Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 03:41 PM EST

PDB ID	:	4KB8
Title	:	CK1d in complex with 1-{4-[3-(4-FLUOROPHENYL)-1-METHYL-1H-PYRAZOL-4-YL]PYRIDIN-2-YL}-N-METHYLMETHANAMINE ligand
Authors	:	Liu, S.
Deposited on	:	2013-04-23
Resolution	:	1.95 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 (i) 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 (i)) were used in the production of this report:

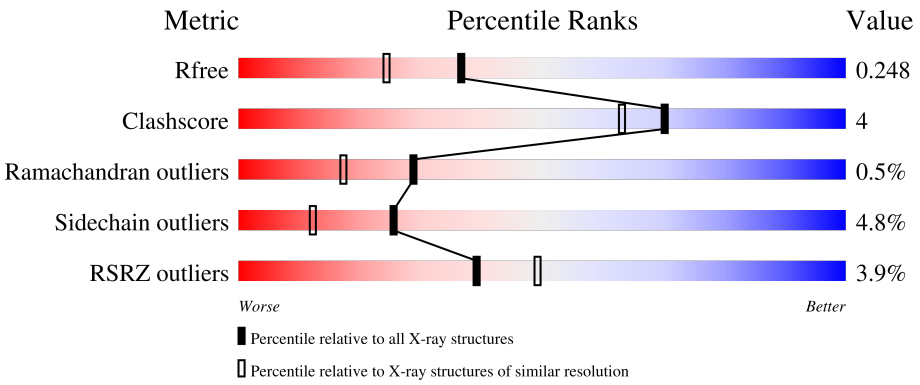
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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 <=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	2%, 73%, 7%, 20%
1	B	331	4%, 79%, 6%, 14%
1	C	331	4%, 76%, 7%, 16%
1	D	331	3%, 74%, 8%, 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9447 atoms, of which 62 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
			Total	C	N	O	S			
1	A	265	2144	1382	365	383	14	0	0	0
1	B	285	2316	1485	403	414	14	0	0	0
1	C	277	2262	1455	389	404	14	0	0	0
1	D	278	2285	1468	398	405	14	0	1	0

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

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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

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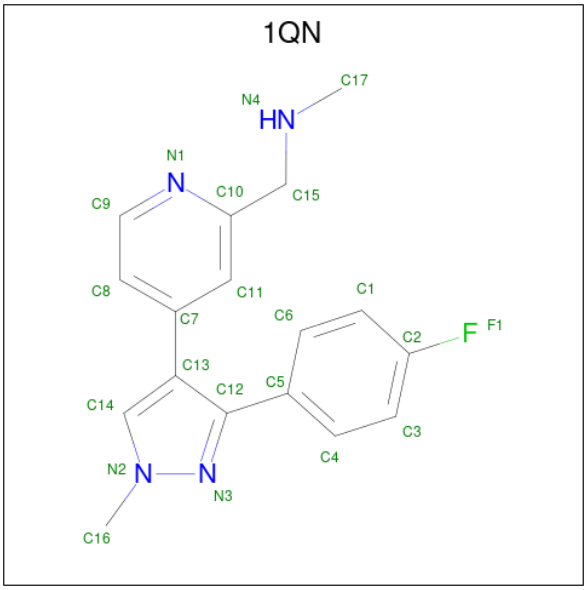
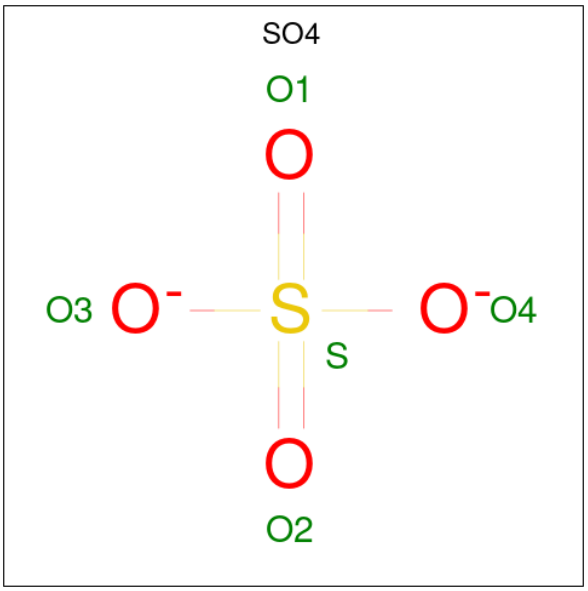
Chain	Residue	Modelled	Actual	Comment	Reference
D	2	SER	-	expression tag	UNP P48730

- Molecule 2 is 1-{4-[3-(4-fluorophenyl)-1-methyl-1H-pyrazol-4-yl]pyridin-2-yl}-N-methylmethanamine (three-letter code: 1QN) (formula: $C_{17}H_{17}FN_4$).



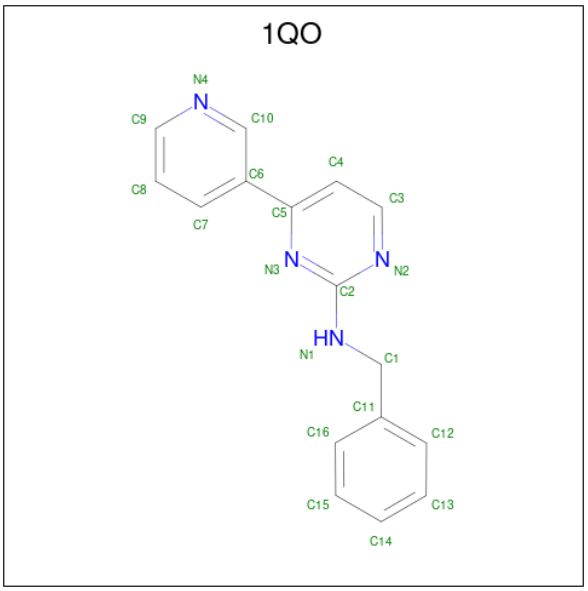
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	17	0
			39	17	1	17	4		
2	C	1	Total	C	F	H	N	17	0
			39	17	1	17	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is N-benzyl-4-(pyridin-3-yl)pyrimidin-2-amine (three-letter code: 1QO) (formula: $C_{16}H_{14}N_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
4	B	1	34	16	14	4	14	0
			Total	C	H	N		
4	D	1	34	16	14	4	14	0

- Molecule 5 is water.

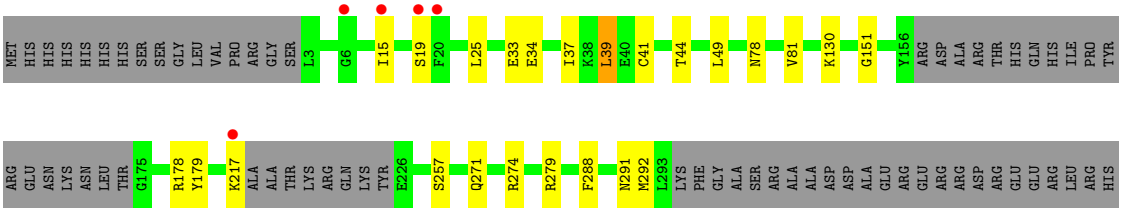
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	63	63	63	0	0
			Total	O		
5	B	62	62	62	0	0
			Total	O		
5	C	74	74	74	0	0
			Total	O		
5	D	55	55	55	0	0

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.

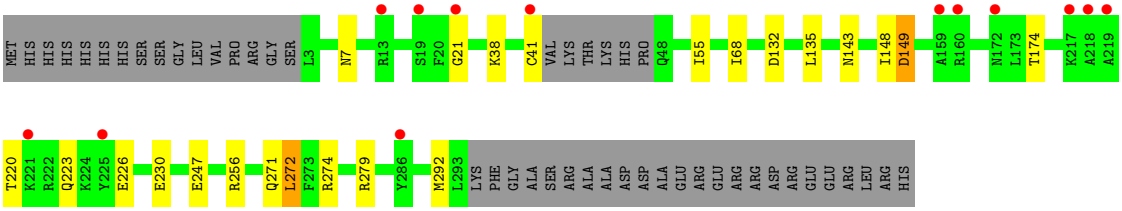
• Molecule 1: Casein kinase I isoform delta

Chain A:



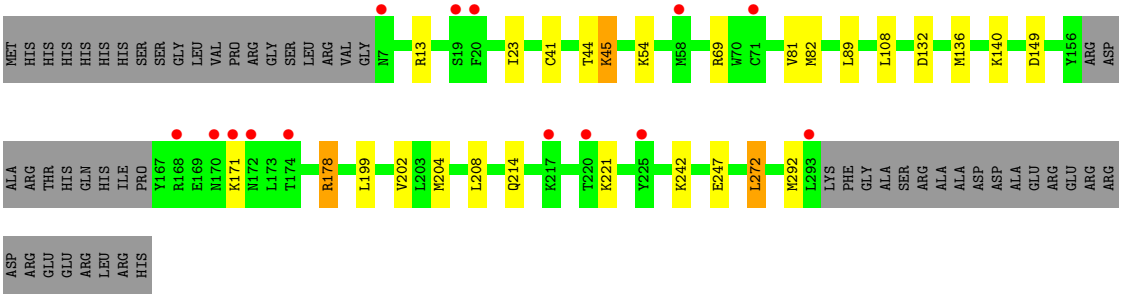
• Molecule 1: Casein kinase I isoform delta

Chain B:



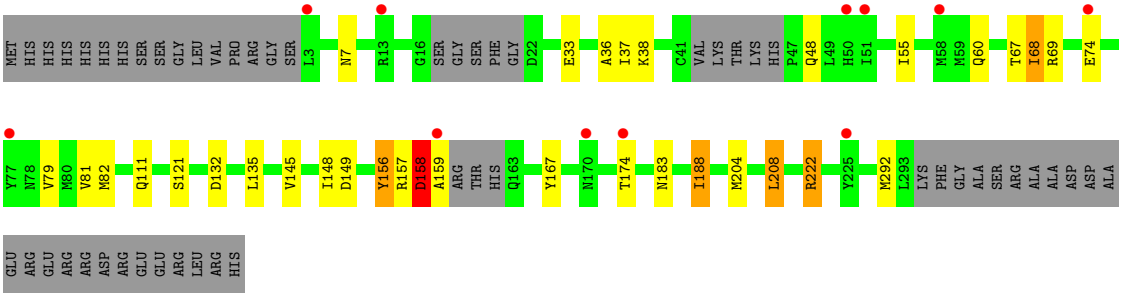
• Molecule 1: Casein kinase I isoform delta

Chain C:



• Molecule 1: Casein kinase I isoform delta

Chain D:


MET HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER L3 N7 R13 G16 SER GLY SER PHE GLY D22 E33 A36 I37 K38 C41 VAL LYS THR LYS HIS P47 Q48 L49 H50 I51 I55 M58 M59 Q60 T67 I68 R69 E74
Y77 N78 V79 M80 V81 M82 Q111 S121 D132 L135 V145 I148 D149 Y156 R157 D158 A159 ARG THR HIS Q163 Y167 N170 T174 M183 I188 M204 L208 R222 Y225 M292 L293 LYS PHE GLY ALA SER ARG ALA ALA ASP ASP ALA
GLU ARG GLU ARG ARG ASP ARG GLU GLU ARG LEU ARG HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.01Å 84.54Å 89.52Å 107.90° 105.87° 93.08°	Depositor
Resolution (Å)	19.66 – 1.95 19.61 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.66-1.95) 96.4 (19.61-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.94Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.205 , 0.232 0.218 , 0.248	Depositor DCC
R_{free} test set	4636 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9447	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 1QO, 1QN

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	0.51	0/2192	0.65	0/2944
1	B	0.48	0/2368	0.64	0/3182
1	C	0.53	0/2313	0.66	0/3106
1	D	0.50	0/2337	0.67	1/3136 (0.0%)
All	All	0.51	0/9210	0.65	1/12368 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	156	TYR	C-N-CA	7.83	141.27	121.70

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	2144	0	2134	13	0
1	B	2316	0	2299	9	0
1	C	2262	0	2263	24	0
1	D	2285	0	2292	20	0
2	A	22	17	17	0	0
2	C	22	17	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	3	0
3	D	10	0	0	0	0
4	B	20	14	14	1	0
4	D	20	14	14	3	0
5	A	63	0	0	1	0
5	B	62	0	0	0	0
5	C	74	0	0	0	0
5	D	55	0	0	0	0
All	All	9385	62	9050	66	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 4.

All (66) 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:89:LEU:HD21	1:C:136:MET:HE1	1.46	0.98
1:C:89:LEU:HD21	1:C:136:MET:CE	2.06	0.84
1:C:178:ARG:HD3	3:C:403:SO4:O3	1.78	0.83
1:A:49:LEU:HD22	1:A:78:ASN:HB3	1.67	0.77
1:C:204:MET:HE3	1:C:208:LEU:CD2	2.18	0.74
1:B:247:GLU:HG3	1:B:272:LEU:HD22	1.74	0.69
1:C:204:MET:HE3	1:C:208:LEU:HD23	1.74	0.69
1:C:247:GLU:HG3	1:C:272:LEU:HD22	1.75	0.67
1:C:41:CYS:HB2	1:C:44:THR:HG23	1.78	0.66
1:D:111:GLN:HB3	1:D:145:VAL:HG22	1.78	0.65
1:D:60:GLN:HE22	1:D:67:THR:HA	1.61	0.65
1:A:288:PHE:H	1:A:291:ASN:HD22	1.42	0.65
1:A:41:CYS:HB2	1:A:44:THR:HG23	1.82	0.62
1:C:204:MET:CE	1:C:208:LEU:HD21	2.29	0.62
1:C:178:ARG:CD	3:C:403:SO4:O3	2.48	0.59
1:D:38:LYS:HB2	4:D:401:1QO:H12	1.84	0.59
1:D:60:GLN:NE2	1:D:68:ILE:H	2.01	0.58
1:C:204:MET:CE	1:C:208:LEU:CD2	2.83	0.56
1:B:271:GLN:NE2	1:B:274:ARG:HH11	2.04	0.56
1:B:226:GLU:O	1:B:230:GLU:HG2	2.06	0.55
1:C:199:LEU:O	1:C:202:VAL:HG22	2.06	0.55
1:B:220:THR:HB	1:B:223:GLN:HG2	1.89	0.54
1:A:271:GLN:NE2	1:A:274:ARG:HH11	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:GLN:HE22	1:D:68:ILE:H	1.54	0.53
1:A:15:ILE:HD11	1:A:25:LEU:HB2	1.91	0.53
1:D:156:TYR:CE1	1:D:158:ASP:CB	2.92	0.53
1:D:156:TYR:CE1	1:D:158:ASP:HB2	2.44	0.52
1:D:135:LEU:HD13	1:D:148:ILE:HG12	1.92	0.51
1:D:204:MET:HE3	1:D:208:LEU:HD13	1.93	0.51
1:C:89:LEU:CD2	1:C:136:MET:CE	2.85	0.50
1:B:279:ARG:NH2	3:C:402:SO4:O3	2.42	0.50
1:A:279:ARG:HD2	5:A:543:HOH:O	2.13	0.49
1:B:38:LYS:HB2	4:B:401:1QO:H12	1.94	0.49
1:C:204:MET:O	1:C:208:LEU:HD23	2.13	0.48
1:C:82:MET:HE2	2:C:401:1QN:H5	1.97	0.47
1:B:135:LEU:HD13	1:B:148:ILE:HG12	1.95	0.47
1:A:37:ILE:HG12	1:A:81:VAL:HG22	1.97	0.47
1:A:271:GLN:HE22	1:A:274:ARG:HH11	1.63	0.46
1:D:111:GLN:HB3	1:D:145:VAL:CG2	2.44	0.46
1:C:89:LEU:CD2	1:C:136:MET:HE2	2.46	0.46
1:C:108:LEU:HD21	1:C:136:MET:HE3	1.97	0.46
1:D:167:TYR:CE1	1:D:188:ILE:HD13	2.50	0.46
1:C:82:MET:HE2	2:C:401:1QN:H6	1.97	0.45
1:D:121:SER:O	1:D:159:ALA:HA	2.15	0.45
1:B:271:GLN:HE22	1:B:274:ARG:HH11	1.62	0.45
1:C:89:LEU:HD21	1:C:136:MET:HE2	1.96	0.44
1:C:23:ILE:HG12	2:C:401:1QN:C12	2.48	0.44
1:D:183:ASN:HB3	1:D:188:ILE:HG12	1.99	0.44
1:B:271:GLN:NE2	1:B:274:ARG:NH1	2.66	0.43
1:A:178:ARG:HD2	1:A:179:TYR:CZ	2.54	0.43
1:D:222:ARG:HA	1:D:222:ARG:HD3	1.73	0.43
1:A:25:LEU:HD11	1:A:34:GLU:OE1	2.18	0.43
1:A:19:SER:OG	1:A:151:GLY:HA3	2.19	0.42
1:D:156:TYR:CE1	1:D:158:ASP:HB3	2.54	0.42
1:C:45:LYS:H	1:C:45:LYS:HG2	1.61	0.42
1:C:178:ARG:HD2	1:C:214:GLN:HG3	2.01	0.42
1:A:271:GLN:NE2	1:A:274:ARG:NH1	2.68	0.42
1:C:82:MET:HE2	2:C:401:1QN:C8	2.49	0.42
1:D:37:ILE:HG12	1:D:81:VAL:HG22	2.01	0.42
1:D:82:MET:HB2	4:D:401:1QO:C16	2.50	0.42
1:D:204:MET:HE3	1:D:208:LEU:CD1	2.49	0.42
1:A:37:ILE:HG22	1:A:39:LEU:HD13	2.02	0.42
1:D:36:ALA:HB3	4:D:401:1QO:H14	2.01	0.41
1:D:156:TYR:HE1	1:D:158:ASP:CB	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:MET:HE2	2:C:401:1QN:C9	2.51	0.41
1:C:199:LEU:HD12	1:C:202:VAL:CG2	2.52	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	259/331 (78%)	253 (98%)	6 (2%)	0	100	100
1	B	281/331 (85%)	275 (98%)	4 (1%)	2 (1%)	22	11
1	C	273/331 (82%)	269 (98%)	3 (1%)	1 (0%)	34	22
1	D	271/331 (82%)	261 (96%)	8 (3%)	2 (1%)	22	11
All	All	1084/1324 (82%)	1058 (98%)	21 (2%)	5 (0%)	29	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	GLY
1	D	158	ASP
1	B	149	ASP
1	D	149	ASP
1	C	149	ASP

5.3.2 Protein sidechains (i)

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	230/288 (80%)	224 (97%)	6 (3%)	46 36
1	B	246/288 (85%)	235 (96%)	11 (4%)	27 15
1	C	243/288 (84%)	230 (95%)	13 (5%)	22 10
1	D	245/288 (85%)	229 (94%)	16 (6%)	17 6
All	All	964/1152 (84%)	918 (95%)	46 (5%)	25 12

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	39	LEU
1	A	130	LYS
1	A	217	LYS
1	A	257	SER
1	A	292	MET
1	B	7	ASN
1	B	41	CYS
1	B	55	ILE
1	B	68	ILE
1	B	132	ASP
1	B	143	ASN
1	B	149	ASP
1	B	174	THR
1	B	256	ARG
1	B	272	LEU
1	B	292	MET
1	C	13	ARG
1	C	45	LYS
1	C	54	LYS
1	C	69	ARG
1	C	81	VAL
1	C	132	ASP
1	C	140	LYS
1	C	171	LYS
1	C	178	ARG
1	C	221	LYS
1	C	242	LYS
1	C	272	LEU
1	C	292	MET
1	D	7	ASN

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Mol	Chain	Res	Type
1	D	33	GLU
1	D	48	GLN
1	D	55	ILE
1	D	68	ILE
1	D	69	ARG
1	D	74	GLU
1	D	79	VAL
1	D	132	ASP
1	D	157	ARG
1	D	158	ASP
1	D	174	THR
1	D	188	ILE
1	D	208	LEU
1	D	222	ARG
1	D	292	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	183	ASN
1	A	271	GLN
1	A	275	ASN
1	A	280	GLN
1	A	291	ASN
1	B	271	GLN
1	B	275	ASN
1	B	280	GLN
1	C	50	HIS
1	C	183	ASN
1	C	207	ASN
1	D	60	GLN
1	D	271	GLN
1	D	280	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	SO4	B	402	-	4,4,4	0.12	0	6,6,6	0.13	0
3	SO4	B	403	-	4,4,4	0.12	0	6,6,6	0.22	0
4	1QO	D	401	-	22,22,22	0.24	0	28,28,28	0.52	0
3	SO4	A	402	-	4,4,4	0.17	0	6,6,6	0.27	0
3	SO4	C	402	-	4,4,4	0.30	0	6,6,6	0.32	0
3	SO4	D	402	-	4,4,4	0.16	0	6,6,6	0.21	0
3	SO4	D	403	-	4,4,4	0.18	0	6,6,6	0.25	0
3	SO4	A	403	-	4,4,4	0.20	0	6,6,6	0.28	0
3	SO4	C	403	-	4,4,4	0.36	0	6,6,6	0.42	0
2	1QN	A	401	-	21,24,24	1.54	4 (19%)	24,33,33	0.72	0
2	1QN	C	401	-	21,24,24	1.50	4 (19%)	24,33,33	0.77	0
4	1QO	B	401	-	22,22,22	0.24	0	28,28,28	0.50	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	1QN	A	401	-	-	2/10/11/11	0/3/3/3
2	1QN	C	401	-	-	2/10/11/11	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1QO	D	401	-	-	0/9/9/9	0/3/3/3
4	1QO	B	401	-	-	1/9/9/9	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1QN	C14-N2	3.71	1.39	1.35
2	C	401	1QN	C14-N2	3.49	1.39	1.35
2	A	401	1QN	C5-C12	-2.95	1.45	1.49
2	C	401	1QN	C5-C12	-2.85	1.45	1.49
2	C	401	1QN	C13-C7	-2.79	1.44	1.49
2	A	401	1QN	C13-C7	-2.77	1.44	1.49
2	C	401	1QN	C12-N3	2.75	1.37	1.35
2	A	401	1QN	C12-N3	2.68	1.37	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	1QN	N3-C12-C5-C4
4	B	401	1QO	C11-C1-N1-C2
2	A	401	1QN	C11-C10-C15-N4
2	A	401	1QN	N1-C10-C15-N4
2	C	401	1QN	N1-C10-C15-N4

There are no ring outliers.

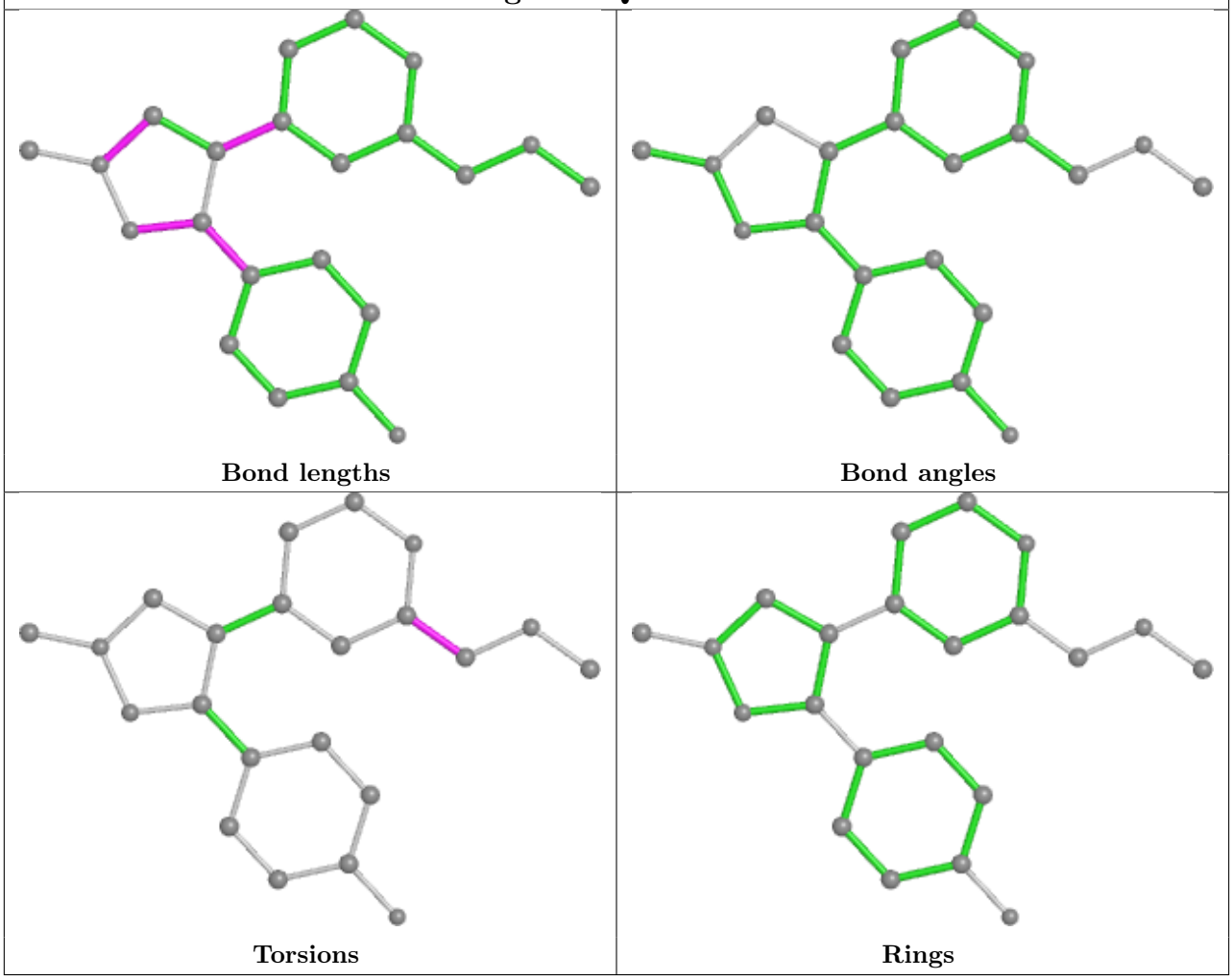
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	1QO	3	0
3	C	402	SO4	1	0
3	C	403	SO4	2	0
2	C	401	1QN	5	0
4	B	401	1QO	1	0

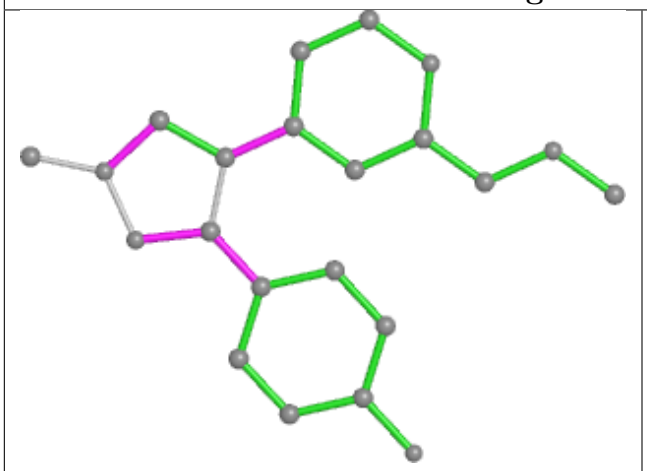
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

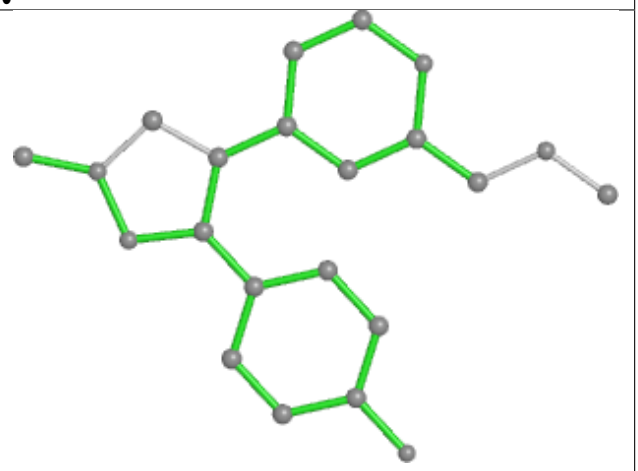
Ligand 1QN A 401



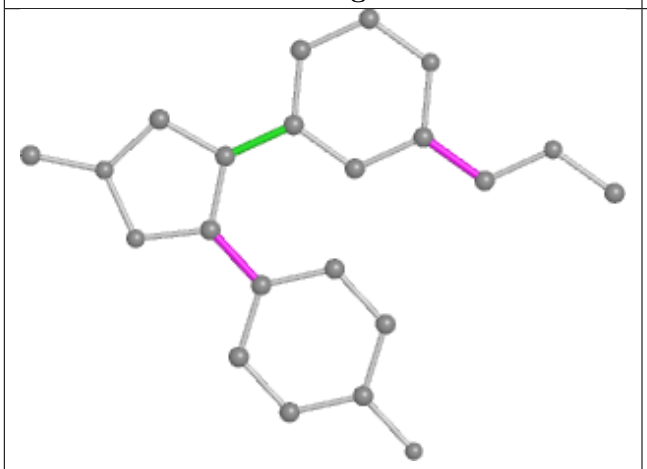
Ligand 1QN C 401



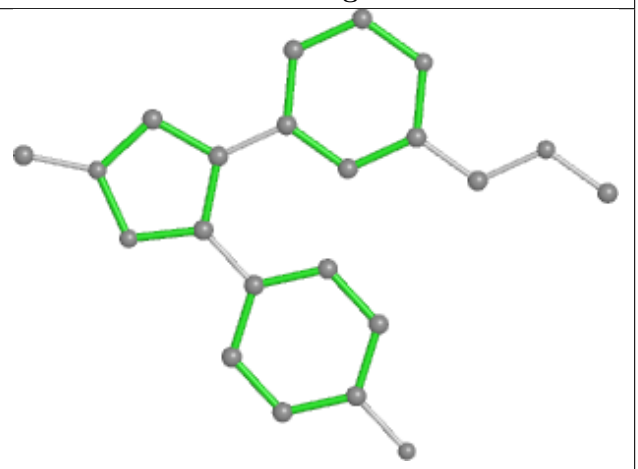
Bond lengths



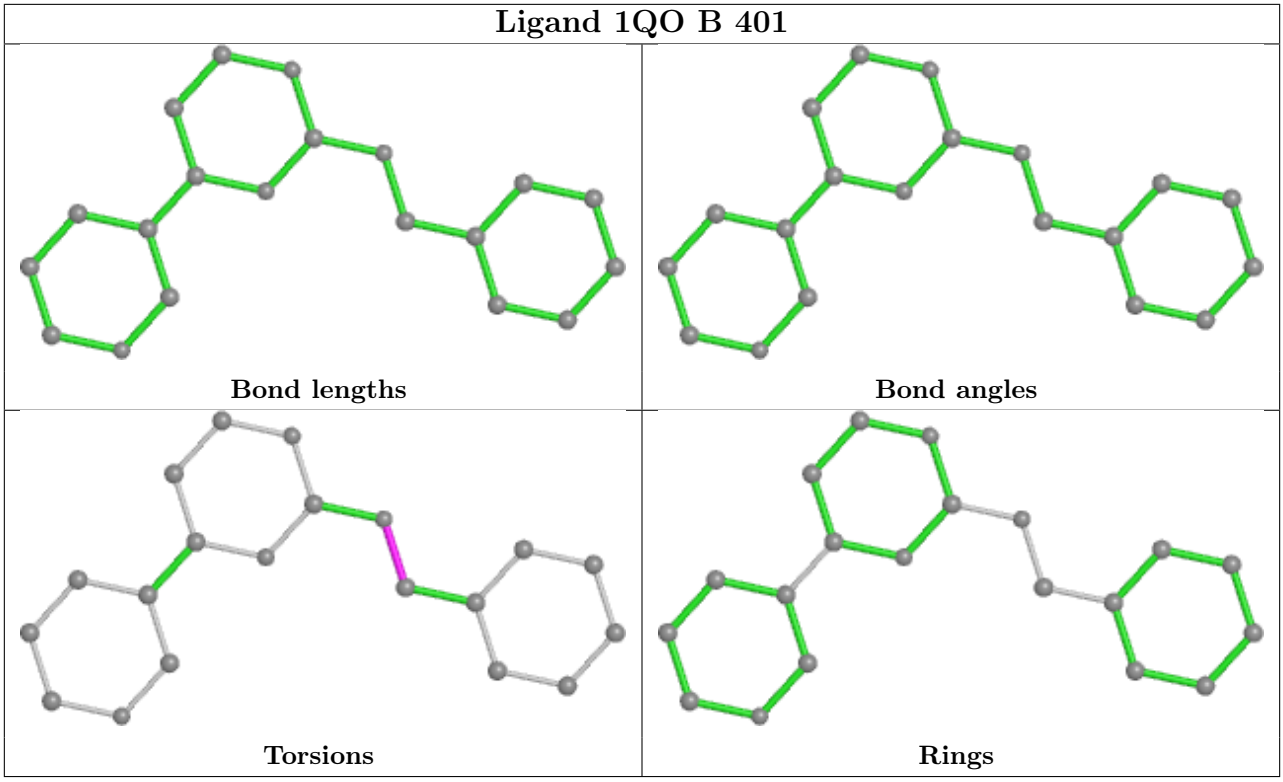
Bond angles



Torsions



Rings



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	265/331 (80%)	-0.15	5 (1%)	66	74	18, 33, 59, 97	0
1	B	285/331 (86%)	-0.04	13 (4%)	32	42	18, 34, 74, 92	0
1	C	277/331 (83%)	-0.05	14 (5%)	28	37	17, 32, 72, 85	0
1	D	278/331 (83%)	-0.05	11 (3%)	38	48	19, 34, 68, 90	0
All	All	1105/1324 (83%)	-0.07	43 (3%)	39	49	17, 34, 68, 97	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	ASN	5.2
1	B	217	LYS	4.9
1	C	293	LEU	4.6
1	D	159	ALA	4.4
1	D	170	ASN	4.4
1	B	19	SER	3.7
1	C	171	LYS	3.2
1	B	41	CYS	3.1
1	C	174	THR	3.0
1	C	168	ARG	3.0
1	D	50	HIS	2.9
1	C	172	ASN	2.9
1	A	6	GLY	2.8
1	B	21	GLY	2.8
1	C	220	THR	2.7
1	A	217	LYS	2.7
1	B	13	ARG	2.7
1	B	159	ALA	2.6
1	B	221	LYS	2.5
1	C	7	ASN	2.5
1	C	58	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	19	SER	2.5
1	B	218	ALA	2.4
1	B	225	TYR	2.4
1	C	225	TYR	2.4
1	D	58	MET	2.4
1	A	15	ILE	2.4
1	C	71	CYS	2.3
1	A	19	SER	2.3
1	D	174	THR	2.2
1	D	225	TYR	2.2
1	D	13	ARG	2.2
1	B	286	TYR	2.2
1	D	74	GLU	2.2
1	C	20	PHE	2.2
1	A	20	PHE	2.1
1	D	3	LEU	2.1
1	D	77	TYR	2.1
1	C	217	LYS	2.1
1	B	160	ARG	2.1
1	B	219	ALA	2.0
1	D	51	ILE	2.0
1	B	172	ASN	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 (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(Å^2)	Q<0.9
4	1QO	B	401	20/20	0.82	0.16	75,85,92,94	14

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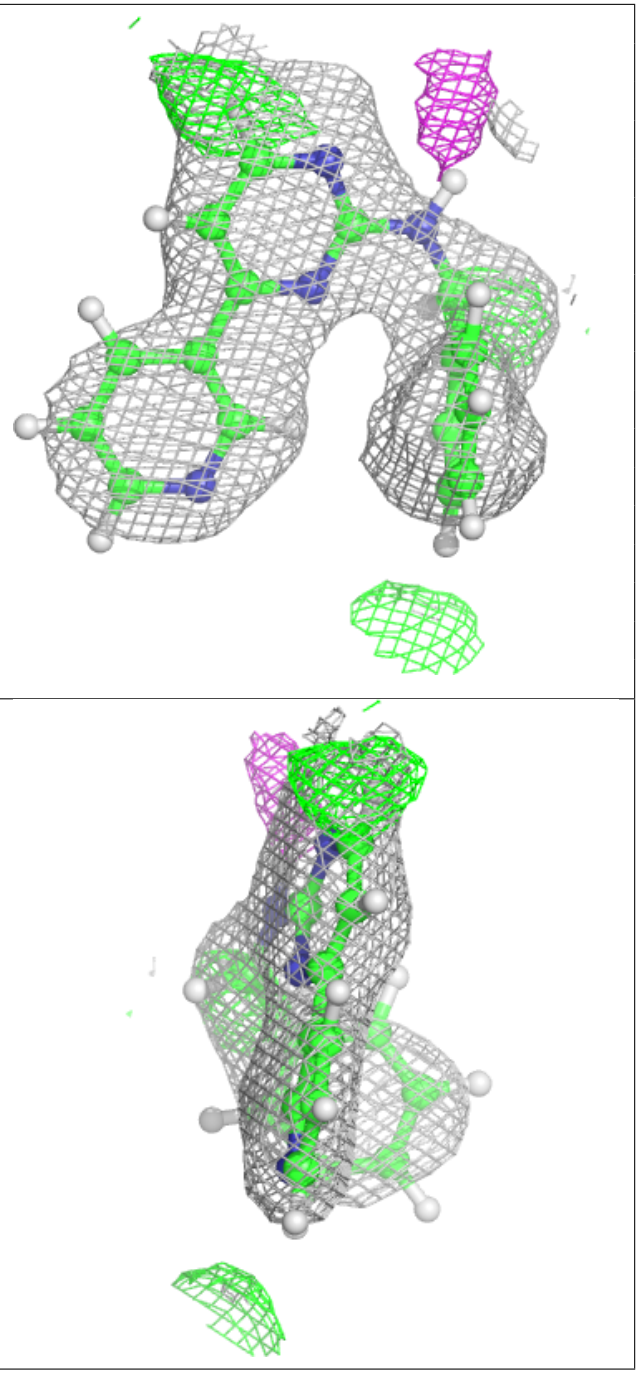
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1QO	D	401	20/20	0.84	0.15	87,95,101,103	14
2	1QN	C	401	22/22	0.92	0.11	29,34,46,47	17
3	SO4	B	403	5/5	0.93	0.08	57,58,59,59	0
2	1QN	A	401	22/22	0.95	0.10	30,38,51,52	17
3	SO4	D	403	5/5	0.98	0.08	56,57,58,59	0
3	SO4	C	402	5/5	0.99	0.09	39,39,42,46	0
3	SO4	C	403	5/5	0.99	0.08	42,43,45,46	0
3	SO4	D	402	5/5	0.99	0.05	37,38,39,39	0
3	SO4	A	403	5/5	0.99	0.10	43,46,49,50	0
3	SO4	B	402	5/5	0.99	0.05	38,40,42,42	0
3	SO4	A	402	5/5	0.99	0.07	45,46,48,48	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.

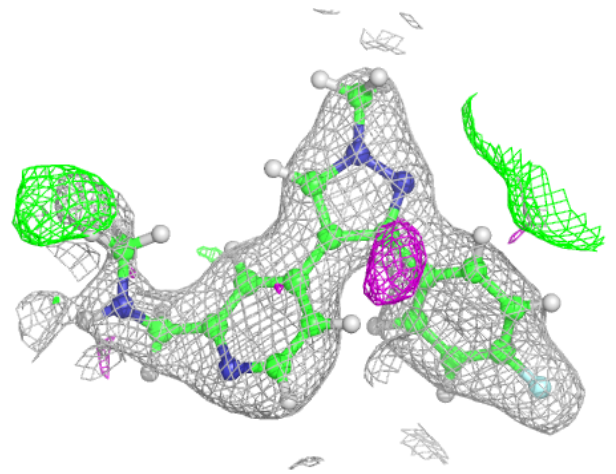
Electron density around 1QO B 401:

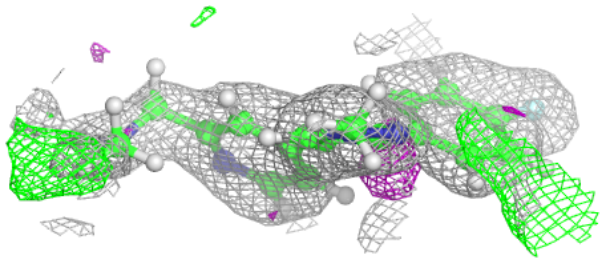
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

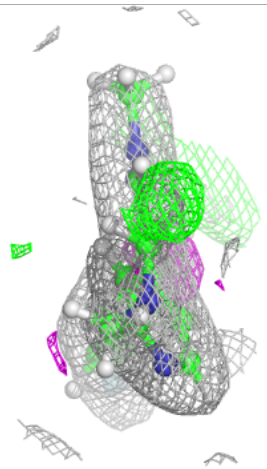


Electron density around 1QN C 401:

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

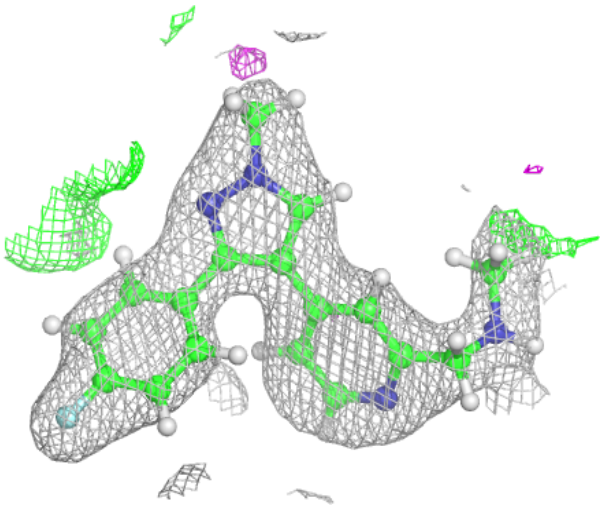


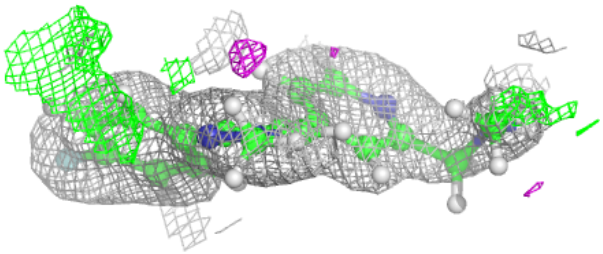


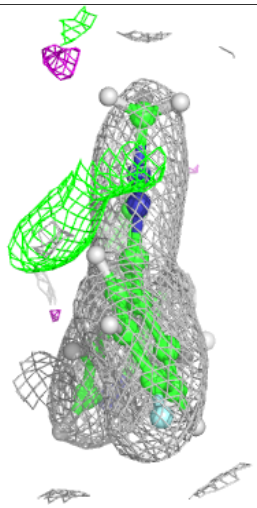


Electron density around 1QN A 401:

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 (i)

There are no such residues in this entry.