



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:30 AM UTC

PDB ID : 2HXX / pdb_00002hxx
Title : KIF1A head-microtubule complex structure in adp-form
Authors : Kikkawa, M.; Hirokawa, N.
Deposited on : 2006-08-03
Resolution : 11.00 Å(reported)
Based on initial models : 1JFF, 1I5S

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

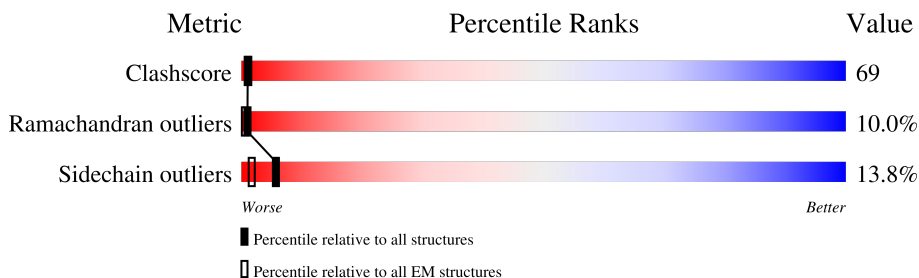
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 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	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	
3	C	394	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9388 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 a protein called Kinesin-like protein KIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	330	Total	C	N	O	S	8	0
			2659	1645	467	532	15		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	MET	-	cloning artifact	UNP P33173
C	-14	ALA	-	cloning artifact	UNP P33173
C	-13	SER	-	cloning artifact	UNP P33173
C	-12	MET	-	cloning artifact	UNP P33173
C	-11	THR	-	cloning artifact	UNP P33173
C	-10	GLY	-	cloning artifact	UNP P33173
C	-9	GLY	-	cloning artifact	UNP P33173
C	-8	GLN	-	cloning artifact	UNP P33173
C	-7	GLN	-	cloning artifact	UNP P33173
C	-6	MET	-	cloning artifact	UNP P33173
C	-5	GLY	-	cloning artifact	UNP P33173
C	-4	ARG	-	cloning artifact	UNP P33173
C	-3	ASP	-	cloning artifact	UNP P33173
C	-2	PRO	-	cloning artifact	UNP P33173
C	-1	ILE	-	cloning artifact	UNP P33173

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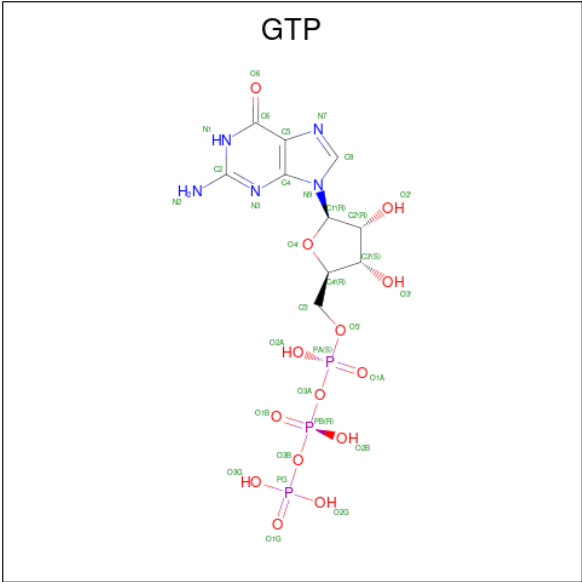
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ASN	-	cloning artifact	UNP P33173
C	1	MET	-	cloning artifact	UNP P33173
C	2	PRO	-	cloning artifact	UNP P33173
C	202	ALA	PRO	engineered mutation	UNP P33173
C	356	ASN	-	linker	UNP P33173
C	357	THR	-	linker	UNP P33173
C	358	VAL	-	linker	UNP P33173
C	359	SER	-	linker	UNP P33173
C	360	VAL	-	linker	UNP P33173
C	361	ASN	-	linker	UNP P33173
C	362	LEU	-	linker	UNP P33173
C	363	GLU	-	linker	UNP P33173
C	364	LEU	-	linker	UNP P33173
C	365	THR	-	linker	UNP P33173
C	366	ALA	-	linker	UNP P33173
C	367	GLU	-	linker	UNP P33173
C	368	GLU	-	linker	UNP P33173
C	369	TRP	-	linker	UNP P33173
C	370	LYS	-	linker	UNP P33173
C	371	LYS	-	linker	UNP P33173
C	372	LYS	-	linker	UNP P33173
C	373	HIS	-	expression tag	UNP P33173
C	374	HIS	-	expression tag	UNP P33173
C	375	HIS	-	expression tag	UNP P33173
C	376	HIS	-	expression tag	UNP P33173
C	377	HIS	-	expression tag	UNP P33173
C	378	HIS	-	expression tag	UNP P33173

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

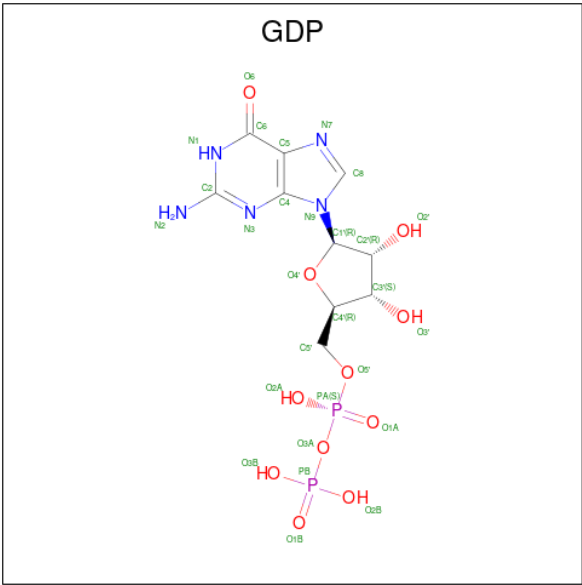
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0

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



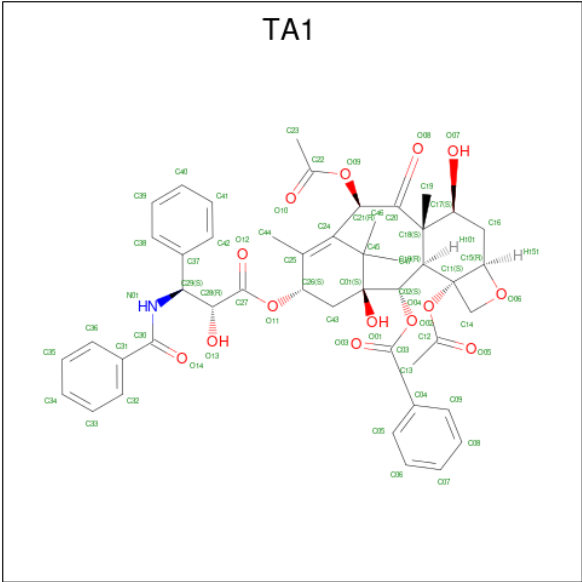
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	32	10	5	14	3	0

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



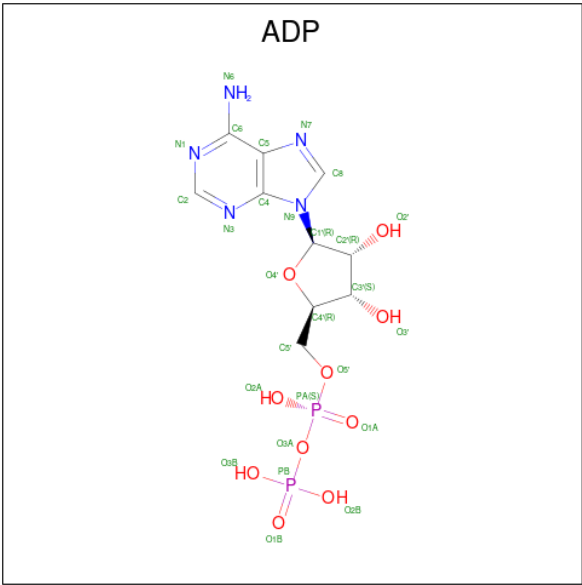
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	B	1	28	10	5	11	2	0

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



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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

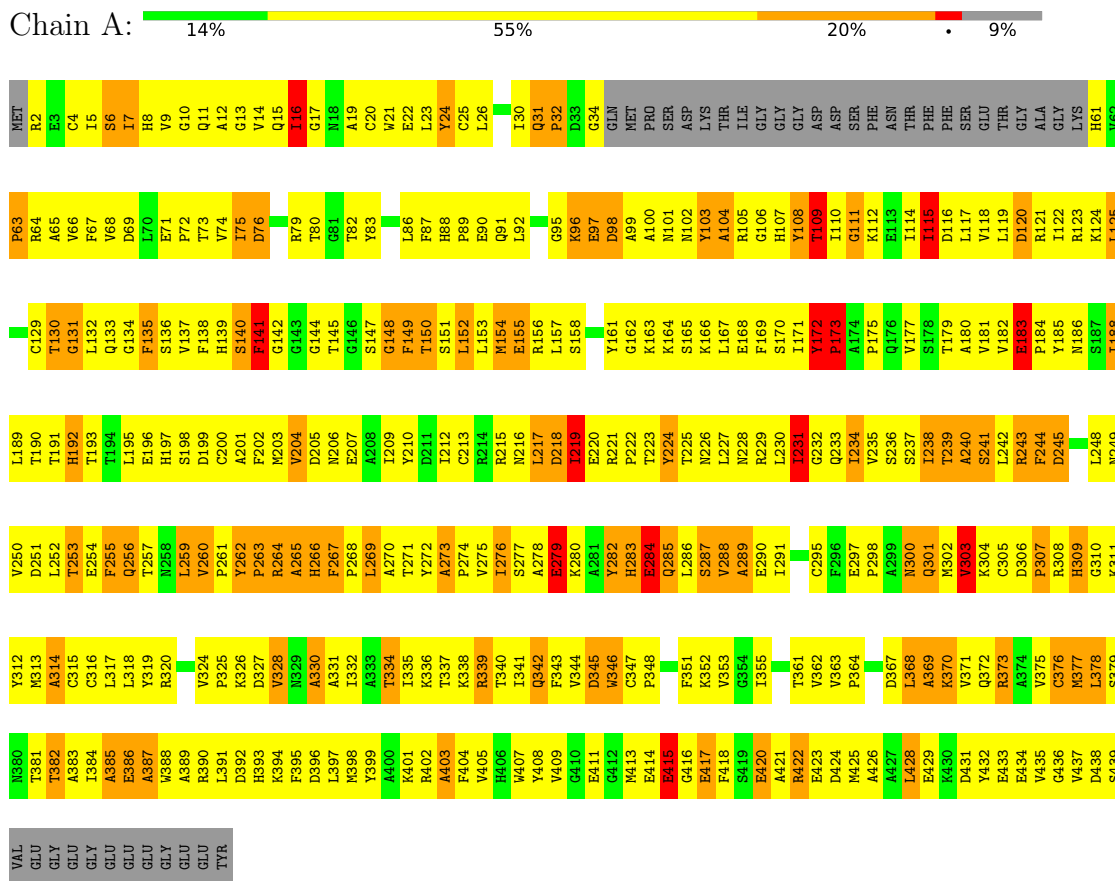


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	C	1	27	10	5	10	2	0

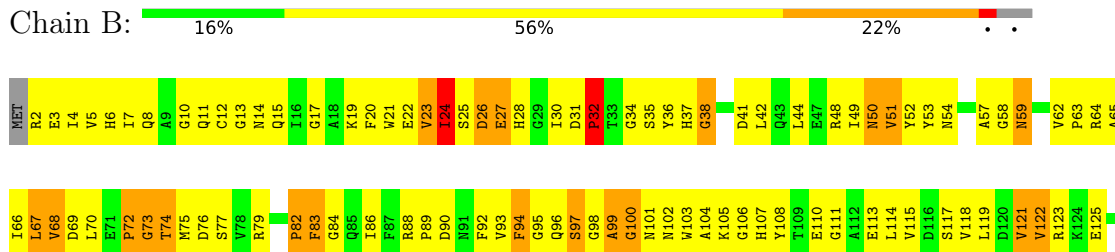
3 Residue-property plots

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



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	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 11.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-11.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9388	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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%)
3	C	0.58	0/2700	1.08	14/3643 (0.4%)
All	All	0.61	1/9426 (0.0%)	1.10	58/12767 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	TYR	CA-C	-5.48	1.48	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	CA-C-N	10.69	133.20	119.84
1	A	172	TYR	C-N-CA	10.69	133.20	119.84
2	B	262	PHE	CA-C-N	10.02	132.36	119.84
2	B	262	PHE	C-N-CA	10.02	132.36	119.84
1	A	283	HIS	N-CA-C	-8.23	101.27	113.61
2	B	77	SER	N-CA-C	-7.87	104.28	114.04
2	B	159	GLU	N-CA-C	-7.77	104.28	114.31
3	C	247	VAL	N-CA-C	7.71	119.58	108.48
2	B	313	LEU	N-CA-C	-7.69	103.86	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	LEU	N-CA-C	-7.54	104.32	113.97
2	B	208	ALA	N-CA-C	-7.53	102.74	112.23
2	B	293	GLN	N-CA-C	-7.41	102.90	110.97
2	B	385	GLN	N-CA-C	-7.12	103.45	111.14
2	B	388	PHE	N-CA-C	-7.02	103.98	112.54
1	A	301	GLN	N-CA-C	7.01	121.53	112.41
2	B	22	GLU	N-CA-C	-6.98	103.37	110.97
2	B	399	PHE	N-CA-C	-6.96	103.62	111.07
2	B	389	LYS	N-CA-C	-6.85	103.50	110.97
1	A	422	ARG	N-CA-C	-6.81	103.09	111.40
1	A	385	ALA	N-CA-C	-6.80	103.10	111.33
1	A	188	ILE	N-CA-C	-6.68	103.21	113.16
1	A	123	ARG	N-CA-C	-6.49	105.93	114.31
2	B	217	LEU	N-CA-C	-6.41	96.53	107.23
3	C	114	ASP	O-C-N	-6.34	114.16	122.59
2	B	27	GLU	N-CA-C	-6.29	105.98	113.21
2	B	181	VAL	N-CA-C	6.02	116.77	111.90
2	B	88	ARG	N-CA-C	-5.96	102.26	109.83
2	B	243	ARG	N-CA-C	-5.93	106.68	112.97
1	A	264	ARG	N-CA-C	-5.90	101.56	110.24
1	A	231	ILE	N-CA-C	-5.85	103.95	110.62
2	B	296	PHE	N-CA-C	5.82	120.01	113.02
3	C	332	SER	N-CA-C	-5.79	102.75	109.93
2	B	247	GLN	N-CA-C	-5.78	104.98	111.28
1	A	415	GLU	N-CA-C	-5.64	105.50	112.38
3	C	115	GLN	N-CA-C	5.64	119.47	112.59
1	A	75	ILE	N-CA-C	-5.53	104.18	111.09
3	C	77[A]	ILE	N-CA-C	5.52	116.59	111.45
3	C	77[B]	ILE	N-CA-C	5.52	116.59	111.45
3	C	34	THR	N-CA-C	5.51	118.80	109.76
1	A	262	TYR	CA-C-N	5.50	126.72	119.84
1	A	262	TYR	C-N-CA	5.50	126.72	119.84
1	A	297	GLU	N-CA-C	-5.49	101.43	109.50
2	B	59	ASN	N-CA-C	-5.47	105.61	114.09
3	C	267	GLU	N-CA-C	-5.46	105.24	111.14
3	C	152	GLU	CA-C-N	-5.42	113.36	122.29
3	C	152	GLU	C-N-CA	-5.42	113.36	122.29
1	A	259	LEU	N-CA-C	5.40	120.89	113.97
2	B	436	GLN	N-CA-C	-5.37	106.42	112.87
3	C	114	ASP	CA-C-N	-5.33	114.19	122.67
3	C	114	ASP	C-N-CA	-5.33	114.19	122.67
1	A	429	GLU	N-CA-C	-5.30	105.96	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	289	PRO	N-CA-C	-5.15	107.15	113.84
3	C	234	THR	O-C-N	5.10	129.85	123.12
3	C	153	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	A	241	SER	N-CA-C	5.07	116.81	111.28
1	A	140	SER	N-CA-C	5.07	116.30	109.11
1	A	421	ALA	N-CA-C	-5.05	107.15	113.72
1	A	16	ILE	N-CA-C	-5.02	105.50	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	47	PRO	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3141	602	0
2	B	3351	0	3229	608	0
3	C	2659	0	2604	122	0
4	A	1	0	0	0	0
4	C	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
8	C	27	0	12	0	0
All	All	9388	0	9061	1271	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 69.

All (1271) 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)
1:A:409:VAL:HG12	3:C:272:ASN:CG	1.22	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:THR:CG2	3:C:172:PRO:O	1.65	1.44
1:A:409:VAL:CG1	3:C:272:ASN:OD1	1.65	1.43
1:A:409:VAL:HG12	3:C:272:ASN:ND2	1.21	1.43
1:A:409:VAL:CG1	3:C:272:ASN:CG	2.01	1.33
1:A:409:VAL:CG1	3:C:272:ASN:ND2	1.95	1.27
2:B:419:THR:HG21	3:C:172:PRO:O	1.24	1.24
1:A:423:GLU:OE2	3:C:346:ARG:NH2	1.71	1.24
3:C:261:LYS:HD2	3:C:262:GLY:N	1.56	1.18
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.17
1:A:409:VAL:CG1	3:C:272:ASN:HD21	1.51	1.17
3:C:163:LYS:HE3	3:C:163:LYS:HA	1.19	1.16
3:C:163:LYS:HE3	3:C:163:LYS:CA	1.77	1.15
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.14
3:C:163:LYS:HA	3:C:163:LYS:CE	1.78	1.10
2:B:419:THR:HB	3:C:172:PRO:HB2	1.16	1.10
2:B:419:THR:HG22	3:C:172:PRO:O	1.48	1.09
3:C:261:LYS:CD	3:C:262:GLY:H	1.67	1.07
1:A:409:VAL:HG11	3:C:272:ASN:OD1	1.29	1.07
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.30	1.06
1:A:109:THR:HG22	1:A:110:ILE:N	1.70	1.03
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.37	1.03
1:A:243:ARG:HH21	1:A:252:LEU:N	1.57	1.02
3:C:113:LYS:O	3:C:114:ASP:HB2	1.56	1.01
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.43	1.01
2:B:236:SER:O	2:B:240:THR:HG23	1.61	1.01
3:C:235:ASN:O	3:C:236:ILE:HD12	1.59	1.00
2:B:299:LYS:H	2:B:299:LYS:HD3	1.24	1.00
2:B:419:THR:HB	3:C:172:PRO:CB	1.94	0.98
3:C:161:LYS:O	3:C:161:LYS:HG2	1.62	0.96
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.47	0.96
1:A:98:ASP:HB2	1:A:105:ARG:HH21	1.31	0.96
1:A:316:CYS:HB3	1:A:378:LEU:HD11	1.48	0.95
2:B:332:MET:HE3	2:B:351:VAL:HG11	1.45	0.95
1:A:251:ASP:N	1:A:254:GLU:HG3	1.82	0.95
2:B:281:GLN:O	2:B:283:TYR:N	2.00	0.94
1:A:237:SER:HB2	1:A:376:CYS:SG	2.08	0.94
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.48	0.94
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.50	0.93
1:A:251:ASP:H	1:A:254:GLU:HG3	1.33	0.93
1:A:109:THR:HG22	1:A:110:ILE:H	1.33	0.92
3:C:216:ARG:HH21	3:C:254:ARG:NH1	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ARG:O	2:B:265:LEU:HB3	1.69	0.92
1:A:409:VAL:HG13	3:C:272:ASN:HD21	1.34	0.92
1:A:409:VAL:HG12	3:C:272:ASN:OD1	1.42	0.91
2:B:70:LEU:H	2:B:145:THR:HG21	1.33	0.90
1:A:151:SER:HB3	1:A:193:THR:HG21	1.51	0.90
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.51	0.90
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.53	0.89
1:A:343:PHE:CZ	1:A:351:PHE:CE1	2.61	0.89
1:A:147:SER:HB2	1:A:190:THR:OG1	1.73	0.89
2:B:102:ASN:HD21	2:B:408:TYR:HA	1.38	0.89
2:B:264:ARG:HB2	2:B:266:HIS:CD2	2.08	0.89
1:A:110:ILE:HG23	1:A:111:GLY:H	1.38	0.88
1:A:122:ILE:HD12	1:A:157:LEU:HD21	1.54	0.88
3:C:163:LYS:HE3	3:C:163:LYS:C	1.98	0.88
2:B:8:GLN:OE1	2:B:67:LEU:HD22	1.72	0.88
2:B:147:SER:O	2:B:151:THR:HB	1.71	0.88
2:B:93:VAL:HG11	2:B:118:VAL:CG2	2.03	0.88
2:B:323:MET:HE2	2:B:328:VAL:HG22	1.54	0.88
2:B:311:ARG:HD3	2:B:342:TYR:HA	1.56	0.88
2:B:276:THR:HB	2:B:281:GLN:HG3	1.56	0.87
2:B:10:GLY:HA2	2:B:145:THR:HB	1.55	0.87
2:B:101:ASN:HD21	2:B:143:GLY:HA2	1.38	0.87
1:A:407:TRP:HE1	2:B:260:VAL:HG23	1.38	0.85
1:A:420:GLU:OE1	3:C:342:LEU:CD2	2.24	0.85
2:B:6:HIS:CE1	2:B:8:GLN:HG2	2.10	0.85
2:B:242:LEU:HD22	2:B:250:ALA:H	1.41	0.85
1:A:220:GLU:C	1:A:222:PRO:HD3	2.02	0.85
2:B:360:PRO:HG2	2:B:371:LEU:HB3	1.56	0.85
2:B:234:THR:HG21	2:B:270:PRO:CB	2.06	0.85
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.57	0.85
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.59	0.84
2:B:153:LEU:O	2:B:157:ILE:HG12	1.75	0.84
1:A:234:ILE:HG13	1:A:270:ALA:HB1	1.59	0.84
1:A:264:ARG:O	1:A:266:HIS:N	2.09	0.84
1:A:415:GLU:CB	3:C:350:ARG:NH2	2.40	0.84
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.13	0.84
2:B:4:ILE:HD13	2:B:136:GLN:HE21	1.42	0.84
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.57	0.84
2:B:324:SER:HB3	2:B:327:GLU:HG2	1.60	0.83
2:B:20:PHE:CD2	2:B:235:MET:SD	2.71	0.83
2:B:101:ASN:ND2	2:B:143:GLY:HA2	1.94	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
2:B:3:GLU:O	2:B:133:GLN:HB3	1.78	0.83
2:B:209:LEU:HB3	2:B:227:LEU:HD22	1.59	0.83
2:B:287:THR:O	2:B:288:VAL:HG23	1.78	0.82
1:A:106:GLY:O	1:A:111:GLY:HA3	1.78	0.82
2:B:148:GLY:O	2:B:151:THR:HG22	1.79	0.82
1:A:151:SER:CB	1:A:193:THR:HG21	2.09	0.82
1:A:172:TYR:C	1:A:172:TYR:HD1	1.87	0.82
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.60	0.82
2:B:156:LYS:HE2	2:B:156:LYS:HA	1.61	0.81
2:B:110:GLU:O	2:B:113:GLU:HG2	1.79	0.81
2:B:20:PHE:CZ	2:B:24:ILE:HD12	2.15	0.81
2:B:150:GLY:HA2	2:B:153:LEU:HD22	1.59	0.81
1:A:6:SER:HB3	1:A:136:SER:OG	1.81	0.81
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.61	0.81
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.46	0.81
1:A:234:ILE:HD13	1:A:234:ILE:O	1.81	0.80
2:B:147:SER:HB2	2:B:190:SER:HB3	1.60	0.80
1:A:248:LEU:HD23	1:A:353:VAL:O	1.80	0.80
1:A:267:PHE:N	1:A:267:PHE:CD1	2.49	0.80
2:B:68:VAL:HG12	2:B:149:MET:SD	2.22	0.80
2:B:236:SER:O	2:B:240:THR:CG2	2.29	0.80
2:B:413:MET:HG3	2:B:414:ASP:H	1.47	0.80
1:A:313:MET:HB3	1:A:344:VAL:HG21	1.63	0.80
3:C:205:VAL:HG23	3:C:208:THR:HG23	1.64	0.80
2:B:264:ARG:HB2	2:B:266:HIS:HD2	1.45	0.79
1:A:264:ARG:C	1:A:266:HIS:H	1.91	0.79
2:B:217:LEU:C	2:B:219:LEU:H	1.91	0.79
1:A:11:GLN:HG3	1:A:74:VAL:CG1	2.13	0.79
2:B:265:LEU:HD12	2:B:265:LEU:O	1.83	0.78
1:A:69:ASP:HA	1:A:145:THR:HG21	1.66	0.78
1:A:184:PRO:HG2	1:A:398:MET:HE1	1.64	0.78
1:A:7:ILE:HG22	1:A:66:VAL:HG22	1.63	0.78
2:B:8:GLN:CD	2:B:67:LEU:HD22	2.08	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
1:A:109:THR:CG2	1:A:110:ILE:N	2.44	0.78
1:A:132:LEU:HD23	1:A:132:LEU:H	1.46	0.78
1:A:241:SER:O	1:A:244:PHE:HB3	1.82	0.78
2:B:259:MET:HA	2:B:314:THR:HG21	1.65	0.78
2:B:242:LEU:HD13	2:B:250:ALA:C	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:HA	1:A:197:HIS:ND1	1.99	0.77
2:B:396:THR:HG23	2:B:422:GLU:OE2	1.83	0.77
1:A:172:TYR:C	1:A:172:TYR:CD1	2.61	0.77
2:B:205:ASP:OD1	2:B:304:ALA:HB2	1.84	0.77
2:B:234:THR:CG2	2:B:270:PRO:HB2	2.11	0.77
2:B:259:MET:HG2	2:B:314:THR:HG21	1.67	0.77
1:A:243:ARG:HH21	1:A:252:LEU:H	0.79	0.77
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.67	0.77
1:A:231:ILE:HA	1:A:234:ILE:HG22	1.66	0.76
1:A:223:THR:HB	1:A:225:THR:HG22	1.67	0.76
1:A:331:ALA:O	1:A:335:ILE:HG12	1.86	0.76
1:A:221:ARG:O	1:A:221:ARG:HD3	1.85	0.76
1:A:110:ILE:HG23	1:A:111:GLY:N	1.99	0.76
1:A:163:LYS:O	1:A:164:LYS:HG2	1.86	0.76
2:B:198:THR:O	2:B:265:LEU:HD22	1.85	0.76
1:A:225:THR:O	1:A:229:ARG:HG3	1.86	0.76
2:B:35:SER:HB3	2:B:59:ASN:HA	1.65	0.76
2:B:192:HIS:ND1	2:B:424:ASN:OD1	2.18	0.75
3:C:145[B]:SER:OG	3:C:181:LEU:HD21	1.86	0.75
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.68	0.75
2:B:250:ALA:HA	2:B:254:LYS:HE2	1.67	0.75
1:A:362:VAL:HG13	1:A:368:LEU:HD12	1.68	0.75
2:B:209:LEU:HG	2:B:230:LEU:HD22	1.69	0.75
1:A:205:ASP:CB	1:A:303:VAL:HA	2.17	0.75
1:A:88:HIS:C	1:A:90:GLU:H	1.95	0.75
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.52	0.75
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.21	0.75
1:A:381:THR:C	1:A:383:ALA:H	1.95	0.75
2:B:176:LYS:HE3	2:B:207:GLU:HG3	1.68	0.75
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.68	0.75
1:A:276:ILE:HG23	1:A:369:ALA:CB	2.16	0.74
2:B:19:LYS:HG3	2:B:228:ASN:CB	2.17	0.74
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.87	0.74
1:A:306:ASP:O	1:A:308:ARG:N	2.20	0.74
3:C:163:LYS:HE3	3:C:164:GLY:N	2.02	0.74
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.18	0.74
1:A:101:ASN:ND2	2:B:254:LYS:HD2	2.02	0.74
1:A:63:PRO:C	1:A:64:ARG:HG2	2.12	0.74
2:B:168:THR:HB	2:B:201:THR:HG23	1.68	0.74
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.27	0.73
1:A:63:PRO:O	1:A:64:ARG:HG2	1.88	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
2:B:76:ASP:HA	2:B:79:ARG:HG2	1.71	0.73
1:A:415:GLU:CG	3:C:350:ARG:NH2	2.30	0.73
1:A:105:ARG:O	1:A:110:ILE:HG22	1.89	0.73
2:B:6:HIS:HE1	2:B:8:GLN:HG2	1.52	0.73
2:B:103:TRP:CZ3	2:B:108:TYR:HE1	2.05	0.73
2:B:217:LEU:O	2:B:219:LEU:N	2.22	0.73
2:B:274:PRO:HG2	2:B:371:LEU:HD21	1.69	0.73
1:A:242:LEU:HG	1:A:250:VAL:O	1.88	0.73
1:A:104:ALA:HB2	1:A:413:MET:HG3	1.71	0.73
1:A:415:GLU:HB3	3:C:350:ARG:HH22	1.54	0.73
2:B:111:GLY:O	2:B:115:VAL:HG23	1.89	0.73
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.19	0.73
3:C:235:ASN:O	3:C:236:ILE:CD1	2.36	0.73
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:103:TYR:CD2	1:A:189:LEU:HD13	2.24	0.72
2:B:419:THR:CB	3:C:172:PRO:HB2	2.09	0.72
1:A:7:ILE:HD11	1:A:137:VAL:HG22	1.71	0.72
1:A:112:LYS:O	1:A:115:ILE:HG22	1.89	0.72
1:A:25:CYS:HB2	1:A:30:ILE:O	1.89	0.72
3:C:288:MET:O	3:C:289:ASP:HB2	1.89	0.72
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.20	0.72
1:A:242:LEU:HD21	1:A:250:VAL:HB	1.71	0.72
2:B:237:GLY:O	2:B:241:CYS:HB3	1.90	0.71
1:A:154:MET:HE1	1:A:166:LYS:HB3	1.70	0.71
2:B:269:MET:HE2	2:B:381:SER:OG	1.91	0.71
2:B:325:MET:HE3	2:B:325:MET:HA	1.72	0.71
2:B:356:CYS:SG	2:B:357:ASP:N	2.62	0.71
1:A:343:PHE:CZ	1:A:351:PHE:HE1	2.08	0.71
2:B:48:ARG:HG2	2:B:243:ARG:O	1.90	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
2:B:66:ILE:C	2:B:67:LEU:HD23	2.15	0.71
2:B:70:LEU:HG	2:B:145:THR:CG2	2.20	0.71
2:B:299:LYS:HD3	2:B:299:LYS:N	2.04	0.71
3:C:216:ARG:HH21	3:C:254:ARG:HH11	1.39	0.71
1:A:166:LYS:HE3	1:A:199:ASP:OD1	1.90	0.71
2:B:255:LEU:O	2:B:259:MET:HG3	1.91	0.71
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.73	0.71
2:B:265:LEU:HD12	2:B:265:LEU:C	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:ILE:HD12	3:C:243:LYS:HE2	1.72	0.70
1:A:259:LEU:HD11	1:A:378:LEU:CD1	2.20	0.70
2:B:201:THR:OG1	2:B:265:LEU:HD11	1.90	0.70
1:A:317:LEU:HD12	1:A:351:PHE:HD2	1.55	0.70
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.06	0.70
2:B:70:LEU:HG	2:B:145:THR:HG23	1.74	0.70
1:A:5:ILE:HG22	1:A:6:SER:N	2.07	0.70
3:C:92:CYS:SG	3:C:318:ASN:HB3	2.32	0.70
3:C:161:LYS:O	3:C:161:LYS:CG	2.39	0.70
3:C:261:LYS:HD2	3:C:262:GLY:H	0.72	0.70
1:A:312:TYR:O	1:A:344:VAL:HG23	1.90	0.70
2:B:10:GLY:O	2:B:14:ASN:HB2	1.90	0.70
2:B:175:PRO:HD2	2:B:207:GLU:OE2	1.91	0.70
2:B:230:LEU:HD21	2:B:302:MET:HE2	1.74	0.70
1:A:148:GLY:O	1:A:151:SER:HB2	1.91	0.70
1:A:244:PHE:HD2	1:A:245:ASP:N	1.89	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:HE1	1.72	0.69
1:A:243:ARG:NH2	1:A:252:LEU:N	2.28	0.69
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.69
1:A:199:ASP:HB3	1:A:256:GLN:HE21	1.57	0.69
2:B:234:THR:O	2:B:238:VAL:HG23	1.92	0.69
2:B:24:ILE:HD11	2:B:52:TYR:CE1	2.28	0.69
2:B:180:THR:HG22	2:B:181:VAL:N	2.07	0.69
2:B:209:LEU:HD23	2:B:227:LEU:HB3	1.75	0.69
2:B:251:ASP:O	2:B:253:ARG:N	2.26	0.69
2:B:301:MET:HE1	2:B:377:PHE:HE2	1.58	0.69
1:A:237:SER:CB	1:A:376:CYS:SG	2.80	0.69
1:A:234:ILE:HD13	1:A:234:ILE:C	2.18	0.68
1:A:222:PRO:HD2	2:B:326:LYS:HB3	1.74	0.68
1:A:371:VAL:HG12	1:A:372:GLN:H	1.57	0.68
2:B:242:LEU:CD2	2:B:250:ALA:H	2.07	0.68
3:C:229:ARG:O	3:C:237:THR:HA	1.93	0.68
1:A:71:GLU:HG3	2:B:2:ARG:HH21	1.58	0.68
1:A:141:PHE:O	1:A:147:SER:HB3	1.94	0.68
1:A:221:ARG:N	1:A:222:PRO:HD3	2.09	0.68
2:B:172:VAL:HG11	2:B:387:LEU:CD2	2.22	0.68
2:B:243:ARG:HH22	2:B:252:LEU:HG	1.59	0.68
2:B:256:ALA:O	2:B:260:VAL:HG22	1.94	0.68
1:A:133:GLN:HG2	1:A:243:ARG:HH22	1.57	0.68
1:A:394:LYS:HG2	2:B:348:PRO:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:MET:CE	2:B:355:VAL:HG21	2.24	0.68
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.74	0.68
2:B:250:ALA:HB1	2:B:254:LYS:HB2	1.75	0.68
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.29	0.68
1:A:234:ILE:CB	1:A:302:MET:HE1	2.24	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.94	0.67
1:A:407:TRP:HE1	2:B:260:VAL:CG2	2.07	0.67
1:A:115:ILE:CD1	1:A:119:LEU:HG	2.23	0.67
1:A:175:PRO:HG3	1:A:304:LYS:HG2	1.76	0.67
1:A:217:LEU:HD12	1:A:277:SER:HB3	1.75	0.67
1:A:402:ARG:O	1:A:403:ALA:C	2.36	0.67
1:A:251:ASP:O	1:A:254:GLU:HB2	1.94	0.67
2:B:267:PHE:N	2:B:267:PHE:CD1	2.62	0.67
2:B:230:LEU:HD23	2:B:231:VAL:N	2.10	0.67
2:B:257:VAL:O	2:B:257:VAL:HG12	1.93	0.67
1:A:7:ILE:HD12	1:A:153:LEU:CD2	2.24	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
3:C:264:ARG:HG3	3:C:264:ARG:HH11	1.60	0.67
2:B:44:LEU:HD12	2:B:49:ILE:HD13	1.76	0.67
2:B:182:VAL:HG23	2:B:186:ASN:HD21	1.60	0.67
1:A:68:VAL:HG11	1:A:149:PHE:CZ	2.30	0.66
1:A:152:LEU:HA	1:A:155:GLU:HB2	1.77	0.66
2:B:107:HIS:CD2	2:B:151:THR:CG2	2.77	0.66
2:B:242:LEU:CD1	2:B:255:LEU:HD11	2.25	0.66
1:A:172:TYR:HD1	1:A:173:PRO:N	1.93	0.66
2:B:310:GLY:HA3	2:B:436:GLN:HE21	1.59	0.66
1:A:420:GLU:OE1	3:C:342:LEU:HD23	1.95	0.66
2:B:204:ILE:HD13	2:B:231:VAL:HG22	1.76	0.66
1:A:276:ILE:O	1:A:369:ALA:HB2	1.95	0.66
2:B:276:THR:HB	2:B:281:GLN:CG	2.25	0.66
2:B:324:SER:C	2:B:326:LYS:H	2.03	0.66
2:B:4:ILE:HG21	2:B:136:GLN:HG2	1.76	0.66
2:B:93:VAL:CG1	2:B:118:VAL:HG22	2.19	0.66
1:A:100:ALA:CB	1:A:105:ARG:HD3	2.25	0.65
1:A:313:MET:HB3	1:A:344:VAL:CG2	2.26	0.65
2:B:420:GLU:OE1	3:C:170:GLU:O	2.14	0.65
1:A:345:ASP:C	1:A:347:CYS:H	2.04	0.65
2:B:66:ILE:CD1	2:B:122:VAL:HG12	2.26	0.65
1:A:341:ILE:HG12	1:A:341:ILE:O	1.95	0.65
1:A:415:GLU:HB3	3:C:350:ARG:NH2	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:ARG:HG3	3:C:264:ARG:NH1	2.12	0.65
2:B:413:MET:HG2	2:B:418:PHE:HE1	1.61	0.65
1:A:217:LEU:HD11	1:A:367:ASP:O	1.96	0.65
1:A:315:CYS:HB3	1:A:377:MET:HE1	1.78	0.65
1:A:423:GLU:CD	3:C:346:ARG:NH2	2.54	0.65
2:B:422:GLU:O	2:B:426:ASN:HB2	1.97	0.65
2:B:35:SER:HB3	2:B:59:ASN:CA	2.26	0.65
2:B:158:ARG:NE	2:B:197:ASN:O	2.30	0.65
2:B:161:TYR:C	2:B:163:ASP:H	2.05	0.65
2:B:427:ASP:O	2:B:430:SER:HB3	1.97	0.65
1:A:317:LEU:HD12	1:A:351:PHE:CD2	2.32	0.65
1:A:372:GLN:O	1:A:373:ARG:HB3	1.96	0.65
2:B:281:GLN:O	2:B:283:TYR:HB2	1.96	0.65
2:B:431:GLU:O	2:B:434:GLN:HG2	1.97	0.65
2:B:242:LEU:HD12	2:B:255:LEU:HD11	1.78	0.64
2:B:299:LYS:O	2:B:300:ASN:HB2	1.97	0.64
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.79	0.64
2:B:103:TRP:HZ3	2:B:108:TYR:HE1	1.42	0.64
2:B:114:LEU:O	2:B:118:VAL:HG23	1.97	0.64
2:B:229:HIS:HD1	2:B:229:HIS:C	2.05	0.64
2:B:243:ARG:HH21	2:B:252:LEU:H	1.45	0.64
1:A:311:LYS:HE3	1:A:342:GLN:CD	2.22	0.64
2:B:241:CYS:O	2:B:244:PHE:HB2	1.97	0.64
1:A:206:ASN:OD1	1:A:227:LEU:HD13	1.96	0.64
2:B:105:LYS:O	2:B:110:GLU:HB2	1.97	0.64
3:C:84[B]:HIS:CD2	3:C:324:ARG:HG3	2.33	0.64
1:A:224:TYR:CD1	2:B:325:MET:HG2	2.33	0.64
1:A:271:THR:HG23	1:A:300:ASN:O	1.97	0.64
1:A:305:CYS:SG	1:A:384:ILE:HD13	2.37	0.64
2:B:284:ARG:O	2:B:286:LEU:N	2.31	0.64
1:A:234:ILE:CG2	1:A:302:MET:HE1	2.27	0.64
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.32	0.64
2:B:192:HIS:O	2:B:195:VAL:HG12	1.98	0.64
1:A:155:GLU:HA	1:A:197:HIS:HD1	1.63	0.64
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.64
1:A:343:PHE:HZ	1:A:351:PHE:CE1	2.10	0.64
2:B:180:THR:CG2	2:B:181:VAL:N	2.61	0.64
1:A:276:ILE:HG23	1:A:369:ALA:HB2	1.80	0.64
7:B:601:TA1:H463	7:B:601:TA1:H261	1.80	0.64
1:A:317:LEU:HD11	1:A:351:PHE:HE2	1.63	0.64
1:A:344:VAL:HG12	1:A:345:ASP:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:LEU:C	2:B:219:LEU:N	2.55	0.64
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.33	0.63
2:B:349:ASN:C	2:B:349:ASN:HD22	2.06	0.63
1:A:151:SER:O	1:A:155:GLU:HB2	1.98	0.63
3:C:322:ASN:OD1	3:C:323[A]:SER:N	2.31	0.63
1:A:115:ILE:HG23	1:A:116:ASP:N	2.12	0.63
2:B:318:VAL:HA	2:B:354:ALA:HB3	1.81	0.63
3:C:60:THR:O	3:C:61:SER:HB3	1.96	0.63
2:B:137:LEU:HD22	2:B:154:ILE:CG2	2.28	0.63
1:A:152:LEU:HD12	1:A:153:LEU:N	2.14	0.63
1:A:6:SER:HB3	1:A:136:SER:HG	1.64	0.63
1:A:7:ILE:HG22	1:A:66:VAL:CG2	2.28	0.63
1:A:386:GLU:O	1:A:389:ALA:N	2.31	0.63
2:B:133:GLN:HG3	2:B:165:ILE:HD11	1.80	0.62
1:A:236:SER:O	1:A:240:ALA:HB3	1.99	0.62
2:B:4:ILE:HA	2:B:134:GLY:O	1.99	0.62
2:B:253:ARG:O	2:B:254:LYS:C	2.42	0.62
1:A:175:PRO:HG2	1:A:207:GLU:OE1	1.98	0.62
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.82	0.62
1:A:7:ILE:CD1	1:A:137:VAL:HG22	2.29	0.62
2:B:253:ARG:O	2:B:256:ALA:N	2.33	0.62
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.34	0.62
2:B:107:HIS:HD2	2:B:151:THR:CG2	2.12	0.62
1:A:269:LEU:O	1:A:378:LEU:HA	1.99	0.62
2:B:230:LEU:O	2:B:233:ALA:HB3	2.00	0.62
2:B:63:PRO:HD2	2:B:86:ILE:HG12	1.80	0.62
2:B:205:ASP:OD1	2:B:304:ALA:N	2.32	0.62
2:B:282:GLN:O	2:B:282:GLN:HG2	1.97	0.62
1:A:23:LEU:HD22	1:A:232:GLY:O	1.99	0.62
1:A:118:VAL:HG11	1:A:149:PHE:HZ	1.65	0.62
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.81	0.62
2:B:70:LEU:H	2:B:145:THR:CG2	2.10	0.62
1:A:288:VAL:O	1:A:290:GLU:N	2.33	0.62
1:A:315:CYS:HB3	1:A:377:MET:CE	2.29	0.62
1:A:267:PHE:HD1	1:A:267:PHE:H	1.47	0.62
1:A:381:THR:C	1:A:383:ALA:N	2.56	0.62
2:B:70:LEU:C	2:B:99:ALA:HB2	2.24	0.61
2:B:154:ILE:HG22	2:B:166:MET:HE2	1.81	0.61
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.30	0.61
1:A:88:HIS:O	1:A:90:GLU:N	2.33	0.61
1:A:278:ALA:HA	1:A:282:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ILE:CD1	2:B:231:VAL:HG13	2.30	0.61
3:C:43:PRO:HG2	3:C:44:LYS:HE3	1.83	0.61
1:A:102:ASN:OD1	1:A:105:ARG:HB3	1.99	0.61
1:A:177:VAL:HG11	2:B:329:ASP:HB3	1.83	0.61
2:B:283:TYR:C	2:B:284:ARG:HG2	2.25	0.61
1:A:179:THR:HG22	2:B:352:LYS:NZ	2.15	0.61
2:B:4:ILE:HG23	2:B:134:GLY:O	2.00	0.61
2:B:70:LEU:CG	2:B:145:THR:HG23	2.30	0.61
2:B:114:LEU:HD23	2:B:149:MET:CE	2.30	0.61
1:A:181:VAL:HG21	2:B:258:ASN:O	2.01	0.61
1:A:248:LEU:CD2	1:A:353:VAL:O	2.49	0.61
2:B:128:SER:OG	2:B:129:CYS:N	2.34	0.61
1:A:115:ILE:HG13	1:A:152:LEU:HD13	1.81	0.61
2:B:299:LYS:H	2:B:299:LYS:CD	2.07	0.61
1:A:179:THR:HG21	2:B:248:LEU:HD21	1.81	0.61
1:A:177:VAL:CG1	2:B:329:ASP:HB3	2.31	0.61
2:B:279:GLY:O	2:B:282:GLN:HB3	2.01	0.61
1:A:167:LEU:HA	1:A:200:CYS:O	2.01	0.60
1:A:362:VAL:HG13	1:A:368:LEU:HB2	1.83	0.60
1:A:436:GLY:C	1:A:438:ASP:H	2.08	0.60
1:A:407:TRP:NE1	2:B:260:VAL:HG23	2.14	0.60
2:B:211:ASP:OD1	2:B:212:ILE:N	2.33	0.60
2:B:230:LEU:CD2	2:B:302:MET:HE2	2.31	0.60
1:A:119:LEU:CD2	1:A:122:ILE:HD11	2.28	0.60
1:A:191:THR:HG21	1:A:425:MET:SD	2.41	0.60
2:B:19:LYS:CG	2:B:228:ASN:HB3	2.31	0.60
1:A:169:PHE:CE1	1:A:235:VAL:HG22	2.36	0.60
2:B:31:ASP:O	2:B:32:PRO:C	2.44	0.60
2:B:324:SER:O	2:B:328:VAL:HG23	2.01	0.60
1:A:168:GLU:OE1	1:A:198:SER:HB2	2.00	0.60
1:A:179:THR:HG21	2:B:248:LEU:CD2	2.30	0.60
2:B:49:ILE:O	2:B:51:VAL:N	2.35	0.60
2:B:70:LEU:N	2:B:145:THR:HG21	2.11	0.60
1:A:229:ARG:NH1	1:A:363:VAL:HG21	2.16	0.60
1:A:435:VAL:HG12	1:A:435:VAL:O	2.02	0.60
2:B:285:ALA:HB1	2:B:290:GLU:HG2	1.82	0.60
3:C:113:LYS:O	3:C:114:ASP:CB	2.34	0.60
1:A:11:GLN:HE21	1:A:74:VAL:HG22	1.66	0.60
1:A:115:ILE:HD13	1:A:115:ILE:O	2.02	0.60
1:A:284:GLU:O	1:A:286:LEU:N	2.35	0.60
1:A:401:LYS:HZ2	2:B:346:TRP:CD1	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:THR:HA	2:B:425:MET:HE2	1.83	0.60
2:B:324:SER:CB	2:B:327:GLU:HG2	2.30	0.60
2:B:419:THR:HG21	3:C:172:PRO:C	2.20	0.60
3:C:169:ARG:O	3:C:176:PRO:HA	2.01	0.60
1:A:344:VAL:HG11	1:A:346:TRP:NE1	2.16	0.60
2:B:205:ASP:OD1	2:B:304:ALA:CB	2.50	0.60
1:A:119:LEU:O	1:A:122:ILE:HG12	2.02	0.60
2:B:68:VAL:CG1	2:B:149:MET:SD	2.90	0.60
2:B:102:ASN:ND2	2:B:407:TRP:O	2.35	0.60
2:B:424:ASN:C	2:B:424:ASN:HD22	2.09	0.60
1:A:409:VAL:C	1:A:411:GLU:H	2.09	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
1:A:101:ASN:CG	2:B:254:LYS:HD2	2.28	0.59
1:A:413:MET:O	1:A:414:GLU:HG3	2.02	0.59
2:B:89:PRO:HA	2:B:92:PHE:CD1	2.38	0.59
2:B:115:VAL:HG21	2:B:152:LEU:HD23	1.84	0.59
2:B:141:LEU:CD1	2:B:141:LEU:N	2.65	0.59
1:A:371:VAL:HG12	1:A:372:GLN:N	2.17	0.59
1:A:420:GLU:OE1	3:C:342:LEU:HD21	2.01	0.59
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.85	0.59
2:B:299:LYS:O	2:B:300:ASN:CB	2.51	0.59
2:B:324:SER:C	2:B:326:LYS:N	2.59	0.59
1:A:6:SER:HA	1:A:136:SER:O	2.02	0.59
1:A:242:LEU:C	1:A:244:PHE:H	2.09	0.59
2:B:30:ILE:HD13	2:B:53:TYR:CE2	2.38	0.59
3:C:273:LYS:HE2	3:C:308:ASP:O	2.03	0.59
1:A:278:ALA:HB2	1:A:369:ALA:HA	1.85	0.59
2:B:151:THR:OG1	2:B:193:GLN:HB3	2.03	0.59
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.29	0.59
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.33	0.58
2:B:194:LEU:C	2:B:196:GLU:H	2.11	0.58
2:B:229:HIS:C	2:B:229:HIS:ND1	2.62	0.58
2:B:307:PRO:HB3	2:B:312:TYR:OH	2.04	0.58
1:A:150:THR:O	1:A:151:SER:C	2.47	0.58
1:A:264:ARG:C	1:A:266:HIS:N	2.60	0.58
2:B:180:THR:CG2	2:B:181:VAL:H	2.17	0.58
1:A:2:ARG:N	1:A:131:GLY:O	2.36	0.58
1:A:215:ARG:C	1:A:216:ASN:HD22	2.12	0.58
1:A:234:ILE:HB	1:A:302:MET:HE1	1.85	0.58
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HD13	1:A:115:ILE:C	2.28	0.58
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.15	0.58
1:A:339:ARG:C	1:A:341:ILE:H	2.11	0.58
1:A:407:TRP:O	1:A:411:GLU:HG2	2.02	0.58
1:A:218:ASP:O	1:A:219:ILE:HG23	2.04	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.04	0.58
2:B:320:ARG:O	2:B:359:PRO:HA	2.04	0.58
1:A:166:LYS:HD2	1:A:197:HIS:O	2.04	0.57
1:A:369:ALA:O	1:A:370:LYS:HB3	2.03	0.57
2:B:30:ILE:HA	2:B:35:SER:O	2.04	0.57
1:A:317:LEU:HD11	1:A:351:PHE:CE2	2.38	0.57
1:A:362:VAL:HG11	1:A:368:LEU:O	2.04	0.57
2:B:226:ASP:O	2:B:227:LEU:C	2.46	0.57
2:B:319:PHE:HA	2:B:375:ALA:HA	1.86	0.57
2:B:345:GLU:C	2:B:347:ILE:H	2.13	0.57
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.40	0.57
1:A:202:PHE:CE2	1:A:378:LEU:HD22	2.38	0.57
2:B:273:ALA:CB	2:B:274:PRO:HD3	2.30	0.57
1:A:63:PRO:HD3	1:A:86:LEU:O	2.04	0.57
2:B:132:LEU:CD2	2:B:164:ARG:HG3	2.32	0.57
2:B:253:ARG:O	2:B:257:VAL:N	2.33	0.57
1:A:165:SER:HA	1:A:199:ASP:OD2	2.04	0.57
1:A:362:VAL:CG1	1:A:368:LEU:HB2	2.35	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
1:A:196:GLU:C	1:A:197:HIS:CD2	2.82	0.57
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.18	0.57
2:B:182:VAL:HG23	2:B:186:ASN:ND2	2.20	0.57
2:B:14:ASN:OD1	2:B:75:MET:HG2	2.05	0.57
2:B:198:THR:HG22	2:B:265:LEU:HD22	1.86	0.57
3:C:322:ASN:OD1	3:C:323[B]:SER:N	2.31	0.57
2:B:270:PRO:HA	2:B:377:PHE:O	2.04	0.57
2:B:424:ASN:C	2:B:424:ASN:ND2	2.61	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:239:THR:O	1:A:240:ALA:C	2.48	0.56
1:A:283:HIS:O	1:A:284:GLU:C	2.47	0.56
2:B:70:LEU:CD1	2:B:145:THR:HG23	2.35	0.56
2:B:149:MET:O	2:B:153:LEU:HD13	2.05	0.56
1:A:175:PRO:HG3	1:A:304:LYS:CG	2.35	0.56
1:A:210:TYR:CE2	1:A:227:LEU:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HB2	1:A:266:HIS:HD2	1.67	0.56
1:A:331:ALA:O	1:A:334:THR:HG22	2.05	0.56
2:B:50:ASN:O	2:B:64:ARG:NH2	2.38	0.56
3:C:112[B]:GLU:OE1	3:C:113:LYS:HG2	2.05	0.56
1:A:117:LEU:HD11	1:A:121:ARG:HH22	1.69	0.56
1:A:152:LEU:HA	1:A:155:GLU:CB	2.35	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.56
1:A:420:GLU:CD	3:C:346:ARG:HD2	2.30	0.56
2:B:49:ILE:O	2:B:50:ASN:C	2.48	0.56
2:B:319:PHE:CD2	2:B:375:ALA:HB2	2.40	0.56
2:B:422:GLU:O	2:B:426:ASN:N	2.37	0.56
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.35	0.56
1:A:313:MET:O	1:A:314:ALA:HB2	2.04	0.56
2:B:6:HIS:HB3	2:B:65:ALA:HB2	1.87	0.56
2:B:151:THR:OG1	2:B:193:GLN:CB	2.54	0.56
2:B:216:THR:O	2:B:217:LEU:HD12	2.05	0.56
3:C:216:ARG:HH21	3:C:254:ARG:HH12	1.50	0.56
2:B:19:LYS:O	2:B:23:VAL:HG23	2.06	0.56
1:A:11:GLN:HE22	2:B:249:ASN:ND2	2.03	0.56
1:A:19:ALA:CB	1:A:228:ASN:HB3	2.35	0.56
1:A:394:LYS:HG2	2:B:348:PRO:CG	2.35	0.56
2:B:259:MET:CA	2:B:314:THR:HG21	2.35	0.56
2:B:311:ARG:HD2	2:B:344:VAL:H	1.71	0.56
3:C:151:CYS:O	3:C:152:GLU:HB2	2.05	0.56
2:B:139:HIS:HE1	2:B:168:THR:HG23	1.71	0.56
2:B:190:SER:O	2:B:194:LEU:HG	2.06	0.56
2:B:204:ILE:HG21	2:B:231:VAL:CG2	2.36	0.56
2:B:223:THR:HG22	2:B:224:TYR:N	2.21	0.56
3:C:108:MET:HG2	3:C:200:ASN:ND2	2.21	0.56
1:A:172:TYR:OH	1:A:387:ALA:O	2.24	0.56
2:B:119:LEU:O	2:B:123:ARG:HG3	2.06	0.56
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.56
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.87	0.56
1:A:88:HIS:C	1:A:90:GLU:N	2.57	0.56
1:A:110:ILE:CG2	1:A:111:GLY:H	2.15	0.55
1:A:253:THR:O	1:A:256:GLN:HG2	2.06	0.55
2:B:108:TYR:CE1	2:B:413:MET:HE1	2.40	0.55
2:B:272:PHE:HB3	2:B:275:LEU:HD22	1.88	0.55
1:A:244:PHE:C	1:A:244:PHE:CD2	2.83	0.55
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.41	0.55
2:B:166:MET:HB3	2:B:198:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:OE2	3:C:346:ARG:CZ	2.50	0.55
2:B:67:LEU:HD23	2:B:67:LEU:N	2.22	0.55
2:B:209:LEU:O	2:B:210:TYR:C	2.48	0.55
2:B:312:TYR:O	2:B:344:VAL:HB	2.05	0.55
1:A:382:THR:O	1:A:382:THR:HG22	2.05	0.55
2:B:165:ILE:HD13	2:B:165:ILE:H	1.71	0.55
2:B:311:ARG:HG2	2:B:311:ARG:HH11	1.71	0.55
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.42	0.55
2:B:369:ARG:C	2:B:369:ARG:HD2	2.32	0.55
3:C:108:MET:HG2	3:C:200:ASN:HD21	1.70	0.55
1:A:150:THR:O	1:A:153:LEU:N	2.40	0.55
2:B:191:VAL:HG11	2:B:425:MET:HE2	1.89	0.55
2:B:310:GLY:CA	2:B:436:GLN:HE21	2.19	0.55
1:A:231:ILE:HA	1:A:234:ILE:CG2	2.36	0.55
1:A:381:THR:OG1	1:A:383:ALA:HB3	2.07	0.55
2:B:210:TYR:HD2	2:B:227:LEU:HD21	1.71	0.55
3:C:134:THR:HG23	3:C:134:THR:O	2.06	0.55
1:A:216:ASN:O	1:A:217:LEU:HB2	2.05	0.55
2:B:191:VAL:HA	2:B:194:LEU:HD12	1.88	0.55
1:A:6:SER:O	1:A:65:ALA:HB1	2.07	0.55
1:A:408:TYR:O	1:A:411:GLU:N	2.39	0.55
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.42	0.54
1:A:408:TYR:CD1	1:A:418:PHE:HZ	2.24	0.54
2:B:68:VAL:HG12	2:B:149:MET:CE	2.38	0.54
1:A:9:VAL:CG1	1:A:139:HIS:HB3	2.38	0.54
1:A:305:CYS:O	1:A:306:ASP:C	2.49	0.54
2:B:4:ILE:HD13	2:B:136:GLN:NE2	2.18	0.54
2:B:20:PHE:CE2	2:B:24:ILE:HD12	2.43	0.54
2:B:147:SER:O	2:B:151:THR:CB	2.52	0.54
3:C:261:LYS:CD	3:C:262:GLY:N	2.45	0.54
1:A:163:LYS:O	1:A:163:LYS:HG2	2.08	0.54
2:B:239:THR:HG22	2:B:240:THR:N	2.22	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:431:GLU:O	2:B:434:GLN:CG	2.56	0.54
1:A:17:GLY:O	1:A:21:TRP:HB2	2.08	0.54
1:A:179:THR:HG22	2:B:352:LYS:HZ1	1.72	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:107:HIS:HD2	2:B:151:THR:HG22	1.72	0.54
2:B:213:CYS:SG	2:B:219:LEU:HD23	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:THR:O	2:B:241:CYS:N	2.41	0.54
1:A:5:ILE:O	1:A:136:SER:N	2.40	0.54
1:A:98:ASP:O	1:A:110:ILE:HD13	2.08	0.54
2:B:179:ASP:HB2	6:B:600:GDP:H3'	1.90	0.54
1:A:5:ILE:O	1:A:135:PHE:HA	2.09	0.53
2:B:259:MET:CG	2:B:314:THR:HG21	2.36	0.53
2:B:298:ALA:O	2:B:299:LYS:C	2.50	0.53
2:B:322:ARG:HG3	2:B:322:ARG:HH11	1.73	0.53
2:B:4:ILE:CG2	2:B:136:GLN:HG2	2.38	0.53
2:B:259:MET:HG2	2:B:314:THR:CG2	2.38	0.53
1:A:163:LYS:C	1:A:164:LYS:HG2	2.33	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
1:A:121:ARG:O	1:A:125:LEU:HB2	2.08	0.53
1:A:328:VAL:C	1:A:330:ALA:H	2.16	0.53
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.44	0.53
3:C:81:MET:HE2	3:C:326:ALA:HB2	1.91	0.53
1:A:324:VAL:O	1:A:327:ASP:HB2	2.08	0.53
1:A:101:ASN:ND2	5:A:500:GTP:O3G	2.42	0.53
1:A:110:ILE:O	1:A:112:LYS:N	2.41	0.53
1:A:242:LEU:C	1:A:244:PHE:N	2.66	0.53
1:A:243:ARG:CZ	1:A:252:LEU:HG	2.39	0.53
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.53
3:C:108:MET:CG	3:C:200:ASN:HD21	2.21	0.53
3:C:216:ARG:NH2	3:C:254:ARG:NH1	2.47	0.53
1:A:173:PRO:HB2	1:A:391:LEU:CD1	2.38	0.53
2:B:5:VAL:HG23	2:B:5:VAL:O	2.09	0.53
1:A:5:ILE:CG2	1:A:6:SER:N	2.70	0.53
1:A:182:VAL:O	1:A:184:PRO:N	2.41	0.53
1:A:338:LYS:O	1:A:340:THR:N	2.34	0.53
2:B:141:LEU:HA	2:B:147:SER:HB3	1.91	0.53
2:B:323:MET:HG3	2:B:328:VAL:HG21	1.90	0.53
3:C:13:ARG:HG3	3:C:13:ARG:HH11	1.73	0.53
3:C:36:THR:HB	3:C:47:PRO:HB2	1.91	0.53
1:A:248:LEU:HB3	1:A:355:ILE:H	1.73	0.53
2:B:70:LEU:HD12	2:B:145:THR:HG23	1.91	0.53
2:B:210:TYR:CD2	2:B:227:LEU:HD21	2.44	0.53
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.90	0.53
2:B:343:PHE:O	2:B:344:VAL:O	2.26	0.53
1:A:98:ASP:CB	1:A:105:ARG:HH21	2.14	0.52
1:A:206:ASN:OD1	1:A:227:LEU:CD1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HD13	1:A:231:ILE:N	2.25	0.52
1:A:339:ARG:C	1:A:341:ILE:N	2.68	0.52
1:A:344:VAL:HG12	1:A:345:ASP:H	1.74	0.52
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.73	0.52
2:B:172:VAL:CG1	2:B:387:LEU:HD21	2.24	0.52
2:B:226:ASP:O	2:B:229:HIS:N	2.43	0.52
2:B:250:ALA:CA	2:B:254:LYS:HE2	2.35	0.52
1:A:173:PRO:HB2	1:A:391:LEU:HD11	1.91	0.52
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.43	0.52
2:B:297:ASP:OD1	2:B:298:ALA:N	2.39	0.52
1:A:115:ILE:O	1:A:116:ASP:C	2.51	0.52
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.42	0.52
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.40	0.52
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.89	0.52
1:A:345:ASP:OD2	1:A:439:SER:HB3	2.10	0.52
1:A:434:GLU:C	1:A:436:GLY:H	2.18	0.52
2:B:175:PRO:O	2:B:176:LYS:C	2.52	0.52
2:B:198:THR:HG22	2:B:265:LEU:CD2	2.39	0.52
3:C:84[B]:HIS:NE2	3:C:89:TYR:HB2	2.25	0.52
1:A:4:CYS:HA	1:A:134:GLY:O	2.10	0.52
2:B:107:HIS:CD2	2:B:151:THR:HG22	2.45	0.52
1:A:8:HIS:HB3	1:A:13:GLY:O	2.10	0.52
1:A:34:GLY:C	1:A:61:HIS:N	2.68	0.52
2:B:188:THR:HA	2:B:425:MET:CE	2.40	0.52
2:B:212:ILE:O	2:B:216:THR:HB	2.09	0.52
2:B:346:TRP:CD1	2:B:346:TRP:H	2.27	0.52
2:B:425:MET:O	2:B:428:LEU:HB3	2.09	0.52
1:A:63:PRO:C	1:A:64:ARG:CG	2.83	0.52
1:A:253:THR:O	1:A:254:GLU:C	2.52	0.52
2:B:277:SER:OG	2:B:281:GLN:HB2	2.10	0.52
3:C:264:ARG:NH1	3:C:264:ARG:CG	2.72	0.52
2:B:200:GLU:N	2:B:265:LEU:HD13	2.25	0.52
2:B:314:THR:CG2	2:B:315:VAL:N	2.73	0.52
1:A:9:VAL:HG21	1:A:149:PHE:CD1	2.46	0.51
2:B:242:LEU:HD22	2:B:250:ALA:N	2.19	0.51
2:B:320:ARG:HA	2:B:356:CYS:HB3	1.92	0.51
2:B:331:GLN:O	2:B:335:VAL:HG23	2.08	0.51
2:B:149:MET:O	2:B:153:LEU:HD22	2.10	0.51
2:B:416:MET:HG2	3:C:171:HIS:CG	2.45	0.51
1:A:201:ALA:O	1:A:267:PHE:HA	2.10	0.51
1:A:243:ARG:NH2	1:A:251:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:HG21	1:A:300:ASN:OD1	2.09	0.51
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.92	0.51
3:C:41:LYS:C	3:C:42:GLN:HG3	2.35	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:417:GLU:HA	1:A:417:GLU:OE1	2.10	0.51
1:A:244:PHE:CD2	1:A:245:ASP:N	2.76	0.51
1:A:396:ASP:O	1:A:397:LEU:C	2.53	0.51
2:B:296:PHE:CZ	2:B:315:VAL:HG11	2.46	0.51
2:B:103:TRP:CE2	2:B:189:LEU:HB3	2.45	0.51
2:B:264:ARG:HE	2:B:264:ARG:HA	1.75	0.51
2:B:360:PRO:O	2:B:369:ARG:C	2.54	0.51
3:C:255:ALA:HB1	3:C:272:ASN:HA	1.93	0.51
2:B:263:PRO:O	2:B:264:ARG:C	2.52	0.51
1:A:67:PHE:HE1	1:A:87:PHE:CE2	2.29	0.51
2:B:295:MET:SD	2:B:375:ALA:O	2.68	0.51
2:B:360:PRO:HB2	7:B:601:TA1:H281	1.91	0.51
1:A:115:ILE:HD11	1:A:119:LEU:HG	1.92	0.51
1:A:133:GLN:HB3	1:A:243:ARG:HH12	1.76	0.51
1:A:140:SER:O	1:A:142:GLY:N	2.44	0.51
1:A:231:ILE:CA	1:A:234:ILE:HG22	2.38	0.51
1:A:171:ILE:O	1:A:171:ILE:HG22	2.10	0.51
1:A:310:GLY:HA3	1:A:383:ALA:N	2.26	0.51
1:A:362:VAL:HG13	1:A:368:LEU:CD1	2.38	0.51
2:B:21:TRP:HZ2	2:B:65:ALA:HB2	1.76	0.51
2:B:175:PRO:HD2	2:B:207:GLU:CD	2.35	0.51
2:B:288:VAL:CG2	2:B:323:MET:HE3	2.40	0.51
2:B:323:MET:HG3	2:B:328:VAL:CG2	2.41	0.51
3:C:134:THR:O	3:C:134:THR:CG2	2.59	0.51
1:A:22:GLU:O	1:A:23:LEU:C	2.54	0.50
1:A:196:GLU:O	1:A:197:HIS:CD2	2.64	0.50
2:B:113:GLU:HG3	2:B:114:LEU:N	2.26	0.50
1:A:238:ILE:O	1:A:242:LEU:HB2	2.11	0.50
1:A:132:LEU:CD2	1:A:164:LYS:HE3	2.41	0.50
1:A:196:GLU:C	1:A:197:HIS:HD2	2.19	0.50
1:A:119:LEU:HA	1:A:122:ILE:HG12	1.93	0.50
1:A:191:THR:HG23	1:A:192:HIS:N	2.25	0.50
1:A:255:PHE:O	1:A:256:GLN:C	2.53	0.50
2:B:399:PHE:O	2:B:402:LYS:N	2.29	0.50
1:A:10:GLY:O	1:A:11:GLN:C	2.53	0.50
1:A:122:ILE:CD1	1:A:157:LEU:HD21	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:THR:HG23	2:B:241:CYS:H	1.76	0.50
1:A:110:ILE:CG2	1:A:111:GLY:N	2.71	0.50
1:A:402:ARG:O	1:A:403:ALA:O	2.29	0.50
2:B:260:VAL:HG23	2:B:260:VAL:O	2.10	0.50
2:B:307:PRO:C	2:B:309:HIS:H	2.18	0.50
2:B:387:LEU:HD23	2:B:388:PHE:CD2	2.47	0.50
2:B:431:GLU:OE1	2:B:432:TYR:CA	2.57	0.50
1:A:115:ILE:CG2	1:A:116:ASP:N	2.75	0.50
1:A:133:GLN:CB	1:A:243:ARG:HH12	2.24	0.50
2:B:176:LYS:CE	2:B:207:GLU:HG3	2.39	0.50
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.43	0.50
2:B:333:LEU:O	2:B:336:GLN:N	2.45	0.50
1:A:16:ILE:HG23	1:A:17:GLY:N	2.26	0.50
1:A:95:GLY:C	1:A:97:GLU:N	2.69	0.50
1:A:241:SER:C	1:A:244:PHE:HB3	2.36	0.50
2:B:149:MET:O	2:B:149:MET:HG2	2.10	0.50
2:B:168:THR:O	2:B:201:THR:HA	2.12	0.50
2:B:224:TYR:O	2:B:225:GLY:C	2.53	0.50
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.94	0.50
2:B:8:GLN:HB3	2:B:14:ASN:HA	1.94	0.50
2:B:49:ILE:HG13	2:B:50:ASN:H	1.76	0.50
2:B:336:GLN:HE22	2:B:349:ASN:ND2	2.10	0.50
1:A:11:GLN:O	1:A:14:VAL:HB	2.12	0.49
2:B:262:PHE:O	2:B:264:ARG:N	2.45	0.49
2:B:345:GLU:O	2:B:347:ILE:N	2.45	0.49
3:C:156:ASP:H	3:C:162:ASN:ND2	2.10	0.49
1:A:413:MET:C	1:A:414:GLU:HG3	2.36	0.49
1:A:414:GLU:OE1	1:A:414:GLU:N	2.46	0.49
2:B:82:PRO:C	2:B:84:GLY:H	2.20	0.49
2:B:265:LEU:O	2:B:266:HIS:O	2.29	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
3:C:163:LYS:CA	3:C:163:LYS:CE	2.53	0.49
2:B:3:GLU:HA	2:B:51:VAL:HA	1.93	0.49
2:B:4:ILE:HD12	2:B:239:THR:CG2	2.42	0.49
2:B:69:ASP:HA	2:B:145:THR:HG21	1.95	0.49
2:B:242:LEU:C	2:B:244:PHE:H	2.19	0.49
1:A:149:PHE:HE1	1:A:153:LEU:HD22	1.77	0.49
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.46	0.49
1:A:148:GLY:O	1:A:149:PHE:C	2.55	0.49
2:B:4:ILE:HG22	2:B:5:VAL:N	2.27	0.49
2:B:332:MET:CE	2:B:351:VAL:HG11	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:GLU:HA	2:B:434:GLN:CG	2.42	0.49
1:A:152:LEU:HD12	1:A:152:LEU:C	2.38	0.49
1:A:286:LEU:O	1:A:287:SER:C	2.55	0.49
2:B:265:LEU:HD12	2:B:266:HIS:O	2.12	0.49
3:C:125:ASP:O	3:C:129:ARG:HG3	2.12	0.49
1:A:23:LEU:HD23	1:A:236:SER:CB	2.37	0.49
1:A:188:ILE:O	1:A:191:THR:HG22	2.13	0.49
1:A:192:HIS:CD2	1:A:424:ASP:OD2	2.66	0.49
1:A:234:ILE:C	1:A:234:ILE:CD1	2.86	0.49
2:B:142:GLY:HA3	2:B:183:GLU:OE2	2.13	0.49
1:A:101:ASN:ND2	2:B:254:LYS:CD	2.76	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
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.49
1:A:274:PRO:CB	1:A:371:VAL:HG21	2.43	0.49
2:B:173:PRO:HB3	2:B:183:GLU:HG2	1.93	0.49
2:B:431:GLU:OE1	2:B:432:TYR:N	2.46	0.49
1:A:158:SER:OG	1:A:197:HIS:HB3	2.13	0.49
1:A:191:THR:CG2	1:A:192:HIS:N	2.76	0.49
1:A:227:LEU:O	1:A:231:ILE:HG12	2.12	0.49
1:A:392:ASP:O	1:A:395:PHE:HB3	2.13	0.49
2:B:24:ILE:HG22	2:B:25:SER:N	2.27	0.49
2:B:173:PRO:HB3	2:B:183:GLU:CG	2.42	0.49
2:B:413:MET:HG3	2:B:414:ASP:N	2.22	0.49
3:C:19:GLU:HG2	3:C:334:ALA:CB	2.42	0.49
1:A:147:SER:CB	1:A:190:THR:OG1	2.52	0.48
1:A:149:PHE:O	1:A:150:THR:C	2.56	0.48
1:A:283:HIS:O	1:A:285:GLN:N	2.45	0.48
1:A:11:GLN:CG	1:A:74:VAL:HG11	2.28	0.48
1:A:104:ALA:CB	1:A:408:TYR:HD2	2.26	0.48
1:A:218:ASP:C	1:A:219:ILE:HG12	2.37	0.48
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.28	0.48
2:B:199:ASP:O	2:B:200:GLU:HG3	2.13	0.48
2:B:269:MET:HB3	2:B:303:ALA:HB2	1.94	0.48
1:A:9:VAL:HG11	1:A:150:THR:OG1	2.14	0.48
2:B:154:ILE:HG22	2:B:166:MET:CE	2.44	0.48
2:B:176:LYS:HG3	2:B:177:VAL:H	1.78	0.48
2:B:239:THR:O	2:B:240:THR:C	2.56	0.48
3:C:161:LYS:O	3:C:163:LYS:N	2.46	0.48
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.96	0.48
1:A:204:VAL:CG1	1:A:209:ILE:HD11	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:O	1:A:231:ILE:C	2.57	0.48
1:A:252:LEU:O	1:A:253:THR:C	2.56	0.48
1:A:316:CYS:HB3	1:A:378:LEU:HD12	1.95	0.48
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.94	0.48
2:B:209:LEU:O	2:B:213:CYS:N	2.47	0.48
2:B:296:PHE:HZ	2:B:315:VAL:HG11	1.78	0.48
1:A:263:PRO:O	1:A:264:ARG:C	2.56	0.48
1:A:288:VAL:C	1:A:290:GLU:N	2.71	0.48
1:A:317:LEU:CD1	1:A:351:PHE:CD2	2.97	0.48
2:B:325:MET:CE	2:B:355:VAL:HG11	2.38	0.48
1:A:13:GLY:C	1:A:16:ILE:HG22	2.38	0.48
1:A:151:SER:OG	1:A:193:THR:HG21	2.13	0.48
1:A:369:ALA:O	1:A:370:LYS:CB	2.62	0.48
2:B:168:THR:CB	2:B:201:THR:HG23	2.38	0.48
2:B:187:ALA:O	2:B:188:THR:C	2.57	0.48
2:B:191:VAL:HG13	2:B:192:HIS:N	2.28	0.48
2:B:209:LEU:CD2	2:B:227:LEU:HD13	2.44	0.48
2:B:237:GLY:O	2:B:241:CYS:CB	2.61	0.48
1:A:12:ALA:CB	1:A:140:SER:OG	2.59	0.48
1:A:132:LEU:HD21	1:A:164:LYS:HE3	1.96	0.48
2:B:175:PRO:CD	2:B:207:GLU:OE1	2.61	0.48
2:B:182:VAL:O	2:B:183:GLU:C	2.56	0.48
2:B:287:THR:O	2:B:288:VAL:CG2	2.58	0.48
2:B:20:PHE:CG	2:B:235:MET:SD	3.07	0.48
1:A:203:MET:SD	1:A:267:PHE:HB3	2.53	0.48
1:A:210:TYR:CE2	1:A:227:LEU:HD21	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:C:335:ASP:N	3:C:335:ASP:OD1	2.46	0.48
1:A:5:ILE:HG22	1:A:6:SER:H	1.78	0.48
1:A:97:GLU:HB2	1:A:110:ILE:HD11	1.96	0.48
1:A:217:LEU:CD1	1:A:277:SER:HA	2.44	0.48
2:B:243:ARG:N	2:B:243:ARG:HD3	2.26	0.48
3:C:92:CYS:SG	3:C:318:ASN:CB	3.02	0.48
1:A:115:ILE:HG23	1:A:116:ASP:H	1.79	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:137:LEU:HD22	2:B:154:ILE:HG21	1.94	0.47
1:A:19:ALA:HB2	1:A:228:ASN:HB3	1.96	0.47
1:A:96:LYS:O	1:A:97:GLU:O	2.31	0.47
1:A:103:TYR:O	1:A:104:ALA:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.45	0.47
2:B:297:ASP:OD2	2:B:299:LYS:HE2	2.14	0.47
2:B:308:ARG:HG3	2:B:342:TYR:OH	2.13	0.47
3:C:153:ARG:HB3	3:C:165:ASN:HB3	1.96	0.47
1:A:99:ALA:O	1:A:100:ALA:HB3	2.14	0.47
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.47
1:A:224:TYR:CG	2:B:325:MET:HG2	2.50	0.47
2:B:101:ASN:ND2	2:B:101:ASN:O	2.48	0.47
2:B:264:ARG:HA	2:B:264:ARG:NE	2.29	0.47
2:B:333:LEU:O	2:B:334:ASN:C	2.58	0.47
1:A:6:SER:OG	1:A:65:ALA:HB2	2.14	0.47
1:A:110:ILE:O	1:A:111:GLY:C	2.57	0.47
1:A:147:SER:O	1:A:190:THR:HG23	2.14	0.47
2:B:49:ILE:HG13	2:B:50:ASN:N	2.28	0.47
2:B:156:LYS:HA	2:B:156:LYS:CE	2.38	0.47
2:B:185:TYR:HD2	2:B:395:PHE:CE1	2.33	0.47
1:A:117:LEU:HD12	1:A:121:ARG:HH12	1.80	0.47
2:B:210:TYR:O	2:B:211:ASP:C	2.57	0.47
1:A:115:ILE:CD1	1:A:115:ILE:C	2.87	0.47
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.49	0.47
1:A:226:ASN:O	1:A:229:ARG:N	2.48	0.47
1:A:241:SER:HB3	1:A:320:ARG:NH2	2.30	0.47
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.97	0.47
1:A:286:LEU:CD1	1:A:290:GLU:HG2	2.44	0.47
2:B:115:VAL:CG2	2:B:152:LEU:HD23	2.44	0.47
2:B:211:ASP:OD1	2:B:212:ILE:HG13	2.13	0.47
2:B:259:MET:HE1	2:B:378:ILE:CG2	2.45	0.47
2:B:419:THR:CG2	3:C:172:PRO:C	2.70	0.47
3:C:137:ASN:HA	3:C:230:HIS:HB3	1.96	0.47
1:A:25:CYS:SG	1:A:83:TYR:HE2	2.38	0.47
1:A:175:PRO:HD2	1:A:207:GLU:HB3	1.97	0.47
1:A:224:TYR:HD1	2:B:247:GLN:HB3	1.80	0.47
2:B:24:ILE:CD1	2:B:52:TYR:CE1	2.97	0.47
2:B:70:LEU:O	2:B:99:ALA:HB2	2.15	0.47
2:B:134:GLY:HA3	2:B:165:ILE:HG12	1.97	0.47
2:B:242:LEU:HD11	2:B:250:ALA:HB3	1.97	0.47
2:B:310:GLY:HA3	2:B:436:GLN:NE2	2.29	0.47
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.79	0.47
1:A:392:ASP:OD2	1:A:422:ARG:NE	2.48	0.47
1:A:409:VAL:C	1:A:411:GLU:N	2.71	0.47
2:B:272:PHE:CE1	7:B:601:TA1:H391	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:CE1	1:A:152:LEU:HB3	2.49	0.47
1:A:386:GLU:O	1:A:388:TRP:N	2.47	0.47
1:A:436:GLY:O	1:A:438:ASP:N	2.48	0.47
2:B:168:THR:N	2:B:200:GLU:O	2.43	0.47
2:B:226:ASP:O	2:B:229:HIS:HB3	2.14	0.47
2:B:383:ALA:C	2:B:385:GLN:N	2.72	0.47
2:B:384:ILE:O	2:B:384:ILE:HG23	2.14	0.47
2:B:416:MET:SD	3:C:171:HIS:ND1	2.88	0.47
1:A:9:VAL:HG21	1:A:149:PHE:HD1	1.80	0.46
1:A:151:SER:HB3	1:A:193:THR:CG2	2.34	0.46
1:A:154:MET:HA	1:A:157:LEU:HD12	1.96	0.46
1:A:384:ILE:HG22	1:A:384:ILE:O	2.15	0.46
2:B:2:ARG:NH1	2:B:251:ASP:CG	2.73	0.46
2:B:72:PRO:O	2:B:73:GLY:C	2.58	0.46
1:A:243:ARG:NH2	1:A:252:LEU:HB2	2.31	0.46
2:B:20:PHE:O	2:B:24:ILE:HB	2.14	0.46
2:B:259:MET:HE1	2:B:378:ILE:HG21	1.98	0.46
1:A:4:CYS:SG	1:A:252:LEU:CD1	3.02	0.46
1:A:99:ALA:H	2:B:2:ARG:HH22	1.63	0.46
1:A:114:ILE:O	1:A:118:VAL:HG23	2.16	0.46
1:A:191:THR:O	1:A:195:LEU:HB2	2.15	0.46
1:A:210:TYR:CZ	1:A:227:LEU:HD11	2.51	0.46
2:B:26:ASP:C	2:B:28:HIS:H	2.21	0.46
2:B:198:THR:HG23	2:B:200:GLU:H	1.79	0.46
2:B:416:MET:HG2	3:C:171:HIS:ND1	2.29	0.46
1:A:148:GLY:O	1:A:151:SER:CB	2.61	0.46
1:A:152:LEU:C	1:A:152:LEU:CD1	2.89	0.46
1:A:324:VAL:HG12	1:A:326:LYS:H	1.81	0.46
1:A:415:GLU:CG	3:C:350:ARG:NH1	1.87	0.46
2:B:192:HIS:HD1	2:B:424:ASN:CG	2.20	0.46
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.46
2:B:408:TYR:O	2:B:411:GLU:HB2	2.16	0.46
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.46
1:A:286:LEU:O	1:A:287:SER:O	2.34	0.46
1:A:381:THR:O	1:A:383:ALA:N	2.49	0.46
1:A:436:GLY:C	1:A:438:ASP:N	2.72	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
2:B:287:THR:N	2:B:290:GLU:OE1	2.48	0.46
3:C:134:THR:O	3:C:135:ASN:HB2	2.15	0.46
1:A:119:LEU:HD11	1:A:156:ARG:HD2	1.97	0.46
1:A:120:ASP:O	1:A:124:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HA	1:A:291:ILE:HG12	1.97	0.46
1:A:335:ILE:C	1:A:337:THR:N	2.73	0.46
2:B:12:CYS:C	2:B:14:ASN:N	2.71	0.46
2:B:196:GLU:O	2:B:197:ASN:OD1	2.34	0.46
2:B:427:ASP:OD1	2:B:427:ASP:C	2.58	0.46
1:A:166:LYS:CE	1:A:199:ASP:OD1	2.62	0.46
1:A:180:ALA:HA	2:B:352:LYS:NZ	2.31	0.46
1:A:328:VAL:C	1:A:330:ALA:N	2.73	0.46
1:A:423:GLU:CD	3:C:346:ARG:HH21	2.14	0.46
2:B:113:GLU:CG	2:B:114:LEU:N	2.79	0.46
2:B:307:PRO:C	2:B:309:HIS:N	2.71	0.46
1:A:5:ILE:CG2	1:A:6:SER:H	2.29	0.46
1:A:203:MET:SD	1:A:267:PHE:CB	3.04	0.46
1:A:265:ALA:O	1:A:266:HIS:O	2.33	0.46
1:A:288:VAL:O	1:A:289:ALA:C	2.59	0.46
1:A:317:LEU:CD1	1:A:351:PHE:CE2	2.99	0.46
2:B:380:ASN:C	2:B:380:ASN:HD22	2.24	0.46
1:A:243:ARG:NH2	1:A:252:LEU:CB	2.78	0.46
1:A:407:TRP:O	1:A:411:GLU:CG	2.63	0.46
2:B:288:VAL:C	2:B:290:GLU:N	2.70	0.46
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.81	0.46
2:B:194:LEU:O	2:B:265:LEU:HD23	2.16	0.46
2:B:199:ASP:C	2:B:265:LEU:HD13	2.40	0.46
2:B:409:THR:C	2:B:411:GLU:H	2.22	0.46
7:B:601:TA1:H463	7:B:601:TA1:C26	2.46	0.46
3:C:288:MET:O	3:C:289:ASP:CB	2.62	0.46
1:A:95:GLY:C	1:A:97:GLU:H	2.23	0.45
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.97	0.45
1:A:226:ASN:O	1:A:227:LEU:C	2.59	0.45
1:A:260:VAL:O	1:A:260:VAL:CG2	2.63	0.45
1:A:401:LYS:C	1:A:403:ALA:H	2.24	0.45
2:B:324:SER:OG	2:B:326:LYS:HB3	2.16	0.45
2:B:360:PRO:HG2	2:B:371:LEU:CB	2.38	0.45
1:A:130:THR:O	1:A:131:GLY:C	2.59	0.45
1:A:344:VAL:CG1	1:A:345:ASP:N	2.78	0.45
2:B:98:GLY:C	2:B:100:GLY:H	2.24	0.45
2:B:161:TYR:C	2:B:163:ASP:N	2.71	0.45
2:B:409:THR:HA	2:B:413:MET:HB3	1.99	0.45
1:A:212:ILE:HD11	1:A:302:MET:H	1.82	0.45
1:A:256:GLN:O	1:A:260:VAL:HG13	2.15	0.45
1:A:278:ALA:O	1:A:279:GLU:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:O	1:A:385:ALA:C	2.59	0.45
2:B:11:GLN:O	2:B:14:ASN:HB3	2.16	0.45
2:B:23:VAL:O	2:B:25:SER:N	2.50	0.45
2:B:135:PHE:CD1	2:B:135:PHE:N	2.84	0.45
2:B:137:LEU:HD22	2:B:154:ILE:HG23	1.97	0.45
2:B:154:ILE:HD12	2:B:155:SER:N	2.31	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:CD	2.80	0.45
1:A:308:ARG:O	1:A:309:HIS:HB3	2.16	0.45
1:A:11:GLN:HE21	1:A:74:VAL:CG2	2.29	0.45
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.30	0.45
1:A:145:THR:O	1:A:149:PHE:HB3	2.15	0.45
1:A:185:TYR:OH	1:A:399:TYR:HA	2.15	0.45
1:A:210:TYR:CD2	1:A:227:LEU:HD21	2.51	0.45
1:A:271:THR:O	1:A:376:CYS:HA	2.17	0.45
1:A:276:ILE:HG12	1:A:277:SER:N	2.32	0.45
1:A:278:ALA:HB2	1:A:369:ALA:CA	2.45	0.45
2:B:12:CYS:O	2:B:13:GLY:C	2.59	0.45
2:B:133:GLN:O	2:B:165:ILE:CD1	2.64	0.45
2:B:210:TYR:CE2	2:B:227:LEU:HD11	2.52	0.45
2:B:359:PRO:CB	2:B:360:PRO:HD2	2.45	0.45
2:B:106:GLY:O	2:B:149:MET:HB2	2.17	0.45
2:B:208:ALA:O	2:B:212:ILE:HG13	2.16	0.45
2:B:209:LEU:HD23	2:B:227:LEU:HD13	1.98	0.45
2:B:319:PHE:CD2	2:B:323:MET:HE1	2.52	0.45
1:A:11:GLN:NE2	1:A:74:VAL:HG22	2.30	0.45
1:A:104:ALA:HB1	1:A:413:MET:HG3	1.95	0.45
1:A:229:ARG:NH1	1:A:229:ARG:HG2	2.31	0.45
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.31	0.45
2:B:230:LEU:CG	2:B:302:MET:HE2	2.46	0.45
1:A:100:ALA:C	1:A:102:ASN:H	2.24	0.45
2:B:67:LEU:HD12	2:B:92:PHE:CD2	2.51	0.45
2:B:99:ALA:O	2:B:100:GLY:C	2.60	0.45
2:B:167:ASN:HA	2:B:200:GLU:O	2.17	0.45
2:B:242:LEU:HD22	2:B:250:ALA:O	2.17	0.45
2:B:313:LEU:O	2:B:347:ILE:HD12	2.16	0.45
2:B:324:SER:O	2:B:326:LYS:N	2.50	0.45
1:A:287:SER:O	1:A:288:VAL:C	2.60	0.45
2:B:14:ASN:O	2:B:17:GLY:N	2.50	0.45
2:B:274:PRO:HG2	2:B:371:LEU:CD2	2.43	0.45
1:A:234:ILE:CG1	1:A:270:ALA:HB1	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:C	1:A:347:CYS:N	2.68	0.45
3:C:216:ARG:NH2	3:C:254:ARG:HH11	2.08	0.45
1:A:182:VAL:O	1:A:183:GLU:C	2.60	0.44
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.47	0.44
1:A:334:THR:CG2	1:A:335:ILE:N	2.79	0.44
1:A:408:TYR:CG	1:A:418:PHE:HZ	2.34	0.44
2:B:175:PRO:HG2	2:B:207:GLU:OE1	2.16	0.44
3:C:193:GLN:HA	3:C:196:MET:HE3	1.98	0.44
1:A:204:VAL:O	1:A:204:VAL:HG12	2.17	0.44
1:A:231:ILE:C	1:A:233:GLN:N	2.73	0.44
1:A:268:PRO:CA	1:A:379:SER:O	2.65	0.44
1:A:286:LEU:HG	1:A:290:GLU:HB2	1.97	0.44
1:A:392:ASP:OD2	1:A:422:ARG:CZ	2.65	0.44
1:A:413:MET:C	1:A:414:GLU:CG	2.90	0.44
2:B:52:TYR:HE1	2:B:240:THR:HB	1.82	0.44
2:B:102:ASN:OD1	2:B:408:TYR:CZ	2.70	0.44
2:B:288:VAL:N	2:B:289:PRO:HD2	2.32	0.44
2:B:409:THR:C	2:B:411:GLU:N	2.73	0.44
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.97	0.44
1:A:423:GLU:O	1:A:426:ALA:HB3	2.16	0.44
2:B:6:HIS:HB3	2:B:21:TRP:HZ2	1.81	0.44
2:B:23:VAL:O	2:B:24:ILE:C	2.60	0.44
2:B:141:LEU:N	2:B:141:LEU:HD12	2.33	0.44
2:B:423:SER:O	2:B:424:ASN:C	2.60	0.44
2:B:435:TYR:C	2:B:437:ASP:N	2.72	0.44
1:A:272:TYR:CE2	1:A:274:PRO:HD2	2.53	0.44
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.99	0.44
2:B:281:GLN:C	2:B:283:TYR:N	2.67	0.44
2:B:390:ARG:O	2:B:391:ILE:C	2.61	0.44
1:A:283:HIS:O	1:A:283:HIS:ND1	2.49	0.44
2:B:72:PRO:HG2	2:B:73:GLY:H	1.83	0.44
2:B:188:THR:HG23	2:B:425:MET:HE3	1.98	0.44
2:B:312:TYR:HA	2:B:381:SER:HA	1.99	0.44
2:B:421:ALA:O	2:B:422:GLU:C	2.58	0.44
1:A:23:LEU:CD2	1:A:232:GLY:O	2.64	0.44
1:A:115:ILE:CG1	1:A:152:LEU:HD13	2.46	0.44
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.83	0.44
1:A:144:GLY:N	5:A:500:GTP:O3G	2.48	0.44
1:A:384:ILE:C	1:A:386:GLU:N	2.72	0.44
1:A:393:HIS:O	1:A:394:LYS:C	2.60	0.44
1:A:398:MET:HE3	1:A:398:MET:HB2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:HD12	2:B:239:THR:HG21	1.98	0.44
2:B:24:ILE:CG2	2:B:25:SER:N	2.80	0.44
3:C:137:ASN:CB	3:C:230:HIS:HB3	2.48	0.44
1:A:12:ALA:HB2	5:A:500:GTP:C8	2.52	0.44
1:A:230:LEU:O	1:A:233:GLN:N	2.35	0.44
1:A:287:SER:N	1:A:290:GLU:OE1	2.51	0.44
1:A:388:TRP:CD2	1:A:425:MET:HE1	2.52	0.44
2:B:8:GLN:CG	2:B:67:LEU:HD22	2.47	0.44
2:B:189:LEU:HD23	2:B:421:ALA:CB	2.47	0.44
1:A:31:GLN:CB	1:A:32:PRO:CD	2.91	0.44
1:A:72:PRO:HG2	1:A:73:THR:H	1.83	0.44
1:A:182:VAL:O	1:A:184:PRO:CD	2.65	0.44
1:A:184:PRO:HG2	1:A:398:MET:CE	2.41	0.44
1:A:278:ALA:CA	1:A:282:TYR:OH	2.65	0.44
1:A:404:PHE:CD1	1:A:404:PHE:N	2.83	0.44
2:B:42:LEU:C	2:B:44:LEU:H	2.26	0.44
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.52	0.44
2:B:72:PRO:O	2:B:74:THR:N	2.50	0.44
2:B:161:TYR:CD1	2:B:161:TYR:N	2.86	0.44
2:B:168:THR:CG2	2:B:201:THR:HG23	2.48	0.44
2:B:204:ILE:HD13	2:B:231:VAL:CG2	2.45	0.44
2:B:269:MET:HB2	2:B:301:MET:HE3	2.00	0.44
3:C:130:ILE:O	3:C:133:THR:HB	2.18	0.44
1:A:100:ALA:O	1:A:102:ASN:N	2.49	0.44
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.52	0.44
1:A:121:ARG:HG2	1:A:121:ARG:NH1	2.33	0.44
1:A:144:GLY:H	5:A:500:GTP:PG	2.41	0.44
1:A:153:LEU:O	1:A:157:LEU:HG	2.18	0.44
1:A:295:CYS:HB3	1:A:377:MET:HG2	1.99	0.44
1:A:303:VAL:O	1:A:303:VAL:CG1	2.65	0.44
1:A:328:VAL:O	1:A:330:ALA:N	2.38	0.44
1:A:362:VAL:HG13	1:A:368:LEU:CG	2.48	0.44
2:B:243:ARG:HH21	2:B:252:LEU:N	2.12	0.44
2:B:273:ALA:CB	2:B:274:PRO:CD	2.93	0.44
1:A:343:PHE:CE1	1:A:351:PHE:HE1	2.36	0.43
2:B:95:GLY:C	2:B:97:SER:H	2.25	0.43
3:C:284:ALA:O	3:C:287:GLU:HB3	2.18	0.43
1:A:21:TRP:HE1	1:A:63:PRO:HB3	1.83	0.43
1:A:172:TYR:CD1	1:A:173:PRO:N	2.80	0.43
1:A:255:PHE:O	1:A:259:LEU:N	2.50	0.43
2:B:37:HIS:O	2:B:38:GLY:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:VAL:HG11	2:B:153:LEU:HD21	2.00	0.43
2:B:103:TRP:HZ3	2:B:108:TYR:CE1	2.27	0.43
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.98	0.43
2:B:161:TYR:O	2:B:163:ASP:N	2.51	0.43
1:A:377:MET:O	1:A:377:MET:HG3	2.18	0.43
2:B:167:ASN:HD21	2:B:252:LEU:HD22	1.82	0.43
2:B:330:GLU:O	2:B:331:GLN:C	2.61	0.43
2:B:402:LYS:O	2:B:403:ALA:C	2.61	0.43
1:A:23:LEU:O	1:A:26:LEU:HB3	2.17	0.43
1:A:274:PRO:HB2	1:A:371:VAL:HG21	1.98	0.43
1:A:363:VAL:CG1	1:A:364:PRO:HD2	2.48	0.43
3:C:219:ALA:HB3	3:C:248:ASP:HB3	1.99	0.43
3:C:226:THR:CG2	3:C:239[B]:GLU:HG3	2.48	0.43
1:A:63:PRO:HG2	1:A:91:GLN:OE1	2.18	0.43
1:A:310:GLY:HA3	1:A:383:ALA:CA	2.49	0.43
1:A:409:VAL:HG13	3:C:272:ASN:ND2	2.01	0.43
2:B:70:LEU:HB2	2:B:99:ALA:CB	2.48	0.43
2:B:70:LEU:HD21	2:B:149:MET:HE3	1.98	0.43
2:B:82:PRO:HB2	2:B:83:PHE:H	1.56	0.43
2:B:240:THR:HG23	2:B:241:CYS:N	2.34	0.43
2:B:332:MET:HE3	2:B:351:VAL:CG1	2.32	0.43
3:C:224:ILE:CD1	3:C:243:LYS:HD3	2.48	0.43
1:A:25:CYS:SG	1:A:26:LEU:N	2.92	0.43
1:A:414:GLU:C	1:A:416:GLY:N	2.74	0.43
1:A:8:HIS:HA	1:A:138:PHE:HB2	2.00	0.43
1:A:108:TYR:O	1:A:109:THR:C	2.61	0.43
1:A:304:LYS:O	1:A:304:LYS:HG3	2.19	0.43
2:B:147:SER:HB2	2:B:190:SER:CB	2.41	0.43
1:A:119:LEU:O	1:A:120:ASP:C	2.60	0.43
1:A:231:ILE:HD13	1:A:231:ILE:H	1.82	0.43
1:A:238:ILE:O	1:A:242:LEU:CB	2.67	0.43
2:B:295:MET:SD	2:B:375:ALA:HB3	2.57	0.43
2:B:301:MET:C	2:B:303:ALA:N	2.77	0.43
3:C:306:TYR:CD2	3:C:316:ARG:HG3	2.53	0.43
1:A:184:PRO:O	1:A:185:TYR:C	2.62	0.43
2:B:239:THR:CG2	2:B:240:THR:N	2.80	0.43
2:B:422:GLU:O	2:B:426:ASN:CB	2.67	0.43
1:A:12:ALA:C	1:A:14:VAL:N	2.75	0.43
1:A:207:GLU:O	1:A:210:TYR:N	2.51	0.43
2:B:121:VAL:C	2:B:123:ARG:N	2.77	0.43
1:A:15:GLN:NE2	5:A:500:GTP:N7	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:HB2	1:A:186:ASN:O	2.19	0.42
1:A:209:ILE:CD1	1:A:231:ILE:CD1	2.97	0.42
1:A:262:TYR:HB3	1:A:263:PRO:HD2	2.00	0.42
1:A:390:ARG:HG3	1:A:390:ARG:HH11	1.83	0.42
2:B:7:ILE:N	2:B:136:GLN:O	2.51	0.42
2:B:48:ARG:HG2	2:B:243:ARG:HB3	2.01	0.42
2:B:105:LYS:HG2	2:B:110:GLU:CG	2.48	0.42
2:B:178:SER:C	2:B:180:THR:H	2.27	0.42
2:B:210:TYR:O	2:B:214:PHE:N	2.52	0.42
2:B:212:ILE:O	2:B:212:ILE:HG22	2.18	0.42
2:B:389:LYS:O	2:B:390:ARG:C	2.62	0.42
1:A:378:LEU:HD12	1:A:378:LEU:O	2.19	0.42
2:B:301:MET:O	2:B:303:ALA:N	2.51	0.42
1:A:343:PHE:HZ	1:A:351:PHE:CZ	2.36	0.42
2:B:103:TRP:HB2	2:B:186:ASN:HA	2.01	0.42
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.42
1:A:425:MET:O	1:A:426:ALA:C	2.60	0.42
1:A:425:MET:O	1:A:428:LEU:N	2.45	0.42
1:A:434:GLU:C	1:A:436:GLY:N	2.74	0.42
2:B:118:VAL:O	2:B:119:LEU:C	2.62	0.42
2:B:138:THR:O	2:B:139:HIS:HB3	2.20	0.42
2:B:352:LYS:HD3	2:B:352:LYS:C	2.43	0.42
3:C:22:ARG:HG2	3:C:336:ILE:HG21	2.01	0.42
1:A:8:HIS:CD2	1:A:138:PHE:CD1	3.07	0.42
1:A:268:PRO:C	1:A:269:LEU:HD23	2.44	0.42
2:B:194:LEU:C	2:B:196:GLU:N	2.70	0.42
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.76	0.42
2:B:250:ALA:CB	2:B:254:LYS:HE2	2.49	0.42
3:C:189:TYR:O	3:C:192:ILE:HG22	2.20	0.42
1:A:428:LEU:HD12	1:A:428:LEU:HA	1.79	0.42
2:B:106:GLY:O	2:B:149:MET:CA	2.68	0.42
2:B:192:HIS:NE2	2:B:420:GLU:HG2	2.34	0.42
2:B:242:LEU:HB3	2:B:250:ALA:O	2.20	0.42
1:A:104:ALA:HB3	1:A:408:TYR:HD2	1.84	0.42
1:A:132:LEU:H	1:A:132:LEU:CD2	2.23	0.42
1:A:255:PHE:O	1:A:257:THR:N	2.53	0.42
1:A:305:CYS:SG	1:A:383:ALA:HB1	2.60	0.42
2:B:6:HIS:HB3	2:B:65:ALA:CB	2.48	0.42
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.42
2:B:262:PHE:HA	2:B:263:PRO:HD2	1.65	0.42
2:B:343:PHE:CD2	2:B:350:ASN:ND2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:O	1:A:79:ARG:N	2.52	0.42
1:A:175:PRO:CG	1:A:304:LYS:HG2	2.47	0.42
1:A:210:TYR:OH	2:B:325:MET:HB3	2.20	0.42
1:A:231:ILE:C	1:A:233:GLN:H	2.28	0.42
2:B:82:PRO:C	2:B:84:GLY:N	2.78	0.42
2:B:118:VAL:O	2:B:122:VAL:HG13	2.19	0.42
2:B:297:ASP:CG	2:B:299:LYS:HE2	2.45	0.42
2:B:435:TYR:C	2:B:437:ASP:H	2.27	0.42
3:C:59:HIS:O	3:C:59:HIS:CG	2.72	0.42
1:A:140:SER:O	1:A:141:PHE:C	2.62	0.42
1:A:251:ASP:CA	1:A:254:GLU:HG3	2.48	0.42
1:A:383:ALA:C	1:A:385:ALA:N	2.78	0.42
2:B:307:PRO:O	2:B:309:HIS:N	2.53	0.42
1:A:76:ASP:O	1:A:80:THR:N	2.53	0.42
1:A:175:PRO:HG3	1:A:304:LYS:CB	2.50	0.42
1:A:199:ASP:OD2	1:A:256:GLN:NE2	2.46	0.42
1:A:238:ILE:HD11	1:A:378:LEU:HD23	2.01	0.42
1:A:386:GLU:O	1:A:387:ALA:C	2.63	0.42
1:A:402:ARG:O	1:A:405:VAL:N	2.49	0.42
2:B:25:SER:O	2:B:28:HIS:N	2.53	0.42
2:B:35:SER:CB	2:B:59:ASN:HA	2.42	0.42
2:B:333:LEU:HD11	2:B:337:ASN:HD21	1.85	0.42
2:B:399:PHE:O	2:B:401:ARG:N	2.53	0.42
2:B:153:LEU:HD13	2:B:153:LEU:N	2.34	0.41
2:B:276:THR:O	7:B:601:TA1:H192	2.21	0.41
1:A:242:LEU:HD11	1:A:250:VAL:HG23	2.02	0.41
1:A:289:ALA:HB3	1:A:290:GLU:OE2	2.20	0.41
2:B:94:PHE:N	2:B:94:PHE:CD2	2.84	0.41
2:B:265:LEU:C	2:B:265:LEU:CD1	2.83	0.41
3:C:152:GLU:O	3:C:153:ARG:HG3	2.19	0.41
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.50	0.41
1:A:335:ILE:C	1:A:337:THR:H	2.28	0.41
1:A:409:VAL:O	3:C:272:ASN:ND2	2.54	0.41
2:B:44:LEU:HD12	2:B:49:ILE:CD1	2.49	0.41
3:C:46:THR:HA	3:C:47:PRO:HD3	1.90	0.41
3:C:231:ASP:O	3:C:235:ASN:HA	2.21	0.41
1:A:7:ILE:HD11	1:A:137:VAL:CG2	2.44	0.41
1:A:318:LEU:HB2	1:A:376:CYS:SG	2.61	0.41
1:A:363:VAL:HG13	1:A:364:PRO:HD2	2.02	0.41
2:B:135:PHE:CD1	2:B:166:MET:SD	3.14	0.41
2:B:171:VAL:HG12	2:B:171:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:O	2:B:387:LEU:HG	2.15	0.41
3:C:13:ARG:HB2	3:C:14:PRO:CD	2.50	0.41
1:A:213:CYS:O	1:A:219:ILE:HG13	2.20	0.41
2:B:274:PRO:HD3	2:B:374:SER:HA	2.03	0.41
2:B:417:GLU:O	2:B:420:GLU:HB3	2.20	0.41
3:C:162:ASN:O	3:C:164:GLY:N	2.53	0.41
1:A:23:LEU:HD11	1:A:361:THR:O	2.21	0.41
1:A:115:ILE:CG2	1:A:116:ASP:H	2.32	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HD3	2.02	0.41
1:A:399:TYR:C	1:A:401:LYS:N	2.77	0.41
2:B:98:GLY:O	2:B:100:GLY:N	2.49	0.41
2:B:119:LEU:O	2:B:122:VAL:HG22	2.21	0.41
3:C:226:THR:CG2	3:C:239[A]:GLU:HG2	2.50	0.41
1:A:173:PRO:HG3	1:A:183:GLU:CD	2.45	0.41
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.92	0.41
2:B:175:PRO:O	2:B:177:VAL:N	2.53	0.41
2:B:273:ALA:HB1	2:B:291:LEU:HG	2.01	0.41
2:B:395:PHE:HB3	2:B:396:THR:H	1.73	0.41
3:C:112[A]:GLU:H	3:C:112[A]:GLU:HG2	1.54	0.41
3:C:148:GLU:HB2	3:C:155:ARG:HB3	2.02	0.41
1:A:24:TYR:O	1:A:25:CYS:C	2.63	0.41
1:A:161:TYR:O	1:A:162:GLY:C	2.64	0.41
2:B:19:LYS:HG3	2:B:228:ASN:HB2	2.01	0.41
2:B:210:TYR:O	2:B:213:CYS:N	2.49	0.41
1:A:101:ASN:HD21	2:B:254:LYS:NZ	2.19	0.41
1:A:105:ARG:O	1:A:110:ILE:CG2	2.64	0.41
1:A:332:ILE:CD1	1:A:353:VAL:HG22	2.51	0.41
1:A:408:TYR:O	1:A:409:VAL:C	2.63	0.41
2:B:52:TYR:C	2:B:53:TYR:CD1	2.99	0.41
2:B:168:THR:HB	2:B:198:THR:HG21	2.03	0.41
2:B:168:THR:O	2:B:202:TYR:N	2.44	0.41
2:B:291:LEU:HD21	2:B:373:MET:HG2	2.03	0.41
3:C:135:ASN:OD1	3:C:137:ASN:N	2.50	0.41
3:C:137:ASN:HB3	3:C:230:HIS:HB3	2.02	0.41
3:C:228:LYS:HG2	3:C:239[A]:GLU:HG3	2.03	0.41
2:B:70:LEU:HB2	2:B:99:ALA:HB2	2.03	0.41
2:B:125:GLU:O	2:B:128:SER:HB3	2.21	0.41
2:B:132:LEU:O	2:B:164:ARG:HD2	2.21	0.41
2:B:139:HIS:HE1	2:B:168:THR:CG2	2.34	0.41
2:B:143:GLY:O	2:B:147:SER:OG	2.38	0.41
2:B:182:VAL:O	2:B:184:PRO:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LEU:HD23	2:B:227:LEU:CB	2.49	0.41
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.98	0.40
1:A:67:PHE:HB2	1:A:92:LEU:HD23	2.02	0.40
1:A:166:LYS:HB2	1:A:199:ASP:OD1	2.20	0.40
1:A:276:ILE:C	1:A:369:ALA:HB2	2.45	0.40
2:B:26:ASP:C	2:B:26:ASP:OD1	2.64	0.40
2:B:114:LEU:HD12	2:B:117:SER:OG	2.21	0.40
2:B:311:ARG:HG2	2:B:311:ARG:NH1	2.34	0.40
3:C:127:PHE:HZ	3:C:186:VAL:HG23	1.86	0.40
1:A:149:PHE:CD1	1:A:150:THR:N	2.89	0.40
1:A:243:ARG:NH2	1:A:252:LEU:HG	2.35	0.40
1:A:265:ALA:O	1:A:266:HIS:C	2.63	0.40
1:A:401:LYS:O	1:A:402:ARG:HB2	2.21	0.40
2:B:48:ARG:CG	2:B:243:ARG:O	2.66	0.40
2:B:175:PRO:HG2	2:B:207:GLU:CD	2.47	0.40
2:B:191:VAL:HG11	2:B:425:MET:CG	2.43	0.40
3:C:112[B]:GLU:OE1	3:C:113:LYS:CE	2.69	0.40
1:A:95:GLY:O	1:A:96:LYS:C	2.64	0.40
1:A:207:GLU:C	1:A:209:ILE:H	2.29	0.40
1:A:301:GLN:O	1:A:302:MET:C	2.61	0.40
2:B:11:GLN:HA	2:B:74:THR:HG21	2.03	0.40
2:B:14:ASN:O	2:B:15:GLN:C	2.64	0.40
2:B:153:LEU:HD12	2:B:153:LEU:HA	1.88	0.40
2:B:359:PRO:HB2	2:B:360:PRO:CD	2.49	0.40
1:A:14:VAL:HG11	1:A:75:ILE:HD13	2.04	0.40
1:A:147:SER:OG	1:A:148:GLY:N	2.54	0.40
1:A:209:ILE:HD13	1:A:231:ILE:HD11	2.04	0.40
1:A:272:TYR:O	1:A:300:ASN:ND2	2.54	0.40
1:A:273:ALA:HB2	1:A:375:VAL:HB	2.02	0.40
2:B:20:PHE:CD2	2:B:235:MET:CG	3.04	0.40
2:B:35:SER:HB3	2:B:59:ASN:OD1	2.22	0.40
2:B:102:ASN:ND2	2:B:408:TYR:HA	2.20	0.40
2:B:202:TYR:CE2	2:B:268:PHE:HD1	2.38	0.40
2:B:239:THR:CG2	2:B:240:THR:H	2.34	0.40
2:B:282:GLN:O	2:B:282:GLN:CG	2.65	0.40
1:A:362:VAL:HG13	1:A:368:LEU:CB	2.50	0.40
1:A:392:ASP:OD2	1:A:392:ASP:C	2.64	0.40
2:B:409:THR:O	2:B:412:GLY:N	2.48	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	3
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	4
3	C	332/394 (84%)	317 (96%)	14 (4%)	1 (0%)	36	72
All	All	1164/1290 (90%)	856 (74%)	192 (16%)	116 (10%)	1	7

All (116) 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
1	A	265	ALA
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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	34	GLY
2	B	83	PHE
2	B	99	ALA
2	B	100	GLY
2	B	302	MET
2	B	386	GLU
3	C	135	ASN
1	A	89	PRO
1	A	300	ASN
1	A	348	PRO
2	B	96	GLN
2	B	395	PHE
1	A	129	CYS
1	A	256	GLN
1	A	303	VAL
1	A	307	PRO
2	B	57	ALA
2	B	74	THR
2	B	285	ALA
2	B	424	ASN
1	A	31	GLN
1	A	273	ALA
1	A	382	THR

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Mol	Chain	Res	Type
2	B	51	VAL
2	B	58	GLY
2	B	145	THR
2	B	162	PRO
2	B	400	ARG
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	12
2	B	367/381 (96%)	306 (83%)	61 (17%)	2	10
3	C	298/345 (86%)	271 (91%)	27 (9%)	9	27
All	All	1012/1103 (92%)	871 (86%)	141 (14%)	6	14

All (141) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	158	ARG
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
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

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Mol	Chain	Res	Type
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
3	C	22	ARG
3	C	25	LYS
3	C	44	LYS
3	C	111	GLN
3	C	112[A]	GLU
3	C	112[B]	GLU
3	C	113	LYS
3	C	133	THR
3	C	134	THR
3	C	153	ARG
3	C	161	LYS
3	C	163	LYS
3	C	205	VAL
3	C	233	GLU
3	C	235	ASN
3	C	236	ILE
3	C	239[A]	GLU
3	C	239[B]	GLU
3	C	240	LYS
3	C	254	ARG
3	C	261	LYS
3	C	266	LYS
3	C	273	LYS
3	C	285	LEU
3	C	289	ASP
3	C	317	GLU

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Mol	Chain	Res	Type
3	C	352	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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
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	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	385	GLN
2	B	406	HIS
2	B	434	GLN
2	B	436	GLN
3	C	42	GLN
3	C	115	GLN
3	C	162	ASN
3	C	165	ASN
3	C	222	ASN
3	C	227	GLN

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Mol	Chain	Res	Type
3	C	235	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	GDP	B	600	-	29,30,30	2.86	11 (37%)	45,47,47	3.47	16 (35%)
8	ADP	C	2000	4	28,29,29	2.38	9 (32%)	43,45,45	2.43	12 (27%)
7	TA1	B	601	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
5	GTP	A	500	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)

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
8	ADP	C	2000	4	-	4/16/32/32	0/3/3/3
7	TA1	B	601	-	-	9/41/127/127	0/7/7/7
5	GTP	A	500	4	-	4/22/38/38	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2000	ADP	PA-O3A	8.09	1.68	1.59
6	B	600	GDP	PA-O3A	7.54	1.67	1.59
7	B	601	TA1	C06-C05	6.52	1.50	1.38
5	A	500	GTP	PA-O3A	-6.04	1.53	1.59
6	B	600	GDP	O6-C6	5.99	1.34	1.23
6	B	600	GDP	C8-N9	5.88	1.50	1.37
5	A	500	GTP	PB-O3A	-5.71	1.53	1.59
7	B	601	TA1	C08-C07	-5.65	1.25	1.38
5	A	500	GTP	PB-O3B	5.43	1.65	1.59
7	B	601	TA1	C18-C10	5.35	1.69	1.57
7	B	601	TA1	C05-C04	4.80	1.46	1.39
6	B	600	GDP	C2-N1	4.79	1.49	1.37
8	C	2000	ADP	PA-O5'	4.29	1.76	1.59
7	B	601	TA1	C45-C24	4.23	1.61	1.54
6	B	600	GDP	PB-O2B	-3.91	1.40	1.54
8	C	2000	ADP	PA-O2A	-3.82	1.37	1.55
7	B	601	TA1	C36-C31	3.72	1.45	1.39
7	B	601	TA1	O02-C03	3.51	1.41	1.34
6	B	600	GDP	O4'-C1'	3.38	1.49	1.42
7	B	601	TA1	C25-C24	3.35	1.39	1.34
7	B	601	TA1	C46-C45	3.27	1.60	1.53
7	B	601	TA1	C43-C01	3.20	1.60	1.54
7	B	601	TA1	C11-C10	3.09	1.61	1.54
8	C	2000	ADP	C5-C6	3.05	1.49	1.41
6	B	600	GDP	C8-N7	3.00	1.41	1.32
6	B	600	GDP	C5-N7	-2.82	1.33	1.39
7	B	601	TA1	C43-C26	2.82	1.58	1.52
6	B	600	GDP	C5-C4	2.63	1.45	1.38
7	B	601	TA1	C26-C25	2.55	1.56	1.51
7	B	601	TA1	C01-C45	2.53	1.66	1.56
7	B	601	TA1	C18-C20	2.53	1.62	1.55
8	C	2000	ADP	C2'-C3'	2.49	1.60	1.53
8	C	2000	ADP	O5'-C5'	2.48	1.54	1.44
7	B	601	TA1	C04-C03	-2.47	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	GDP	PB-O3B	2.45	1.63	1.54
6	B	600	GDP	C2-N3	-2.43	1.27	1.33
8	C	2000	ADP	C8-N9	-2.38	1.33	1.37
8	C	2000	ADP	O4'-C1'	2.36	1.47	1.42
7	B	601	TA1	C16-C15	2.31	1.56	1.52
7	B	601	TA1	C41-C42	2.31	1.42	1.38
7	B	601	TA1	O09-C21	2.17	1.49	1.44
7	B	601	TA1	C37-C29	2.16	1.54	1.52
7	B	601	TA1	C33-C32	2.15	1.42	1.38
7	B	601	TA1	C08-C09	2.13	1.42	1.38
7	B	601	TA1	C10-C02	2.13	1.62	1.57
7	B	601	TA1	C39-C38	2.09	1.42	1.38
7	B	601	TA1	C07-C06	2.05	1.42	1.38
7	B	601	TA1	C34-C33	2.04	1.42	1.38
8	C	2000	ADP	C5-C4	-2.01	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	N9-C8-N7	-10.74	93.48	113.40
6	B	600	GDP	C8-N7-C5	9.22	120.68	104.26
6	B	600	GDP	C6-C5-N7	8.57	145.90	130.29
8	C	2000	ADP	O5'-PA-O1A	-8.33	75.93	108.94
8	C	2000	ADP	O2A-PA-O5'	-6.81	76.69	107.57
6	B	600	GDP	N2-C2-N3	6.30	131.97	119.67
6	B	600	GDP	C6-C5-C4	-6.16	109.56	118.83
6	B	600	GDP	C8-N9-C4	5.84	116.97	106.03
7	B	601	TA1	C06-C05-C04	-5.82	114.64	120.36
7	B	601	TA1	C07-C08-C09	5.72	127.30	120.24
8	C	2000	ADP	C4'-O4'-C1'	5.31	121.19	109.47
8	C	2000	ADP	O2A-PA-O1A	4.58	133.74	112.44
6	B	600	GDP	C5-C6-N1	4.51	124.73	113.25
6	B	600	GDP	N2-C2-N1	-4.26	107.78	116.76
6	B	600	GDP	C2-N3-C4	4.09	119.34	112.30
7	B	601	TA1	C05-C04-C03	-4.03	111.52	120.40
8	C	2000	ADP	O2B-PB-O3A	3.95	117.88	104.64
6	B	600	GDP	O6-C6-C5	-3.95	116.11	126.53
6	B	600	GDP	C4-C5-N7	-3.87	104.54	110.67
6	B	600	GDP	C2-N1-C6	-3.82	118.18	125.11
7	B	601	TA1	C09-C04-C03	3.60	128.34	120.40
6	B	600	GDP	C2'-C3'-C4'	3.44	109.25	102.61
7	B	601	TA1	C17-C18-C20	3.20	109.77	102.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2000	ADP	O3A-PB-O1B	-3.13	94.59	111.04
8	C	2000	ADP	O4'-C4'-C3'	-3.02	99.15	105.15
7	B	601	TA1	O04-C11-C14	-3.02	101.73	108.13
7	B	601	TA1	C45-C01-C02	2.96	115.19	111.93
8	C	2000	ADP	C2'-C3'-C4'	2.75	107.93	102.61
5	A	500	GTP	O2G-PG-O3B	2.66	113.56	104.64
6	B	600	GDP	C1'-N9-C8	-2.66	119.18	126.73
7	B	601	TA1	O01-C01-C43	2.48	113.39	107.04
8	C	2000	ADP	C5'-C4'-C3'	2.44	123.98	115.21
8	C	2000	ADP	O4'-C1'-C2'	-2.37	101.55	106.62
7	B	601	TA1	C08-C09-C04	-2.32	118.09	120.36
6	B	600	GDP	O2'-C2'-C3'	2.31	119.21	111.82
7	B	601	TA1	C10-C18-C17	-2.22	102.33	106.55
7	B	601	TA1	C14-C11-C15	-2.21	83.10	85.38
7	B	601	TA1	O06-C15-C11	2.20	92.98	90.58
5	A	500	GTP	O5'-C5'-C4'	2.10	116.14	108.99
8	C	2000	ADP	O2B-PB-O1B	2.07	118.92	110.83
6	B	600	GDP	C4'-O4'-C1'	2.06	114.02	109.47
8	C	2000	ADP	C4-N9-C8	2.06	107.90	105.74
7	B	601	TA1	C21-O09-C22	2.04	120.17	115.95
5	A	500	GTP	O3G-PG-O3B	2.01	111.38	104.64

There are no chirality outliers.

All (21) 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'
8	C	2000	ADP	PA-O3A-PB-O1B
8	C	2000	ADP	C3'-C4'-C5'-O5'
5	A	500	GTP	C5'-O5'-PA-O1A
5	A	500	GTP	O4'-C4'-C5'-O5'

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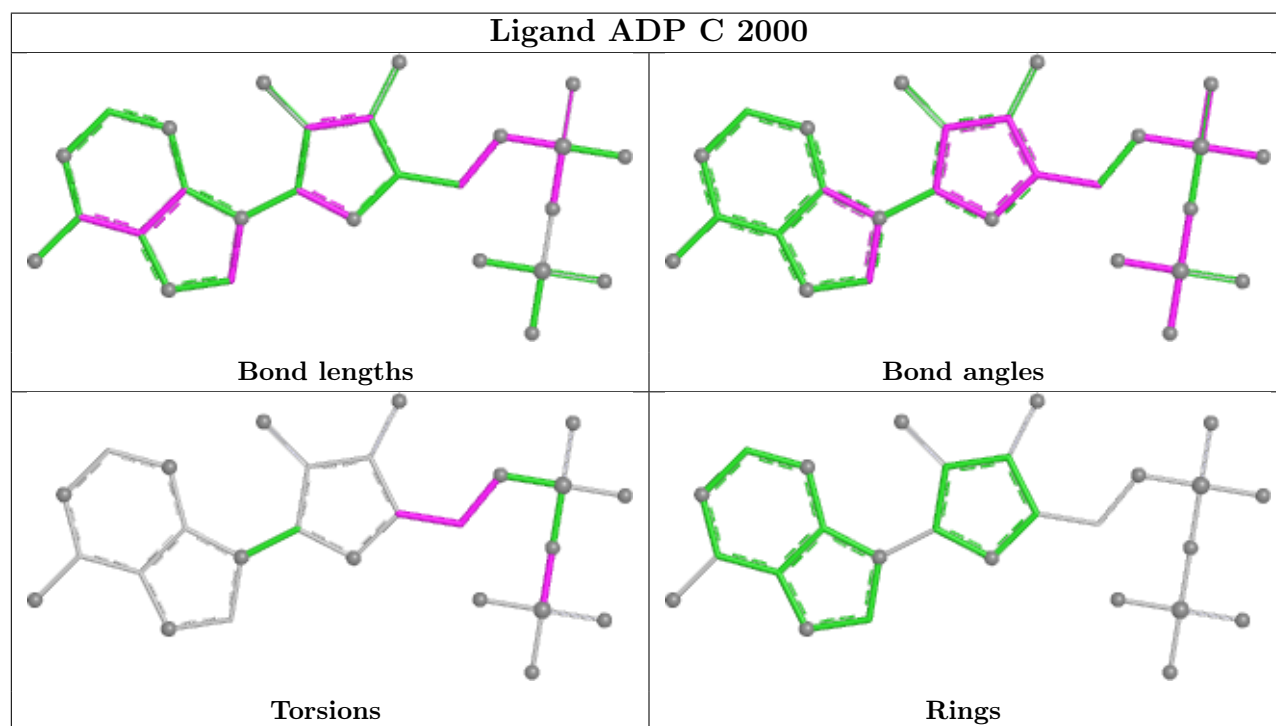
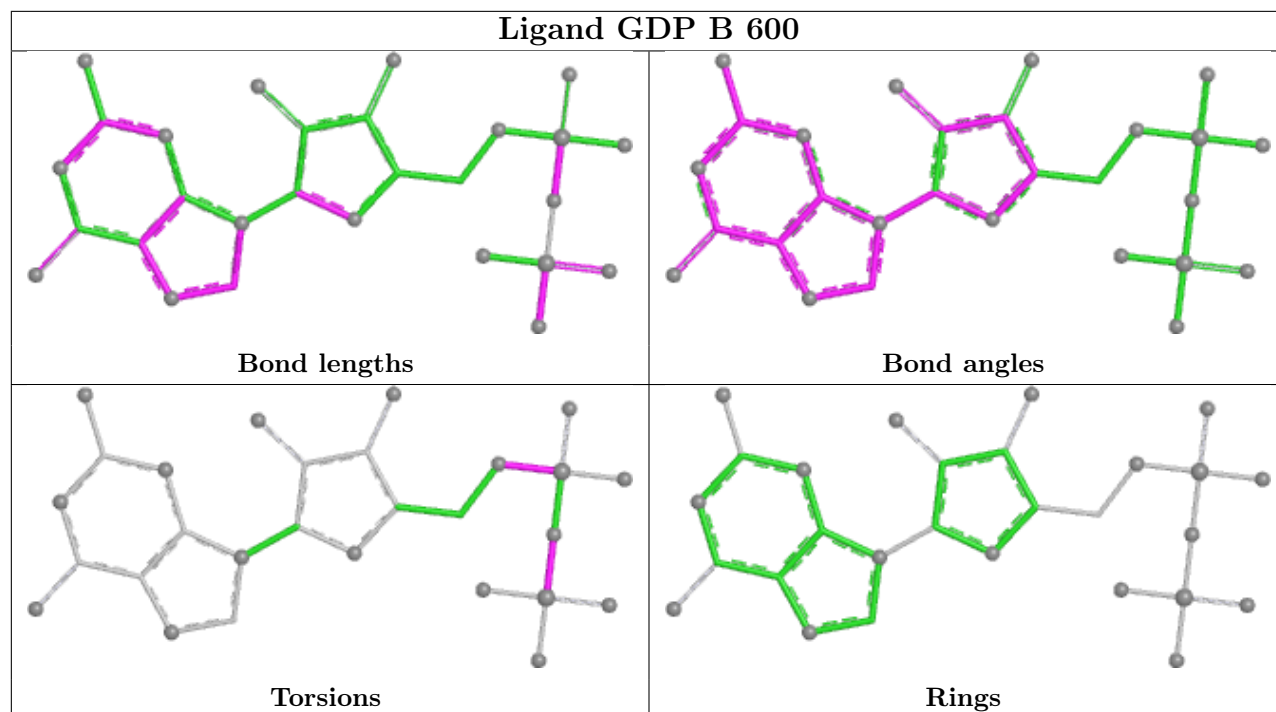
Mol	Chain	Res	Type	Atoms
8	C	2000	ADP	C4'-C5'-O5'-PA
8	C	2000	ADP	O4'-C4'-C5'-O5'
6	B	600	GDP	PA-O3A-PB-O3B
7	B	601	TA1	C15-C11-O04-C12
5	A	500	GTP	PG-O3B-PB-O2B

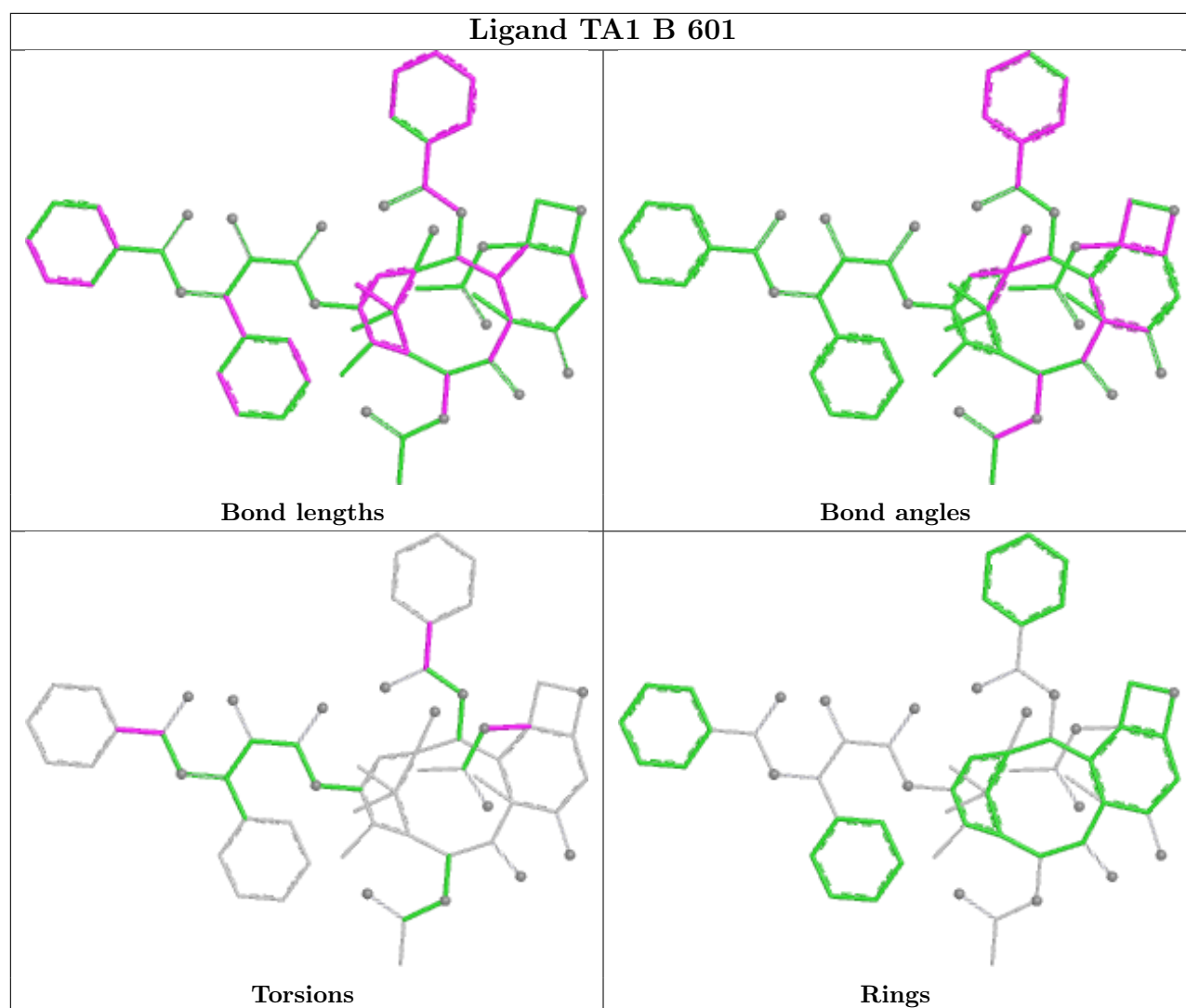
There are no ring outliers.

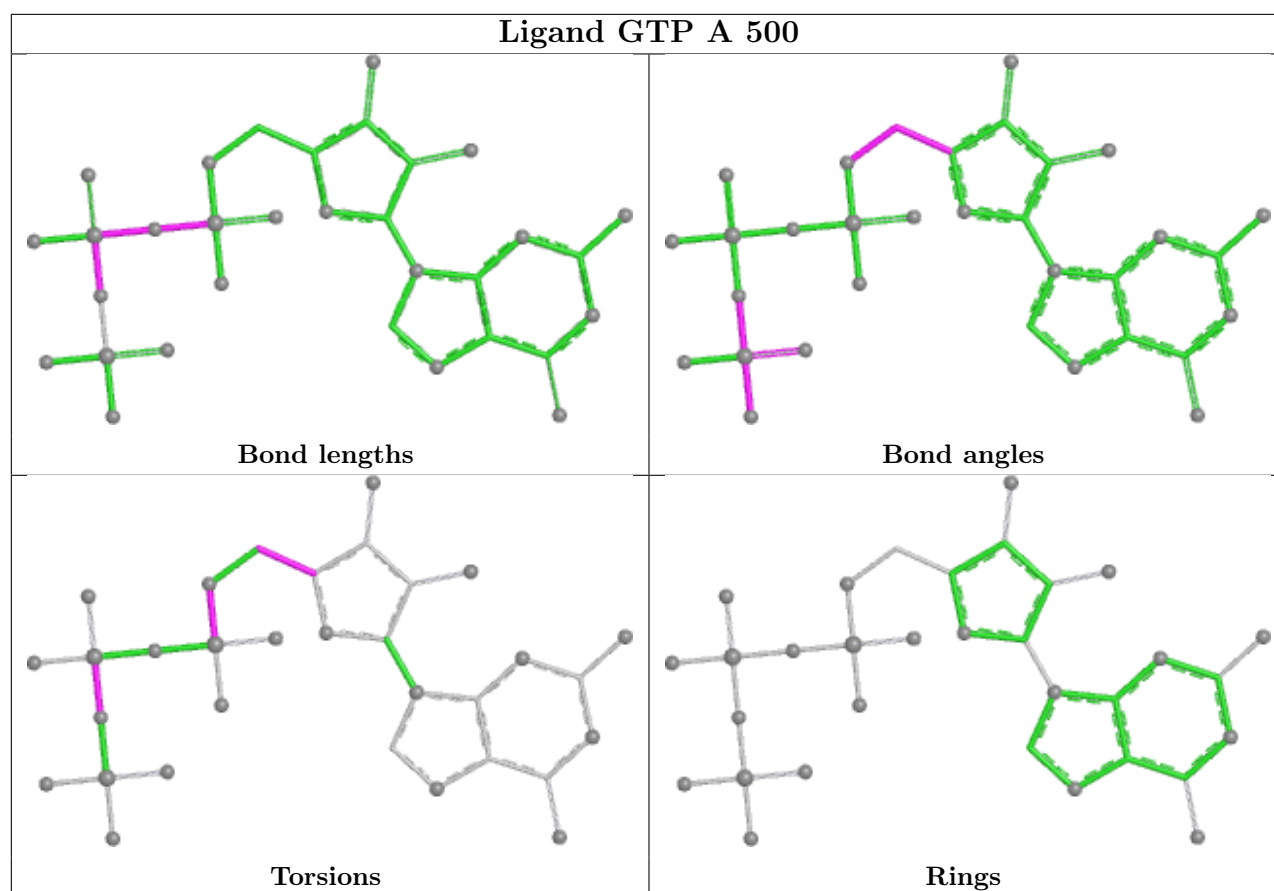
3 monomers are involved in 11 short contacts:

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