



Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 01:24 PM JST

PDB ID : 8ZT1 / pdb_00008zt1
EMDB ID : EMD-60438
Title : sStructure of calcium preference ATP-gated channel P2X1 in complex with BTFA
Authors : Zhang, H.; Xu, H.E.
Deposited on : 2024-06-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

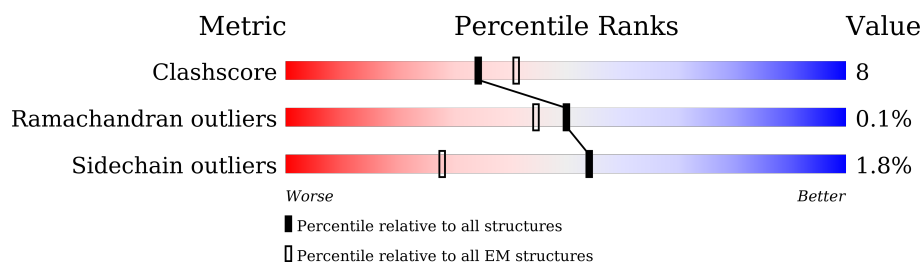
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	428	
1	B	428	
1	C	428	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7919 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called P2X purinoceptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	330	Total	C	N	O	S	0	0
			2576	1660	446	456	14		
1	B	329	Total	C	N	O	S	0	0
			2577	1666	443	453	15		
1	C	326	Total	C	N	O	S	0	0
			2551	1645	440	452	14		

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P51576
A	400	LYS	-	expression tag	UNP P51576
A	401	LEU	-	expression tag	UNP P51576
A	402	LEU	-	expression tag	UNP P51576
A	403	GLU	-	expression tag	UNP P51576
A	404	VAL	-	expression tag	UNP P51576
A	405	LEU	-	expression tag	UNP P51576
A	406	PHE	-	expression tag	UNP P51576
A	407	GLN	-	expression tag	UNP P51576
A	408	GLY	-	expression tag	UNP P51576
A	409	PRO	-	expression tag	UNP P51576
A	410	HIS	-	expression tag	UNP P51576
A	411	HIS	-	expression tag	UNP P51576
A	412	HIS	-	expression tag	UNP P51576
A	413	HIS	-	expression tag	UNP P51576
A	414	HIS	-	expression tag	UNP P51576
A	415	HIS	-	expression tag	UNP P51576
A	416	HIS	-	expression tag	UNP P51576
A	417	HIS	-	expression tag	UNP P51576
A	418	HIS	-	expression tag	UNP P51576
A	419	HIS	-	expression tag	UNP P51576
A	420	ASP	-	expression tag	UNP P51576
A	421	TYR	-	expression tag	UNP P51576
A	422	LYS	-	expression tag	UNP P51576

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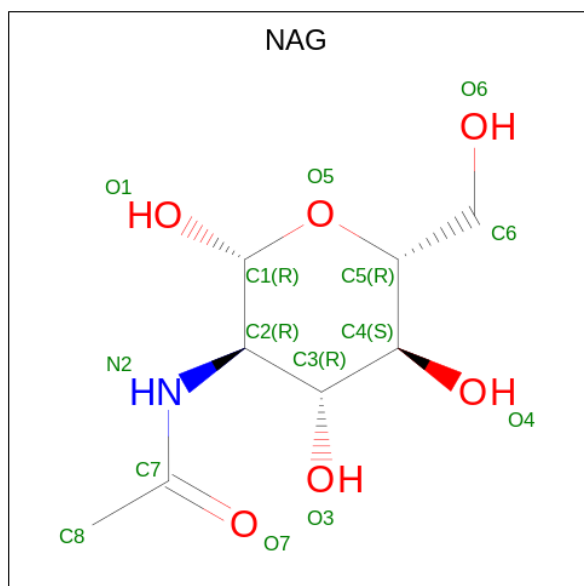
Chain	Residue	Modelled	Actual	Comment	Reference
A	423	ASP	-	expression tag	UNP P51576
A	424	ASP	-	expression tag	UNP P51576
A	425	ASP	-	expression tag	UNP P51576
A	426	ASP	-	expression tag	UNP P51576
A	427	LYS	-	expression tag	UNP P51576
B	0	MET	-	initiating methionine	UNP P51576
B	400	LYS	-	expression tag	UNP P51576
B	401	LEU	-	expression tag	UNP P51576
B	402	LEU	-	expression tag	UNP P51576
B	403	GLU	-	expression tag	UNP P51576
B	404	VAL	-	expression tag	UNP P51576
B	405	LEU	-	expression tag	UNP P51576
B	406	PHE	-	expression tag	UNP P51576
B	407	GLN	-	expression tag	UNP P51576
B	408	GLY	-	expression tag	UNP P51576
B	409	PRO	-	expression tag	UNP P51576
B	410	HIS	-	expression tag	UNP P51576
B	411	HIS	-	expression tag	UNP P51576
B	412	HIS	-	expression tag	UNP P51576
B	413	HIS	-	expression tag	UNP P51576
B	414	HIS	-	expression tag	UNP P51576
B	415	HIS	-	expression tag	UNP P51576
B	416	HIS	-	expression tag	UNP P51576
B	417	HIS	-	expression tag	UNP P51576
B	418	HIS	-	expression tag	UNP P51576
B	419	HIS	-	expression tag	UNP P51576
B	420	ASP	-	expression tag	UNP P51576
B	421	TYR	-	expression tag	UNP P51576
B	422	LYS	-	expression tag	UNP P51576
B	423	ASP	-	expression tag	UNP P51576
B	424	ASP	-	expression tag	UNP P51576
B	425	ASP	-	expression tag	UNP P51576
B	426	ASP	-	expression tag	UNP P51576
B	427	LYS	-	expression tag	UNP P51576
C	0	MET	-	initiating methionine	UNP P51576
C	400	LYS	-	expression tag	UNP P51576
C	401	LEU	-	expression tag	UNP P51576
C	402	LEU	-	expression tag	UNP P51576
C	403	GLU	-	expression tag	UNP P51576
C	404	VAL	-	expression tag	UNP P51576
C	405	LEU	-	expression tag	UNP P51576
C	406	PHE	-	expression tag	UNP P51576

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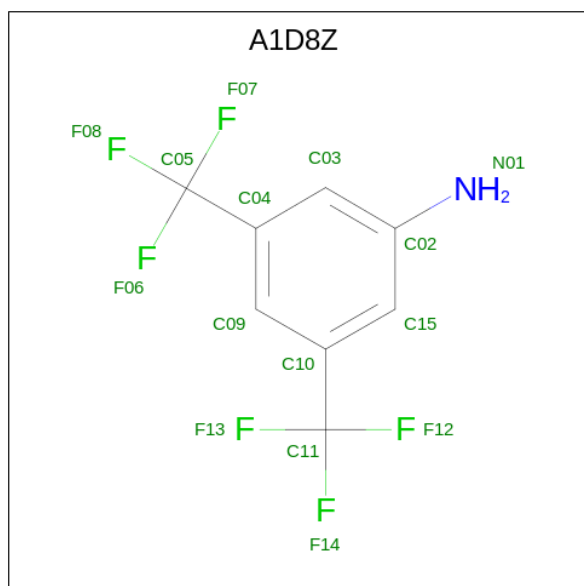
Chain	Residue	Modelled	Actual	Comment	Reference
C	407	GLN	-	expression tag	UNP P51576
C	408	GLY	-	expression tag	UNP P51576
C	409	PRO	-	expression tag	UNP P51576
C	410	HIS	-	expression tag	UNP P51576
C	411	HIS	-	expression tag	UNP P51576
C	412	HIS	-	expression tag	UNP P51576
C	413	HIS	-	expression tag	UNP P51576
C	414	HIS	-	expression tag	UNP P51576
C	415	HIS	-	expression tag	UNP P51576
C	416	HIS	-	expression tag	UNP P51576
C	417	HIS	-	expression tag	UNP P51576
C	418	HIS	-	expression tag	UNP P51576
C	419	HIS	-	expression tag	UNP P51576
C	420	ASP	-	expression tag	UNP P51576
C	421	TYR	-	expression tag	UNP P51576
C	422	LYS	-	expression tag	UNP P51576
C	423	ASP	-	expression tag	UNP P51576
C	424	ASP	-	expression tag	UNP P51576
C	425	ASP	-	expression tag	UNP P51576
C	426	ASP	-	expression tag	UNP P51576
C	427	LYS	-	expression tag	UNP P51576

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



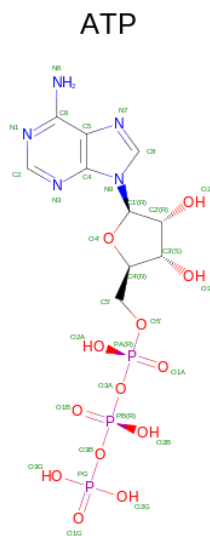
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	C	1	Total 14	C 8	N 1	O 5	0

- Molecule 3 is 3,5-bis(trifluoromethyl)aniline (CCD ID: A1D8Z) (formula: $\text{C}_8\text{H}_5\text{F}_6\text{N}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	F	N	0
			15	8	6	1	

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



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Ca 1 1	0
5	B	1	Total Ca 1 1	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Mg 1 1	0
6	B	1	Total Mg 1 1	0
6	C	1	Total Mg 1 1	0

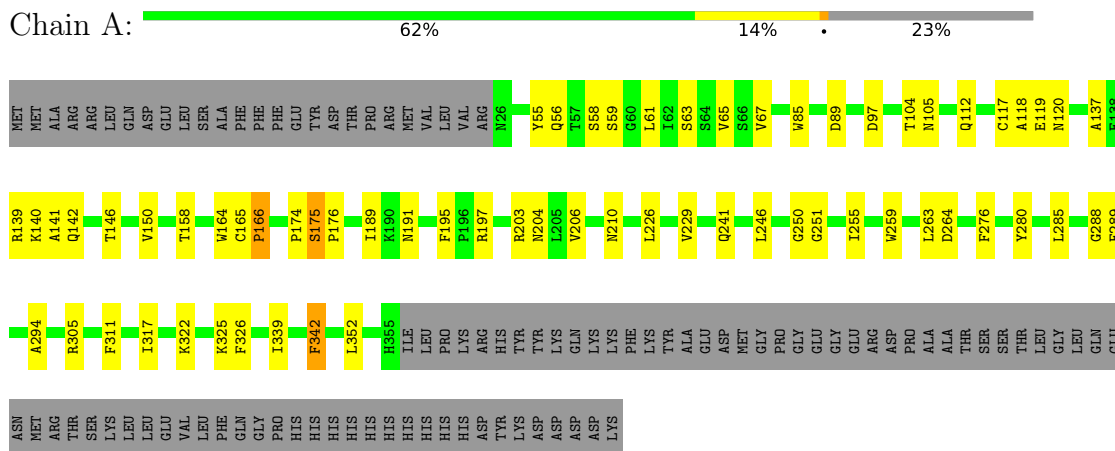
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total 2	O 2	0
7	B	1	Total 1	O 1	0
7	C	1	Total 1	O 1	0

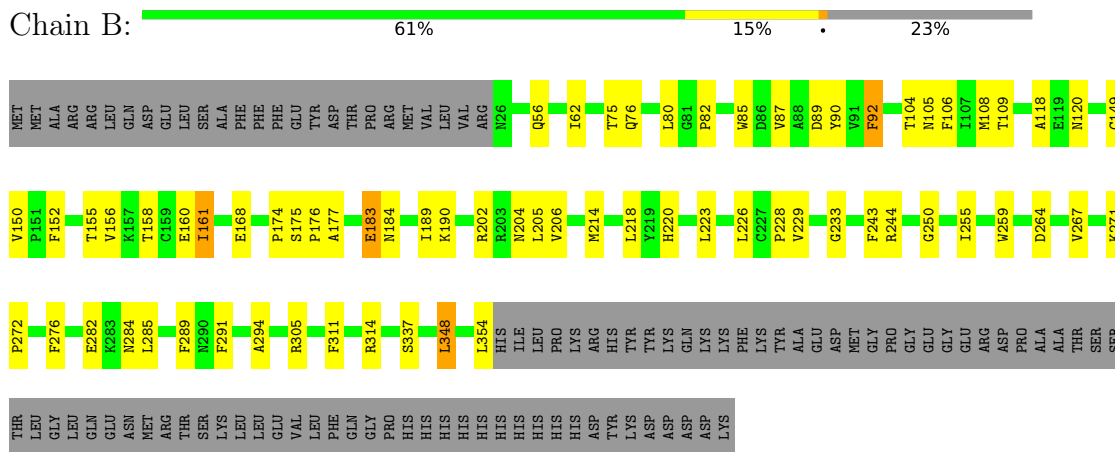
3 Residue-property plots

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

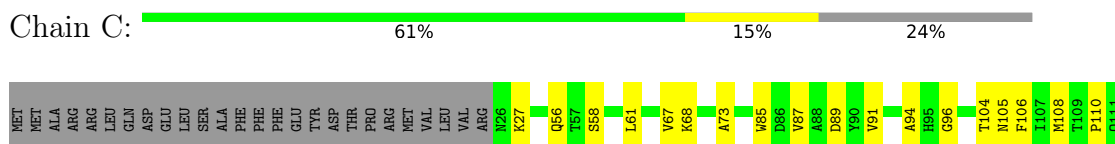
• Molecule 1: P2X purinoceptor 1



• Molecule 1: P2X purinoceptor 1



• Molecule 1: P2X purinoceptor 1



ARG	V253	Q112
ASP	G254	R139
PRO	G255	
ALA	T256	T146
ALA	I257	
THR		
SER	D264	F151
SER		F152
THR	F276	
LEU		K157
GLY	Y280	
LEU	G281	G165
GLN		P166
GLU	P287	
ASN		K172
MET	R305	
ARG		S175
THR	F311	P176
SER	G312	
LYS	I313	E181
LEU		A182
LEU	V319	E183
GLU		N184
VAL	I339	F185
LEU	G340	
PHE	I341	I189
GLN	F342	
GLY		
PRO	T346	F195
HIS		P196
HIS	L351	R197
HIS	LEU	
HIS	LEU	V200
HIS	LEU	
HIS	LEU	N204
HIS	HIS	L205
HIS	HIS	V206
HIS	ILE	
HIS	LEU	
HIS	PRO	N210
HIS	LYS	
ASP	ARG	W214
TYR	HIS	W215
LYS	TYR	K216
ASP	TYR	G217
ASP	LYS	
ASP	GLN	L223
ASP	LYS	
LYS	PHE	L226
	LYS	V235
	TYR	
	ALA	Q241
	GLU	D242
	ASP	F243
	MET	
	GLY	L246
	PRO	
	GLY	K249
	GLU	G250
	GLY	G251
	GLU	V255

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A1D8Z, NAG, CA, 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	0.30	0/2643	0.59	3/3581 (0.1%)
1	B	0.29	0/2643	0.59	7/3580 (0.2%)
1	C	0.23	0/2617	0.56	5/3545 (0.1%)
All	All	0.28	0/7903	0.58	15/10706 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	SER	N-CA-C	-7.12	103.52	111.71
1	C	341	ILE	N-CA-C	-7.08	102.24	111.09
1	B	348	LEU	N-CA-C	6.94	118.85	111.28
1	B	90	TYR	N-CA-C	6.70	118.58	111.28
1	B	149	CYS	N-CA-C	6.60	120.50	111.39
1	C	27	LYS	N-CA-C	-6.28	106.83	114.75
1	A	175	SER	CA-C-N	-6.23	113.10	119.83
1	A	175	SER	C-N-CA	-6.23	113.10	119.83
1	B	152	PHE	N-CA-C	-6.00	103.51	111.96
1	A	352	LEU	N-CA-C	-5.83	105.67	112.89
1	C	217	CYS	N-CA-C	5.73	118.24	108.90
1	B	92	PHE	N-CA-C	5.52	122.02	109.81
1	C	181	GLU	N-CA-C	-5.46	106.47	113.02
1	B	218	LEU	N-CA-C	-5.26	100.33	108.90
1	C	152	PHE	N-CA-C	-5.20	105.68	112.23

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	2576	0	2533	41	0
1	B	2577	0	2563	47	0
1	C	2551	0	2518	42	0
2	A	42	0	39	0	0
2	B	42	0	39	1	0
2	C	14	0	13	0	0
3	A	15	0	0	1	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
All	All	7919	0	7741	123	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 8.

All (123) 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:B:76:GLN:HE22	1:B:82:PRO:HG3	1.18	1.06
1:B:76:GLN:NE2	1:B:82:PRO:HG3	1.71	1.04
1:A:285:LEU:HD21	1:B:205:LEU:HD23	1.47	0.95
1:B:76:GLN:HE22	1:B:82:PRO:CG	1.87	0.87
1:B:205:LEU:HD21	1:B:214:MET:HE1	1.56	0.85
1:B:205:LEU:HD21	1:B:214:MET:CE	2.09	0.82
1:B:155:THR:HG23	1:B:156:VAL:HG13	1.61	0.81
1:A:285:LEU:CD2	1:B:205:LEU:HD23	2.11	0.81
1:C:216:LYS:O	1:C:216:LYS:HG2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ILE:O	1:C:204:ASN:ND2	2.27	0.68
1:C:249:LYS:HD2	1:C:287:PRO:HB2	1.75	0.67
1:B:226:LEU:HD11	1:B:271:LYS:HE3	1.77	0.66
1:A:105:ASN:HD21	1:A:174:PRO:HD2	1.60	0.66
1:B:354:LEU:HG	1:B:354:LEU:O	1.94	0.65
1:A:189:ILE:O	1:A:204:ASN:ND2	2.30	0.64
1:C:56:GLN:NE2	1:C:264:ASP:OD2	2.31	0.63
1:A:339:ILE:HA	1:A:342:PHE:HB2	1.80	0.62
1:A:139:ARG:HG2	1:A:140:LYS:HG3	1.82	0.62
1:B:189:ILE:O	1:B:204:ASN:ND2	2.33	0.61
1:B:205:LEU:HD11	1:B:228:PRO:HG3	1.83	0.60
1:C:91:VAL:HG12	1:C:94:ALA:H	1.67	0.60
1:C:146:THR:HG22	1:C:146:THR:O	2.01	0.60
1:C:195:PHE:HD2	1:C:200:VAL:HG13	1.69	0.57
1:A:97:ASP:OD2	3:A:504:A1D8Z:C03	2.53	0.56
1:B:314:ARG:NH1	1:C:96:GLY:O	2.36	0.56
1:C:342:PHE:O	1:C:346:THR:HG23	2.05	0.56
1:C:58:SER:O	1:C:197:ARG:NH2	2.39	0.56
1:A:112:GLN:HB3	1:A:164:TRP:HB3	1.88	0.56
1:B:80:LEU:HD22	1:B:108:MET:HE1	1.86	0.56
1:B:56:GLN:NE2	1:B:264:ASP:OD2	2.38	0.55
1:A:175:SER:HB2	1:A:176:PRO:HD3	1.87	0.55
1:B:76:GLN:HE22	1:B:82:PRO:CD	2.20	0.55
1:C:85:TRP:HE3	1:C:89:ASP:HB3	1.72	0.55
1:A:85:TRP:HE3	1:A:89:ASP:HB3	1.72	0.55
1:B:85:TRP:HE3	1:B:89:ASP:HB3	1.72	0.55
1:A:229:VAL:HG11	1:C:139:ARG:HH12	1.71	0.54
1:A:67:VAL:HG12	1:A:189:ILE:HG12	1.89	0.54
1:A:58:SER:O	1:A:197:ARG:NH1	2.41	0.53
1:A:165:CYS:SG	1:A:166:PRO:HD3	2.48	0.53
1:C:206:VAL:HG21	1:C:226:LEU:HD13	1.91	0.53
1:C:342:PHE:CD2	1:C:346:THR:CG2	2.91	0.53
1:A:65:VAL:HG11	1:A:317:ILE:HG21	1.90	0.53
1:A:146:THR:HG22	1:A:146:THR:O	2.09	0.53
1:A:61:LEU:HD13	1:A:63:SER:HB3	1.90	0.52
1:B:105:ASN:HD21	1:B:174:PRO:HD2	1.74	0.52
1:A:206:VAL:HG21	1:A:226:LEU:HD13	1.90	0.52
1:C:342:PHE:CE2	1:C:346:THR:HG22	2.45	0.52
1:A:119:GLU:HG2	1:A:158:THR:HB	1.92	0.52
1:A:120:ASN:HB3	1:A:142:GLN:HE22	1.75	0.52
1:B:104:THR:OG1	1:B:311:PHE:O	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:THR:OG1	1:C:311:PHE:O	2.25	0.52
1:C:246:LEU:HG	1:C:251:GLY:HA3	1.92	0.51
1:A:56:GLN:NE2	1:A:264:ASP:OD2	2.43	0.51
1:C:151:PRO:HA	1:C:157:LYS:HA	1.92	0.51
1:B:205:LEU:CD2	1:B:214:MET:CE	2.86	0.50
1:B:282:GLU:N	1:B:282:GLU:OE1	2.45	0.50
1:C:241:GLN:HE21	1:C:280:TYR:HB3	1.75	0.50
1:C:342:PHE:CE2	1:C:346:THR:CG2	2.95	0.50
1:C:183:GLU:CG	1:C:243:PHE:CD1	2.95	0.49
1:A:288:GLY:O	1:B:190:LYS:NZ	2.45	0.49
1:B:205:LEU:CD2	1:B:214:MET:HE1	2.34	0.49
1:A:104:THR:OG1	1:A:311:PHE:O	2.28	0.49
1:A:241:GLN:HE21	1:A:280:TYR:HB3	1.77	0.49
1:A:250:GLY:HA3	1:A:289:PHE:H	1.78	0.48
1:C:183:GLU:HG2	1:C:243:PHE:CD1	2.47	0.48
1:B:75:THR:HG21	1:B:106:PHE:HE1	1.78	0.48
1:C:67:VAL:HG12	1:C:189:ILE:HG12	1.95	0.48
1:A:191:ASN:ND2	1:A:259:TRP:HE1	2.12	0.47
1:B:202:ARG:HD2	1:B:267:VAL:HG22	1.96	0.47
1:C:183:GLU:HG3	1:C:243:PHE:CE1	2.49	0.47
1:A:137:ALA:HB3	1:A:141:ALA:HA	1.97	0.47
1:A:294:ALA:HB1	1:A:305:ARG:HD2	1.97	0.47
1:A:61:LEU:HB3	1:A:195:PHE:CE1	2.51	0.46
1:B:250:GLY:HA3	1:B:289:PHE:H	1.80	0.46
1:C:165:CYS:HB3	1:C:166:PRO:HD3	1.96	0.46
1:B:76:GLN:NE2	1:B:82:PRO:CG	2.54	0.46
1:B:183:GLU:HG3	1:B:243:PHE:CG	2.51	0.46
1:A:61:LEU:CD1	1:A:63:SER:HB3	2.46	0.46
1:A:263:LEU:HB2	1:A:325:LYS:HG2	1.99	0.45
1:C:214:MET:HE2	1:C:214:MET:HB3	1.85	0.45
1:C:108:MET:HE2	1:C:110:PRO:HB3	1.98	0.45
1:C:257:ILE:HB	1:C:319:VAL:HG22	1.99	0.45
1:B:220:HIS:HB3	1:B:223:LEU:HB2	1.99	0.44
1:B:294:ALA:HB1	1:B:305:ARG:HD2	1.97	0.44
1:B:76:GLN:OE1	1:B:80:LEU:O	2.35	0.44
1:B:109:THR:HG21	1:B:168:GLU:HA	1.99	0.44
1:B:118:ALA:HB1	1:B:158:THR:OG1	2.17	0.44
1:C:146:THR:O	1:C:146:THR:CG2	2.66	0.44
1:B:177:ALA:H	1:B:244:ARG:HH22	1.64	0.44
1:B:183:GLU:HG2	1:B:233:GLY:HA3	2.00	0.44
1:B:161:ILE:H	1:B:161:ILE:HG13	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:TRP:CE2	1:B:272:PRO:HB3	2.53	0.44
1:C:183:GLU:HG2	1:C:243:PHE:CG	2.53	0.44
1:A:118:ALA:HB2	1:A:150:VAL:HG23	2.00	0.43
1:B:155:THR:HG23	1:B:156:VAL:N	2.33	0.43
1:C:112:GLN:HA	1:C:166:PRO:HD2	2.01	0.43
1:A:117:CYS:SG	1:A:118:ALA:N	2.91	0.42
1:B:150:VAL:HG22	1:B:160:GLU:HB2	2.01	0.42
1:C:255:ILE:HG12	1:C:276:PHE:HD1	1.84	0.42
1:A:118:ALA:HB1	1:A:158:THR:OG1	2.19	0.42
1:B:175:SER:HB3	1:B:176:PRO:HD3	2.01	0.42
1:A:55:TYR:HD2	1:A:326:PHE:HD1	1.67	0.42
1:A:203:ARG:HD3	1:C:281:GLY:HA3	2.01	0.42
1:A:246:LEU:HG	1:A:251:GLY:HA3	2.01	0.41
1:C:73:ALA:HB2	1:C:185:PHE:HZ	1.84	0.41
1:B:354:LEU:O	1:B:354:LEU:CG	2.67	0.41
1:C:175:SER:HB3	1:C:176:PRO:HD3	2.01	0.41
1:A:59:SER:HB2	1:A:197:ARG:HD2	2.01	0.41
1:B:92:PHE:CD2	1:B:291:PHE:HZ	2.38	0.41
1:C:104:THR:HG21	1:C:313:ILE:HG12	2.02	0.41
1:C:112:GLN:OE1	1:C:305:ARG:NE	2.40	0.41
1:A:139:ARG:HH22	1:B:229:VAL:HG21	1.86	0.41
1:B:244:ARG:HH11	1:B:244:ARG:HA	1.85	0.41
1:B:284:ASN:OD1	1:B:285:LEU:N	2.54	0.41
1:C:339:ILE:O	1:C:342:PHE:HB3	2.21	0.41
1:A:58:SER:HB3	1:A:322:LYS:HD2	2.02	0.41
1:A:255:ILE:HG12	1:A:276:PHE:HD1	1.86	0.41
1:B:184:ASN:HD22	2:B:501:NAG:H61	1.86	0.40
1:C:61:LEU:HB3	1:C:195:PHE:CE1	2.56	0.40
1:C:105:ASN:OD1	1:C:106:PHE:N	2.54	0.40
1:C:216:LYS:O	1:C:216:LYS:CG	2.58	0.40
1:B:255:ILE:HG12	1:B:276:PHE:HD1	1.86	0.40
1:C:235:VAL:HG12	1:C:253:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/428 (77%)	320 (98%)	7 (2%)	1 (0%)	37	67
1	B	327/428 (76%)	318 (97%)	9 (3%)	0	100	100
1	C	324/428 (76%)	315 (97%)	9 (3%)	0	100	100
All	All	979/1284 (76%)	953 (97%)	25 (3%)	1 (0%)	50	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/371 (75%)	275 (99%)	2 (1%)	81	94
1	B	280/371 (76%)	273 (98%)	7 (2%)	42	75
1	C	276/371 (74%)	270 (98%)	6 (2%)	47	79
All	All	833/1113 (75%)	818 (98%)	15 (2%)	54	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	342	PHE
1	B	62	ILE
1	B	87	VAL
1	B	120	ASN
1	B	161	ILE
1	B	183	GLU
1	B	206	VAL

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Mol	Chain	Res	Type
1	B	348	LEU
1	C	68	LYS
1	C	87	VAL
1	C	172	LYS
1	C	210	ASN
1	C	223	LEU
1	C	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	95	HIS
1	A	111	GLN
1	A	116	HIS
1	A	191	ASN
1	A	241	GLN
1	B	37	GLN
1	B	76	GLN
1	B	111	GLN
1	B	116	HIS
1	B	120	ASN
1	B	191	ASN
1	B	220	HIS
1	B	241	GLN
1	B	266	HIS
1	C	26	ASN
1	C	76	GLN
1	C	114	GLN
1	C	241	GLN
1	C	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	$\# Z > 2$
2	NAG	A	501	1	14,14,15	0.27	0	17,19,21	0.40	0
4	ATP	C	501	6	26,33,33	0.91	1 (3%)	31,52,52	1.51	6 (19%)
4	ATP	B	504	6	26,33,33	0.90	1 (3%)	31,52,52	1.47	6 (19%)
2	NAG	B	501	1	14,14,15	0.94	1 (7%)	17,19,21	1.22	1 (5%)
2	NAG	B	502	1	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	A	503	1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	C	502	1	14,14,15	0.28	0	17,19,21	0.42	0
3	A1D8Z	A	504	-	15,15,15	1.05	1 (6%)	24,24,24	1.11	1 (4%)
2	NAG	B	503	1	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	A	502	1	14,14,15	0.22	0	17,19,21	0.40	0
4	ATP	A	505	6	26,33,33	0.91	1 (3%)	31,52,52	1.53	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
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	ATP	C	501	6	-	5/18/38/38	0/3/3/3
4	ATP	B	504	6	-	2/18/38/38	0/3/3/3
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	4/6/23/26	0/1/1/1
2	NAG	A	503	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	502	1	-	2/6/23/26	0/1/1/1
3	A1D8Z	A	504	-	-	0/12/12/12	0/1/1/1
2	NAG	B	503	1	-	2/6/23/26	0/1/1/1
2	NAG	A	502	1	-	2/6/23/26	0/1/1/1
4	ATP	A	505	6	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	O5-C1	3.35	1.49	1.43
4	A	505	ATP	C5-C4	2.40	1.47	1.40
4	C	501	ATP	C5-C4	2.40	1.47	1.40
4	B	504	ATP	C5-C4	2.37	1.47	1.40
3	A	504	A1D8Z	C02-N01	2.04	1.45	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C1-O5-C5	4.81	118.71	112.19
4	B	504	ATP	N3-C2-N1	-3.24	123.61	128.68
4	C	501	ATP	PB-O3B-PG	-3.20	121.83	132.83
4	A	505	ATP	N3-C2-N1	-3.18	123.71	128.68
4	A	505	ATP	PA-O3A-PB	-3.16	121.97	132.83
4	C	501	ATP	N3-C2-N1	-3.15	123.75	128.68
4	A	505	ATP	PB-O3B-PG	-3.03	122.44	132.83
4	A	505	ATP	C3'-C2'-C1'	3.02	105.53	100.98
4	B	504	ATP	C3'-C2'-C1'	2.97	105.45	100.98
4	C	501	ATP	C3'-C2'-C1'	2.88	105.31	100.98
4	C	501	ATP	PA-O3A-PB	-2.85	123.06	132.83
4	B	504	ATP	PB-O3B-PG	-2.77	123.31	132.83
4	A	505	ATP	C4-C5-N7	-2.67	106.61	109.40
4	B	504	ATP	PA-O3A-PB	-2.63	123.78	132.83
4	B	504	ATP	C4-C5-N7	-2.56	106.73	109.40
4	C	501	ATP	C4-C5-N7	-2.55	106.74	109.40
4	A	505	ATP	C2'-C3'-C4'	2.04	106.61	102.64
4	A	505	ATP	C2-N1-C6	2.03	122.23	118.75
4	C	501	ATP	C2-N1-C6	2.03	122.23	118.75
3	A	504	A1D8Z	F08-C05-C04	-2.03	108.48	112.93
4	B	504	ATP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	ATP	C5'-O5'-PA-O2A
4	C	501	ATP	C5'-O5'-PA-O1A
2	C	502	NAG	C4-C5-C6-O6
2	C	502	NAG	O5-C5-C6-O6
2	A	502	NAG	O5-C5-C6-O6
2	A	503	NAG	C8-C7-N2-C2
2	A	503	NAG	O7-C7-N2-C2
2	B	502	NAG	C8-C7-N2-C2
2	B	502	NAG	O7-C7-N2-C2
2	B	503	NAG	C8-C7-N2-C2
2	B	503	NAG	O7-C7-N2-C2
2	A	502	NAG	C4-C5-C6-O6
2	B	502	NAG	O5-C5-C6-O6
2	B	502	NAG	C4-C5-C6-O6
4	B	504	ATP	O4'-C4'-C5'-O5'
4	A	505	ATP	C5'-O5'-PA-O3A
4	C	501	ATP	C5'-O5'-PA-O3A
4	A	505	ATP	C5'-O5'-PA-O1A
4	C	501	ATP	C5'-O5'-PA-O2A
4	A	505	ATP	PB-O3A-PA-O2A
4	B	504	ATP	C3'-C4'-C5'-O5'
4	C	501	ATP	O4'-C4'-C5'-O5'
4	A	505	ATP	PG-O3B-PB-O2B
4	A	505	ATP	PB-O3A-PA-O1A
4	C	501	ATP	PA-O3A-PB-O1B

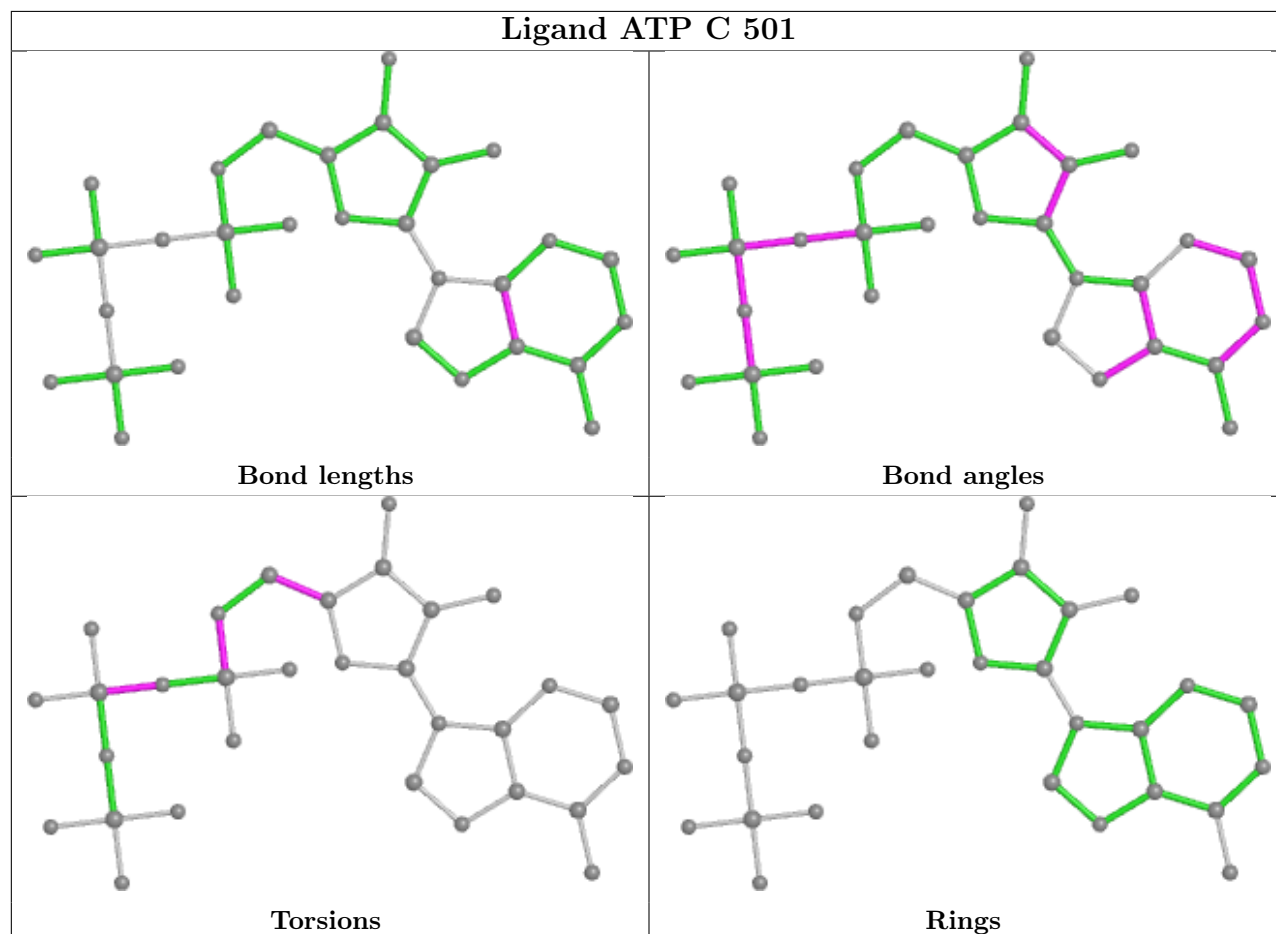
There are no ring outliers.

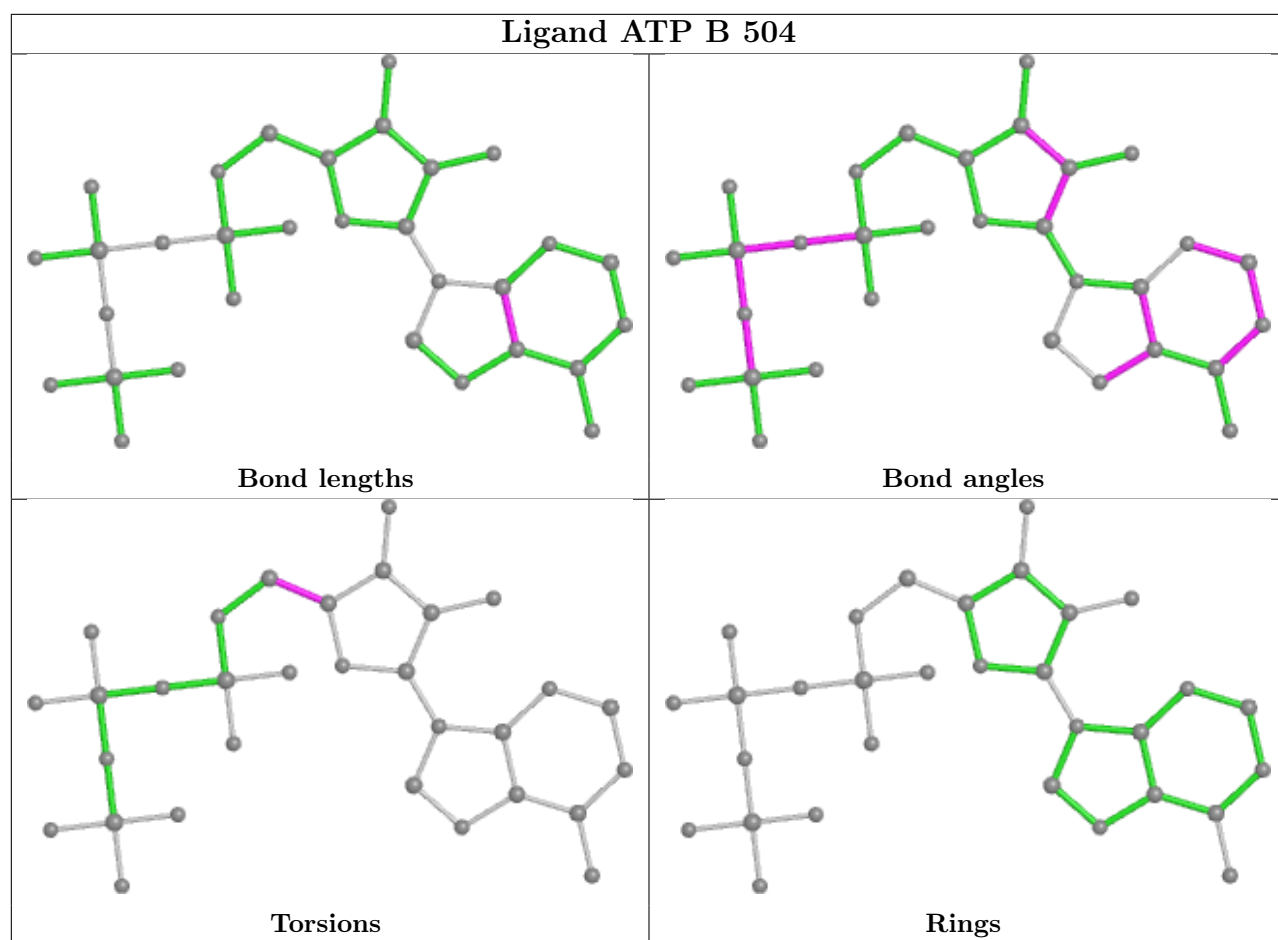
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAG	1	0
3	A	504	A1D8Z	1	0

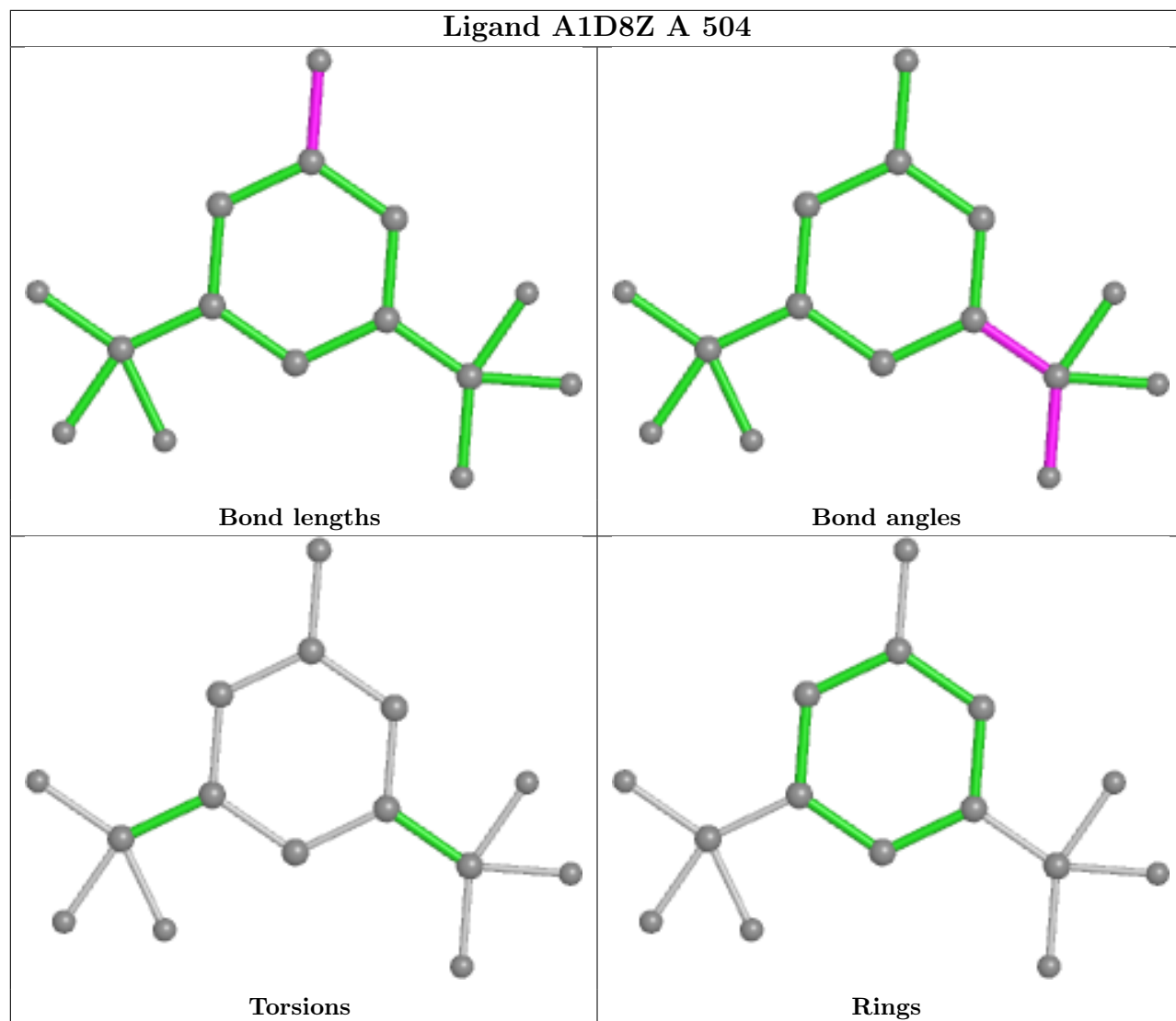
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

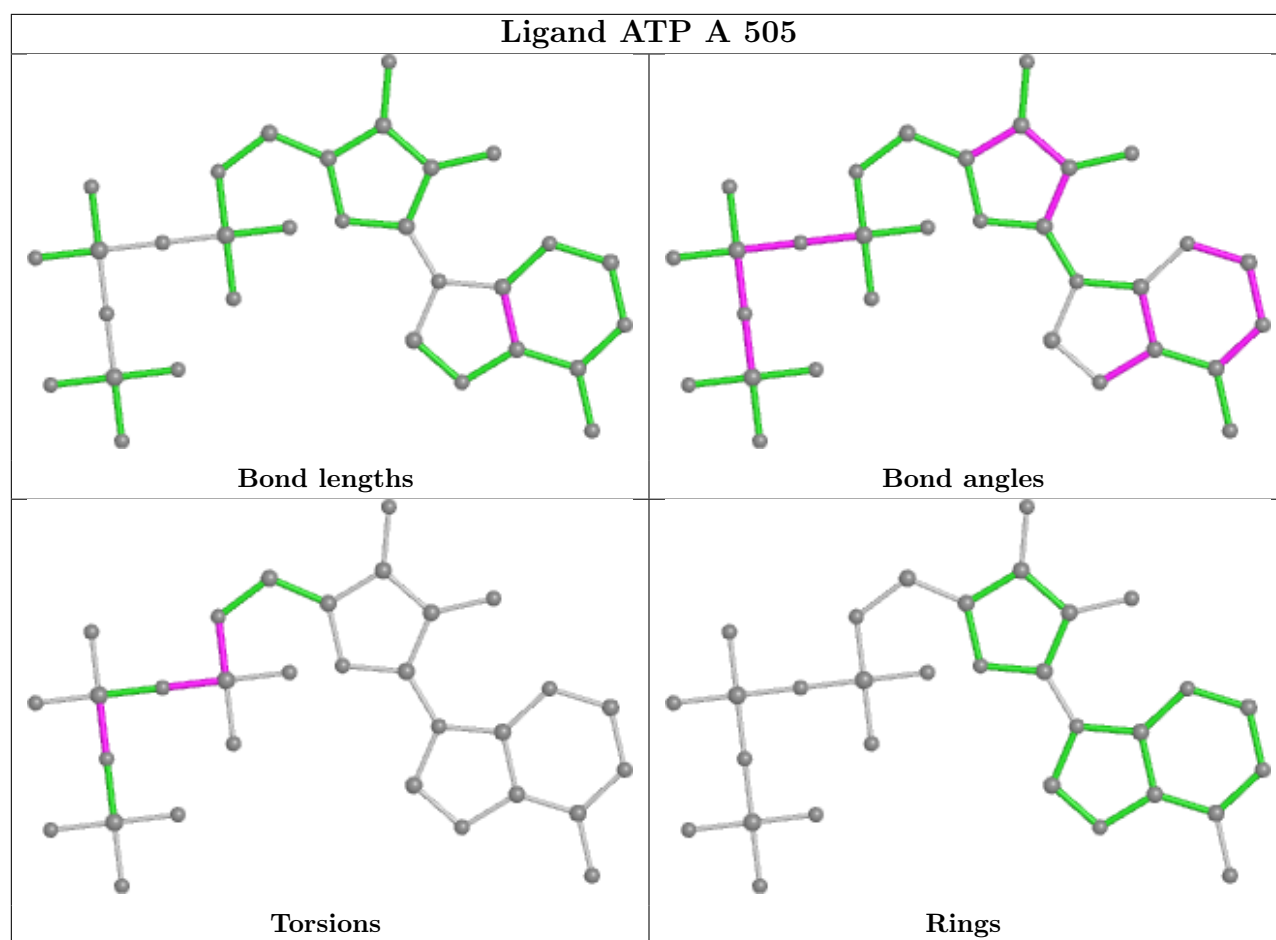
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand A1D8Z A 504





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.