



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:30 pm BST

PDB ID : 2YJF
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

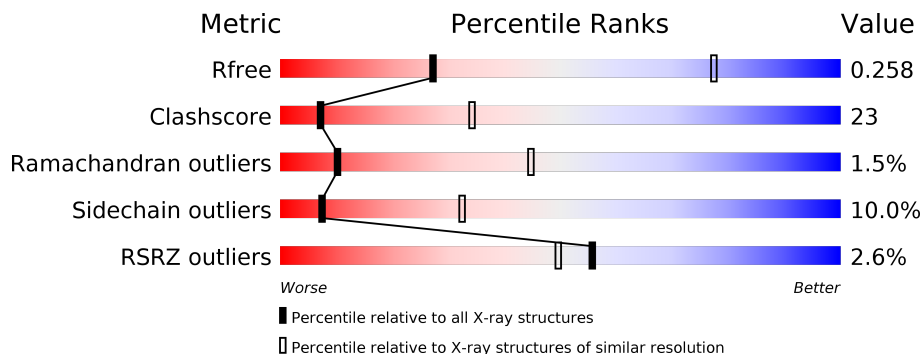
1 Overall quality at a glance i

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	
1	B	377	
1	C	377	
1	D	377	
1	E	377	
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
3	LAB	A	1376	-	-	-	X

2 Entry composition [i](#)

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

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

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

There are 13 discrepancies between the modelled and reference sequences:

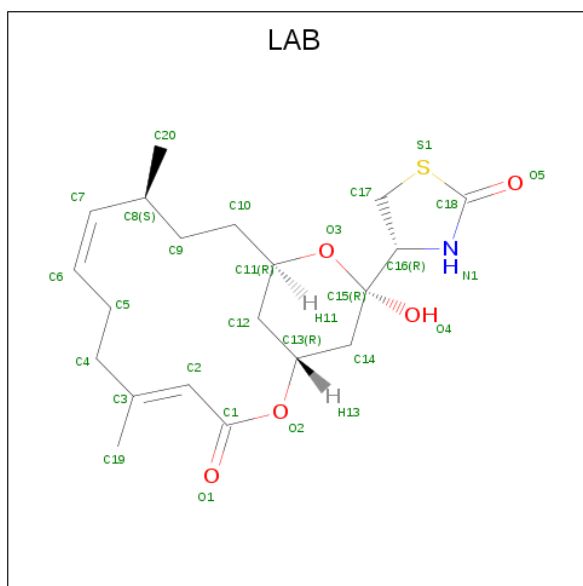
Chain	Residue	Modelled	Actual	Comment	Reference
M	63	ALA	-	expression tag	UNP Q8K4J6
M	64	PRO	-	expression tag	UNP Q8K4J6
M	65	GLY	-	expression tag	UNP Q8K4J6
M	66	SER	-	expression tag	UNP Q8K4J6
M	67	LEU	-	expression tag	UNP Q8K4J6
M	68	SER	-	expression tag	UNP Q8K4J6
M	69	GLU	-	expression tag	UNP Q8K4J6
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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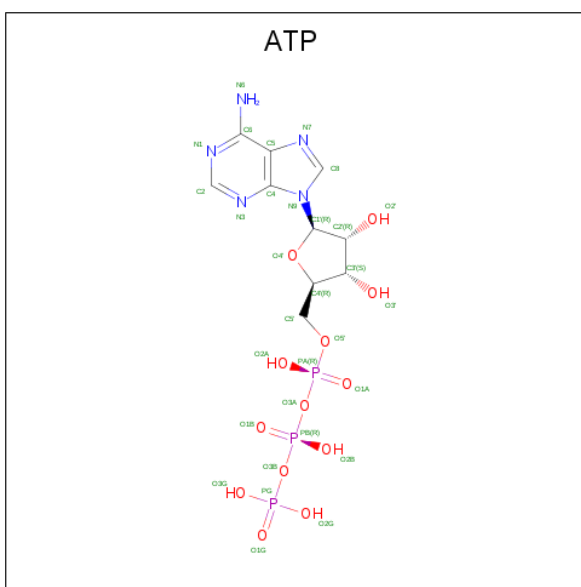
Chain	Residue	Modelled	Actual	Comment	Reference
M	172	ARG	PRO	engineered mutation	UNP Q8K4J6

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



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

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



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

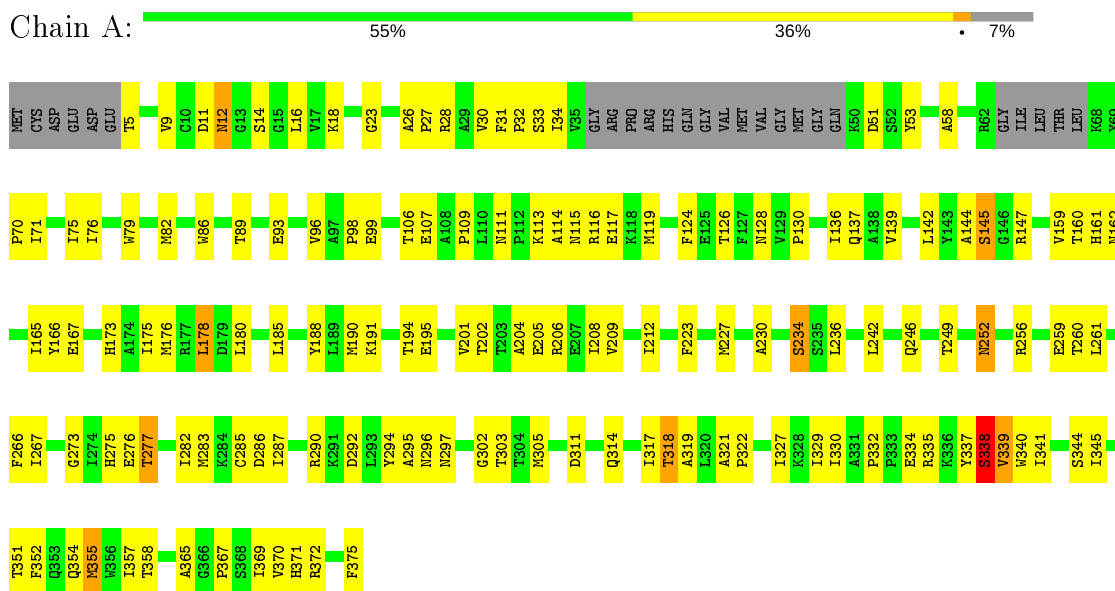
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

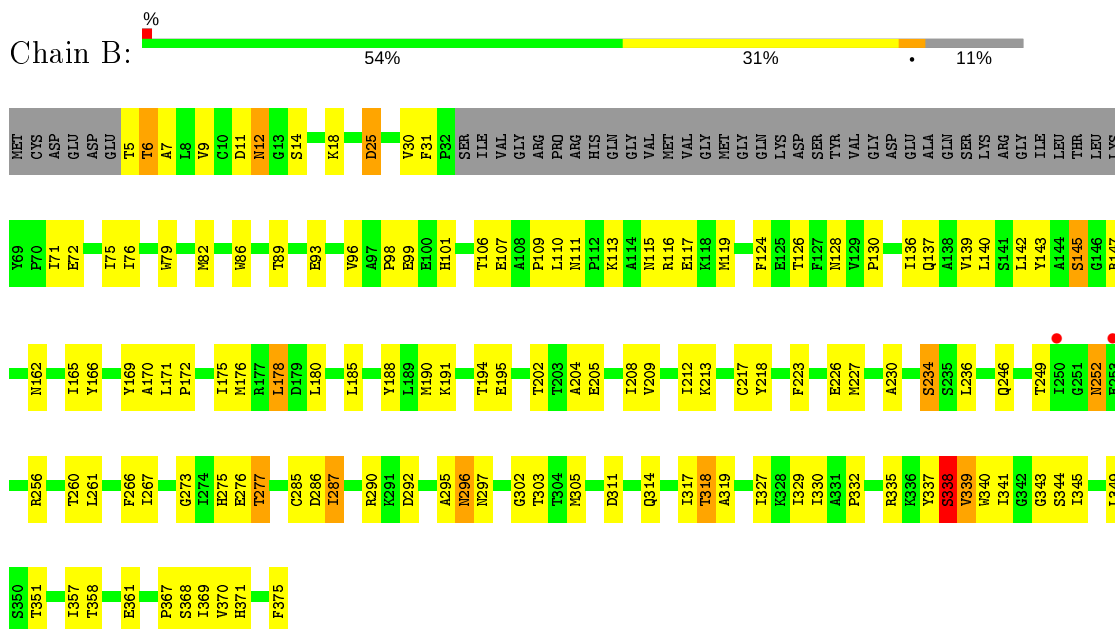
3 Residue-property plots [i](#)

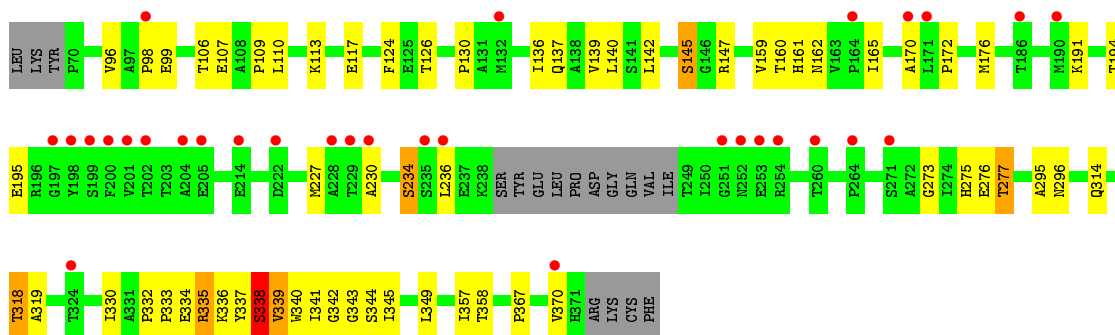
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: ACTIN, ALPHA SKELETAL MUSCLE



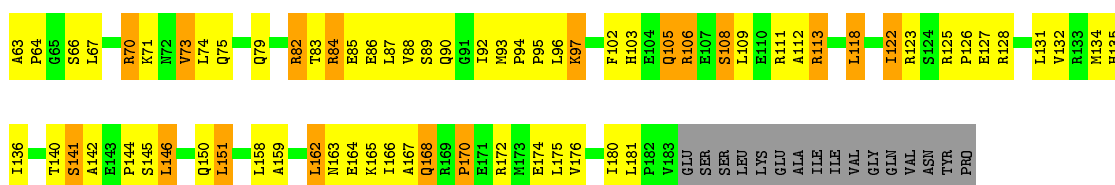
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE





● Molecule 2: MKL/MYOCARDIN-LIKE PROTEIN 1

Chain M: 37% 39% 12% 12%



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) 99.2 (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)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.272 0.232 , 0.258	Depositor DCC
R_{free} test set	2411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 113.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13272	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LAB, ATP

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	0.41	0/2703	0.53	0/3684
1	B	0.35	0/2545	0.50	0/3477
1	C	0.38	0/2583	0.53	0/3523
1	D	0.37	0/2568	0.53	0/3509
1	E	0.28	0/1989	0.47	0/2746
2	M	0.44	0/933	0.68	0/1262
All	All	0.37	0/13321	0.53	0/18201

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2645	0	2492	119	0
1	B	2487	0	2291	105	0
1	C	2531	0	2363	133	0
1	D	2514	0	2292	104	0
1	E	1959	0	1496	56	0
2	M	922	0	899	95	0
3	A	27	0	29	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	569	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 23.

All (569) 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
2:M:84:ARG:HA	2:M:87:LEU:HD12	1.55	0.87
1:C:287:ILE:HA	1:C:290:ARG:HG3	1.57	0.86
1:C:6:THR:HG22	1:C:7:ALA:H	1.38	0.86
2:M:168:GLN:HG2	2:M:168:GLN:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	2:M:106:ARG:HH11	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
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
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:295:ALA:C	1:C:296:ASN:HD22	1.94	0.69
1:C:334:GLU:OE1	1:C:334:GLU:N	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:C:191:LYS:O	1:C:194:THR:HG22	1.96	0.66
1:A:351:THR:OG1	2:M:75:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PHE:HZ	1:B:89:THR:HG1	1.43	0.66
1:A:31:PHE:HZ	1:A:89:THR:HG1	1.43	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: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: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
1:C:349:LEU:HD11	2:M:162:LEU:HB3	1.79	0.64
1:A:365:ALA:HB3	1:A:369:ILE:HD12	1.79	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:A:330:ILE:HG22	1:A:332:PRO:HD3	1.80	0.63
1:A:136:ILE:HD12	1:A:136:ILE:N	2.14	0.63
1:C:145:SER:OG	1:C:147:ARG:HD2	1.99	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:NH1	2:M:106:ARG:HG2	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:A:242:LEU:HD12	1:A:246:GLN:NE2	2.07	0.62
1:D:115:ASN:ND2	1:D:119:MET:HE2	2.15	0.61
2:M:141:SER:CB	2:M:142:ALA:HA	2.29	0.61
1:D:273:GLY:O	1:D:277:THR:HG23	2.00	0.61
1:D:9:VAL:HG12	1:D:340:TRP:CD1	2.35	0.61
1:E:136:ILE:N	1:E:136:ILE:HD12	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:151:LEU:HD13	2:M:151:LEU:C	2.21	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:295:ALA:C	1:A:296:ASN:HD22	2.05	0.60
1:C:352:PHE:C	1:C:354:GLN:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:LYS:O	1:A:194:THR:HG22	2.02	0.60
1:A:12:ASN:ND2	1:A:86:TRP:HE1	1.99	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
2:M:112:ALA:O	2:M:113:ARG:C	2.40	0.59
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
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:E:295:ALA:C	1:E:296:ASN:HD22	2.05	0.59
1:C:136:ILE:N	1:C:136:ILE:HD12	2.16	0.59
1:C:349:LEU:HD13	2:M:163:ASN:HA	1.84	0.59
1:E:191:LYS:O	1:E:194:THR:HG22	2.02	0.59
1:B:205:GLU:O	1:B:209:VAL:HG23	2.02	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: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
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:A:115:ASN:ND2	1:A:119:MET:HE2	2.19	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:107:GLU:O	1:B:137:GLN:HG3	2.05	0.57
1:B:96:VAL:O	1:B:98:PRO:HD3	2.05	0.57
1:C:236:LEU:HD12	1:C:236:LEU:C	2.23	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:171:LEU:HD12	1:B:285:CYS:SG	2.44	0.57
1:B:76:ILE:HD13	1:B:82:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	2:M:168:GLN:O	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:180:LEU:HD21	1:B:260:THR:HG22	1.86	0.57
1:B:9:VAL:HG12	1:B:340:TRP:CD1	2.39	0.57
2:M:88:VAL:HG23	2:M:93:MET:O	2.05	0.57
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: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: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:76:ILE:HG21	1:B:79:TRP:CZ3	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:106:ARG:CG	2:M:106:ARG:NH1	2.66	0.55
1:D:69:TYR:CE2	1:D:183:ARG:NH1	2.75	0.55
1:A:166:TYR:CD1	1:A:167:GLU:HG3	2.42	0.55
1:C:330:ILE:HG22	1:C:332:PRO:HD3	1.89	0.55
1:C:55:GLY:O	1:C:58:ALA:HB3	2.06	0.55
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
2:M:180:ILE:C	2:M:181:LEU:HG	2.28	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:B:115:ASN:ND2	1:B:119:MET:HE2	2.23	0.54
1:E:23:GLY:CA	2:M:142:ALA:HB1	2.24	0.54
2:M:63:ALA:N	2:M:64:PRO:HD2	2.23	0.54
1:A:345:ILE:HD13	2:M:70:ARG:HB3	1.89	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:D:248:ILE:HG12	1:D:249:THR:H	1.74	0.53
2:M:164:GLU:CD	2:M:165:LYS:N	2.62	0.53
1:C:166:TYR:CD1	2:M:175:LEU:HD21	2.43	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: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:107:GLU:O	1:C:137:GLN:HG3	2.09	0.52
1:C:191:LYS:O	1:C:194:THR:CG2	2.56	0.52
1:C:33:SER:O	1:C:70:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:SER:C	1:E:236:LEU:H	2.12	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:335:ARG:C	1:D:337:TYR:N	2.61	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: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:O	1:B:303:THR:HG22	2.10	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: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:234:SER:C	1:A:236:LEU:H	2.13	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:173:HIS:ND1	2:M:94:PRO:CG	2.70	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: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:234:SER:C	1:B:236:LEU:H	2.14	0.51
1:B:297:ASN:HB3	1:B:329:ILE:HD13	1.91	0.51
1:C:349:LEU:HD11	2:M:162:LEU:HD12	1.92	0.51
2:M:170:PRO:HB3	2:M:174:GLU:CD	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:HB3	1:A:329:ILE:HD13	1.93	0.51
1:B:117:GLU:CD	1:B:371:HIS:HE2	2.14	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: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:A:31:PHE:CE1	1:A:93:GLU:HG3	2.47	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: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
2:M:128:ARG:HH12	2:M:140:THR:HG23	1.76	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:O	2:M:151:LEU:HD13	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:335:ARG:C	1:D:337:TYR:H	2.15	0.49
1:E:339:VAL:HG12	1:E:340:TRP:N	2.27	0.49
1:B:166:TYR:HD1	2:M:131:LEU:HD11	1.75	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:115:ASN:ND2	1:C:119:MET:HE3	2.27	0.49
1:C:27:PRO:HA	1:C:340:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:LYS:HZ2	1:D:215:LYS:HB3	1.77	0.49
1:D:317:ILE:HG22	1:D:327:ILE:CD1	2.43	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:C:335:ARG:C	1:C:337:TYR:N	2.66	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: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:D:227:MET:O	1:D:230:ALA:HB3	2.13	0.48
1:E:318:THR:HG22	1:E:319:ALA:N	2.28	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
1:D:318:THR:HG22	1:D:319:ALA:N	2.29	0.48
2:M:86:GLU:O	2:M:89:SER:HB3	2.14	0.48
3:A:1376:LAB:H51	3:A:1376:LAB:H11	1.95	0.48
1:A:53:TYR:O	1:A:58:ALA:HB2	2.14	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:D:215:LYS:NZ	1:D:215:LYS:HB3	2.29	0.48
1:A:352:PHE:HA	1:A:355:MET:CE	2.44	0.47
1:E:341:ILE:O	1:E:345:ILE:HG13	2.14	0.47
1:A:126:THR:O	1:A:126:THR:HG22	2.15	0.47
1:B:208:ILE:O	1:B:212:ILE:HG13	2.15	0.47
1:C:111:ASN:ND2	1:C:115:ASN:HD22	2.08	0.47
1:C:18:LYS:HG3	1:C:30:VAL:CG2	2.32	0.47
1:A:335:ARG:C	1:A:337:TYR:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ILE:O	1:A:212:ILE:HG13	2.14	0.47
1:A:124:PHE:HZ	1:A:357:ILE:O	1.98	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
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:73:VAL:HG22	2:M:74:LEU:N	2.29	0.47
1:C:337:TYR:O	1:C:338:SER:C	2.53	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:99:GLU:H	1:D:99:GLU:CD	2.18	0.47
1:B:9:VAL:HG21	1:B:344:SER:HA	1.97	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
1:A:275:HIS:CG	1:A:276:GLU:N	2.82	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:D:202:THR:CB	1:D:205:GLU:HG3	2.45	0.47
1:E:9:VAL:HG21	1:E:344:SER:HA	1.97	0.47
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:HD12	1:B:330:ILE:N	2.30	0.46
1:D:339:VAL:HG12	1:D:340:TRP:N	2.30	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: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:C:6:THR:HG22	1:C:7:ALA:N	2.17	0.46
1:E:335:ARG:C	1:E:337:TYR:N	2.69	0.46
1:D:159:VAL:HG22	1:D:160:THR:N	2.30	0.46
1:B:335:ARG:C	1:B:337:TYR:N	2.67	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:E:99:GLU:H	1:E:99:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:O	1:A:370:VAL:HG12	2.15	0.46
1:A:99:GLU:CD	1:A:99:GLU:H	2.18	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:HA	2:M:118:LEU:HD12	1.61	0.46
1:C:194:THR:HG23	1:C:195:GLU:N	2.30	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:C:139:VAL:HA	1:C:165:ILE:HD13	1.98	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
1:C:294:TYR:O	1:C:327:ILE:HA	2.16	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
1:A:139:VAL:HG22	1:A:165:ILE:HD13	1.97	0.45
1:A:204:ALA:O	1:A:208:ILE:HG13	2.16	0.45
1:B:178:LEU:HD11	1:B:180:LEU:HB3	1.99	0.45
1:E:275:HIS:CG	1:E:276:GLU:N	2.85	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:126:THR:O	1:E:126:THR:HG22	2.17	0.45
1:E:191:LYS:O	1:E:194:THR:CG2	2.65	0.45
1:D:305:MET:HA	1:D:335:ARG:HH21	1.81	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:334:GLU:OE1	1:D:334:GLU:N	2.50	0.44
1:D:124:PHE:HZ	1:D:357:ILE:O	1.99	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
2:M:151:LEU:CD1	2:M:151:LEU:C	2.85	0.44
1:B:170:ALA:O	1:B:172:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PRO:HB3	1:C:175:ILE:HD13	1.99	0.44
1:B:287:ILE:HD11	1:C:30:VAL:HG21	2.00	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:C:344:SER:O	1:C:345:ILE:C	2.55	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:A:345:ILE:HG23	2:M:71:LYS:HG3	1.99	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
1:B:311:ASP:O	1:B:314:GLN:HB3	2.18	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:E:23:GLY:HA2	2:M:142:ALA:CB	2.25	0.44
1:E:337:TYR:O	1:E:338:SER:C	2.54	0.44
1:C:166:TYR:HD1	2:M:175:LEU:HD21	1.83	0.44
1:A:139:VAL:HA	1:A:165:ILE:HD13	1.99	0.44
1:B:335:ARG:C	1:B:337:TYR:H	2.19	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:B:295:ALA:C	1:B:296:ASN:HD22	2.20	0.44
1:C:341:ILE:O	1:C:344:SER:HB3	2.18	0.44
1:A:194:THR:CG2	1:A:195:GLU:N	2.81	0.43
1:C:230:ALA:HA	1:C:236:LEU:HD23	1.99	0.43
1:C:335:ARG:C	1:C:337:TYR:H	2.20	0.43
1:A:114:ALA:HB2	1:D:28:ARG:CD	2.45	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:355:MET:O	1:C:356:TRP:C	2.56	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
1:D:285:CYS:O	1:D:286:ASP:C	2.55	0.43
2:M:125:ARG:HA	2:M:126:PRO:HD3	1.84	0.43
1:C:334:GLU:HB3	2:M:135:HIS:CD2	2.53	0.43
1:A:23:GLY:O	2:M:67:LEU:HD13	2.19	0.43
2:M:180:ILE:O	2:M:181:LEU:CB	2.66	0.43
1:B:6:THR:O	1:B:101:HIS:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:82:MET:HE3	1:C:86:TRP:CE2	2.53	0.43
1:A:352:PHE:HA	1:A:355:MET:HE3	2.00	0.43
1:B:286:ASP:OD1	1:B:287:ILE:N	2.52	0.43
1:D:139:VAL:HA	1:D:165:ILE:HD13	2.00	0.43
1:B:351:THR:HG21	2:M:122:ILE:HG21	2.01	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
2:M:158:LEU:C	2:M:158:LEU:HD23	2.39	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:A:283:MET:C	1:A:285:CYS:H	2.23	0.42
1:A:82:MET:HE3	1:A:86:TRP:CE2	2.54	0.42
1:D:311:ASP:O	1:D:314:GLN:HB3	2.19	0.42
2:M:127:GLU:O	2:M:128:ARG:C	2.58	0.42
1:A:9:VAL:HG21	1:A:344:SER:HA	2.00	0.42
1:C:159:VAL:HG22	1:C:160:THR:N	2.34	0.42
1:D:338:SER:O	1:D:339:VAL:C	2.57	0.42
2:M:162:LEU:HD13	2:M:166:ILE:CG2	2.50	0.42
1:C:351:THR:HG21	2:M:167:ALA:HA	2.00	0.42
2:M:88:VAL:HG21	2:M:95:PRO:HA	2.00	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:A:317:ILE:HG22	1:A:327:ILE:CD1	2.46	0.42
1:D:337:TYR:O	1:D:338:SER:C	2.57	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:338:SER:O	1:C:339:VAL:C	2.58	0.42
1:E:159:VAL:HG21	1:E:161:HIS:CE1	2.54	0.42
1:E:335:ARG:C	1:E:337:TYR:H	2.22	0.42
1:A:335:ARG:C	1:A:337:TYR:H	2.22	0.42
1:D:140:LEU:HD22	1:D:343:GLY:HA2	2.02	0.42
1:A:145:SER:HG	1:A:147:ARG:HD2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LYS:O	1:C:340:TRP:CD1	2.73	0.42
1:C:9:VAL:HG12	1:C:340:TRP:NE1	2.33	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
1:A:261:LEU:HD11	1:A:303:THR:HG22	2.03	0.41
1:B:337:TYR:O	1:B:338:SER:C	2.58	0.41
1:C:238:LYS:HD2	1:C:238:LYS:HA	1.63	0.41
1:D:178:LEU:CD1	1:D:180:LEU:HB3	2.50	0.41
1:D:66:THR:HG22	1:D:66:THR:O	2.19	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:A:188:TYR:CD1	1:A:267:ILE:HG22	2.55	0.41
1:A:117:GLU:CG	1:A:371:HIS:HE2	2.32	0.41
1:B:292:ASP:O	1:B:296:ASN:HB2	2.19	0.41
1:D:295:ALA:C	1:D:296:ASN:HD22	2.23	0.41
1:D:374:CYS:O	1:D:375:PHE:OXT	2.39	0.41
2:M:74:LEU:HA	2:M:74:LEU:HD12	1.93	0.41
1:A:234:SER:O	1:A:236:LEU:N	2.54	0.41
1:D:215:LYS:CB	1:D:215:LYS:NZ	2.84	0.41
1:D:215:LYS:HZ3	1:D:215:LYS:HA	1.85	0.41
1:E:159:VAL:HG22	1:E:160:THR:N	2.35	0.41
1:A:145:SER:HG	1:A:147:ARG:HH11	1.67	0.41
1:B:111:ASN:ND2	1:B:115:ASN:HD22	2.12	0.41
1:A:109:PRO:HB3	1:A:175:ILE:HD13	2.03	0.41
1:C:178:LEU:CD1	1:C:180:LEU:HB3	2.51	0.41
1:C:15:GLY:HA2	1:C:33:SER:HB2	2.03	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:E:338:SER:O	1:E:339:VAL:C	2.59	0.41
1:B:202:THR:HB	1:B:205:GLU:HG3	2.03	0.41
1:A:117:GLU:OE1	1:A:367:PRO:HB2	2.20	0.41
1:C:321:ALA:HB1	1:C:322:PRO:HD2	2.03	0.41
1:A:302:GLY:O	1:A:305:MET:HG2	2.21	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:D:159:VAL:HG21	1:D:161:HIS:CE1	2.56	0.41
1:D:151:ILE:HB	1:D:293:LEU:HD22	2.02	0.41
1:A:338:SER:O	1:A:339:VAL:C	2.59	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: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:338:SER:O	1:B:339:VAL:C	2.58	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:HD12	1:A:330:ILE:N	2.37	0.40
1:A:337:TYR:O	1:A:338:SER:C	2.59	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:234:SER:O	1:E:236:LEU:N	2.55	0.40
2:M:67:LEU:O	2:M:67:LEU:HD23	2.20	0.40
1:B:178:LEU:CD1	1:B:180:LEU:HB3	2.51	0.40
1:E:136:ILE:H	1:E:136:ILE:HD12	1.86	0.40
1:E:342:GLY:O	1:E:343:GLY:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/377 (92%)	304 (88%)	39 (11%)	3 (1%)	17	56
1	B	331/377 (88%)	287 (87%)	41 (12%)	3 (1%)	17	56
1	C	337/377 (89%)	287 (85%)	41 (12%)	9 (3%)	5	33
1	D	337/377 (89%)	291 (86%)	42 (12%)	4 (1%)	13	50
1	E	312/377 (83%)	270 (86%)	37 (12%)	5 (2%)	9	43
2	M	119/137 (87%)	98 (82%)	18 (15%)	3 (2%)	5	34
All	All	1782/2022 (88%)	1537 (86%)	218 (12%)	27 (2%)	10	45

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 [i](#)

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%)	242 (91%)	24 (9%)	9 37
1	B	247/320 (77%)	225 (91%)	22 (9%)	9 37
1	C	252/320 (79%)	227 (90%)	25 (10%)	8 33
1	D	242/320 (76%)	218 (90%)	24 (10%)	8 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	128/320 (40%)	120 (94%)	8 (6%)	18	51
2	M	90/123 (73%)	71 (79%)	19 (21%)	1	5
All	All	1225/1723 (71%)	1103 (90%)	122 (10%)	7	32

All (122) 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	51	ASP
1	A	71	ILE
1	A	75	ILE
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	249	THR
1	A	252	ASN
1	A	277	THR
1	A	292	ASP
1	A	318	THR
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	25	ASP
1	B	71	ILE
1	B	72	GLU
1	B	75	ILE
1	B	128	ASN
1	B	145	SER

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Mol	Chain	Res	Type
1	B	178	LEU
1	B	185	LEU
1	B	246	GLN
1	B	249	THR
1	B	252	ASN
1	B	277	THR
1	B	287	ILE
1	B	296	ASN
1	B	318	THR
1	B	338	SER
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	191	LYS
1	C	196	ARG
1	C	206	ARG
1	C	229	THR
1	C	236	LEU
1	C	238	LYS
1	C	248	ILE
1	C	249	THR
1	C	252	ASN
1	C	270	GLU
1	C	277	THR
1	C	287	ILE
1	C	296	ASN
1	C	318	THR
1	C	338	SER
1	C	351	THR
1	C	354	GLN
1	C	358	THR
1	D	5	THR
1	D	6	THR
1	D	12	ASN
1	D	14	SER
1	D	24	ASP

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Mol	Chain	Res	Type
1	D	25	ASP
1	D	28	ARG
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	145	SER
1	D	178	LEU
1	D	185	LEU
1	D	229	THR
1	D	248	ILE
1	D	277	THR
1	D	318	THR
1	D	338	SER
1	D	355	MET
1	D	358	THR
1	D	374	CYS
1	E	6	THR
1	E	12	ASN
1	E	14	SER
1	E	145	SER
1	E	277	THR
1	E	318	THR
1	E	338	SER
1	E	358	THR
2	M	66	SER
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

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Mol	Chain	Res	Type
2	M	146	LEU
2	M	151	LEU
2	M	162	LEU
2	M	168	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	115	ASN
1	A	161	HIS
1	A	246	GLN
1	A	252	ASN
1	A	296	ASN
1	B	12	ASN
1	B	115	ASN
1	B	161	HIS
1	B	246	GLN
1	B	252	ASN
1	C	12	ASN
1	C	115	ASN
1	C	161	HIS
1	C	246	GLN
1	C	252	ASN
1	C	296	ASN
1	C	371	HIS
1	D	12	ASN
1	D	115	ASN
1	D	161	HIS
1	E	161	HIS
2	M	72	ASN
2	M	79	GLN
2	M	150	GLN

5.3.3 RNA

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 carbohydrates 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	B	1377	5	26,33,33	1.71	5 (19%)	31,52,52	1.74	7 (22%)
4	ATP	C	1377	5	26,33,33	1.84	6 (23%)	31,52,52	1.78	8 (25%)
4	ATP	A	1377	5	26,33,33	1.75	5 (19%)	31,52,52	1.79	6 (19%)
4	ATP	E	1377	5	26,33,33	1.76	5 (19%)	31,52,52	1.66	6 (19%)
3	LAB	C	1376	-	28,29,29	1.64	4 (14%)	30,41,41	2.16	5 (16%)
3	LAB	A	1376	-	28,29,29	1.59	3 (10%)	30,41,41	2.42	9 (30%)
4	ATP	D	1377	5	26,33,33	1.72	4 (15%)	31,52,52	1.69	7 (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	B	1377	5	-	5/18/38/38	0/3/3/3
4	ATP	C	1377	5	-	6/18/38/38	0/3/3/3
4	ATP	A	1377	5	-	6/18/38/38	0/3/3/3
4	ATP	E	1377	5	-	6/18/38/38	0/3/3/3
3	LAB	C	1376	-	-	6/21/49/49	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LAB	A	1376	-	-	4/21/49/49	0/2/3/3
4	ATP	D	1377	5	-	5/18/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1376	LAB	O2-C1	5.48	1.45	1.34
3	A	1376	LAB	O2-C1	5.39	1.45	1.34
3	C	1376	LAB	C18-S1	-5.21	1.66	1.77
3	A	1376	LAB	C18-S1	-5.14	1.66	1.77
4	E	1377	ATP	C2'-C3'	-4.98	1.39	1.53
4	D	1377	ATP	C2'-C3'	-4.89	1.40	1.53
4	C	1377	ATP	C2'-C3'	-4.85	1.40	1.53
4	B	1377	ATP	C2'-C3'	-4.81	1.40	1.53
4	A	1377	ATP	C2'-C3'	-4.80	1.40	1.53
4	C	1377	ATP	C2'-C1'	-4.17	1.47	1.53
4	E	1377	ATP	C2'-C1'	-4.13	1.47	1.53
4	B	1377	ATP	C2'-C1'	-4.11	1.47	1.53
4	D	1377	ATP	C2'-C1'	-4.09	1.47	1.53
4	A	1377	ATP	C2'-C1'	-3.87	1.47	1.53
4	A	1377	ATP	O4'-C4'	-2.84	1.38	1.45
4	C	1377	ATP	O4'-C1'	-2.83	1.37	1.41
4	D	1377	ATP	O4'-C4'	-2.82	1.38	1.45
4	E	1377	ATP	O4'-C4'	-2.75	1.38	1.45
4	C	1377	ATP	O4'-C4'	-2.72	1.38	1.45
4	B	1377	ATP	O4'-C4'	-2.72	1.38	1.45
4	E	1377	ATP	C6-N6	2.45	1.43	1.34
3	C	1376	LAB	O4-C15	2.45	1.44	1.40
4	D	1377	ATP	C6-N6	2.41	1.42	1.34
4	B	1377	ATP	C6-N6	2.41	1.42	1.34
4	C	1377	ATP	C3'-C4'	-2.39	1.46	1.53
4	A	1377	ATP	C3'-C4'	-2.32	1.47	1.53
4	A	1377	ATP	C6-N6	2.30	1.42	1.34
4	E	1377	ATP	C3'-C4'	-2.20	1.47	1.53
4	C	1377	ATP	C6-N6	2.18	1.42	1.34
3	A	1376	LAB	C17-S1	-2.05	1.76	1.81
4	B	1377	ATP	C3'-C4'	-2.02	1.47	1.53
3	C	1376	LAB	C17-S1	-2.01	1.77	1.81

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1376	LAB	C17-S1-C18	8.98	96.82	92.00
3	A	1376	LAB	C17-S1-C18	8.80	96.72	92.00
4	A	1377	ATP	PB-O3B-PG	-5.54	113.82	132.83
3	A	1376	LAB	O3-C15-C16	5.04	110.71	104.25
4	D	1377	ATP	PB-O3B-PG	-4.84	116.21	132.83
4	C	1377	ATP	PB-O3B-PG	-4.81	116.32	132.83
4	B	1377	ATP	PB-O3B-PG	-4.76	116.48	132.83
3	A	1376	LAB	O2-C1-C2	4.35	121.49	111.27
4	E	1377	ATP	PB-O3B-PG	-4.35	117.90	132.83
4	C	1377	ATP	PA-O3A-PB	-4.12	118.70	132.83
4	B	1377	ATP	N3-C2-N1	-4.06	122.33	128.68
4	B	1377	ATP	PA-O3A-PB	-4.00	119.08	132.83
4	E	1377	ATP	PA-O3A-PB	-3.82	119.73	132.83
4	E	1377	ATP	N3-C2-N1	-3.76	122.81	128.68
4	D	1377	ATP	PA-O3A-PB	-3.75	119.96	132.83
3	C	1376	LAB	O3-C15-C16	3.73	109.03	104.25
4	D	1377	ATP	N3-C2-N1	-3.68	122.92	128.68
4	A	1377	ATP	PA-O3A-PB	-3.63	120.37	132.83
4	A	1377	ATP	N3-C2-N1	-3.52	123.17	128.68
4	C	1377	ATP	N3-C2-N1	-3.25	123.59	128.68
4	C	1377	ATP	C4-C5-N7	-3.16	106.10	109.40
4	C	1377	ATP	O5'-C5'-C4'	3.11	119.68	108.99
3	A	1376	LAB	O2-C1-O1	-3.10	118.30	123.35
3	C	1376	LAB	O2-C1-C2	3.09	118.52	111.27
4	B	1377	ATP	O5'-C5'-C4'	3.08	119.61	108.99
4	A	1377	ATP	O3G-PG-O3B	2.88	114.29	104.64
4	D	1377	ATP	O5'-C5'-C4'	2.87	118.85	108.99
4	E	1377	ATP	O5'-C5'-C4'	2.75	118.44	108.99
4	A	1377	ATP	C4-C5-N7	-2.70	106.59	109.40
3	A	1376	LAB	C12-C13-C14	-2.69	105.09	111.00
4	C	1377	ATP	C3'-C2'-C1'	2.63	104.94	100.98
3	A	1376	LAB	C14-C15-C16	-2.57	108.74	113.75
4	C	1377	ATP	O3G-PG-O3B	2.47	112.93	104.64
4	D	1377	ATP	C4-C5-N7	-2.46	106.83	109.40
4	C	1377	ATP	O4'-C1'-C2'	-2.44	103.36	106.93
4	E	1377	ATP	C4-C5-N7	-2.42	106.88	109.40
4	A	1377	ATP	O5'-C5'-C4'	2.41	117.30	108.99
3	A	1376	LAB	O1-C1-C2	-2.40	120.18	126.23
4	B	1377	ATP	C3'-C2'-C1'	2.38	104.56	100.98
4	B	1377	ATP	O3G-PG-O3B	2.30	112.36	104.64
4	E	1377	ATP	C3'-C2'-C1'	2.25	104.37	100.98
3	C	1376	LAB	C19-C3-C4	2.23	119.02	115.27
3	A	1376	LAB	C4-C5-C6	-2.15	107.94	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1377	ATP	C4-C5-N7	-2.13	107.18	109.40
4	D	1377	ATP	O3G-PG-O3B	2.13	111.77	104.64
3	A	1376	LAB	C19-C3-C4	2.11	118.83	115.27
4	D	1377	ATP	C3'-C2'-C1'	2.06	104.08	100.98
3	C	1376	LAB	O1-C1-C2	-2.06	121.04	126.23

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C	1377	ATP	C5'-O5'-PA-O3A
4	A	1377	ATP	C5'-O5'-PA-O1A
4	A	1377	ATP	C5'-O5'-PA-O3A
4	E	1377	ATP	C5'-O5'-PA-O1A
4	E	1377	ATP	C5'-O5'-PA-O3A
3	C	1376	LAB	O3-C15-C16-C17
4	D	1377	ATP	C5'-O5'-PA-O1A
4	D	1377	ATP	C5'-O5'-PA-O3A
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	B	1377	ATP	C3'-C4'-C5'-O5'
4	A	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	B	1377	ATP	O4'-C4'-C5'-O5'
4	A	1377	ATP	O4'-C4'-C5'-O5'
4	D	1377	ATP	O4'-C4'-C5'-O5'
3	C	1376	LAB	C9-C10-C11-C12
3	C	1376	LAB	O2-C1-C2-C3
3	A	1376	LAB	O2-C1-C2-C3
3	A	1376	LAB	C2-C1-O2-C13
3	C	1376	LAB	O1-C1-C2-C3
3	A	1376	LAB	O1-C1-C2-C3
3	C	1376	LAB	C11-C10-C9-C8
4	B	1377	ATP	PG-O3B-PB-O2B
4	C	1377	ATP	PG-O3B-PB-O2B

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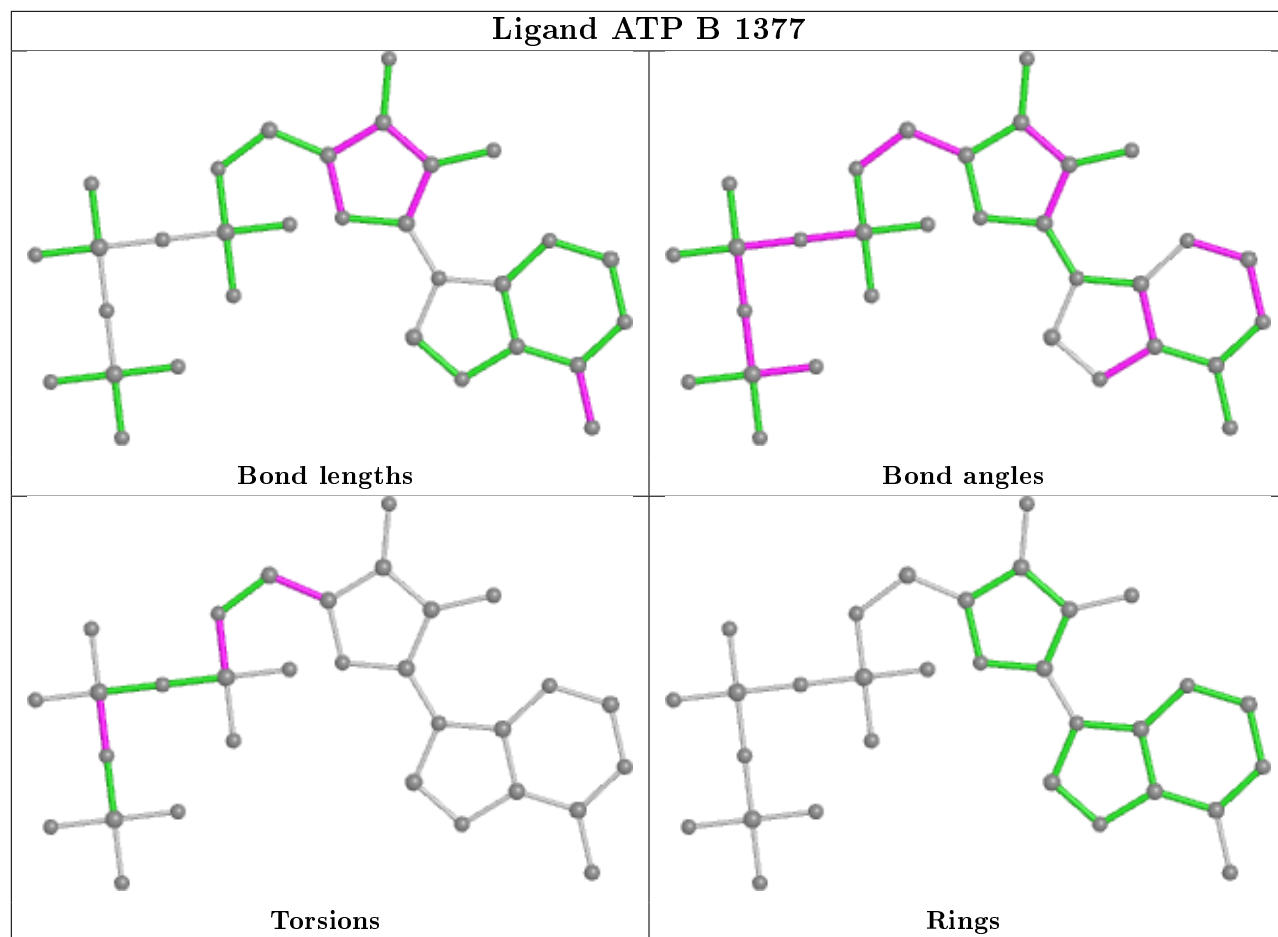
Mol	Chain	Res	Type	Atoms
4	A	1377	ATP	PG-O3B-PB-O2B
4	A	1377	ATP	PA-O3A-PB-O1B
4	E	1377	ATP	PG-O3B-PB-O2B
4	E	1377	ATP	PA-O3A-PB-O1B
4	D	1377	ATP	PG-O3B-PB-O2B
4	C	1377	ATP	C5'-O5'-PA-O2A

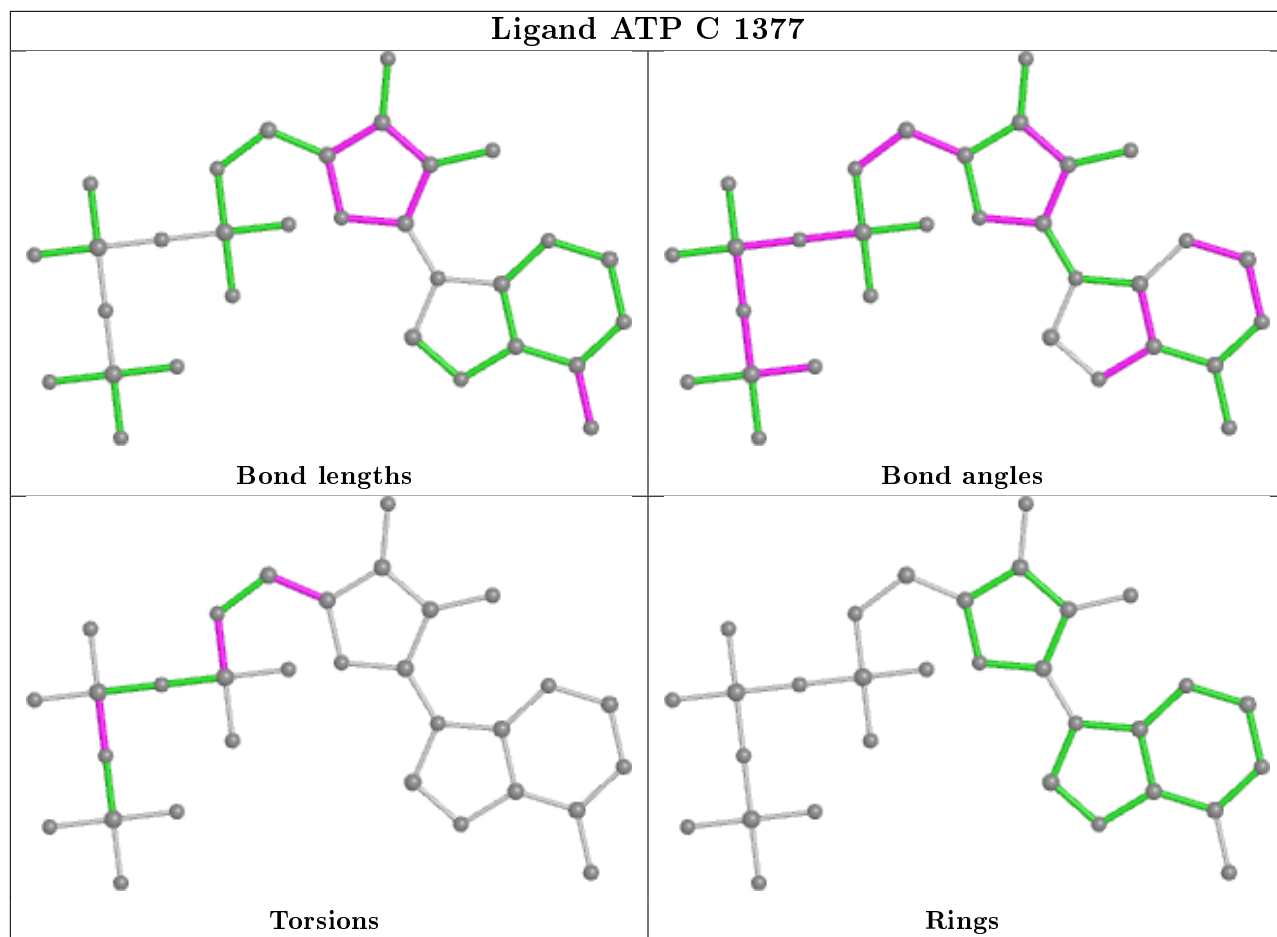
There are no ring outliers.

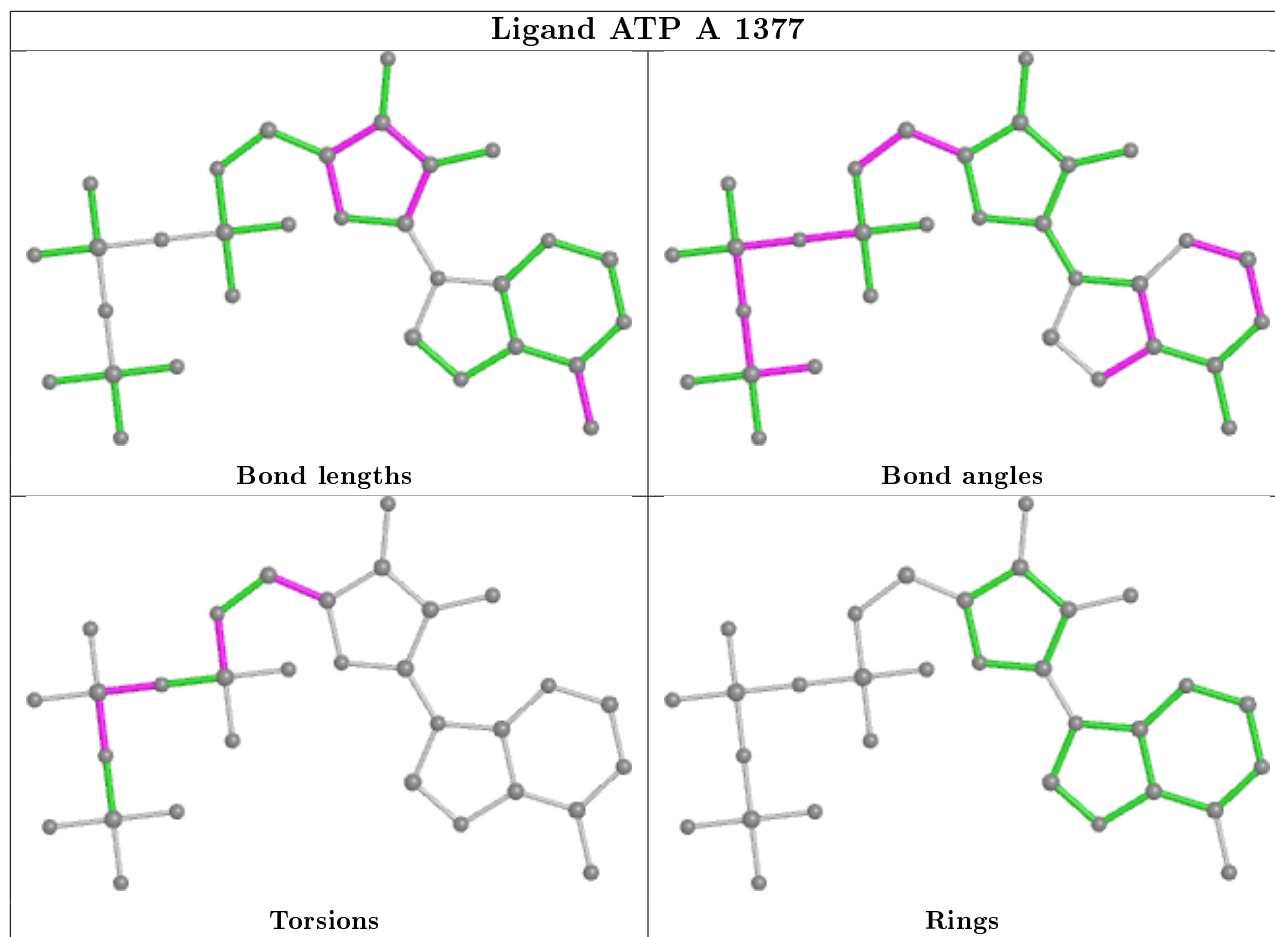
6 monomers are involved in 12 short contacts:

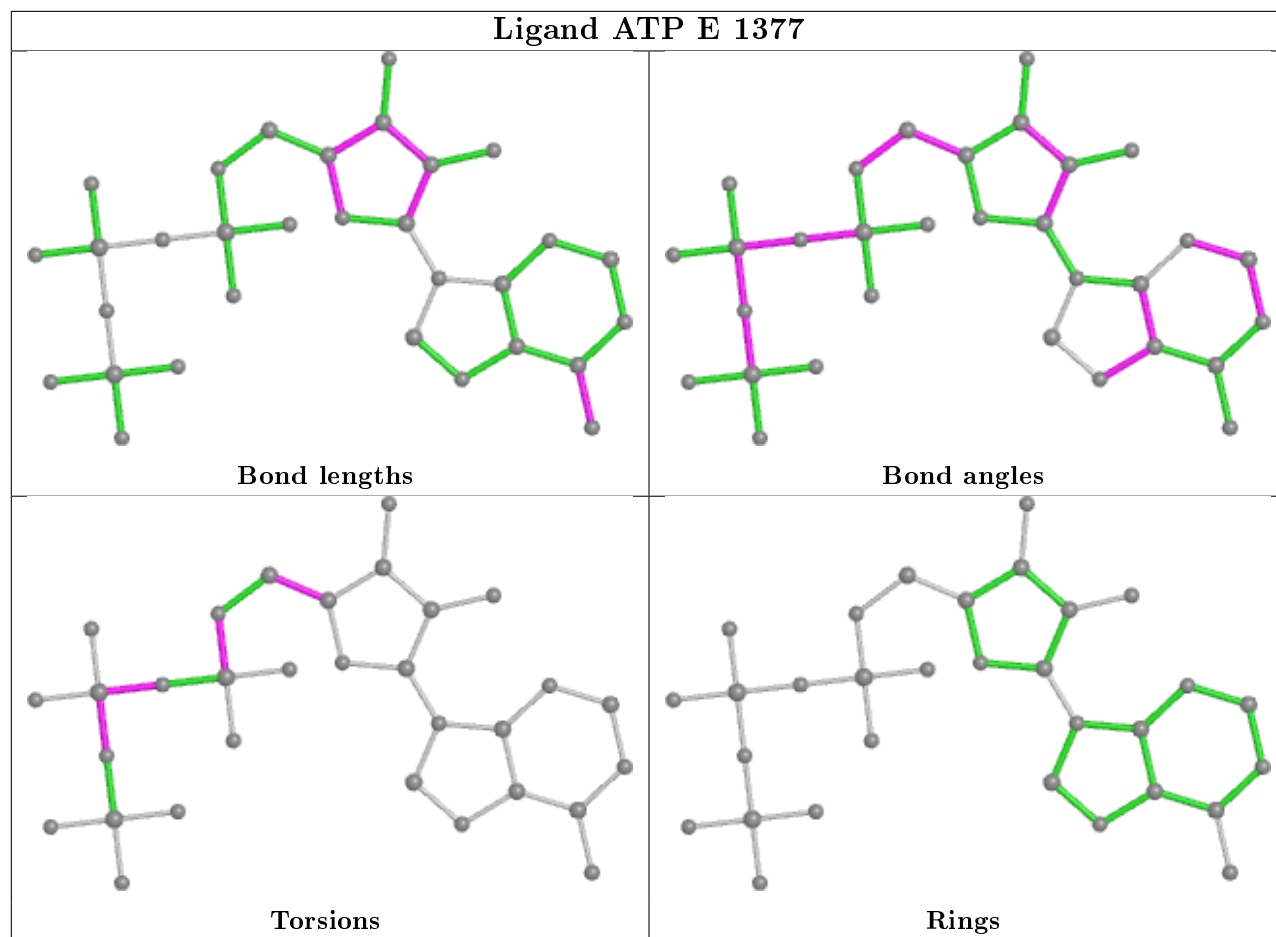
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1377	ATP	1	0
4	A	1377	ATP	1	0
4	E	1377	ATP	1	0
3	C	1376	LAB	4	0
3	A	1376	LAB	4	0
4	D	1377	ATP	1	0

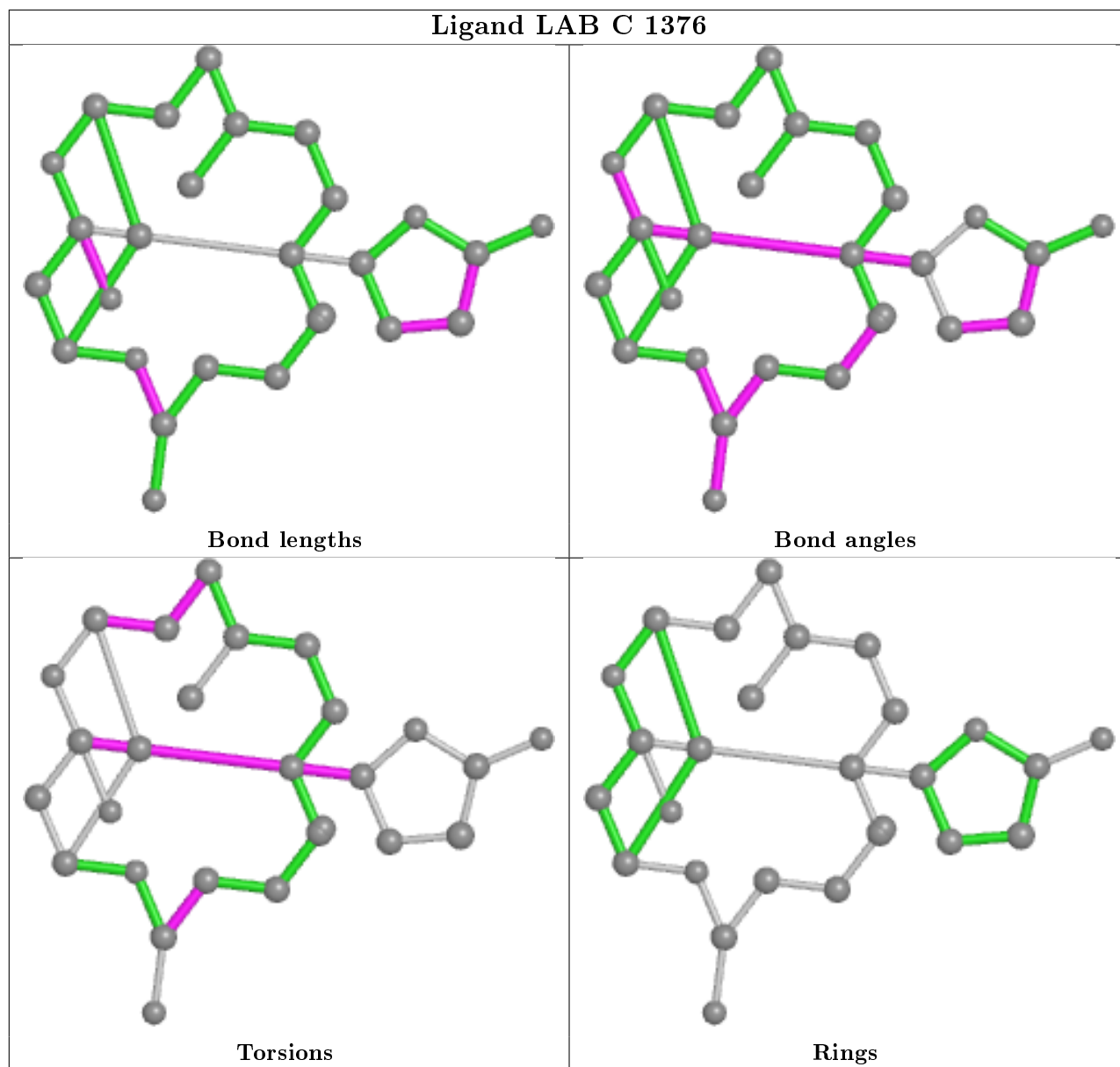
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

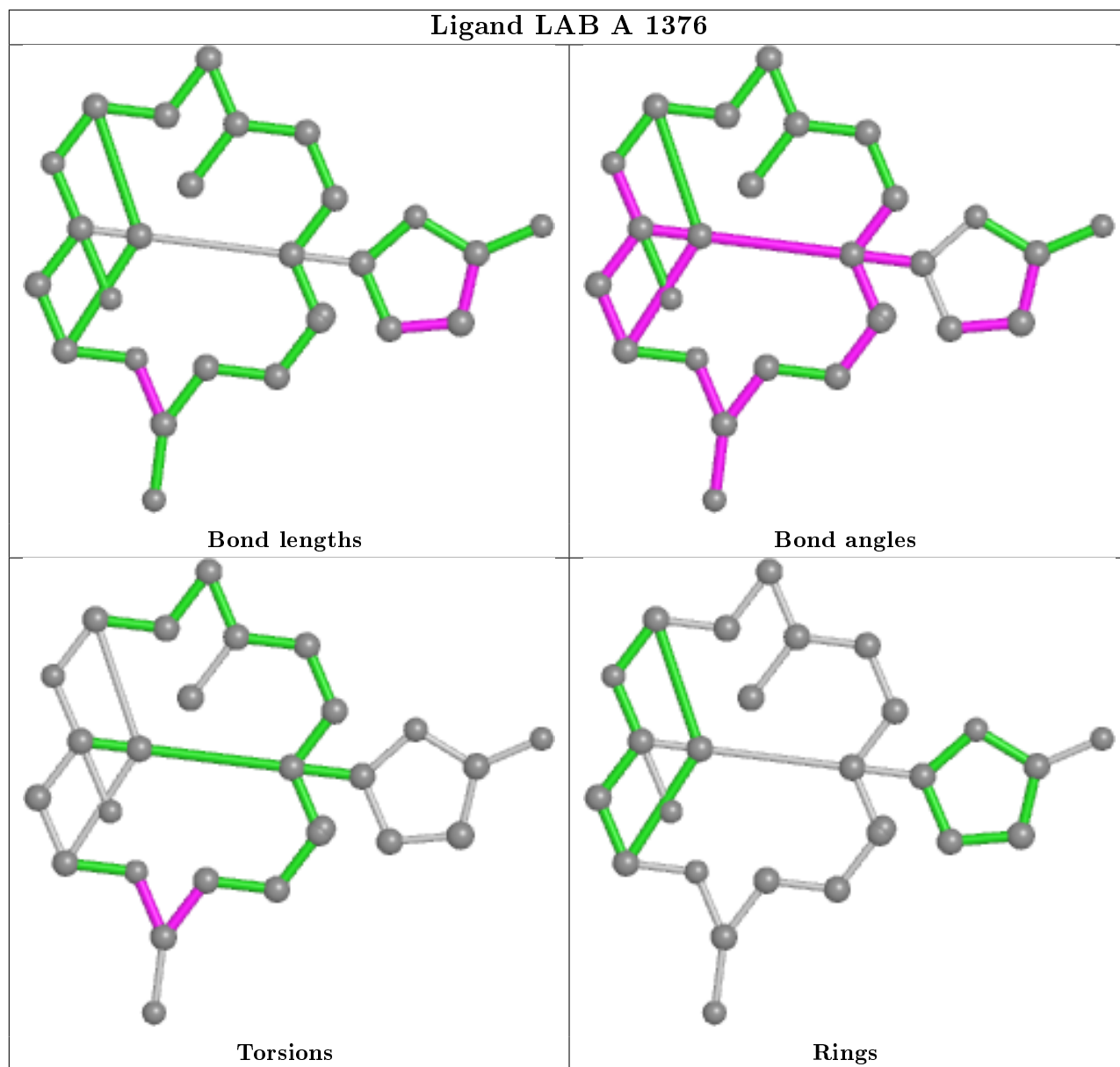


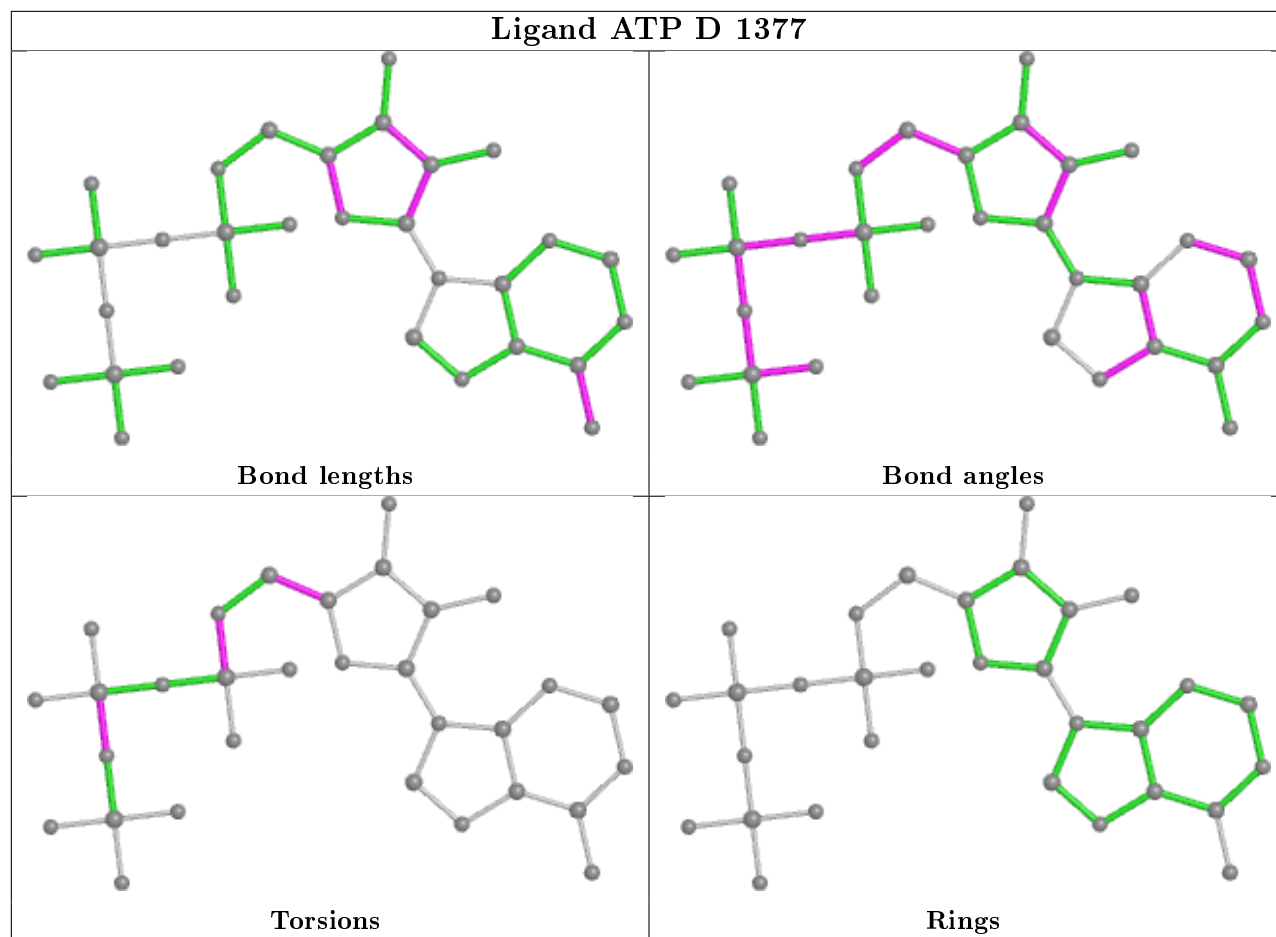












5.7 Other polymers [i](#)

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%)	-0.19	0 100 100	58, 110, 176, 238	0
1	B	335/377 (88%)	-0.08	2 (0%) 89 86	83, 142, 206, 291	0
1	C	343/377 (90%)	-0.19	4 (1%) 79 73	61, 117, 197, 268	0
1	D	345/377 (91%)	-0.14	9 (2%) 56 49	72, 125, 213, 264	0
1	E	318/377 (84%)	0.50	32 (10%) 7 7	110, 220, 311, 473	0
2	M	121/137 (88%)	-0.37	0 100 100	80, 122, 172, 199	0
All	All	1814/2022 (89%)	-0.05	47 (2%) 56 49	58, 134, 249, 473	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	200	PHE	5.9
1	E	204	ALA	5.6
1	E	197	GLY	5.1
1	E	253	GLU	4.8
1	E	199	SER	4.4
1	E	252	ASN	4.4
1	D	250	ILE	4.0
1	E	205	GLU	4.0
1	D	243	PRO	3.9
1	D	240	TYR	3.6
1	C	76	ILE	3.4
1	D	251	GLY	3.3
1	B	250	ILE	3.0
1	E	235	SER	3.0
1	E	170	ALA	3.0
1	E	260	THR	2.9
1	D	252	ASN	2.8
1	E	230	ALA	2.8
1	D	248	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	228	ALA	2.8
1	E	202	THR	2.7
1	E	251	GLY	2.7
1	E	190	MET	2.5
1	E	254	ARG	2.5
1	E	370	VAL	2.5
1	C	25	ASP	2.5
1	E	132	MET	2.5
1	E	10	CYS	2.4
1	C	103	THR	2.4
1	D	249	THR	2.4
1	E	229	THR	2.3
1	D	317	ILE	2.3
1	E	186	THR	2.3
1	E	271	SER	2.3
1	E	201	VAL	2.3
1	E	222	ASP	2.2
1	E	236	LEU	2.2
1	E	98	PRO	2.2
1	E	324	THR	2.2
1	D	239	SER	2.1
1	E	171	LEU	2.1
1	E	264	PRO	2.1
1	E	164	PRO	2.1
1	E	214	GLU	2.1
1	B	253	GLU	2.0
1	C	55	GLY	2.0
1	E	198	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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,

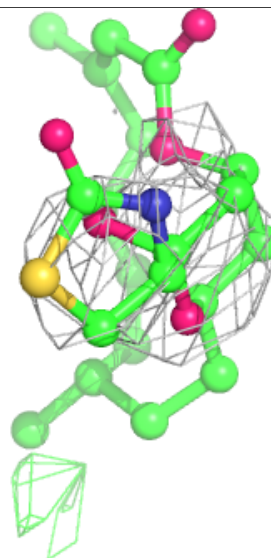
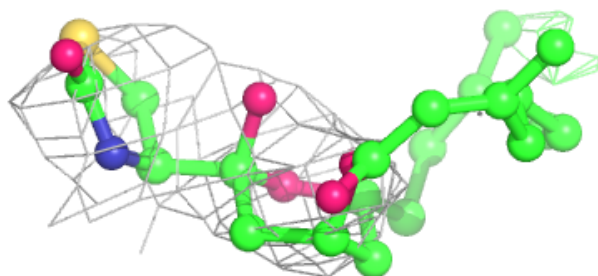
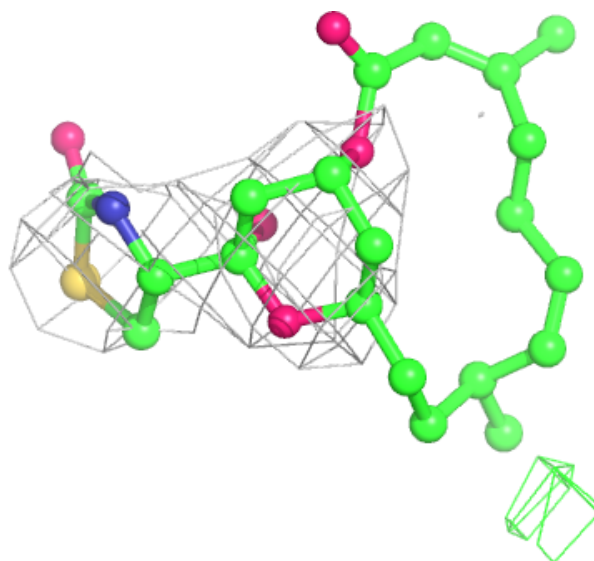
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LAB	A	1376	27/27	0.78	0.70	198,198,198,198	0
4	ATP	E	1377	31/31	0.86	0.19	207,207,207,207	0
5	MG	B	1378	1/1	0.87	0.39	105,105,105,105	0
5	MG	E	1378	1/1	0.88	0.15	158,158,158,158	0
4	ATP	D	1377	31/31	0.88	0.26	143,143,143,143	0
5	MG	C	1378	1/1	0.91	0.38	105,105,105,105	0
4	ATP	B	1377	31/31	0.91	0.22	146,146,146,146	0
3	LAB	C	1376	27/27	0.93	0.40	117,117,117,117	0
4	ATP	A	1377	31/31	0.94	0.23	105,105,105,105	0
5	MG	D	1378	1/1	0.95	0.44	105,105,105,105	0
5	MG	A	1378	1/1	0.96	0.54	105,105,105,105	0
4	ATP	C	1377	31/31	0.96	0.23	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.

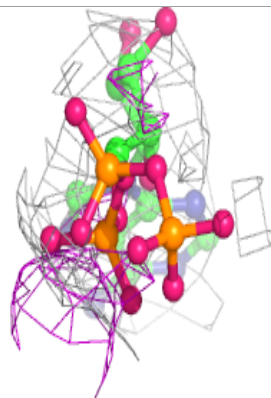
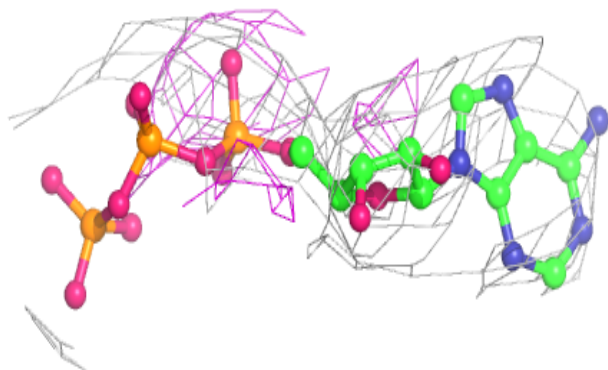
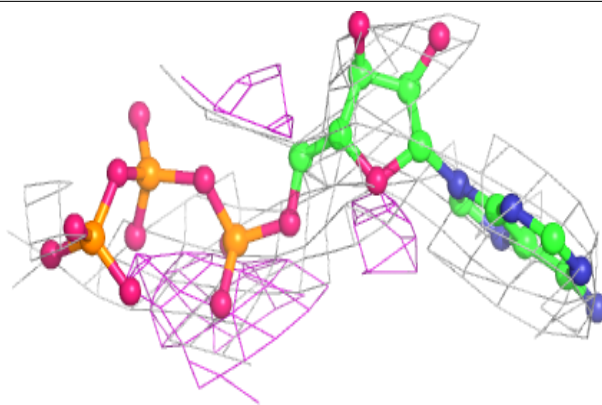
Electron density around LAB A 1376:

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

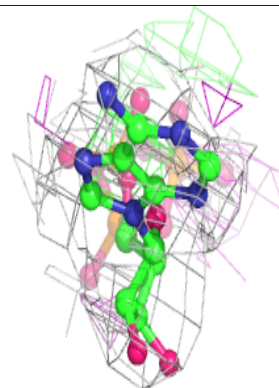
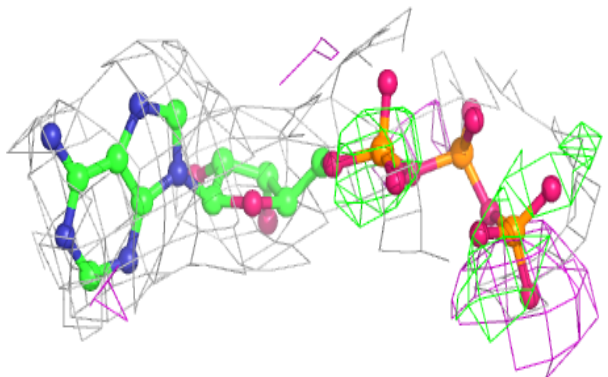
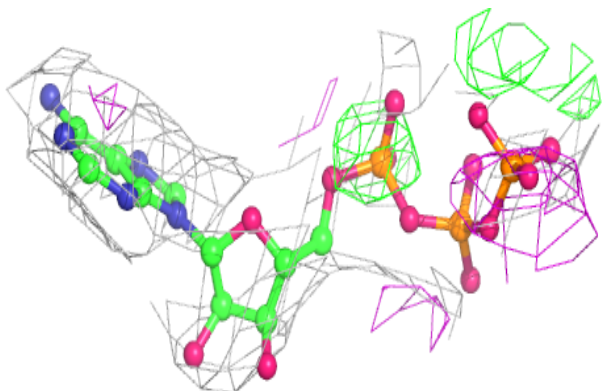


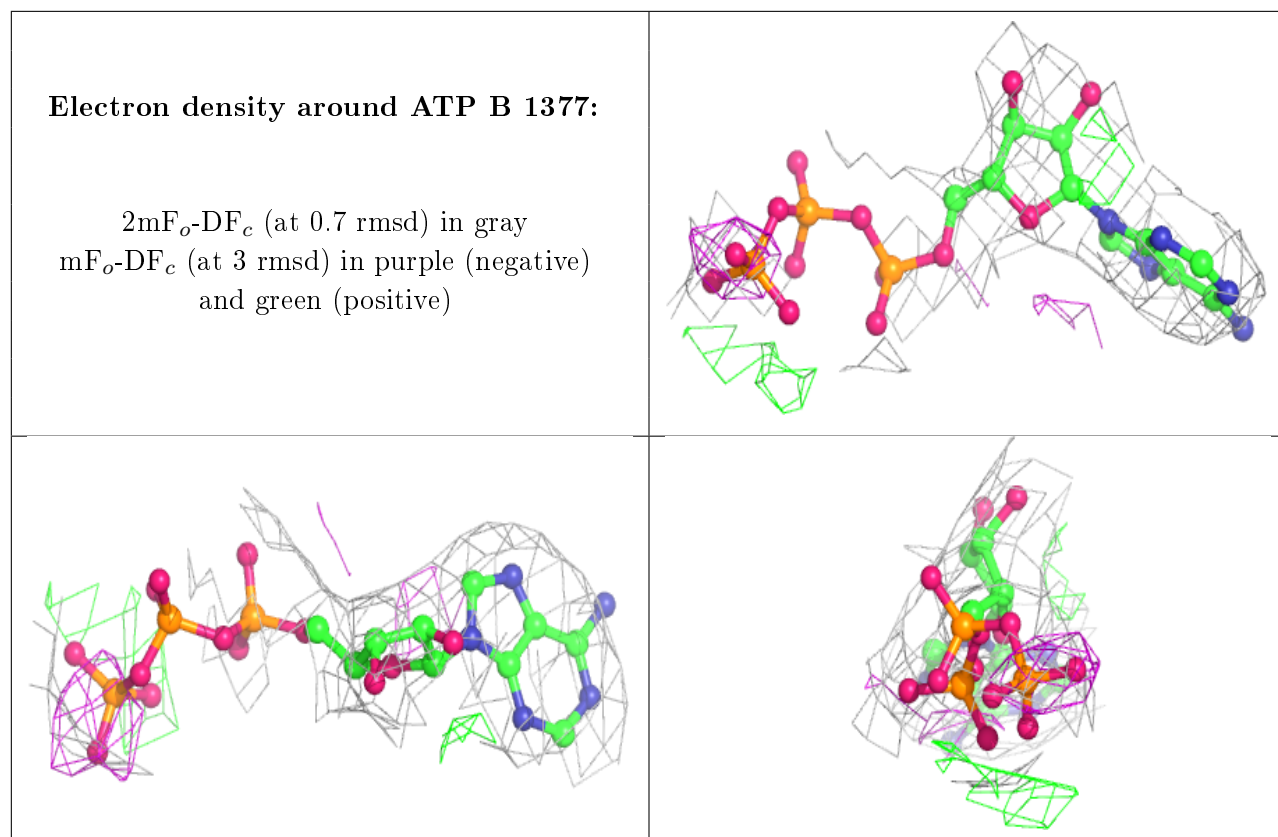
Electron density around ATP E 1377:

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

**Electron density around ATP D 1377:**

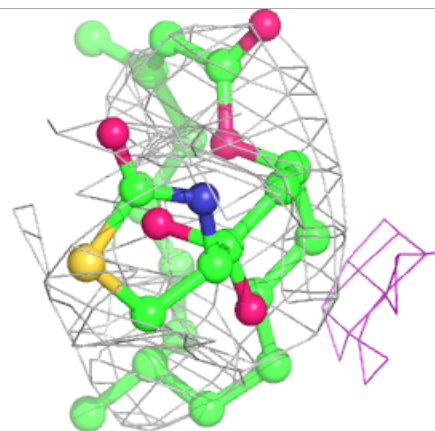
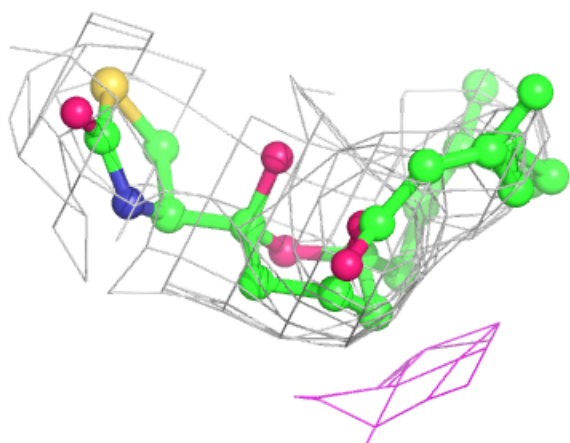
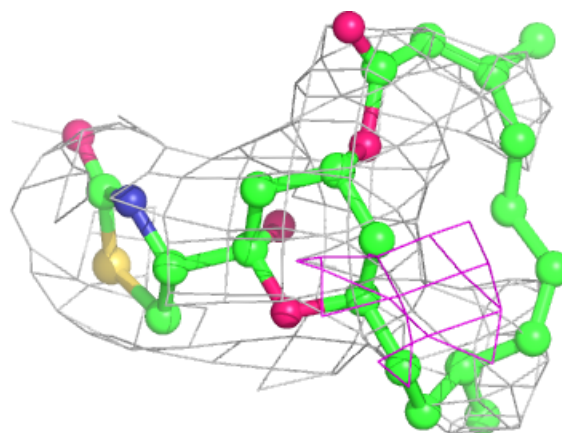
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





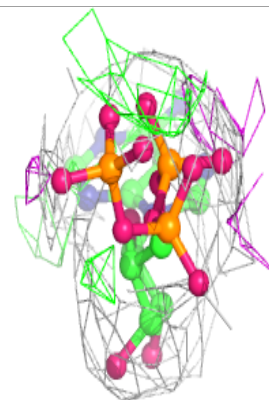
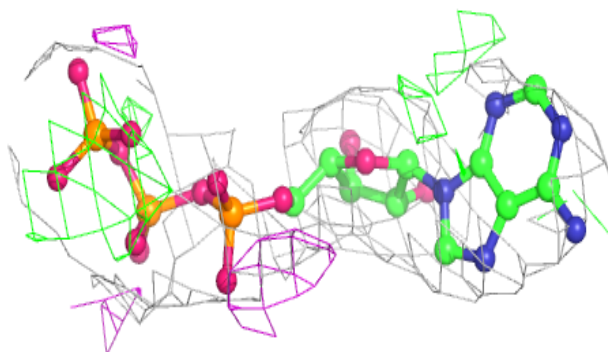
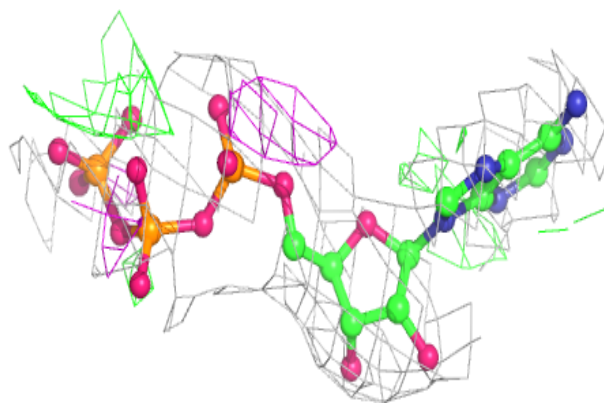
Electron density around LAB C 1376:

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

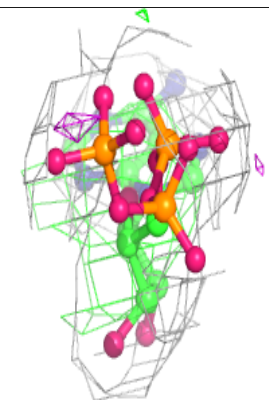
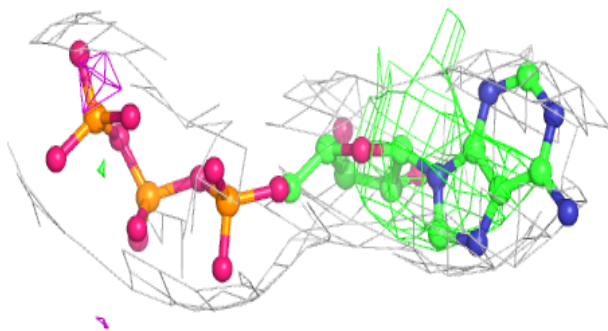
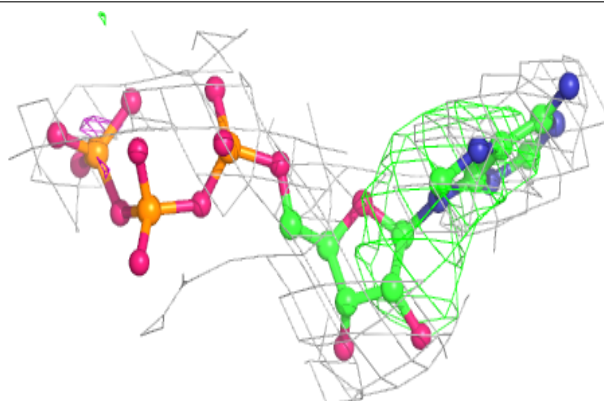


Electron density around ATP A 1377:

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

**Electron density around ATP C 1377:**

$2mF_o-DF_c$ (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.