:GLU:O	1:A:426:ALA:HB3	2.16	0.45
2:B:23:VAL:O	2:B:25:SER:N	2.50	0.45
2:B:72:PRO:O	2:B:74:THR:N	2.50	0.45
2:B:102:ASN:ND2	2:B:408:TYR:HA	2.20	0.45
1:A:182:VAL:O	1:A:184:PRO:CD	2.65	0.45
1:A:244:PHE:HD2	1:A:244:PHE:C	2.24	0.45
1:A:255:PHE:O	1:A:259:LEU:N	2.50	0.45
2:B:14:ASN:O	2:B:17:GLY:N	2.50	0.45
2:B:137:LEU:HD22	2:B:154:ILE:HG23	1.98	0.45
2:B:196:GLU:O	2:B:197:ASN:OD1	2.34	0.45
2:B:242:LEU:HD22	2:B:250:ALA:O	2.17	0.45
1:A:4:CYS:SG	1:A:252:LEU:CD1	3.02	0.45
1:A:184:PRO:HG2	1:A:398:MET:CE	2.41	0.45
1:A:278:ALA:CA	1:A:282:TYR:OH	2.65	0.45
1:A:288:VAL:HA	1:A:291:ILE:HG12	1.98	0.45
1:A:303:VAL:O	1:A:303:VAL:CG1	2.65	0.45
1:A:425:MET:O	1:A:426:ALA:C	2.60	0.45
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.52	0.45
2:B:167:ASN:HA	2:B:200:GLU:O	2.17	0.45
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.98	0.44
1:A:260:VAL:O	1:A:260:VAL:CG2	2.63	0.44
1:A:316:CYS:HB3	1:A:378:LEU:HD12	1.95	0.44
2:B:4:ILE:HD12	2:B:239:THR:HG21	1.98	0.44
2:B:8:GLN:CG	2:B:67:LEU:HD22	2.47	0.44
2:B:95:GLY:C	2:B:97:SER:H	2.25	0.44
1:A:11:GLN:HE21	1:A:74:VAL:CG2	2.29	0.44
1:A:287:SER:O	1:A:288:VAL:C	2.60	0.44
1:A:288:VAL:O	1:A:289:ALA:C	2.59	0.44
1:A:295:CYS:HB3	1:A:377:MET:HG2	1.99	0.44
2:B:42:LEU:C	2:B:44:LEU:H	2.26	0.44
2:B:98:GLY:C	2:B:100:GLY:H	2.24	0.44
2:B:288:VAL:N	2:B:289:PRO:CD	2.80	0.44
1:A:280:LYS:HB3	1:A:281:ALA:H	1.49	0.44
1:A:388:TRP:CD2	1:A:425:MET:HE1	2.52	0.44
2:B:23:VAL:O	2:B:24:ILE:C	2.60	0.44
2:B:52:TYR:HE1	2:B:240:THR:HB	1.82	0.44
2:B:99:ALA:O	2:B:100:GLY:C	2.60	0.44
2:B:175:PRO:HG2	2:B:207:GLU:OE1	2.16	0.44
2:B:288:VAL:N	2:B:289:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:MET:SD	2:B:375:ALA:HB3	2.57	0.44
2:B:325:MET:HE1	2:B:355:VAL:HG21	1.99	0.44
1:A:119:LEU:O	1:A:120:ASP:C	2.60	0.44
2:B:189:LEU:HD23	2:B:421:ALA:CB	2.47	0.44
2:B:390:ARG:O	2:B:391:ILE:C	2.61	0.44
1:A:8:HIS:HA	1:A:138:PHE:HB2	2.00	0.44
1:A:101:ASN:ND2	2:B:254:LYS:CD	2.75	0.44
1:A:105:ARG:O	1:A:110:ILE:CG2	2.64	0.44
1:A:204:VAL:HG12	1:A:204:VAL:O	2.17	0.44
1:A:226:ASN:O	1:A:227:LEU:C	2.59	0.44
1:A:287:SER:N	1:A:290:GLU:OE1	2.51	0.44
2:B:212:ILE:O	2:B:212:ILE:HG22	2.18	0.44
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.83	0.44
1:A:271:THR:O	1:A:376:CYS:HA	2.17	0.44
1:A:301:GLN:O	1:A:302:MET:C	2.61	0.44
1:A:363:VAL:CG1	1:A:364:PRO:HD2	2.48	0.44
1:A:384:ILE:O	1:A:385:ALA:C	2.59	0.44
2:B:70:LEU:HD21	2:B:149:MET:HE3	1.98	0.44
2:B:167:ASN:HD21	2:B:252:LEU:HD22	1.82	0.44
2:B:312:TYR:HA	2:B:381:SER:HA	1.99	0.44
2:B:423:SER:O	2:B:424:ASN:C	2.60	0.44
1:A:12:ALA:HB2	5:A:500:GTP:C8	2.52	0.44
1:A:23:LEU:O	1:A:26:LEU:HB3	2.17	0.44
1:A:23:LEU:CD2	1:A:232:GLY:O	2.64	0.44
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.52	0.44
1:A:182:VAL:O	1:A:183:GLU:C	2.60	0.44
2:B:280:SER:OG	2:B:281:GLN:N	2.49	0.44
1:A:72:PRO:HG2	1:A:73:THR:H	1.83	0.44
1:A:343:PHE:HZ	1:A:351:PHE:CZ	2.36	0.44
2:B:102:ASN:OD1	2:B:408:TYR:CZ	2.70	0.44
2:B:161:TYR:O	2:B:163:ASP:N	2.51	0.44
2:B:168:THR:CG2	2:B:201:THR:HG23	2.48	0.44
1:A:153:LEU:O	1:A:157:LEU:HG	2.18	0.44
2:B:37:HIS:O	2:B:38:GLY:C	2.61	0.44
2:B:402:LYS:O	2:B:403:ALA:C	2.61	0.44
1:A:108:TYR:O	1:A:109:THR:C	2.61	0.43
1:A:121:ARG:HG2	1:A:121:ARG:NH1	2.33	0.43
1:A:343:PHE:CE1	1:A:351:PHE:HE1	2.36	0.43
2:B:330:GLU:O	2:B:331:GLN:C	2.61	0.43
2:B:352:LYS:HD3	2:B:352:LYS:C	2.43	0.43
1:A:104:ALA:HB1	1:A:413:MET:HG3	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:CD1	1:A:157:LEU:HD21	2.35	0.43
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.47	0.43
1:A:268:PRO:CA	1:A:379:SER:O	2.65	0.43
1:A:362:VAL:HG13	1:A:368:LEU:CG	2.48	0.43
2:B:240:THR:HG23	2:B:241:CYS:N	2.33	0.43
2:B:431:GLU:O	2:B:434:GLN:N	2.48	0.43
1:A:63:PRO:HG2	1:A:91:GLN:OE1	2.18	0.43
1:A:231:ILE:HD13	1:A:231:ILE:H	1.82	0.43
1:A:304:LYS:O	1:A:304:LYS:HG3	2.19	0.43
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.81	0.43
2:B:282:GLN:HB3	2:B:282:GLN:HE21	1.51	0.43
1:A:390:ARG:HG3	1:A:390:ARG:HH11	1.83	0.43
1:A:12:ALA:C	1:A:14:VAL:N	2.75	0.43
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.99	0.43
1:A:310:GLY:HA3	1:A:383:ALA:CA	2.49	0.43
2:B:7:ILE:N	2:B:136:GLN:O	2.51	0.43
2:B:141:LEU:N	2:B:141:LEU:HD12	2.32	0.43
2:B:310:GLY:HA3	2:B:436:GLN:NE2	2.29	0.43
1:A:21:TRP:HE1	1:A:63:PRO:HB3	1.83	0.43
1:A:104:ALA:HB3	1:A:408:TYR:HD2	1.84	0.43
1:A:262:TYR:HB3	1:A:263:PRO:HD2	2.00	0.43
1:A:344:VAL:CG1	1:A:345:ASP:N	2.78	0.43
1:A:384:ILE:C	1:A:386:GLU:N	2.72	0.43
2:B:105:LYS:HG2	2:B:110:GLU:CG	2.48	0.43
1:A:144:GLY:H	5:A:500:GTP:PG	2.41	0.43
1:A:328:VAL:O	1:A:330:ALA:N	2.38	0.43
1:A:378:LEU:HD12	1:A:378:LEU:O	2.19	0.43
2:B:121:VAL:C	2:B:123:ARG:N	2.77	0.43
2:B:153:LEU:HD13	2:B:153:LEU:N	2.34	0.43
1:A:377:MET:O	1:A:377:MET:HG3	2.18	0.43
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.76	0.43
2:B:269:MET:HB2	2:B:301:MET:HE3	2.00	0.43
2:B:345:GLU:C	2:B:347:ILE:N	2.77	0.43
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.93	0.43
1:A:184:PRO:O	1:A:185:TYR:C	2.62	0.43
2:B:192:HIS:NE2	2:B:420:GLU:HG2	2.34	0.43
1:A:8:HIS:CD2	1:A:138:PHE:CD1	3.07	0.43
1:A:25:CYS:SG	1:A:26:LEU:N	2.92	0.43
1:A:76:ASP:O	1:A:79:ARG:N	2.52	0.43
1:A:238:ILE:O	1:A:242:LEU:CB	2.67	0.43
1:A:238:ILE:HD11	1:A:378:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:CD1	1:A:231:ILE:CD1	2.97	0.42
1:A:283:HIS:O	1:A:283:HIS:ND1	2.49	0.42
2:B:6:HIS:HB3	2:B:65:ALA:CB	2.48	0.42
2:B:12:CYS:O	2:B:13:GLY:C	2.59	0.42
2:B:48:ARG:HG2	2:B:243:ARG:HB3	2.01	0.42
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.42
2:B:301:MET:O	2:B:303:ALA:N	2.51	0.42
1:A:15:GLN:NE2	5:A:500:GTP:N7	2.67	0.42
1:A:115:ILE:CG2	1:A:116:ASP:H	2.32	0.42
1:A:272:TYR:CE2	1:A:274:PRO:HD2	2.53	0.42
1:A:399:TYR:C	1:A:401:LYS:N	2.77	0.42
2:B:70:LEU:HB2	2:B:99:ALA:CB	2.48	0.42
2:B:161:TYR:CD1	2:B:161:TYR:N	2.86	0.42
2:B:282:GLN:O	2:B:282:GLN:CG	2.65	0.42
2:B:435:TYR:C	2:B:437:ASP:H	2.27	0.42
1:A:268:PRO:C	1:A:269:LEU:HD23	2.44	0.42
2:B:360:PRO:HG2	2:B:371:LEU:CB	2.38	0.42
1:A:383:ALA:C	1:A:385:ALA:N	2.78	0.42
2:B:138:THR:O	2:B:139:HIS:HB3	2.20	0.42
1:A:251:ASP:CA	1:A:254:GLU:HG3	2.49	0.42
1:A:265:GLY:O	1:A:266:HIS:C	2.63	0.42
1:A:363:VAL:HG13	1:A:364:PRO:HD2	2.02	0.42
2:B:98:GLY:O	2:B:100:GLY:N	2.49	0.42
2:B:106:GLY:O	2:B:149:MET:CA	2.68	0.42
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.42
1:A:173:PRO:HG3	1:A:183:GLU:CD	2.45	0.42
2:B:178:SER:C	2:B:180:THR:H	2.27	0.42
2:B:301:MET:C	2:B:303:ALA:N	2.77	0.42
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.50	0.42
2:B:72:PRO:HG2	2:B:73:GLY:H	1.83	0.42
2:B:250:ALA:CB	2:B:254:LYS:HE2	2.49	0.42
2:B:297:ASP:CG	2:B:299:LYS:HE2	2.45	0.42
1:A:166:LYS:HB2	1:A:199:ASP:OD1	2.20	0.42
2:B:103:TRP:HB2	2:B:186:ASN:HA	2.01	0.42
2:B:273:ALA:HB1	2:B:291:LEU:HG	2.01	0.42
1:A:147:SER:HB2	1:A:186:ASN:O	2.19	0.42
1:A:305:CYS:SG	1:A:383:ALA:HB1	2.60	0.42
1:A:335:ILE:C	1:A:337:THR:H	2.28	0.42
2:B:68:VAL:HG11	2:B:153:LEU:HD21	2.00	0.42
2:B:171:VAL:HG12	2:B:171:VAL:O	2.20	0.42
2:B:281:GLN:C	2:B:283:TYR:N	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:LYS:O	2:B:390:ARG:C	2.62	0.42
1:A:67:PHE:HB2	1:A:92:LEU:HD23	2.02	0.42
1:A:204:VAL:CG1	1:A:231:ILE:HD12	2.42	0.42
1:A:231:ILE:C	1:A:233:GLN:H	2.28	0.42
2:B:343:PHE:CD2	2:B:350:ASN:ND2	2.88	0.42
1:A:276:ILE:C	1:A:369:ALA:HB2	2.45	0.41
2:B:82:PRO:C	2:B:84:GLY:N	2.78	0.41
2:B:118:VAL:O	2:B:122:VAL:HG13	2.19	0.41
2:B:161:TYR:C	2:B:163:ASP:N	2.71	0.41
2:B:307:PRO:O	2:B:309:HIS:N	2.53	0.41
1:A:161:TYR:C	1:A:163:LYS:N	2.77	0.41
1:A:289:ALA:HB3	1:A:290:GLU:OE2	2.21	0.41
2:B:143:GLY:O	2:B:147:SER:OG	2.38	0.41
2:B:274:PRO:HD3	2:B:374:SER:HA	2.03	0.41
2:B:311:ARG:HG2	2:B:311:ARG:NH1	2.34	0.41
1:A:24:TYR:O	1:A:25:CYS:C	2.63	0.41
1:A:144:GLY:N	5:A:500:GTP:O3G	2.48	0.41
1:A:255:PHE:O	1:A:257:THR:N	2.53	0.41
2:B:264:ARG:O	2:B:265:LEU:CB	2.53	0.41
1:A:140:SER:O	1:A:141:PHE:C	2.62	0.41
1:A:210:TYR:OH	2:B:325:MET:HB3	2.20	0.41
1:A:243:ARG:NH2	1:A:252:LEU:HG	2.35	0.41
2:B:165:ILE:H	2:B:165:ILE:CD1	2.31	0.41
2:B:262:PHE:HA	2:B:263:PRO:HD2	1.65	0.41
1:A:76:ASP:O	1:A:80:THR:N	2.53	0.41
2:B:333:LEU:HD11	2:B:337:ASN:HD21	1.85	0.41
1:A:213:CYS:O	1:A:219:ILE:HG13	2.20	0.41
1:A:273:ALA:HB2	1:A:375:VAL:HB	2.03	0.41
2:B:20:PHE:CD2	2:B:235:MET:CG	3.04	0.41
2:B:118:VAL:O	2:B:119:LEU:C	2.62	0.41
2:B:202:TYR:CE2	2:B:268:PHE:HD1	2.38	0.41
2:B:276:THR:O	7:B:601:TA1:H192	2.21	0.41
1:A:101:ASN:HD21	2:B:254:LYS:NZ	2.18	0.41
1:A:175:PRO:HG3	1:A:304:LYS:CB	2.50	0.41
1:A:204:VAL:CG1	1:A:209:ILE:HD11	2.42	0.41
2:B:168:THR:O	2:B:202:TYR:N	2.44	0.41
2:B:175:PRO:O	2:B:177:VAL:N	2.53	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HD3	2.01	0.41
2:B:25:SER:O	2:B:28:HIS:N	2.53	0.41
2:B:105:LYS:HG2	2:B:110:GLU:HG3	2.03	0.41
2:B:192:HIS:HD1	2:B:424:ASN:CG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:PHE:O	2:B:401:ARG:N	2.53	0.41
2:B:417:GLU:O	2:B:420:GLU:HB3	2.21	0.41
1:A:23:LEU:HD11	1:A:361:THR:O	2.21	0.41
1:A:30:ILE:O	1:A:30:ILE:HG22	2.21	0.41
1:A:95:GLY:O	1:A:96:LYS:C	2.64	0.41
1:A:132:LEU:H	1:A:132:LEU:CD2	2.23	0.41
1:A:172:TYR:OH	1:A:387:ALA:C	2.64	0.41
1:A:332:ILE:CD1	1:A:353:VAL:HG22	2.51	0.41
2:B:14:ASN:O	2:B:15:GLN:C	2.64	0.41
2:B:52:TYR:C	2:B:53:TYR:CD1	2.99	0.41
2:B:135:PHE:CD1	2:B:166:MET:SD	3.14	0.41
2:B:139:HIS:HE1	2:B:168:THR:CG2	2.34	0.41
2:B:147:SER:HB2	2:B:190:SER:CB	2.41	0.41
2:B:168:THR:HB	2:B:198:THR:HG21	2.03	0.41
2:B:210:TYR:O	2:B:214:PHE:N	2.52	0.41
2:B:242:LEU:HB3	2:B:250:ALA:O	2.20	0.41
2:B:259:MET:HE3	2:B:268:PHE:CZ	2.56	0.41
2:B:274:PRO:HG2	2:B:371:LEU:CD2	2.43	0.41
2:B:292:THR:O	2:B:293:GLN:C	2.64	0.41
1:A:100:ALA:HB2	1:A:105:ARG:HD3	2.02	0.41
1:A:181:VAL:HG23	2:B:258:ASN:HB3	2.03	0.41
1:A:199:ASP:CB	1:A:256:GLN:NE2	2.77	0.41
1:A:386:GLU:O	1:A:387:ALA:C	2.63	0.41
2:B:78:VAL:O	2:B:84:GLY:HA3	2.22	0.41
2:B:238:VAL:HB	2:B:239:THR:H	1.65	0.41
2:B:291:LEU:HD21	2:B:373:MET:HG2	2.03	0.41
1:A:207:GLU:C	1:A:209:ILE:H	2.29	0.40
1:A:414:GLU:C	1:A:416:GLY:N	2.74	0.40
1:A:425:MET:O	1:A:428:LEU:N	2.45	0.40
2:B:125:GLU:O	2:B:128:SER:HB3	2.22	0.40
2:B:132:LEU:O	2:B:164:ARG:HD2	2.21	0.40
2:B:332:MET:HE3	2:B:351:VAL:CG1	2.32	0.40
1:A:149:PHE:CD1	1:A:150:THR:N	2.89	0.40
1:A:272:TYR:O	1:A:300:ASN:ND2	2.54	0.40
1:A:398:MET:HE3	1:A:398:MET:HB2	1.78	0.40
1:A:408:TYR:O	1:A:409:VAL:C	2.63	0.40
2:B:19:LYS:HG3	2:B:228:ASN:HB2	2.01	0.40
2:B:24:ILE:CG2	2:B:25:SER:N	2.80	0.40
2:B:188:THR:O	2:B:191:VAL:HG12	2.21	0.40
2:B:422:GLU:O	2:B:426:ASN:CB	2.67	0.40
1:A:179:THR:HG21	2:B:248:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HG	1:A:290:GLU:CB	2.52	0.40
2:B:359:PRO:HB2	2:B:360:PRO:CD	2.49	0.40
1:A:207:GLU:O	1:A:210:TYR:N	2.51	0.40
1:A:318:LEU:HB2	1:A:376:CYS:SG	2.61	0.40
2:B:118:VAL:O	2:B:121:VAL:N	2.54	0.40
2:B:204:ILE:HG23	2:B:209:LEU:HD11	2.03	0.40
2:B:286:LEU:O	2:B:287:THR:C	2.65	0.40
2:B:12:CYS:O	2:B:14:ASN:N	2.55	0.40
2:B:268:PHE:HA	2:B:379:GLY:O	2.22	0.40
2:B:405:LEU:O	2:B:405:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	3
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	3
All	All	832/896 (93%)	539 (65%)	178 (21%)	115 (14%)	0	3

All (115) Ramachandran outliers are listed below:

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

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

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

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	294 (85%)	53 (15%)	3	16
2	B	367/381 (96%)	307 (84%)	60 (16%)	2	14
All	All	714/758 (94%)	601 (84%)	113 (16%)	4	15

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	7	ILE
1	A	16	ILE
1	A	20	CYS
1	A	32	PRO
1	A	76	ASP
1	A	82	THR
1	A	98	ASP
1	A	109	THR
1	A	115	ILE
1	A	120	ASP
1	A	125	LEU
1	A	130	THR
1	A	135	PHE
1	A	141	PHE
1	A	150	THR
1	A	152	LEU
1	A	154	MET
1	A	155	GLU
1	A	172	TYR
1	A	173	PRO
1	A	183	GLU
1	A	192	HIS
1	A	204	VAL
1	A	219	ILE
1	A	224	TYR
1	A	231	ILE
1	A	234	ILE
1	A	243	ARG
1	A	244	PHE
1	A	253	THR
1	A	260	VAL
1	A	267	PHE
1	A	269	LEU
1	A	276	ILE
1	A	279	GLU
1	A	284	GLU
1	A	303	VAL
1	A	325	PRO
1	A	328	VAL
1	A	334	THR
1	A	345	ASP
1	A	352	LYS

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Mol	Chain	Res	Type
1	A	368	LEU
1	A	376	CYS
1	A	377	MET
1	A	378	LEU
1	A	415	GLU
1	A	417	GLU
1	A	420	GLU
1	A	431	ASP
1	A	432	TYR
1	A	433	GLU
2	B	24	ILE
2	B	26	ASP
2	B	32	PRO
2	B	41	ASP
2	B	67	LEU
2	B	68	VAL
2	B	90	ASP
2	B	94	PHE
2	B	121	VAL
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	151	THR
2	B	153	LEU
2	B	161	TYR
2	B	163	ASP
2	B	165	ILE
2	B	174	SER
2	B	193	GLN
2	B	198	THR
2	B	201	THR
2	B	203	CYS
2	B	207	GLU
2	B	211	ASP
2	B	214	PHE
2	B	227	LEU
2	B	229	HIS
2	B	230	LEU
2	B	232	SER

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Mol	Chain	Res	Type
2	B	236	SER
2	B	240	THR
2	B	265	LEU
2	B	267	PHE
2	B	275	LEU
2	B	282	GLN
2	B	284	ARG
2	B	299	LYS
2	B	306	ASP
2	B	309	HIS
2	B	314	THR
2	B	322	ARG
2	B	324	SER
2	B	325	MET
2	B	331	GLN
2	B	343	PHE
2	B	344	VAL
2	B	352	LYS
2	B	353	THR
2	B	369	ARG
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

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

Mol	Chain	Res	Type
1	A	8	HIS
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

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	301	GLN
1	A	309	HIS
2	B	14	ASN
2	B	43	GLN
2	B	91	ASN
2	B	101	ASN
2	B	102	ASN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	186	ASN
2	B	266	HIS
2	B	282	GLN
2	B	331	GLN
2	B	334	ASN
2	B	336	GLN
2	B	337	ASN
2	B	349	ASN
2	B	380	ASN
2	B	406	HIS
2	B	434	GLN
2	B	436	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	GDP	B	600	-	29,30,30	2.86	11 (37%)	45,47,47	3.48	16 (35%)
5	GTP	A	500	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
7	TA1	B	601	-	68,68,68	2.20	26 (38%)	105,105,105	1.50	13 (12%)

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
6	GDP	B	600	-	-	4/16/32/32	0/3/3/3
5	GTP	A	500	4	-	4/22/38/38	0/3/3/3
7	TA1	B	601	-	-	9/41/127/127	0/7/7/7

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	GDP	PA-O3A	7.55	1.67	1.59
7	B	601	TA1	C06-C05	6.50	1.50	1.38
5	A	500	GTP	PA-O3A	-6.00	1.53	1.59
6	B	600	GDP	O6-C6	5.96	1.34	1.23
6	B	600	GDP	C8-N9	5.87	1.50	1.37
5	A	500	GTP	PB-O3A	-5.69	1.53	1.59
7	B	601	TA1	C08-C07	-5.66	1.25	1.38
5	A	500	GTP	PB-O3B	5.41	1.65	1.59
7	B	601	TA1	C18-C10	5.36	1.69	1.57
7	B	601	TA1	C05-C04	4.84	1.46	1.39
6	B	600	GDP	C2-N1	4.76	1.49	1.37
7	B	601	TA1	C45-C24	4.27	1.61	1.54
6	B	600	GDP	PB-O2B	-3.91	1.40	1.54
7	B	601	TA1	C36-C31	3.74	1.45	1.39
7	B	601	TA1	O02-C03	3.53	1.41	1.34
6	B	600	GDP	O4'-C1'	3.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	TA1	C25-C24	3.36	1.39	1.34
7	B	601	TA1	C46-C45	3.24	1.60	1.53
7	B	601	TA1	C43-C01	3.19	1.60	1.54
7	B	601	TA1	C11-C10	3.11	1.61	1.54
6	B	600	GDP	C8-N7	3.03	1.41	1.32
6	B	600	GDP	C5-N7	-2.86	1.33	1.39
7	B	601	TA1	C43-C26	2.83	1.58	1.52
6	B	600	GDP	C5-C4	2.64	1.46	1.38
7	B	601	TA1	C26-C25	2.58	1.56	1.51
7	B	601	TA1	C01-C45	2.53	1.66	1.56
7	B	601	TA1	C18-C20	2.51	1.62	1.55
7	B	601	TA1	C04-C03	-2.46	1.44	1.50
6	B	600	GDP	PB-O3B	2.46	1.63	1.54
6	B	600	GDP	C2-N3	-2.45	1.27	1.33
7	B	601	TA1	C41-C42	2.32	1.42	1.38
7	B	601	TA1	C16-C15	2.32	1.56	1.52
7	B	601	TA1	C37-C29	2.17	1.54	1.52
7	B	601	TA1	O09-C21	2.17	1.49	1.44
7	B	601	TA1	C33-C32	2.15	1.42	1.38
7	B	601	TA1	C08-C09	2.14	1.42	1.38
7	B	601	TA1	C10-C02	2.11	1.62	1.57
7	B	601	TA1	C39-C38	2.08	1.42	1.38
7	B	601	TA1	C07-C06	2.05	1.42	1.38
7	B	601	TA1	C34-C33	2.03	1.42	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	N9-C8-N7	-10.76	93.44	113.40
6	B	600	GDP	C8-N7-C5	9.22	120.69	104.26
6	B	600	GDP	C6-C5-N7	8.59	145.92	130.29
6	B	600	GDP	N2-C2-N3	6.28	131.94	119.67
6	B	600	GDP	C6-C5-C4	-6.19	109.52	118.83
6	B	600	GDP	C8-N9-C4	5.86	117.02	106.03
7	B	601	TA1	C06-C05-C04	-5.86	114.61	120.36
7	B	601	TA1	C07-C08-C09	5.76	127.35	120.24
6	B	600	GDP	C5-C6-N1	4.51	124.72	113.25
6	B	600	GDP	N2-C2-N1	-4.25	107.80	116.76
6	B	600	GDP	C2-N3-C4	4.10	119.36	112.30
7	B	601	TA1	C05-C04-C03	-4.05	111.46	120.40
6	B	600	GDP	O6-C6-C5	-3.96	116.08	126.53
6	B	600	GDP	C4-C5-N7	-3.85	104.56	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	C2-N1-C6	-3.81	118.20	125.11
7	B	601	TA1	C09-C04-C03	3.62	128.37	120.40
6	B	600	GDP	C2'-C3'-C4'	3.42	109.23	102.61
7	B	601	TA1	C17-C18-C20	3.22	109.82	102.58
7	B	601	TA1	O04-C11-C14	-3.01	101.75	108.13
7	B	601	TA1	C45-C01-C02	2.98	115.20	111.93
6	B	600	GDP	C1'-N9-C8	-2.67	119.15	126.73
5	A	500	GTP	O2G-PG-O3B	2.65	113.52	104.64
7	B	601	TA1	O01-C01-C43	2.48	113.39	107.04
7	B	601	TA1	C08-C09-C04	-2.35	118.06	120.36
6	B	600	GDP	O2'-C2'-C3'	2.29	119.16	111.82
7	B	601	TA1	C14-C11-C15	-2.23	83.08	85.38
7	B	601	TA1	C10-C18-C17	-2.23	102.32	106.55
7	B	601	TA1	O06-C15-C11	2.20	92.98	90.58
5	A	500	GTP	O5'-C5'-C4'	2.09	116.12	108.99
6	B	600	GDP	C4'-O4'-C1'	2.07	114.04	109.47
7	B	601	TA1	C21-O09-C22	2.03	120.13	115.95
5	A	500	GTP	O3G-PG-O3B	2.02	111.41	104.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

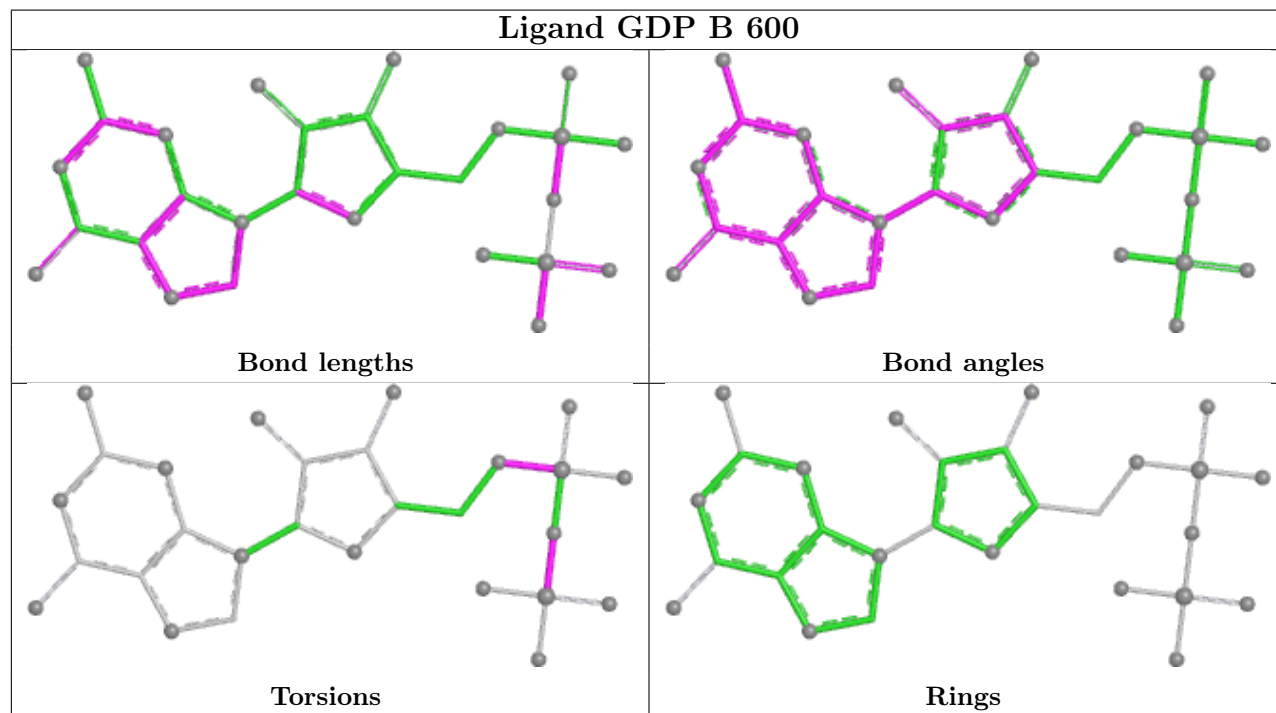
Mol	Chain	Res	Type	Atoms
6	B	600	GDP	PA-O3A-PB-O2B
6	B	600	GDP	C5'-O5'-PA-O3A
6	B	600	GDP	C5'-O5'-PA-O1A
7	B	601	TA1	O02-C03-C04-C05
7	B	601	TA1	O02-C03-C04-C09
7	B	601	TA1	O03-C03-C04-C09
7	B	601	TA1	O03-C03-C04-C05
7	B	601	TA1	N01-C30-C31-C36
7	B	601	TA1	O14-C30-C31-C36
7	B	601	TA1	N01-C30-C31-C32
7	B	601	TA1	O14-C30-C31-C32
5	A	500	GTP	C3'-C4'-C5'-O5'
5	A	500	GTP	C5'-O5'-PA-O1A
5	A	500	GTP	O4'-C4'-C5'-O5'
6	B	600	GDP	PA-O3A-PB-O3B
7	B	601	TA1	C15-C11-O04-C12
5	A	500	GTP	PG-O3B-PB-O2B

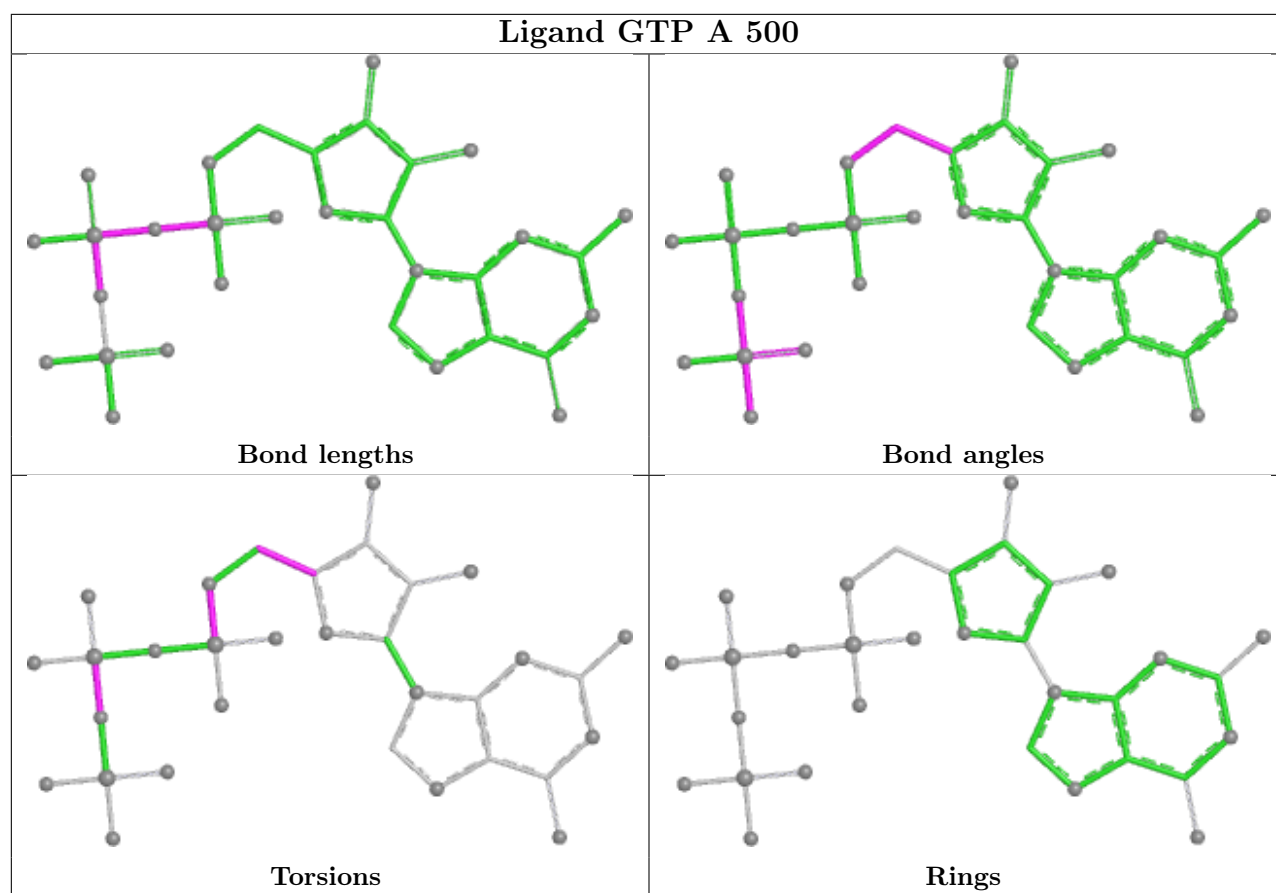
There are no ring outliers.

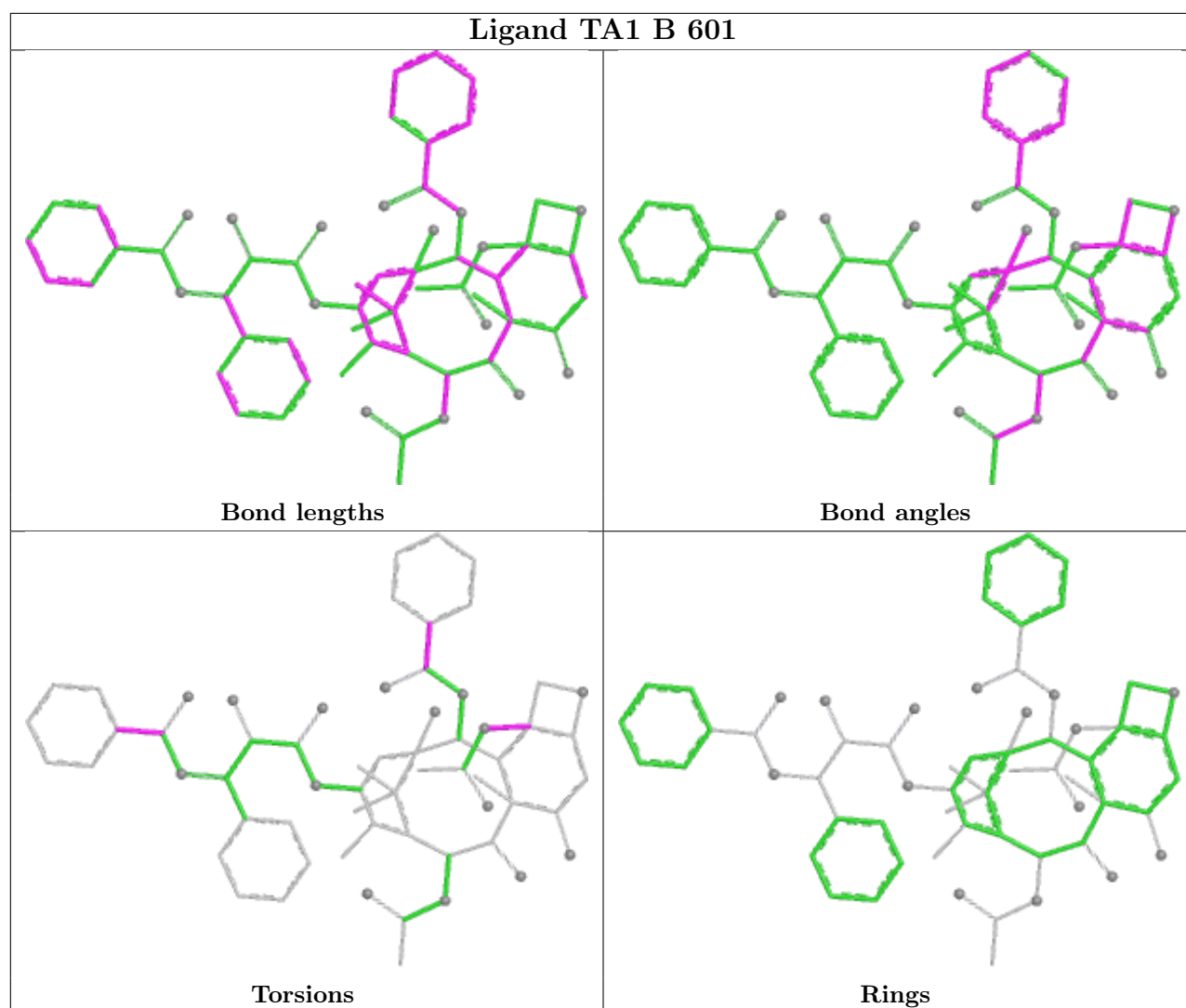
3 monomers are involved in 11 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.