



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:44 AM BST

PDB ID : 4KBA
Title : CK1d in complex with 9-[3-(4-fluorophenyl)-1-methyl-1H-pyrazol-4-yl]-2,3,4,5-tetrahydropyrido[2,3-f][1,4]oxazepine inhibitor
Authors : Liu, S.
Deposited on : 2013-04-23
Resolution : 1.98 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 : 2.13.1
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) : 2.13.1

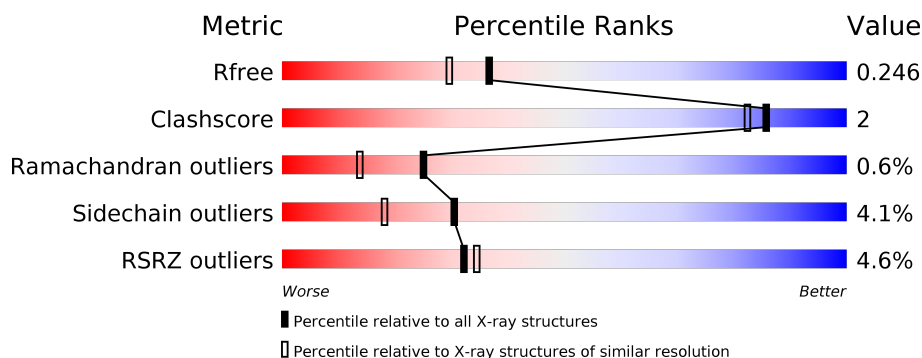
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 74%, yellow 74%, yellow 79%, green 79%, green 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 74% 5% 21% </div> </div>
1	B	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 7%, orange 7%, orange 78%, yellow 78%, yellow 85%, green 85%, green 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 78% 7% 14% </div> </div>
1	C	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, orange 5%, orange 77%, yellow 77%, yellow 83%, green 83%, green 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 77% 6% 16% </div> </div>
1	D	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 75%, yellow 75%, yellow 82%, green 82%, green 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 75% 7% 17% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9346 atoms, of which 68 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 Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2126	1371	362	379	14			
1	B	285	Total	C	N	O	S	0	0	0
			2316	1485	403	414	14			
1	C	277	Total	C	N	O	S	0	0	0
			2262	1455	389	404	14			
1	D	274	Total	C	N	O	S	0	2	0
			2257	1454	390	398	15			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P48730
A	-12	HIS	-	EXPRESSION TAG	UNP P48730
A	-11	HIS	-	EXPRESSION TAG	UNP P48730
A	-10	HIS	-	EXPRESSION TAG	UNP P48730
A	-9	HIS	-	EXPRESSION TAG	UNP P48730
A	-8	HIS	-	EXPRESSION TAG	UNP P48730
A	-7	HIS	-	EXPRESSION TAG	UNP P48730
A	-6	SER	-	EXPRESSION TAG	UNP P48730
A	-5	SER	-	EXPRESSION TAG	UNP P48730
A	-4	GLY	-	EXPRESSION TAG	UNP P48730
A	-3	LEU	-	EXPRESSION TAG	UNP P48730
A	-2	VAL	-	EXPRESSION TAG	UNP P48730
A	-1	PRO	-	EXPRESSION TAG	UNP P48730
A	0	ARG	-	EXPRESSION TAG	UNP P48730
A	1	GLY	-	EXPRESSION TAG	UNP P48730
A	2	SER	-	EXPRESSION TAG	UNP P48730
B	-13	MET	-	EXPRESSION TAG	UNP P48730
B	-12	HIS	-	EXPRESSION TAG	UNP P48730
B	-11	HIS	-	EXPRESSION TAG	UNP P48730
B	-10	HIS	-	EXPRESSION TAG	UNP P48730
B	-9	HIS	-	EXPRESSION TAG	UNP P48730

Continued on next page...

Continued from previous page...

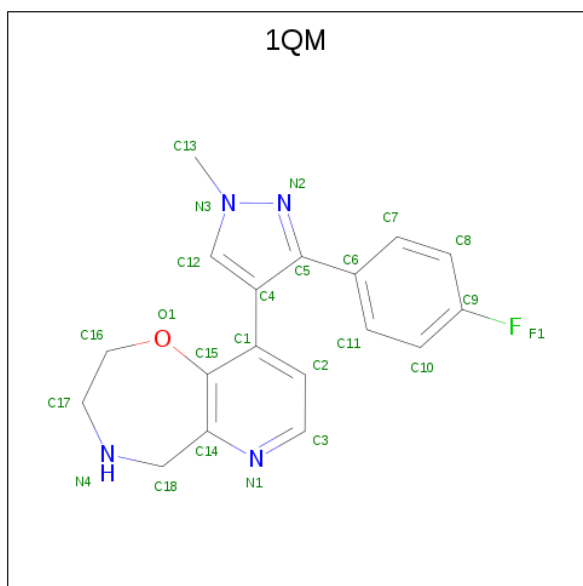
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	EXPRESSION TAG	UNP P48730
B	-7	HIS	-	EXPRESSION TAG	UNP P48730
B	-6	SER	-	EXPRESSION TAG	UNP P48730
B	-5	SER	-	EXPRESSION TAG	UNP P48730
B	-4	GLY	-	EXPRESSION TAG	UNP P48730
B	-3	LEU	-	EXPRESSION TAG	UNP P48730
B	-2	VAL	-	EXPRESSION TAG	UNP P48730
B	-1	PRO	-	EXPRESSION TAG	UNP P48730
B	0	ARG	-	EXPRESSION TAG	UNP P48730
B	1	GLY	-	EXPRESSION TAG	UNP P48730
B	2	SER	-	EXPRESSION TAG	UNP P48730
C	-13	MET	-	EXPRESSION TAG	UNP P48730
C	-12	HIS	-	EXPRESSION TAG	UNP P48730
C	-11	HIS	-	EXPRESSION TAG	UNP P48730
C	-10	HIS	-	EXPRESSION TAG	UNP P48730
C	-9	HIS	-	EXPRESSION TAG	UNP P48730
C	-8	HIS	-	EXPRESSION TAG	UNP P48730
C	-7	HIS	-	EXPRESSION TAG	UNP P48730
C	-6	SER	-	EXPRESSION TAG	UNP P48730
C	-5	SER	-	EXPRESSION TAG	UNP P48730
C	-4	GLY	-	EXPRESSION TAG	UNP P48730
C	-3	LEU	-	EXPRESSION TAG	UNP P48730
C	-2	VAL	-	EXPRESSION TAG	UNP P48730
C	-1	PRO	-	EXPRESSION TAG	UNP P48730
C	0	ARG	-	EXPRESSION TAG	UNP P48730
C	1	GLY	-	EXPRESSION TAG	UNP P48730
C	2	SER	-	EXPRESSION TAG	UNP P48730
D	-13	MET	-	EXPRESSION TAG	UNP P48730
D	-12	HIS	-	EXPRESSION TAG	UNP P48730
D	-11	HIS	-	EXPRESSION TAG	UNP P48730
D	-10	HIS	-	EXPRESSION TAG	UNP P48730
D	-9	HIS	-	EXPRESSION TAG	UNP P48730
D	-8	HIS	-	EXPRESSION TAG	UNP P48730
D	-7	HIS	-	EXPRESSION TAG	UNP P48730
D	-6	SER	-	EXPRESSION TAG	UNP P48730
D	-5	SER	-	EXPRESSION TAG	UNP P48730
D	-4	GLY	-	EXPRESSION TAG	UNP P48730
D	-3	LEU	-	EXPRESSION TAG	UNP P48730
D	-2	VAL	-	EXPRESSION TAG	UNP P48730
D	-1	PRO	-	EXPRESSION TAG	UNP P48730
D	0	ARG	-	EXPRESSION TAG	UNP P48730
D	1	GLY	-	EXPRESSION TAG	UNP P48730

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	SER	-	EXPRESSION TAG	UNP P48730

- Molecule 2 is 9-[3-(4-fluorophenyl)-1-methyl-1H-pyrazol-4-yl]-2,3,4,5-tetrahydropyrido[2,3-f][1,4]oxazepine (three-letter code: 1QM) (formula: C₁₈H₁₇FN₄O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	17	0
			41	18	1	17	4	1		
2	B	1	Total	C	F	H	N	O	17	0
			41	18	1	17	4	1		
2	C	1	Total	C	F	H	N	O	17	0
			41	18	1	17	4	1		
2	D	1	Total	C	F	H	N	O	17	0
			41	18	1	17	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

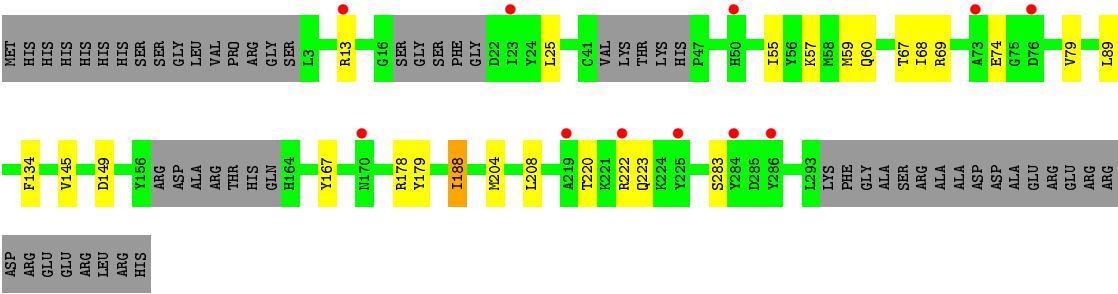
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	33	Total	O	0	0
			33	33		
4	C	56	Total	O	0	0
			56	56		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	40	Total	O	0	0
			40	40		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.69Å 83.96Å 89.29Å 108.00° 105.71° 93.00°	Depositor
Resolution (Å)	19.96 – 1.98 19.74 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.96-1.98) 96.4 (19.74-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.97Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.208 , 0.237 0.226 , 0.246	Depositor DCC
R_{free} test set	4379 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9346	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1QM, 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	0.52	0/2174	0.65	1/2921 (0.0%)
1	B	0.49	0/2368	0.65	0/3182
1	C	0.53	0/2313	0.67	0/3106
1	D	0.50	0/2312	0.66	0/3102
All	All	0.51	0/9167	0.66	1/12311 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	N-CA-CB	5.41	123.39	111.50

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	2126	0	2115	10	0
1	B	2316	0	2299	10	0
1	C	2262	0	2263	12	0
1	D	2257	0	2271	8	0
2	A	24	17	17	2	0
2	B	24	17	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	17	17	0	0
2	D	24	17	17	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	1	0
3	D	15	0	0	0	0
4	A	47	0	0	1	0
4	B	33	0	0	0	0
4	C	56	0	0	0	0
4	D	40	0	0	0	0
All	All	9278	68	9016	40	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 2.

All (40) 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:288:PHE:H	1:A:291:ASN:HD22	1.28	0.82
1:B:226:GLU:O	1:B:230:GLU:HG2	1.83	0.77
1:D:60:GLN:HE22	1:D:67:THR:HA	1.51	0.76
1:C:48:GLN:HE22	1:C:151:GLY:HA2	1.54	0.73
1:C:89:LEU:HD21	1:C:136:MET:HE1	1.75	0.68
1:C:40:GLU:O	1:C:41:CYS:HB2	1.97	0.64
1:C:89:LEU:HD21	1:C:136:MET:CE	2.28	0.63
1:A:82:MET:HE1	2:A:401:1QM:H1	1.82	0.60
1:C:199:LEU:O	1:C:202:VAL:HG22	2.02	0.60
1:C:204:MET:HE3	1:C:208:LEU:CD2	2.32	0.59
1:B:236:PRO:O	1:B:239:VAL:HG22	2.04	0.58
1:A:199:LEU:O	1:A:202:VAL:HG22	2.04	0.57
1:D:204:MET:HE3	1:D:208:LEU:HD13	1.89	0.55
1:C:41:CYS:CB	1:C:44:THR:HG23	2.38	0.53
1:C:41:CYS:HB2	1:C:44:THR:HG23	1.90	0.53
1:D:167:TYR:CE1	1:D:188:ILE:HD13	2.43	0.53
1:B:216:LEU:HD23	1:B:227:ARG:HB3	1.93	0.51
1:B:271:GLN:NE2	1:B:274:ARG:HH11	2.09	0.50
1:A:178:ARG:HD2	1:A:179:TYR:CZ	2.47	0.49
1:B:160:ARG:HD3	1:B:161:THR:HG23	1.95	0.49
1:A:82:MET:HE1	2:A:401:1QM:C2	2.42	0.49
1:B:279:ARG:NH2	3:C:402:SO4:O3	2.46	0.48
1:B:178:ARG:HD2	1:B:179:TYR:CZ	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:O	1:A:41:CYS:HB2	2.14	0.47
1:D:178:ARG:HD2	1:D:179:TYR:CZ	2.51	0.45
1:A:288:PHE:H	1:A:291:ASN:ND2	2.06	0.45
1:A:199:LEU:HA	1:A:202:VAL:HG22	1.99	0.44
1:C:178:ARG:HD2	1:C:214:GLN:HG3	1.98	0.44
1:D:89:LEU:HD13	1:D:134:PHE:O	2.17	0.44
1:C:199:LEU:HD12	1:C:202:VAL:CG2	2.47	0.44
1:C:199:LEU:HA	1:C:202:VAL:HG22	2.00	0.43
1:D:204:MET:HE3	1:D:208:LEU:CD1	2.48	0.43
1:B:158:ASP:HB3	1:B:161:THR:OG1	2.19	0.43
1:D:220:THR:OG1	1:D:223:GLN:HG2	2.18	0.43
1:B:55:ILE:O	1:B:59:MET:HG2	2.19	0.42
1:A:199:LEU:HD12	1:A:202:VAL:CG2	2.49	0.42
1:C:204:MET:CE	1:C:208:LEU:CD2	2.98	0.42
1:A:279:ARG:HD2	4:A:545:HOH:O	2.18	0.42
1:B:271:GLN:HE22	1:B:274:ARG:HH11	1.67	0.41
1:D:55:ILE:O	1:D:59:MET:HG2	2.22	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	257/331 (78%)	249 (97%)	6 (2%)	2 (1%)	19	9
1	B	281/331 (85%)	277 (99%)	3 (1%)	1 (0%)	34	22
1	C	273/331 (82%)	266 (97%)	5 (2%)	2 (1%)	22	11
1	D	268/331 (81%)	260 (97%)	6 (2%)	2 (1%)	22	11
All	All	1079/1324 (82%)	1052 (98%)	20 (2%)	7 (1%)	25	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	CYS
1	C	41	CYS
1	D	74	GLU
1	B	149	ASP
1	D	149	ASP
1	A	149	ASP
1	C	149	ASP

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	228/288 (79%)	223 (98%)	5 (2%)	52	46
1	B	246/288 (85%)	233 (95%)	13 (5%)	22	10
1	C	243/288 (84%)	232 (96%)	11 (4%)	27	15
1	D	243/288 (84%)	233 (96%)	10 (4%)	30	18
All	All	960/1152 (83%)	921 (96%)	39 (4%)	30	18

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	39	LEU
1	A	57	LYS
1	A	227	ARG
1	A	292	MET
1	B	13	ARG
1	B	14	LYS
1	B	22	ASP
1	B	25	LEU
1	B	63	VAL
1	B	68	ILE
1	B	132	ASP
1	B	149	ASP
1	B	160	ARG
1	B	171	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	220	THR
1	B	230	GLU
1	B	256	ARG
1	C	7	ASN
1	C	25	LEU
1	C	48	GLN
1	C	54	LYS
1	C	57	LYS
1	C	69	ARG
1	C	81	VAL
1	C	171	LYS
1	C	178	ARG
1	C	221	LYS
1	C	242	LYS
1	D	13	ARG
1	D	25	LEU
1	D	57	LYS
1	D	68	ILE
1	D	69	ARG
1	D	79	VAL
1	D	145	VAL
1	D	188	ILE
1	D	222	ARG
1	D	283	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	183	ASN
1	A	275	ASN
1	A	280	GLN
1	A	291	ASN
1	B	271	GLN
1	B	275	ASN
1	C	48	GLN
1	C	183	ASN
1	C	207	ASN
1	D	60	GLN
1	D	271	GLN
1	D	280	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 ⓘ

13 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	1QM	D	401	-	22,27,27	1.68	5 (22%)	26,38,38	0.80	0
2	1QM	B	401	-	22,27,27	1.67	5 (22%)	26,38,38	0.85	0
2	1QM	C	401	-	22,27,27	1.63	5 (22%)	26,38,38	0.83	0
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.42	0
3	SO4	C	402	-	4,4,4	0.21	0	6,6,6	0.47	0
3	SO4	B	403	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	A	403	-	4,4,4	0.15	0	6,6,6	0.25	0
3	SO4	D	403	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	D	404	-	4,4,4	0.22	0	6,6,6	0.15	0
2	1QM	A	401	-	22,27,27	1.64	5 (22%)	26,38,38	0.86	1 (3%)
3	SO4	B	402	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	C	403	-	4,4,4	0.33	0	6,6,6	0.18	0
3	SO4	D	402	-	4,4,4	0.27	0	6,6,6	0.17	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
2	1QM	D	401	-	-	2/8/16/16	0/3/4/4
2	1QM	B	401	-	-	3/8/16/16	0/3/4/4
2	1QM	C	401	-	-	3/8/16/16	0/3/4/4
2	1QM	A	401	-	-	3/8/16/16	0/3/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	1QM	C12-N3	3.77	1.39	1.35
2	A	401	1QM	C12-N3	3.77	1.39	1.35
2	B	401	1QM	C12-N3	3.72	1.39	1.35
2	D	401	1QM	C12-N3	3.62	1.39	1.35
2	D	401	1QM	C6-C5	-3.12	1.45	1.49
2	A	401	1QM	C6-C5	-3.10	1.45	1.49
2	B	401	1QM	C1-C4	-3.09	1.44	1.49
2	A	401	1QM	C1-C4	-3.09	1.44	1.49
2	B	401	1QM	C6-C5	-3.08	1.45	1.49
2	C	401	1QM	C6-C5	-3.08	1.45	1.49
2	C	401	1QM	C1-C4	-3.06	1.44	1.49
2	D	401	1QM	C1-C4	-3.03	1.44	1.49
2	D	401	1QM	C5-N2	2.63	1.37	1.35
2	D	401	1QM	C17-C16	2.61	1.54	1.51
2	B	401	1QM	C5-N2	2.59	1.37	1.35
2	B	401	1QM	C17-C16	2.50	1.54	1.51
2	A	401	1QM	C17-C16	2.48	1.54	1.51
2	C	401	1QM	C5-N2	2.39	1.37	1.35
2	A	401	1QM	C5-N2	2.34	1.37	1.35
2	C	401	1QM	C17-C16	2.30	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	1QM	C16-O1-C15	-2.15	112.36	116.21

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	1QM	C15-C1-C4-C5
2	B	401	1QM	C15-C1-C4-C5

Continued on next page...

Continued from previous page...

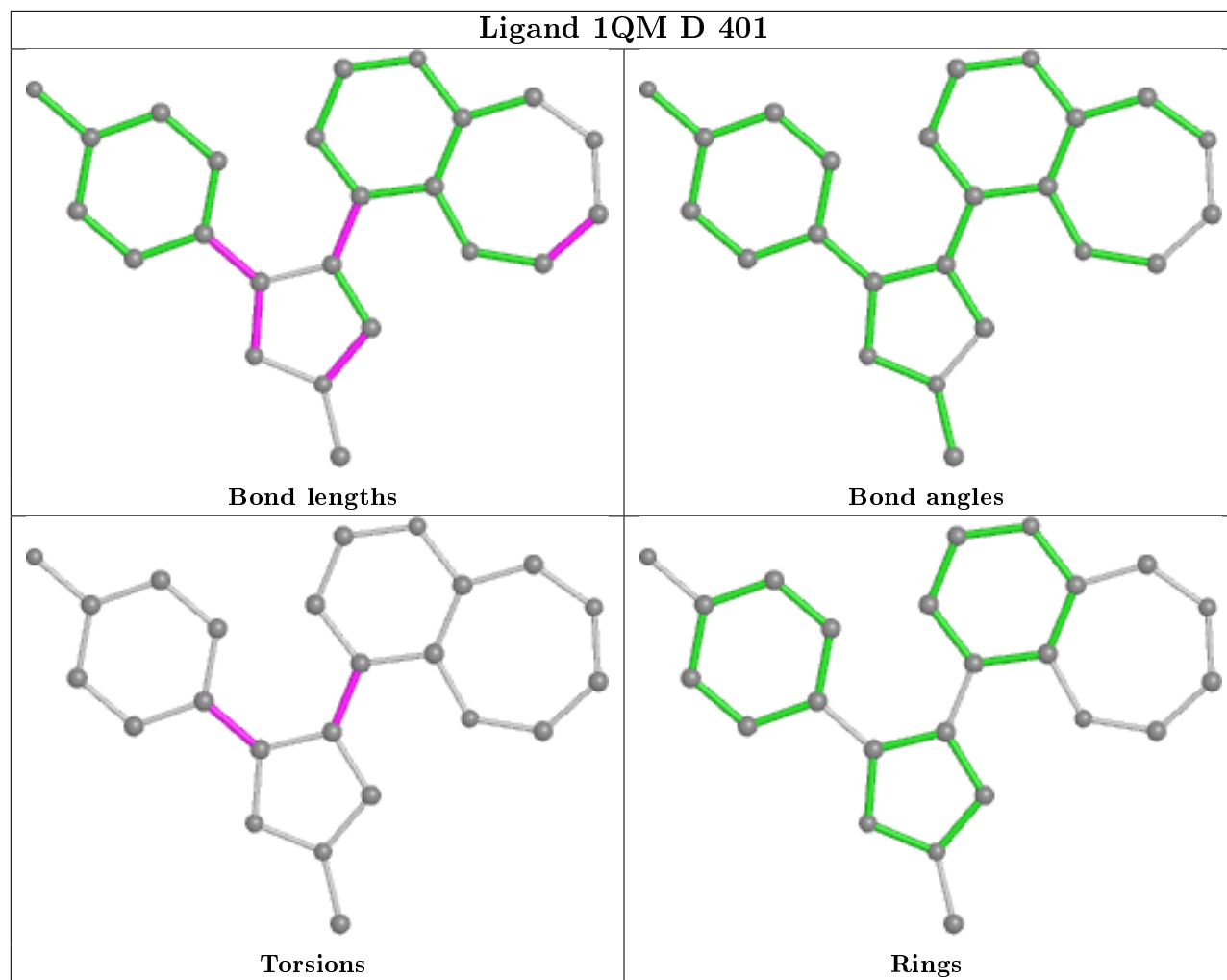
Mol	Chain	Res	Type	Atoms
2	C	401	1QM	C15-C1-C4-C5
2	A	401	1QM	C15-C1-C4-C5
2	C	401	1QM	N2-C5-C6-C11
2	B	401	1QM	N2-C5-C6-C11
2	A	401	1QM	N2-C5-C6-C11
2	D	401	1QM	N2-C5-C6-C11
2	B	401	1QM	N2-C5-C6-C7
2	C	401	1QM	N2-C5-C6-C7
2	A	401	1QM	N2-C5-C6-C7

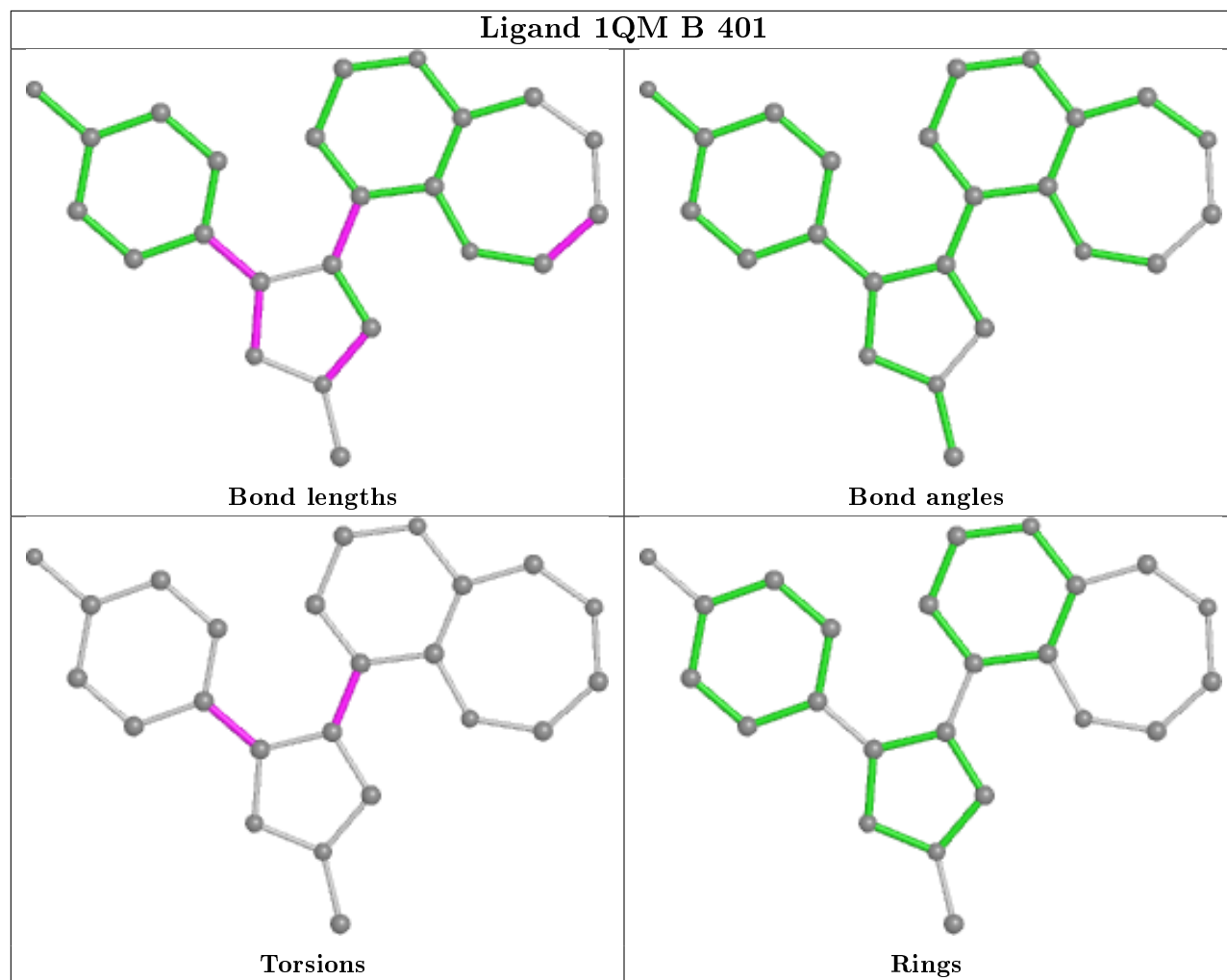
There are no ring outliers.

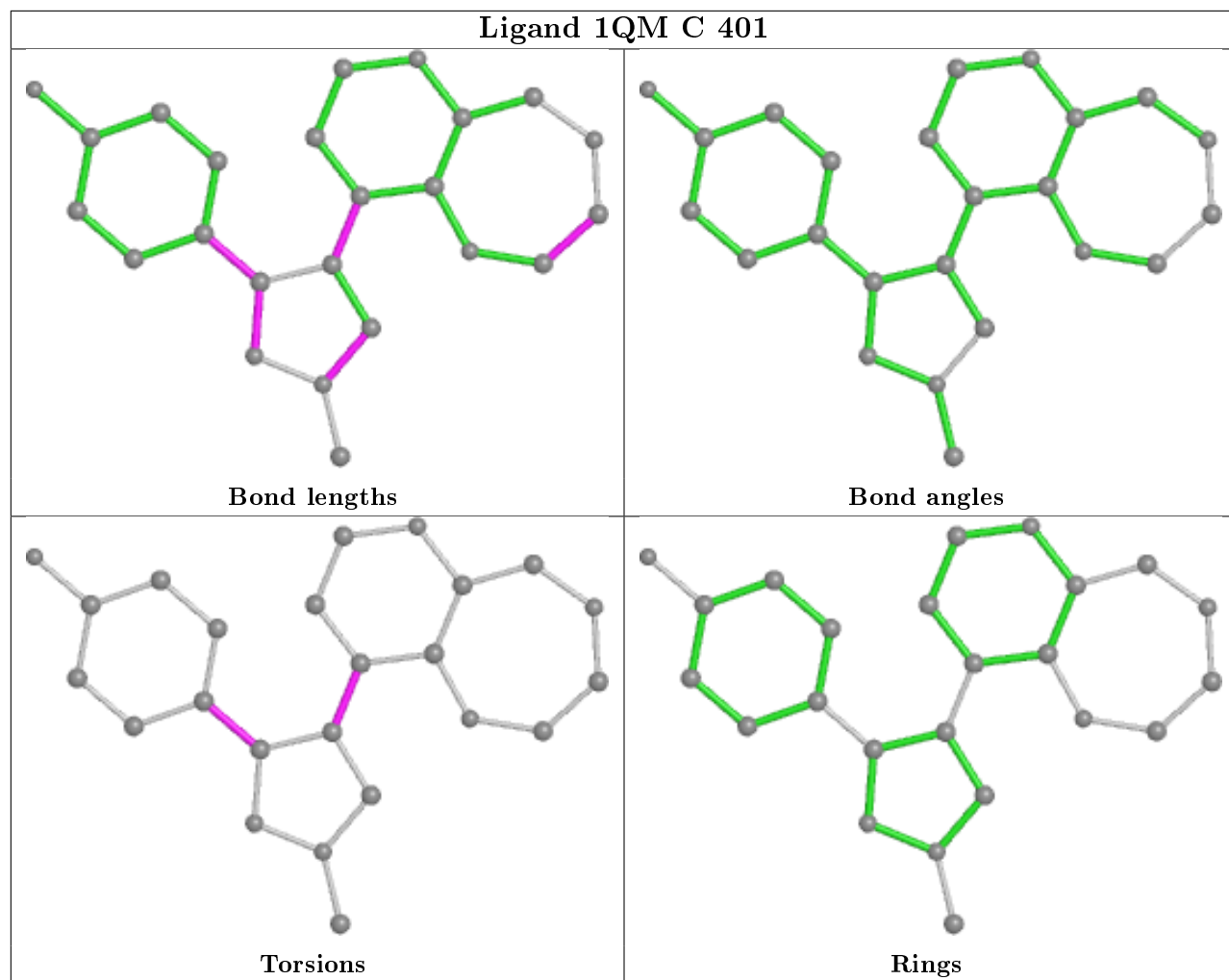
2 monomers are involved in 3 short contacts:

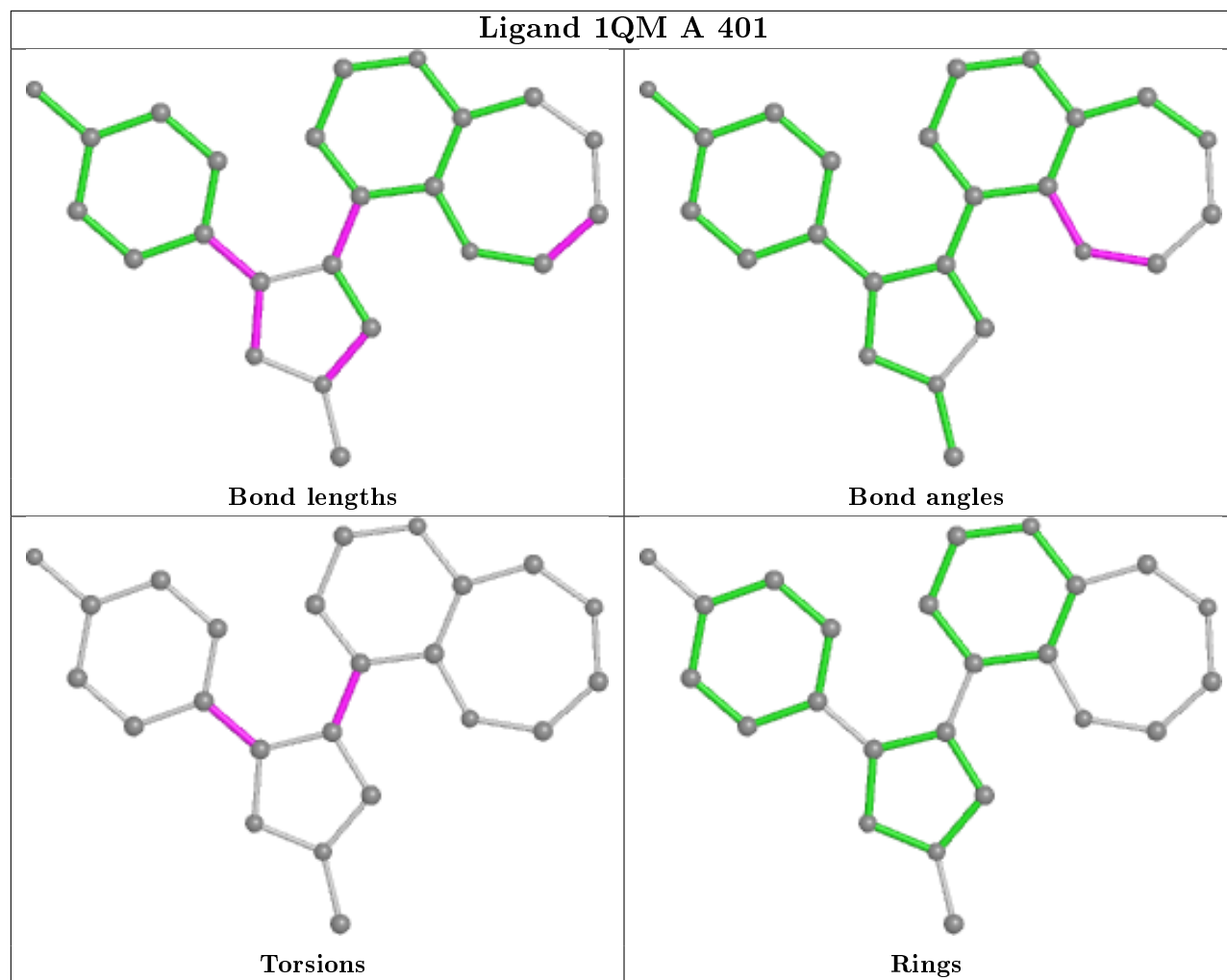
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	SO4	1	0
2	A	401	1QM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/331 (79%)	-0.08	3 (1%) 80 82	19, 31, 50, 63	0
1	B	285/331 (86%)	0.19	22 (7%) 13 15	18, 34, 71, 90	0
1	C	277/331 (83%)	0.05	15 (5%) 25 28	16, 30, 60, 81	0
1	D	274/331 (82%)	0.09	11 (4%) 38 40	19, 34, 66, 81	0
All	All	1099/1324 (83%)	0.07	51 (4%) 32 34	16, 32, 63, 90	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	ALA	5.4
1	C	172	ASN	4.8
1	B	220	THR	4.6
1	B	217	LYS	4.3
1	B	225	TYR	4.2
1	B	161	THR	4.1
1	C	170	ASN	4.1
1	D	170	ASN	3.9
1	D	73	ALA	3.9
1	B	16	GLY	3.7
1	B	284	TYR	3.7
1	D	225	TYR	3.6
1	B	221	LYS	3.5
1	C	171	LYS	3.5
1	B	173	LEU	3.3
1	B	159	ALA	3.2
1	B	222	ARG	3.1
1	A	71	CYS	2.9
1	B	170	ASN	2.9
1	B	41	CYS	2.8
1	D	219	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	95	PHE	2.8
1	B	223	GLN	2.8
1	D	286	TYR	2.7
1	B	21	GLY	2.7
1	C	221	LYS	2.6
1	C	219	ALA	2.6
1	C	222	ARG	2.6
1	B	19	SER	2.6
1	B	293	LEU	2.6
1	D	222	ARG	2.6
1	C	20	PHE	2.6
1	B	7	ASN	2.5
1	D	50	HIS	2.5
1	C	217	LYS	2.4
1	C	225	TYR	2.4
1	D	284	TYR	2.4
1	C	174	THR	2.3
1	B	160	ARG	2.3
1	C	168	ARG	2.3
1	C	169	GLU	2.3
1	A	177	ALA	2.3
1	B	162	HIS	2.3
1	D	13	ARG	2.2
1	C	16	GLY	2.1
1	D	23	ILE	2.1
1	C	7	ASN	2.1
1	B	219	ALA	2.1
1	B	76	ASP	2.1
1	A	60	GLN	2.1
1	D	76	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

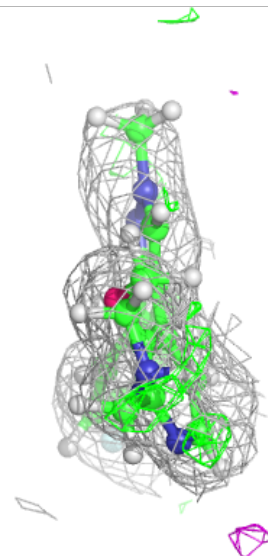
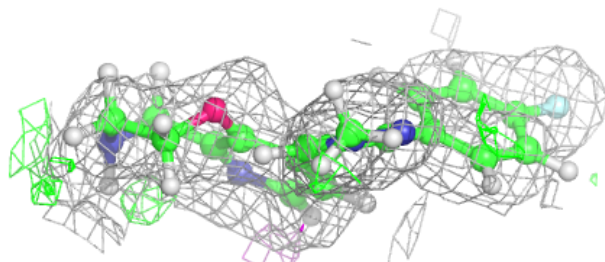
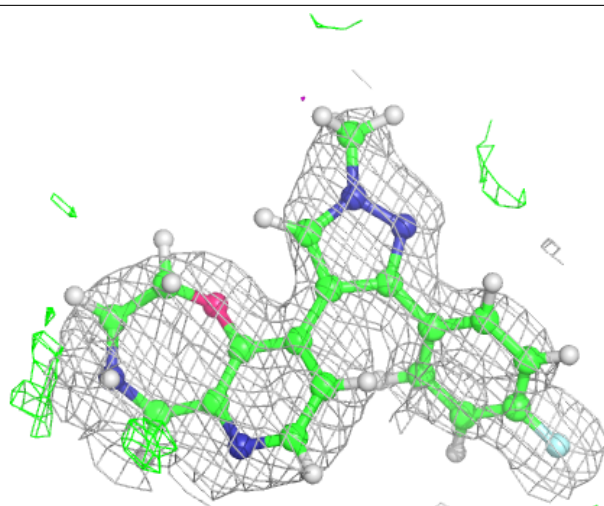
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	D	404	5/5	0.84	0.16	74,76,77,78	0
2	1QM	B	401	24/24	0.94	0.10	26,32,39,40	17
2	1QM	D	401	24/24	0.94	0.11	28,31,37,40	17
2	1QM	C	401	24/24	0.95	0.10	24,28,32,32	17
3	SO4	C	402	5/5	0.96	0.11	36,39,43,43	0
3	SO4	A	402	5/5	0.96	0.09	34,36,40,40	0
3	SO4	D	403	5/5	0.96	0.09	54,55,56,56	0
3	SO4	A	403	5/5	0.97	0.13	34,36,38,40	0
2	1QM	A	401	24/24	0.97	0.09	22,28,32,33	17
3	SO4	C	403	5/5	0.97	0.13	49,49,50,53	0
3	SO4	B	403	5/5	0.98	0.07	52,53,54,54	0
3	SO4	B	402	5/5	0.98	0.07	39,39,40,41	0
3	SO4	D	402	5/5	0.99	0.07	38,39,40,42	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.

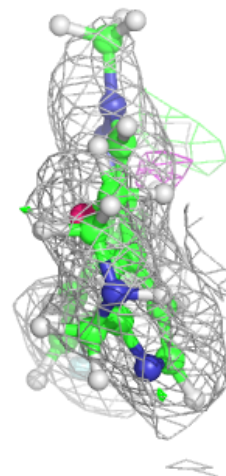
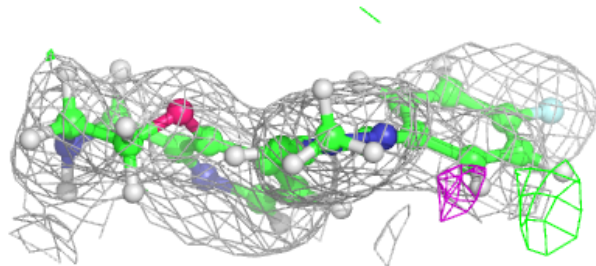
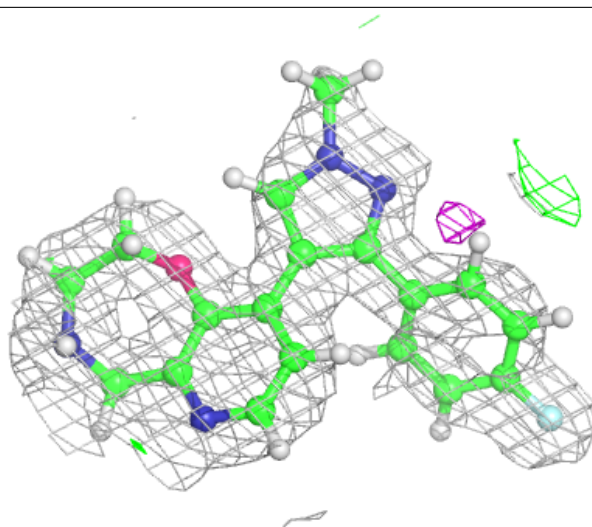
Electron density around 1QM B 401:

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



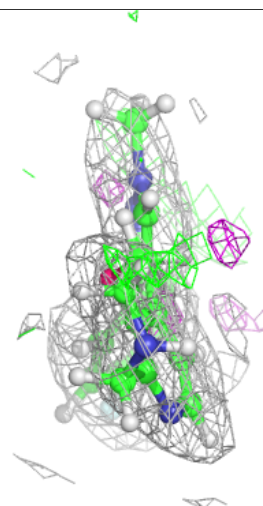
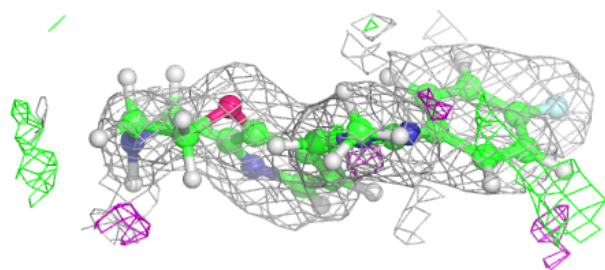
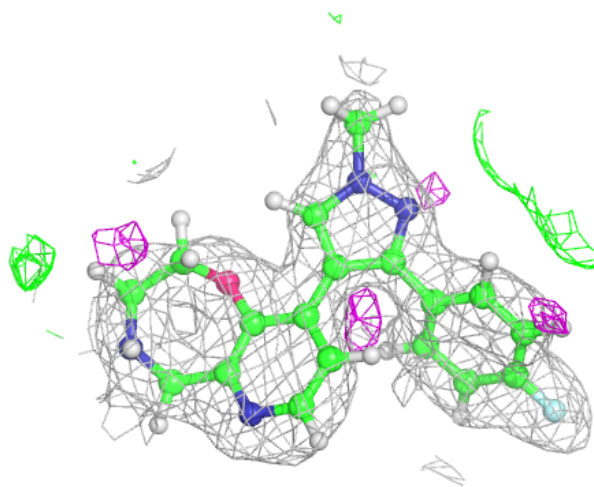
Electron density around 1QM D 401:

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



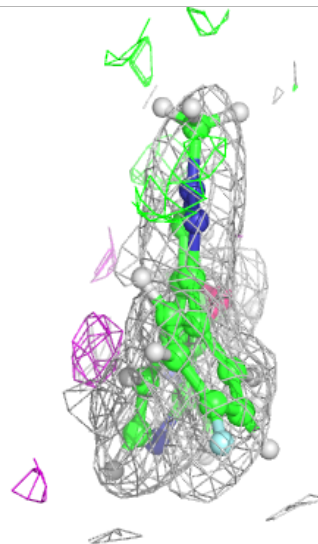
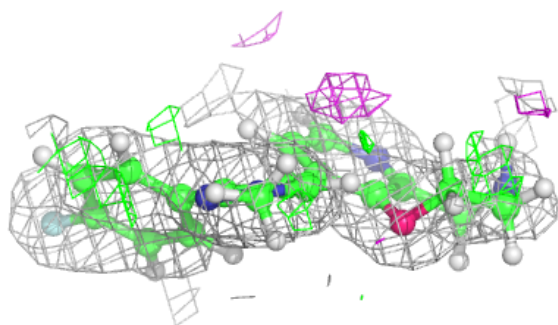
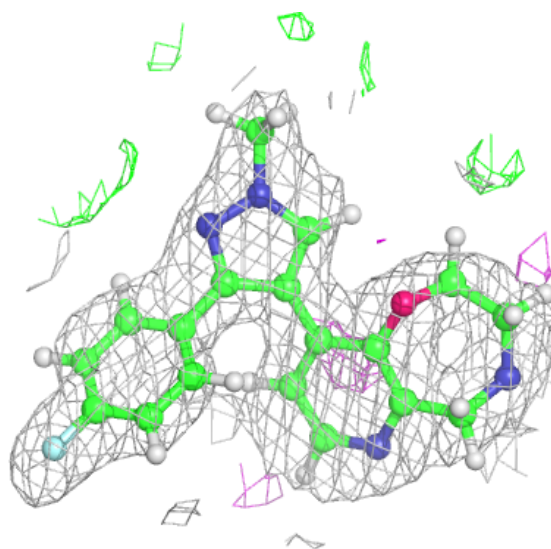
Electron density around 1QM C 401:

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



Electron density around 1QM A 401:

$2mF_o-DF_c$ (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.