



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:16 PM BST

PDB ID : 5VJA
Title : Crystal Structure of human zipper-interacting protein kinase (ZIPK, alias DAPK3) in complex with a pyrazolo[3,4-d]pyrimidinone ligand (HS38)
Authors : Carlson, D.A.; Singer, M.R.; Sutherland, C.; Redondo, C.; Alexander, L.; Hughes, P.F.; Knapp, S.; MacDonald, J.A.; Haystead, T.A.J.
Deposited on : 2017-04-19
Resolution : 2.46 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 : 2.14.4.dev1
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) : 2.14.4.dev1

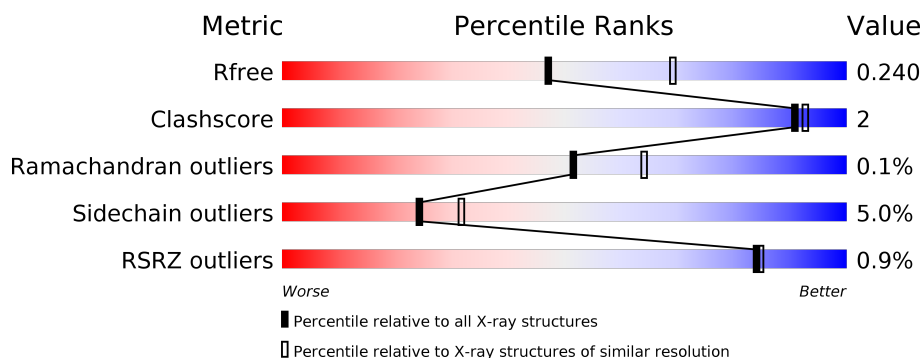
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	283	<div> <div>87%</div> <div>7% • 6%</div> </div>
1	B	283	<div> <div>88%</div> <div>6% 6%</div> </div>
1	C	283	<div> <div>2%</div> <div>87%</div> <div>6% • 6%</div> </div>
1	D	283	<div> <div>%</div> <div>80%</div> <div>11% • 8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9163 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 Death-associated protein kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2156	1378	367	405	6			
1	B	266	Total	C	N	O	S	0	0	0
			2153	1378	364	405	6			
1	C	265	Total	C	N	O	S	0	0	0
			2143	1371	361	405	6			
1	D	261	Total	C	N	O	S	0	1	0
			2119	1354	358	401	6			

There are 8 discrepancies between the modelled and reference sequences:

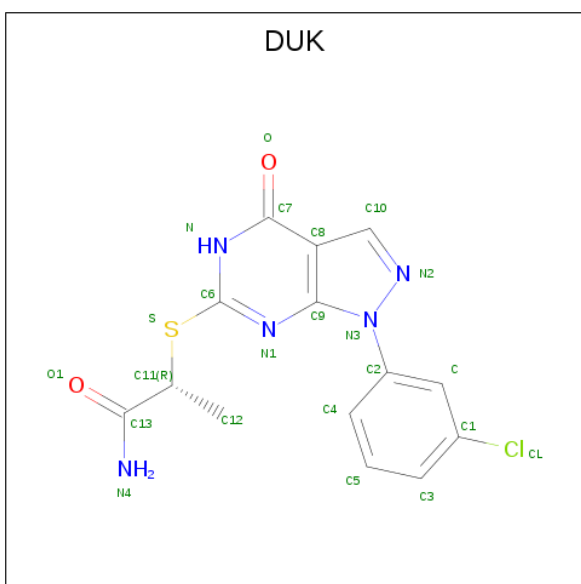
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	-	expression tag	UNP O43293
A	8	MET	-	expression tag	UNP O43293
B	7	SER	-	expression tag	UNP O43293
B	8	MET	-	expression tag	UNP O43293
C	7	SER	-	expression tag	UNP O43293
C	8	MET	-	expression tag	UNP O43293
D	7	SER	-	expression tag	UNP O43293
D	8	MET	-	expression tag	UNP O43293

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



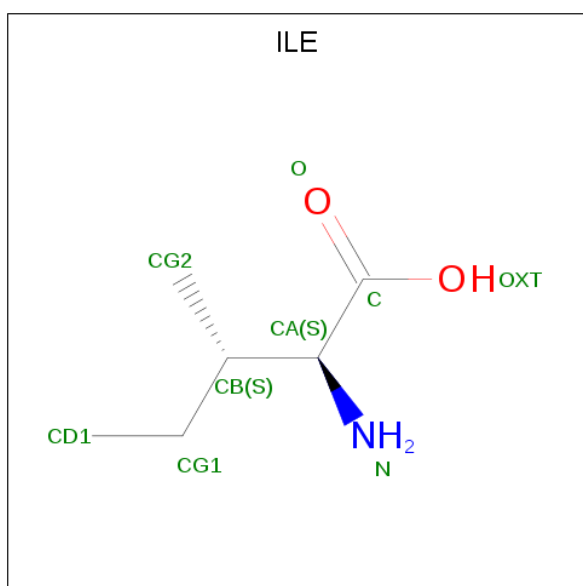
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is (2R)-2-{{1-(3-chlorophenyl)-4-oxo-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-6-yl}sulfanyl}propanamide (three-letter code: DUK) (formula: C₁₄H₁₂ClN₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	
			23	14	1	5	2	1	
3	B	1	Total	C	Cl	N	O	S	
			23	14	1	5	2	1	
3	C	1	Total	C	Cl	N	O	S	
			23	14	1	5	2	1	
3	D	1	Total	C	Cl	N	O	S	
			23	14	1	5	2	1	

- Molecule 4 is ISOLEUCINE (three-letter code: ILE) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O		
			8	6	1	1	0	0

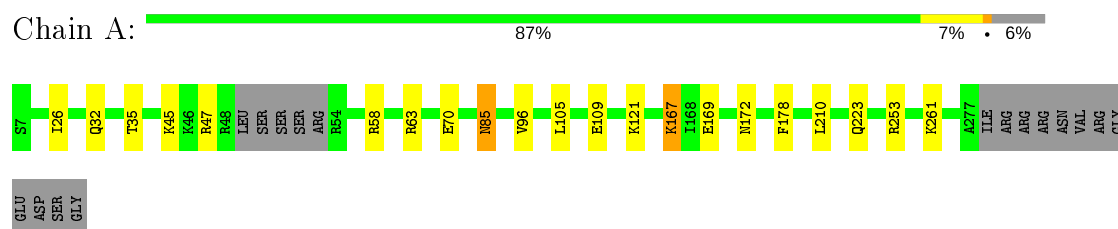
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O		
			137	137	0	0
5	B	142	Total	O		
			142	142	0	0
5	C	98	Total	O		
			98	98	0	0
5	D	99	Total	O		
			99	99	0	0

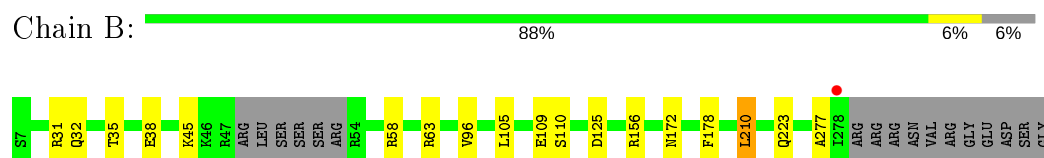
3 Residue-property plots

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 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.

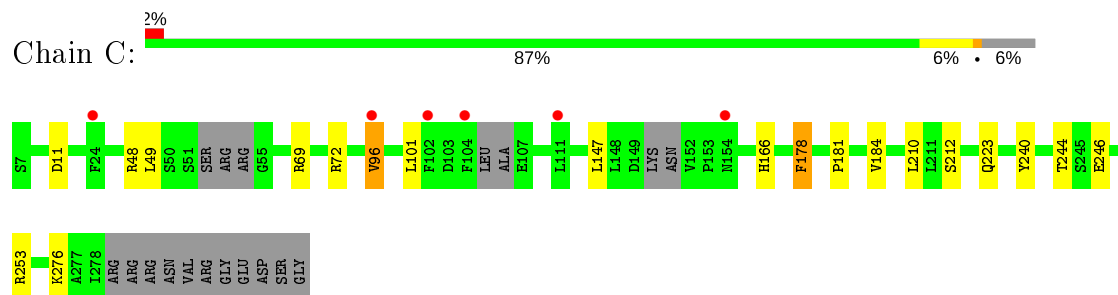
- Molecule 1: Death-associated protein kinase 3



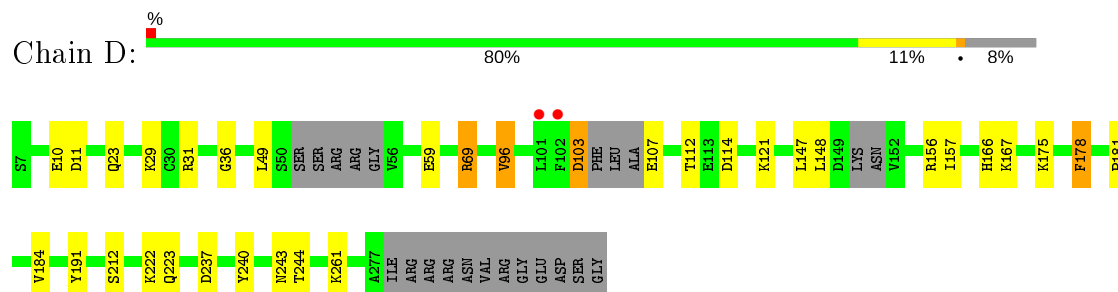
- Molecule 1: Death-associated protein kinase 3



- Molecule 1: Death-associated protein kinase 3



- Molecule 1: Death-associated protein kinase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.49Å 98.49Å 115.02Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	115.02 – 2.46 39.14 – 2.46	Depositor EDS
% Data completeness (in resolution range)	96.8 (115.02-2.46) 96.6 (39.14-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.188 , 0.237 0.193 , 0.240	Depositor DCC
R_{free} test set	2092 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.417 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9163	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DUK, DMS

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	0.75	0/2197	0.89	2/2958 (0.1%)
1	B	0.75	0/2194	0.90	3/2955 (0.1%)
1	C	0.74	0/2182	0.94	3/2936 (0.1%)
1	D	0.77	0/2160	0.94	7/2907 (0.2%)
All	All	0.75	0/8733	0.91	15/11756 (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	A	253	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	63	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	63	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	125	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	C	69	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	D	237	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	D	237	ASP	CB-CG-OD1	5.77	123.50	118.30
1	D	11	ASP	CB-CG-OD1	5.62	123.35	118.30
1	C	11	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	210	LEU	CA-CB-CG	5.11	127.04	115.30
1	D	69	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	114	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	178	PHE	CB-CG-CD1	5.05	124.34	120.80
1	D	243	ASN	N-CA-CB	-5.04	101.52	110.60
1	D	178	PHE	CB-CG-CD1	5.03	124.32	120.80

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	2156	0	2160	5	0
1	B	2153	0	2158	4	0
1	C	2143	0	2142	7	0
1	D	2119	0	2120	13	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
3	A	23	0	0	0	0
3	B	23	0	0	0	0
3	C	23	0	0	0	0
3	D	23	0	0	0	0
4	D	8	0	10	0	0
5	A	137	0	0	0	0
5	B	142	0	0	0	1
5	C	98	0	0	2	0
5	D	99	0	0	2	0
All	All	9163	0	8614	29	1

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 2.

All (29) 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:D:103:ASP:N	1:D:103:ASP:OD1	2.19	0.76
1:A:85:ASN:H	1:A:85:ASN:HD22	1.34	0.74
1:C:244:THR:N	5:C:1101:HOH:O	2.20	0.73
1:B:31:ARG:NH2	1:B:38:GLU:OE2	2.25	0.69
1:D:244:THR:N	5:D:403:HOH:O	2.33	0.61
1:D:96:VAL:HG12	1:D:147:LEU:O	2.01	0.60
1:D:212:SER:HB2	1:D:240:TYR:HB3	1.85	0.58
1:C:212:SER:HB2	1:C:240:TYR:HB3	1.86	0.58
1:C:96:VAL:HG12	1:C:147:LEU:O	2.06	0.55
1:B:32:GLN:NE2	1:B:35:THR:OG1	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:NE2	1:A:35:THR:OG1	2.30	0.53
1:D:31:ARG:HD3	1:D:36:GLY:HA2	1.93	0.51
1:D:175:LYS:HE2	1:D:191:TYR:O	2.12	0.50
1:D:112:THR:HG22	5:D:437:HOH:O	2.12	0.49
1:C:246:GLU:OE1	1:C:253:ARG:NH2	2.45	0.49
1:B:32:GLN:HE21	1:B:35:THR:HG1	1.58	0.48
1:A:70:GLU:OE2	1:A:167:LYS:NZ	2.47	0.47
1:A:96:VAL:HG23	1:A:96:VAL:O	2.14	0.47
1:D:147:LEU:HD23	1:D:157:ILE:HG22	1.97	0.47
1:B:96:VAL:HG23	1:B:96:VAL:O	2.15	0.46
1:D:148:LEU:HD21	1:D:156:ARG:HB3	2.00	0.43
1:C:72:ARG:NH2	5:C:1106:HOH:O	2.41	0.43
1:C:101:LEU:HD21	1:C:210:LEU:HD21	2.00	0.43
1:D:147:LEU:CD2	1:D:157:ILE:HG22	2.49	0.43
1:D:31:ARG:CD	1:D:36:GLY:HA2	2.48	0.42
1:D:175:LYS:CE	1:D:191:TYR:O	2.68	0.41
1:A:261:LYS:HA	1:A:261:LYS:HD3	1.91	0.41
1:D:181:PRO:O	1:D:184:VAL:HG22	2.20	0.41
1:C:181:PRO:O	1:C:184:VAL:HG22	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1176:HOH:O	5:B:1236:HOH:O[2_455]	2.15	0.05

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	262/283 (93%)	258 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	262/283 (93%)	257 (98%)	4 (2%)	1 (0%)	34	41
1	C	257/283 (91%)	251 (98%)	6 (2%)	0	100	100
1	D	254/283 (90%)	249 (98%)	5 (2%)	0	100	100
All	All	1035/1132 (91%)	1015 (98%)	19 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	277	ALA

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	235/250 (94%)	221 (94%)	14 (6%)	19	24
1	B	235/250 (94%)	225 (96%)	10 (4%)	29	38
1	C	235/250 (94%)	228 (97%)	7 (3%)	41	52
1	D	233/250 (93%)	217 (93%)	16 (7%)	15	18
All	All	938/1000 (94%)	891 (95%)	47 (5%)	24	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	45	LYS
1	A	47	ARG
1	A	58	ARG
1	A	85	ASN
1	A	105	LEU
1	A	109	GLU
1	A	121	LYS
1	A	167	LYS
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	172	ASN
1	A	178	PHE
1	A	210	LEU
1	A	223	GLN
1	B	45	LYS
1	B	58	ARG
1	B	105	LEU
1	B	109	GLU
1	B	110	SER
1	B	156	ARG
1	B	172	ASN
1	B	178	PHE
1	B	210	LEU
1	B	223	GLN
1	C	48	ARG
1	C	49	LEU
1	C	96	VAL
1	C	166	HIS
1	C	178	PHE
1	C	223	GLN
1	C	276	LYS
1	D	10	GLU
1	D	23	GLN
1	D	29	LYS
1	D	49	LEU
1	D	59	GLU
1	D	69	ARG
1	D	96	VAL
1	D	103	ASP
1	D	107	GLU
1	D	121	LYS
1	D	166	HIS
1	D	167	LYS
1	D	178	PHE
1	D	222	LYS
1	D	223	GLN
1	D	261	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	80	HIS
1	A	85	ASN
1	A	151	ASN
1	A	243	ASN
1	B	32	GLN
1	B	80	HIS
1	B	118	GLN
1	B	172	ASN
1	B	243	ASN
1	D	23	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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
3	DUK	A	1002	-	21,25,25	2.81	7 (33%)	23,36,36	4.28	9 (39%)
3	DUK	B	1002	-	21,25,25	2.75	6 (28%)	23,36,36	3.97	8 (34%)
3	DUK	C	1002	-	21,25,25	2.69	7 (33%)	23,36,36	3.69	10 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DUK	D	303	-	21,25,25	2.64	7 (33%)	23,36,36	3.70	11 (47%)
2	DMS	A	1001	-	3,3,3	0.48	0	3,3,3	0.99	0
2	DMS	D	302	-	3,3,3	0.41	0	3,3,3	0.98	0
2	DMS	C	1001	-	3,3,3	0.46	0	3,3,3	1.05	0
4	ILE	D	301	-	6,7,8	0.72	0	5,8,10	0.84	0
2	DMS	B	1001	-	3,3,3	0.40	0	3,3,3	1.01	0

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
3	DUK	C	1002	-	-	4/11/12/12	0/3/3/3
3	DUK	B	1002	-	-	4/11/12/12	0/3/3/3
4	ILE	D	301	-	-	3/7/8/10	-
3	DUK	A	1002	-	-	4/11/12/12	0/3/3/3
3	DUK	D	303	-	-	4/11/12/12	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	DUK	C9-N1	7.62	1.47	1.35
3	B	1002	DUK	N2-N3	-7.39	1.25	1.39
3	B	1002	DUK	C9-N1	7.00	1.46	1.35
3	C	1002	DUK	C9-N1	6.90	1.46	1.35
3	D	303	DUK	C9-N1	6.68	1.46	1.35
3	C	1002	DUK	N2-N3	-6.60	1.26	1.39
3	D	303	DUK	N2-N3	-6.35	1.27	1.39
3	A	1002	DUK	N2-N3	-6.24	1.27	1.39
3	A	1002	DUK	C6-N	4.90	1.41	1.34
3	D	303	DUK	C6-N	4.24	1.40	1.34
3	A	1002	DUK	C7-N	4.20	1.40	1.33
3	C	1002	DUK	C6-N	4.03	1.40	1.34
3	B	1002	DUK	C6-N	3.82	1.39	1.34
3	D	303	DUK	C7-N	3.48	1.39	1.33
3	B	1002	DUK	C7-N	3.31	1.38	1.33
3	C	1002	DUK	C7-N	3.22	1.38	1.33
3	C	1002	DUK	C8-C9	-3.12	1.35	1.43
3	D	303	DUK	C8-C9	-3.10	1.35	1.43
3	B	1002	DUK	C8-C9	-2.95	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	DUK	C13-N4	2.76	1.39	1.32
3	A	1002	DUK	C8-C9	-2.51	1.37	1.43
3	C	1002	DUK	C13-N4	2.33	1.38	1.32
3	A	1002	DUK	C13-N4	2.32	1.38	1.32
3	D	303	DUK	C13-N4	2.16	1.38	1.32
3	D	303	DUK	C6-N1	-2.16	1.30	1.34
3	C	1002	DUK	C6-N1	-2.07	1.30	1.34
3	A	1002	DUK	C1-CL	-2.02	1.70	1.74

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	DUK	C8-C7-N	-15.76	113.41	124.40
3	B	1002	DUK	C8-C7-N	-13.79	114.78	124.40
3	D	303	DUK	C8-C7-N	-12.89	115.41	124.40
3	C	1002	DUK	C8-C7-N	-12.34	115.79	124.40
3	A	1002	DUK	C7-N-C6	7.66	124.57	115.79
3	B	1002	DUK	C7-N-C6	7.19	124.04	115.79
3	B	1002	DUK	C11-C13-N4	6.41	123.21	116.92
3	D	303	DUK	C7-N-C6	6.16	122.85	115.79
3	C	1002	DUK	C7-N-C6	6.00	122.67	115.79
3	C	1002	DUK	C10-N2-N3	5.94	111.72	103.93
3	B	1002	DUK	C10-N2-N3	5.94	111.71	103.93
3	A	1002	DUK	C11-C13-N4	5.86	122.66	116.92
3	A	1002	DUK	C10-N2-N3	5.68	111.37	103.93
3	D	303	DUK	C10-N2-N3	5.57	111.23	103.93
3	C	1002	DUK	C11-C13-N4	5.47	122.28	116.92
3	D	303	DUK	C11-C13-N4	4.00	120.84	116.92
3	C	1002	DUK	C4-C2-C	-3.15	118.01	121.74
3	B	1002	DUK	N1-C6-N	-3.03	121.40	126.95
3	A	1002	DUK	C10-C8-C9	2.95	107.93	105.20
3	D	303	DUK	C4-C2-C	-2.91	118.29	121.74
3	D	303	DUK	N1-C6-N	-2.88	121.67	126.95
3	A	1002	DUK	C8-C10-N2	-2.85	104.53	110.43
3	C	1002	DUK	N1-C6-N	-2.84	121.75	126.95
3	B	1002	DUK	C8-C10-N2	-2.71	104.80	110.43
3	A	1002	DUK	C4-C2-C	-2.66	118.59	121.74
3	C	1002	DUK	C8-C10-N2	-2.61	105.02	110.43
3	A	1002	DUK	N1-C6-N	-2.60	122.18	126.95
3	D	303	DUK	C6-N1-C9	2.59	118.89	115.32
3	D	303	DUK	C-C1-CL	-2.56	115.95	119.15
3	D	303	DUK	C8-C10-N2	-2.56	105.12	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	DUK	C6-N1-C9	2.56	118.85	115.32
3	A	1002	DUK	O1-C13-N4	-2.48	118.68	123.00
3	D	303	DUK	C3-C1-CL	2.41	123.11	119.35
3	B	1002	DUK	C4-C2-C	-2.39	118.91	121.74
3	D	303	DUK	C4-C2-N3	2.32	124.03	119.61
3	C	1002	DUK	C-C1-CL	-2.16	116.45	119.15
3	C	1002	DUK	C4-C2-N3	2.09	123.61	119.61
3	B	1002	DUK	C10-C8-C9	2.08	107.12	105.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

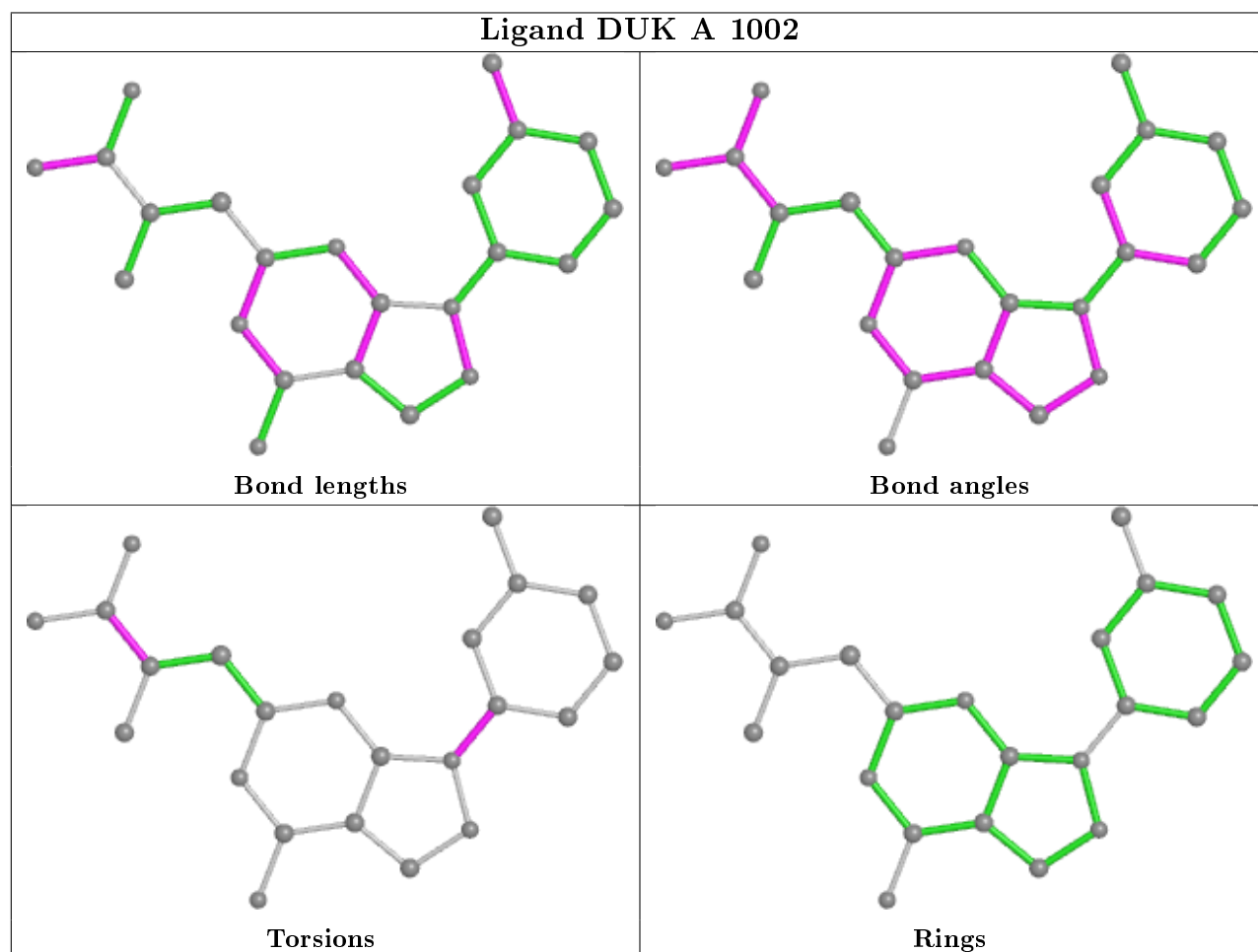
Mol	Chain	Res	Type	Atoms
3	A	1002	DUK	S-C11-C13-O1
3	A	1002	DUK	C-C2-N3-C9
3	A	1002	DUK	C4-C2-N3-C9
3	B	1002	DUK	C-C2-N3-C9
3	B	1002	DUK	C4-C2-N3-C9
3	C	1002	DUK	S-C11-C13-O1
3	C	1002	DUK	C-C2-N3-C9
3	C	1002	DUK	C4-C2-N3-C9
3	D	303	DUK	S-C11-C13-O1
3	D	303	DUK	C-C2-N3-C9
3	D	303	DUK	C4-C2-N3-C9
4	D	301	ILE	CA-CB-CG1-CD1
3	D	303	DUK	C-C2-N3-N2
4	D	301	ILE	CG2-CB-CG1-CD1
3	B	1002	DUK	S-C11-C13-O1
4	D	301	ILE	C-CA-CB-CG1
3	C	1002	DUK	C-C2-N3-N2
3	B	1002	DUK	C-C2-N3-N2
3	A	1002	DUK	C-C2-N3-N2

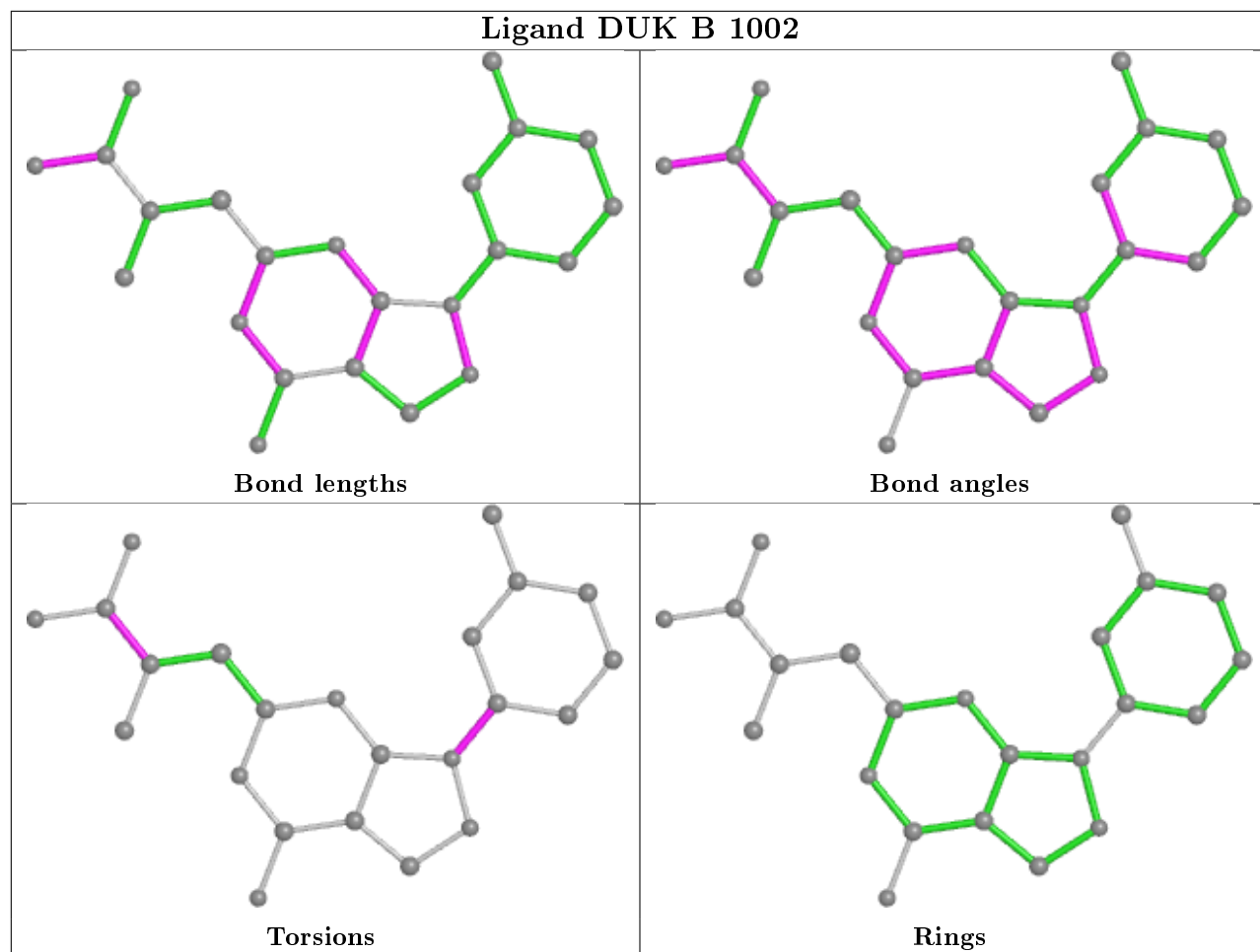
There are no ring outliers.

No monomer is involved in short contacts.

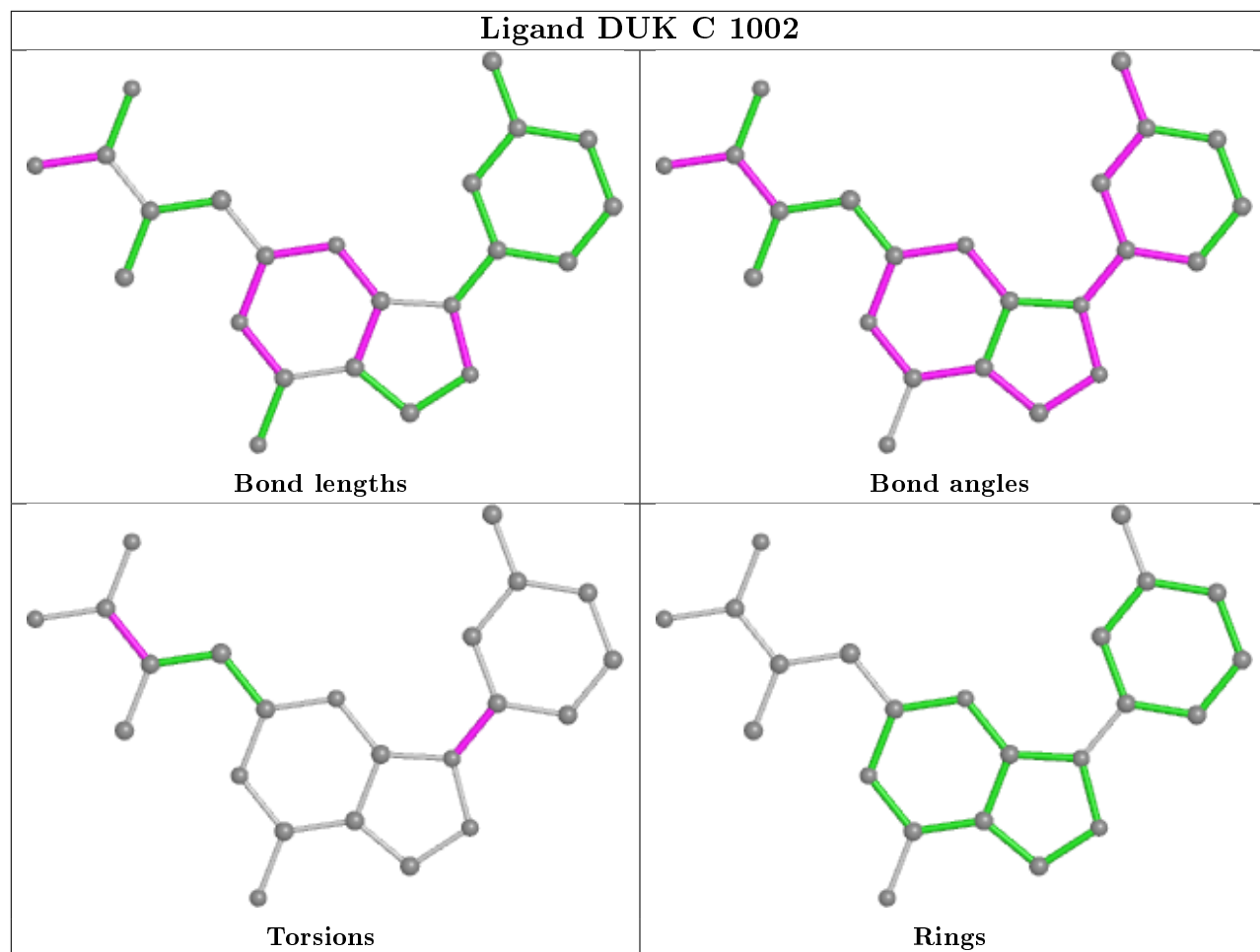
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

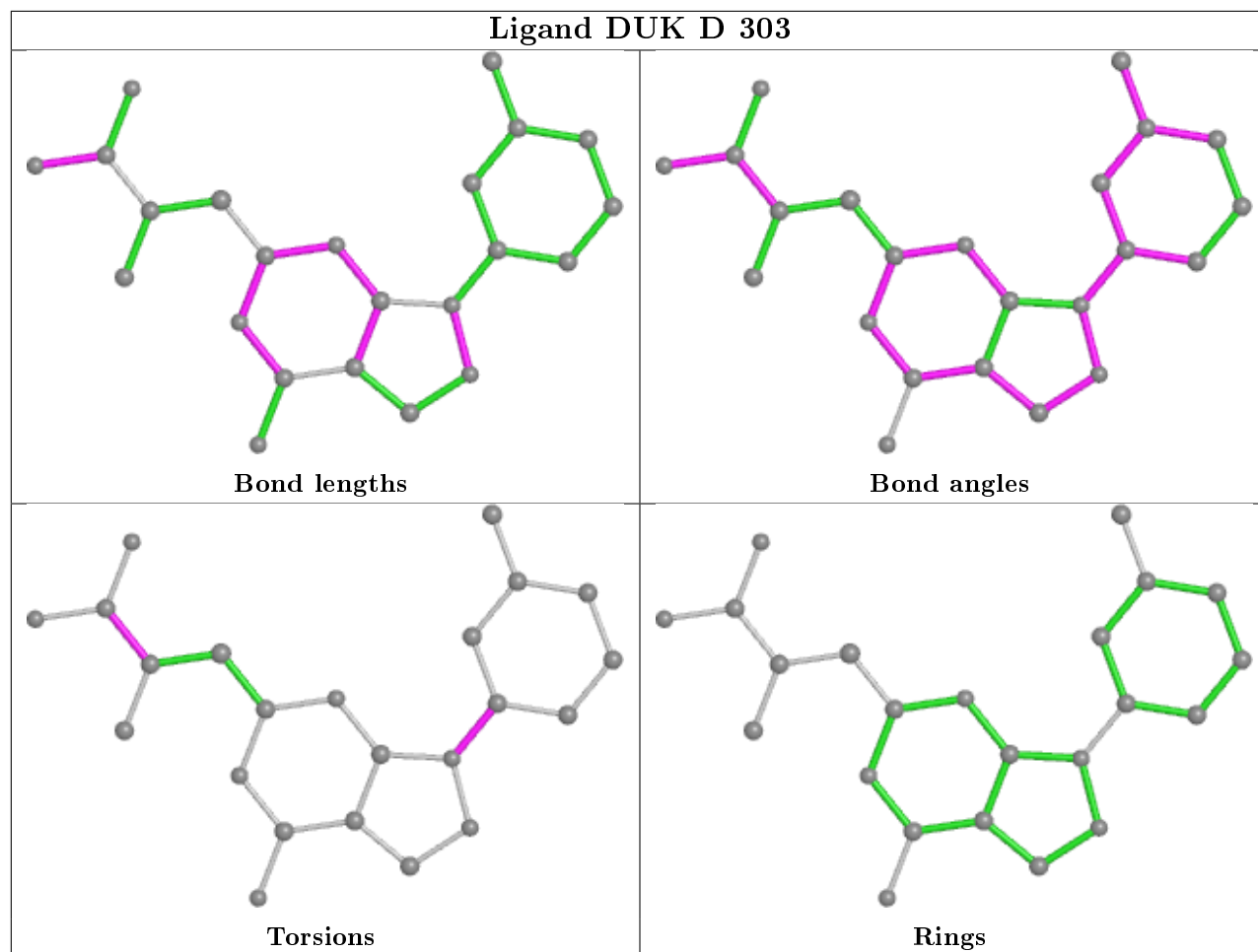
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 DUK C 1002





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	266/283 (93%)	-0.46	0 100 100	19, 32, 58, 83	0
1	B	266/283 (93%)	-0.48	1 (0%) 92 93	18, 31, 59, 84	0
1	C	265/283 (93%)	-0.18	6 (2%) 60 56	19, 40, 83, 113	0
1	D	261/283 (92%)	-0.24	2 (0%) 86 86	18, 38, 75, 94	0
All	All	1058/1132 (93%)	-0.34	9 (0%) 84 85	18, 35, 73, 113	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	PHE	4.3
1	C	104	PHE	3.5
1	C	96	VAL	2.7
1	D	102	PHE	2.5
1	C	111	LEU	2.3
1	D	101	LEU	2.3
1	C	154	ASN	2.1
1	C	24	PHE	2.0
1	B	278	ILE	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 monosaccharides in this entry.

6.4 Ligands

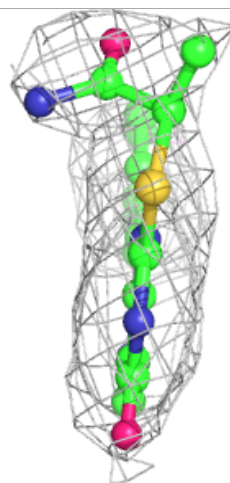
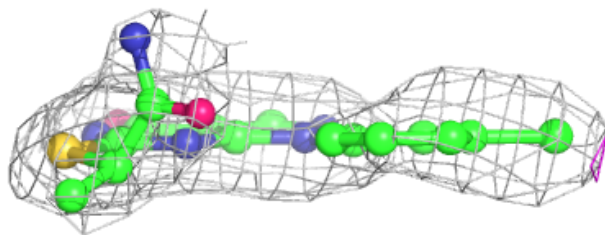
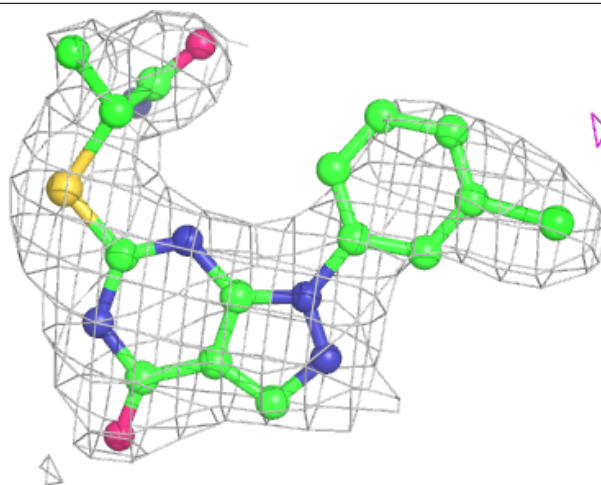
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ILE	D	301	8/9	0.64	0.31	69,88,94,95	0
2	DMS	D	302	4/4	0.83	0.20	53,56,58,79	0
2	DMS	C	1001	4/4	0.90	0.16	44,48,50,70	0
3	DUK	C	1002	23/23	0.93	0.16	52,58,66,69	0
2	DMS	B	1001	4/4	0.93	0.12	47,50,50,71	0
3	DUK	B	1002	23/23	0.95	0.12	25,33,46,48	0
3	DUK	D	303	23/23	0.95	0.18	38,47,67,72	0
3	DUK	A	1002	23/23	0.96	0.13	24,30,62,67	0
2	DMS	A	1001	4/4	0.97	0.15	42,44,48,51	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.

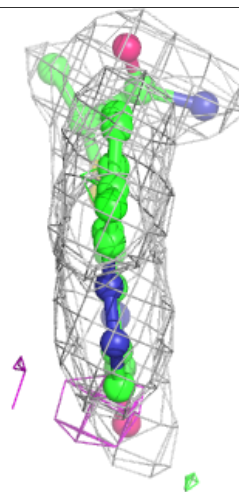
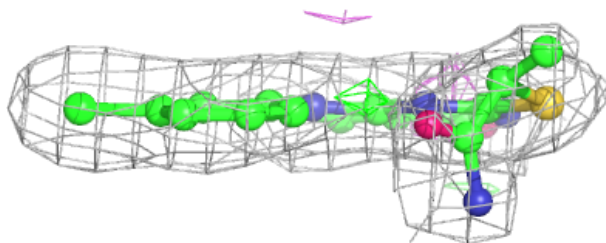
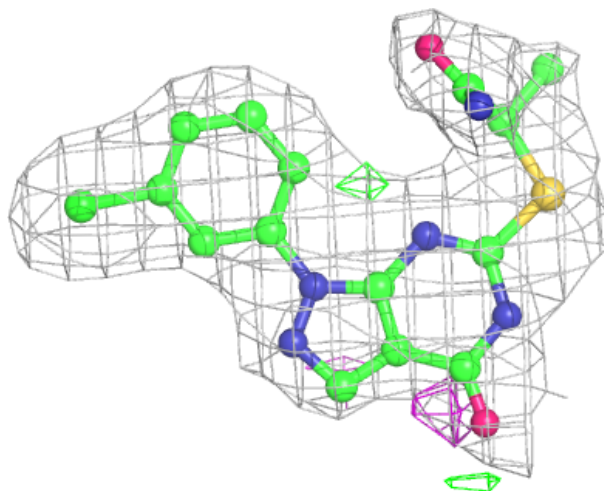
Electron density around DUK C 1002:

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



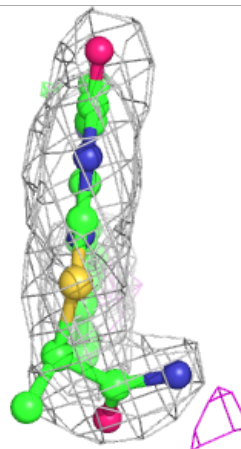
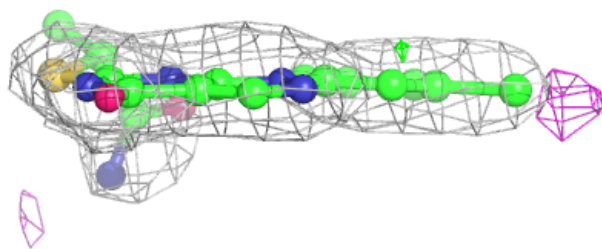
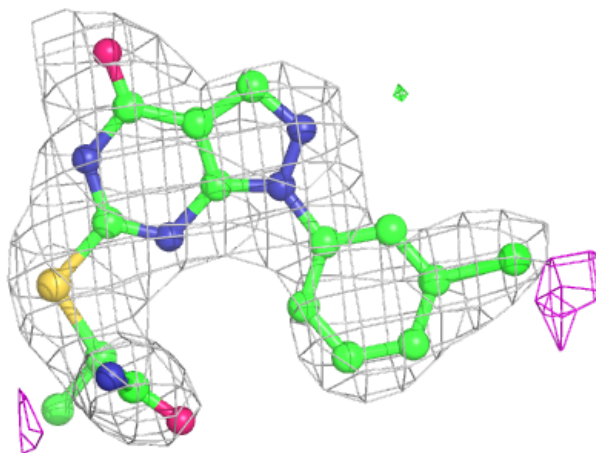
Electron density around DUK B 1002:

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



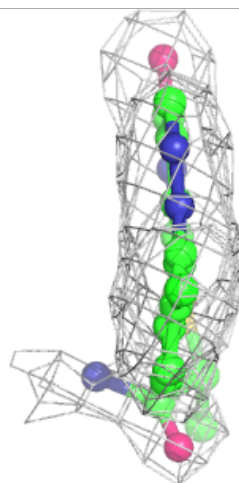
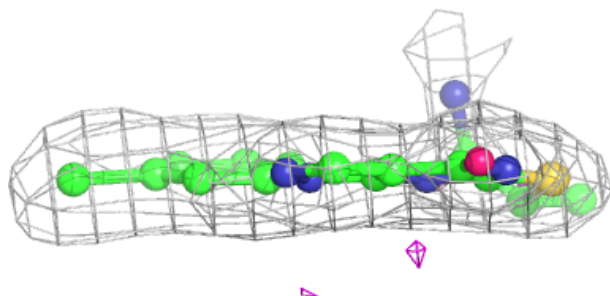
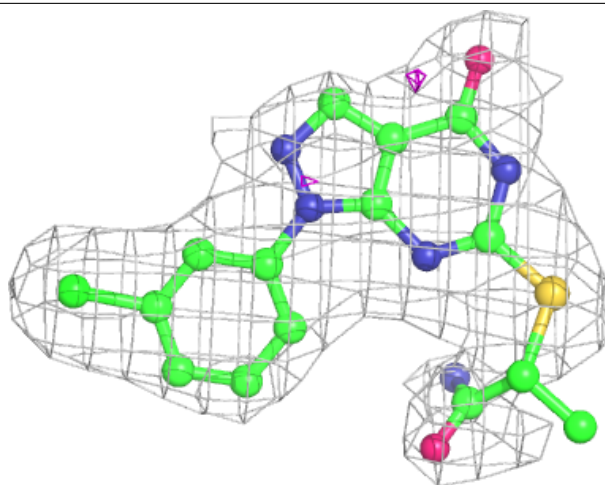
Electron density around DUK D 303:

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



Electron density around DUK A 1002:

$2mF_o-DF_c$ (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.