



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:30 PM UTC

PDB ID : 2YJF / pdb_00002yjf
Title : Oligomeric assembly of actin bound to MRTF-A
Authors : Mouilleron, S.; Langer, C.A.; Guettler, S.; McDonald, N.Q.; Treisman, R.
Deposited on : 2011-05-19
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

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)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

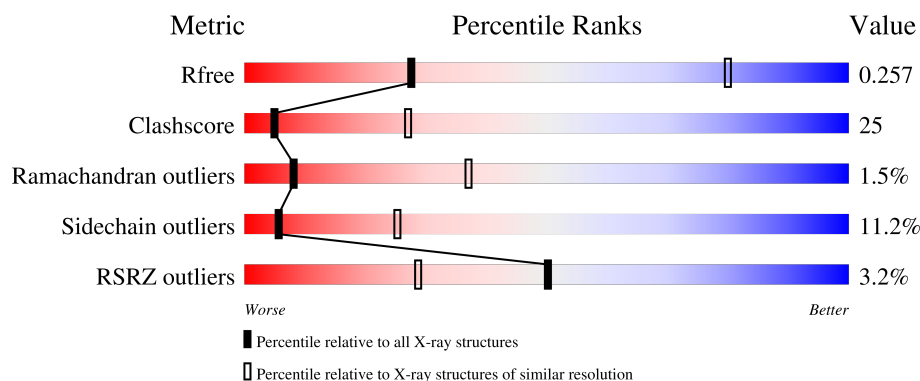
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



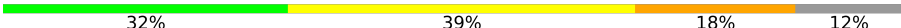
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	377	2% 53% 38% 7%
1	B	377	% 51% 34% 11%
1	C	377	3% 49% 38% 5% 9%
1	D	377	% 55% 32% 8%
1	E	377	8% 64% 19% 16%

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Mol	Chain	Length	Quality of chain
2	M	137	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	A	1378	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2645	1682	442	502	19			
1	B	335	Total	C	N	O	S	0	0	0
			2487	1580	407	481	19			
1	C	343	Total	C	N	O	S	0	0	0
			2531	1604	417	491	19			
1	D	345	Total	C	N	O	S	0	0	0
			2514	1596	416	483	19			
1	E	318	Total	C	N	O	S	0	0	0
			1959	1216	345	389	9			

- Molecule 2 is a protein called MKL/MYOCARDIN-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	121	Total	C	N	O	S	0	0	0
			922	567	183	170	2			

There are 13 discrepancies between the modelled and reference sequences:

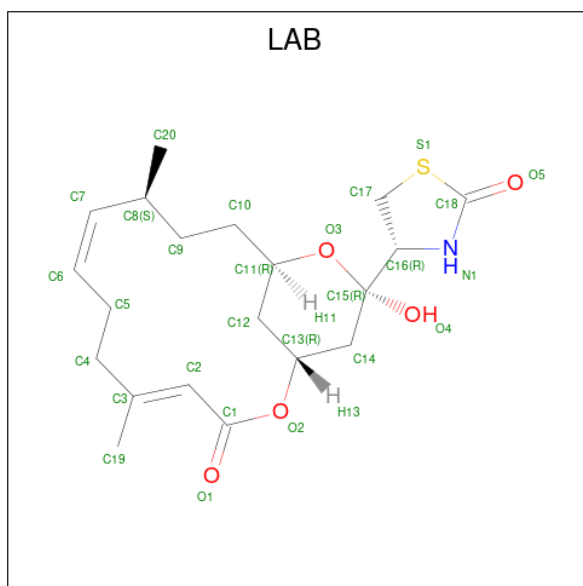
Chain	Residue	Modelled	Actual	Comment	Reference
M	63	ALA	-	expression tag	UNP Q8K4J6
M	64	PRO	-	expression tag	UNP Q8K4J6
M	65	GLY	-	expression tag	UNP Q8K4J6
M	66	SER	-	expression tag	UNP Q8K4J6
M	67	LEU	-	expression tag	UNP Q8K4J6
M	68	SER	-	expression tag	UNP Q8K4J6
M	69	GLU	-	expression tag	UNP Q8K4J6
M	70	ARG	-	expression tag	UNP Q8K4J6
M	71	LYS	-	expression tag	UNP Q8K4J6
M	72	ASN	-	expression tag	UNP Q8K4J6
M	107	GLU	ARG	conflict	UNP Q8K4J6
M	171	GLU	GLY	engineered mutation	UNP Q8K4J6

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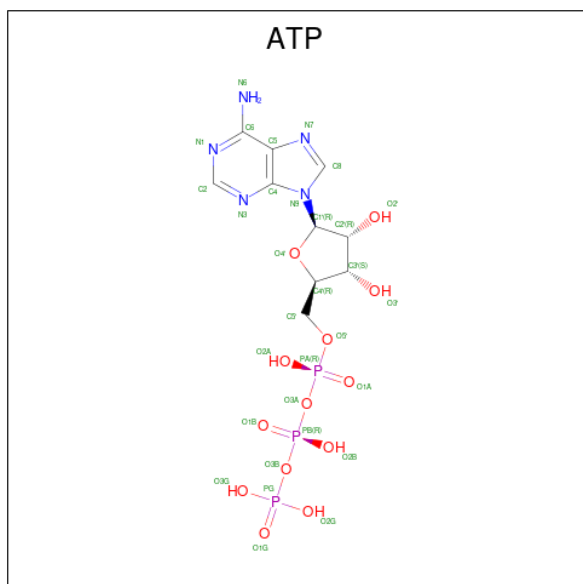
Chain	Residue	Modelled	Actual	Comment	Reference
M	172	ARG	PRO	engineered mutation	UNP Q8K4J6

- Molecule 3 is LATRUNCULIN B (CCD ID: LAB) (formula: $C_{20}H_{29}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



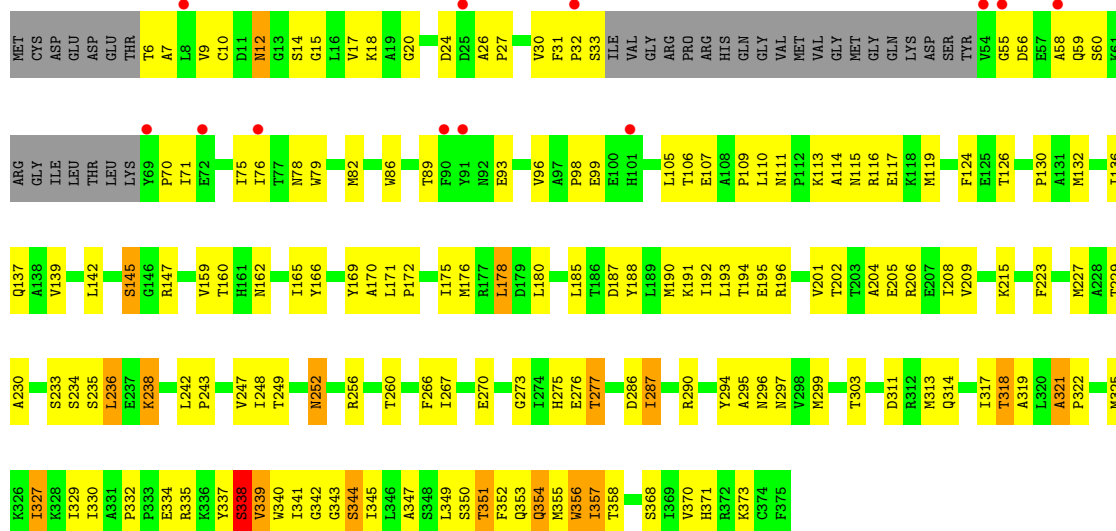
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

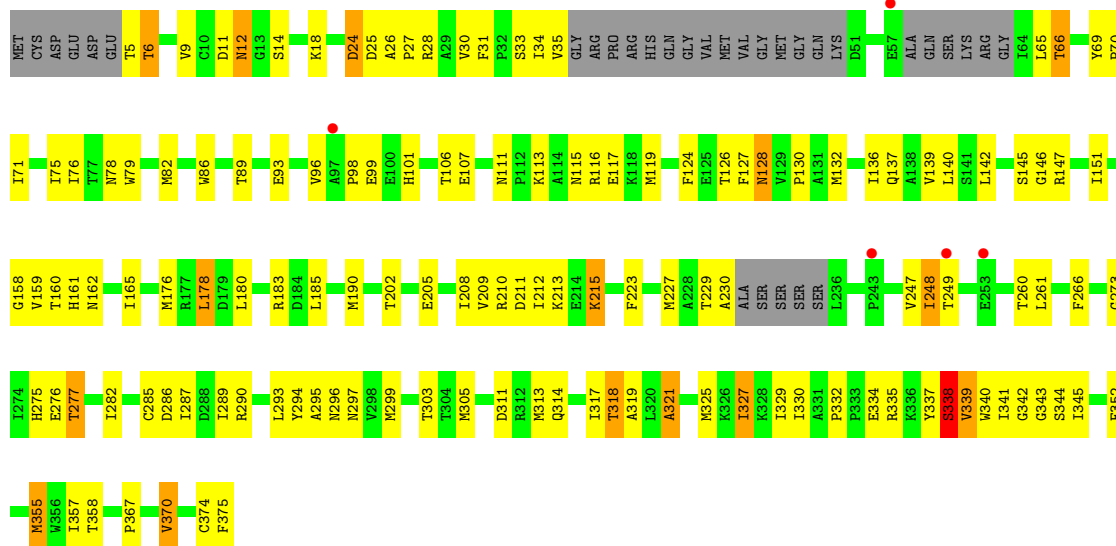
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

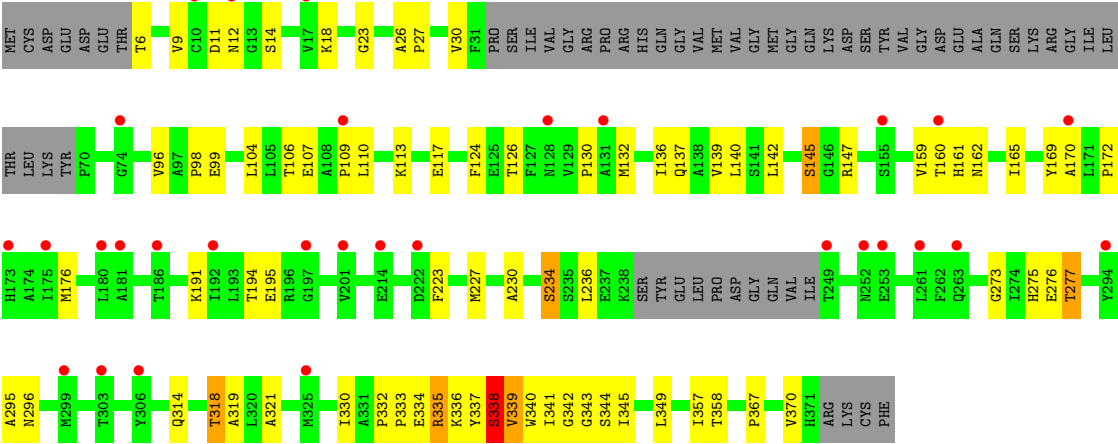


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

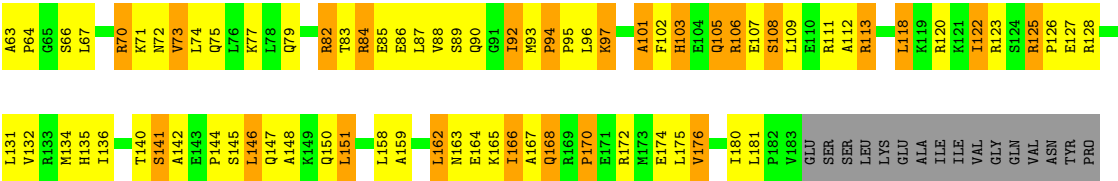
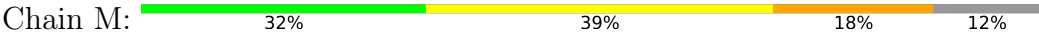


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE





● Molecule 2: MKL/MYOCARDIN-LIKE PROTEIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	182.91Å 182.91Å 378.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.52 – 3.50 46.52 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (46.52-3.50) 99.1 (46.52-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.272 0.231 , 0.257	Depositor DCC
R_{free} test set	2411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 138.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13272	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, LAB, 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	0.52	0/2703	0.86	3/3684 (0.1%)
1	B	0.44	0/2545	0.82	2/3477 (0.1%)
1	C	0.49	0/2583	0.85	3/3523 (0.1%)
1	D	0.47	0/2568	0.86	2/3509 (0.1%)
1	E	0.38	0/1989	0.84	2/2746 (0.1%)
2	M	0.58	0/933	1.07	8/1262 (0.6%)
All	All	0.48	0/13321	0.86	20/18201 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	103	HIS	N-CA-C	-6.59	104.27	112.90
2	M	101	ALA	N-CA-C	-6.37	101.52	110.50
2	M	94	PRO	CA-C-N	-6.27	113.04	120.13
2	M	94	PRO	C-N-CA	-6.27	113.04	120.13
2	M	125	ARG	CA-C-N	5.87	126.68	120.11
2	M	125	ARG	C-N-CA	5.87	126.68	120.11
1	E	321	ALA	CA-C-N	5.76	126.09	119.93
1	E	321	ALA	C-N-CA	5.76	126.09	119.93
1	C	321	ALA	CA-C-N	5.75	126.09	119.93
1	C	321	ALA	C-N-CA	5.75	126.09	119.93
1	D	321	ALA	CA-C-N	5.75	126.08	119.93
1	D	321	ALA	C-N-CA	5.75	126.08	119.93
1	B	321	ALA	CA-C-N	5.51	125.83	119.93
1	B	321	ALA	C-N-CA	5.51	125.83	119.93
1	C	193	LEU	N-CA-C	-5.40	106.53	113.01
1	A	321	ALA	CA-C-N	5.26	125.56	119.93
1	A	321	ALA	C-N-CA	5.26	125.56	119.93
2	M	92	ILE	N-CA-C	-5.14	106.67	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	77	LYS	N-CA-C	-5.13	107.05	113.72
1	A	24	ASP	N-CA-C	5.08	117.41	110.24

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	2645	0	2492	128	0
1	B	2487	0	2291	120	0
1	C	2531	0	2363	147	0
1	D	2514	0	2292	117	0
1	E	1959	0	1496	61	0
2	M	922	0	899	103	0
3	A	27	0	29	4	0
3	C	27	0	29	4	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
4	C	31	0	12	0	0
4	D	31	0	12	1	0
4	E	31	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	13272	0	11951	633	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 25.

All (633) 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:E:23:GLY:HA2	2:M:142:ALA:HB1	1.34	1.08
1:C:202:THR:HB	1:C:205:GLU:HG3	1.42	1.02
1:A:242:LEU:HD12	1:A:246:GLN:HE21	1.24	1.01
2:M:106:ARG:HH11	2:M:106:ARG:HG2	1.25	1.01
1:C:18:LYS:HG3	1:C:30:VAL:HG22	1.49	0.95
1:C:202:THR:CB	1:C:205:GLU:HG3	2.02	0.89
1:A:18:LYS:HG3	1:A:30:VAL:HG22	1.55	0.88
1:C:352:PHE:HA	1:C:355:MET:SD	2.14	0.88
1:A:352:PHE:HA	1:A:355:MET:HE3	1.53	0.88
2:M:84:ARG:HA	2:M:87:LEU:HD12	1.55	0.87
1:C:6:THR:HG22	1:C:7:ALA:H	1.38	0.86
1:C:287:ILE:HA	1:C:290:ARG:HG3	1.57	0.86
2:M:168:GLN:O	2:M:168:GLN:HG2	1.75	0.86
1:D:18:LYS:HG3	1:D:30:VAL:HG22	1.58	0.85
1:E:18:LYS:HG3	1:E:30:VAL:HG22	1.57	0.85
1:C:192:ILE:O	1:C:195:GLU:HG2	1.77	0.84
2:M:131:LEU:HD12	2:M:136:ILE:HG21	1.59	0.82
2:M:180:ILE:HG22	2:M:181:LEU:HG	1.62	0.81
1:B:18:LYS:HG3	1:B:30:VAL:HG22	1.62	0.81
1:C:351:THR:HB	2:M:166:ILE:HD11	1.62	0.80
1:A:111:ASN:HD21	1:A:115:ASN:HD22	1.28	0.80
1:A:173:HIS:ND1	2:M:94:PRO:HG3	1.96	0.80
1:C:111:ASN:HD21	1:C:115:ASN:HD22	1.32	0.77
1:C:171:LEU:HD22	2:M:181:LEU:HD21	1.67	0.77
1:D:111:ASN:HD21	1:D:115:ASN:HD22	1.28	0.77
1:B:166:TYR:CD1	2:M:131:LEU:HD11	2.20	0.76
2:M:106:ARG:HH11	2:M:106:ARG:CG	1.97	0.76
1:D:357:ILE:CD1	1:D:370:VAL:HA	2.16	0.76
1:D:357:ILE:HD11	1:D:370:VAL:HA	1.65	0.76
1:C:357:ILE:HD11	1:C:373:LYS:CB	2.15	0.76
1:B:205:GLU:HA	1:B:208:ILE:HD12	1.67	0.75
1:B:111:ASN:HD21	1:B:115:ASN:HD22	1.35	0.74
1:D:31:PHE:HZ	1:D:89:THR:HG1	1.33	0.74
1:C:295:ALA:C	1:C:296:ASN:HD22	1.94	0.74
2:M:108:SER:O	2:M:111:ARG:HB3	1.87	0.73
1:B:190:MET:HG2	1:B:209:VAL:HG21	1.70	0.73
1:B:252:ASN:HD22	1:B:256:ARG:HD3	1.54	0.73
1:A:252:ASN:HD22	1:A:256:ARG:HD3	1.55	0.72
1:C:317:ILE:HG22	1:C:327:ILE:HD13	1.72	0.71
1:C:252:ASN:HD22	1:C:256:ARG:HD3	1.55	0.71
1:D:317:ILE:HG22	1:D:327:ILE:HD13	1.72	0.71
1:B:317:ILE:HG22	1:B:327:ILE:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:O	1:C:236:LEU:HD12	1.91	0.70
1:C:252:ASN:ND2	1:C:256:ARG:HD3	2.06	0.70
1:D:190:MET:HG2	1:D:209:VAL:HG21	1.73	0.70
1:A:167:GLU:OE1	2:M:82:ARG:HG3	1.90	0.70
1:C:334:GLU:N	1:C:334:GLU:OE1	2.26	0.69
1:A:12:ASN:HD21	1:A:86:TRP:HE1	1.40	0.69
1:C:205:GLU:HA	1:C:208:ILE:HD12	1.75	0.68
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.74	0.68
1:D:285:CYS:HB3	1:D:289:ILE:HD11	1.74	0.68
1:B:349:LEU:HD11	2:M:118:LEU:HB3	1.75	0.68
1:B:252:ASN:ND2	1:B:256:ARG:HD3	2.08	0.68
1:C:347:ALA:HA	1:C:352:PHE:CD1	2.28	0.68
1:C:12:ASN:ND2	1:C:86:TRP:HE1	1.92	0.67
1:B:12:ASN:HD21	1:B:86:TRP:HE1	1.42	0.67
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.76	0.67
1:A:252:ASN:ND2	1:A:256:ARG:HD3	2.10	0.67
1:A:114:ALA:HB2	1:D:28:ARG:HD2	1.77	0.67
1:A:317:ILE:HG22	1:A:327:ILE:HD13	1.77	0.66
1:A:351:THR:OG1	2:M:75:GLN:HG3	1.96	0.66
1:C:191:LYS:O	1:C:194:THR:HG22	1.96	0.66
1:A:273:GLY:O	1:A:277:THR:HG23	1.96	0.66
1:D:202:THR:HB	1:D:205:GLU:HG3	1.78	0.66
2:M:151:LEU:C	2:M:151:LEU:HD13	2.21	0.66
1:A:166:TYR:CE1	1:A:167:GLU:HG3	2.31	0.66
1:C:190:MET:HG2	1:C:209:VAL:HG21	1.78	0.65
1:E:106:THR:HB	1:E:137:GLN:HG2	1.79	0.65
1:A:106:THR:HB	1:A:137:GLN:HG2	1.78	0.65
1:D:12:ASN:HD21	1:D:86:TRP:HE1	1.43	0.65
1:A:295:ALA:C	1:A:296:ASN:HD22	2.05	0.65
1:C:352:PHE:C	1:C:354:GLN:H	2.05	0.65
1:D:106:THR:HB	1:D:137:GLN:HG2	1.79	0.65
1:E:273:GLY:O	1:E:277:THR:HG23	1.97	0.65
1:C:273:GLY:O	1:C:277:THR:HG23	1.98	0.65
1:D:115:ASN:HD22	1:D:119:MET:HE3	1.61	0.65
1:A:31:PHE:HZ	1:A:89:THR:HG1	1.44	0.64
1:B:273:GLY:O	1:B:277:THR:HG23	1.96	0.64
1:C:32:PRO:HB3	3:C:1376:LAB:H102	1.79	0.64
2:M:112:ALA:O	2:M:113:ARG:C	2.40	0.64
1:C:349:LEU:HD11	2:M:162:LEU:HB3	1.79	0.64
1:A:115:ASN:HD22	1:A:119:MET:HE3	1.62	0.64
1:D:215:LYS:HB3	1:D:215:LYS:HZ2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:ALA:C	1:E:296:ASN:HD22	2.05	0.64
1:A:365:ALA:HB3	1:A:369:ILE:HD12	1.79	0.64
1:B:115:ASN:HD22	1:B:119:MET:HE3	1.63	0.64
1:C:351:THR:CB	2:M:166:ILE:HD11	2.27	0.64
1:C:106:THR:HB	1:C:137:GLN:HG2	1.80	0.63
1:D:115:ASN:ND2	1:D:119:MET:HE3	2.14	0.63
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.80	0.63
1:A:136:ILE:N	1:A:136:ILE:HD12	2.14	0.63
1:C:145:SER:OG	1:C:147:ARG:HD2	1.99	0.63
1:B:31:PHE:HZ	1:B:89:THR:HG1	1.47	0.63
1:B:106:THR:HB	1:B:137:GLN:HG2	1.80	0.62
1:D:96:VAL:O	1:D:98:PRO:HD3	1.99	0.62
2:M:106:ARG:HG2	2:M:106:ARG:NH1	2.05	0.62
1:A:16:LEU:HD11	3:A:1376:LAB:O1	1.99	0.62
1:B:191:LYS:O	1:B:194:THR:HG22	2.00	0.62
1:C:236:LEU:HD12	1:C:236:LEU:C	2.23	0.62
1:A:242:LEU:HD12	1:A:246:GLN:NE2	2.07	0.62
2:M:141:SER:CB	2:M:142:ALA:HA	2.29	0.61
1:D:9:VAL:HG12	1:D:340:TRP:CD1	2.35	0.61
1:D:273:GLY:O	1:D:277:THR:HG23	2.00	0.61
1:E:136:ILE:HD12	1:E:136:ILE:N	2.16	0.61
1:C:347:ALA:HA	1:C:352:PHE:CE1	2.33	0.61
1:A:145:SER:OG	1:A:147:ARG:HD2	2.01	0.61
1:D:26:ALA:HB1	1:D:27:PRO:HD2	1.82	0.61
2:M:94:PRO:HB2	2:M:103:HIS:NE2	2.16	0.61
1:E:9:VAL:HG12	1:E:340:TRP:CD1	2.36	0.61
1:C:32:PRO:HB3	3:C:1376:LAB:H122	1.81	0.61
1:C:116:ARG:HH12	1:C:370:VAL:HG22	1.66	0.61
1:A:116:ARG:NH1	1:A:370:VAL:HG22	2.16	0.60
1:A:115:ASN:ND2	1:A:119:MET:HE3	2.15	0.60
1:E:330:ILE:HG22	1:E:332:PRO:HD3	1.83	0.60
1:C:31:PHE:HZ	1:C:89:THR:HG1	1.48	0.60
1:B:330:ILE:HG22	1:B:332:PRO:HD3	1.84	0.60
1:A:12:ASN:ND2	1:A:86:TRP:HE1	1.99	0.60
1:A:191:LYS:O	1:A:194:THR:HG22	2.02	0.60
1:B:31:PHE:HZ	1:B:89:THR:OG1	1.85	0.60
1:D:330:ILE:HG22	1:D:332:PRO:HD3	1.82	0.60
1:D:205:GLU:O	1:D:209:VAL:HG23	2.03	0.59
1:C:17:VAL:O	1:C:30:VAL:HA	2.02	0.59
1:D:162:ASN:HB2	1:D:176:MET:HB2	1.85	0.59
1:D:375:PHE:O	2:M:113:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG12	1:A:340:TRP:CD1	2.37	0.59
1:E:162:ASN:HB2	1:E:176:MET:HB2	1.83	0.59
1:C:136:ILE:HD12	1:C:136:ILE:N	2.16	0.59
1:C:349:LEU:HD13	2:M:163:ASN:HA	1.84	0.59
1:D:223:PHE:CZ	1:D:227:MET:HE2	2.37	0.59
1:E:191:LYS:O	1:E:194:THR:HG22	2.02	0.59
2:M:180:ILE:C	2:M:181:LEU:HG	2.28	0.59
1:B:205:GLU:O	1:B:209:VAL:HG23	2.02	0.58
1:B:223:PHE:CZ	1:B:227:MET:HE2	2.38	0.58
1:B:162:ASN:HB2	1:B:176:MET:HB2	1.86	0.58
1:C:99:GLU:O	1:C:130:PRO:HD3	2.04	0.58
1:A:31:PHE:HZ	1:A:89:THR:OG1	1.86	0.58
1:E:96:VAL:O	1:E:98:PRO:HD3	2.04	0.58
1:B:115:ASN:ND2	1:B:119:MET:HE3	2.18	0.58
1:D:180:LEU:HD21	1:D:260:THR:HG22	1.85	0.58
1:C:252:ASN:HD21	1:C:256:ARG:HH11	1.51	0.58
2:M:164:GLU:CD	2:M:165:LYS:N	2.62	0.58
1:C:115:ASN:HD22	1:C:119:MET:HE3	1.68	0.58
1:A:230:ALA:HA	1:A:236:LEU:HD23	1.86	0.58
1:C:124:PHE:HZ	1:C:357:ILE:O	1.85	0.58
1:B:136:ILE:N	1:B:136:ILE:HD12	2.19	0.57
1:C:180:LEU:HD21	1:C:260:THR:HG22	1.86	0.57
1:D:31:PHE:HZ	1:D:89:THR:OG1	1.86	0.57
1:C:286:ASP:OD1	1:C:287:ILE:N	2.37	0.57
1:A:287:ILE:HA	1:A:290:ARG:HG3	1.85	0.57
1:D:341:ILE:HD13	2:M:102:PHE:CE2	2.39	0.57
1:B:96:VAL:O	1:B:98:PRO:HD3	2.05	0.57
1:B:107:GLU:O	1:B:137:GLN:HG3	2.05	0.57
1:C:116:ARG:NH1	1:C:370:VAL:HG22	2.19	0.57
1:D:145:SER:OG	1:D:147:ARG:HD2	2.04	0.57
1:B:76:ILE:HD13	1:B:82:MET:HG2	1.86	0.57
1:B:171:LEU:HD12	1:B:285:CYS:SG	2.44	0.57
1:C:76:ILE:HD13	1:C:82:MET:HG2	1.86	0.57
1:D:136:ILE:N	1:D:136:ILE:HD12	2.20	0.57
2:M:168:GLN:O	2:M:168:GLN:CG	2.50	0.57
1:A:107:GLU:O	1:A:137:GLN:HG3	2.04	0.57
1:A:205:GLU:O	1:A:209:VAL:HG23	2.03	0.57
1:B:9:VAL:HG12	1:B:340:TRP:CD1	2.39	0.57
1:B:180:LEU:HD21	1:B:260:THR:HG22	1.86	0.57
1:E:234:SER:C	1:E:236:LEU:H	2.12	0.57
2:M:88:VAL:HG23	2:M:93:MET:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:96:LEU:O	2:M:97:LYS:CB	2.53	0.57
1:B:139:VAL:HG22	1:B:165:ILE:HD13	1.86	0.56
1:A:223:PHE:CZ	1:A:227:MET:HE2	2.40	0.56
1:C:20:GLY:HA3	1:C:340:TRP:CZ2	2.39	0.56
1:D:341:ILE:HD13	2:M:102:PHE:CZ	2.40	0.56
1:B:145:SER:OG	1:B:147:ARG:HD2	2.05	0.56
1:C:31:PHE:HZ	1:C:89:THR:OG1	1.87	0.56
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.85	0.56
1:D:107:GLU:O	1:D:137:GLN:HG3	2.06	0.56
1:E:145:SER:OG	1:E:147:ARG:HD2	2.04	0.56
1:E:223:PHE:CZ	1:E:227:MET:HE2	2.41	0.56
1:B:12:ASN:ND2	1:B:86:TRP:HE1	2.03	0.56
1:D:248:ILE:HG12	1:D:249:THR:N	2.19	0.56
2:M:131:LEU:HD12	2:M:136:ILE:CG2	2.32	0.56
1:C:368:SER:O	1:C:371:HIS:HD2	1.88	0.56
1:D:76:ILE:HG21	1:D:79:TRP:CZ3	2.41	0.56
1:B:139:VAL:HA	1:B:165:ILE:HD13	1.88	0.56
1:A:32:PRO:HB3	3:A:1376:LAB:H122	1.89	0.56
1:B:110:LEU:HD22	2:M:145:SER:HA	1.88	0.56
1:D:178:LEU:HD12	1:D:180:LEU:H	1.71	0.56
1:A:96:VAL:O	1:A:98:PRO:HD3	2.06	0.55
1:B:234:SER:C	1:B:236:LEU:H	2.14	0.55
1:C:223:PHE:CZ	1:C:227:MET:HE2	2.41	0.55
2:M:170:PRO:HB3	2:M:174:GLU:CD	2.32	0.55
1:B:76:ILE:HG21	1:B:79:TRP:CZ3	2.42	0.55
1:B:117:GLU:CD	1:B:371:HIS:HE2	2.14	0.55
1:C:12:ASN:HD21	1:C:86:TRP:HE1	1.53	0.55
1:C:178:LEU:HD12	1:C:180:LEU:H	1.71	0.55
1:A:116:ARG:HH12	1:A:370:VAL:HG22	1.69	0.55
2:M:172:ARG:O	2:M:176:VAL:HG23	2.07	0.55
1:C:20:GLY:HA3	1:C:340:TRP:HZ2	1.71	0.55
1:E:26:ALA:HB1	1:E:27:PRO:HD2	1.89	0.55
1:E:345:ILE:HG12	2:M:146:LEU:HD13	1.88	0.55
1:B:116:ARG:NH1	1:B:370:VAL:HG22	2.22	0.55
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.87	0.55
1:B:361:GLU:HB3	1:B:369:ILE:CD1	2.37	0.55
1:D:76:ILE:HD13	1:D:82:MET:HG2	1.89	0.55
1:A:234:SER:C	1:A:236:LEU:H	2.13	0.55
1:B:31:PHE:CE2	1:B:93:GLU:HG3	2.41	0.55
1:E:107:GLU:O	1:E:137:GLN:HG3	2.05	0.55
2:M:106:ARG:CG	2:M:106:ARG:NH1	2.66	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:TYR:CE2	1:D:183:ARG:NH1	2.75	0.55
1:D:335:ARG:C	1:D:337:TYR:N	2.61	0.55
1:A:166:TYR:CD1	1:A:167:GLU:HG3	2.42	0.55
1:C:55:GLY:O	1:C:58:ALA:HB3	2.06	0.55
1:C:330:ILE:HG22	1:C:332:PRO:HD3	1.89	0.55
1:C:115:ASN:ND2	1:C:119:MET:HE3	2.22	0.54
1:B:6:THR:HG22	1:B:7:ALA:H	1.73	0.54
2:M:170:PRO:HA	2:M:174:GLU:OE2	2.07	0.54
1:A:145:SER:HG	1:A:147:ARG:HD2	1.72	0.54
1:A:11:ASP:HA	1:A:106:THR:OG1	2.07	0.54
1:C:114:ALA:O	1:C:117:GLU:HG2	2.08	0.54
1:D:335:ARG:C	1:D:337:TYR:H	2.15	0.54
1:E:23:GLY:CA	2:M:142:ALA:HB1	2.24	0.54
1:A:345:ILE:HD13	2:M:70:ARG:HB3	1.89	0.54
2:M:63:ALA:N	2:M:64:PRO:HD2	2.23	0.54
1:C:96:VAL:O	1:C:98:PRO:HD3	2.08	0.54
1:A:180:LEU:HD21	1:A:260:THR:HG22	1.88	0.54
1:D:11:ASP:HA	1:D:106:THR:OG1	2.08	0.54
1:D:18:LYS:NZ	4:D:1377:ATP:O1B	2.41	0.54
1:A:282:ILE:O	1:A:285:CYS:HB2	2.08	0.53
1:C:9:VAL:HG12	1:C:340:TRP:CD1	2.43	0.53
1:B:143:TYR:HB3	2:M:118:LEU:HD21	1.90	0.53
1:C:56:ASP:O	1:C:59:GLN:N	2.41	0.53
1:D:12:ASN:ND2	1:D:86:TRP:HE1	2.04	0.53
1:B:99:GLU:O	1:B:130:PRO:HD3	2.09	0.53
1:B:370:VAL:HG13	1:B:371:HIS:N	2.24	0.53
1:C:166:TYR:CD1	2:M:175:LEU:HD21	2.43	0.53
1:D:248:ILE:HG12	1:D:249:THR:H	1.74	0.53
1:A:99:GLU:O	1:A:130:PRO:HD3	2.08	0.53
1:B:252:ASN:HD21	1:B:256:ARG:HH11	1.57	0.53
1:B:318:THR:HA	1:B:327:ILE:HD12	1.91	0.53
1:D:99:GLU:O	1:D:130:PRO:HD3	2.09	0.53
1:C:335:ARG:C	1:C:337:TYR:N	2.66	0.53
1:B:339:VAL:HG12	1:B:340:TRP:N	2.24	0.53
1:B:341:ILE:O	1:B:345:ILE:HG13	2.09	0.53
1:D:31:PHE:CE1	1:D:93:GLU:HG3	2.43	0.53
1:A:76:ILE:HD13	1:A:82:MET:HG2	1.90	0.53
1:B:18:LYS:NZ	4:B:1377:ATP:O1B	2.40	0.53
2:M:83:THR:HG23	2:M:86:GLU:H	1.73	0.53
1:C:33:SER:O	1:C:70:PRO:HD2	2.09	0.52
1:C:107:GLU:O	1:C:137:GLN:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LYS:O	1:C:194:THR:CG2	2.56	0.52
1:E:11:ASP:HA	1:E:106:THR:OG1	2.09	0.52
1:E:99:GLU:O	1:E:130:PRO:HD3	2.08	0.52
1:A:318:THR:HA	1:A:327:ILE:HD12	1.91	0.52
1:C:76:ILE:HG21	1:C:79:TRP:CZ3	2.45	0.52
1:E:314:GLN:O	1:E:318:THR:HB	2.08	0.52
1:A:341:ILE:O	1:A:345:ILE:HG13	2.09	0.52
1:D:287:ILE:HA	1:D:290:ARG:HG3	1.91	0.52
1:D:299:MET:HE3	1:D:313:MET:HG2	1.92	0.52
1:D:341:ILE:O	1:D:345:ILE:HG13	2.10	0.52
2:M:158:LEU:HD23	2:M:159:ALA:N	2.24	0.52
1:B:116:ARG:HH12	1:B:370:VAL:HG22	1.75	0.52
1:C:337:TYR:O	1:C:338:SER:C	2.53	0.52
1:D:314:GLN:O	1:D:318:THR:HB	2.10	0.52
2:M:85:GLU:O	2:M:89:SER:HB2	2.09	0.52
1:B:303:THR:HG22	1:B:303:THR:O	2.10	0.52
1:D:99:GLU:H	1:D:99:GLU:CD	2.18	0.52
1:A:252:ASN:HD21	1:A:256:ARG:HH11	1.58	0.52
1:B:202:THR:HB	1:B:205:GLU:H	1.74	0.51
1:A:303:THR:O	1:A:303:THR:HG22	2.09	0.51
1:C:318:THR:HA	1:C:327:ILE:HD12	1.93	0.51
1:D:6:THR:O	1:D:101:HIS:HB3	2.09	0.51
1:A:178:LEU:HD12	1:A:180:LEU:H	1.74	0.51
1:A:202:THR:HB	1:A:205:GLU:H	1.75	0.51
1:D:145:SER:HG	1:D:147:ARG:HD2	1.76	0.51
1:C:295:ALA:O	1:C:296:ASN:ND2	2.40	0.51
1:D:142:LEU:O	1:D:145:SER:HB3	2.10	0.51
1:D:211:ASP:O	1:D:215:LYS:HG2	2.10	0.51
1:A:173:HIS:ND1	2:M:94:PRO:CG	2.70	0.51
1:C:31:PHE:CE2	1:C:93:GLU:HG3	2.45	0.51
1:D:303:THR:HG22	1:D:303:THR:O	2.10	0.51
1:A:339:VAL:HG12	1:A:340:TRP:N	2.26	0.51
1:B:178:LEU:HD12	1:B:180:LEU:H	1.76	0.51
1:C:318:THR:HG22	1:C:319:ALA:N	2.25	0.51
2:M:73:VAL:CG2	2:M:74:LEU:N	2.73	0.51
1:A:335:ARG:C	1:A:337:TYR:N	2.67	0.51
1:B:113:LYS:CB	1:B:371:HIS:HE1	2.24	0.51
1:C:314:GLN:O	1:C:318:THR:HB	2.11	0.51
1:D:294:TYR:CE1	1:D:321:ALA:HB2	2.45	0.51
2:M:88:VAL:N	2:M:93:MET:HB2	2.26	0.51
1:B:297:ASN:HB3	1:B:329:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ARG:C	1:B:337:TYR:N	2.67	0.51
1:C:349:LEU:HD11	2:M:162:LEU:HD12	1.92	0.51
1:E:99:GLU:H	1:E:99:GLU:CD	2.19	0.51
1:A:99:GLU:H	1:A:99:GLU:CD	2.18	0.51
1:A:297:ASN:HB3	1:A:329:ILE:HD13	1.93	0.51
1:C:252:ASN:ND2	1:C:256:ARG:HH11	2.09	0.51
1:A:32:PRO:HB3	3:A:1376:LAB:H102	1.93	0.51
1:C:202:THR:OG1	1:C:205:GLU:HG3	2.10	0.51
1:C:349:LEU:HB3	2:M:163:ASN:OD1	2.11	0.51
1:B:76:ILE:HD12	1:B:119:MET:HE2	1.92	0.50
1:A:31:PHE:CE1	1:A:93:GLU:HG3	2.47	0.50
1:A:194:THR:HG23	1:A:195:GLU:N	2.26	0.50
1:A:227:MET:O	1:A:230:ALA:HB3	2.11	0.50
1:B:314:GLN:O	1:B:318:THR:HB	2.11	0.50
1:D:357:ILE:HD13	1:D:370:VAL:HA	1.93	0.50
1:B:227:MET:O	1:B:230:ALA:HB3	2.11	0.50
1:E:335:ARG:C	1:E:337:TYR:N	2.69	0.50
1:C:227:MET:O	1:C:230:ALA:HB3	2.12	0.50
1:E:227:MET:O	1:E:230:ALA:HB3	2.12	0.50
1:C:205:GLU:O	1:C:209:VAL:HG23	2.12	0.50
1:A:144:ALA:O	2:M:70:ARG:HD2	2.12	0.50
1:B:25:ASP:OD1	1:B:25:ASP:N	2.44	0.50
1:D:318:THR:HA	1:D:327:ILE:HD12	1.93	0.50
1:A:314:GLN:O	1:A:318:THR:HB	2.12	0.50
1:A:318:THR:HG22	1:A:319:ALA:N	2.27	0.50
1:D:113:LYS:O	1:D:117:GLU:HG3	2.12	0.50
1:D:117:GLU:OE1	1:D:367:PRO:HB2	2.11	0.50
1:E:18:LYS:NZ	4:E:1377:ATP:O1B	2.43	0.50
1:A:76:ILE:HG21	1:A:79:TRP:CZ3	2.47	0.49
1:A:299:MET:HE3	1:A:313:MET:HG2	1.93	0.49
2:M:128:ARG:HH12	2:M:140:THR:HG23	1.76	0.49
2:M:151:LEU:C	2:M:151:LEU:CD1	2.85	0.49
1:D:158:GLY:HA3	1:D:183:ARG:HH21	1.76	0.49
1:A:113:LYS:O	1:A:117:GLU:HG3	2.12	0.49
1:B:318:THR:HG22	1:B:319:ALA:N	2.27	0.49
2:M:151:LEU:HD13	2:M:151:LEU:O	2.11	0.49
1:D:297:ASN:HB3	1:D:329:ILE:HD13	1.93	0.49
1:B:223:PHE:HE2	1:B:266:PHE:HZ	1.61	0.49
1:B:287:ILE:HA	1:B:290:ARG:HG3	1.95	0.49
1:B:351:THR:HG21	2:M:122:ILE:CG2	2.42	0.49
1:D:76:ILE:HD12	1:D:119:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:TYR:HD1	2:M:131:LEU:HD11	1.75	0.49
1:B:299:MET:HE3	1:B:313:MET:HG2	1.94	0.49
1:E:339:VAL:HG12	1:E:340:TRP:N	2.27	0.49
1:B:169:TYR:HE1	1:B:375:PHE:HD2	1.61	0.49
1:D:208:ILE:O	1:D:212:ILE:HG13	2.13	0.49
1:D:33:SER:O	1:D:70:PRO:HD2	2.13	0.49
1:C:344:SER:O	1:C:345:ILE:C	2.55	0.49
1:A:76:ILE:HD12	1:A:119:MET:HE2	1.93	0.49
1:C:27:PRO:HA	1:C:340:TRP:CZ2	2.48	0.49
1:D:317:ILE:HG22	1:D:327:ILE:CD1	2.43	0.49
1:E:337:TYR:O	1:E:338:SER:C	2.54	0.49
1:B:117:GLU:OE1	1:B:367:PRO:HB2	2.12	0.48
1:C:297:ASN:HB3	1:C:329:ILE:HD13	1.95	0.48
2:M:175:LEU:CD2	2:M:180:ILE:HD12	2.43	0.48
1:A:370:VAL:HG13	1:A:371:HIS:N	2.28	0.48
1:C:303:THR:HG22	1:C:303:THR:O	2.13	0.48
1:D:111:ASN:ND2	1:D:115:ASN:HD22	2.05	0.48
1:D:202:THR:HB	1:D:205:GLU:H	1.78	0.48
1:B:295:ALA:C	1:B:296:ASN:HD22	2.20	0.48
1:B:335:ARG:C	1:B:337:TYR:H	2.19	0.48
1:B:145:SER:HG	1:B:147:ARG:HD2	1.78	0.48
1:C:113:LYS:CB	1:C:371:HIS:HE1	2.26	0.48
1:A:286:ASP:OD2	2:M:92:ILE:HD13	2.14	0.48
1:C:299:MET:HE3	1:C:313:MET:HG2	1.96	0.48
1:A:159:VAL:HG22	1:A:160:THR:N	2.28	0.48
1:A:178:LEU:HD11	1:A:180:LEU:HB3	1.94	0.48
1:B:227:MET:HE1	1:B:256:ARG:HD2	1.96	0.48
1:C:335:ARG:C	1:C:337:TYR:H	2.20	0.48
1:C:355:MET:O	1:C:356:TRP:C	2.56	0.48
1:D:227:MET:O	1:D:230:ALA:HB3	2.13	0.48
1:D:285:CYS:O	1:D:286:ASP:C	2.55	0.48
1:A:33:SER:O	1:A:70:PRO:HD2	2.13	0.48
1:C:142:LEU:O	1:C:145:SER:HB3	2.14	0.48
1:C:126:THR:HG22	1:C:126:THR:O	2.14	0.48
1:C:275:HIS:CG	1:C:276:GLU:N	2.82	0.48
1:D:24:ASP:OD1	1:D:24:ASP:N	2.44	0.48
1:E:124:PHE:HZ	1:E:357:ILE:O	1.97	0.48
1:B:191:LYS:O	1:B:194:THR:CG2	2.62	0.48
1:B:361:GLU:HB3	1:B:369:ILE:HD11	1.95	0.48
2:M:86:GLU:O	2:M:89:SER:HB3	2.14	0.48
1:A:53:TYR:O	1:A:58:ALA:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1376:LAB:H51	3:A:1376:LAB:H11	1.95	0.48
1:C:317:ILE:HG22	1:C:327:ILE:CD1	2.42	0.48
1:C:339:VAL:HG12	1:C:340:TRP:N	2.28	0.48
1:E:318:THR:HG22	1:E:319:ALA:N	2.28	0.48
1:E:341:ILE:O	1:E:345:ILE:HG13	2.14	0.47
1:B:208:ILE:O	1:B:212:ILE:HG13	2.15	0.47
1:C:18:LYS:HG3	1:C:30:VAL:CG2	2.32	0.47
1:C:111:ASN:ND2	1:C:115:ASN:HD22	2.08	0.47
1:B:252:ASN:ND2	1:B:256:ARG:HH11	2.12	0.47
1:E:345:ILE:HG23	2:M:150:GLN:HG3	1.97	0.47
2:M:162:LEU:HD13	2:M:166:ILE:HG23	1.95	0.47
1:A:124:PHE:HZ	1:A:357:ILE:O	1.98	0.47
1:A:208:ILE:O	1:A:212:ILE:HG13	2.14	0.47
1:B:204:ALA:O	1:B:208:ILE:HG13	2.14	0.47
1:B:275:HIS:CG	1:B:276:GLU:N	2.83	0.47
2:M:158:LEU:HD23	2:M:158:LEU:C	2.39	0.47
1:A:283:MET:C	1:A:285:CYS:H	2.23	0.47
1:B:113:LYS:CB	1:B:371:HIS:CE1	2.97	0.47
1:B:162:ASN:OD1	1:B:277:THR:OG1	2.31	0.47
1:C:10:CYS:HB3	1:C:105:LEU:HD23	1.96	0.47
1:E:139:VAL:HA	1:E:165:ILE:HD13	1.96	0.47
2:M:127:GLU:O	2:M:128:ARG:C	2.58	0.47
1:D:338:SER:O	1:D:339:VAL:C	2.57	0.47
1:D:352:PHE:HA	1:D:355:MET:HE3	1.97	0.47
1:A:227:MET:HE1	1:A:256:ARG:HD2	1.96	0.47
1:B:9:VAL:HG21	1:B:344:SER:HA	1.97	0.47
1:B:317:ILE:HG22	1:B:327:ILE:CD1	2.42	0.47
1:D:223:PHE:HE2	1:D:266:PHE:HZ	1.63	0.47
1:D:318:THR:HG22	1:D:319:ALA:N	2.29	0.47
1:D:337:TYR:O	1:D:338:SER:C	2.57	0.47
1:D:178:LEU:HD11	1:D:180:LEU:HB3	1.96	0.47
1:E:349:LEU:HD23	2:M:150:GLN:NE2	2.29	0.47
2:M:73:VAL:HG22	2:M:74:LEU:N	2.29	0.47
1:A:275:HIS:CG	1:A:276:GLU:N	2.82	0.47
1:C:338:SER:O	1:C:339:VAL:C	2.58	0.47
2:M:141:SER:OG	2:M:142:ALA:HA	2.14	0.47
2:M:180:ILE:HG22	2:M:181:LEU:CG	2.41	0.47
1:A:223:PHE:HE2	1:A:266:PHE:HZ	1.62	0.47
1:C:178:LEU:HD11	1:C:180:LEU:HB3	1.96	0.47
1:C:325:MET:HE2	1:C:325:MET:HB2	1.76	0.47
1:D:202:THR:CB	1:D:205:GLU:HG3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:VAL:HG21	1:E:344:SER:HA	1.97	0.47
1:A:126:THR:HG22	1:A:126:THR:O	2.15	0.46
1:A:252:ASN:ND2	1:A:256:ARG:HH11	2.13	0.46
1:B:126:THR:O	1:B:126:THR:HG22	2.15	0.46
1:B:330:ILE:N	1:B:330:ILE:HD12	2.30	0.46
1:D:339:VAL:HG12	1:D:340:TRP:N	2.30	0.46
1:E:335:ARG:C	1:E:337:TYR:H	2.22	0.46
1:A:159:VAL:HG21	1:A:161:HIS:CE1	2.50	0.46
1:A:294:TYR:CE1	1:A:321:ALA:HB2	2.51	0.46
2:M:88:VAL:CA	2:M:93:MET:HB2	2.45	0.46
1:C:6:THR:HG22	1:C:7:ALA:N	2.17	0.46
1:C:162:ASN:OD1	1:C:277:THR:OG1	2.31	0.46
1:C:223:PHE:HE2	1:C:266:PHE:HZ	1.62	0.46
1:D:215:LYS:HB3	1:D:215:LYS:NZ	2.29	0.46
1:B:337:TYR:O	1:B:338:SER:C	2.58	0.46
1:D:295:ALA:C	1:D:296:ASN:HD22	2.23	0.46
1:A:335:ARG:C	1:A:337:TYR:H	2.22	0.46
1:C:124:PHE:CZ	1:C:357:ILE:HG22	2.50	0.46
1:C:202:THR:HB	1:C:205:GLU:H	1.80	0.46
1:C:311:ASP:O	1:C:314:GLN:HB3	2.16	0.46
1:E:113:LYS:O	1:E:117:GLU:HG3	2.14	0.46
1:A:367:PRO:O	1:A:370:VAL:HG12	2.15	0.46
1:D:286:ASP:OD1	1:D:287:ILE:N	2.48	0.46
1:E:145:SER:HG	1:E:147:ARG:HD2	1.81	0.46
2:M:118:LEU:HD12	2:M:118:LEU:HA	1.61	0.46
1:D:275:HIS:CG	1:D:276:GLU:N	2.84	0.46
1:A:191:LYS:O	1:A:194:THR:CG2	2.63	0.46
1:C:113:LYS:CB	1:C:371:HIS:CE1	2.99	0.46
1:B:99:GLU:CD	1:B:99:GLU:H	2.19	0.46
1:C:139:VAL:HA	1:C:165:ILE:HD13	1.98	0.46
1:C:194:THR:HG23	1:C:195:GLU:N	2.30	0.46
1:D:111:ASN:HD21	1:D:119:MET:HE3	1.81	0.46
1:E:338:SER:O	1:E:339:VAL:C	2.59	0.46
1:A:173:HIS:HB3	2:M:103:HIS:CD2	2.51	0.46
1:A:372:ARG:O	1:A:375:PHE:HE1	1.99	0.46
1:B:109:PRO:O	1:B:110:LEU:HB2	2.15	0.46
1:B:142:LEU:O	1:B:145:SER:HB3	2.16	0.45
1:C:139:VAL:HG22	1:C:165:ILE:HD13	1.98	0.45
1:E:194:THR:HG23	1:E:195:GLU:N	2.30	0.45
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.98	0.45
1:B:113:LYS:O	1:B:117:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:TYR:O	1:C:327:ILE:HA	2.16	0.45
1:A:338:SER:O	1:A:339:VAL:C	2.59	0.45
1:C:32:PRO:HB3	3:C:1376:LAB:C12	2.45	0.45
1:D:126:THR:HG22	1:D:126:THR:O	2.16	0.45
2:M:102:PHE:HA	2:M:105:GLN:HG2	1.99	0.45
2:M:120:ARG:C	2:M:122:ILE:N	2.74	0.45
1:A:139:VAL:HG22	1:A:165:ILE:HD13	1.97	0.45
1:B:338:SER:O	1:B:339:VAL:C	2.58	0.45
1:A:204:ALA:O	1:A:208:ILE:HG13	2.16	0.45
1:A:337:TYR:O	1:A:338:SER:C	2.59	0.45
1:B:178:LEU:HD11	1:B:180:LEU:HB3	1.99	0.45
1:B:11:ASP:HA	1:B:106:THR:OG1	2.17	0.45
2:M:82:ARG:HG3	2:M:82:ARG:H	1.45	0.45
1:D:282:ILE:HG22	1:D:290:ARG:HD3	1.98	0.45
1:E:191:LYS:O	1:E:194:THR:CG2	2.65	0.45
1:E:342:GLY:O	1:E:343:GLY:C	2.60	0.45
1:B:342:GLY:O	1:B:343:GLY:C	2.59	0.45
1:D:305:MET:HA	1:D:335:ARG:HH21	1.81	0.45
1:E:275:HIS:CG	1:E:276:GLU:N	2.85	0.45
1:A:295:ALA:O	1:A:296:ASN:ND2	2.50	0.45
1:B:169:TYR:CE1	2:M:125:ARG:NH2	2.85	0.45
1:E:109:PRO:O	1:E:110:LEU:HB2	2.17	0.45
1:D:124:PHE:HZ	1:D:357:ILE:O	1.99	0.44
1:D:132:MET:HE2	1:D:132:MET:HB2	1.89	0.44
1:D:159:VAL:HG22	1:D:160:THR:N	2.30	0.44
1:D:334:GLU:OE1	1:D:334:GLU:N	2.50	0.44
1:A:111:ASN:ND2	1:A:115:ASN:HD22	2.06	0.44
1:C:356:TRP:O	1:C:357:ILE:HD13	2.17	0.44
1:A:234:SER:C	1:A:236:LEU:N	2.75	0.44
1:B:170:ALA:O	1:B:172:PRO:HD3	2.18	0.44
1:B:287:ILE:HD11	1:C:30:VAL:HG21	2.00	0.44
1:C:109:PRO:HB3	1:C:175:ILE:HD13	1.99	0.44
1:D:335:ARG:O	1:D:337:TYR:N	2.50	0.44
2:M:122:ILE:HG22	2:M:123:ARG:N	2.33	0.44
2:M:134:MET:O	2:M:135:HIS:HB3	2.17	0.44
1:A:345:ILE:HG23	2:M:71:LYS:HG3	1.99	0.44
1:D:9:VAL:HG21	1:D:344:SER:HA	1.98	0.44
1:E:170:ALA:O	1:E:172:PRO:HD3	2.18	0.44
1:E:367:PRO:O	1:E:370:VAL:HG12	2.17	0.44
1:B:117:GLU:CG	1:B:371:HIS:HE2	2.31	0.44
1:B:124:PHE:HZ	1:B:357:ILE:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ASP:O	1:B:314:GLN:HB3	2.18	0.44
1:C:166:TYR:HD1	2:M:175:LEU:HD21	1.83	0.44
1:C:170:ALA:O	1:C:172:PRO:HD3	2.18	0.44
1:C:204:ALA:O	1:C:208:ILE:HG13	2.16	0.44
1:D:342:GLY:O	1:D:343:GLY:C	2.60	0.44
1:E:23:GLY:HA2	2:M:142:ALA:CB	2.25	0.44
1:A:139:VAL:HA	1:A:165:ILE:HD13	1.99	0.44
1:C:32:PRO:CB	3:C:1376:LAB:H102	2.46	0.44
1:D:305:MET:HA	1:D:335:ARG:NH2	2.33	0.44
1:A:311:ASP:O	1:A:314:GLN:HB3	2.18	0.44
1:C:111:ASN:HD21	1:C:119:MET:HE3	1.83	0.44
1:C:341:ILE:O	1:C:344:SER:HB3	2.18	0.44
1:A:114:ALA:HB2	1:D:28:ARG:CD	2.45	0.43
1:A:194:THR:CG2	1:A:195:GLU:N	2.81	0.43
1:B:166:TYR:O	1:B:167:GLU:C	2.61	0.43
1:C:230:ALA:HA	1:C:236:LEU:HD23	1.99	0.43
1:E:139:VAL:HG22	1:E:165:ILE:HD13	2.00	0.43
2:M:86:GLU:O	2:M:90:GLN:HG3	2.18	0.43
1:C:109:PRO:O	1:C:110:LEU:HB2	2.18	0.43
1:C:334:GLU:H	1:C:334:GLU:CD	2.25	0.43
1:A:23:GLY:O	2:M:67:LEU:HD13	2.19	0.43
1:C:178:LEU:HD12	1:C:178:LEU:C	2.44	0.43
1:C:334:GLU:HB3	2:M:135:HIS:CD2	2.53	0.43
1:D:139:VAL:HG22	1:D:165:ILE:HD13	2.01	0.43
1:D:146:GLY:O	2:M:108:SER:HB3	2.19	0.43
2:M:125:ARG:HA	2:M:126:PRO:HD3	1.84	0.43
1:C:58:ALA:C	1:C:60:SER:N	2.75	0.43
1:C:227:MET:HE1	1:C:256:ARG:HD2	2.01	0.43
2:M:180:ILE:O	2:M:181:LEU:CB	2.66	0.43
1:A:111:ASN:HD21	1:A:119:MET:HE3	1.83	0.43
1:B:6:THR:O	1:B:101:HIS:HB3	2.19	0.43
1:C:187:ASP:O	1:C:190:MET:HB2	2.19	0.43
1:E:349:LEU:HD21	2:M:150:GLN:CG	2.49	0.43
1:B:302:GLY:O	1:B:305:MET:HG2	2.18	0.43
1:B:261:LEU:HD11	1:B:303:THR:HG22	2.01	0.43
1:E:126:THR:O	1:E:126:THR:HG22	2.17	0.43
2:M:147:GLN:O	2:M:148:ALA:C	2.61	0.43
1:B:286:ASP:OD1	1:B:287:ILE:N	2.52	0.43
1:B:351:THR:HG21	2:M:122:ILE:HG21	2.01	0.43
1:D:139:VAL:HA	1:D:165:ILE:HD13	2.00	0.43
2:M:164:GLU:CD	2:M:165:LYS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASN:OD1	1:B:78:ASN:C	2.62	0.43
1:B:188:TYR:CD1	1:B:267:ILE:HG22	2.54	0.43
1:C:351:THR:CG2	2:M:166:ILE:HD11	2.49	0.43
1:E:142:LEU:O	1:E:145:SER:HB3	2.18	0.43
1:D:293:LEU:HD23	1:D:293:LEU:HA	1.90	0.42
1:D:330:ILE:N	1:D:330:ILE:HD12	2.34	0.42
1:A:18:LYS:NZ	4:A:1377:ATP:O1B	2.50	0.42
1:A:142:LEU:O	1:A:145:SER:HB3	2.19	0.42
1:D:311:ASP:O	1:D:314:GLN:HB3	2.19	0.42
2:M:72:ASN:O	2:M:73:VAL:C	2.62	0.42
2:M:120:ARG:C	2:M:122:ILE:H	2.26	0.42
1:A:9:VAL:HG21	1:A:344:SER:HA	2.00	0.42
1:A:325:MET:HE2	1:A:325:MET:HB2	1.76	0.42
1:B:234:SER:C	1:B:236:LEU:N	2.77	0.42
1:C:159:VAL:HG22	1:C:160:THR:N	2.34	0.42
1:C:351:THR:HG21	2:M:167:ALA:HA	2.00	0.42
1:E:234:SER:C	1:E:236:LEU:N	2.75	0.42
2:M:88:VAL:HG21	2:M:95:PRO:HA	2.00	0.42
2:M:162:LEU:HD13	2:M:166:ILE:CG2	2.50	0.42
1:A:178:LEU:CD1	1:A:180:LEU:HB3	2.50	0.42
1:B:194:THR:HG23	1:B:195:GLU:N	2.33	0.42
1:B:358:THR:HG23	1:B:361:GLU:CD	2.45	0.42
1:E:132:MET:HE2	1:E:132:MET:HB2	1.94	0.42
1:A:317:ILE:HG22	1:A:327:ILE:CD1	2.46	0.42
1:C:76:ILE:HD12	1:C:119:MET:HE2	2.00	0.42
1:A:321:ALA:HB1	1:A:322:PRO:HD2	2.02	0.42
1:B:140:LEU:HD22	1:B:343:GLY:HA2	2.01	0.42
1:C:342:GLY:O	1:C:343:GLY:C	2.63	0.42
1:E:159:VAL:HG21	1:E:161:HIS:CE1	2.54	0.42
1:A:178:LEU:HD12	1:A:178:LEU:C	2.45	0.42
1:C:350:SER:O	1:C:351:THR:C	2.63	0.42
1:D:140:LEU:HD22	1:D:343:GLY:HA2	2.02	0.42
1:E:165:ILE:HG23	1:E:169:TYR:C	2.44	0.42
1:A:78:ASN:OD1	1:A:78:ASN:C	2.63	0.42
1:C:9:VAL:HG12	1:C:340:TRP:NE1	2.33	0.42
1:C:18:LYS:O	1:C:340:TRP:CD1	2.73	0.42
1:C:145:SER:HG	1:C:147:ARG:HD2	1.83	0.42
1:C:330:ILE:HD12	1:C:330:ILE:N	2.34	0.42
1:B:109:PRO:HB3	1:B:175:ILE:HD13	2.02	0.42
1:E:334:GLU:O	1:E:336:LYS:N	2.53	0.42
2:M:83:THR:OG1	2:M:85:GLU:OE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD11	1:A:303:THR:HG22	2.03	0.41
1:C:238:LYS:HD2	1:C:238:LYS:HA	1.63	0.41
1:D:66:THR:O	1:D:66:THR:HG22	2.19	0.41
1:D:178:LEU:CD1	1:D:180:LEU:HB3	2.50	0.41
2:M:111:ARG:O	2:M:112:ALA:C	2.62	0.41
1:C:188:TYR:CD1	1:C:267:ILE:HG22	2.55	0.41
1:D:107:GLU:OE1	1:D:116:ARG:HG2	2.20	0.41
1:D:261:LEU:HD11	1:D:303:THR:HG22	2.01	0.41
1:E:344:SER:O	1:E:345:ILE:C	2.62	0.41
2:M:107:GLU:O	2:M:108:SER:C	2.62	0.41
1:A:136:ILE:O	1:A:137:GLN:C	2.63	0.41
1:A:188:TYR:CD1	1:A:267:ILE:HG22	2.55	0.41
1:B:292:ASP:O	1:B:296:ASN:HB2	2.19	0.41
1:D:325:MET:HB2	1:D:325:MET:HE2	1.77	0.41
1:D:374:CYS:O	1:D:375:PHE:OXT	2.39	0.41
2:M:74:LEU:HD12	2:M:74:LEU:HA	1.93	0.41
1:A:234:SER:O	1:A:236:LEU:N	2.54	0.41
1:A:344:SER:O	1:A:345:ILE:C	2.63	0.41
1:B:352:PHE:HA	1:B:355:MET:HE3	2.02	0.41
1:D:215:LYS:NZ	1:D:215:LYS:CB	2.84	0.41
1:B:111:ASN:ND2	1:B:115:ASN:HD22	2.12	0.41
1:D:127:PHE:O	1:D:128:ASN:C	2.62	0.41
1:D:344:SER:O	1:D:345:ILE:C	2.63	0.41
1:A:109:PRO:HB3	1:A:175:ILE:HD13	2.03	0.41
1:C:15:GLY:HA2	1:C:33:SER:HB2	2.03	0.41
1:C:132:MET:HE2	1:C:132:MET:HB2	1.94	0.41
1:C:178:LEU:CD1	1:C:180:LEU:HB3	2.51	0.41
1:D:210:ARG:O	1:D:213:LYS:HB3	2.20	0.41
1:E:330:ILE:N	1:E:330:ILE:HD12	2.35	0.41
1:A:342:GLY:O	1:A:343:GLY:C	2.63	0.41
1:B:202:THR:HB	1:B:205:GLU:HG3	2.03	0.41
1:C:165:ILE:HG23	1:C:169:TYR:C	2.45	0.41
1:A:117:GLU:OE1	1:A:367:PRO:HB2	2.20	0.41
1:A:302:GLY:O	1:A:305:MET:HG2	2.21	0.41
1:B:325:MET:HB2	1:B:325:MET:HE2	1.73	0.41
1:C:114:ALA:HA	1:C:117:GLU:HG2	2.02	0.41
1:C:242:LEU:HB3	1:C:243:PRO:HD2	2.03	0.41
1:C:321:ALA:HB1	1:C:322:PRO:HD2	2.03	0.41
1:D:151:ILE:HB	1:D:293:LEU:HD22	2.02	0.41
1:D:159:VAL:HG21	1:D:161:HIS:CE1	2.56	0.41
1:B:218:TYR:OH	1:B:226:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASN:OD1	1:C:78:ASN:C	2.63	0.41
1:D:162:ASN:OD1	1:D:277:THR:OG1	2.33	0.41
1:A:256:ARG:O	1:A:259:GLU:HB3	2.21	0.40
1:B:274:ILE:HG13	1:B:313:MET:HE1	2.04	0.40
1:D:332:PRO:C	1:D:334:GLU:H	2.30	0.40
1:E:140:LEU:HD22	1:E:343:GLY:HA2	2.03	0.40
2:M:82:ARG:HD3	2:M:87:LEU:HD21	2.03	0.40
1:A:330:ILE:N	1:A:330:ILE:HD12	2.37	0.40
1:B:213:LYS:O	1:B:217:CYS:HB2	2.21	0.40
1:C:24:ASP:OD1	1:C:24:ASP:N	2.55	0.40
1:E:159:VAL:HG22	1:E:160:THR:N	2.35	0.40
1:D:78:ASN:OD1	1:D:78:ASN:C	2.64	0.40
1:E:234:SER:O	1:E:236:LEU:N	2.55	0.40
2:M:67:LEU:HD23	2:M:67:LEU:O	2.20	0.40
1:B:178:LEU:CD1	1:B:180:LEU:HB3	2.51	0.40
1:E:136:ILE:HD12	1:E:136:ILE:H	1.86	0.40
2:M:101:ALA:C	2:M:102:PHE:CG	3.00	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/377 (92%)	304 (88%)	39 (11%)	3 (1%)	14	47
1	B	331/377 (88%)	287 (87%)	41 (12%)	3 (1%)	14	47
1	C	337/377 (89%)	287 (85%)	41 (12%)	9 (3%)	4	27
1	D	337/377 (89%)	291 (86%)	42 (12%)	4 (1%)	10	41
1	E	312/377 (83%)	270 (86%)	37 (12%)	5 (2%)	7	36
2	M	119/137 (87%)	98 (82%)	18 (15%)	3 (2%)	4	28
All	All	1782/2022 (88%)	1537 (86%)	218 (12%)	27 (2%)	8	37

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	233	SER
1	C	235	SER
1	A	234	SER
1	A	339	VAL
1	B	339	VAL
1	C	356	TRP
1	D	66	THR
1	D	338	SER
1	D	339	VAL
1	E	234	SER
1	E	339	VAL
2	M	97	LYS
1	A	338	SER
1	B	234	SER
1	B	338	SER
1	C	234	SER
1	C	338	SER
1	C	339	VAL
1	E	338	SER
1	C	353	GLN
2	M	144	PRO
1	C	26	ALA
1	C	344	SER
1	D	370	VAL
1	E	335	ARG
2	M	170	PRO
1	E	333	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/320 (83%)	238 (90%)	28 (10%)	6	27
1	B	247/320 (77%)	220 (89%)	27 (11%)	6	26
1	C	252/320 (79%)	224 (89%)	28 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	242/320 (76%)	218 (90%)	24 (10%)	7	29
1	E	128/320 (40%)	119 (93%)	9 (7%)	14	39
2	M	90/123 (73%)	69 (77%)	21 (23%)	1	5
All	All	1225/1723 (71%)	1088 (89%)	137 (11%)	6	25

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	12	ASN
1	A	14	SER
1	A	28	ARG
1	A	34	ILE
1	A	35	VAL
1	A	51	ASP
1	A	71	ILE
1	A	75	ILE
1	A	104	LEU
1	A	128	ASN
1	A	145	SER
1	A	178	LEU
1	A	185	LEU
1	A	201	VAL
1	A	206	ARG
1	A	247	VAL
1	A	249	THR
1	A	252	ASN
1	A	263	GLN
1	A	277	THR
1	A	318	THR
1	A	327	ILE
1	A	334	GLU
1	A	338	SER
1	A	354	GLN
1	A	355	MET
1	A	358	THR
1	B	5	THR
1	B	6	THR
1	B	12	ASN
1	B	14	SER
1	B	24	ASP

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Mol	Chain	Res	Type
1	B	25	ASP
1	B	71	ILE
1	B	72	GLU
1	B	75	ILE
1	B	104	LEU
1	B	128	ASN
1	B	178	LEU
1	B	185	LEU
1	B	201	VAL
1	B	246	GLN
1	B	249	THR
1	B	252	ASN
1	B	263	GLN
1	B	277	THR
1	B	287	ILE
1	B	296	ASN
1	B	318	THR
1	B	327	ILE
1	B	338	SER
1	B	355	MET
1	B	358	THR
1	B	368	SER
1	C	12	ASN
1	C	14	SER
1	C	71	ILE
1	C	75	ILE
1	C	145	SER
1	C	178	LEU
1	C	185	LEU
1	C	196	ARG
1	C	201	VAL
1	C	206	ARG
1	C	215	LYS
1	C	229	THR
1	C	236	LEU
1	C	238	LYS
1	C	247	VAL
1	C	248	ILE
1	C	249	THR
1	C	252	ASN
1	C	270	GLU
1	C	277	THR

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Mol	Chain	Res	Type
1	C	287	ILE
1	C	318	THR
1	C	327	ILE
1	C	338	SER
1	C	351	THR
1	C	354	GLN
1	C	357	ILE
1	C	358	THR
1	D	5	THR
1	D	6	THR
1	D	12	ASN
1	D	14	SER
1	D	24	ASP
1	D	25	ASP
1	D	34	ILE
1	D	35	VAL
1	D	65	LEU
1	D	71	ILE
1	D	75	ILE
1	D	128	ASN
1	D	178	LEU
1	D	185	LEU
1	D	215	LYS
1	D	229	THR
1	D	247	VAL
1	D	248	ILE
1	D	277	THR
1	D	318	THR
1	D	327	ILE
1	D	338	SER
1	D	355	MET
1	D	358	THR
1	E	6	THR
1	E	12	ASN
1	E	14	SER
1	E	104	LEU
1	E	145	SER
1	E	277	THR
1	E	318	THR
1	E	338	SER
1	E	358	THR
2	M	66	SER

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Mol	Chain	Res	Type
2	M	70	ARG
2	M	73	VAL
2	M	79	GLN
2	M	82	ARG
2	M	84	ARG
2	M	105	GLN
2	M	106	ARG
2	M	108	SER
2	M	109	LEU
2	M	113	ARG
2	M	118	LEU
2	M	122	ILE
2	M	132	VAL
2	M	141	SER
2	M	146	LEU
2	M	151	LEU
2	M	162	LEU
2	M	166	ILE
2	M	168	GLN
2	M	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	92	ASN
1	A	115	ASN
1	A	161	HIS
1	A	246	GLN
1	A	252	ASN
1	A	280	ASN
1	A	296	ASN
1	A	297	ASN
1	B	12	ASN
1	B	92	ASN
1	B	101	HIS
1	B	115	ASN
1	B	161	HIS
1	B	246	GLN
1	B	252	ASN
1	B	280	ASN
1	C	12	ASN

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Mol	Chain	Res	Type
1	C	92	ASN
1	C	115	ASN
1	C	161	HIS
1	C	246	GLN
1	C	252	ASN
1	C	280	ASN
1	C	297	ASN
1	C	371	HIS
1	D	12	ASN
1	D	73	HIS
1	D	92	ASN
1	D	101	HIS
1	D	115	ASN
1	D	161	HIS
1	D	280	ASN
1	D	297	ASN
1	E	161	HIS
2	M	72	ASN
2	M	79	GLN
2	M	103	HIS
2	M	105	GLN
2	M	150	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	1377	5	32,33,33	1.75	7 (21%)	48,52,52	1.83	12 (25%)
3	LAB	A	1376	-	28,29,29	1.62	2 (7%)	29,41,41	2.39	9 (31%)
4	ATP	D	1377	5	32,33,33	1.67	4 (12%)	48,52,52	1.74	12 (25%)
4	ATP	B	1377	5	32,33,33	1.63	6 (18%)	48,52,52	1.77	11 (22%)
4	ATP	E	1377	5	32,33,33	1.62	5 (15%)	48,52,52	1.75	10 (20%)
3	LAB	C	1376	-	28,29,29	1.68	3 (10%)	29,41,41	2.11	5 (17%)
4	ATP	C	1377	5	32,33,33	1.75	8 (25%)	48,52,52	1.85	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	1377	5	-	7/22/38/38	0/3/3/3
3	LAB	A	1376	-	-	4/21/49/49	0/2/3/3
4	ATP	D	1377	5	-	6/22/38/38	0/3/3/3
4	ATP	B	1377	5	-	5/22/38/38	0/3/3/3
4	ATP	E	1377	5	-	6/22/38/38	0/3/3/3
3	LAB	C	1376	-	-	6/21/49/49	0/2/3/3
4	ATP	C	1377	5	-	6/22/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1376	LAB	C18-S1	-5.54	1.66	1.77
3	C	1376	LAB	O2-C1	5.47	1.45	1.34
3	A	1376	LAB	C18-S1	-5.46	1.66	1.77
3	A	1376	LAB	O2-C1	5.37	1.45	1.34
4	E	1377	ATP	C2'-C3'	-5.04	1.39	1.53
4	D	1377	ATP	C2'-C3'	-4.95	1.40	1.53
4	C	1377	ATP	C2'-C3'	-4.90	1.40	1.53
4	B	1377	ATP	C2'-C3'	-4.86	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1377	ATP	C2'-C3'	-4.86	1.40	1.53
4	A	1377	ATP	PB-O3B	-3.92	1.55	1.59
4	D	1377	ATP	PB-O3B	-3.50	1.55	1.59
4	E	1377	ATP	C6-N6	3.43	1.43	1.34
4	D	1377	ATP	C6-N6	3.37	1.42	1.34
4	B	1377	ATP	C6-N6	3.37	1.42	1.34
4	A	1377	ATP	C6-N6	3.22	1.42	1.34
4	B	1377	ATP	PB-O3B	-3.13	1.56	1.59
4	C	1377	ATP	C6-N6	3.04	1.42	1.34
4	A	1377	ATP	O4'-C4'	-2.85	1.38	1.45
4	D	1377	ATP	O4'-C4'	-2.83	1.38	1.45
4	E	1377	ATP	O4'-C4'	-2.76	1.38	1.45
4	C	1377	ATP	O4'-C4'	-2.73	1.38	1.45
4	B	1377	ATP	O4'-C4'	-2.73	1.38	1.45
4	C	1377	ATP	PB-O3B	-2.72	1.56	1.59
4	C	1377	ATP	C8-N9	-2.64	1.33	1.37
4	C	1377	ATP	C5-N7	-2.53	1.34	1.39
3	C	1376	LAB	O4-C15	2.44	1.44	1.40
4	C	1377	ATP	C3'-C4'	-2.41	1.46	1.53
4	A	1377	ATP	C5-N7	-2.36	1.34	1.39
4	A	1377	ATP	C3'-C4'	-2.34	1.47	1.53
4	E	1377	ATP	C3'-C4'	-2.21	1.47	1.53
4	E	1377	ATP	PB-O3B	-2.11	1.57	1.59
4	C	1377	ATP	O4'-C1'	-2.11	1.37	1.42
4	A	1377	ATP	C8-N9	-2.10	1.34	1.37
4	B	1377	ATP	C5-N7	-2.07	1.35	1.39
4	B	1377	ATP	C3'-C4'	-2.03	1.47	1.53

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1376	LAB	C17-S1-C18	8.25	96.82	92.04
3	A	1376	LAB	C17-S1-C18	8.08	96.72	92.04
4	C	1377	ATP	C5-C4-N3	-5.48	119.18	126.72
3	A	1376	LAB	O3-C15-C16	5.04	110.71	104.25
4	A	1377	ATP	C5-C4-N3	-4.93	119.93	126.72
4	E	1377	ATP	C5-C4-N3	-4.85	120.04	126.72
4	D	1377	ATP	C5-C4-N3	-4.62	120.35	126.72
4	B	1377	ATP	C5-C4-N3	-4.58	120.41	126.72
3	A	1376	LAB	O2-C1-C2	4.44	121.49	111.20
4	B	1377	ATP	N3-C2-N1	-4.13	122.33	128.58
4	C	1377	ATP	C4-C5-N7	-3.92	106.10	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1377	ATP	N3-C2-N1	-3.81	122.81	128.58
4	D	1377	ATP	N3-C2-N1	-3.74	122.92	128.58
3	C	1376	LAB	O3-C15-C16	3.73	109.03	104.25
4	A	1377	ATP	N3-C2-N1	-3.57	123.17	128.58
4	A	1377	ATP	C4-C5-N7	-3.49	106.59	110.58
4	A	1377	ATP	N9-C8-N7	-3.37	109.16	113.94
4	B	1377	ATP	N9-C8-N7	-3.32	109.23	113.94
4	C	1377	ATP	N3-C2-N1	-3.30	123.59	128.58
4	D	1377	ATP	C4-C5-N7	-3.28	106.83	110.58
4	E	1377	ATP	C4-C5-N7	-3.24	106.88	110.58
4	A	1377	ATP	C5-N7-C8	3.22	108.51	103.45
3	C	1376	LAB	O2-C1-C2	3.16	118.52	111.20
3	A	1376	LAB	O2-C1-O1	-3.15	118.30	123.34
4	C	1377	ATP	N9-C8-N7	-3.15	109.47	113.94
4	C	1377	ATP	O5'-C5'-C4'	3.14	119.68	108.99
4	B	1377	ATP	O5'-C5'-C4'	3.12	119.61	108.99
4	C	1377	ATP	C5-N7-C8	3.11	108.33	103.45
4	C	1377	ATP	C2-N3-C4	3.11	119.42	111.83
4	B	1377	ATP	C2-N3-C4	3.06	119.30	111.83
4	D	1377	ATP	N9-C8-N7	-3.04	109.62	113.94
4	E	1377	ATP	C2-N3-C4	3.01	119.18	111.83
3	A	1376	LAB	C12-C13-C14	-3.01	105.09	111.02
4	A	1377	ATP	N3-C4-N9	2.98	132.24	127.17
4	E	1377	ATP	N3-C4-N9	2.98	132.24	127.17
4	B	1377	ATP	C4-C5-N7	-2.98	107.18	110.58
4	E	1377	ATP	N9-C8-N7	-2.97	109.72	113.94
4	C	1377	ATP	N3-C4-N9	2.97	132.21	127.17
4	B	1377	ATP	N3-C4-N9	2.94	132.17	127.17
4	D	1377	ATP	C5-N7-C8	2.93	108.06	103.45
4	D	1377	ATP	N3-C4-N9	2.91	132.12	127.17
4	D	1377	ATP	O5'-C5'-C4'	2.90	118.85	108.99
4	B	1377	ATP	C5-N7-C8	2.89	107.99	103.45
4	A	1377	ATP	O3G-PG-O3B	2.88	114.29	104.64
4	A	1377	ATP	C2-N3-C4	2.87	118.84	111.83
4	E	1377	ATP	C5-N7-C8	2.85	107.93	103.45
4	D	1377	ATP	C2-N3-C4	2.82	118.71	111.83
4	B	1377	ATP	O2B-PB-O3A	2.81	114.88	107.27
4	D	1377	ATP	O2B-PB-O3A	2.81	114.86	107.27
4	E	1377	ATP	O5'-C5'-C4'	2.77	118.44	108.99
4	A	1377	ATP	O2A-PA-O3A	2.63	114.38	107.27
4	C	1377	ATP	C5-C4-N9	2.57	108.61	105.81
3	A	1376	LAB	C14-C15-C16	-2.57	108.74	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1377	ATP	O2B-PB-O3A	2.48	113.97	107.27
4	C	1377	ATP	O3G-PG-O3B	2.47	112.93	104.64
4	A	1377	ATP	O5'-C5'-C4'	2.44	117.30	108.99
3	A	1376	LAB	O1-C1-C2	-2.43	120.18	126.23
4	B	1377	ATP	C4-N9-C8	2.33	108.19	105.74
4	B	1377	ATP	O3G-PG-O3B	2.30	112.36	104.64
4	E	1377	ATP	O2B-PB-O3B	2.27	113.42	107.27
4	A	1377	ATP	O2B-PB-O3A	2.22	113.27	107.27
3	C	1376	LAB	C19-C3-C4	2.18	119.02	115.23
4	D	1377	ATP	O2A-PA-O3A	2.14	113.06	107.27
3	A	1376	LAB	C4-C5-C6	-2.13	107.94	112.57
4	D	1377	ATP	O3G-PG-O3B	2.13	111.77	104.64
4	D	1377	ATP	C4-N9-C8	2.12	107.96	105.74
3	C	1376	LAB	O1-C1-C2	-2.08	121.04	126.23
3	A	1376	LAB	C19-C3-C4	2.07	118.83	115.23
4	A	1377	ATP	C4-N9-C8	2.07	107.91	105.74
4	E	1377	ATP	O2B-PB-O3A	2.01	112.69	107.27

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1376	LAB	O3-C15-C16-C17
4	A	1377	ATP	C5'-O5'-PA-O1A
4	B	1377	ATP	C5'-O5'-PA-O1A
4	B	1377	ATP	C5'-O5'-PA-O3A
4	C	1377	ATP	C5'-O5'-PA-O1A
4	D	1377	ATP	C5'-O5'-PA-O1A
4	D	1377	ATP	C5'-O5'-PA-O3A
4	E	1377	ATP	C5'-O5'-PA-O1A
3	C	1376	LAB	C9-C10-C11-O3
4	C	1377	ATP	C3'-C4'-C5'-O5'
4	E	1377	ATP	C3'-C4'-C5'-O5'
3	A	1376	LAB	O1-C1-O2-C13
4	A	1377	ATP	C3'-C4'-C5'-O5'
4	B	1377	ATP	C3'-C4'-C5'-O5'
4	D	1377	ATP	C3'-C4'-C5'-O5'
4	C	1377	ATP	O4'-C4'-C5'-O5'
4	E	1377	ATP	O4'-C4'-C5'-O5'
4	D	1377	ATP	O4'-C4'-C5'-O5'
4	A	1377	ATP	O4'-C4'-C5'-O5'
4	B	1377	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	1377	ATP	C5'-O5'-PA-O3A
4	C	1377	ATP	C5'-O5'-PA-O3A
4	E	1377	ATP	C5'-O5'-PA-O3A
3	C	1376	LAB	C9-C10-C11-C12
3	A	1376	LAB	O2-C1-C2-C3
3	C	1376	LAB	O2-C1-C2-C3
3	A	1376	LAB	C2-C1-O2-C13
3	A	1376	LAB	O1-C1-C2-C3
3	C	1376	LAB	O1-C1-C2-C3
3	C	1376	LAB	C11-C10-C9-C8
4	A	1377	ATP	PG-O3B-PB-O2B
4	A	1377	ATP	PA-O3A-PB-O1B
4	B	1377	ATP	PG-O3B-PB-O2B
4	C	1377	ATP	PG-O3B-PB-O2B
4	D	1377	ATP	PG-O3B-PB-O2B
4	E	1377	ATP	PG-O3B-PB-O2B
4	E	1377	ATP	PA-O3A-PB-O1B
4	A	1377	ATP	PA-O3A-PB-O2B
4	C	1377	ATP	PA-O3A-PB-O1B
4	D	1377	ATP	PA-O3A-PB-O1B

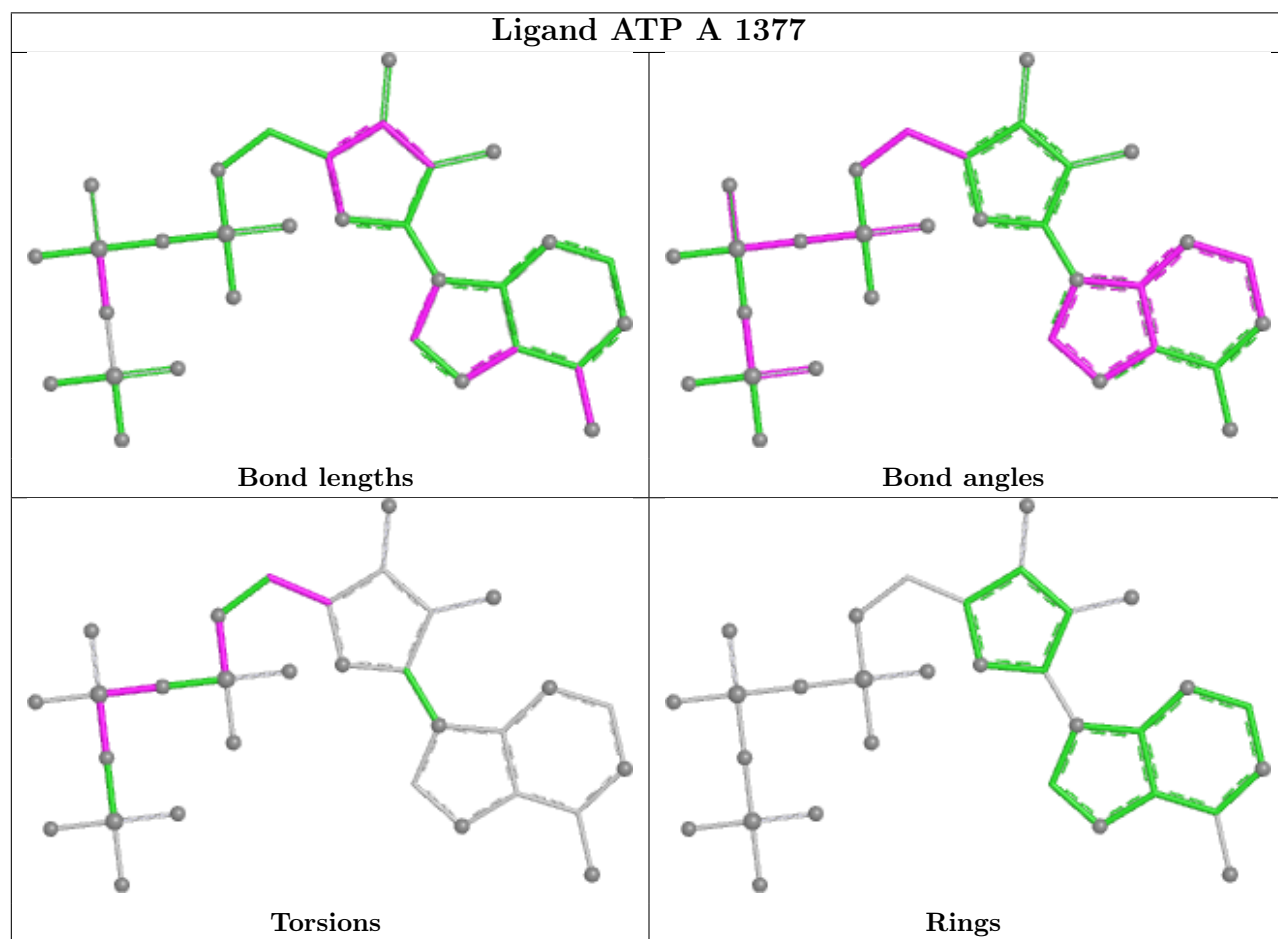
There are no ring outliers.

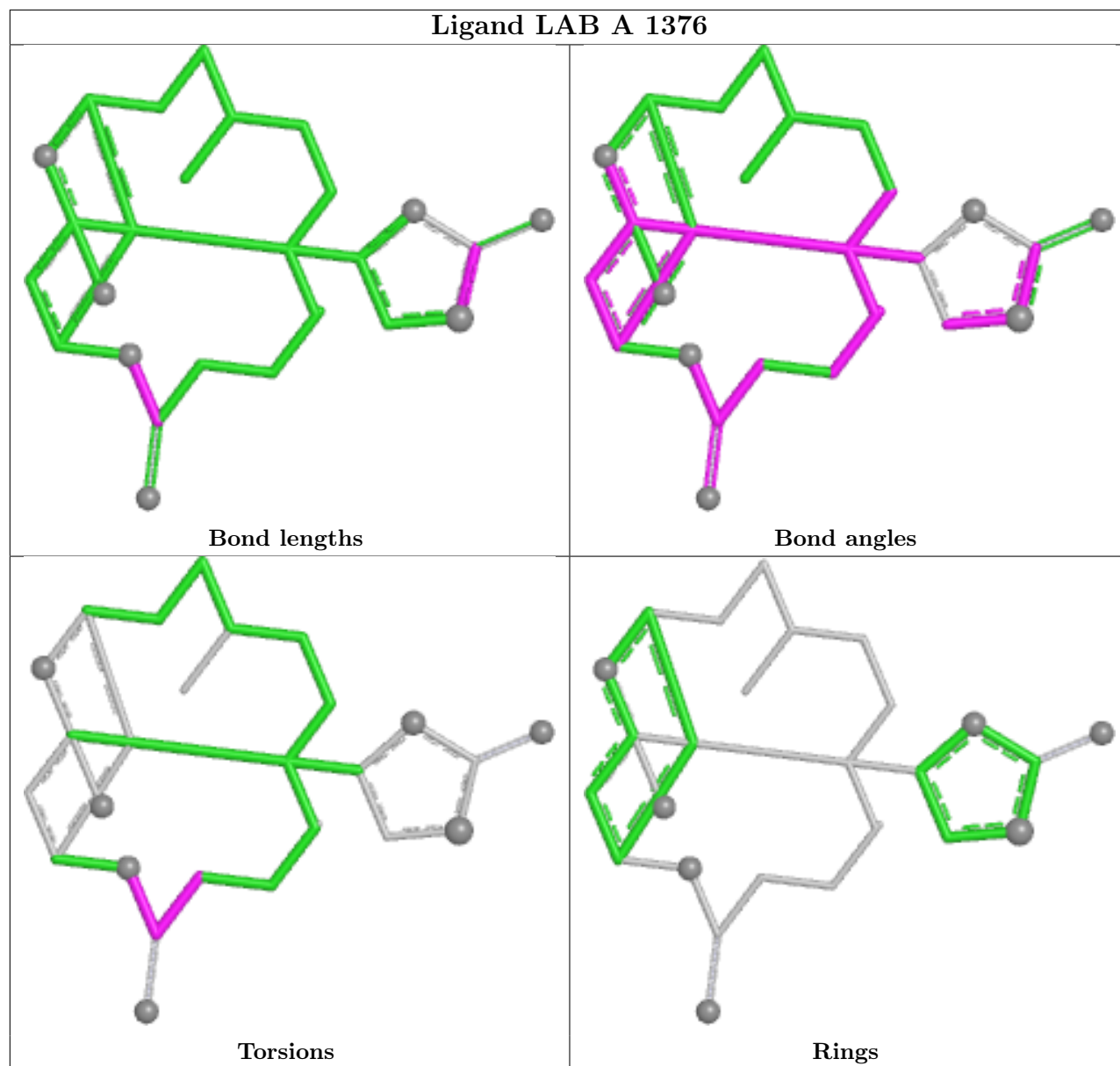
6 monomers are involved in 12 short contacts:

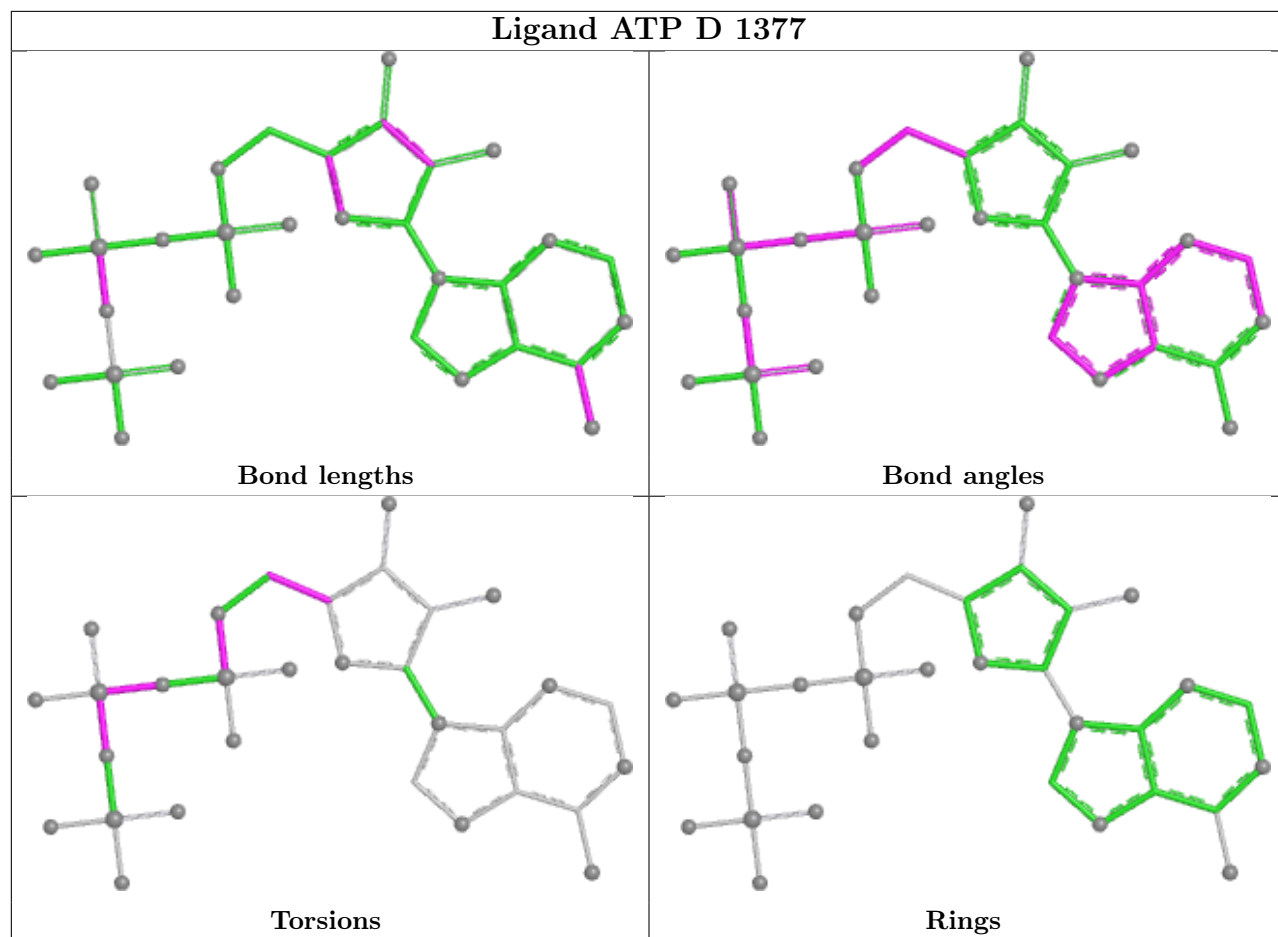
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1377	ATP	1	0
3	A	1376	LAB	4	0
4	D	1377	ATP	1	0
4	B	1377	ATP	1	0
4	E	1377	ATP	1	0
3	C	1376	LAB	4	0

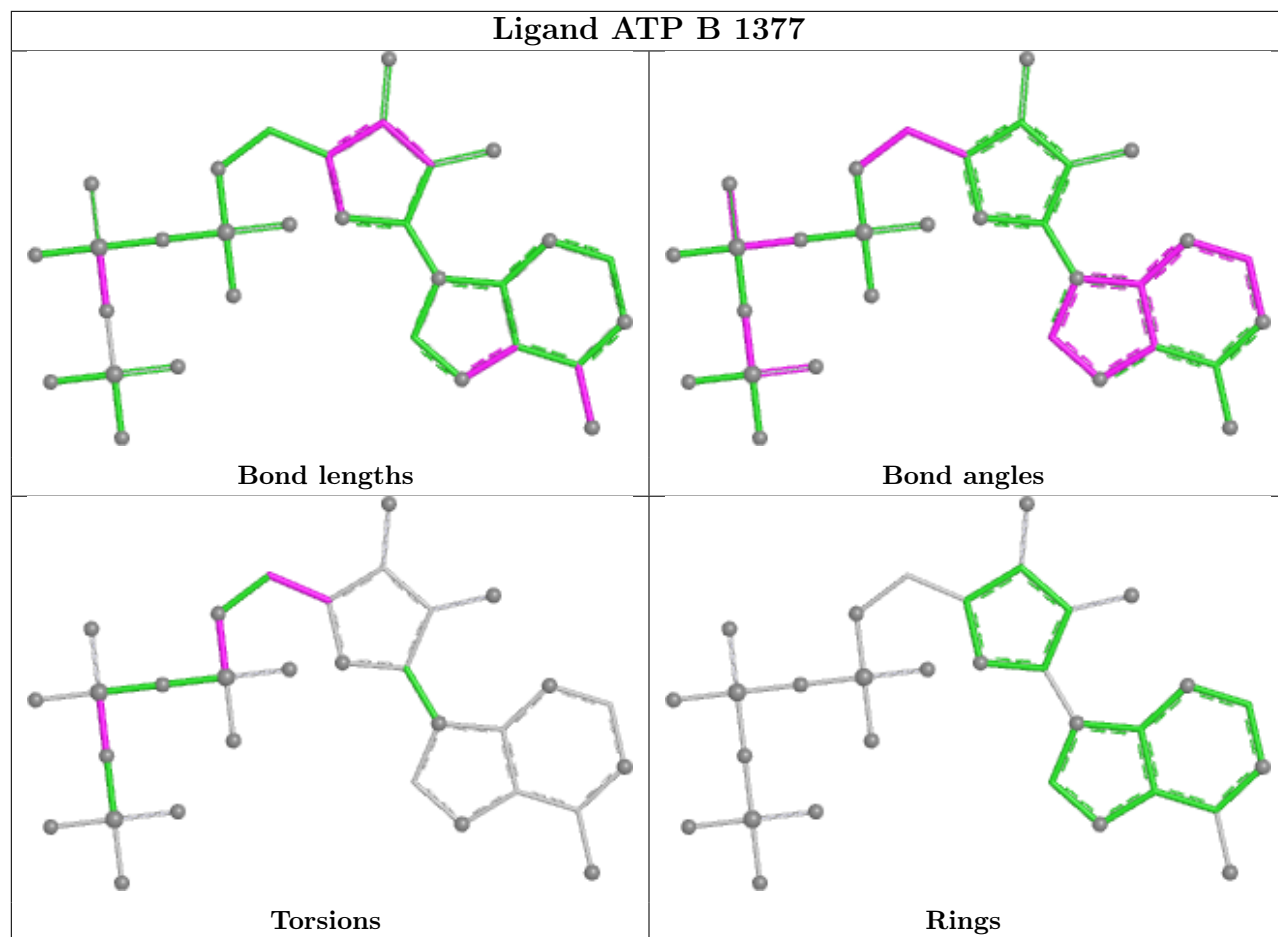
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

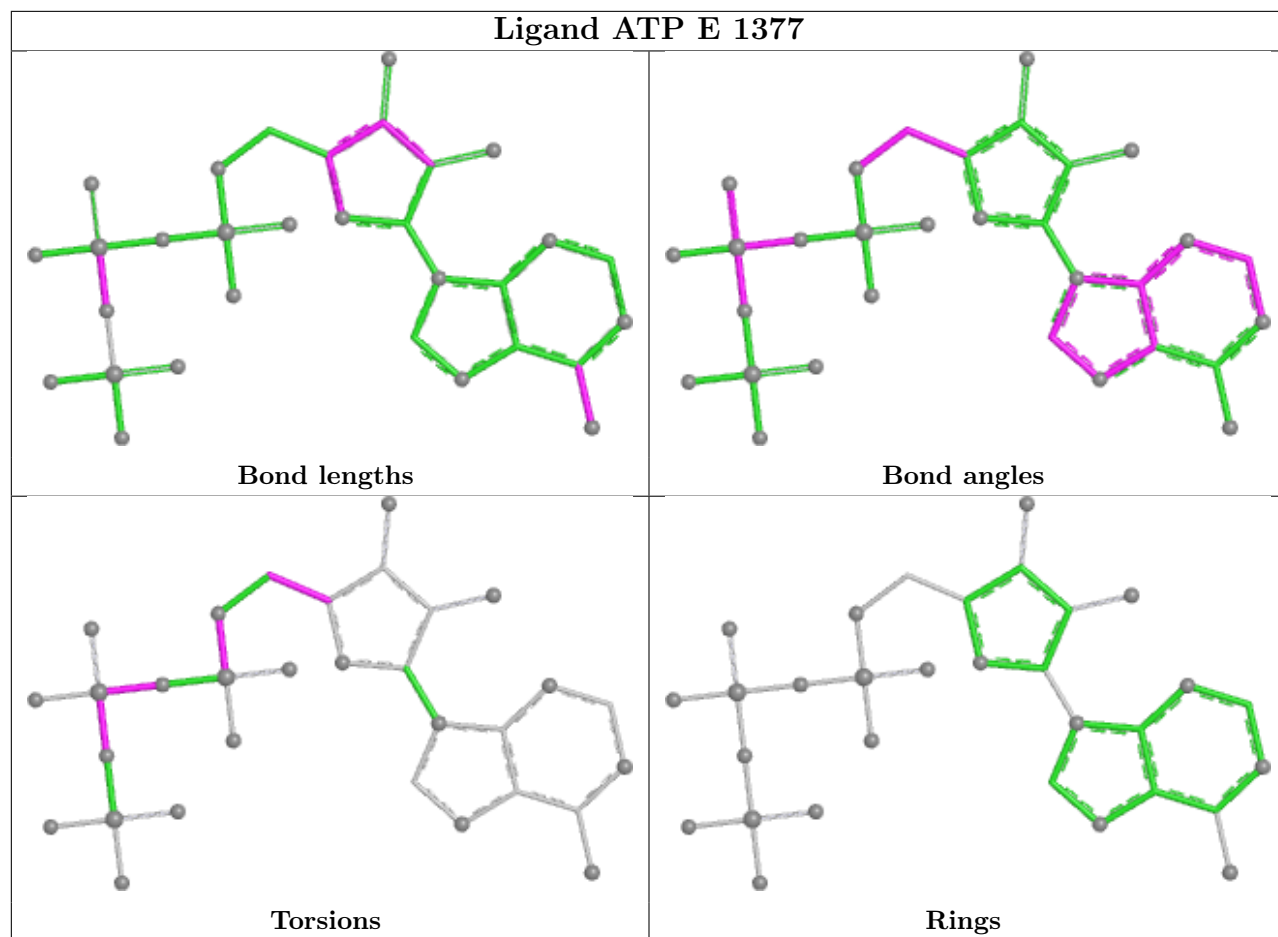
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

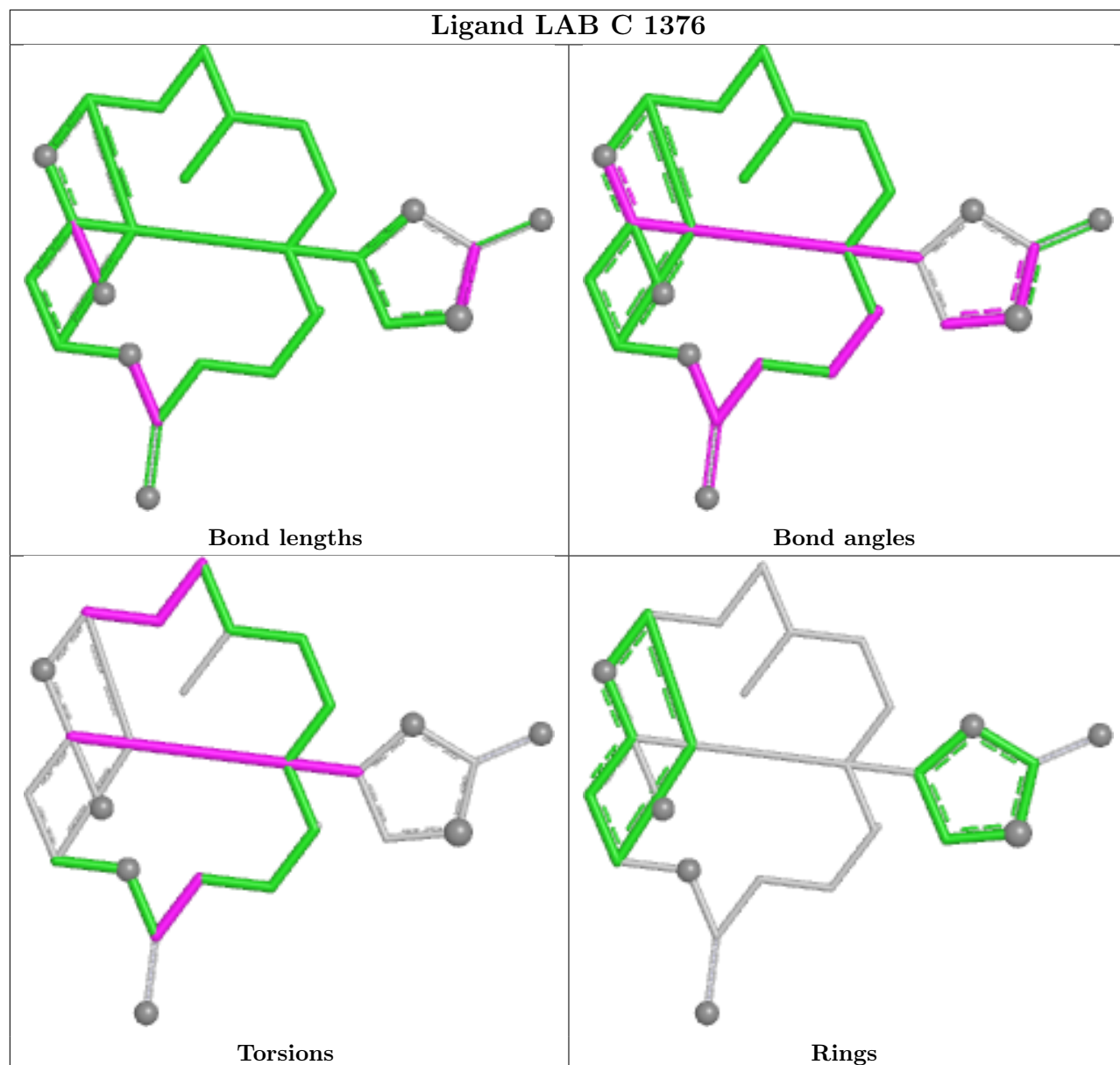


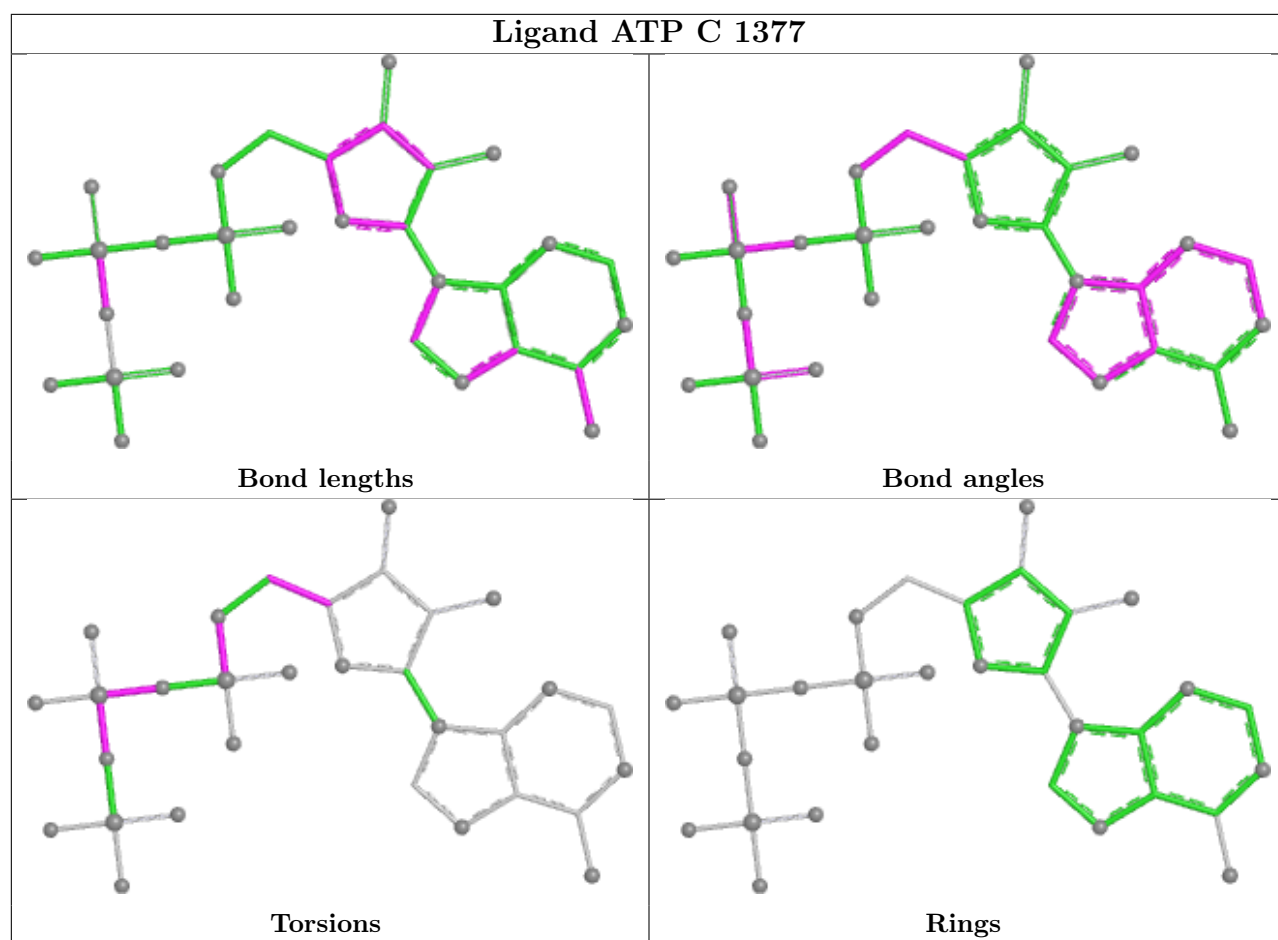












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/377 (93%)	-0.05	8 (2%) 61 37	58, 110, 176, 238	0
1	B	335/377 (88%)	0.02	3 (0%) 81 58	83, 142, 206, 291	0
1	C	343/377 (90%)	0.10	12 (3%) 47 26	61, 116, 197, 268	0
1	D	345/377 (91%)	0.11	5 (1%) 73 48	72, 125, 213, 264	0
1	E	318/377 (84%)	0.71	30 (9%) 14 9	110, 220, 311, 473	0
2	M	121/137 (88%)	-0.20	0 100 100	80, 122, 172, 199	0
All	All	1814/2022 (89%)	0.14	58 (3%) 50 29	58, 134, 249, 473	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	GLY	5.7
1	E	10	CYS	5.7
1	E	261	LEU	4.6
1	E	74	GLY	4.3
1	E	303	THR	4.1
1	E	253	GLU	4.1
1	E	160	THR	4.0
1	E	12	ASN	3.7
1	A	199	SER	3.4
1	C	69	TYR	3.4
1	E	128	ASN	3.4
1	E	155	SER	3.1
1	C	25	ASP	3.1
1	A	130	PRO	2.9
1	E	306	TYR	2.9
1	E	201	VAL	2.8
1	E	192	ILE	2.8
1	B	30	VAL	2.7
1	A	58	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	214	GLU	2.7
1	C	76	ILE	2.6
1	E	173	HIS	2.6
1	E	197	GLY	2.6
1	C	54	VAL	2.6
1	E	109	PRO	2.6
1	E	299	MET	2.6
1	E	186	THR	2.5
1	D	57	GLU	2.5
1	E	170	ALA	2.5
1	E	181	ALA	2.5
1	D	243	PRO	2.5
1	E	17	VAL	2.4
1	A	121	GLN	2.4
1	B	28	ARG	2.4
1	D	249	THR	2.4
1	E	180	LEU	2.3
1	A	62	ARG	2.3
1	D	253	GLU	2.3
1	E	294	TYR	2.3
1	E	252	ASN	2.3
1	C	58	ALA	2.3
1	A	252	ASN	2.2
1	A	237	GLU	2.2
1	B	253	GLU	2.2
1	A	69	TYR	2.2
1	E	175	ILE	2.2
1	C	90	PHE	2.1
1	E	222	ASP	2.1
1	C	8	LEU	2.1
1	C	101	HIS	2.1
1	D	97	ALA	2.1
1	E	325	MET	2.1
1	E	249	THR	2.0
1	E	131	ALA	2.0
1	C	32	PRO	2.0
1	E	263	GLN	2.0
1	C	91	TYR	2.0
1	C	72	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

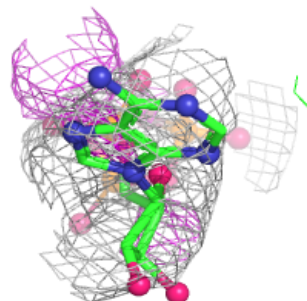
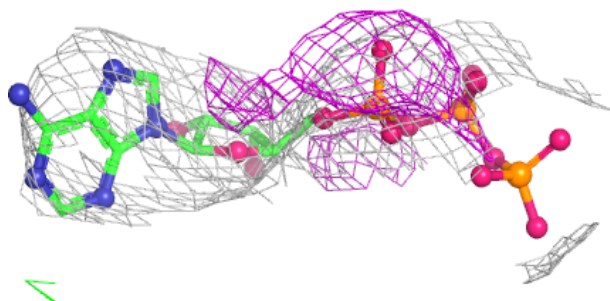
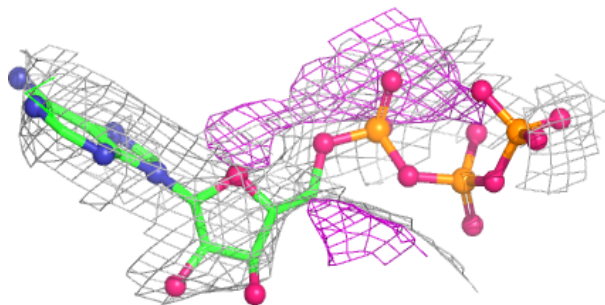
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	E	1377	31/31	0.73	0.14	207,207,207,207	0
5	MG	A	1378	1/1	0.80	0.48	105,105,105,105	0
5	MG	B	1378	1/1	0.83	0.27	105,105,105,105	0
5	MG	C	1378	1/1	0.86	0.26	105,105,105,105	0
3	LAB	A	1376	27/27	0.89	0.23	198,198,198,198	0
5	MG	E	1378	1/1	0.89	0.13	158,158,158,158	0
4	ATP	D	1377	31/31	0.90	0.13	143,143,143,143	0
4	ATP	A	1377	31/31	0.91	0.12	105,105,105,105	0
4	ATP	B	1377	31/31	0.91	0.13	146,146,146,146	0
5	MG	D	1378	1/1	0.92	0.27	105,105,105,105	0
3	LAB	C	1376	27/27	0.93	0.12	117,117,117,117	0
4	ATP	C	1377	31/31	0.94	0.13	105,105,105,105	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

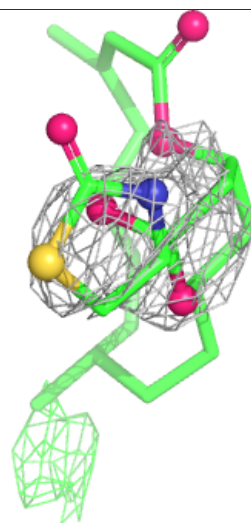
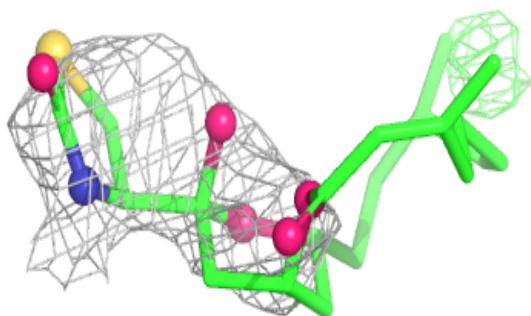
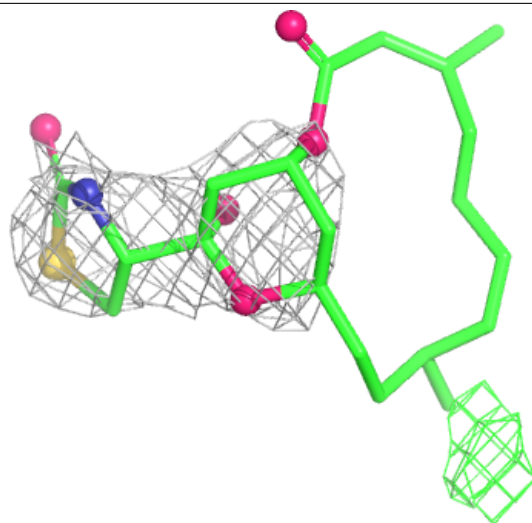
Electron density around ATP E 1377:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



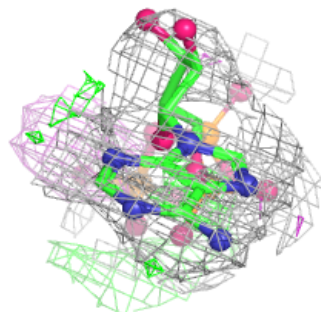
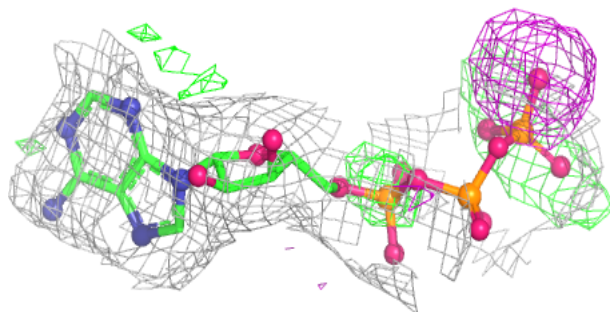
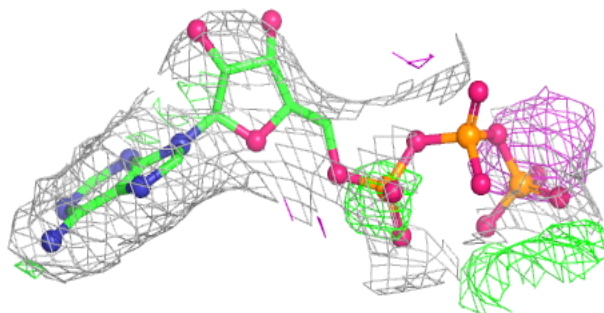
Electron density around LAB A 1376:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

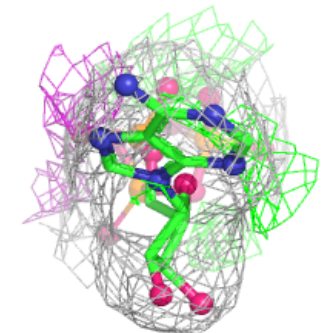
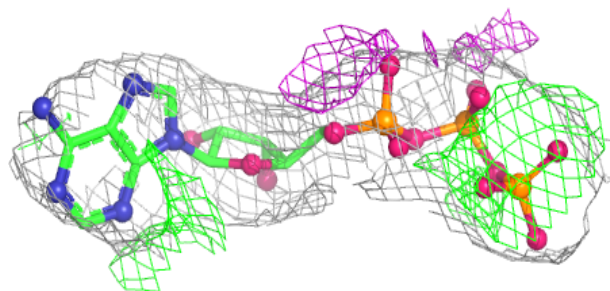
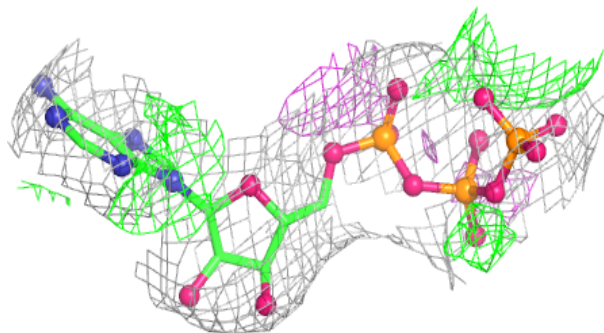


Electron density around ATP D 1377:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

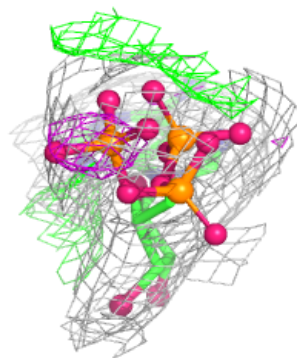
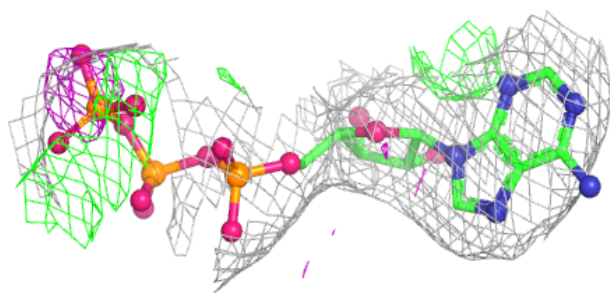
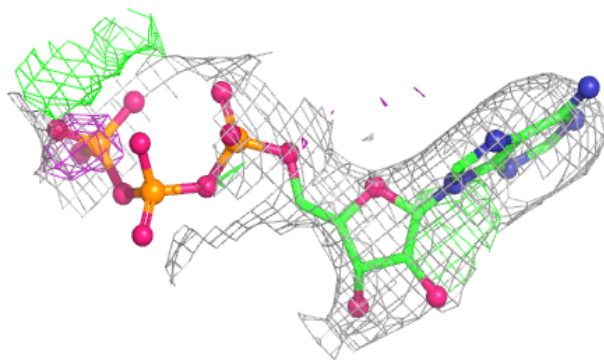
**Electron density around ATP A 1377:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

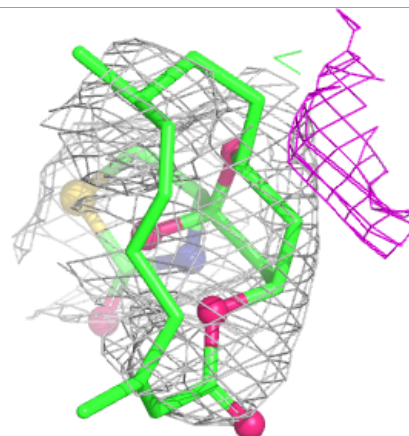
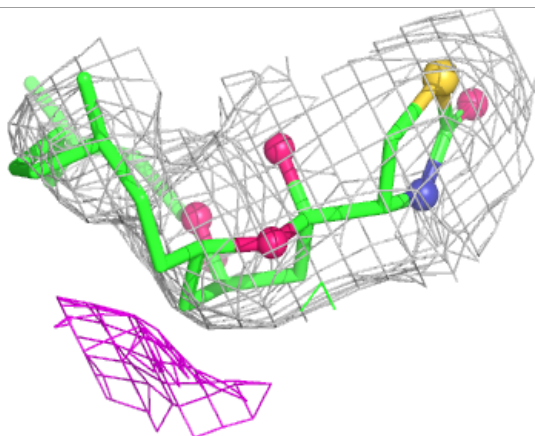
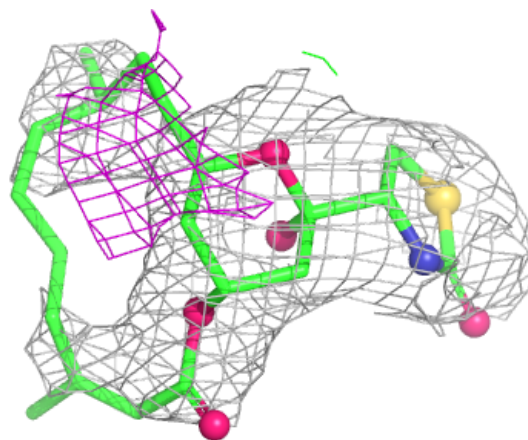


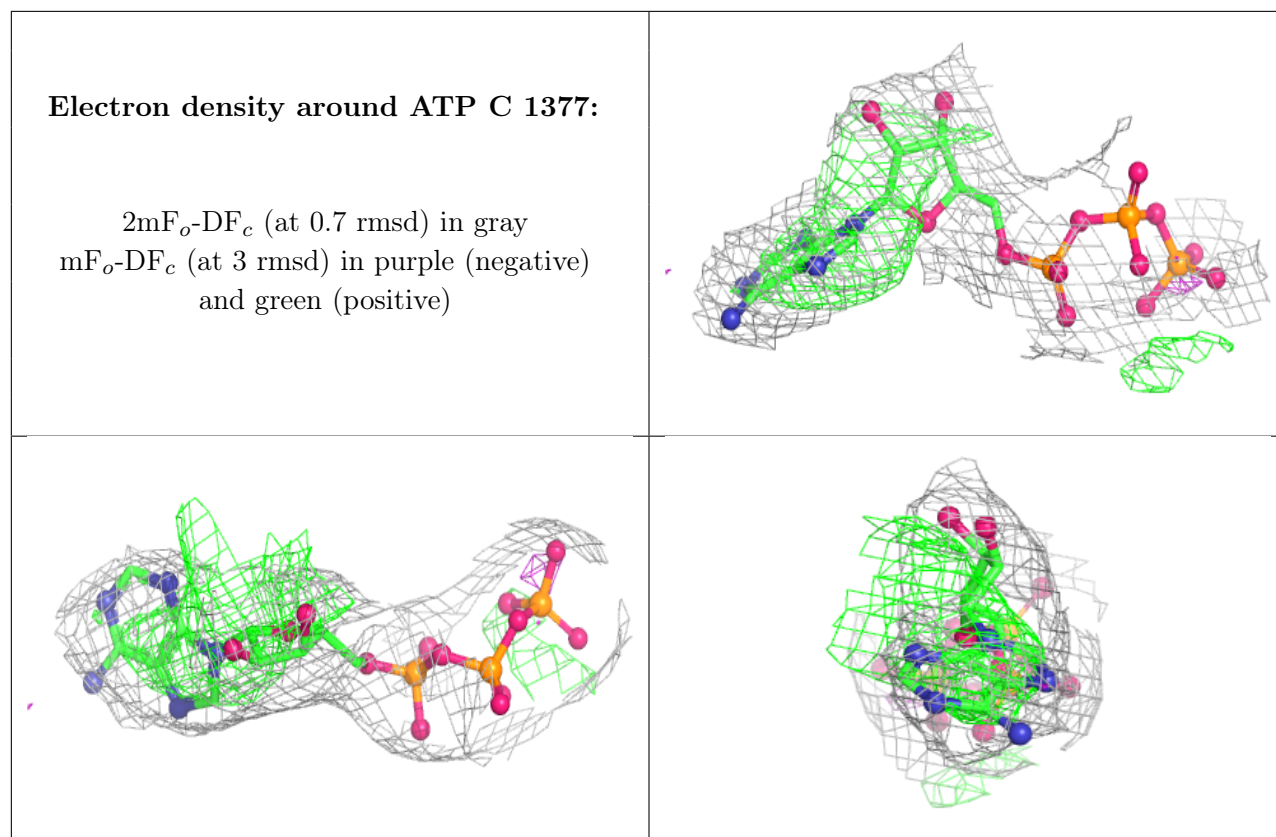
Electron density around ATP B 1377:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LAB C 1376:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.