



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:19 pm BST

PDB ID : 2GM1
Title : Crystal structure of the mitotic kinesin eg5 in complex with mg-adp and n-(3-aminopropyl)-n-((3-benzyl-5-chloro-4-oxo-3,4-dihydropyrrolo[2,1-f][1,2,4]triazin-2-yl)(cyclopropyl)methyl)-4-methylbenzamide
Authors : Sheriff, S.
Deposited on : 2006-04-05
Resolution : 2.30 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

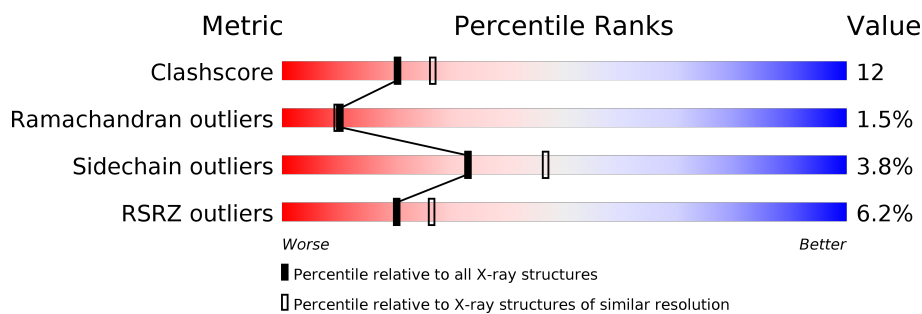
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	368	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	368	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>••</div> <div>13%</div> </div> </div>
1	D	368	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	368	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10443 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.

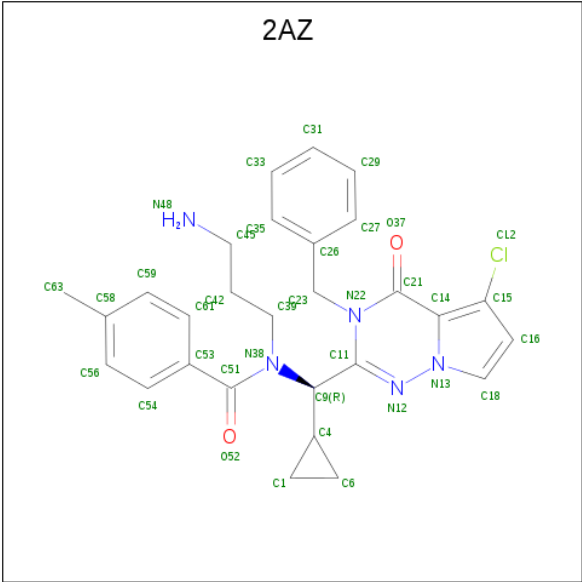
- Molecule 1 is a protein called KINESIN-RELATED MOTOR PROTEIN EG5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	1
			2505	1570	435	490	10			
1	B	321	Total	C	N	O	S	0	0	1
			2467	1550	427	480	10			
1	D	325	Total	C	N	O	S	0	0	1
			2483	1561	432	480	10			
1	E	323	Total	C	N	O	S	0	0	1
			2492	1563	436	483	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

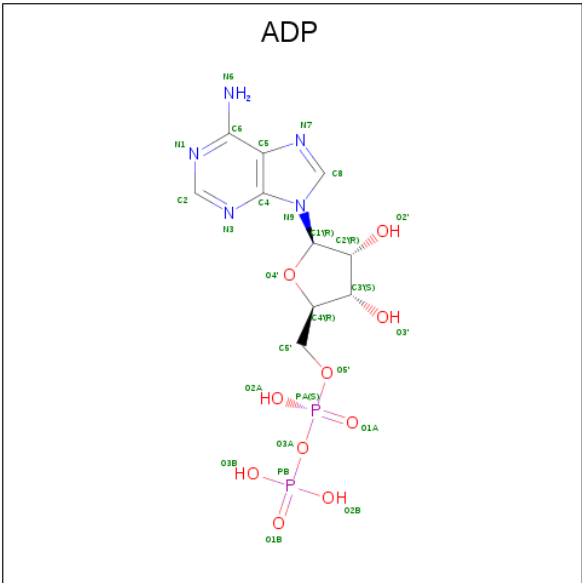
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		

- Molecule 3 is N-(3-AMINOPROPYL)-N-[(R)-(3-BENZYL-5-CHLORO-4-OXO-3,4-DIHYDROPYRROLO[2,1-F][1,2,4]TRIAZIN-2-YL)(CYCLOPROPYL)METHYL]-4-METHYLBENZAMIDE (three-letter code: 2AZ) (formula: C₂₈H₃₀ClN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			36	28	1	5	2		
3	B	1	Total	C	Cl	N	O	0	0
			36	28	1	5	2		
3	D	1	Total	C	Cl	N	O	0	0
			36	28	1	5	2		
3	E	1	Total	C	Cl	N	O	0	0
			36	28	1	5	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

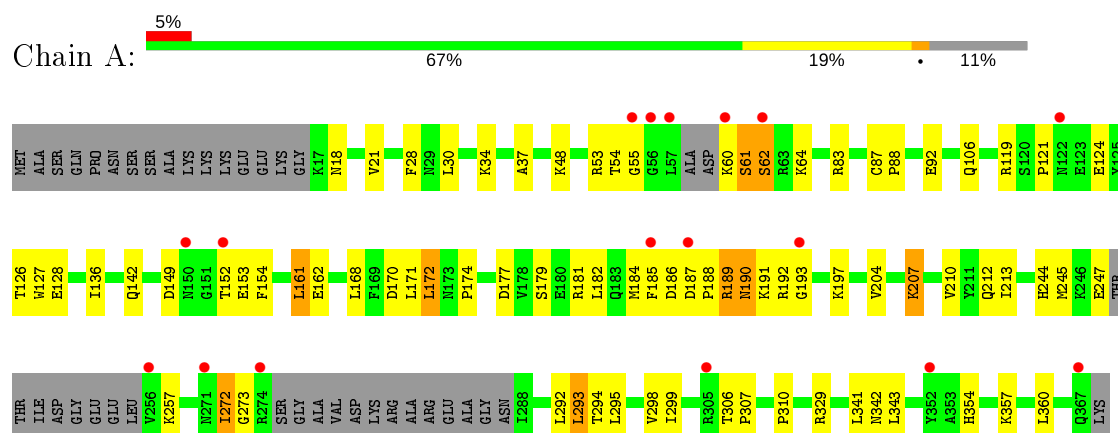
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	44	Total	O	0	0
			44	44		
5	D	55	Total	O	0	0
			55	55		
5	E	68	Total	O	0	0
			68	68		

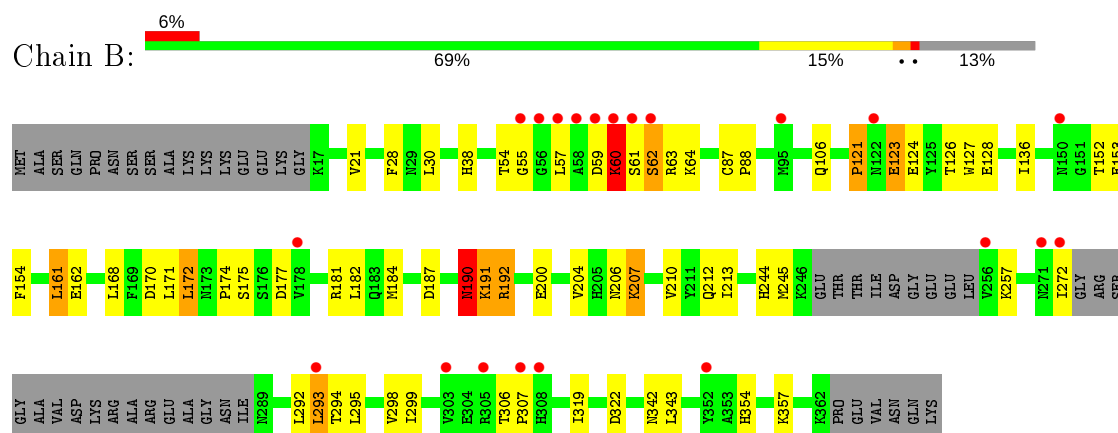
3 Residue-property plots [i](#)

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.

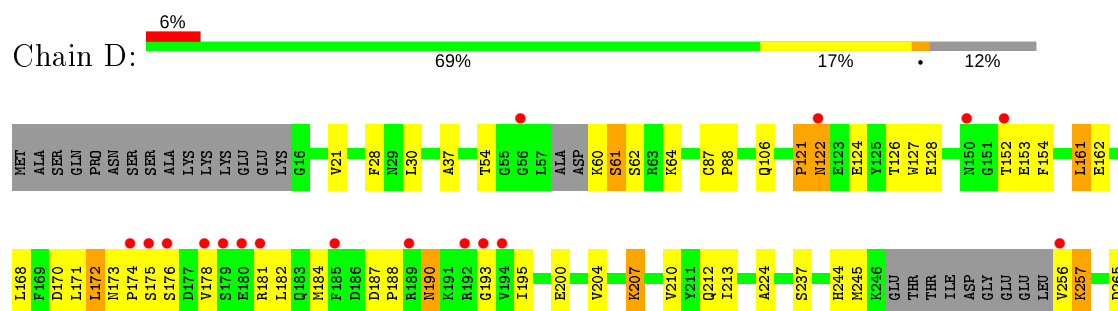
• Molecule 1: KINESIN-RELATED MOTOR PROTEIN EG5



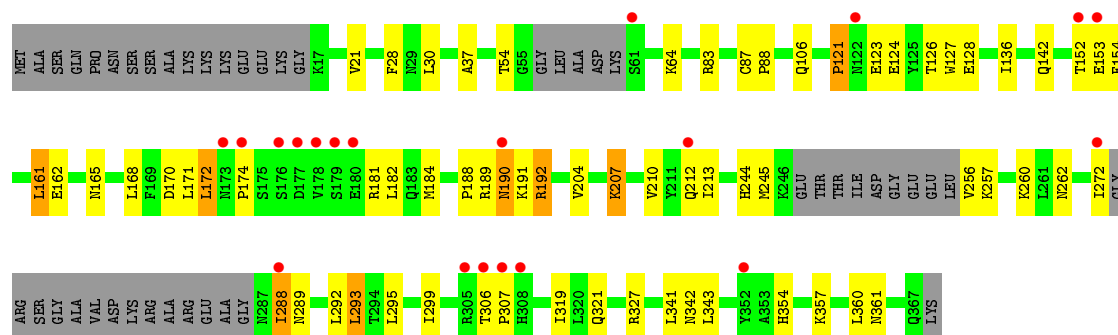
• Molecule 1: KINESIN-RELATED MOTOR PROTEIN EG5



• Molecule 1: KINESIN-RELATED MOTOR PROTEIN EG5



- Molecule 1: KINESIN-RELATED MOTOR PROTEIN EG5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.70 Å 112.60 Å 108.10 Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	49.86 – 2.30 49.85 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.86-2.30) 96.3 (49.85-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.32 Å)	Xtriage
Refinement program	CNS, CNX 2005	Depositor
R, R_{free}	0.230 , 0.269 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,-l,-k 0.000 for -h,l,k 0.167 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10443	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9059e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, 2AZ, ADP

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	0.31	0/2542	0.49	0/3447
1	B	0.31	0/2504	0.49	0/3394
1	D	0.32	0/2520	0.50	0/3416
1	E	0.32	0/2529	0.50	0/3427
All	All	0.31	0/10095	0.50	0/13684

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	1
1	E	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLU	Peptide
1	B	123	GLU	Peptide
1	B	124	GLU	Peptide
1	D	124	GLU	Peptide
1	E	124	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	E	191	LYS	Peptide

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	2505	0	2460	69	0
1	B	2467	0	2446	62	0
1	D	2483	0	2460	64	0
1	E	2492	0	2470	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	36	0	30	1	0
3	B	36	0	30	1	0
3	D	36	0	30	0	0
3	E	36	0	30	1	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	2	0
5	A	69	0	0	2	0
5	B	44	0	0	0	0
5	D	55	0	0	1	0
5	E	68	0	0	5	0
All	All	10443	0	10004	251	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 12.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG22	1:A:153:GLU:H	1.19	1.08
1:B:152:THR:HG22	1:B:153:GLU:H	1.20	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:THR:HG22	1:E:153:GLU:H	1.20	1.04
1:D:152:THR:HG22	1:D:153:GLU:H	1.20	1.04
1:D:60:LYS:HA	1:D:61:SER:CB	1.88	1.03
1:E:192:ARG:HH12	1:E:327:ARG:NH1	1.66	0.94
1:E:192:ARG:NH1	1:E:327:ARG:HH11	1.67	0.91
1:D:256:VAL:HG12	1:D:257:LYS:H	1.37	0.88
1:D:60:LYS:HA	1:D:61:SER:HB2	1.54	0.88
1:A:83:ARG:NH1	1:B:200:GLU:OE1	2.10	0.84
1:D:60:LYS:HA	1:D:61:SER:HB3	1.62	0.80
1:D:175:SER:HB3	1:E:142:GLN:NE2	1.96	0.80
1:B:168:LEU:HD21	1:B:184:MET:HE2	1.65	0.79
1:D:152:THR:HG22	1:D:153:GLU:N	1.98	0.78
1:A:272:ILE:HG13	1:A:273:GLY:H	1.49	0.78
1:E:152:THR:HG22	1:E:153:GLU:N	1.98	0.77
1:D:245:MET:HB2	1:D:256:VAL:HG12	1.67	0.77
1:A:152:THR:HG22	1:A:153:GLU:N	1.97	0.77
1:A:272:ILE:HG13	1:A:273:GLY:N	1.99	0.77
1:B:152:THR:HG22	1:B:153:GLU:N	1.98	0.76
1:A:186:ASP:O	1:A:188:PRO:HD3	1.86	0.75
1:D:168:LEU:HD21	1:D:184:MET:HE2	1.67	0.74
1:B:60:LYS:CD	1:B:63:ARG:HH21	1.99	0.74
1:B:60:LYS:NZ	1:B:60:LYS:HB2	2.03	0.74
1:B:245:MET:O	1:B:257:LYS:HA	1.88	0.73
1:D:245:MET:O	1:D:257:LYS:HA	1.88	0.73
1:E:168:LEU:HD21	1:E:184:MET:HE2	1.68	0.73
1:D:188:PRO:HD3	1:D:195:ILE:HD11	1.71	0.72
1:B:190:ASN:HD22	1:B:190:ASN:C	1.92	0.72
1:D:190:ASN:HD21	1:D:193:GLY:N	1.86	0.72
1:E:245:MET:O	1:E:257:LYS:HA	1.88	0.72
1:E:192:ARG:HH12	1:E:327:ARG:HH11	0.83	0.72
1:D:60:LYS:CA	1:D:61:SER:CB	2.67	0.72
1:A:245:MET:O	1:A:257:LYS:HA	1.89	0.72
1:A:119:ARG:NH1	5:A:425:HOH:O	2.22	0.71
1:A:190:ASN:HD22	1:A:193:GLY:N	1.89	0.69
1:A:60:LYS:O	1:A:61:SER:HB2	1.92	0.67
1:E:162:GLU:HG3	1:E:171:LEU:CD2	2.25	0.67
1:E:192:ARG:NH1	1:E:327:ARG:HD2	2.09	0.67
1:B:60:LYS:HZ3	1:B:60:LYS:HB2	1.59	0.67
1:A:162:GLU:HG3	1:A:171:LEU:CD2	2.25	0.67
1:B:162:GLU:HG3	1:B:171:LEU:CD2	2.25	0.67
1:D:162:GLU:HG3	1:D:171:LEU:CD2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:H	1:A:257:LYS:NZ	1.94	0.65
1:A:55:GLY:HA3	1:A:61:SER:HB3	1.77	0.65
1:A:168:LEU:HD21	1:A:184:MET:HE2	1.79	0.64
1:B:152:THR:CG2	1:B:153:GLU:H	1.98	0.64
1:D:170:ASP:HB2	1:D:182:LEU:HD11	1.82	0.62
1:E:170:ASP:HB2	1:E:182:LEU:HD11	1.82	0.61
1:D:60:LYS:CA	1:D:61:SER:HB3	2.30	0.61
1:B:60:LYS:HD2	1:B:63:ARG:HH21	1.65	0.61
1:D:256:VAL:HG12	1:D:257:LYS:N	2.13	0.61
1:B:61:SER:O	1:B:62:SER:CB	2.48	0.61
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.83	0.60
1:E:189:ARG:O	1:E:190:ASN:C	2.39	0.60
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.83	0.60
1:D:152:THR:CG2	1:D:153:GLU:H	1.98	0.59
1:A:247:GLU:H	1:A:257:LYS:HZ3	1.50	0.59
1:A:161:LEU:HD12	1:A:161:LEU:C	2.22	0.59
1:A:18:ASN:ND2	1:A:360:LEU:HD23	2.17	0.59
1:B:161:LEU:C	1:B:161:LEU:HD12	2.22	0.58
1:D:161:LEU:HD12	1:D:161:LEU:C	2.23	0.58
1:A:272:ILE:CG1	1:A:273:GLY:H	2.15	0.58
1:A:172:LEU:O	1:A:174:PRO:HD3	2.04	0.58
1:A:152:THR:HG23	1:A:154:PHE:CE2	2.39	0.58
1:B:172:LEU:O	1:B:174:PRO:HD3	2.04	0.58
1:D:126:THR:HB	1:D:128:GLU:OE1	2.03	0.58
1:D:188:PRO:HD3	1:D:195:ILE:CD1	2.32	0.58
1:D:152:THR:HG23	1:D:154:PHE:CE2	2.39	0.57
1:E:126:THR:HB	1:E:128:GLU:OE1	2.03	0.57
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.86	0.57
1:B:152:THR:HG23	1:B:154:PHE:CE2	2.40	0.57
1:B:126:THR:HB	1:B:128:GLU:OE1	2.04	0.57
1:A:126:THR:HB	1:A:128:GLU:OE1	2.04	0.57
1:E:161:LEU:C	1:E:161:LEU:HD12	2.25	0.57
1:B:162:GLU:HG3	1:B:171:LEU:HD23	1.87	0.56
1:E:204:VAL:HG11	1:E:210:VAL:CG2	2.35	0.56
1:D:204:VAL:HG11	1:D:210:VAL:CG2	2.35	0.56
1:E:152:THR:HG23	1:E:154:PHE:CE2	2.40	0.56
1:A:185:PHE:CD2	1:A:197:LYS:HE2	2.40	0.56
1:A:48:LYS:HE2	1:B:206:ASN:ND2	2.21	0.56
1:B:190:ASN:O	1:B:191:LYS:CB	2.54	0.56
1:D:172:LEU:O	1:D:174:PRO:HD3	2.04	0.56
1:E:162:GLU:HG3	1:E:171:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:C	1:A:192:ARG:H	2.07	0.56
1:A:187:ASP:HB3	1:A:190:ASN:HB3	1.87	0.56
1:E:152:THR:HG22	5:E:414:HOH:O	2.05	0.56
1:A:190:ASN:O	1:A:192:ARG:N	2.38	0.55
1:E:172:LEU:O	1:E:174:PRO:HD3	2.05	0.55
1:D:162:GLU:HG3	1:D:171:LEU:HD23	1.88	0.55
1:D:175:SER:HB3	1:E:142:GLN:HE21	1.71	0.55
1:A:188:PRO:O	1:A:189:ARG:CB	2.55	0.55
1:A:204:VAL:HG11	1:A:210:VAL:CG2	2.37	0.54
1:D:200:GLU:OE1	1:E:83:ARG:NH1	2.41	0.54
1:A:61:SER:O	1:A:62:SER:CB	2.56	0.54
1:B:187:ASP:HB3	1:B:190:ASN:HB3	1.89	0.54
4:D:372:ADP:H2'	4:D:372:ADP:O5'	2.07	0.54
1:B:204:VAL:HG11	1:B:210:VAL:CG2	2.38	0.54
1:B:60:LYS:HE3	1:B:63:ARG:NH2	2.23	0.53
1:A:185:PHE:HD2	1:A:197:LYS:HE2	1.73	0.53
1:A:295:LEU:O	1:A:299:ILE:HG12	2.07	0.53
1:A:92:GLU:HG3	1:A:329:ARG:NH1	2.23	0.53
1:B:295:LEU:O	1:B:299:ILE:HG12	2.08	0.53
1:D:295:LEU:O	1:D:299:ILE:HG12	2.09	0.53
1:A:168:LEU:HD21	1:A:184:MET:CE	2.40	0.52
1:B:127:TRP:HZ2	1:B:207:LYS:HG2	1.75	0.52
1:B:60:LYS:HE3	1:B:63:ARG:HH21	1.75	0.52
1:B:168:LEU:HD21	1:B:184:MET:CE	2.40	0.51
4:B:372:ADP:O5'	4:B:372:ADP:H2'	2.10	0.51
1:D:204:VAL:HG11	1:D:210:VAL:HG23	1.93	0.51
1:E:168:LEU:HD21	1:E:184:MET:CE	2.39	0.51
1:E:295:LEU:O	1:E:299:ILE:HG12	2.10	0.51
1:B:106:GLN:HE22	1:B:342:ASN:ND2	2.09	0.51
1:E:204:VAL:HG11	1:E:210:VAL:HG23	1.93	0.51
1:E:244:HIS:HD2	5:E:418:HOH:O	1.94	0.51
4:E:372:ADP:O5'	4:E:372:ADP:H2'	2.09	0.51
4:A:372:ADP:O5'	4:A:372:ADP:H2'	2.11	0.51
1:D:245:MET:SD	1:D:256:VAL:HG13	2.50	0.51
1:A:127:TRP:HZ2	1:A:207:LYS:HG2	1.76	0.50
1:B:60:LYS:CE	1:B:63:ARG:HH21	2.24	0.50
1:E:121:PRO:C	1:E:123:GLU:H	2.14	0.50
1:D:244:HIS:HD2	5:D:415:HOH:O	1.94	0.50
1:A:187:ASP:HB3	1:A:190:ASN:CB	2.41	0.50
1:B:354:HIS:O	1:B:357:LYS:HG2	2.11	0.50
1:A:152:THR:HG23	1:A:154:PHE:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:PRO:O	1:E:123:GLU:N	2.43	0.49
1:B:190:ASN:ND2	1:B:190:ASN:C	2.64	0.49
1:B:38:HIS:CE1	1:B:57:LEU:HB2	2.48	0.49
1:D:152:THR:HG23	1:D:154:PHE:HE2	1.77	0.49
1:A:34:LYS:HG3	4:E:372:ADP:C2	2.47	0.49
1:A:190:ASN:HD22	1:A:193:GLY:H	1.59	0.49
1:D:168:LEU:HD21	1:D:184:MET:CE	2.39	0.49
1:A:106:GLN:HE22	1:A:342:ASN:ND2	2.11	0.49
1:D:354:HIS:O	1:D:357:LYS:HG2	2.12	0.49
1:E:188:PRO:HG2	1:E:189:ARG:NH1	2.27	0.49
1:E:354:HIS:O	1:E:357:LYS:HG2	2.12	0.49
1:A:204:VAL:HG11	1:A:210:VAL:HG23	1.95	0.49
1:A:354:HIS:O	1:A:357:LYS:HG2	2.12	0.49
1:B:192:ARG:NH2	1:B:322:ASP:OD1	2.46	0.49
1:B:152:THR:HG23	1:B:154:PHE:HE2	1.78	0.49
1:D:306:THR:HB	1:D:307:PRO:HD2	1.95	0.49
1:E:192:ARG:HB2	1:E:321:GLN:CD	2.34	0.48
1:B:306:THR:HB	1:B:307:PRO:HD2	1.95	0.48
1:E:306:THR:HB	1:E:307:PRO:HD2	1.95	0.48
1:A:177:ASP:OD2	1:A:179:SER:HB3	2.14	0.48
1:A:306:THR:HB	1:A:307:PRO:HD2	1.95	0.48
1:B:55:GLY:HA3	1:B:61:SER:CB	2.43	0.48
1:B:54:THR:HG21	1:B:64:LYS:HG3	1.95	0.48
1:A:149:ASP:OD2	1:B:177:ASP:HB2	2.14	0.48
1:D:54:THR:HG21	1:D:64:LYS:HG3	1.95	0.47
1:B:204:VAL:HG11	1:B:210:VAL:HG23	1.97	0.47
1:E:152:THR:HG23	1:E:154:PHE:HE2	1.79	0.47
1:E:127:TRP:HZ2	1:E:207:LYS:HG2	1.79	0.47
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.95	0.47
1:E:212:GLN:HG3	1:E:213:ILE:N	2.28	0.47
1:D:127:TRP:HZ2	1:D:207:LYS:HG2	1.79	0.47
1:B:60:LYS:HD2	1:B:63:ARG:HE	1.80	0.47
1:A:60:LYS:O	1:A:61:SER:CB	2.63	0.47
1:A:142:GLN:CD	1:B:175:SER:HB3	2.34	0.46
1:D:21:VAL:CG2	1:D:357:LYS:HB3	2.46	0.46
1:E:54:THR:HG21	1:E:64:LYS:HG3	1.96	0.46
1:E:106:GLN:HE22	1:E:342:ASN:ND2	2.13	0.46
1:D:187:ASP:CB	1:D:190:ASN:HD22	2.29	0.46
1:D:60:LYS:HE2	1:D:62:SER:HB2	1.97	0.46
1:D:106:GLN:HE22	1:D:342:ASN:ND2	2.13	0.46
1:A:152:THR:CG2	1:A:153:GLU:N	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:CG2	1:B:357:LYS:HB3	2.45	0.46
1:A:53:ARG:HD2	1:A:60:LYS:N	2.31	0.45
1:A:189:ARG:O	1:A:190:ASN:HB2	2.16	0.45
1:B:121:PRO:C	1:B:123:GLU:H	2.20	0.45
1:D:256:VAL:O	1:D:257:LYS:HB3	2.16	0.45
1:A:212:GLN:HG3	1:A:213:ILE:N	2.31	0.45
1:B:127:TRP:CZ2	1:B:207:LYS:HG2	2.52	0.45
1:B:212:GLN:HG3	1:B:213:ILE:N	2.31	0.45
1:E:288:ILE:HA	1:E:289:ASN:HA	1.46	0.44
1:E:87:CYS:HB2	1:E:88:PRO:HD3	1.98	0.44
1:D:121:PRO:O	1:D:122:ASN:C	2.55	0.44
1:E:165:ASN:HA	1:E:288:ILE:HG23	1.98	0.44
1:E:172:LEU:HA	1:E:172:LEU:HD12	1.75	0.44
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.77	0.44
1:B:60:LYS:CB	1:B:60:LYS:NZ	2.76	0.44
1:D:212:GLN:HG3	1:D:213:ILE:N	2.31	0.44
1:E:152:THR:CG2	1:E:153:GLU:H	1.98	0.44
1:E:207:LYS:HB3	5:E:395:HOH:O	2.18	0.44
1:E:21:VAL:CG2	1:E:357:LYS:HB3	2.48	0.44
1:B:61:SER:O	1:B:62:SER:OG	2.31	0.44
1:B:136:ILE:HD13	3:B:371:2AZ:CL2	2.54	0.44
1:B:87:CYS:HB2	1:B:88:PRO:HD3	1.99	0.44
1:D:204:VAL:HG11	1:D:210:VAL:HG22	1.99	0.44
1:E:136:ILE:HD13	3:E:371:2AZ:CL2	2.55	0.44
1:E:204:VAL:HG11	1:E:210:VAL:HG22	2.00	0.44
1:D:87:CYS:HB2	1:D:88:PRO:HD3	1.99	0.44
1:E:272:ILE:HG22	1:E:293:LEU:HD22	1.99	0.43
1:A:127:TRP:CZ2	1:A:207:LYS:HG2	2.53	0.43
1:E:256:VAL:O	1:E:257:LYS:HB3	2.18	0.43
1:B:184:MET:HE3	1:B:319:ILE:HD11	2.01	0.43
1:A:207:LYS:O	1:A:210:VAL:HB	2.18	0.43
1:D:256:VAL:O	1:D:257:LYS:CB	2.65	0.43
1:A:272:ILE:HG22	1:A:293:LEU:HD22	2.00	0.43
1:B:272:ILE:HG22	1:B:293:LEU:HD22	2.00	0.43
1:D:190:ASN:HD21	1:D:193:GLY:CA	2.31	0.43
1:A:18:ASN:HD22	1:A:360:LEU:HD23	1.83	0.43
1:A:87:CYS:HB2	1:A:88:PRO:HD3	2.01	0.43
1:E:37:ALA:HB2	1:E:341:LEU:HD22	2.01	0.43
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.76	0.42
1:B:207:LYS:O	1:B:210:VAL:HB	2.19	0.42
1:E:207:LYS:CB	5:E:395:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:O	1:B:61:SER:N	2.52	0.42
1:E:207:LYS:O	1:E:210:VAL:HB	2.20	0.42
1:B:21:VAL:HG21	1:B:357:LYS:HB3	2.02	0.42
1:D:152:THR:CG2	1:D:153:GLU:N	2.68	0.42
1:D:153:GLU:OE2	1:D:153:GLU:HA	2.20	0.42
1:A:153:GLU:OE2	1:A:153:GLU:HA	2.20	0.42
1:D:244:HIS:HA	1:D:257:LYS:O	2.20	0.42
1:A:21:VAL:CG2	1:A:357:LYS:HB3	2.49	0.42
1:B:154:PHE:HA	1:B:244:HIS:O	2.20	0.42
1:B:294:THR:O	1:B:298:VAL:HG23	2.20	0.42
1:D:37:ALA:HB2	1:D:341:LEU:HD22	2.01	0.42
1:A:310:PRO:HA	5:A:437:HOH:O	2.19	0.42
1:D:327:ARG:HA	1:D:362:LYS:O	2.20	0.42
1:E:184:MET:HE3	1:E:319:ILE:HD11	2.02	0.42
1:A:154:PHE:HA	1:A:244:HIS:O	2.20	0.41
1:A:294:THR:O	1:A:298:VAL:HG23	2.21	0.41
1:B:204:VAL:HG11	1:B:210:VAL:HG22	2.01	0.41
1:B:244:HIS:HA	1:B:257:LYS:O	2.20	0.41
1:A:244:HIS:HA	1:A:257:LYS:O	2.20	0.41
1:D:294:THR:O	1:D:298:VAL:HG23	2.19	0.41
1:D:21:VAL:HG21	1:D:357:LYS:HB3	2.02	0.41
1:A:204:VAL:HG11	1:A:210:VAL:HG22	2.01	0.41
1:E:360:LEU:HD13	1:E:361:ASN:O	2.21	0.41
1:D:184:MET:HE3	1:D:319:ILE:HD11	2.03	0.41
1:E:154:PHE:HA	1:E:244:HIS:O	2.20	0.41
1:A:184:MET:HB3	1:A:184:MET:HE2	1.90	0.41
1:D:272:ILE:HG22	1:D:293:LEU:HD22	2.02	0.41
1:B:190:ASN:ND2	1:B:192:ARG:H	2.19	0.41
1:D:207:LYS:O	1:D:210:VAL:HB	2.21	0.41
1:E:244:HIS:CD2	5:E:418:HOH:O	2.72	0.41
1:E:192:ARG:HH11	1:E:327:ARG:HD2	1.85	0.41
1:A:136:ILE:HD13	3:A:371:2AZ:CL2	2.58	0.41
1:D:172:LEU:HD12	1:D:172:LEU:HA	1.73	0.41
1:A:37:ALA:HB2	1:A:341:LEU:HD22	2.02	0.41
1:B:153:GLU:OE2	1:B:153:GLU:HA	2.21	0.41
1:D:237:SER:HB3	1:D:265:ASP:HB3	2.02	0.41
1:E:260:LYS:HE2	1:E:262:ASN:HD21	1.86	0.41
1:D:245:MET:HB2	1:D:256:VAL:CG1	2.44	0.41
1:E:152:THR:CG2	1:E:153:GLU:N	2.68	0.41
1:E:244:HIS:HA	1:E:257:LYS:O	2.21	0.40
1:D:127:TRP:CZ2	1:D:207:LYS:HG2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ASN:ND2	1:D:176:SER:HB2	2.36	0.40
1:E:127:TRP:CZ2	1:E:207:LYS:HG2	2.55	0.40
1:D:178:VAL:HG21	1:D:224:ALA:HB2	2.04	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	320/368 (87%)	306 (96%)	7 (2%)	7 (2%)	6	5
1	B	315/368 (86%)	303 (96%)	7 (2%)	5 (2%)	9	9
1	D	317/368 (86%)	304 (96%)	8 (2%)	5 (2%)	9	9
1	E	315/368 (86%)	304 (96%)	9 (3%)	2 (1%)	25	31
All	All	1267/1472 (86%)	1217 (96%)	31 (2%)	19 (2%)	10	10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	62	SER
1	B	60	LYS
1	B	62	SER
1	B	191	LYS
1	D	61	SER
1	D	122	ASN
1	E	121	PRO
1	A	121	PRO
1	A	189	ARG
1	A	190	ASN
1	B	121	PRO

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Mol	Chain	Res	Type
1	D	121	PRO
1	E	190	ASN
1	A	191	LYS
1	A	272	ILE
1	D	190	ASN
1	D	257	LYS
1	B	190	ASN

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	274/322 (85%)	265 (97%)	9 (3%)	38	53
1	B	271/322 (84%)	259 (96%)	12 (4%)	28	39
1	D	272/322 (84%)	263 (97%)	9 (3%)	38	53
1	E	275/322 (85%)	264 (96%)	11 (4%)	31	44
All	All	1092/1288 (85%)	1051 (96%)	41 (4%)	33	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	30	LEU
1	A	161	LEU
1	A	172	LEU
1	A	181	ARG
1	A	207	LYS
1	A	292	LEU
1	A	293	LEU
1	A	343	LEU
1	B	28	PHE
1	B	30	LEU
1	B	60	LYS
1	B	161	LEU
1	B	172	LEU

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Mol	Chain	Res	Type
1	B	181	ARG
1	B	190	ASN
1	B	192	ARG
1	B	207	LYS
1	B	292	LEU
1	B	293	LEU
1	B	343	LEU
1	D	28	PHE
1	D	30	LEU
1	D	161	LEU
1	D	172	LEU
1	D	181	ARG
1	D	207	LYS
1	D	292	LEU
1	D	293	LEU
1	D	343	LEU
1	E	28	PHE
1	E	30	LEU
1	E	161	LEU
1	E	172	LEU
1	E	181	ARG
1	E	192	ARG
1	E	207	LYS
1	E	288	ILE
1	E	292	LEU
1	E	293	LEU
1	E	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	190	ASN
1	A	205	HIS
1	A	229	ASN
1	A	262	ASN
1	A	321	GLN
1	A	342	ASN
1	A	354	HIS
1	B	190	ASN
1	B	205	HIS
1	B	262	ASN

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Mol	Chain	Res	Type
1	B	321	GLN
1	B	342	ASN
1	D	190	ASN
1	D	205	HIS
1	D	229	ASN
1	D	244	HIS
1	D	262	ASN
1	D	321	GLN
1	D	342	ASN
1	E	142	GLN
1	E	205	HIS
1	E	229	ASN
1	E	262	ASN
1	E	321	GLN
1	E	342	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	ADP	D	372	2	24,29,29	1.32	2 (8%)	29,45,45	1.94	5 (17%)
4	ADP	B	372	2	24,29,29	1.42	3 (12%)	29,45,45	2.02	4 (13%)
3	2AZ	B	371	-	35,40,40	1.73	7 (20%)	39,57,57	1.47	6 (15%)
4	ADP	E	372	2	24,29,29	1.39	3 (12%)	29,45,45	1.89	4 (13%)
3	2AZ	E	371	-	35,40,40	1.64	7 (20%)	39,57,57	1.47	5 (12%)
4	ADP	A	372	2	24,29,29	1.49	3 (12%)	29,45,45	2.02	4 (13%)
3	2AZ	A	371	-	35,40,40	1.78	8 (22%)	39,57,57	1.49	4 (10%)
3	2AZ	D	371	-	35,40,40	1.68	6 (17%)	39,57,57	1.48	5 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	372	2	-	2/12/32/32	0/3/3/3
4	ADP	B	372	2	-	2/12/32/32	0/3/3/3
3	2AZ	B	371	-	-	4/24/30/30	0/5/5/5
4	ADP	E	372	2	-	2/12/32/32	0/3/3/3
3	2AZ	E	371	-	-	5/24/30/30	0/5/5/5
4	ADP	A	372	2	-	3/12/32/32	0/3/3/3
3	2AZ	A	371	-	-	5/24/30/30	0/5/5/5
3	2AZ	D	371	-	-	5/24/30/30	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	371	2AZ	C11-C9	4.75	1.57	1.50
3	B	371	2AZ	C11-C9	4.70	1.57	1.50
3	A	371	2AZ	C11-N12	4.64	1.38	1.31
3	D	371	2AZ	C11-N12	4.42	1.37	1.31
3	B	371	2AZ	C11-N12	4.24	1.37	1.31
3	E	371	2AZ	C11-C9	4.16	1.57	1.50
4	B	372	ADP	C2-N3	4.15	1.38	1.32
3	E	371	2AZ	C11-N12	4.10	1.37	1.31
4	E	372	ADP	C2-N3	3.88	1.38	1.32
4	A	372	ADP	C2-N3	3.85	1.38	1.32
3	D	371	2AZ	C11-C9	3.83	1.56	1.50
4	D	372	ADP	C2-N3	3.68	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	371	2AZ	C21-C14	3.62	1.47	1.41
3	E	371	2AZ	C21-C14	3.49	1.46	1.41
3	D	371	2AZ	C21-C14	3.36	1.46	1.41
3	A	371	2AZ	C21-C14	3.32	1.46	1.41
4	E	372	ADP	C4-N3	3.20	1.40	1.35
3	E	371	2AZ	C51-N38	3.04	1.41	1.34
4	A	372	ADP	C4-N3	3.03	1.39	1.35
3	D	371	2AZ	C51-N38	2.98	1.41	1.34
4	A	372	ADP	PB-O3B	-2.84	1.43	1.54
4	B	372	ADP	C4-N3	2.81	1.39	1.35
4	D	372	ADP	C4-N3	2.74	1.39	1.35
3	B	371	2AZ	C51-N38	2.73	1.41	1.34
3	D	371	2AZ	C39-N38	2.66	1.51	1.46
3	A	371	2AZ	C51-N38	2.62	1.40	1.34
3	B	371	2AZ	C39-N38	2.60	1.51	1.46
3	A	371	2AZ	C15-CL2	-2.51	1.67	1.74
3	A	371	2AZ	C61-C53	2.28	1.43	1.39
3	D	371	2AZ	C61-C53	2.25	1.43	1.39
3	A	371	2AZ	C14-N13	2.23	1.43	1.40
3	B	371	2AZ	C15-CL2	-2.20	1.68	1.74
3	E	371	2AZ	C39-N38	2.20	1.50	1.46
3	E	371	2AZ	C61-C53	2.16	1.43	1.39
4	B	372	ADP	PB-O3B	-2.13	1.46	1.54
3	A	371	2AZ	C39-N38	2.10	1.50	1.46
3	B	371	2AZ	C23-N22	-2.09	1.44	1.48
3	E	371	2AZ	C23-N22	-2.08	1.44	1.48
4	E	372	ADP	PA-O5'	-2.07	1.50	1.59

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	372	ADP	N3-C2-N1	-7.70	116.65	128.68
4	B	372	ADP	N3-C2-N1	-7.47	117.00	128.68
4	D	372	ADP	N3-C2-N1	-7.12	117.54	128.68
4	E	372	ADP	N3-C2-N1	-6.87	117.94	128.68
3	B	371	2AZ	C14-C21-N22	-5.05	115.11	120.30
3	A	371	2AZ	C14-C21-N22	-4.91	115.26	120.30
3	A	371	2AZ	C42-C39-N38	4.79	120.72	113.31
3	D	371	2AZ	C14-C21-N22	-4.79	115.38	120.30
3	E	371	2AZ	C14-C21-N22	-4.79	115.38	120.30
3	E	371	2AZ	C42-C39-N38	4.55	120.34	113.31
4	D	372	ADP	C2'-C3'-C4'	-4.54	93.82	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	371	2AZ	C42-C39-N38	4.46	120.20	113.31
4	B	372	ADP	C2'-C3'-C4'	-4.43	94.03	102.64
4	E	372	ADP	C2'-C3'-C4'	-4.29	94.30	102.64
3	D	371	2AZ	C42-C39-N38	4.25	119.88	113.31
4	A	372	ADP	C2'-C3'-C4'	-4.03	94.81	102.64
4	B	372	ADP	O4'-C1'-C2'	-3.44	101.90	106.93
4	A	372	ADP	O4'-C1'-C2'	-3.17	102.29	106.93
3	E	371	2AZ	C16-C18-N13	-3.06	104.58	106.73
4	D	372	ADP	O4'-C1'-C2'	-3.03	102.50	106.93
3	A	371	2AZ	C18-C16-C15	3.00	109.75	105.88
3	D	371	2AZ	C16-C18-N13	-2.93	104.67	106.73
4	E	372	ADP	O4'-C1'-C2'	-2.89	102.70	106.93
3	D	371	2AZ	C18-C16-C15	2.82	109.51	105.88
4	A	372	ADP	C2-N1-C6	2.79	123.53	118.75
3	B	371	2AZ	C18-C16-C15	2.78	109.47	105.88
3	E	371	2AZ	C18-C16-C15	2.77	109.44	105.88
3	B	371	2AZ	C16-C18-N13	-2.72	104.82	106.73
3	A	371	2AZ	C16-C18-N13	-2.65	104.86	106.73
4	E	372	ADP	C2-N1-C6	2.29	122.67	118.75
4	B	372	ADP	C2-N1-C6	2.27	122.63	118.75
4	D	372	ADP	C2-N1-C6	2.09	122.33	118.75
3	D	371	2AZ	C23-N22-C21	-2.05	115.32	117.79
3	E	371	2AZ	C9-N38-C51	2.04	127.78	121.00
3	B	371	2AZ	C9-N38-C51	2.03	127.73	121.00
3	B	371	2AZ	C1-C4-C9	-2.01	115.44	119.28
4	D	372	ADP	C1'-N9-C4	2.00	130.16	126.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	372	ADP	PA-O3A-PB-O2B
4	D	372	ADP	PA-O3A-PB-O3B
4	B	372	ADP	PA-O3A-PB-O2B
4	B	372	ADP	PA-O3A-PB-O3B
3	E	371	2AZ	C42-C39-N38-C51
3	B	371	2AZ	C42-C39-N38-C51
4	E	372	ADP	PA-O3A-PB-O2B
4	E	372	ADP	PA-O3A-PB-O3B
4	A	372	ADP	PA-O3A-PB-O2B
4	A	372	ADP	PA-O3A-PB-O3B
3	A	371	2AZ	C42-C39-N38-C51

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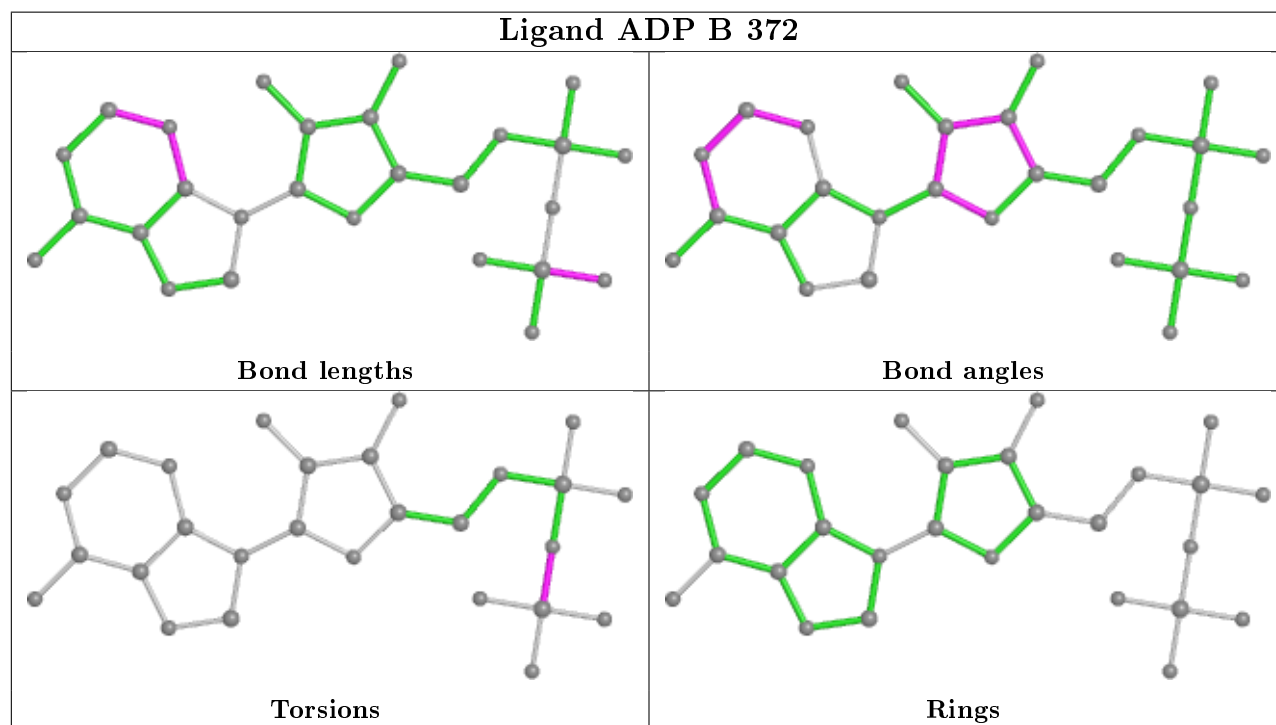
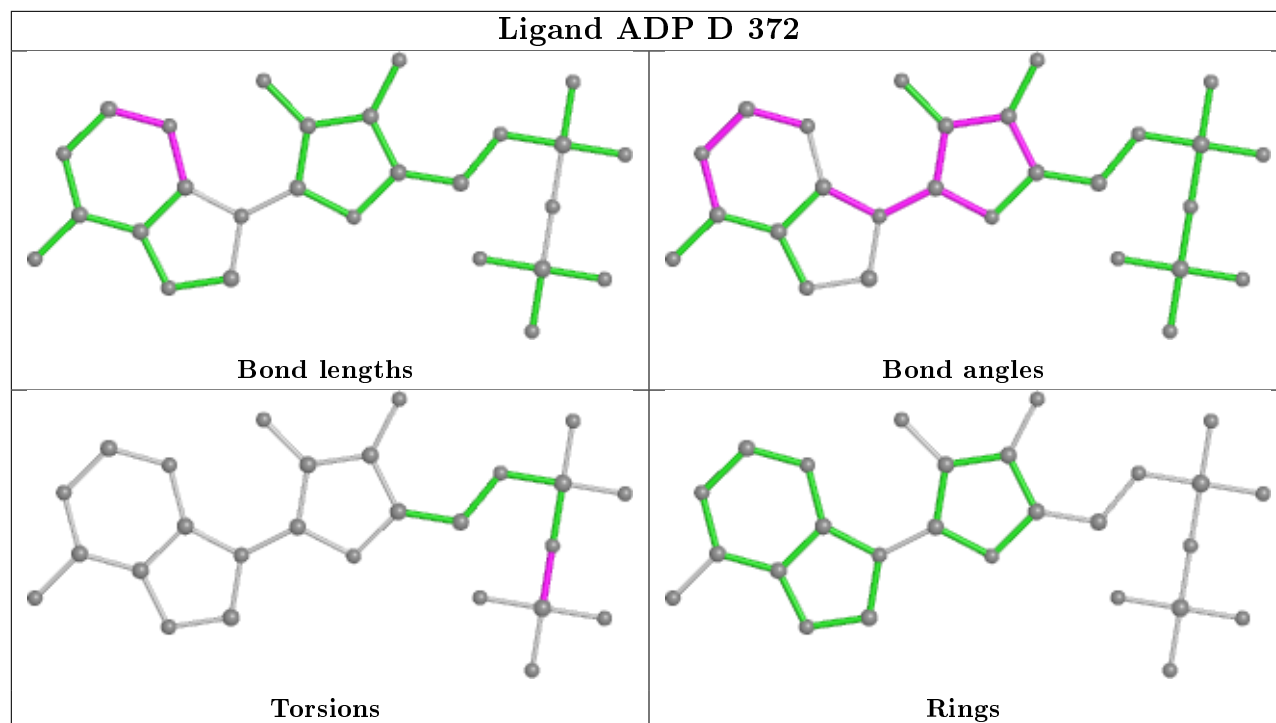
Mol	Chain	Res	Type	Atoms
3	D	371	2AZ	C42-C39-N38-C51
3	B	371	2AZ	N38-C39-C42-C45
3	E	371	2AZ	N38-C39-C42-C45
3	A	371	2AZ	N38-C39-C42-C45
3	D	371	2AZ	N38-C39-C42-C45
3	E	371	2AZ	C39-C42-C45-N48
3	B	371	2AZ	C39-C42-C45-N48
3	A	371	2AZ	C39-C42-C45-N48
3	D	371	2AZ	C39-C42-C45-N48
3	E	371	2AZ	C42-C39-N38-C9
3	B	371	2AZ	C42-C39-N38-C9
3	A	371	2AZ	C42-C39-N38-C9
3	D	371	2AZ	C42-C39-N38-C9
4	A	372	ADP	PA-O3A-PB-O1B
3	D	371	2AZ	N22-C23-C26-C27
3	A	371	2AZ	N22-C23-C26-C27
3	E	371	2AZ	N22-C23-C26-C27

There are no ring outliers.

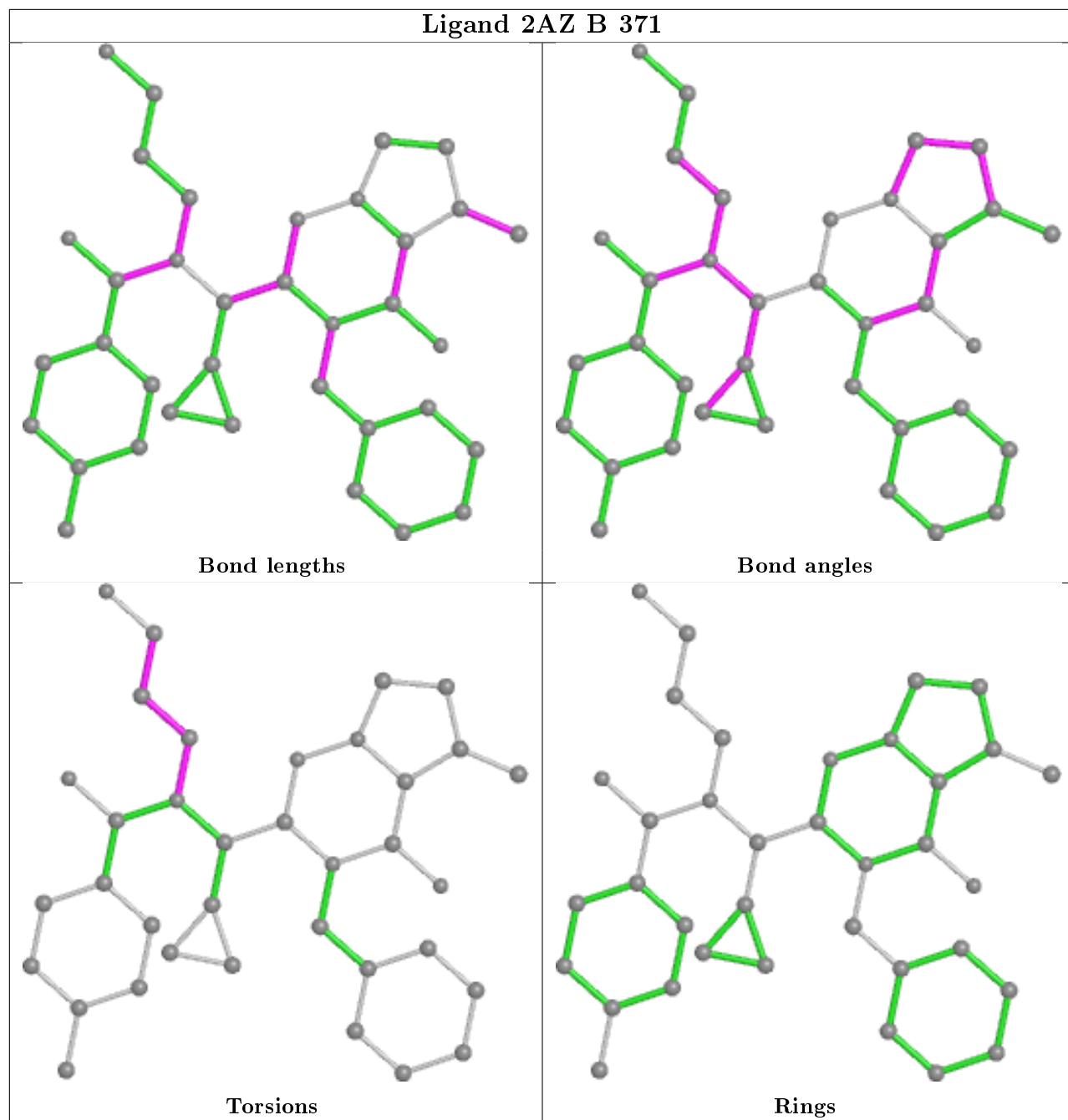
7 monomers are involved in 8 short contacts:

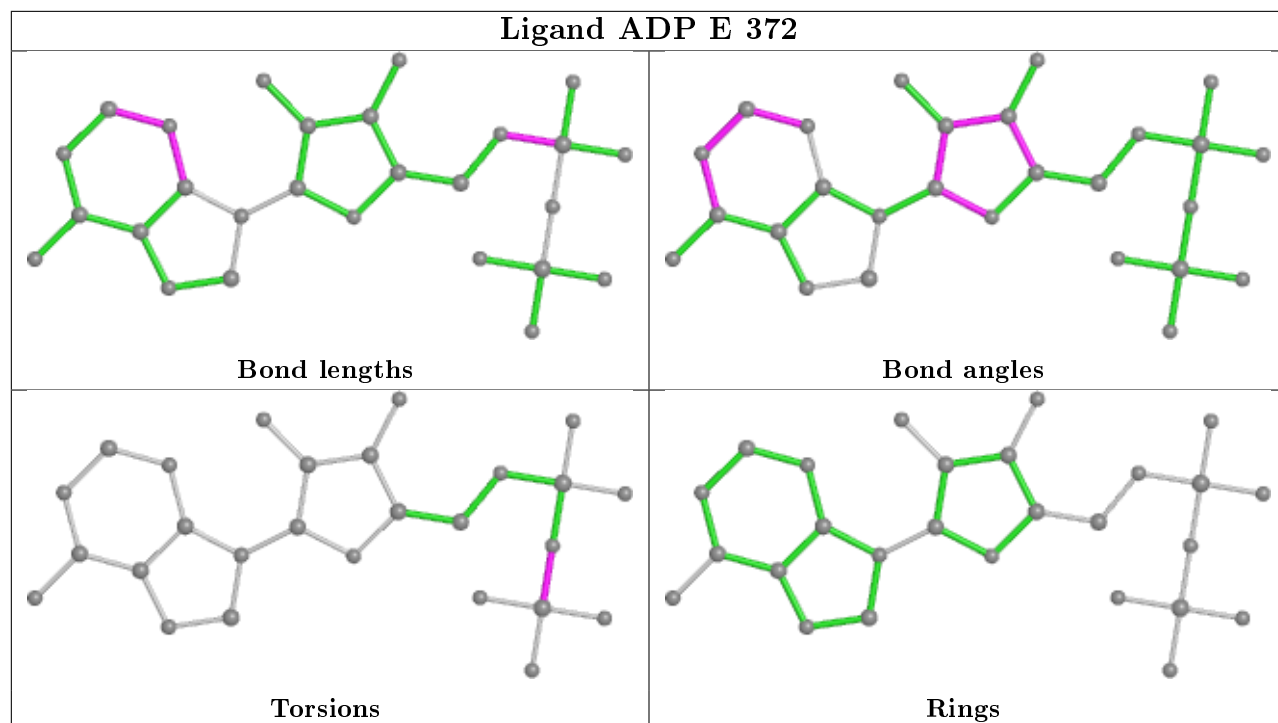
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	372	ADP	1	0
4	B	372	ADP	1	0
3	B	371	2AZ	1	0
4	E	372	ADP	2	0
3	E	371	2AZ	1	0
4	A	372	ADP	1	0
3	A	371	2AZ	1	0

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.

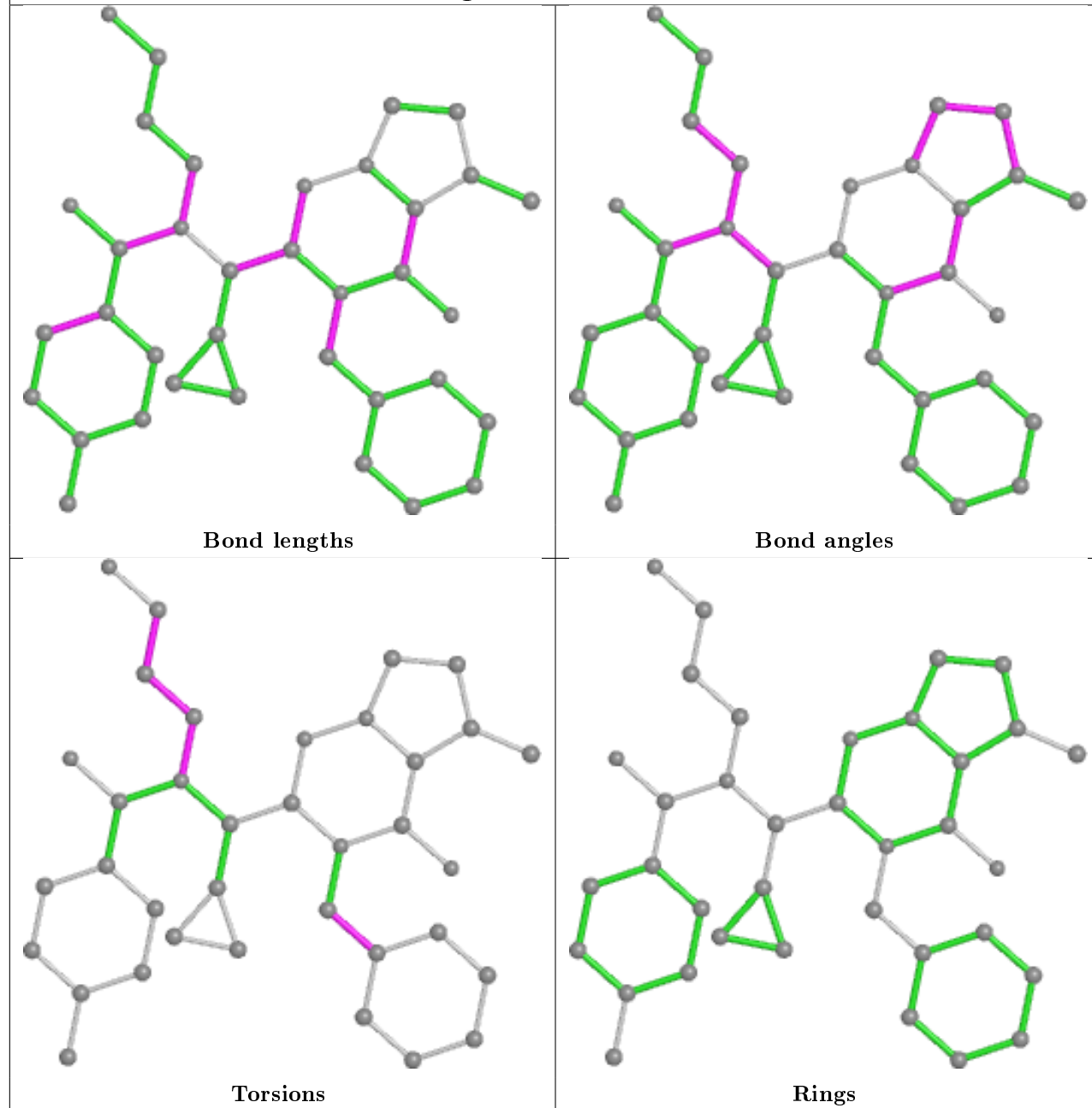


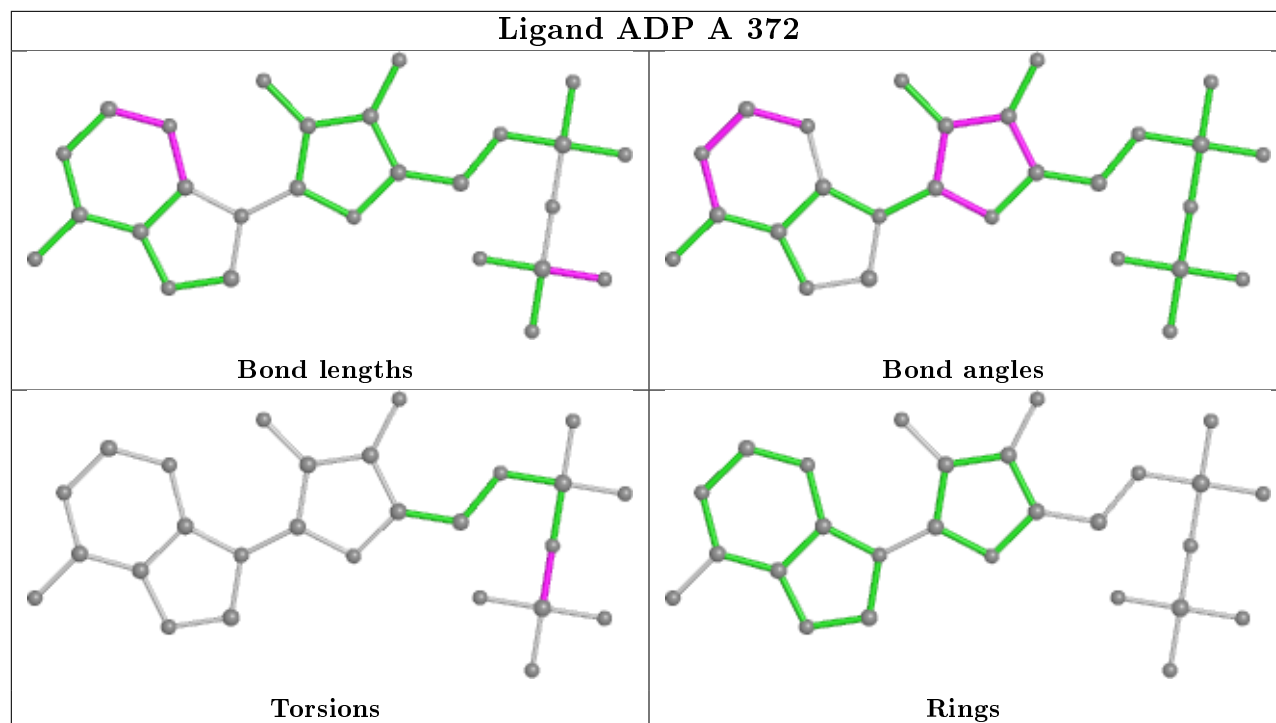
Ligand 2AZ B 371



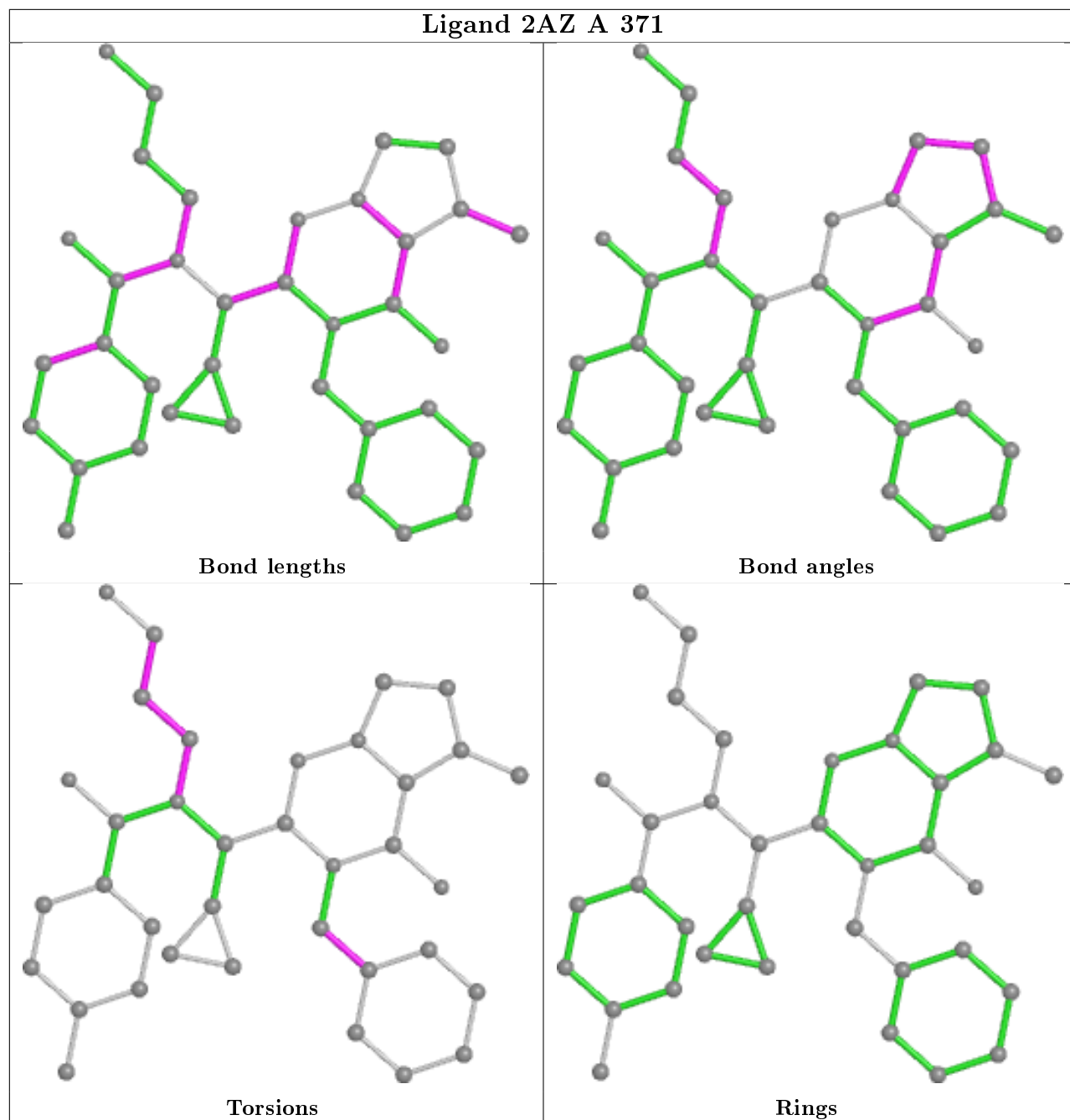


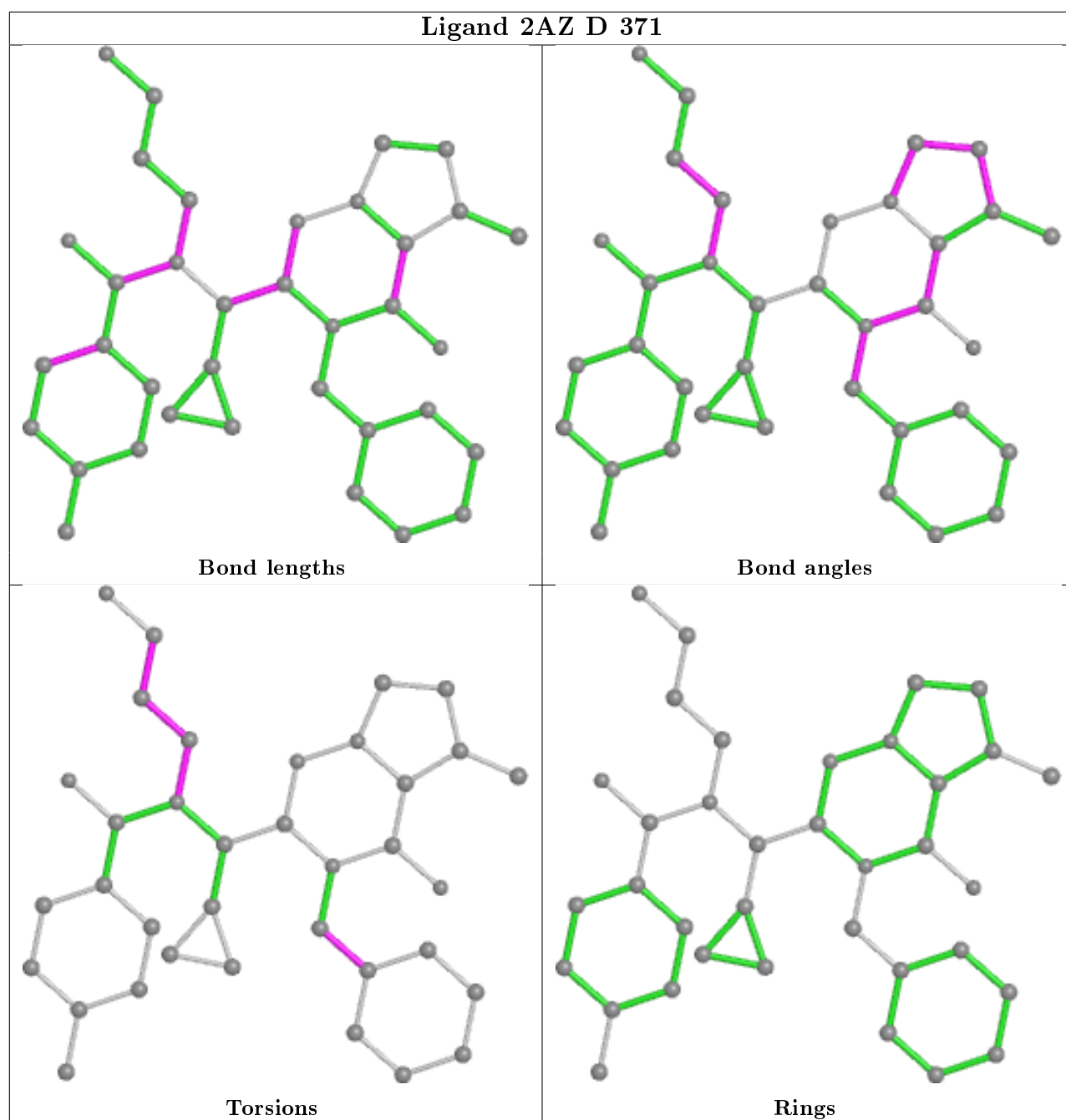
Ligand 2AZ E 371





Ligand 2AZ A 371





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	328/368 (89%)	0.14	17 (5%) 27 34	13, 30, 61, 70	0
1	B	321/368 (87%)	0.16	21 (6%) 18 24	12, 32, 60, 72	0
1	D	325/368 (88%)	0.14	22 (6%) 17 22	13, 31, 61, 73	0
1	E	323/368 (87%)	0.25	20 (6%) 20 26	13, 30, 57, 69	0
All	All	1297/1472 (88%)	0.17	80 (6%) 20 26	12, 31, 60, 73	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	178	VAL	11.7
1	D	178	VAL	10.3
1	D	175	SER	8.3
1	B	58	ALA	7.3
1	D	179	SER	5.9
1	B	308	HIS	5.7
1	D	56	GLY	5.7
1	D	180	GLU	5.1
1	E	152	THR	5.1
1	E	179	SER	4.7
1	A	256	VAL	4.6
1	A	185	PHE	4.6
1	A	56	GLY	4.6
1	D	308	HIS	4.6
1	B	122	ASN	4.3
1	B	57	LEU	4.3
1	E	122	ASN	4.2
1	A	57	LEU	4.2
1	A	274	ARG	4.2
1	B	307	PRO	4.1
1	E	308	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	185	PHE	4.1
1	E	190	ASN	4.0
1	D	174	PRO	4.0
1	B	60	LYS	3.8
1	B	272	ILE	3.8
1	D	307	PRO	3.8
1	E	272	ILE	3.7
1	A	305	ARG	3.7
1	B	352	TYR	3.5
1	E	61	SER	3.5
1	D	152	THR	3.4
1	B	150	ASN	3.4
1	E	352	TYR	3.4
1	A	152	THR	3.3
1	D	176	SER	3.3
1	A	187	ASP	3.3
1	D	181	ARG	3.2
1	E	174	PRO	3.2
1	E	176	SER	3.1
1	B	59	ASP	3.1
1	E	180	GLU	3.1
1	A	122	ASN	3.1
1	D	150	ASN	3.1
1	B	303	VAL	3.0
1	B	55	GLY	2.9
1	A	193	GLY	2.9
1	D	256	VAL	2.8
1	D	271	ASN	2.8
1	D	122	ASN	2.8
1	A	55	GLY	2.7
1	A	352	TYR	2.7
1	A	367	GLN	2.6
1	E	305	ARG	2.6
1	D	189	ARG	2.5
1	E	173	ASN	2.5
1	A	62	SER	2.5
1	B	61	SER	2.5
1	B	305	ARG	2.4
1	B	256	VAL	2.4
1	A	150	ASN	2.4
1	B	95	MET	2.4
1	D	352	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	307	PRO	2.3
1	E	177	ASP	2.3
1	B	293	LEU	2.3
1	D	194	VAL	2.3
1	D	192	ARG	2.3
1	B	56	GLY	2.3
1	D	193	GLY	2.2
1	B	271	ASN	2.2
1	D	305	ARG	2.2
1	A	271	ASN	2.2
1	E	212	GLN	2.2
1	E	288	ILE	2.1
1	B	62	SER	2.1
1	E	153	GLU	2.1
1	E	306	THR	2.1
1	B	178	VAL	2.0
1	A	60	LYS	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(\AA^2)	Q<0.9
2	MG	D	370	1/1	0.84	0.14	41,41,41,41	0
2	MG	B	370	1/1	0.88	0.13	51,51,51,51	0
3	2AZ	B	371	36/36	0.90	0.15	18,25,34,34	0
2	MG	E	370	1/1	0.91	0.08	39,39,39,39	0
3	2AZ	A	371	36/36	0.91	0.14	19,25,35,36	0
3	2AZ	E	371	36/36	0.92	0.14	16,23,33,33	0

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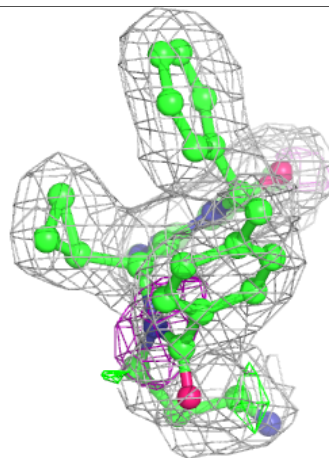
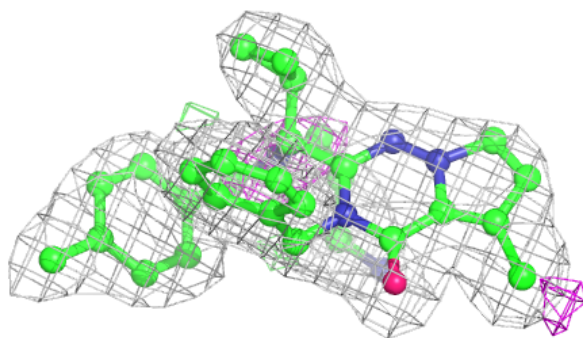
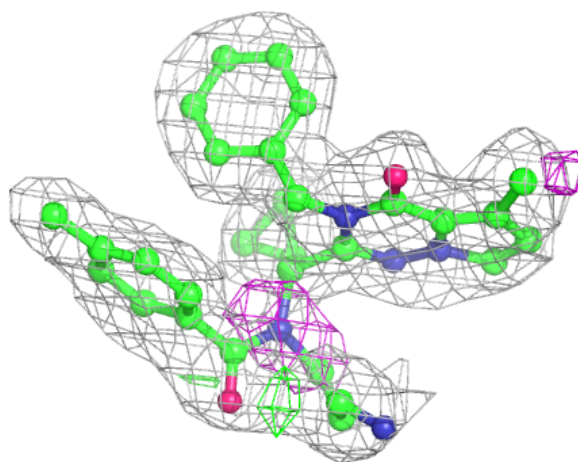
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	2AZ	D	371	36/36	0.92	0.15	16,22,34,35	0
2	MG	A	370	1/1	0.94	0.12	41,41,41,41	0
2	MG	A	369	1/1	0.97	0.14	19,19,19,19	0
4	ADP	B	372	27/27	0.98	0.10	14,15,18,20	0
4	ADP	E	372	27/27	0.98	0.10	12,16,18,20	0
2	MG	E	369	1/1	0.98	0.14	22,22,22,22	0
2	MG	D	369	1/1	0.98	0.16	24,24,24,24	0
4	ADP	D	372	27/27	0.98	0.11	13,15,16,21	0
2	MG	B	369	1/1	0.98	0.16	23,23,23,23	0
4	ADP	A	372	27/27	0.98	0.10	11,14,17,19	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.

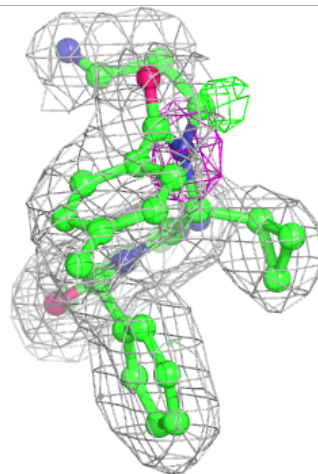
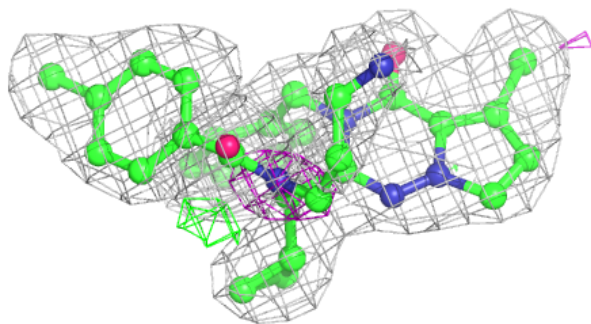
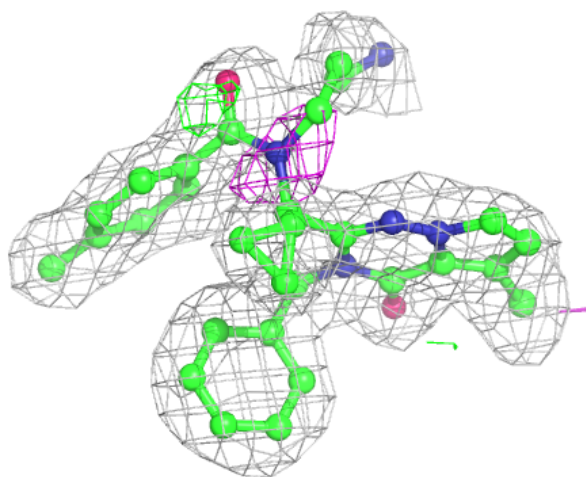
Electron density around 2AZ B 371:

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



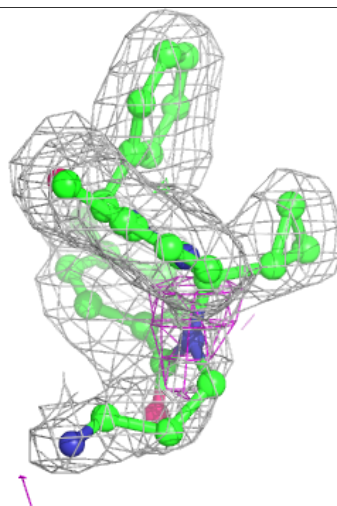
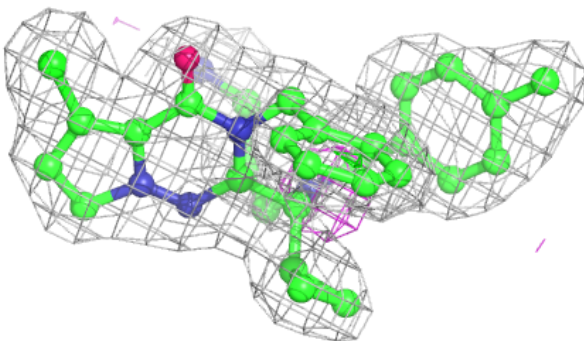
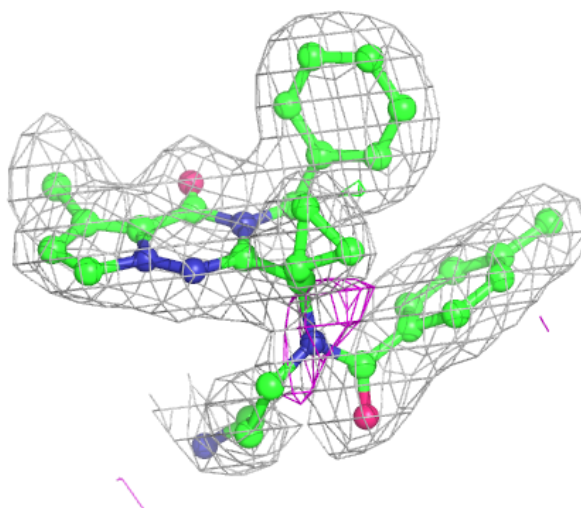
Electron density around 2AZ A 371:

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



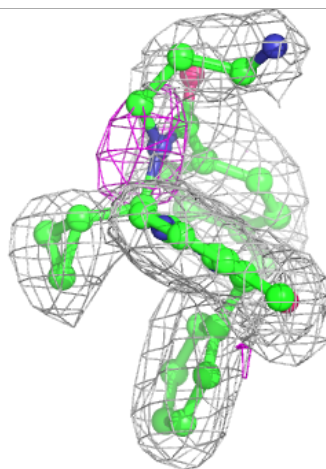
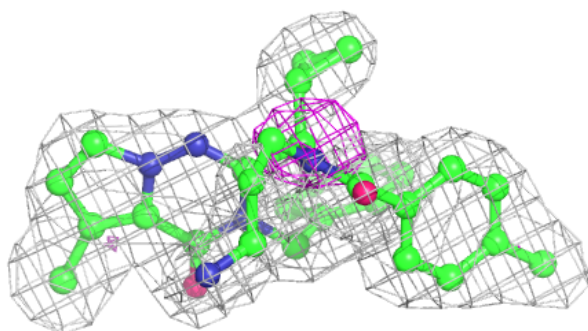
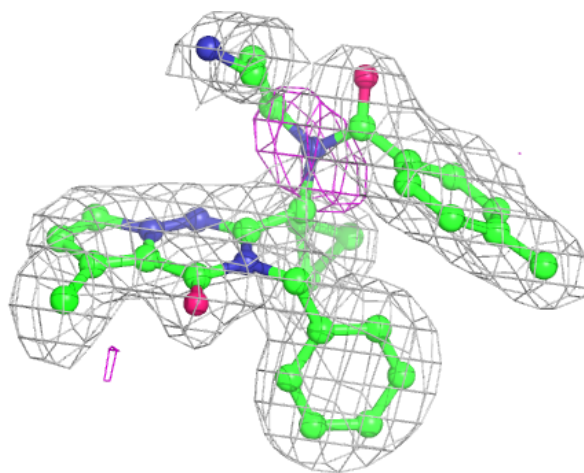
Electron density around 2AZ E 371:

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



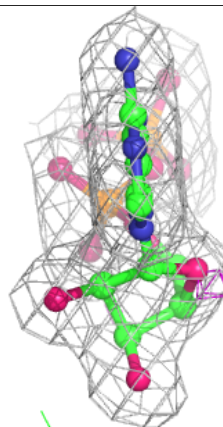
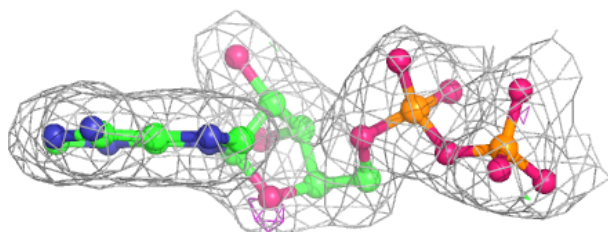
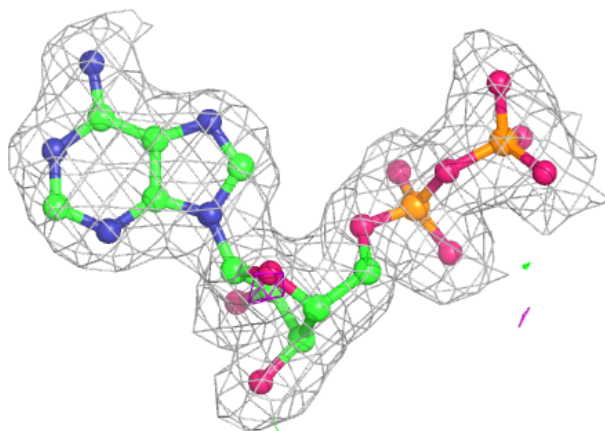
Electron density around 2AZ D 371:

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



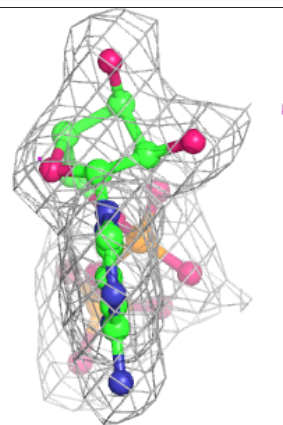
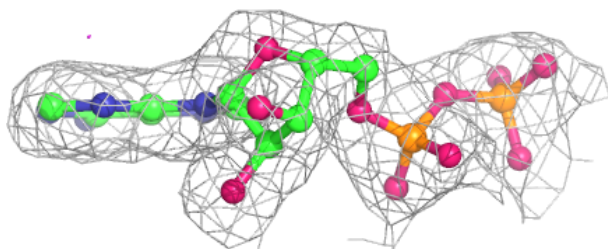
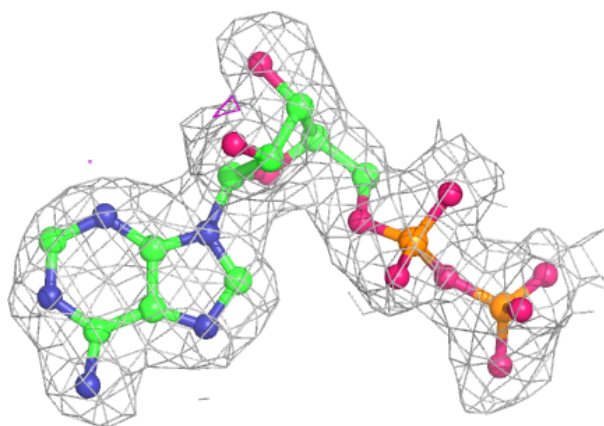
Electron density around ADP B 372:

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

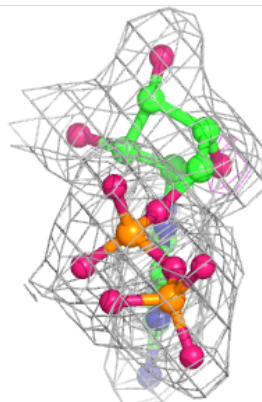
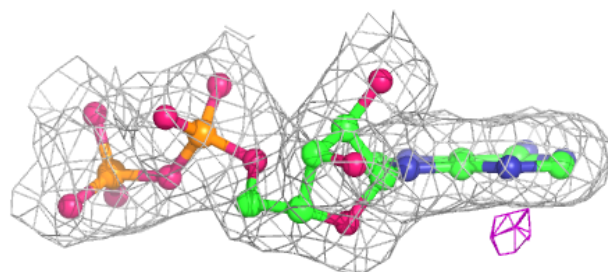
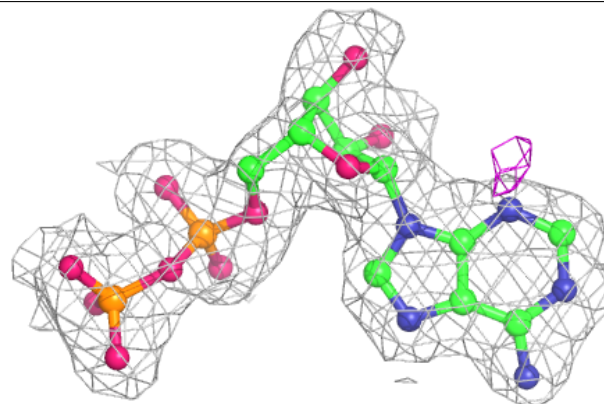


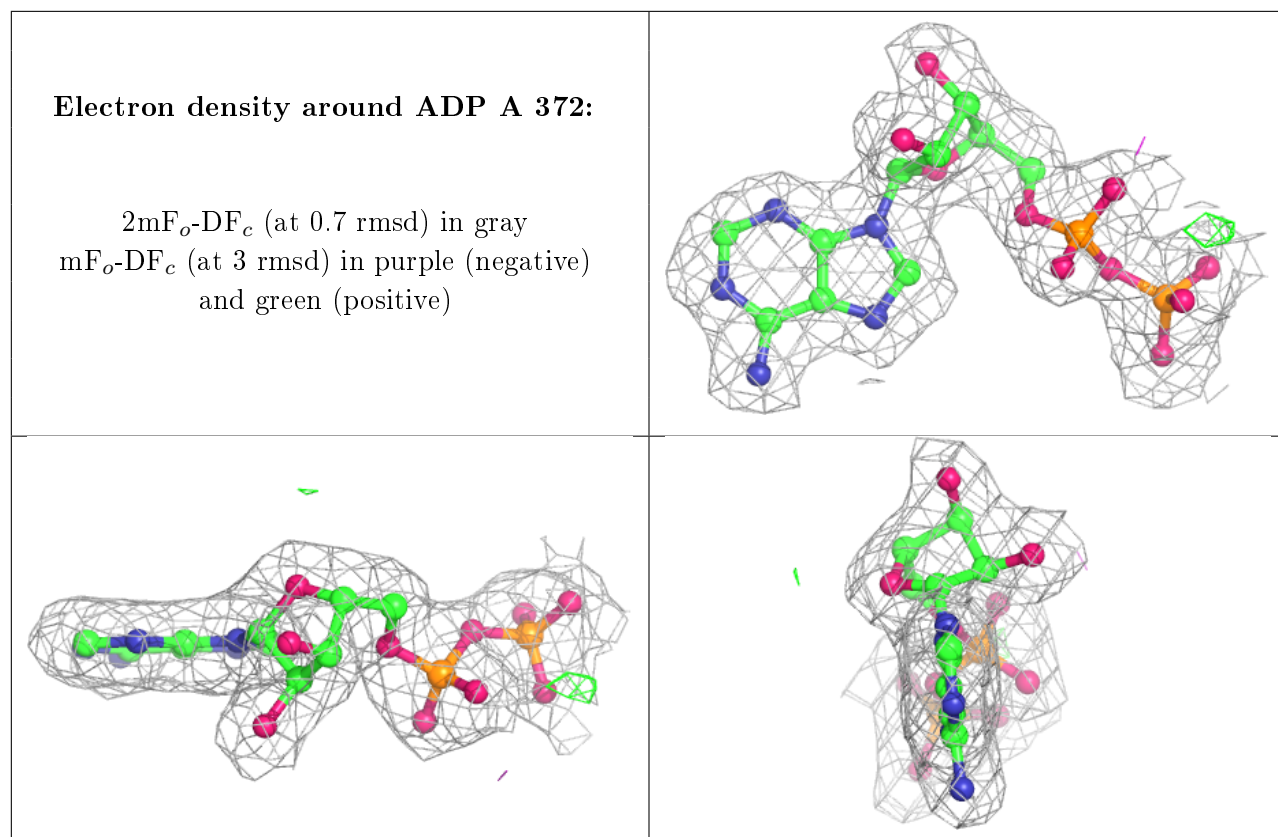
Electron density around ADP E 372:

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

**Electron density around ADP D 372:**

$2mF_o-DF_c$ (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.