



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:38 PM UTC

PDB ID : 4KB8 / pdb_00004kb8
Title : CK1d in complex with 1-{4-[3-(4-FLUOROPHENYL)-1-METHYL-1H-PYR
AZOL-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 ⓘ 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

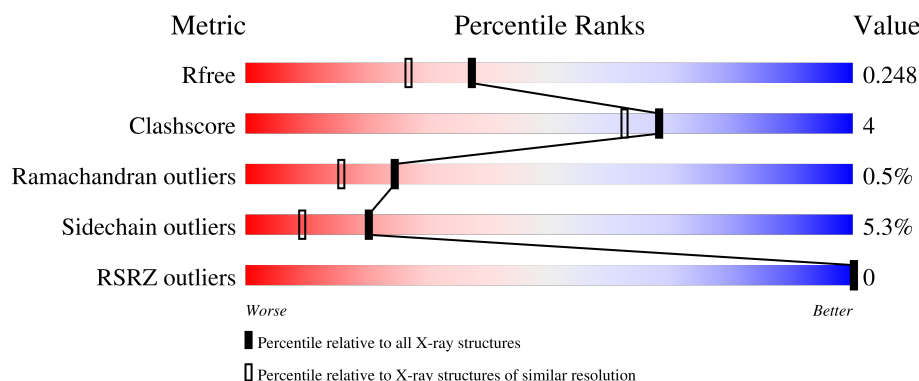
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	
1	B	331	
1	C	331	
1	D	331	

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

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
1	A	265	Total	C	N	O	S	0	0	0
			2144	1382	365	383	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	278	Total	C	N	O	S	0	1	0
			2285	1468	398	405	14			

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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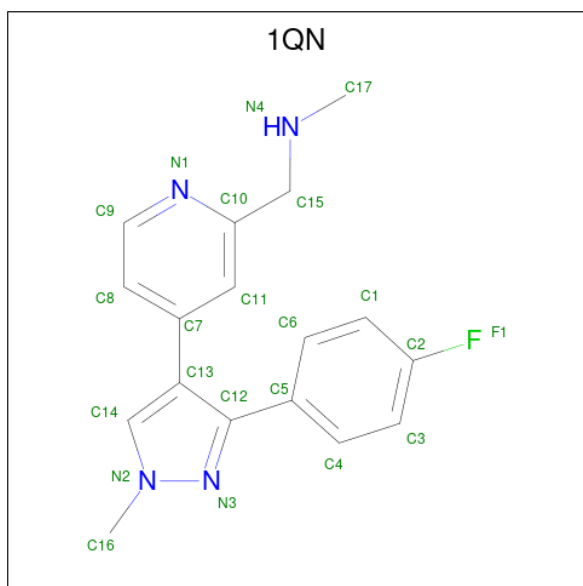
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P48730
B	-7	HIS	-	expression tag	UNP P48730
B	-6	SER	-	expression tag	UNP P48730
B	-5	SER	-	expression tag	UNP P48730
B	-4	GLY	-	expression tag	UNP P48730
B	-3	LEU	-	expression tag	UNP P48730
B	-2	VAL	-	expression tag	UNP P48730
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 (CCD ID: 1QN) (formula: C₁₇H₁₇FN₄).



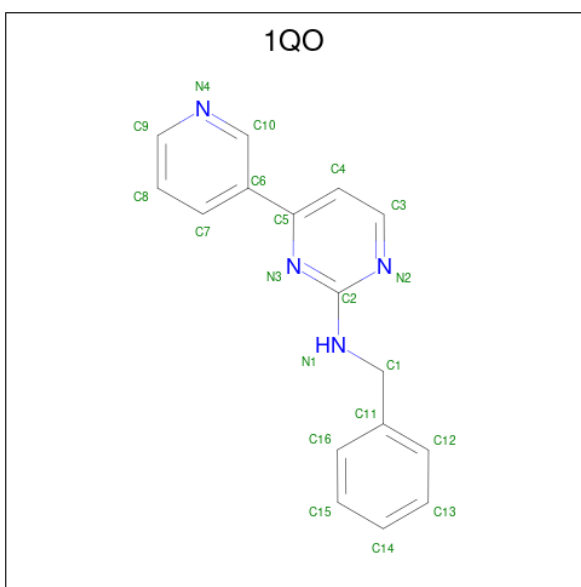
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	17	0
			39	17	1	17	4		
2	C	1	Total	C	F	H	N	17	0
			39	17	1	17	4		

- Molecule 3 is SULFATE ION (CCD ID: 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		

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



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

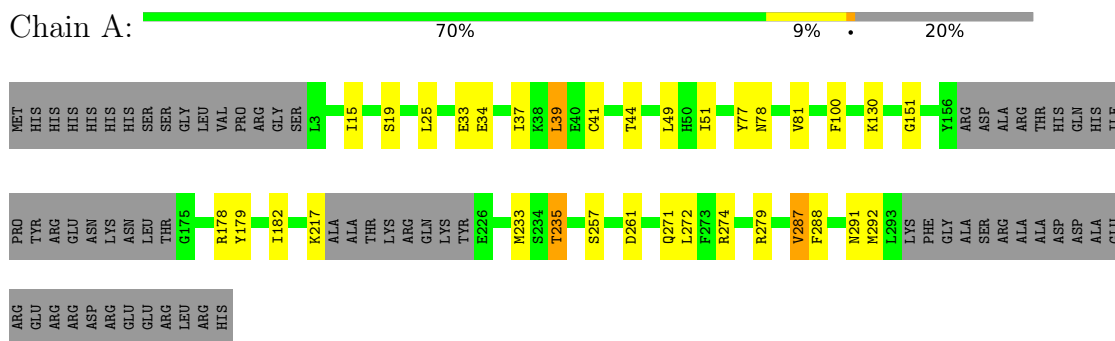
- Molecule 5 is water.

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

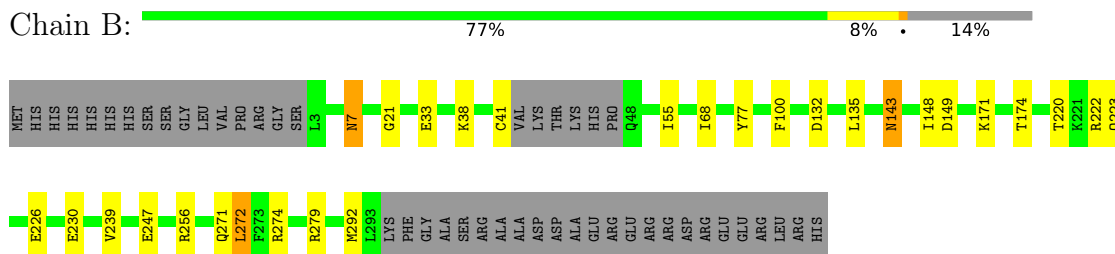
3 Residue-property plots

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.

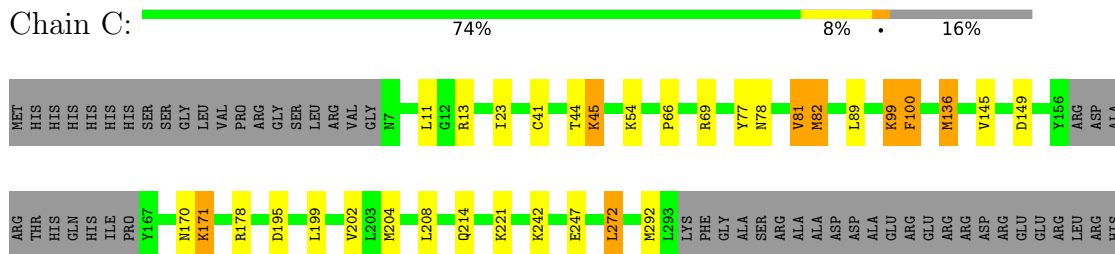
- Molecule 1: Casein kinase I isoform delta



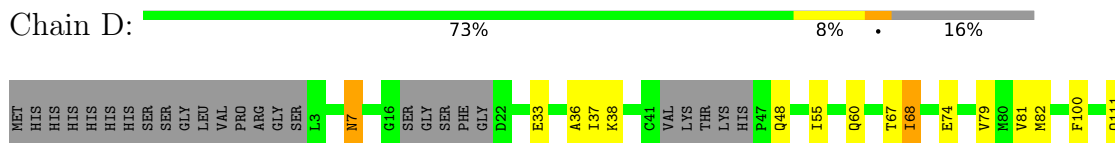
- Molecule 1: Casein kinase I isoform delta

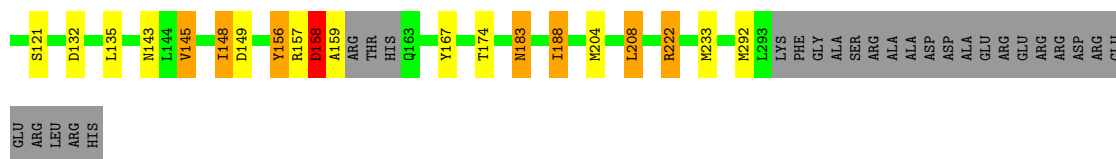


- Molecule 1: Casein kinase I isoform delta



- Molecule 1: Casein kinase I isoform delta





4 Data and refinement statistics

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 19.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.66-1.95) 96.4 (19.66-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.38 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

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: 1QN, SO4, 1QO

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	0.84	0/2192	1.20	7/2944 (0.2%)
1	B	0.79	0/2368	1.20	4/3182 (0.1%)
1	C	0.89	2/2313 (0.1%)	1.21	8/3106 (0.3%)
1	D	0.84	1/2337 (0.0%)	1.22	9/3136 (0.3%)
All	All	0.84	3/9210 (0.0%)	1.21	28/12368 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	MET	SD-CE	-10.65	1.52	1.79
1	C	136	MET	SD-CE	-10.41	1.53	1.79
1	D	233	MET	SD-CE	-5.76	1.65	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	TYR	CA-C-N	10.88	141.27	121.70
1	D	156	TYR	C-N-CA	10.88	141.27	121.70
1	A	287	VAL	N-CA-CB	8.64	121.97	111.60
1	D	158	ASP	CA-CB-CG	7.66	120.26	112.60
1	B	143	ASN	CA-CB-CG	7.21	119.81	112.60
1	B	100	PHE	CA-CB-CG	6.38	120.18	113.80
1	A	261	ASP	CA-CB-CG	6.29	118.89	112.60
1	D	183	ASN	CA-CB-CG	6.14	118.74	112.60
1	D	100	PHE	CA-CB-CG	6.06	119.86	113.80
1	D	143	ASN	CA-CB-CG	5.81	118.41	112.60
1	C	171	LYS	N-CA-C	5.76	118.37	110.24
1	D	7	ASN	CA-CB-CG	5.63	118.23	112.60
1	B	7	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	51	ILE	N-CA-CB	5.50	116.99	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	PHE	CA-CB-CG	5.39	119.19	113.80
1	C	100	PHE	CA-CB-CG	5.38	119.18	113.80
1	D	156	TYR	N-CA-C	5.37	119.96	113.41
1	A	235	THR	CB-CA-C	5.34	115.25	110.44
1	C	78	ASN	N-CA-C	-5.28	101.09	109.96
1	A	77	TYR	N-CA-C	5.27	117.83	109.50
1	C	81	VAL	N-CA-CB	5.26	118.67	111.41
1	D	145	VAL	N-CA-CB	5.13	116.32	110.72
1	C	77	TYR	N-CA-C	5.11	117.44	109.52
1	C	195	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	287	VAL	CB-CA-C	5.07	118.75	111.81
1	B	77	TYR	N-CA-C	5.04	117.33	109.52
1	C	170	ASN	CA-C-N	5.02	127.98	120.90
1	C	170	ASN	C-N-CA	5.02	127.98	120.90

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	2144	0	2134	14	0
1	B	2316	0	2299	9	0
1	C	2262	0	2263	22	0
1	D	2285	0	2292	21	0
2	A	22	17	17	0	0
2	C	22	17	17	2	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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:HE2	1.22	1.13
1:C:89:LEU:CD2	1:C:136:MET:HE2	2.02	0.89
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	2.17	0.75
1:C:204:MET:HE3	1:C:208:LEU:HD23	1.73	0.70
1:B:247:GLU:HG3	1:B:272:LEU:HD22	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:66:PRO:CB	1:C:82:MET:HE3	2.32	0.60
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
1:C:136:MET:HE1	1:C:145:VAL:HG22	1.88	0.54
1:D:60:GLN:HE22	1:D:68:ILE:H	1.54	0.53
1:C:66:PRO:HB3	1:C:82:MET:HE3	1.91	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:204:MET:HE3	1:D:208:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:HD13	1:D:148:ILE:HG12	1.92	0.51
1:B:279:ARG:NH2	3:C:402:SO4:O3	2.42	0.50
1:C:99:LYS:HZ1	1:C:100:PHE:H	1.58	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:A:182:ILE:HG23	1:A:233:MET:HE2	1.96	0.48
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:D:167:TYR:CE1	1:D:188:ILE:HD13	2.50	0.46
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: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:C:82:MET:HE2	2:C:401:1QN:H6	2.01	0.43
1:D:158:ASP:O	1:D:159:ALA:C	2.61	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:D:204:MET:HE3	1:D:208:LEU:CD1	2.48	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: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: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
1:C:199:LEU:HD12	1:C:202:VAL:CG2	2.52	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	259/331 (78%)	253 (98%)	6 (2%)	0	100	100
1	B	281/331 (85%)	275 (98%)	4 (1%)	2 (1%)	18	10
1	C	273/331 (82%)	269 (98%)	3 (1%)	1 (0%)	30	21
1	D	271/331 (82%)	261 (96%)	8 (3%)	2 (1%)	18	10
All	All	1084/1324 (82%)	1058 (98%)	21 (2%)	5 (0%)	24	16

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

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%)	221 (96%)	9 (4%)	28	18
1	B	246/288 (85%)	232 (94%)	14 (6%)	18	8
1	C	243/288 (84%)	231 (95%)	12 (5%)	22	11
1	D	245/288 (85%)	229 (94%)	16 (6%)	15	6
All	All	964/1152 (84%)	913 (95%)	51 (5%)	20	9

All (51) 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	235	THR
1	A	257	SER
1	A	272	LEU
1	A	287	VAL
1	A	292	MET
1	B	7	ASN
1	B	33	GLU
1	B	41	CYS
1	B	55	ILE
1	B	68	ILE
1	B	132	ASP
1	B	143	ASN
1	B	171	LYS
1	B	174	THR
1	B	222	ARG
1	B	239	VAL
1	B	256	ARG
1	B	272	LEU
1	B	292	MET
1	C	11	LEU
1	C	13	ARG
1	C	45	LYS
1	C	54	LYS
1	C	69	ARG
1	C	81	VAL
1	C	99	LYS
1	C	171	LYS
1	C	221	LYS
1	C	242	LYS
1	C	272	LEU
1	C	292	MET
1	D	7	ASN
1	D	33	GLU
1	D	48	GLN
1	D	55	ILE
1	D	68	ILE
1	D	74	GLU
1	D	79	VAL

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Mol	Chain	Res	Type
1	D	132	ASP
1	D	148	ILE
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 (19) 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	190	GLN
1	B	223	GLN
1	B	271	GLN
1	B	275	ASN
1	B	280	GLN
1	C	50	HIS
1	C	170	ASN
1	C	183	ASN
1	C	207	ASN
1	C	223	GLN
1	D	48	GLN
1	D	60	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 [i](#)

There are no oligosaccharides 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	A	403	-	4,4,4	0.22	0	6,6,6	0.28	0
3	SO4	C	402	-	4,4,4	0.31	0	6,6,6	0.29	0
2	1QN	A	401	-	23,24,24	1.49	3 (13%)	31,33,33	0.84	1 (3%)
3	SO4	D	403	-	4,4,4	0.27	0	6,6,6	0.18	0
3	SO4	A	402	-	4,4,4	0.22	0	6,6,6	0.27	0
4	1QO	D	401	-	22,22,22	0.22	0	28,28,28	0.51	0
4	1QO	B	401	-	22,22,22	0.22	0	28,28,28	0.49	0
3	SO4	C	403	-	4,4,4	0.39	0	6,6,6	0.38	0
2	1QN	C	401	-	23,24,24	1.46	3 (13%)	31,33,33	0.89	1 (3%)
3	SO4	B	402	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	D	402	-	4,4,4	0.25	0	6,6,6	0.22	0
3	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.21	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
4	1QO	D	401	-	-	0/9/9/9	0/3/3/3
4	1QO	B	401	-	-	1/9/9/9	0/3/3/3
2	1QN	A	401	-	-	2/10/11/11	0/3/3/3
2	1QN	C	401	-	-	2/10/11/11	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1QN	C14-N2	4.70	1.39	1.34
2	C	401	1QN	C14-N2	4.49	1.39	1.34
2	C	401	1QN	C7-C13	-2.77	1.44	1.48
2	A	401	1QN	C7-C13	-2.75	1.44	1.48
2	C	401	1QN	C12-N3	2.44	1.37	1.33
2	A	401	1QN	C12-N3	2.40	1.37	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	1QN	C14-C13-C12	2.27	106.02	104.71
2	A	401	1QN	C14-C13-C12	2.16	105.95	104.71

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	C	401	1QN	C11-C10-C15-N4

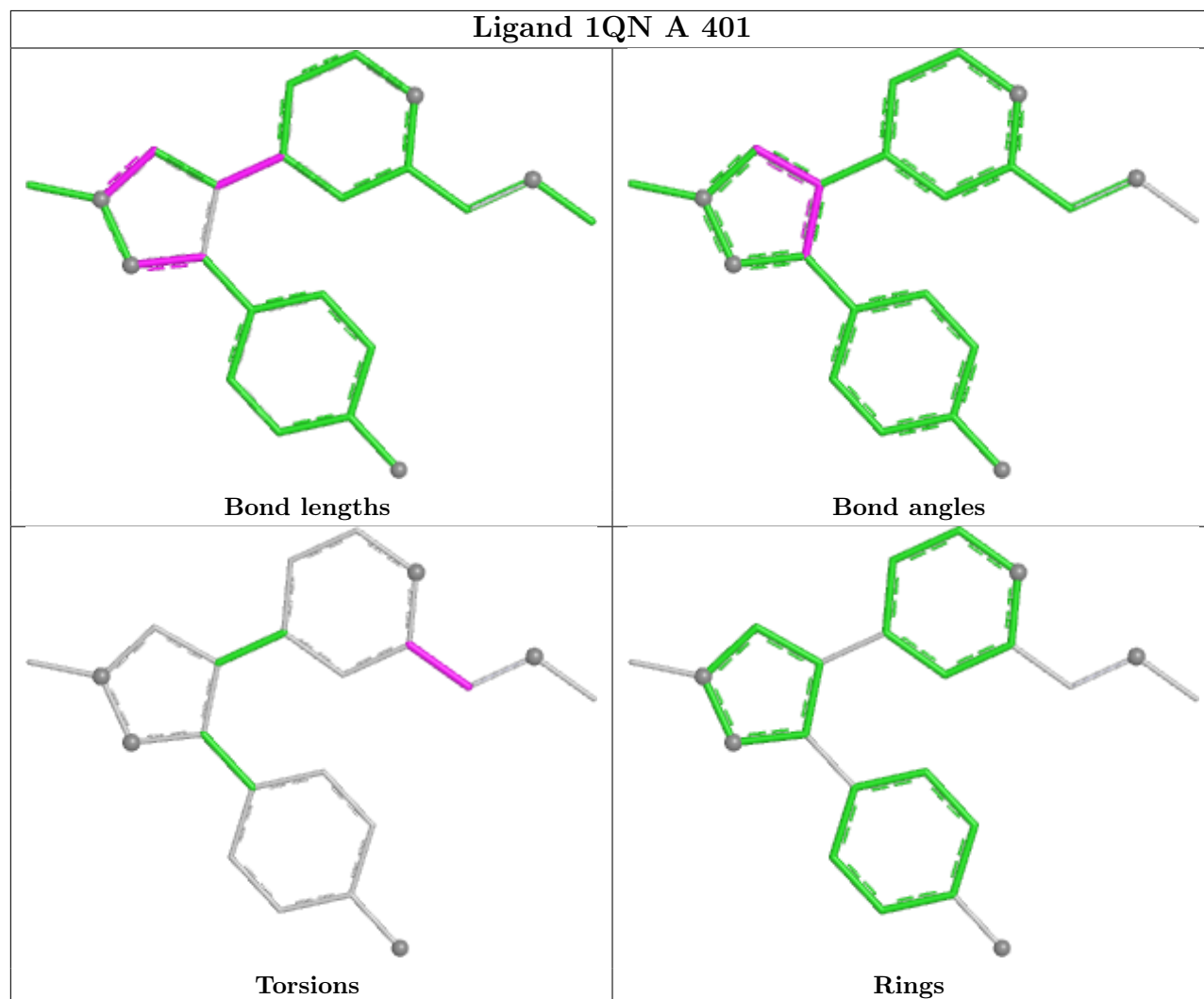
There are no ring outliers.

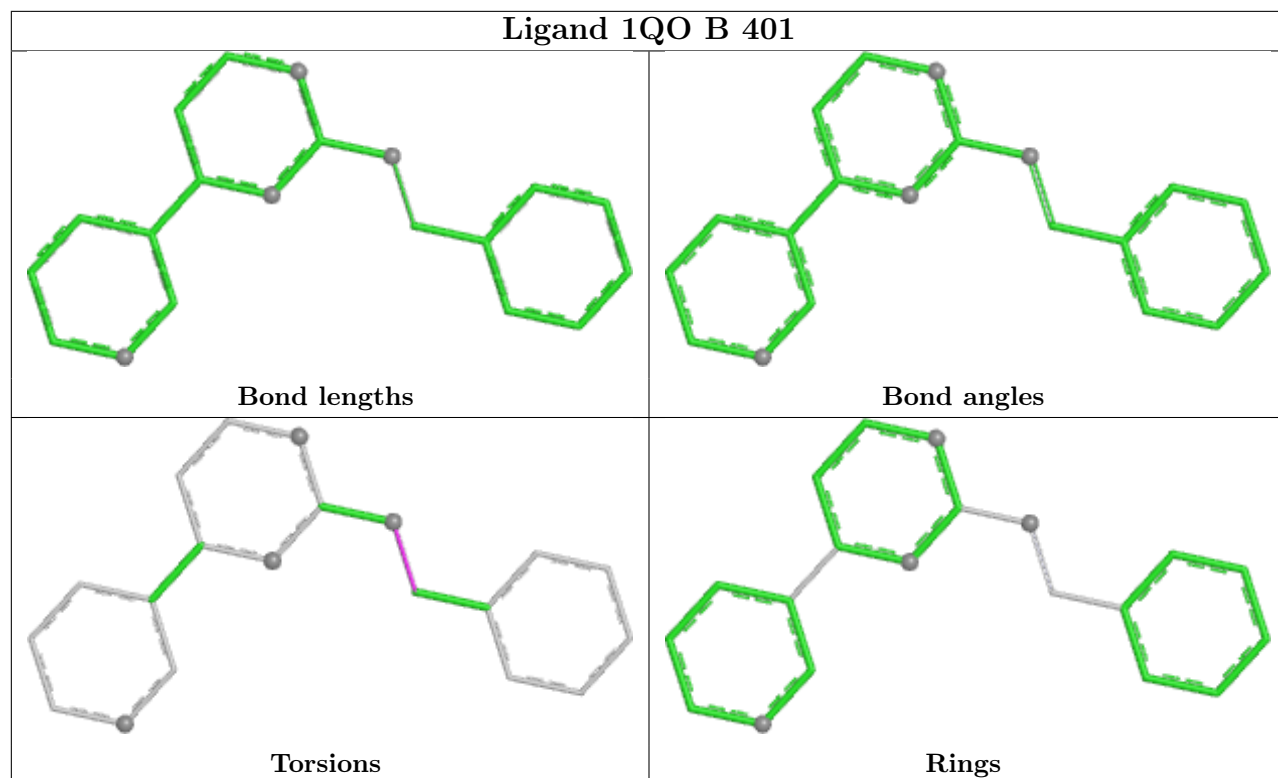
5 monomers are involved in 9 short contacts:

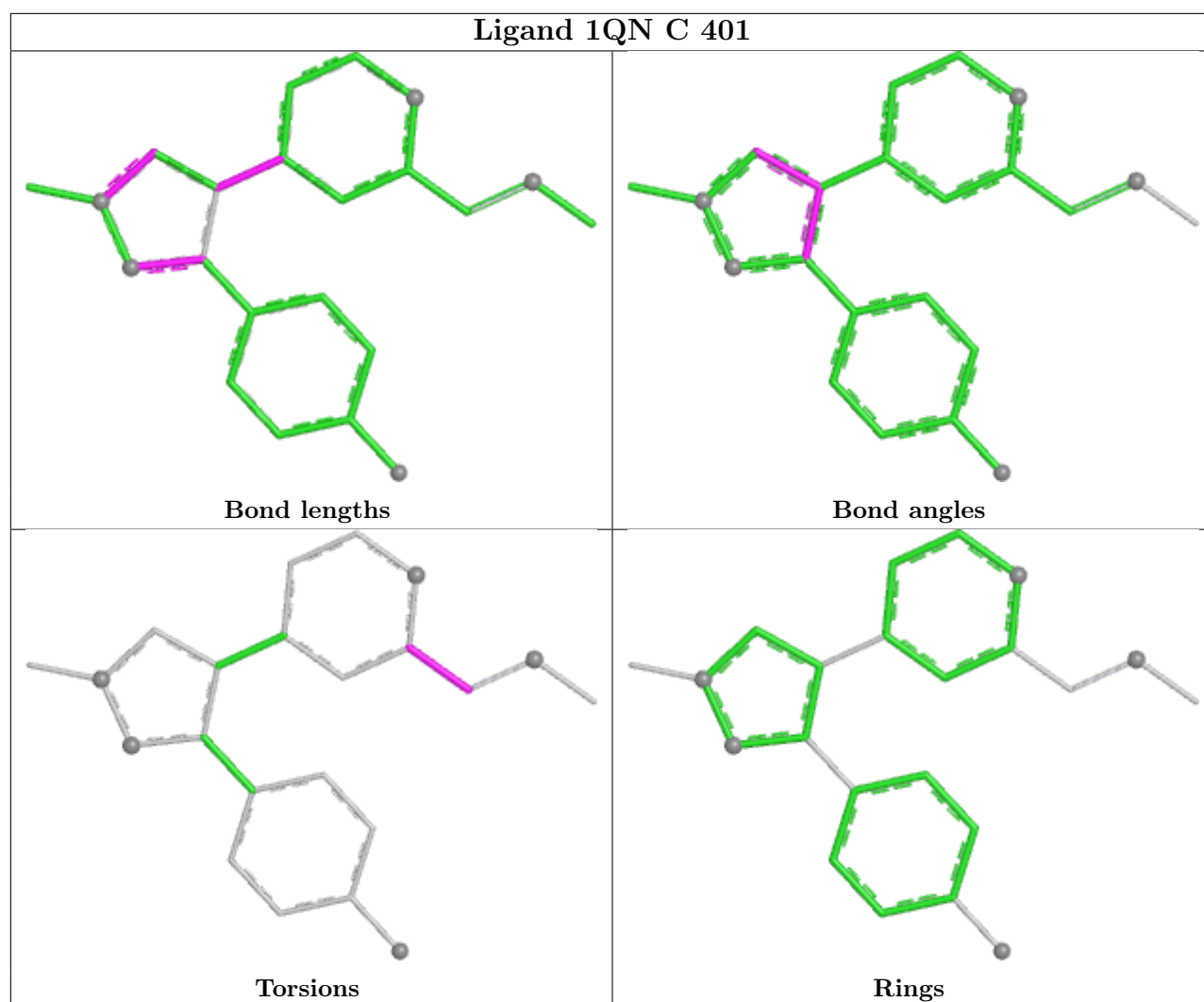
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	SO4	1	0
4	D	401	1QO	3	0
4	B	401	1QO	1	0
3	C	403	SO4	2	0
2	C	401	1QN	2	0

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 [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%)	-1.10	0 100 100	18, 33, 59, 97	0
1	B	285/331 (86%)	-1.07	0 100 100	18, 34, 74, 92	0
1	C	277/331 (83%)	-1.09	0 100 100	17, 32, 72, 85	0
1	D	278/331 (83%)	-1.08	0 100 100	17, 34, 68, 90	1 (0%)
All	All	1105/1324 (83%)	-1.09	0 100 100	17, 34, 68, 97	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	1QO	B	401	20/20	0.93	0.12	75,85,92,94	14
4	1QO	D	401	20/20	0.94	0.14	87,95,101,103	14
2	1QN	C	401	22/22	0.98	0.04	29,34,46,47	17
3	SO4	B	403	5/5	0.99	0.04	57,58,59,59	0

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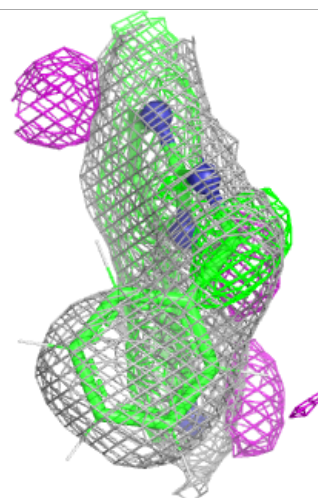
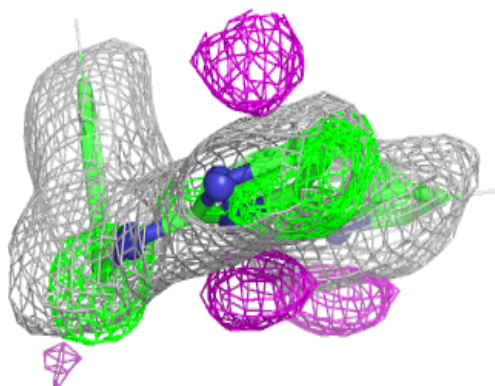
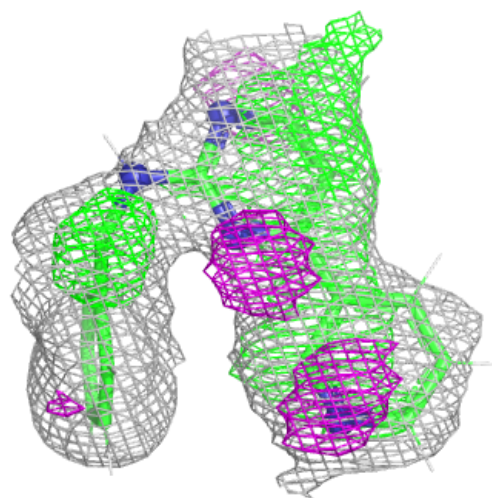
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	403	5/5	0.99	0.03	42,43,45,46	0
3	SO4	D	402	5/5	0.99	0.03	37,38,39,39	0
3	SO4	D	403	5/5	0.99	0.04	56,57,58,59	0
2	1QN	A	401	22/22	0.99	0.04	30,38,51,52	17
3	SO4	B	402	5/5	0.99	0.03	38,40,42,42	0
3	SO4	C	402	5/5	1.00	0.03	39,39,42,46	0
3	SO4	A	402	5/5	1.00	0.02	45,46,48,48	0
3	SO4	A	403	5/5	1.00	0.03	43,46,49,50	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.

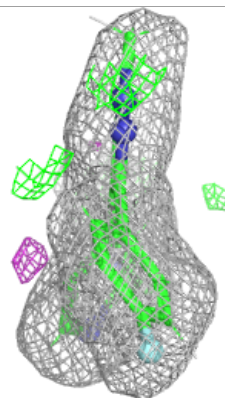
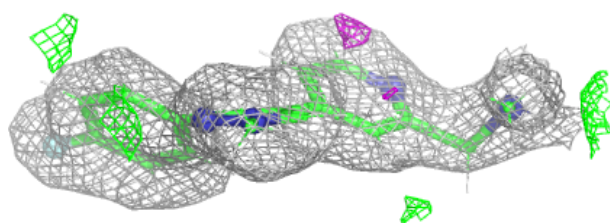
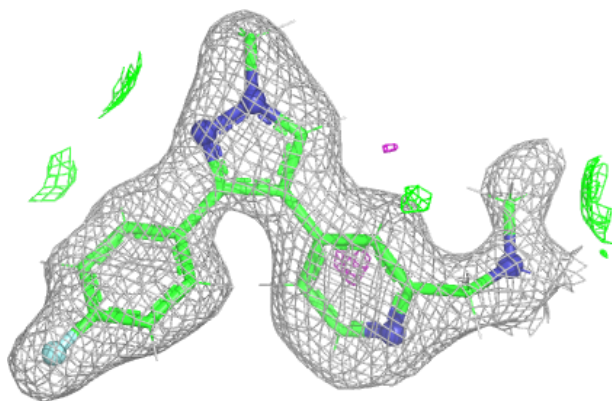
Electron density around 1QO B 401:

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

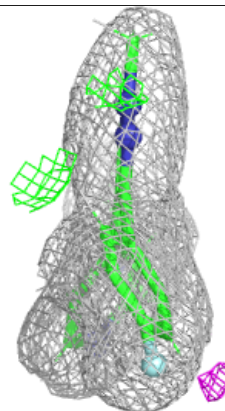
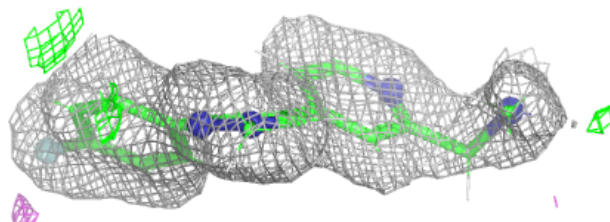
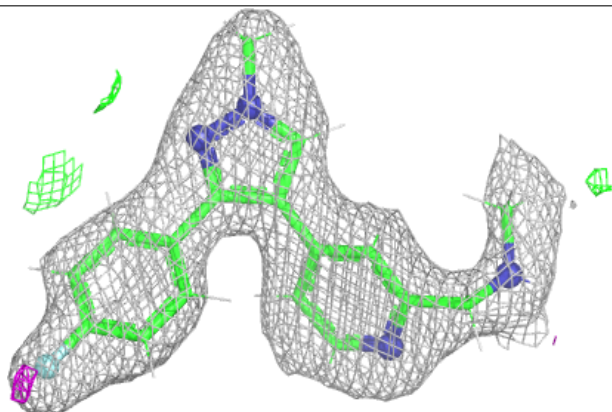


Electron density around 1QN C 401:

$2mF_o-DF_c$ (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.