



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 AM UTC

PDB ID : 6H4W / pdb_00006h4w
Title : Crystal structure of human KDM4A in complex with compound 19d
Authors : Le Bihan, Y.V.; van Montfort, R.L.M.
Deposited on : 2018-07-23
Resolution : 2.81 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

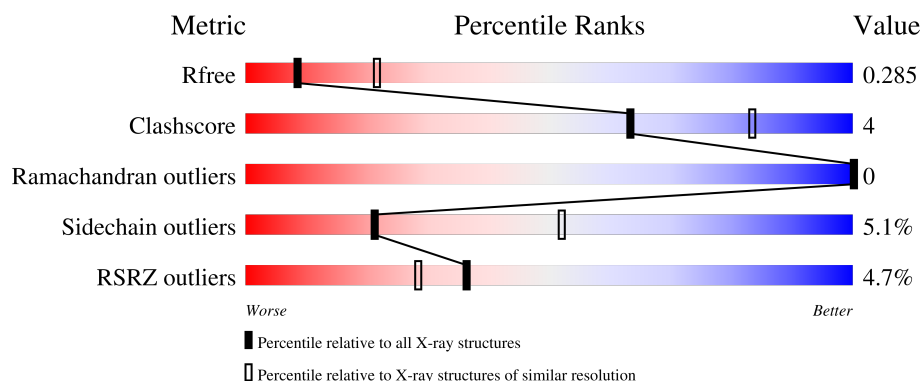
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	360	4% 76% 16% 6%
1	B	360	% 79% 14% 6%
1	C	360	6% 80% 12% 7%
1	D	360	6% 84% 10% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10871 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	1
			2632	1718	423	477	14			
1	B	340	Total	C	N	O	S	0	1	1
			2679	1751	436	477	15			
1	C	335	Total	C	N	O	S	0	0	2
			2585	1683	420	469	13			
1	D	340	Total	C	N	O	S	0	2	0
			2664	1728	436	486	14			

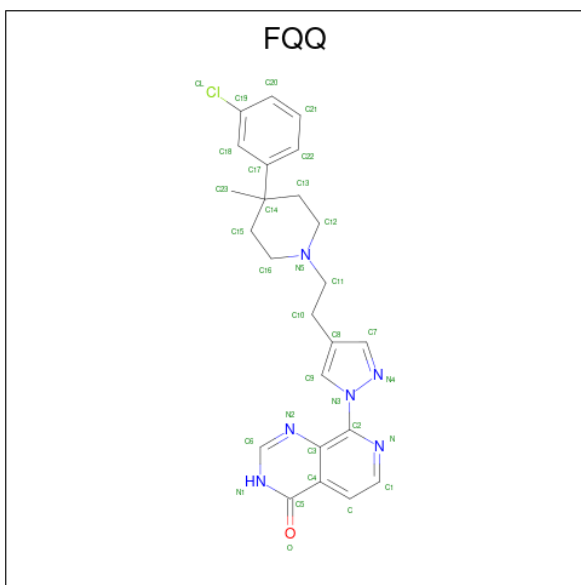
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164
C	0	SER	-	expression tag	UNP O75164
D	0	SER	-	expression tag	UNP O75164

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

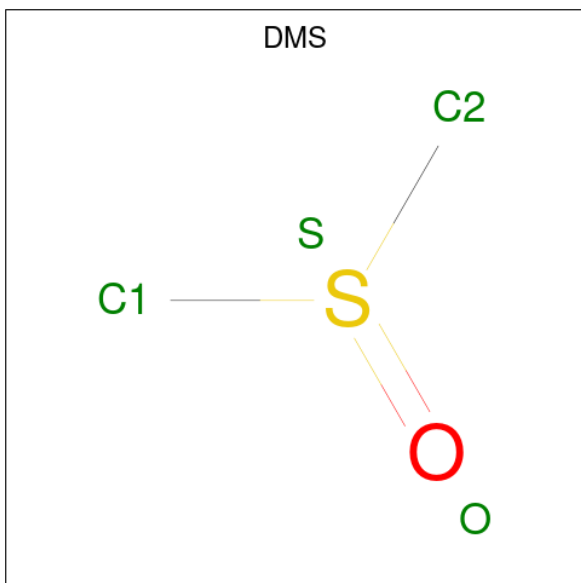
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 8-[4-[2-[4-(3-chlorophenyl)-4-methyl-piperidin-1-yl]ethyl]pyrazol-1-yl]-3 {H}-pyrido[3,4-d]pyrimidin-4-one (CCD ID: FQQ) (formula: C₂₄H₂₅ClN₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 26	C 19	N 6	O 1	0	0	
3	B	1	Total 32	C 24	Cl 1	N 6	O 1	0	0
3	C	1	Total 26	C 19	N 6	O 1	0	0	
3	D	1	Total 26	C 19	N 6	O 1	0	0	

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

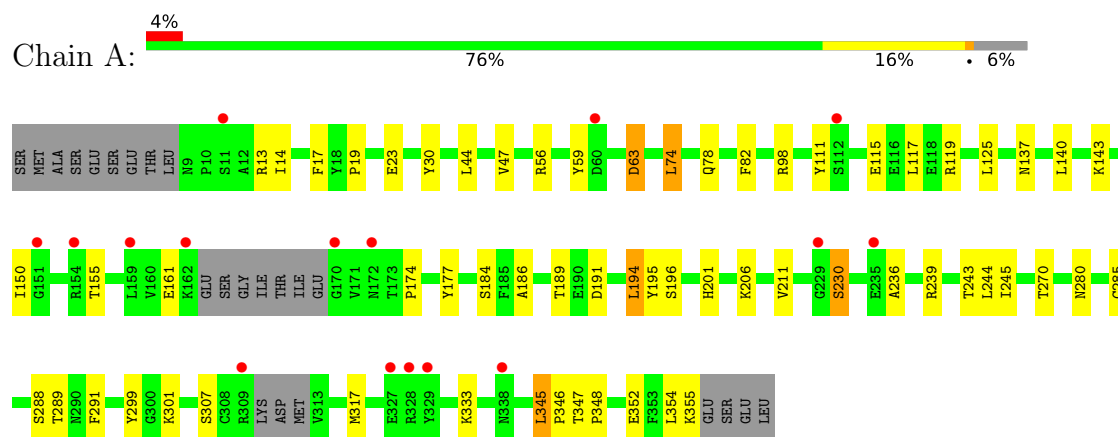
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	59	Total O 59 59	0	0
6	C	33	Total O 33 33	0	0
6	D	41	Total O 41 41	0	0

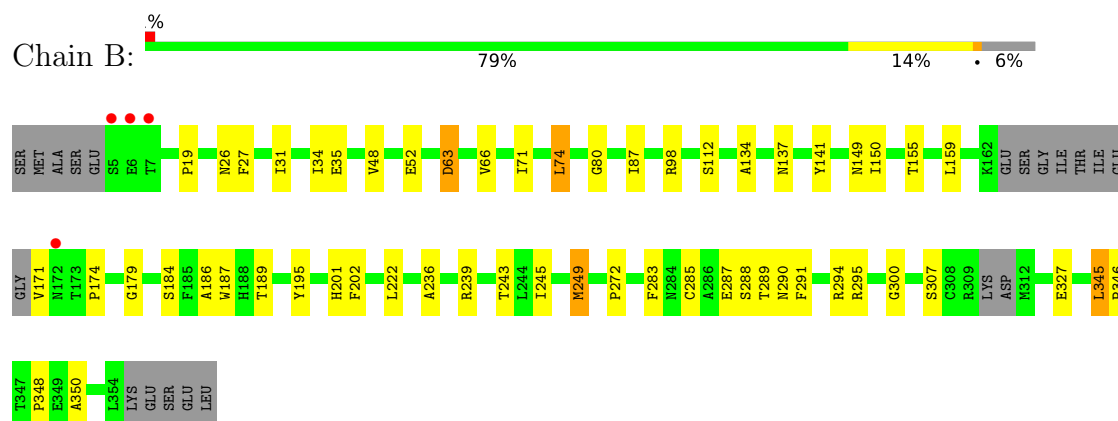
3 Residue-property plots [i](#)

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.

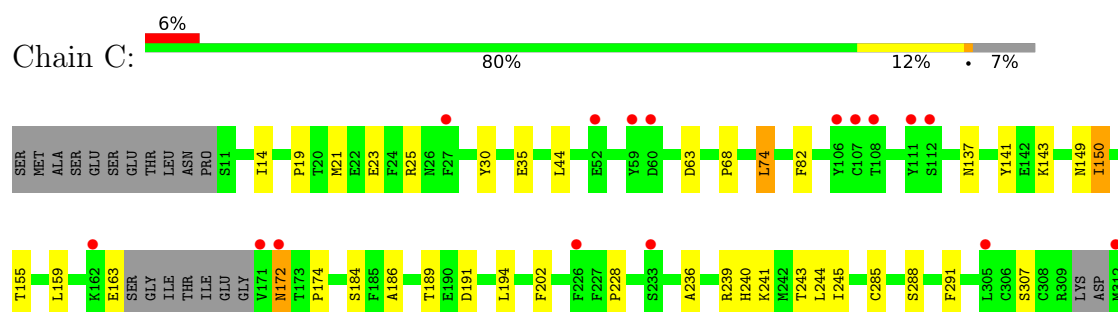
• Molecule 1: Lysine-specific demethylase 4A



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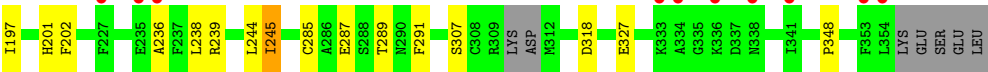
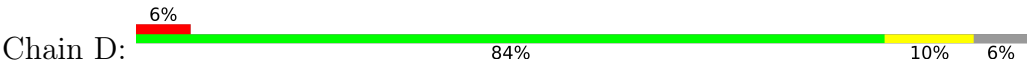


• Molecule 1: Lysine-specific demethylase 4A





● Molecule 1: Lysine-specific demethylase 4A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.56Å 101.49Å 142.31Å 90.00° 99.07° 90.00°	Depositor
Resolution (Å)	48.92 – 2.81 48.92 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.92-2.81) 99.7 (48.92-2.81)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.218 , 0.266 0.237 , 0.285	Depositor DCC
R_{free} test set	2016 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10871	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2186e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, CL, DMS, FQQ

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	0.90	0/2717	1.35	15/3702 (0.4%)
1	B	0.93	0/2764	1.33	16/3763 (0.4%)
1	C	0.85	0/2669	1.32	10/3639 (0.3%)
1	D	0.86	0/2749	1.35	15/3747 (0.4%)
All	All	0.89	0/10899	1.34	56/14851 (0.4%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	THR	CA-C-N	8.65	129.31	120.14
1	D	173	THR	C-N-CA	8.65	129.31	120.14
1	B	189	THR	N-CA-C	-7.37	99.55	110.46
1	A	348	PRO	CA-C-N	7.14	130.80	120.38
1	A	348	PRO	C-N-CA	7.14	130.80	120.38
1	D	189	THR	N-CA-C	-7.14	99.90	110.46
1	A	189	THR	N-CA-C	-6.70	100.55	110.46
1	C	189	THR	N-CA-C	-6.58	100.73	110.46
1	C	184	SER	N-CA-C	6.32	118.78	109.24
1	A	23	GLU	CA-C-N	6.16	128.53	120.28
1	A	23	GLU	C-N-CA	6.16	128.53	120.28
1	A	115	GLU	CB-CG-CD	5.89	122.61	112.60
1	A	184	SER	N-CA-C	5.75	117.93	109.24
1	B	184	SER	N-CA-C	5.64	117.54	109.14
1	B	222	LEU	CA-C-N	5.63	128.10	120.38
1	B	222	LEU	C-N-CA	5.63	128.10	120.38
1	D	173	THR	N-CA-C	5.61	117.82	110.08
1	C	143	LYS	CA-C-N	5.59	128.32	120.28
1	C	143	LYS	C-N-CA	5.59	128.32	120.28
1	A	299	TYR	CA-C-N	5.42	125.96	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	TYR	C-N-CA	5.42	125.96	120.00
1	D	8	LEU	CA-C-N	5.41	128.67	122.83
1	D	8	LEU	C-N-CA	5.41	128.67	122.83
1	C	240	HIS	CA-C-N	5.40	129.85	122.34
1	C	240	HIS	C-N-CA	5.40	129.85	122.34
1	D	348	PRO	CA-C-N	5.36	129.26	120.63
1	D	348	PRO	C-N-CA	5.36	129.26	120.63
1	B	350	ALA	CA-C-N	5.34	127.39	120.44
1	B	350	ALA	C-N-CA	5.34	127.39	120.44
1	B	27	PHE	CA-C-N	5.32	127.66	120.38
1	B	27	PHE	C-N-CA	5.32	127.66	120.38
1	D	184	SER	N-CA-C	5.28	117.22	109.24
1	A	143	LYS	CA-C-N	5.26	127.86	120.28
1	A	143	LYS	C-N-CA	5.26	127.86	120.28
1	D	245	ILE	CA-C-N	5.18	127.60	120.39
1	D	245	ILE	C-N-CA	5.18	127.60	120.39
1	D	143	LYS	CA-C-N	5.14	127.68	120.28
1	D	143	LYS	C-N-CA	5.14	127.68	120.28
1	B	348	PRO	CA-C-N	5.12	128.88	120.63
1	B	348	PRO	C-N-CA	5.12	128.88	120.63
1	A	230	SER	CA-C-N	5.12	127.14	120.28
1	A	230	SER	C-N-CA	5.12	127.14	120.28
1	D	238	LEU	CA-C-N	5.12	127.65	120.28
1	D	238	LEU	C-N-CA	5.12	127.65	120.28
1	B	134	ALA	CA-C-N	5.11	129.62	122.36
1	B	134	ALA	C-N-CA	5.11	129.62	122.36
1	B	294	ARG	CA-C-N	5.10	127.12	120.28
1	B	294	ARG	C-N-CA	5.10	127.12	120.28
1	C	172	ASN	CA-C-N	5.09	131.87	121.48
1	C	172	ASN	C-N-CA	5.09	131.87	121.48
1	B	300	GLY	CA-C-N	5.08	127.09	120.28
1	B	300	GLY	C-N-CA	5.08	127.09	120.28
1	A	211	VAL	N-CA-CB	5.05	117.75	111.39
1	A	347	THR	CB-CA-C	5.03	117.47	109.52
1	C	23	GLU	CA-C-N	5.01	129.20	120.68
1	C	23	GLU	C-N-CA	5.01	129.20	120.68

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	2632	0	2371	23	0
1	B	2679	0	2460	23	0
1	C	2585	0	2279	20	0
1	D	2664	0	2389	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	26	0	0	1	0
3	B	32	0	0	1	0
3	C	26	0	0	3	0
3	D	26	0	0	1	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	C	4	0	6	0	0
5	A	1	0	0	1	0
6	A	43	0	0	0	0
6	B	59	0	0	1	0
6	C	33	0	0	3	0
6	D	41	0	0	0	0
All	All	10871	0	9523	80	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 (80) 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:155:THR:HG21	1:A:291:PHE:HB2	1.56	0.87
1:A:352:GLU:HA	1:A:355:LYS:HE2	1.66	0.77
1:A:196:SER:OG	1:A:270:THR:OG1	2.03	0.76
1:A:150:ILE:HG22	1:A:174:PRO:HB3	1.73	0.70
1:B:80:GLY:HA3	1:B:249:MET:HG2	1.81	0.62
1:B:66:VAL:HG23	1:C:163:GLU:HG2	1.82	0.62
1:B:186:ALA:HB1	1:B:243:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:HD13	1:B:87:ILE:CD1	2.36	0.55
1:D:150:ILE:HG22	1:D:174:PRO:HB3	1.87	0.55
1:B:195:TYR:HB2	1:B:291:PHE:O	2.05	0.55
1:B:272:PRO:HD2	1:B:295:ARG:HH11	1.72	0.54
1:C:150:ILE:HG22	1:C:174:PRO:HB3	1.90	0.54
1:B:150:ILE:HG23	1:B:289:THR:HG22	1.91	0.53
1:D:82:PHE:HB2	1:D:244:LEU:HB2	1.91	0.52
3:C:403:FQQ:N2	3:C:403:FQQ:C9	2.73	0.52
1:C:191:ASP:O	1:C:194:LEU:HD12	2.09	0.52
1:B:236:ALA:HB1	1:B:239:ARG:HG3	1.92	0.51
1:B:345:LEU:HD23	1:B:346:PRO:HD2	1.93	0.51
1:A:345:LEU:HD23	1:A:346:PRO:HD2	1.93	0.51
1:D:201:HIS:HE2	1:D:287:GLU:HB2	1.75	0.50
1:A:191:ASP:O	1:A:194:LEU:HD12	2.11	0.50
1:C:241:LYS:NZ	3:C:403:FQQ:C7	2.74	0.50
1:B:155:THR:HG21	1:B:291:PHE:HB2	1.93	0.50
1:D:236:ALA:HB1	1:D:239:ARG:HG3	1.94	0.49
3:A:403:FQQ:C9	3:A:403:FQQ:N2	2.76	0.49
1:D:155:THR:HG21	1:D:291:PHE:HB2	1.95	0.49
1:A:177:TYR:O	1:A:285:CYS:HA	2.13	0.48
1:A:74:LEU:HB3	1:C:74:LEU:HD22	1.96	0.48
3:D:403:FQQ:C9	3:D:403:FQQ:N2	2.77	0.48
1:C:236:ALA:HB1	1:C:239:ARG:HG3	1.96	0.47
1:A:140:LEU:HB2	1:A:201:HIS:CE1	2.50	0.47
1:A:186:ALA:HB1	1:A:243:THR:O	2.15	0.47
1:A:119:ARG:HD2	5:A:405:CL:CL	2.51	0.47
1:A:195:TYR:HB2	1:A:291:PHE:O	2.14	0.47
1:D:19:PRO:HB3	1:D:30:TYR:CZ	2.50	0.47
1:C:155:THR:HG21	1:C:291:PHE:HB2	1.96	0.47
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.50	0.46
1:B:19:PRO:HD2	1:B:48:VAL:O	2.15	0.46
1:A:111:TYR:CD2	1:A:117:LEU:HB2	2.51	0.45
1:D:150:ILE:HG23	1:D:289:THR:HG22	1.98	0.45
1:B:201:HIS:NE2	1:B:287:GLU:HB2	2.31	0.45
1:C:241:LYS:HZ3	3:C:403:FQQ:C7	2.29	0.45
1:D:202:PHE:CZ	1:D:285:CYS:HB3	2.51	0.45
1:B:150:ILE:HG22	1:B:174:PRO:HB3	1.99	0.45
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.51	0.44
1:A:56:ARG:HD2	1:A:59:TYR:CD1	2.53	0.44
1:D:201:HIS:NE2	1:D:287:GLU:HB2	2.32	0.44
1:A:14:ILE:HD13	1:A:44:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:PHE:HB2	1:C:244:LEU:HB2	2.00	0.44
1:C:21:MET:O	1:C:25:ARG:HG3	2.16	0.43
1:D:150:ILE:HG23	1:D:289:THR:CG2	2.48	0.43
1:C:19:PRO:HB3	1:C:30:TYR:CZ	2.53	0.43
1:A:82:PHE:HB2	1:A:244:LEU:HB2	1.99	0.43
1:C:228:PRO:HD2	6:C:525:HOH:O	2.18	0.43
1:B:187:TRP:CD1	1:B:245:ILE:HD12	2.54	0.43
1:A:150:ILE:HG23	1:A:289:THR:HG22	2.00	0.43
1:C:186:ALA:HB1	1:C:243:THR:O	2.19	0.42
3:B:403:FQQ:N2	3:B:403:FQQ:C9	2.82	0.42
1:C:331:LEU:HD21	6:C:528:HOH:O	2.19	0.42
1:B:31:ILE:HA	1:B:34:ILE:HG12	2.01	0.42
1:B:35:GLU:OE2	1:B:195:TYR:OH	2.34	0.42
1:C:150:ILE:CG2	1:C:174:PRO:HB3	2.49	0.42
1:A:17:PHE:HB2	1:A:47:VAL:HG22	2.01	0.42
1:B:171:VAL:HG22	1:B:290:ASN:HB2	2.02	0.42
1:C:68:PRO:HD2	6:C:516:HOH:O	2.19	0.42
1:C:141:TYR:CE2	1:C:149:ASN:HA	2.55	0.41
1:B:63:ASP:CG	1:B:98:ARG:HH22	2.28	0.41
1:D:114:PHE:O	1:D:115:GLU:C	2.64	0.41
1:A:301:LYS:HA	1:A:317:MET:HG3	2.03	0.41
1:B:74:LEU:HD13	1:B:87:ILE:HD12	2.03	0.41
1:A:236:ALA:HB1	1:A:239:ARG:HG3	2.02	0.41
1:C:14:ILE:HD13	1:C:44:LEU:HD23	2.02	0.41
1:D:153:LEU:HD11	1:D:197:ILE:HG21	2.03	0.41
1:A:63:ASP:CG	1:A:98:ARG:HH22	2.29	0.41
1:B:26:ASN:HB3	6:B:501:HOH:O	2.21	0.41
1:B:179:GLY:O	1:B:283:PHE:HA	2.21	0.41
1:C:345:LEU:HA	1:C:346:PRO:HD3	1.96	0.40
1:B:202:PHE:CZ	1:B:285:CYS:HB3	2.56	0.40
1:C:202:PHE:CZ	1:C:285:CYS:HB3	2.56	0.40
1:A:206:LYS:HG3	1:A:280:ASN:OD1	2.22	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	332/360 (92%)	320 (96%)	12 (4%)	0	100	100
1	B	335/360 (93%)	325 (97%)	10 (3%)	0	100	100
1	C	329/360 (91%)	319 (97%)	10 (3%)	0	100	100
1	D	336/360 (93%)	326 (97%)	10 (3%)	0	100	100
All	All	1332/1440 (92%)	1290 (97%)	42 (3%)	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	252/316 (80%)	237 (94%)	15 (6%)	17	45
1	B	257/316 (81%)	245 (95%)	12 (5%)	23	55
1	C	237/316 (75%)	224 (94%)	13 (6%)	19	49
1	D	256/316 (81%)	245 (96%)	11 (4%)	26	58
All	All	1002/1264 (79%)	951 (95%)	51 (5%)	21	52

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	63	ASP
1	A	74	LEU
1	A	78	GLN
1	A	125	LEU
1	A	137	ASN
1	A	161	GLU
1	A	194	LEU

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Mol	Chain	Res	Type
1	A	230	SER
1	A	245	ILE
1	A	288	SER
1	A	307	SER
1	A	333	LYS
1	A	345	LEU
1	A	354	LEU
1	B	52	GLU
1	B	63	ASP
1	B	71	ILE
1	B	74	LEU
1	B	112	SER
1	B	137	ASN
1	B	159	LEU
1	B	249	MET
1	B	288	SER
1	B	307	SER
1	B	327	GLU
1	B	345	LEU
1	C	35	GLU
1	C	63	ASP
1	C	74	LEU
1	C	137	ASN
1	C	150	ILE
1	C	159	LEU
1	C	172	ASN
1	C	245	ILE
1	C	288	SER
1	C	307	SER
1	C	318	ASP
1	C	321	VAL
1	C	327	GLU
1	D	6	GLU
1	D	63	ASP
1	D	71	ILE
1	D	74	LEU
1	D	137	ASN
1	D	171	VAL
1	D	194	LEU
1	D	245	ILE
1	D	307	SER
1	D	318	ASP

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Mol	Chain	Res	Type
1	D	327	GLU

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

Mol	Chain	Res	Type
1	A	78	GLN
1	A	128	ASN
1	B	102	ASN
1	B	128	ASN
1	C	72	GLN
1	C	78	GLN
1	C	84	GLN
1	C	124	ASN
1	D	78	GLN
1	D	124	ASN
1	D	215	HIS

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](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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
4	DMS	B	405	-	3,3,3	0.35	0	3,3,3	0.24	0
3	FQQ	B	403	2	35,36,36	0.41	0	46,52,52	0.95	2 (4%)
3	FQQ	A	403	2	28,29,36	0.59	1 (3%)	35,42,52	0.97	2 (5%)
4	DMS	C	404	-	3,3,3	0.24	0	3,3,3	0.24	0
4	DMS	A	404	-	3,3,3	0.37	0	3,3,3	0.39	0
3	FQQ	C	403	2	28,29,36	0.73	1 (3%)	35,42,52	1.20	3 (8%)
3	FQQ	D	403	2	28,29,36	0.43	0	35,42,52	1.16	4 (11%)
4	DMS	B	404	-	3,3,3	0.50	0	3,3,3	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
3	FQQ	B	403	2	-	5/15/27/27	0/5/5/5
3	FQQ	A	403	2	-	4/9/21/27	0/4/4/5
3	FQQ	C	403	2	-	5/9/21/27	0/4/4/5
3	FQQ	D	403	2	-	4/9/21/27	0/4/4/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	FQQ	C2-N3	-3.18	1.37	1.41
3	A	403	FQQ	C2-N3	-2.46	1.38	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	FQQ	O-C5-N1	3.84	125.11	120.44
3	D	403	FQQ	O-C5-N1	3.80	125.07	120.44
3	C	403	FQQ	O-C5-N1	3.53	124.74	120.44
3	C	403	FQQ	C4-C5-N1	-3.29	111.57	114.33
3	D	403	FQQ	C4-C5-N1	-3.28	111.58	114.33
3	A	403	FQQ	O-C5-N1	3.24	124.38	120.44
3	B	403	FQQ	C4-C5-N1	-2.73	112.04	114.33
3	C	403	FQQ	C17-C14-C13	2.56	113.73	110.04
3	A	403	FQQ	C4-C5-N1	-2.45	112.28	114.33
3	D	403	FQQ	C17-C14-C13	2.13	113.12	110.04
3	D	403	FQQ	C1-N-C2	2.12	119.85	115.05

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	FQQ	C3-C2-N3-N4
3	A	403	FQQ	N-C2-N3-N4
3	B	403	FQQ	C3-C2-N3-N4
3	B	403	FQQ	N-C2-N3-N4
3	C	403	FQQ	C3-C2-N3-N4
3	C	403	FQQ	N-C2-N3-N4
3	D	403	FQQ	C3-C2-N3-N4
3	D	403	FQQ	N-C2-N3-N4
3	B	403	FQQ	C10-C11-N5-C12
3	C	403	FQQ	C10-C11-N5-C12
3	A	403	FQQ	N-C2-N3-C9
3	B	403	FQQ	N-C2-N3-C9
3	C	403	FQQ	N-C2-N3-C9
3	D	403	FQQ	N-C2-N3-C9
3	A	403	FQQ	C3-C2-N3-C9
3	B	403	FQQ	C3-C2-N3-C9
3	C	403	FQQ	C3-C2-N3-C9
3	D	403	FQQ	C3-C2-N3-C9

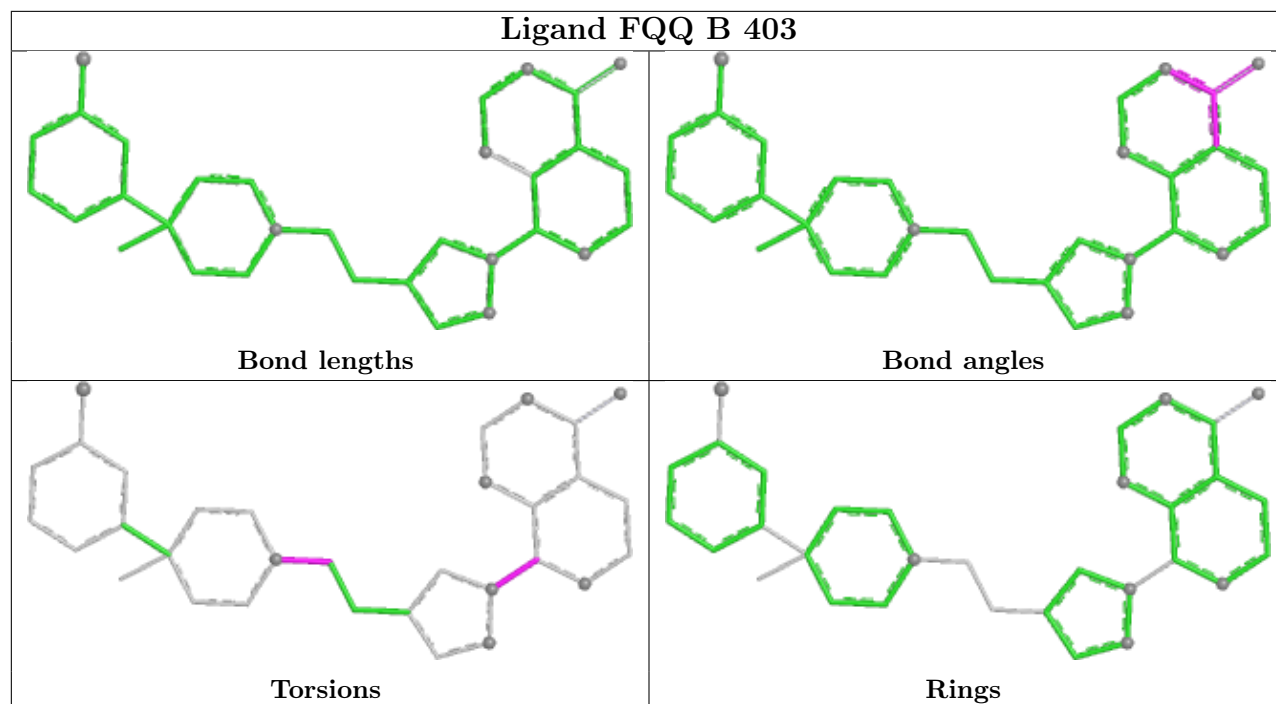
There are no ring outliers.

4 monomers are involved in 6 short contacts:

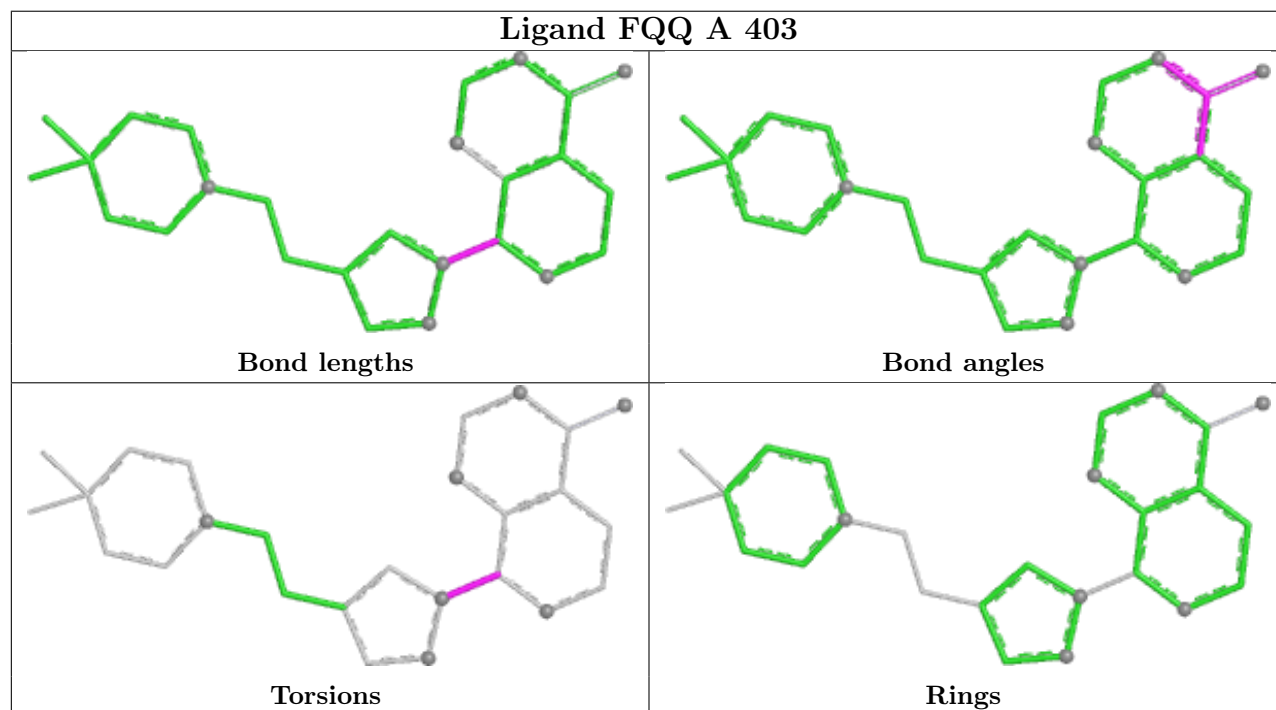
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	FQQ	1	0
3	A	403	FQQ	1	0
3	C	403	FQQ	3	0
3	D	403	FQQ	1	0

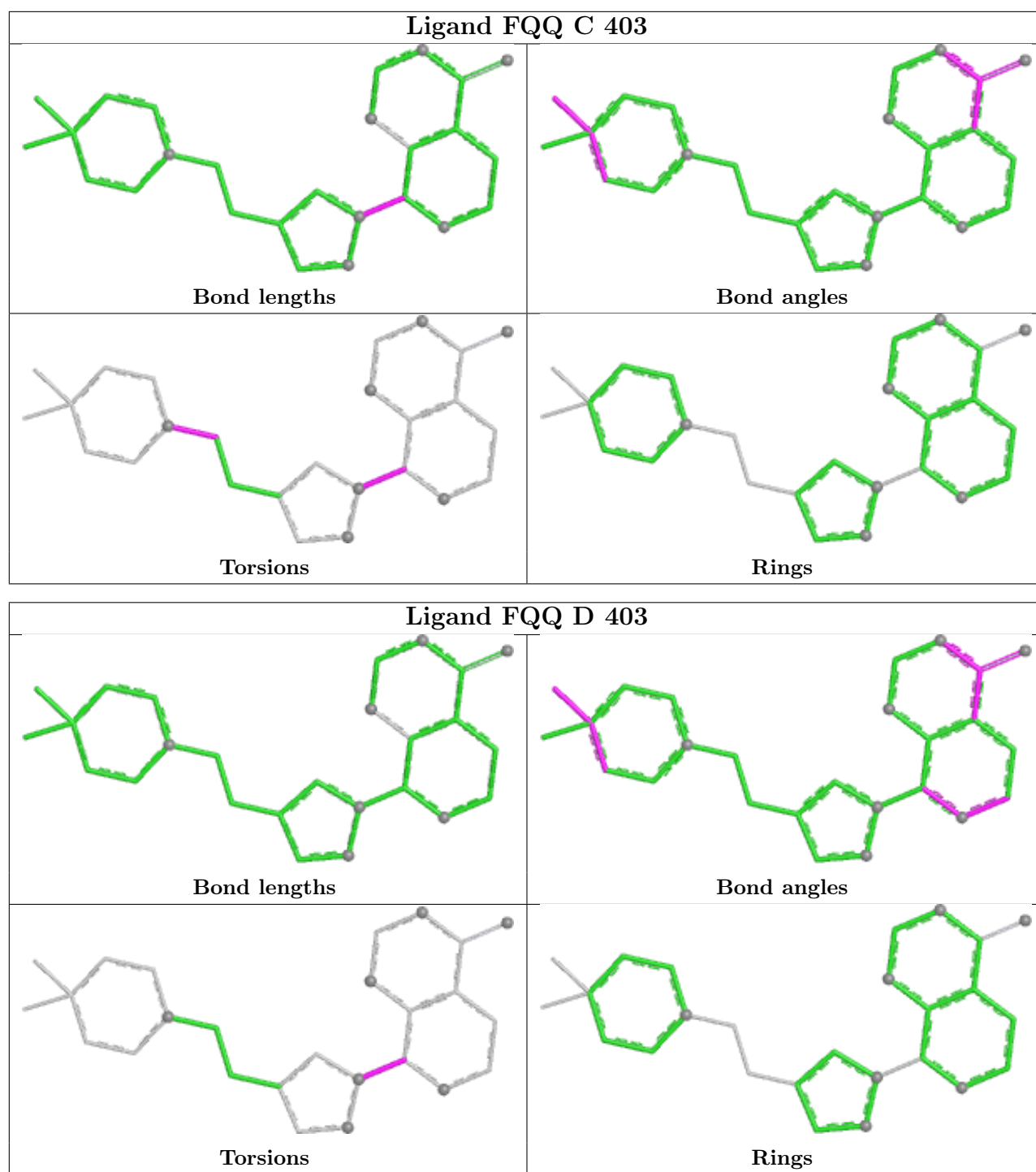
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FQQ B 403



Ligand FQQ A 403





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	337/360 (93%)	0.46	16 (4%) 36 28	26, 50, 87, 114	1 (0%)
1	B	340/360 (94%)	0.24	4 (1%) 76 68	22, 43, 70, 102	1 (0%)
1	C	335/360 (93%)	0.69	23 (6%) 23 16	29, 59, 101, 112	0
1	D	340/360 (94%)	0.50	20 (5%) 28 21	16, 54, 98, 137	2 (0%)
All	All	1352/1440 (93%)	0.47	63 (4%) 36 28	16, 51, 93, 137	4 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	SER	4.9
1	D	11[A]	SER	4.8
1	A	309	ARG	4.3
1	D	161	GLU	3.9
1	A	229	GLY	3.6
1	C	354	LEU	3.5
1	B	7	THR	3.2
1	C	106	TYR	3.2
1	D	5	SER	3.1
1	D	10	PRO	3.1
1	C	312	MET	3.0
1	D	235	GLU	3.0
1	D	354	LEU	3.0
1	C	324	PHE	3.0
1	C	316	SER	2.9
1	A	338	ASN	2.9
1	D	338	ASN	2.8
1	B	172	ASN	2.7
1	B	6	GLU	2.7
1	C	233	SER	2.7
1	D	334	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	172	ASN	2.7
1	A	60[A]	ASP	2.7
1	A	329	TYR	2.7
1	A	11	SER	2.6
1	D	8	LEU	2.6
1	A	162	LYS	2.6
1	C	108	THR	2.6
1	C	313	VAL	2.6
1	D	7	THR	2.6
1	A	235	GLU	2.6
1	D	236	ALA	2.6
1	C	315	ILE	2.5
1	A	170	GLY	2.5
1	D	171	VAL	2.5
1	C	111	TYR	2.5
1	C	162	LYS	2.5
1	C	322	ARG	2.4
1	C	171	VAL	2.4
1	A	154	ARG	2.4
1	A	159	LEU	2.3
1	C	107	CYS	2.3
1	C	112	SER	2.3
1	C	52	GLU	2.3
1	D	336	LYS	2.3
1	D	341	ILE	2.3
1	D	170	GLY	2.2
1	D	353	PHE	2.2
1	C	27	PHE	2.2
1	A	327	GLU	2.2
1	A	328	ARG	2.1
1	C	60	ASP	2.1
1	D	227	PHE	2.1
1	C	305	LEU	2.1
1	D	153	LEU	2.1
1	C	327	GLU	2.1
1	D	113	GLU	2.1
1	D	333	LYS	2.0
1	C	172	ASN	2.0
1	A	151	GLY	2.0
1	C	226	PHE	2.0
1	C	59	TYR	2.0
1	A	112	SER	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](#)

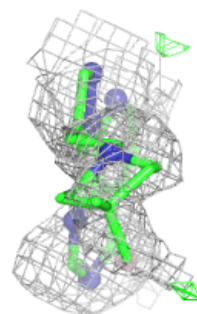
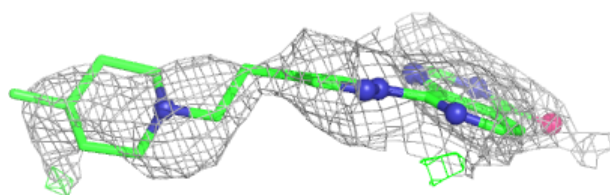
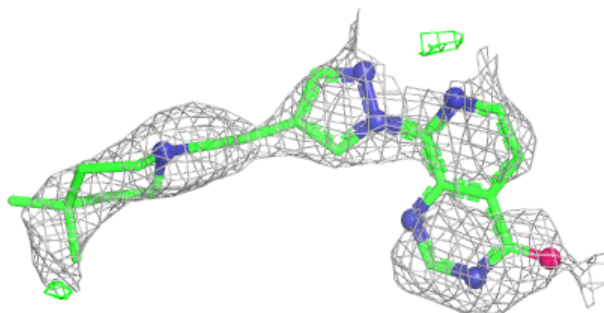
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	DMS	B	404	4/4	0.74	0.29	69,70,71,71	0
3	FQQ	A	403	26/32	0.81	0.18	41,47,55,55	26
4	DMS	B	405	4/4	0.81	0.24	73,73,74,75	4
4	DMS	A	404	4/4	0.82	0.23	71,72,73,73	0
3	FQQ	C	403	26/32	0.85	0.16	44,50,63,65	0
3	FQQ	B	403	32/32	0.85	0.18	37,46,62,71	32
4	DMS	C	404	4/4	0.85	0.19	74,75,76,76	0
3	FQQ	D	403	26/32	0.86	0.18	56,61,64,64	26
5	CL	A	405	1/1	0.87	0.10	74,74,74,74	0
2	ZN	D	402	1/1	0.98	0.04	67,67,67,67	1
2	ZN	A	401	1/1	0.98	0.04	58,58,58,58	0
2	ZN	A	402	1/1	0.98	0.05	86,86,86,86	0
2	ZN	B	401	1/1	0.98	0.04	45,45,45,45	0
2	ZN	C	402	1/1	0.98	0.06	92,92,92,92	0
2	ZN	B	402	1/1	0.99	0.03	37,37,37,37	1
2	ZN	D	401	1/1	0.99	0.03	52,52,52,52	0
2	ZN	C	401	1/1	0.99	0.04	54,54,54,54	0

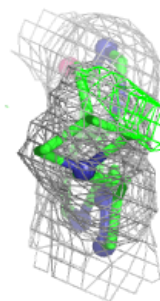
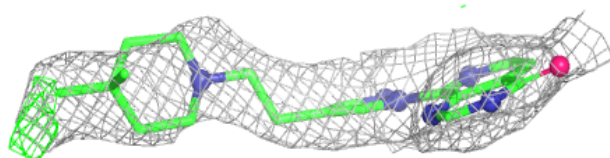
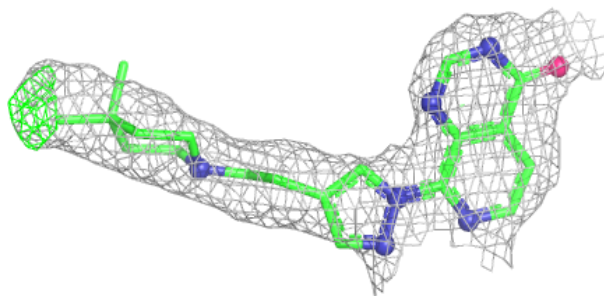
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FQQ A 403:

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

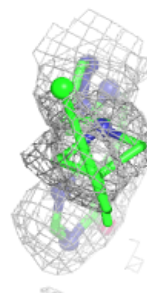
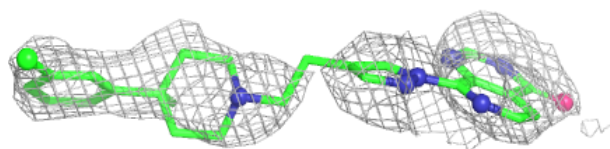
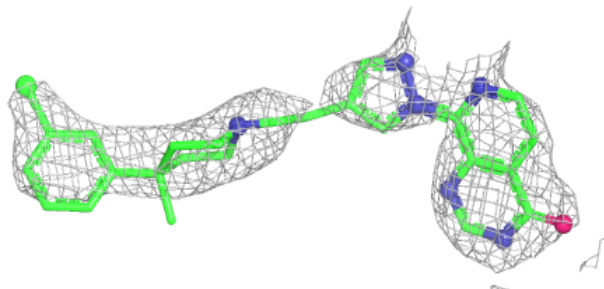
**Electron density around FQQ C 403:**

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

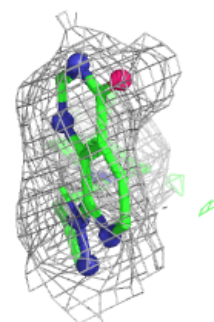
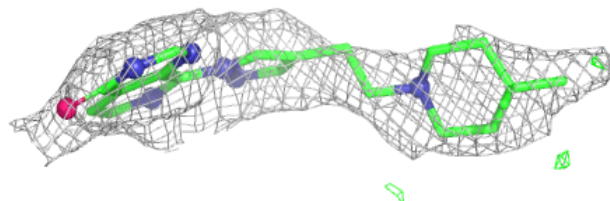
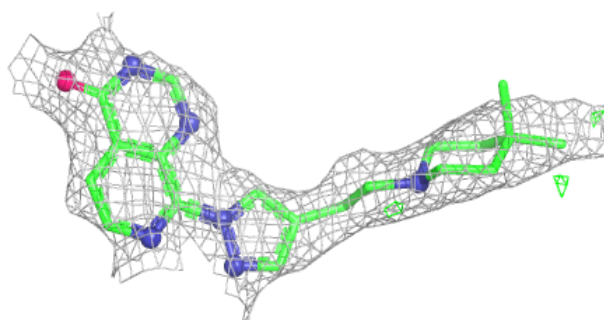


Electron density around FQQ B 403:

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

**Electron density around FQQ D 403:**

$2mF_o-DF_c$ (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.