



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:45 AM UTC

PDB ID : 6YXV / pdb_00006yxv
Title : FOCAL ADHESION KINASE CATALYTIC DOMAIN IN COMPLEX WITH
N-Methyl-N-{3-[(2-phenylamino-5-trifluoromethyl-pyrimidin-4-ylamino)-met
hyl]-pyridin-2-yl}-methanesulfonamide
Authors : Musil, D.; Heinrich, T.; Amaral, M.
Deposited on : 2020-05-04
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

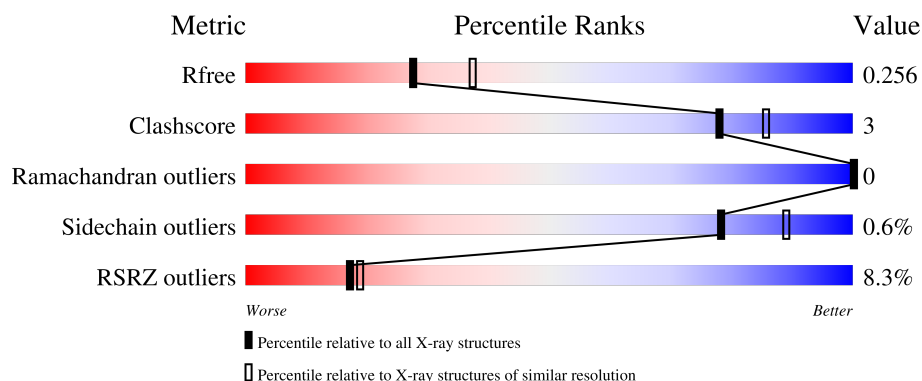
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	7% 85% 7% 7%
1	B	282	6% 84% 8% 8%
1	C	282	8% 84% 9% 6%
1	D	282	10% 78% 13% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8654 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.

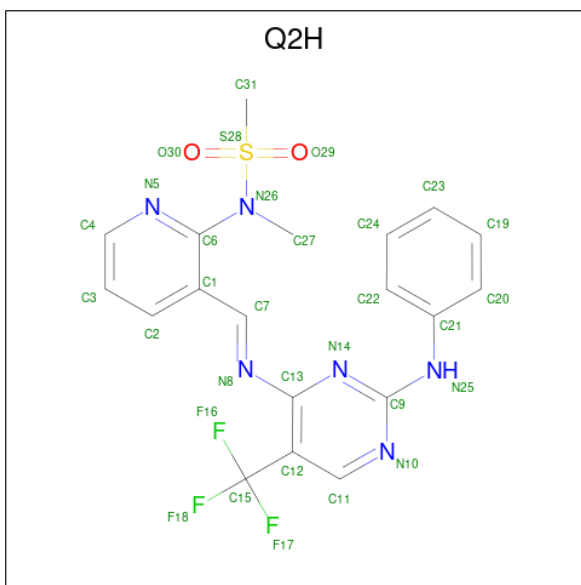
- Molecule 1 is a protein called Focal adhesion kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2101	1342	363	378	18			
1	B	260	Total	C	N	O	S	0	0	0
			2093	1338	362	375	18			
1	C	265	Total	C	N	O	S	0	0	0
			2131	1359	368	386	18			
1	D	257	Total	C	N	O	S	0	0	0
			2062	1318	356	371	17			

There are 12 discrepancies between the modelled and reference sequences:

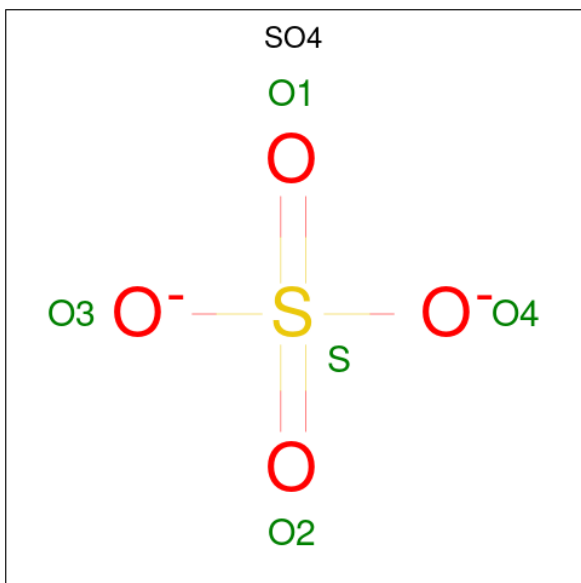
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLY	-	expression tag	UNP Q05397
A	409	SER	-	expression tag	UNP Q05397
A	410	GLY	-	expression tag	UNP Q05397
B	408	GLY	-	expression tag	UNP Q05397
B	409	SER	-	expression tag	UNP Q05397
B	410	GLY	-	expression tag	UNP Q05397
C	408	GLY	-	expression tag	UNP Q05397
C	409	SER	-	expression tag	UNP Q05397
C	410	GLY	-	expression tag	UNP Q05397
D	408	GLY	-	expression tag	UNP Q05397
D	409	SER	-	expression tag	UNP Q05397
D	410	GLY	-	expression tag	UNP Q05397

- Molecule 2 is {N}-methyl- {N}-[3-[({E})-2-phenylazanyl-5-(trifluoromethyl)pyrimidin-4-yl]iminomethyl]pyridin-2-yl]methanesulfonamide (CCD ID: Q2H) (formula: C₁₉H₁₇F₃N₆O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			31	19	3	6	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			31	19	3	6	2	1		
2	C	1	Total	C	F	N	O	S	0	0
			31	19	3	6	2	1		
2	D	1	Total	C	F	N	O	S	0	0
			31	19	3	6	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

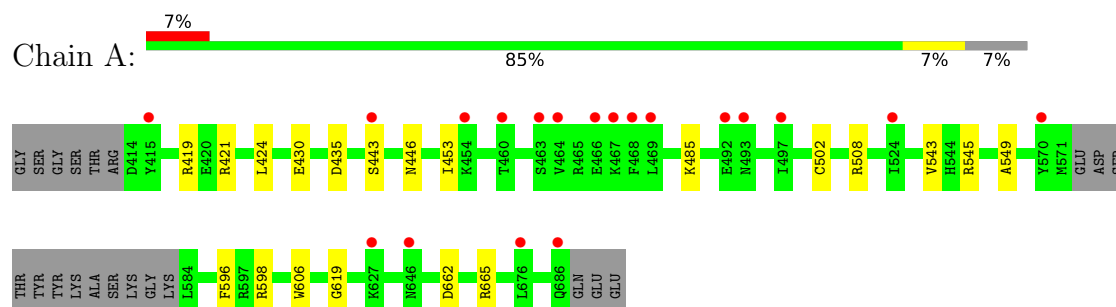
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	46	Total	O	0	0
			46	46		
4	C	30	Total	O	0	0
			30	30		
4	D	29	Total	O	0	0
			29	29		

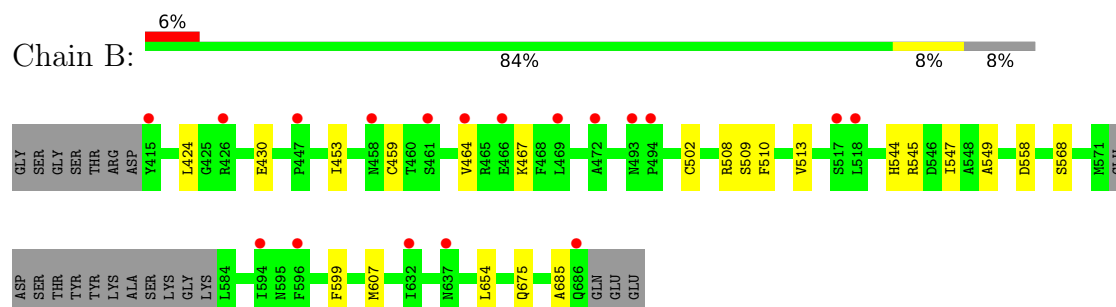
3 Residue-property plots [i](#)

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.

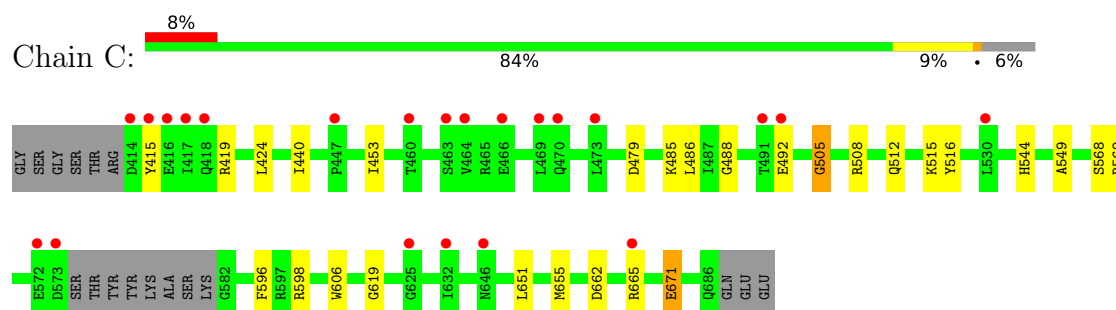
• Molecule 1: Focal adhesion kinase 1



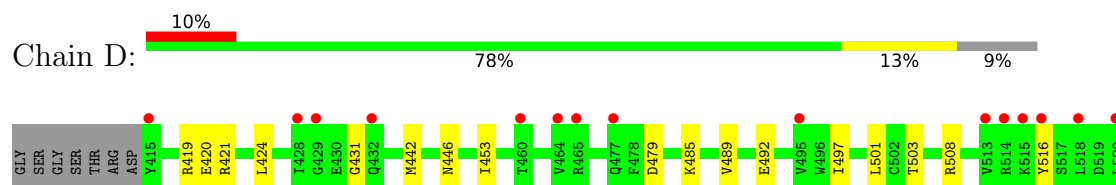
• Molecule 1: Focal adhesion kinase 1

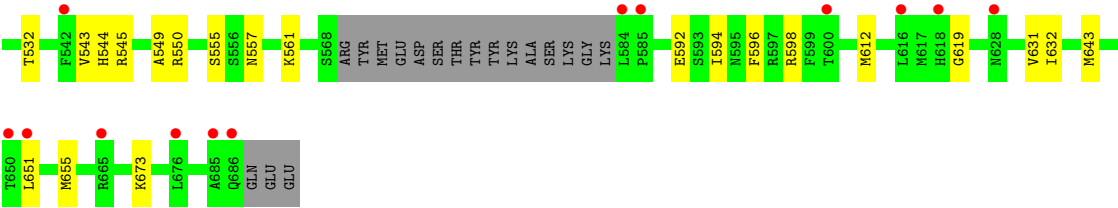


• Molecule 1: Focal adhesion kinase 1



• Molecule 1: Focal adhesion kinase 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.05Å 77.13Å 174.93Å 90.00° 101.34° 90.00°	Depositor
Resolution (Å)	171.52 – 2.30 171.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.6 (171.52-2.30) 64.6 (171.52-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.7 (19-MAR-2020)	Depositor
R, R_{free}	0.202 , 0.232 0.225 , 0.256	Depositor DCC
R_{free} test set	2217 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: Q2H, SO4

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	0.74	0/2148	1.14	6/2904 (0.2%)
1	B	0.78	0/2140	1.19	9/2893 (0.3%)
1	C	0.76	0/2178	1.15	9/2943 (0.3%)
1	D	0.76	1/2108 (0.0%)	1.18	9/2851 (0.3%)
All	All	0.76	1/8574 (0.0%)	1.16	33/11591 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	643	MET	SD-CE	-7.15	1.61	1.79

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	549	ALA	CA-C-N	8.59	131.79	120.28
1	D	549	ALA	C-N-CA	8.59	131.79	120.28
1	B	549	ALA	CA-C-N	8.12	131.50	120.38
1	B	549	ALA	C-N-CA	8.12	131.50	120.38
1	B	510	PHE	CA-CB-CG	7.71	121.51	113.80
1	A	549	ALA	CA-C-N	7.42	130.22	120.28
1	A	549	ALA	C-N-CA	7.42	130.22	120.28
1	C	568	SER	CA-C-N	7.01	130.00	120.54
1	C	568	SER	C-N-CA	7.01	130.00	120.54
1	B	544	HIS	N-CA-C	6.93	118.49	111.07
1	C	549	ALA	CA-C-N	6.49	129.86	120.38
1	C	549	ALA	C-N-CA	6.49	129.86	120.38
1	C	569	ARG	N-CA-C	6.28	118.65	111.11
1	C	544	HIS	N-CA-C	6.24	117.75	111.07
1	D	516	TYR	CA-C-N	6.14	129.12	120.28
1	D	516	TYR	C-N-CA	6.14	129.12	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	568	SER	CA-C-N	5.66	129.31	120.82
1	B	568	SER	C-N-CA	5.66	129.31	120.82
1	C	505	GLY	N-CA-C	5.61	121.98	112.22
1	A	502	CYS	CA-C-N	5.45	127.90	120.54
1	A	502	CYS	C-N-CA	5.45	127.90	120.54
1	D	631	VAL	CA-C-N	5.18	127.29	120.60
1	D	631	VAL	C-N-CA	5.18	127.29	120.60
1	D	431	GLY	CA-C-N	5.18	127.74	120.28
1	D	431	GLY	C-N-CA	5.18	127.74	120.28
1	B	685	ALA	CA-C-N	5.11	130.90	121.70
1	B	685	ALA	C-N-CA	5.11	130.90	121.70
1	A	606	TRP	CA-C-N	5.06	127.06	120.28
1	A	606	TRP	C-N-CA	5.06	127.06	120.28
1	C	606	TRP	CA-C-N	5.04	127.03	120.28
1	C	606	TRP	C-N-CA	5.04	127.03	120.28
1	D	544	HIS	N-CA-C	5.03	116.45	111.07
1	B	502	CYS	N-CA-C	-5.01	97.84	107.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2101	0	2108	10	0
1	B	2093	0	2104	9	0
1	C	2131	0	2134	14	0
1	D	2062	0	2073	17	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	1	0
2	D	31	0	0	0	0
3	B	5	0	0	0	0
4	A	33	0	0	0	0
4	B	46	0	0	1	0
4	C	30	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	29	0	0	1	0
All	All	8654	0	8419	47	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 3.

All (47) 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:C:479:ASP:OD1	1:C:485:LYS:HE3	2.00	0.61
1:D:419:ARG:HH11	1:D:492:GLU:HG3	1.69	0.56
1:D:479:ASP:OD1	1:D:485:LYS:HE3	2.05	0.56
1:D:543:VAL:HG12	1:D:545:ARG:HG3	1.89	0.55
1:B:508:ARG:HD2	4:B:802:HOH:O	2.07	0.53
1:D:501:LEU:HD23	1:D:503:THR:HG22	1.93	0.51
1:A:430:GLU:OE1	1:A:435:ASP:OD1	2.29	0.50
1:D:651:LEU:HG	1:D:655:MET:HE3	1.92	0.50
1:D:424:LEU:HD12	1:D:453:ILE:HD13	1.94	0.49
1:C:651:LEU:HG	1:C:655:MET:HE3	1.95	0.49
1:C:596:PHE:HB2	1:C:598:ARG:HD3	1.95	0.48
1:C:424:LEU:HD12	1:C:453:ILE:HD13	1.94	0.48
1:B:424:LEU:HD12	1:B:453:ILE:HD13	1.96	0.47
1:C:440:ILE:HG21	1:D:503:THR:HG21	1.97	0.47
1:C:508:ARG:NH1	1:C:619:GLY:O	2.48	0.47
1:C:671:GLU:N	1:C:671:GLU:CD	2.73	0.47
1:D:421:ARG:HD2	1:D:442:MET:O	2.14	0.47
1:A:424:LEU:HD12	1:A:453:ILE:HD13	1.96	0.47
1:D:612:MET:HB3	1:D:655:MET:HE2	1.99	0.45
1:B:545:ARG:HG2	1:B:599:PHE:CD1	2.52	0.45
1:C:419:ARG:HH11	1:C:492:GLU:CG	2.29	0.45
1:A:508:ARG:NH1	1:A:619:GLY:O	2.50	0.45
1:B:459:CYS:HB3	1:B:464:VAL:HG12	1.98	0.45
1:D:489:VAL:HG12	1:D:497:ILE:HG12	1.99	0.45
1:C:512:GLN:O	1:C:515:LYS:HE3	2.16	0.44
1:A:596:PHE:HB2	1:A:598:ARG:HD3	1.99	0.44
1:D:508:ARG:NH1	1:D:619:GLY:O	2.50	0.44
1:D:419:ARG:HH11	1:D:492:GLU:CG	2.31	0.44
1:D:532:THR:HG22	1:D:673:LYS:HG3	2.00	0.43
1:D:594:ILE:HG21	1:D:632:ILE:HG12	2.01	0.43
1:A:543:VAL:HG12	1:A:545:ARG:HG3	2.00	0.43
1:C:415:TYR:CE2	1:C:486:LEU:HD21	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:SER:O	1:B:513:VAL:HG23	2.19	0.43
1:A:662:ASP:HB3	1:A:665:ARG:HE	1.85	0.42
1:C:505:GLY:HA2	2:C:701:Q2H:C21	2.50	0.42
1:A:443:SER:HB3	1:A:446:ASN:HB2	2.01	0.42
1:B:654:LEU:HD13	1:B:675:GLN:HG2	2.00	0.42
1:A:421:ARG:NH1	1:B:558:ASP:OD1	2.52	0.42
1:D:555:SER:OG	1:D:561:LYS:HE3	2.19	0.42
1:B:547:ILE:HB	1:B:607:MET:HB3	2.01	0.41
1:C:662:ASP:HB3	1:C:665:ARG:HE	1.85	0.41
1:B:467:LYS:HA	1:B:467:LYS:HD2	1.92	0.41
1:D:550:ARG:HB2	4:D:810:HOH:O	2.20	0.41
1:A:485:LYS:HB2	1:A:485:LYS:HE3	1.91	0.41
1:D:596:PHE:HB2	1:D:598:ARG:HD3	2.03	0.40
1:A:419:ARG:HD3	1:C:516:TYR:HB2	2.04	0.40
1:C:415:TYR:HD2	1:C:488:GLY:HA2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/282 (91%)	252 (98%)	5 (2%)	0	100	100
1	B	256/282 (91%)	252 (98%)	4 (2%)	0	100	100
1	C	261/282 (93%)	255 (98%)	6 (2%)	0	100	100
1	D	253/282 (90%)	248 (98%)	5 (2%)	0	100	100
All	All	1027/1128 (91%)	1007 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	232/249 (93%)	232 (100%)	0	100	100
1	B	231/249 (93%)	230 (100%)	1 (0%)	84	92
1	C	235/249 (94%)	234 (100%)	1 (0%)	84	92
1	D	228/249 (92%)	224 (98%)	4 (2%)	51	70
All	All	926/996 (93%)	920 (99%)	6 (1%)	78	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	430	GLU
1	C	671	GLU
1	D	420	GLU
1	D	446	ASN
1	D	557	ASN
1	D	592	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	A	512	GLN
1	A	618	HIS
1	B	446	ASN
1	B	470	GLN
1	B	512	GLN
1	B	618	HIS
1	C	446	ASN
1	C	493	ASN
1	C	618	HIS
1	C	624	GLN
1	D	446	ASN
1	D	477	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	512	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
2	Q2H	B	701	-	31,33,33	1.57	4 (12%)	40,48,48	1.44	3 (7%)
2	Q2H	D	701	-	31,33,33	1.44	2 (6%)	40,48,48	1.44	4 (10%)
2	Q2H	C	701	-	31,33,33	1.40	2 (6%)	40,48,48	1.33	2 (5%)
3	SO4	B	702	-	4,4,4	0.21	0	6,6,6	0.21	0
2	Q2H	A	701	-	31,33,33	1.50	2 (6%)	40,48,48	1.57	2 (5%)

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	Q2H	C	701	-	-	5/25/25/25	0/3/3/3
2	Q2H	B	701	-	-	6/25/25/25	0/3/3/3
2	Q2H	D	701	-	-	7/25/25/25	0/3/3/3
2	Q2H	A	701	-	-	3/25/25/25	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	Q2H	C7-N8	7.17	1.46	1.27
2	D	701	Q2H	C7-N8	7.00	1.46	1.27
2	B	701	Q2H	C7-N8	6.92	1.46	1.27
2	C	701	Q2H	C7-N8	6.89	1.45	1.27
2	B	701	Q2H	C6-N26	3.41	1.46	1.44
2	A	701	Q2H	C1-C7	3.22	1.52	1.45
2	D	701	Q2H	C1-C7	2.92	1.51	1.45
2	C	701	Q2H	C1-C7	2.77	1.51	1.45
2	B	701	Q2H	C1-C7	2.71	1.51	1.45
2	B	701	Q2H	S28-N26	2.40	1.68	1.64

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	Q2H	N5-C6-N26	-8.21	110.63	116.54
2	D	701	Q2H	N5-C6-N26	-6.98	111.52	116.54
2	B	701	Q2H	N5-C6-N26	-6.93	111.55	116.54
2	C	701	Q2H	N5-C6-N26	-6.09	112.15	116.54
2	B	701	Q2H	C1-C7-N8	-4.43	114.51	122.09
2	A	701	Q2H	C1-C7-N8	-3.92	115.39	122.09
2	C	701	Q2H	C1-C7-N8	-3.77	115.64	122.09
2	D	701	Q2H	C1-C7-N8	-3.43	116.22	122.09
2	D	701	Q2H	C21-N25-C9	2.71	136.69	129.38
2	B	701	Q2H	C15-C12-C13	2.24	126.18	120.95
2	D	701	Q2H	C15-C12-C13	2.16	125.98	120.95

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	Q2H	C2-C1-C7-N8
2	A	701	Q2H	C6-C1-C7-N8
2	A	701	Q2H	C12-C13-N8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	701	Q2H	C2-C1-C7-N8
2	B	701	Q2H	C6-C1-C7-N8
2	C	701	Q2H	C2-C1-C7-N8
2	C	701	Q2H	C6-C1-C7-N8
2	C	701	Q2H	C12-C13-N8-C7
2	D	701	Q2H	C2-C1-C7-N8
2	D	701	Q2H	C6-C1-C7-N8
2	D	701	Q2H	C12-C13-N8-C7
2	B	701	Q2H	C13-C12-C15-F18
2	D	701	Q2H	C13-C12-C15-F18
2	B	701	Q2H	C13-C12-C15-F16
2	B	701	Q2H	C13-C12-C15-F17
2	C	701	Q2H	C13-C12-C15-F17
2	D	701	Q2H	C13-C12-C15-F16
2	D	701	Q2H	C13-C12-C15-F17
2	C	701	Q2H	C1-C6-N26-C27
2	D	701	Q2H	C1-C6-N26-C27
2	B	701	Q2H	C11-C12-C15-F18

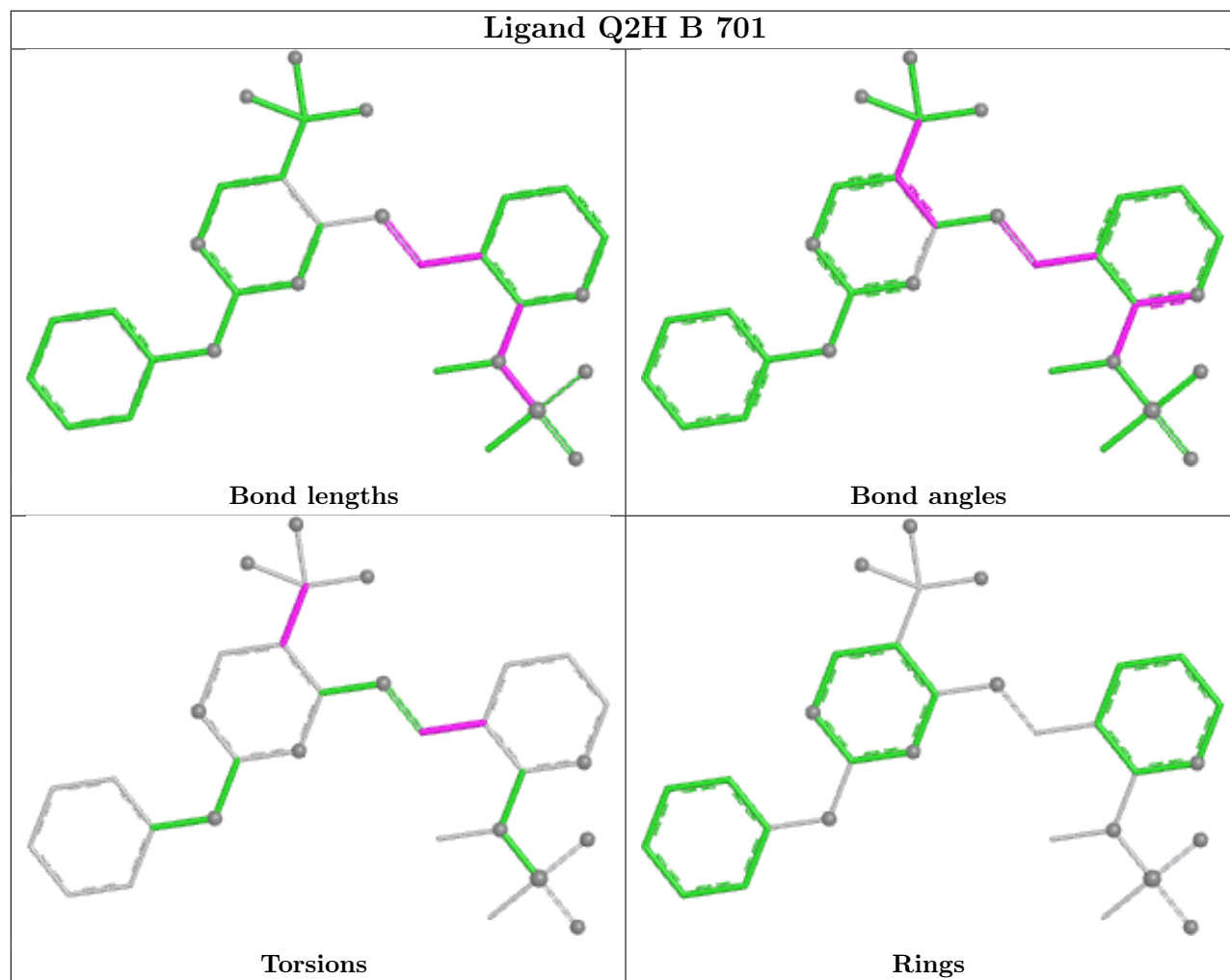
There are no ring outliers.

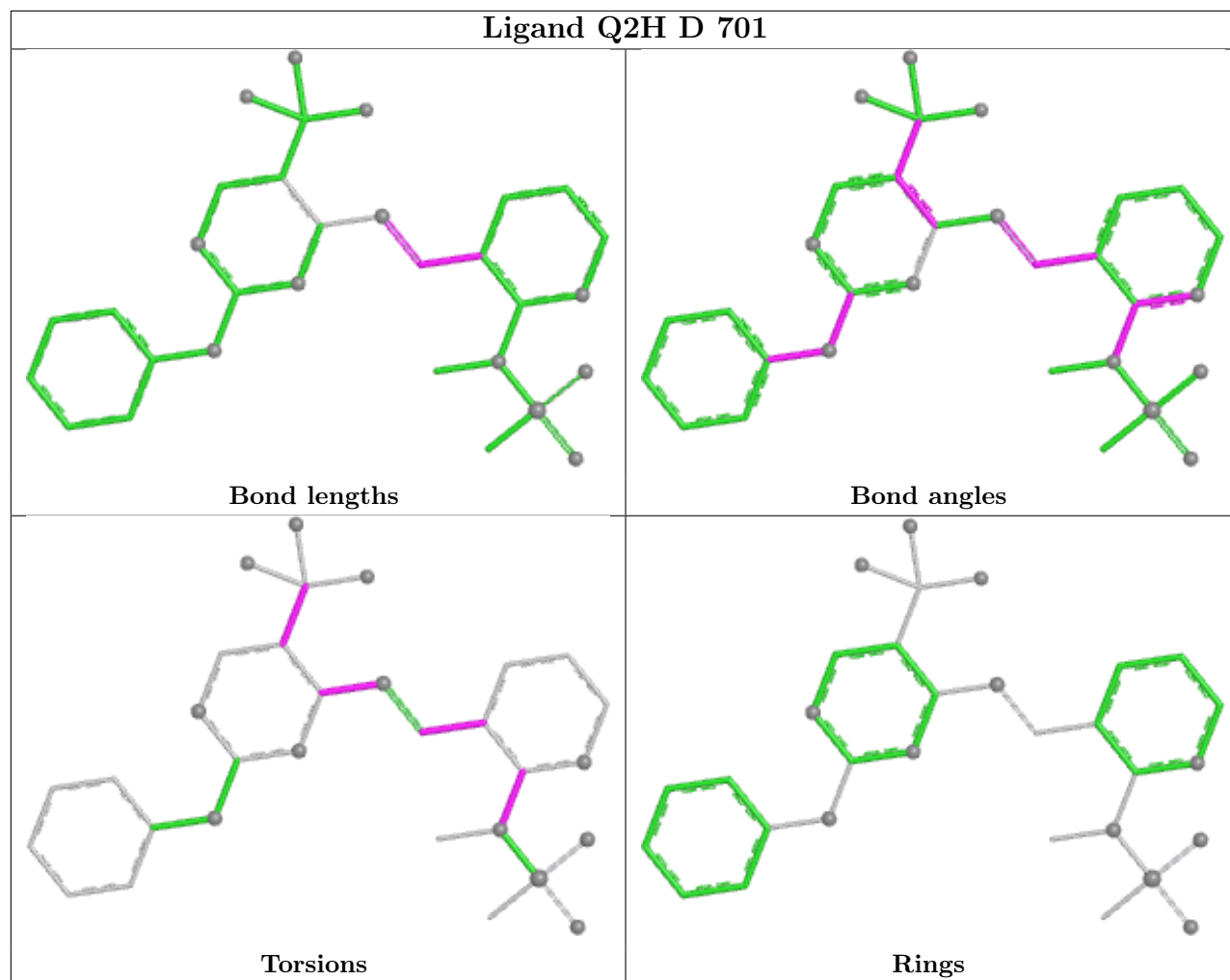
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	Q2H	1	0

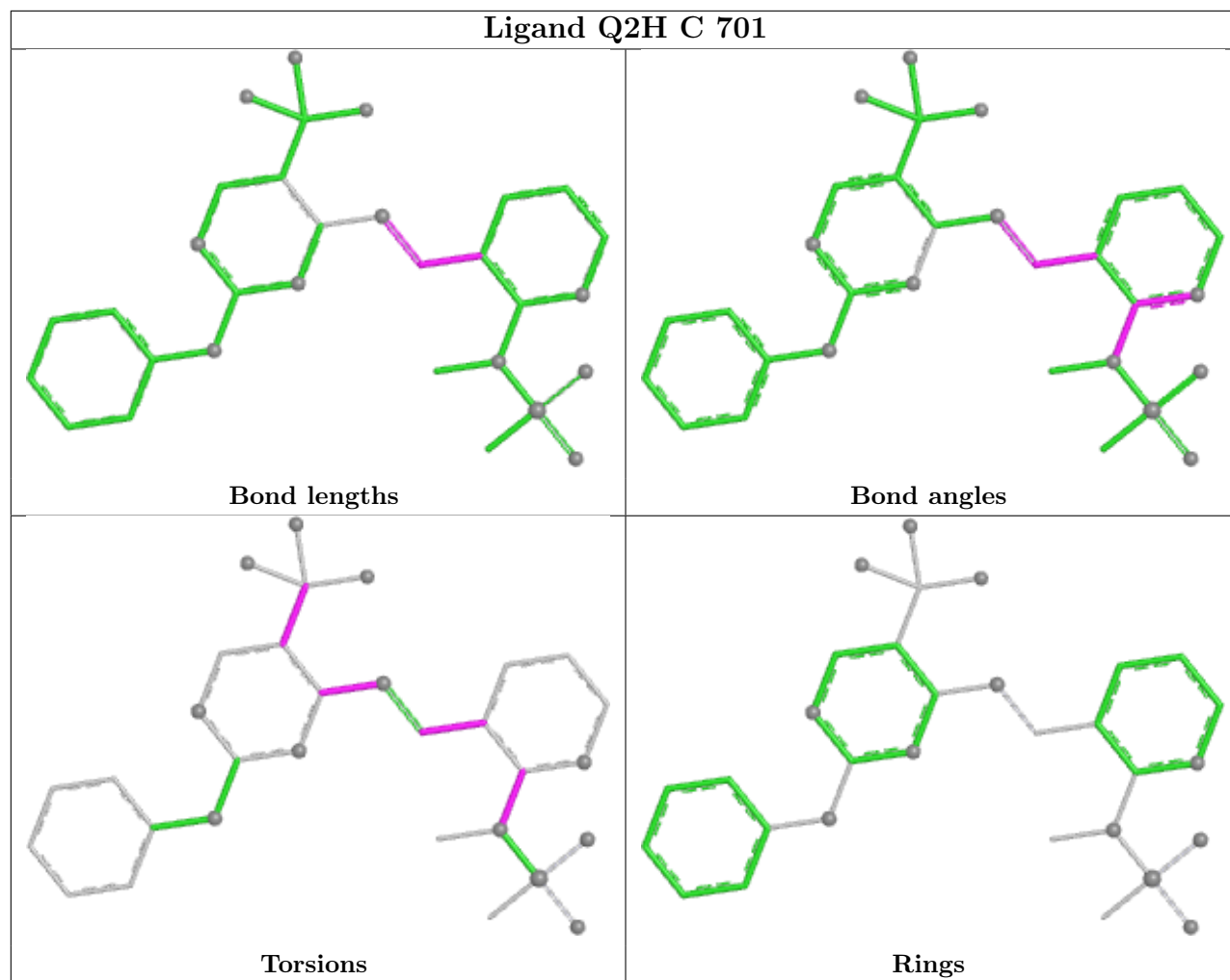
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

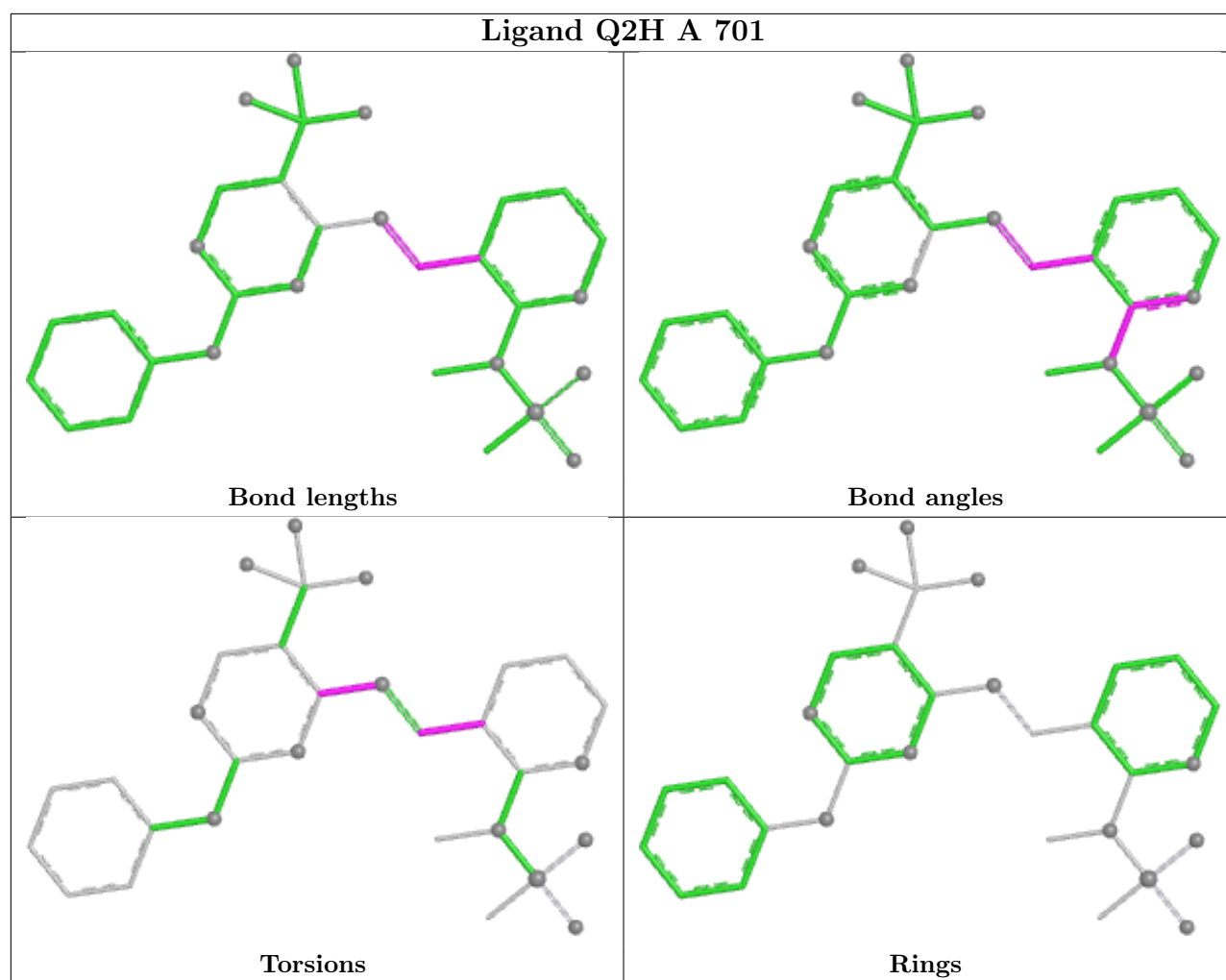
Ligand Q2H B 701





Ligand Q2H C 701





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	261/282 (92%)	0.88	19 (7%) 21 23	37, 58, 96, 111	0
1	B	260/282 (92%)	0.67	18 (6%) 23 25	32, 51, 83, 97	0
1	C	265/282 (93%)	0.72	22 (8%) 17 19	30, 56, 90, 103	0
1	D	257/282 (91%)	1.05	28 (10%) 10 12	44, 66, 101, 115	0
All	All	1043/1128 (92%)	0.83	87 (8%) 17 19	30, 58, 94, 115	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	516	TYR	4.4
1	C	646	ASN	4.4
1	A	415	TYR	4.0
1	A	460	THR	3.9
1	B	464	VAL	3.8
1	C	573	ASP	3.6
1	C	415	TYR	3.5
1	B	596	PHE	3.5
1	A	464	VAL	3.4
1	A	524	ILE	3.4
1	B	493	ASN	3.4
1	A	492	GLU	3.4
1	D	428	ILE	3.3
1	B	466	GLU	3.3
1	A	686	GLN	3.2
1	C	463	SER	3.2
1	D	518	LEU	3.2
1	C	460	THR	3.1
1	B	472	ALA	3.1
1	C	417	ILE	3.1
1	D	650	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	676	LEU	3.0
1	B	447	PRO	2.9
1	D	665	ARG	2.8
1	D	515	LYS	2.8
1	A	570	TYR	2.8
1	C	665	ARG	2.8
1	B	415	TYR	2.7
1	C	469	LEU	2.7
1	C	491	THR	2.7
1	A	463	SER	2.7
1	B	686	GLN	2.6
1	C	466	GLU	2.6
1	D	584	LEU	2.6
1	A	469	LEU	2.6
1	A	493	ASN	2.6
1	D	628	ASN	2.6
1	D	460	THR	2.6
1	D	585	PRO	2.6
1	D	415	TYR	2.6
1	C	464	VAL	2.5
1	D	464	VAL	2.5
1	D	513	VAL	2.5
1	D	520	LEU	2.5
1	D	685	ALA	2.5
1	B	632	ILE	2.5
1	D	432	GLN	2.5
1	A	466	GLU	2.4
1	C	492	GLU	2.4
1	B	637	ASN	2.4
1	A	497	ILE	2.4
1	D	495	VAL	2.3
1	D	542	PHE	2.3
1	C	470	GLN	2.3
1	D	686	GLN	2.3
1	B	469	LEU	2.3
1	D	514	ARG	2.3
1	D	651	LEU	2.3
1	B	426	ARG	2.3
1	C	473	LEU	2.2
1	A	646	ASN	2.2
1	C	414	ASP	2.2
1	B	494	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	625	GLY	2.2
1	D	429	GLY	2.2
1	B	594	ILE	2.2
1	C	632	ILE	2.2
1	C	447	PRO	2.2
1	B	517	SER	2.2
1	A	454	LYS	2.2
1	A	467	LYS	2.2
1	C	572	GLU	2.2
1	D	600	THR	2.2
1	A	443	SER	2.1
1	D	676	LEU	2.1
1	C	418	GLN	2.1
1	D	477	GLN	2.1
1	B	458	ASN	2.1
1	D	618	HIS	2.1
1	D	616	LEU	2.1
1	A	468	PHE	2.1
1	B	518	LEU	2.0
1	D	465	ARG	2.0
1	A	627	LYS	2.0
1	B	461	SER	2.0
1	C	416	GLU	2.0
1	C	530	LEU	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](#)

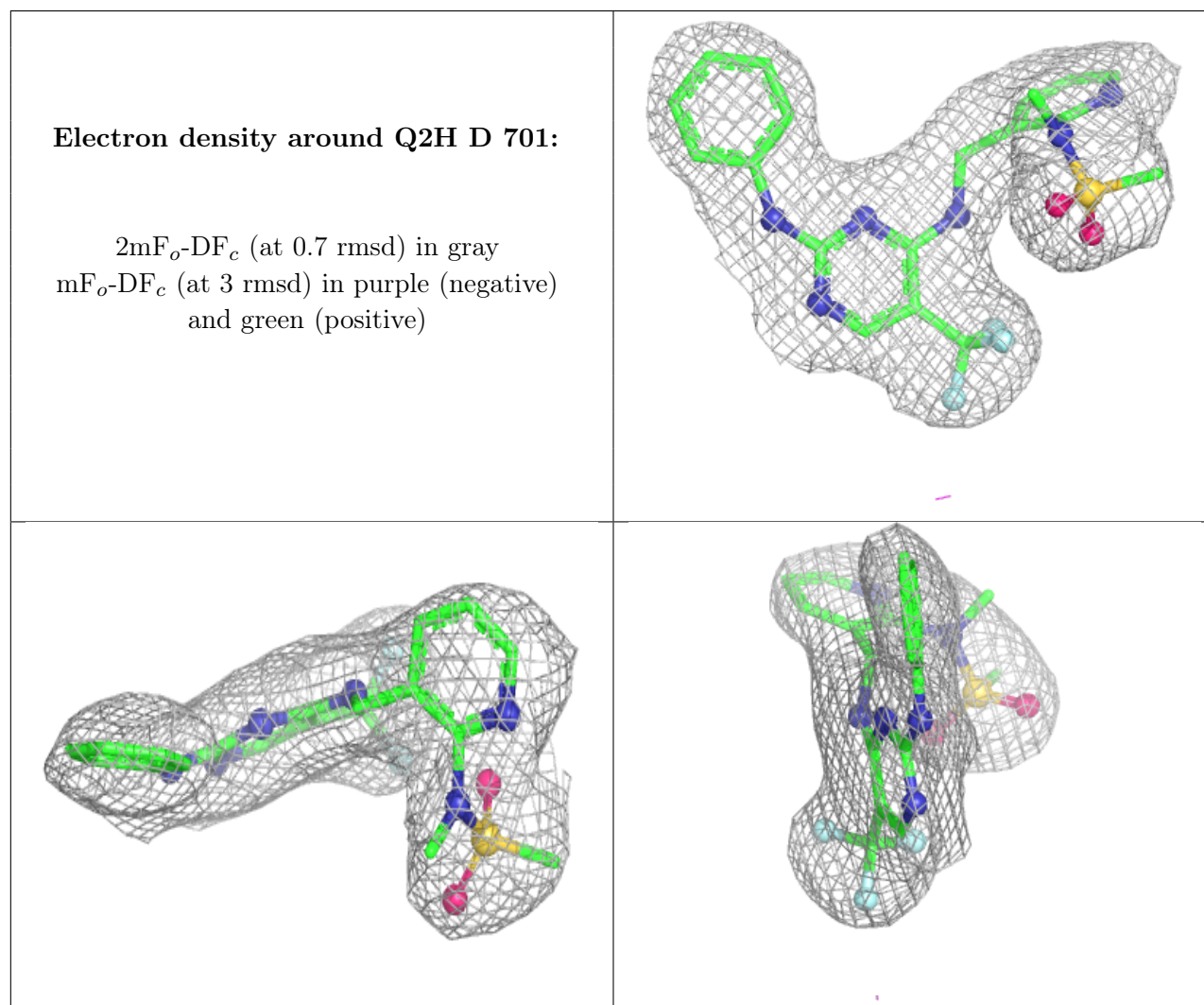
There are no oligosaccharides in this entry.

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.

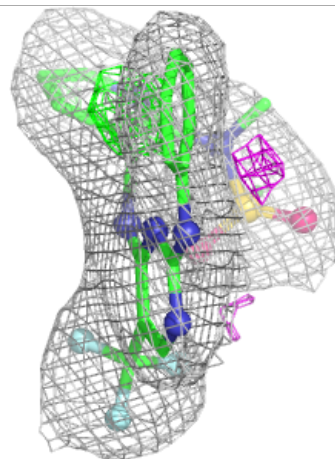
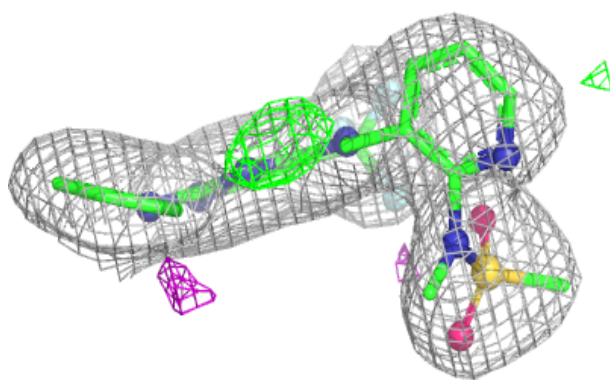
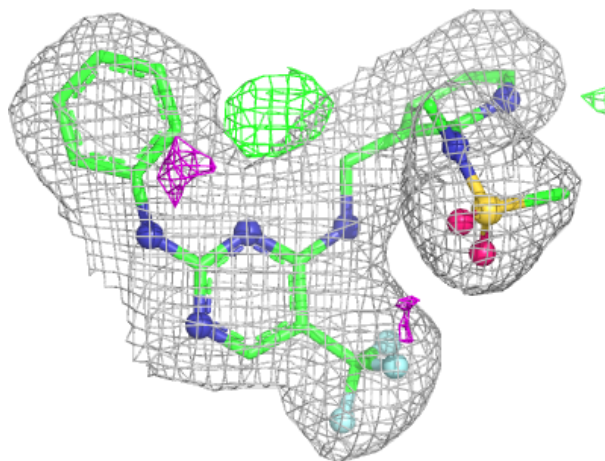
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	702	5/5	0.79	0.17	92,92,93,93	0
2	Q2H	D	701	31/31	0.93	0.11	52,55,64,65	0
2	Q2H	B	701	31/31	0.95	0.09	39,42,46,46	0
2	Q2H	C	701	31/31	0.95	0.08	36,41,45,45	0
2	Q2H	A	701	31/31	0.96	0.08	40,44,47,47	0

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.



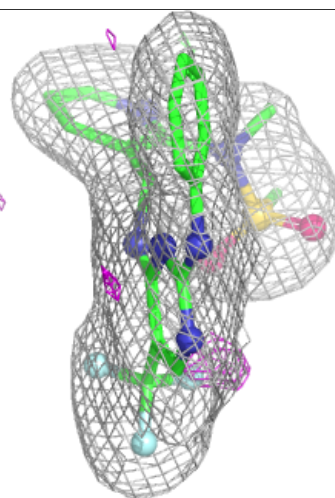
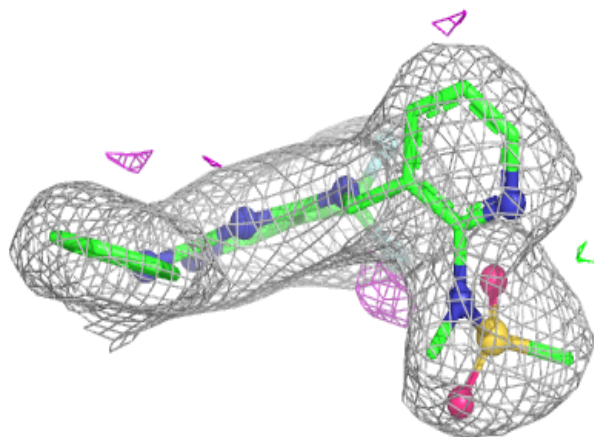
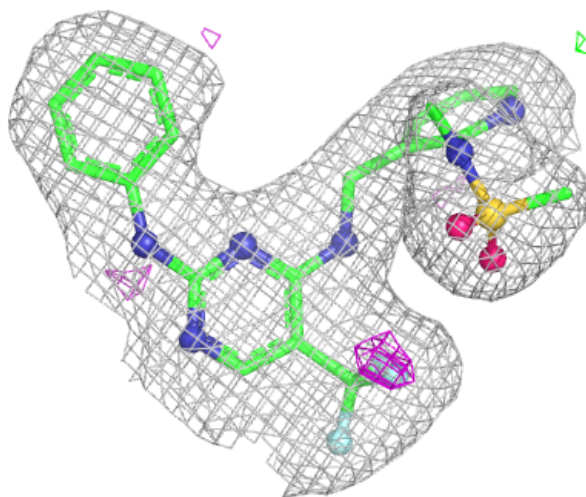
Electron density around Q2H B 701:

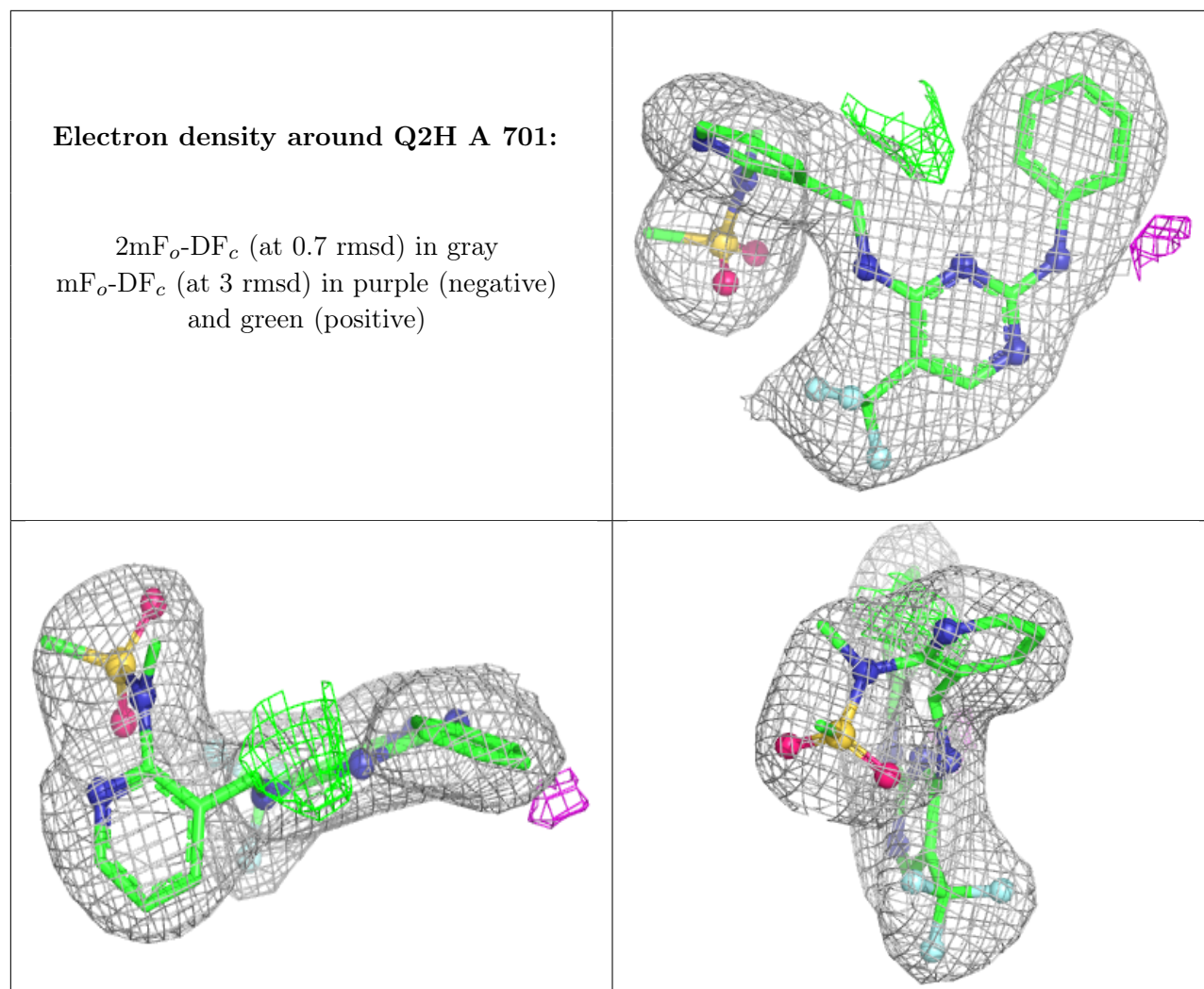
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Q2H C 701:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.