



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:41 am BST

PDB ID : 5VGI
Title : Crystal Structure of KDM4 with the Small Molecule Inhibitor QC6352
Authors : Hosfield, D.J.
Deposited on : 2017-04-11
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

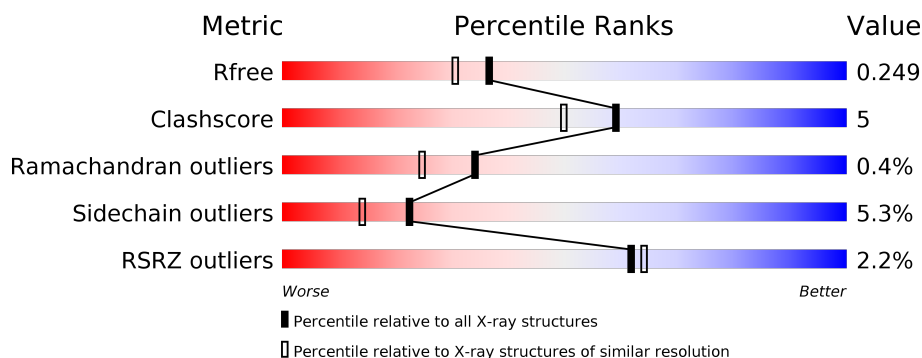
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	370	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	370	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	370	<div> <div>0%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	370	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11655 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	345	Total	C	N	O	S	0	0	0
			2837	1834	478	510	15			
1	B	345	Total	C	N	O	S	0	0	0
			2837	1834	478	510	15			
1	C	337	Total	C	N	O	S	0	0	0
			2777	1797	469	496	15			
1	D	345	Total	C	N	O	S	0	0	0
			2837	1834	478	510	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP O75164
A	-14	GLY	-	expression tag	UNP O75164
A	-13	HIS	-	expression tag	UNP O75164
A	-12	HIS	-	expression tag	UNP O75164
A	-11	HIS	-	expression tag	UNP O75164
A	-10	HIS	-	expression tag	UNP O75164
A	-9	HIS	-	expression tag	UNP O75164
A	-8	HIS	-	expression tag	UNP O75164
A	-7	HIS	-	expression tag	UNP O75164
A	-6	HIS	-	expression tag	UNP O75164
A	-5	GLY	-	expression tag	UNP O75164
A	-4	SER	-	expression tag	UNP O75164
A	-3	GLY	-	expression tag	UNP O75164
A	-2	GLU	-	expression tag	UNP O75164
A	-1	ASN	-	expression tag	UNP O75164
A	0	LEU	-	expression tag	UNP O75164
A	1	TYR	-	expression tag	UNP O75164
A	2	PHE	-	expression tag	UNP O75164
A	3	GLN	-	expression tag	UNP O75164
A	4	SER	-	expression tag	UNP O75164
B	-15	MET	-	expression tag	UNP O75164

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP O75164
B	-13	HIS	-	expression tag	UNP O75164
B	-12	HIS	-	expression tag	UNP O75164
B	-11	HIS	-	expression tag	UNP O75164
B	-10	HIS	-	expression tag	UNP O75164
B	-9	HIS	-	expression tag	UNP O75164
B	-8	HIS	-	expression tag	UNP O75164
B	-7	HIS	-	expression tag	UNP O75164
B	-6	HIS	-	expression tag	UNP O75164
B	-5	GLY	-	expression tag	UNP O75164
B	-4	SER	-	expression tag	UNP O75164
B	-3	GLY	-	expression tag	UNP O75164
B	-2	GLU	-	expression tag	UNP O75164
B	-1	ASN	-	expression tag	UNP O75164
B	0	LEU	-	expression tag	UNP O75164
B	1	TYR	-	expression tag	UNP O75164
B	2	PHE	-	expression tag	UNP O75164
B	3	GLN	-	expression tag	UNP O75164
B	4	SER	-	expression tag	UNP O75164
C	-15	MET	-	expression tag	UNP O75164
C	-14	GLY	-	expression tag	UNP O75164
C	-13	HIS	-	expression tag	UNP O75164
C	-12	HIS	-	expression tag	UNP O75164
C	-11	HIS	-	expression tag	UNP O75164
C	-10	HIS	-	expression tag	UNP O75164
C	-9	HIS	-	expression tag	UNP O75164
C	-8	HIS	-	expression tag	UNP O75164
C	-7	HIS	-	expression tag	UNP O75164
C	-6	HIS	-	expression tag	UNP O75164
C	-5	GLY	-	expression tag	UNP O75164
C	-4	SER	-	expression tag	UNP O75164
C	-3	GLY	-	expression tag	UNP O75164
C	-2	GLU	-	expression tag	UNP O75164
C	-1	ASN	-	expression tag	UNP O75164
C	0	LEU	-	expression tag	UNP O75164
C	1	TYR	-	expression tag	UNP O75164
C	2	PHE	-	expression tag	UNP O75164
C	3	GLN	-	expression tag	UNP O75164
C	4	SER	-	expression tag	UNP O75164
D	-15	MET	-	expression tag	UNP O75164
D	-14	GLY	-	expression tag	UNP O75164
D	-13	HIS	-	expression tag	UNP O75164

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP O75164
D	-11	HIS	-	expression tag	UNP O75164
D	-10	HIS	-	expression tag	UNP O75164
D	-9	HIS	-	expression tag	UNP O75164
D	-8	HIS	-	expression tag	UNP O75164
D	-7	HIS	-	expression tag	UNP O75164
D	-6	HIS	-	expression tag	UNP O75164
D	-5	GLY	-	expression tag	UNP O75164
D	-4	SER	-	expression tag	UNP O75164
D	-3	GLY	-	expression tag	UNP O75164
D	-2	GLU	-	expression tag	UNP O75164
D	-1	ASN	-	expression tag	UNP O75164
D	0	LEU	-	expression tag	UNP O75164
D	1	TYR	-	expression tag	UNP O75164
D	2	PHE	-	expression tag	UNP O75164
D	3	GLN	-	expression tag	UNP O75164
D	4	SER	-	expression tag	UNP O75164

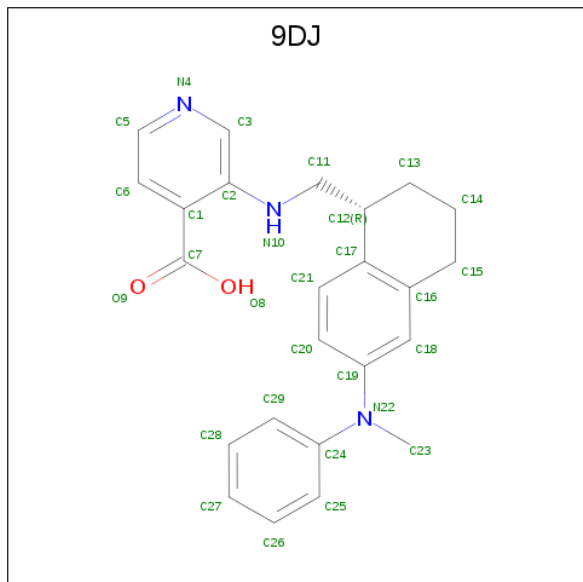
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is 3-[(1R)-6-[methyl(phenyl)amino]-1,2,3,4-tetrahydronaphthalen-1-yl)methyl]amino]pyridine-4-carboxylic acid (three-letter code: 9DJ) (formula: C₂₄H₂₅N₃O₂).

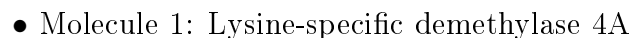
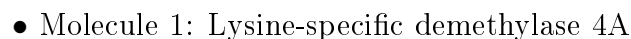


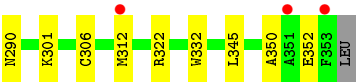
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	24	3	2		
4	B	1	Total	C	N	O	0	0
			29	24	3	2		
4	C	1	Total	C	N	O	0	0
			29	24	3	2		
4	D	1	Total	C	N	O	0	0
			29	24	3	2		

- Molecule 5 is water.

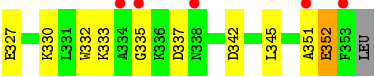
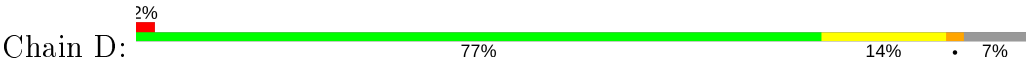
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	58	Total	O	0	0
			58	58		
5	C	80	Total	O	0	0
			80	80		
5	D	58	Total	O	0	0
			58	58		

- 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	57.32Å 101.59Å 141.89Å 90.00° 99.64° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07 47.75 – 2.07	Depositor EDS
% Data completeness (in resolution range)	87.9 (50.00-2.07) 87.9 (47.75-2.07)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.189 , 0.248 0.189 , 0.249	Depositor DCC
R_{free} test set	4274 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11655	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 21.87 % 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 6.4061e-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: NI, ZN, 9DJ

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	1.22	6/2924 (0.2%)	1.10	7/3958 (0.2%)
1	B	1.24	5/2924 (0.2%)	1.19	17/3958 (0.4%)
1	C	1.33	4/2863 (0.1%)	1.19	16/3875 (0.4%)
1	D	1.29	10/2924 (0.3%)	1.12	6/3958 (0.2%)
All	All	1.27	25/11635 (0.2%)	1.15	46/15749 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	TYR	CE1-CZ	8.28	1.49	1.38
1	D	198	ASN	CB-CG	7.94	1.69	1.51
1	D	184	SER	CB-OG	-7.49	1.32	1.42
1	B	209	TYR	CE1-CZ	7.49	1.48	1.38
1	C	93	THR	CB-CG2	7.18	1.76	1.52
1	B	184	SER	CB-OG	-6.95	1.33	1.42
1	D	195	TYR	CE1-CZ	6.87	1.47	1.38
1	D	28	SER	CB-OG	-6.37	1.33	1.42
1	D	185	PHE	CG-CD2	6.09	1.47	1.38
1	C	274	GLY	N-CA	6.00	1.55	1.46
1	D	106	TYR	CG-CD2	5.98	1.47	1.39
1	A	209	TYR	CE1-CZ	5.79	1.46	1.38
1	C	271	PHE	CG-CD1	5.72	1.47	1.38
1	D	61	ASP	CB-CG	5.67	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	SER	CB-OG	-5.64	1.34	1.42
1	B	121	TYR	CG-CD1	5.48	1.46	1.39
1	B	175	TYR	CE1-CZ	5.42	1.45	1.38
1	A	121	TYR	CG-CD2	5.42	1.46	1.39
1	D	106	TYR	CE1-CZ	5.34	1.45	1.38
1	A	296	TRP	CB-CG	5.32	1.59	1.50
1	A	38	GLY	N-CA	5.30	1.53	1.46
1	D	210	SER	CB-OG	5.29	1.49	1.42
1	C	139	THR	CB-CG2	5.23	1.69	1.52
1	A	197	ILE	C-O	5.03	1.32	1.23
1	B	141	TYR	CE1-CZ	5.00	1.45	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASP	CB-CG-OD1	9.47	126.83	118.30
1	B	63	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	B	63	ASP	CB-CG-OD1	8.58	126.02	118.30
1	A	95	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	119	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	51	LYS	CD-CE-NZ	7.87	129.79	111.70
1	C	154	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	B	125	LEU	CB-CG-CD1	-7.58	98.11	111.00
1	D	182	LYS	CD-CE-NZ	-6.89	95.84	111.70
1	C	322	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	345	LEU	CA-CB-CG	6.76	130.84	115.30
1	C	241	LYS	CD-CE-NZ	-6.74	96.20	111.70
1	D	123	LYS	CD-CE-NZ	-6.71	96.28	111.70
1	B	105	LYS	CD-CE-NZ	-6.67	96.35	111.70
1	D	61	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	252	LYS	CD-CE-NZ	-6.62	96.49	111.70
1	A	95	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	92	MET	CG-SD-CE	6.46	110.55	100.20
1	D	63	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	322	ARG	CG-CD-NE	-6.14	98.91	111.80
1	C	119	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	259	LYS	CD-CE-NZ	-5.95	98.02	111.70
1	B	123	LYS	CD-CE-NZ	-5.93	98.07	111.70
1	C	117	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	C	105	LYS	CD-CE-NZ	-5.87	98.21	111.70
1	C	221	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	221	ARG	NE-CZ-NH1	5.86	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	MET	CA-CB-CG	5.86	123.26	113.30
1	C	99	LYS	CD-CE-NZ	-5.83	98.30	111.70
1	D	184	SER	CB-CA-C	-5.78	99.12	110.10
1	B	221	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	13	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	120	LYS	CD-CE-NZ	-5.55	98.93	111.70
1	C	239	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	B	131	ILE	CG1-CB-CG2	-5.48	99.34	111.40
1	A	135	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	322	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	239	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	259	LYS	CD-CE-NZ	5.27	123.81	111.70
1	B	331	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	41	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	218	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	154	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	25	ARG	CG-CD-NE	-5.13	101.03	111.80
1	A	184	SER	CB-CA-C	-5.08	100.44	110.10
1	C	119	ARG	CG-CD-NE	-5.03	101.23	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	351	ALA	Peptide

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	2837	0	2760	28	0
1	B	2837	0	2760	29	0
1	C	2777	0	2697	25	0
1	D	2837	0	2760	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	29	0	0	0	0
4	B	29	0	0	1	0
4	C	29	0	0	0	0
4	D	29	0	0	0	0
5	A	47	0	0	1	0
5	B	58	0	0	4	0
5	C	80	0	0	3	0
5	D	58	0	0	2	0
All	All	11655	0	10977	105	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 5.

All (105) 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:93:THR:CB	1:C:93:THR:CG2	1.76	1.58
1:A:11:SER:HA	5:A:635:HOH:O	1.47	1.14
1:A:74:LEU:HD23	1:A:87:ILE:CD1	2.00	0.91
1:B:9:ASN:N	5:B:601:HOH:O	2.01	0.91
1:C:9:ASN:N	5:C:601:HOH:O	2.10	0.82
1:A:74:LEU:HD23	1:A:87:ILE:HD12	1.63	0.79
1:C:222:LEU:HD11	1:C:226:PHE:CE2	2.23	0.72
1:C:93:THR:CA	1:C:93:THR:CG2	2.72	0.66
1:D:306:CYS:HB3	1:D:312:MET:HG3	1.78	0.66
1:C:312:MET:O	1:C:312:MET:SD	2.54	0.65
1:B:82:PHE:HB2	1:B:244:LEU:HB2	1.78	0.65
1:B:210:SER:HB2	5:B:611:HOH:O	1.98	0.64
1:A:163:GLU:OE1	1:A:319:VAL:CG2	2.46	0.63
1:D:294:ARG:HD3	1:D:324:PHE:CD2	2.35	0.62
1:B:218:ARG:HD2	5:B:656:HOH:O	2.00	0.61
1:A:318:ASP:HB3	1:A:322:ARG:HH12	1.63	0.61
1:D:332:TRP:HA	1:D:337:ASP:HB2	1.82	0.60
1:A:87:ILE:HG22	1:A:89:LYS:HE3	1.84	0.60
1:B:63:ASP:HB3	1:B:95:ARG:HB2	1.84	0.60
1:A:334:ALA:O	1:A:336:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.69	0.57
1:D:154:ARG:HA	1:D:158:ASP:OD2	2.04	0.57
1:A:186:ALA:HA	1:A:244:LEU:HD23	1.87	0.57
1:B:127:PHE:O	1:B:182:LYS:NZ	2.37	0.57
1:B:19:PRO:O	1:B:50:PRO:HG3	2.06	0.55
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.23	0.54
1:C:186:ALA:HA	1:C:244:LEU:HD23	1.90	0.54
1:D:319:VAL:HG13	5:D:646:HOH:O	2.08	0.53
1:B:161:GLU:O	1:B:165:GLY:N	2.42	0.53
1:C:57:ALA:N	1:C:142:GLU:OE1	2.35	0.53
1:B:153:LEU:HD11	1:B:197:ILE:HG21	1.91	0.52
1:B:163:GLU:HG2	1:B:319:VAL:HG21	1.91	0.52
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.43	0.52
1:D:51:LYS:H	1:D:51:LYS:NZ	2.08	0.52
1:C:312:MET:SD	1:C:312:MET:C	2.89	0.52
1:C:301:LYS:HE3	1:C:332:TRP:CD1	2.45	0.52
1:C:11:SER:OG	1:C:13:ARG:HG3	2.11	0.51
1:B:241:LYS:HD2	4:B:503:9DJ:C20	2.41	0.51
1:A:105:LYS:HG3	1:A:106:TYR:CE2	2.46	0.50
1:B:163:GLU:HG3	1:B:163:GLU:O	2.11	0.50
1:A:163:GLU:OE1	1:A:319:VAL:HG23	2.11	0.50
1:A:159:LEU:HD13	1:A:319:VAL:HG22	1.93	0.49
1:C:170:GLY:HA3	1:C:175:TYR:CE2	2.47	0.49
1:C:246:SER:HB2	1:C:247:PRO:HD2	1.94	0.49
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.47	0.49
1:D:163:GLU:O	1:D:164:SER:HB3	2.12	0.49
1:A:137:ASN:OD1	1:A:169:GLU:HG2	2.11	0.49
1:D:19:PRO:HD2	1:D:48:VAL:O	2.13	0.49
1:C:215:HIS:CD2	1:C:218:ARG:HH11	2.30	0.49
1:B:143:LYS:O	1:B:152:ARG:NH1	2.46	0.49
1:D:125:LEU:HD23	1:D:125:LEU:N	2.28	0.49
1:D:294:ARG:CD	1:D:324:PHE:CD2	2.97	0.48
1:D:342:ASP:OD2	1:D:345:LEU:HD13	2.14	0.48
1:B:159:LEU:O	1:B:163:GLU:HB3	2.14	0.48
1:A:218:ARG:HG2	1:A:221:ARG:NH2	2.29	0.48
1:D:90:LYS:HE2	1:D:90:LYS:HB3	1.73	0.47
1:D:150:ILE:HG23	1:D:289:THR:HG22	1.96	0.47
1:B:222:LEU:HD11	1:B:226:PHE:HE2	1.80	0.47
1:C:246:SER:HB2	5:C:673:HOH:O	2.14	0.46
1:B:233:SER:HB2	5:B:602:HOH:O	2.15	0.46
1:B:306:CYS:SG	1:B:312:MET:HG3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:HIS:CD2	1:C:241:LYS:HE3	2.51	0.46
1:B:56:ARG:HD3	1:B:59:TYR:CD1	2.51	0.46
1:D:294:ARG:HD3	1:D:324:PHE:HD2	1.78	0.46
1:A:160:VAL:O	1:A:164:SER:HB2	2.16	0.45
1:A:53:TRP:CZ3	1:A:55:PRO:HD3	2.51	0.45
1:B:327:GLU:OE2	1:B:328:ARG:HG3	2.17	0.45
1:D:312:MET:HE3	5:D:638:HOH:O	2.16	0.45
1:C:217:LYS:HE3	1:C:220:GLU:OE1	2.16	0.45
1:D:333:LYS:C	1:D:335:GLY:H	2.19	0.44
1:D:168:ILE:HB	1:D:171:VAL:HB	1.98	0.44
1:C:144:HIS:H	1:C:144:HIS:CD2	2.36	0.44
1:D:153:LEU:HD11	1:D:197:ILE:HG21	1.99	0.44
1:D:326:PRO:HD2	1:D:327:GLU:OE2	2.18	0.44
1:B:317:MET:O	1:B:318:ASP:C	2.57	0.43
1:B:115:GLU:CD	1:B:115:GLU:H	2.21	0.43
1:A:48:VAL:HA	1:A:49:PRO:HD3	1.89	0.43
1:B:222:LEU:HD11	1:B:226:PHE:CE2	2.54	0.43
1:A:162:LYS:HD2	1:A:162:LYS:HA	1.53	0.43
1:A:295:ARG:HB2	1:A:347:THR:HA	1.99	0.43
1:B:51:LYS:HE2	1:B:51:LYS:HB2	1.81	0.43
1:C:222:LEU:HD11	1:C:226:PHE:HE2	1.78	0.42
1:A:318:ASP:HB3	1:A:322:ARG:NH1	2.33	0.42
1:B:327:GLU:N	1:B:327:GLU:OE1	2.51	0.42
1:B:81:LEU:HD21	1:B:249:MET:HE2	2.02	0.42
1:C:173:THR:HB	1:C:174:PRO:HD2	2.02	0.42
1:A:163:GLU:O	1:C:65:LEU:HD12	2.20	0.42
1:C:171:VAL:O	1:C:290:ASN:HB2	2.21	0.41
1:A:296:TRP:CG	1:A:296:TRP:O	2.73	0.41
1:B:328:ARG:HD3	1:B:337:ASP:OD2	2.19	0.41
1:D:21:MET:HA	1:D:50:PRO:HG3	2.02	0.41
1:A:159:LEU:HD11	1:A:323:LYS:HD3	2.01	0.41
1:A:153:LEU:HD11	1:A:197:ILE:HG21	2.03	0.41
1:B:70:PRO:HG3	1:B:92:MET:HG2	2.02	0.41
1:A:224:LYS:HG3	1:A:231:ALA:CB	2.50	0.41
1:C:154:ARG:HA	1:C:158:ASP:OD2	2.20	0.41
1:D:110:ARG:HD2	1:D:111:TYR:H	1.85	0.41
1:A:317:MET:O	1:A:321:VAL:HG23	2.20	0.41
1:D:18:TYR:CD1	1:D:18:TYR:N	2.89	0.41
1:D:330:LYS:HA	1:D:330:LYS:HD3	1.97	0.41
1:D:99:LYS:HE2	1:D:99:LYS:HB2	1.79	0.41
1:C:32:ALA:HB1	1:C:350:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TRP:HE1	1:C:147:GLU:HB2	1.85	0.41
1:B:147:GLU:CD	1:B:147:GLU:H	2.23	0.40
1:C:171:VAL:N	5:C:605:HOH:O	2.54	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	343/370 (93%)	330 (96%)	12 (4%)	1 (0%)	41	32
1	B	343/370 (93%)	324 (94%)	18 (5%)	1 (0%)	41	32
1	C	333/370 (90%)	322 (97%)	10 (3%)	1 (0%)	41	32
1	D	343/370 (93%)	323 (94%)	18 (5%)	2 (1%)	25	15
All	All	1362/1480 (92%)	1299 (95%)	58 (4%)	5 (0%)	34	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	352	GLU
1	B	161	GLU
1	D	164	SER
1	A	339	THR
1	C	171	VAL

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	302/324 (93%)	284 (94%)	18 (6%)	19	11
1	B	302/324 (93%)	286 (95%)	16 (5%)	22	14
1	C	295/324 (91%)	283 (96%)	12 (4%)	30	23
1	D	302/324 (93%)	284 (94%)	18 (6%)	19	11
All	All	1201/1296 (93%)	1137 (95%)	64 (5%)	22	14

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	90	LYS
1	A	99	LYS
1	A	115	GLU
1	A	123	LYS
1	A	132	TYR
1	A	169	GLU
1	A	175	TYR
1	A	213	PRO
1	A	259	LYS
1	A	263	GLU
1	A	308	CYS
1	A	309	ARG
1	A	311	ASP
1	A	323	LYS
1	A	328	ARG
1	A	330	LYS
1	A	345	LEU
1	B	22	GLU
1	B	74	LEU
1	B	99	LYS
1	B	115	GLU
1	B	125	LEU
1	B	132	TYR
1	B	154	ARG
1	B	175	TYR
1	B	224	LYS
1	B	233	SER
1	B	306	CYS
1	B	310	LYS

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Mol	Chain	Res	Type
1	B	318	ASP
1	B	327	GLU
1	B	352	GLU
1	B	353	PHE
1	C	21	MET
1	C	51	LYS
1	C	88	GLN
1	C	110	ARG
1	C	112	SER
1	C	132	TYR
1	C	143	LYS
1	C	161	GLU
1	C	175	TYR
1	C	306	CYS
1	C	345	LEU
1	C	352	GLU
1	D	11	SER
1	D	28	SER
1	D	61	ASP
1	D	89	LYS
1	D	90	LYS
1	D	110	ARG
1	D	112	SER
1	D	132	TYR
1	D	143	LYS
1	D	163	GLU
1	D	175	TYR
1	D	218	ARG
1	D	233	SER
1	D	272	PRO
1	D	308	CYS
1	D	309	ARG
1	D	310	LYS
1	D	352	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	C	144	HIS
1	C	215	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	9DJ	A	503	2	30,32,32	2.58	11 (36%)	36,44,44	1.98	10 (27%)
4	9DJ	B	503	2	30,32,32	1.93	6 (20%)	36,44,44	1.51	8 (22%)
4	9DJ	C	503	2	30,32,32	2.20	4 (13%)	36,44,44	1.69	9 (25%)
4	9DJ	D	503	2	30,32,32	2.63	6 (20%)	36,44,44	1.51	7 (19%)

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	9DJ	A	503	2	-	0/13/27/27	0/4/4/4
4	9DJ	B	503	2	-	0/13/27/27	0/4/4/4
4	9DJ	C	503	2	-	2/13/27/27	0/4/4/4
4	9DJ	D	503	2	-	0/13/27/27	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	9DJ	C1-C2	8.97	1.53	1.40
4	D	503	9DJ	C16-C17	8.10	1.53	1.40
4	A	503	9DJ	C16-C17	7.36	1.52	1.40
4	A	503	9DJ	C1-C2	6.92	1.50	1.40
4	C	503	9DJ	C1-C2	6.46	1.49	1.40
4	C	503	9DJ	C16-C17	6.10	1.50	1.40
4	B	503	9DJ	C1-C2	5.37	1.48	1.40
4	C	503	9DJ	C1-C7	5.25	1.52	1.47
4	A	503	9DJ	C1-C7	4.70	1.52	1.47
4	B	503	9DJ	C16-C17	4.47	1.47	1.40
4	B	503	9DJ	C1-C7	3.49	1.50	1.47
4	A	503	9DJ	C21-C17	3.14	1.43	1.39
4	A	503	9DJ	C29-C24	2.88	1.45	1.39
4	C	503	9DJ	C11-N10	2.76	1.50	1.45
4	B	503	9DJ	C23-N22	2.72	1.52	1.46
4	D	503	9DJ	C3-N4	2.65	1.40	1.34
4	A	503	9DJ	C3-N4	2.61	1.39	1.34
4	A	503	9DJ	C21-C20	2.59	1.43	1.38
4	D	503	9DJ	C21-C20	2.55	1.43	1.38
4	D	503	9DJ	C1-C7	2.50	1.49	1.47
4	A	503	9DJ	C25-C24	2.49	1.44	1.39
4	D	503	9DJ	C29-C24	2.39	1.44	1.39
4	A	503	9DJ	C20-C19	2.35	1.43	1.39
4	B	503	9DJ	C3-C2	2.35	1.43	1.39
4	A	503	9DJ	C3-C2	2.06	1.42	1.39
4	A	503	9DJ	C19-N22	2.00	1.47	1.42
4	B	503	9DJ	C29-C24	2.00	1.43	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	9DJ	C20-C19-N22	5.98	128.81	120.46
4	C	503	9DJ	C5-C6-C1	-4.19	113.46	118.60
4	C	503	9DJ	C12-C11-N10	-3.96	107.27	112.60
4	A	503	9DJ	C14-C13-C12	3.71	118.74	111.47
4	A	503	9DJ	C18-C19-N22	-3.45	114.36	119.78
4	B	503	9DJ	C14-C15-C16	-3.36	104.19	112.42
4	B	503	9DJ	C13-C12-C11	-3.28	100.24	113.35
4	A	503	9DJ	C5-N4-C3	3.17	122.33	116.85
4	D	503	9DJ	C12-C11-N10	-3.06	108.49	112.60
4	D	503	9DJ	C5-N4-C3	3.03	122.09	116.85
4	C	503	9DJ	C5-N4-C3	2.91	121.88	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	9DJ	C21-C20-C19	2.90	124.14	120.32
4	C	503	9DJ	C19-N22-C24	2.90	124.89	120.74
4	A	503	9DJ	C13-C12-C17	2.87	116.07	109.68
4	D	503	9DJ	C28-C29-C24	2.77	123.31	119.68
4	A	503	9DJ	C13-C12-C11	-2.75	102.35	113.35
4	C	503	9DJ	C6-C1-C2	2.70	120.64	117.92
4	B	503	9DJ	C5-N4-C3	2.70	121.51	116.85
4	B	503	9DJ	C14-C13-C12	-2.70	106.19	111.47
4	D	503	9DJ	C14-C15-C16	-2.68	105.85	112.42
4	B	503	9DJ	C23-N22-C24	2.67	123.04	117.90
4	C	503	9DJ	C18-C19-N22	-2.67	115.58	119.78
4	B	503	9DJ	C20-C19-N22	2.61	124.10	120.46
4	B	503	9DJ	C12-C11-N10	-2.59	109.11	112.60
4	C	503	9DJ	C20-C19-N22	2.45	123.88	120.46
4	A	503	9DJ	C19-N22-C24	2.45	124.25	120.74
4	D	503	9DJ	C14-C13-C12	2.43	116.23	111.47
4	C	503	9DJ	C11-C12-C17	2.26	116.34	111.16
4	B	503	9DJ	C21-C17-C16	-2.22	116.03	118.74
4	A	503	9DJ	C21-C20-C19	2.19	123.21	120.32
4	C	503	9DJ	C14-C13-C12	2.15	115.68	111.47
4	A	503	9DJ	C21-C17-C16	-2.06	116.22	118.74
4	D	503	9DJ	C13-C12-C11	-2.05	105.14	113.35
4	A	503	9DJ	C19-C18-C16	2.05	123.94	120.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503	9DJ	C29-C24-N22-C19
4	C	503	9DJ	C25-C24-N22-C19

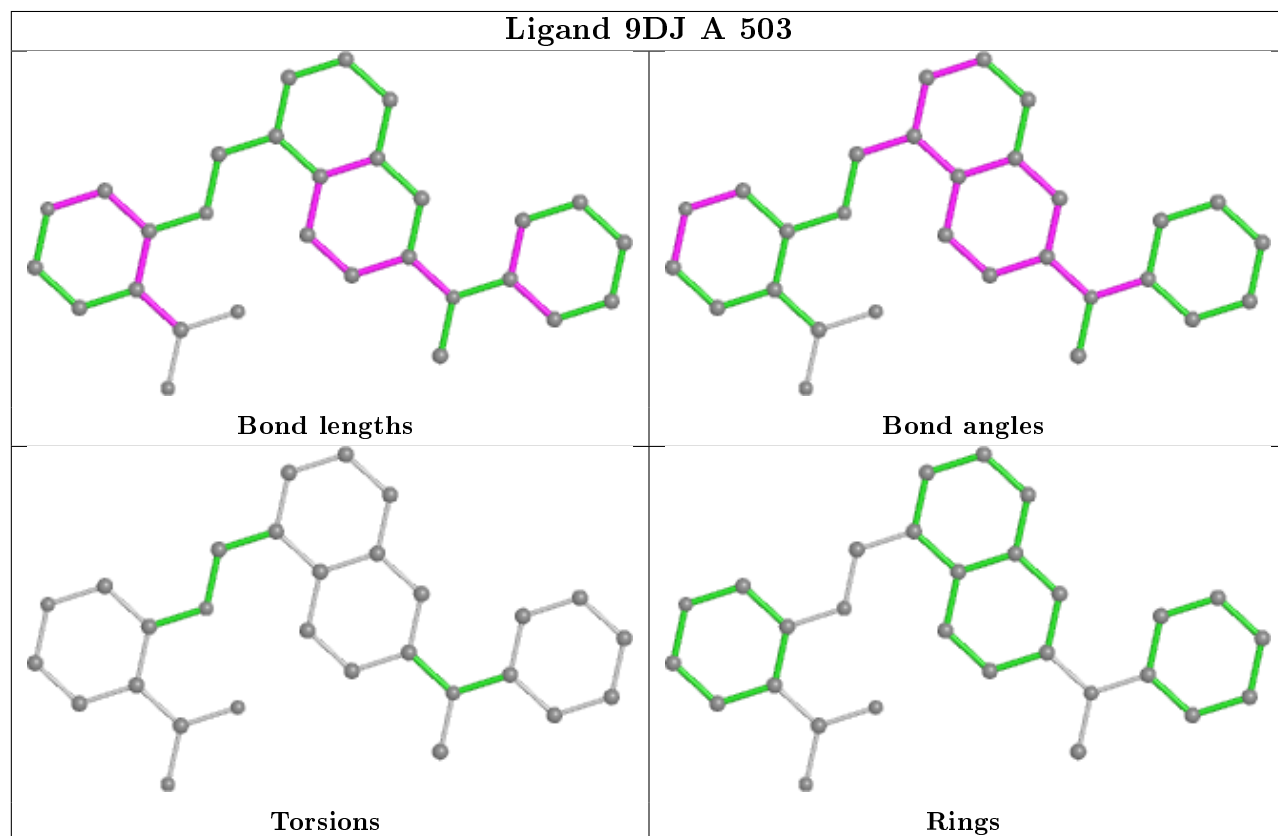
There are no ring outliers.

1 monomer is involved in 1 short contact:

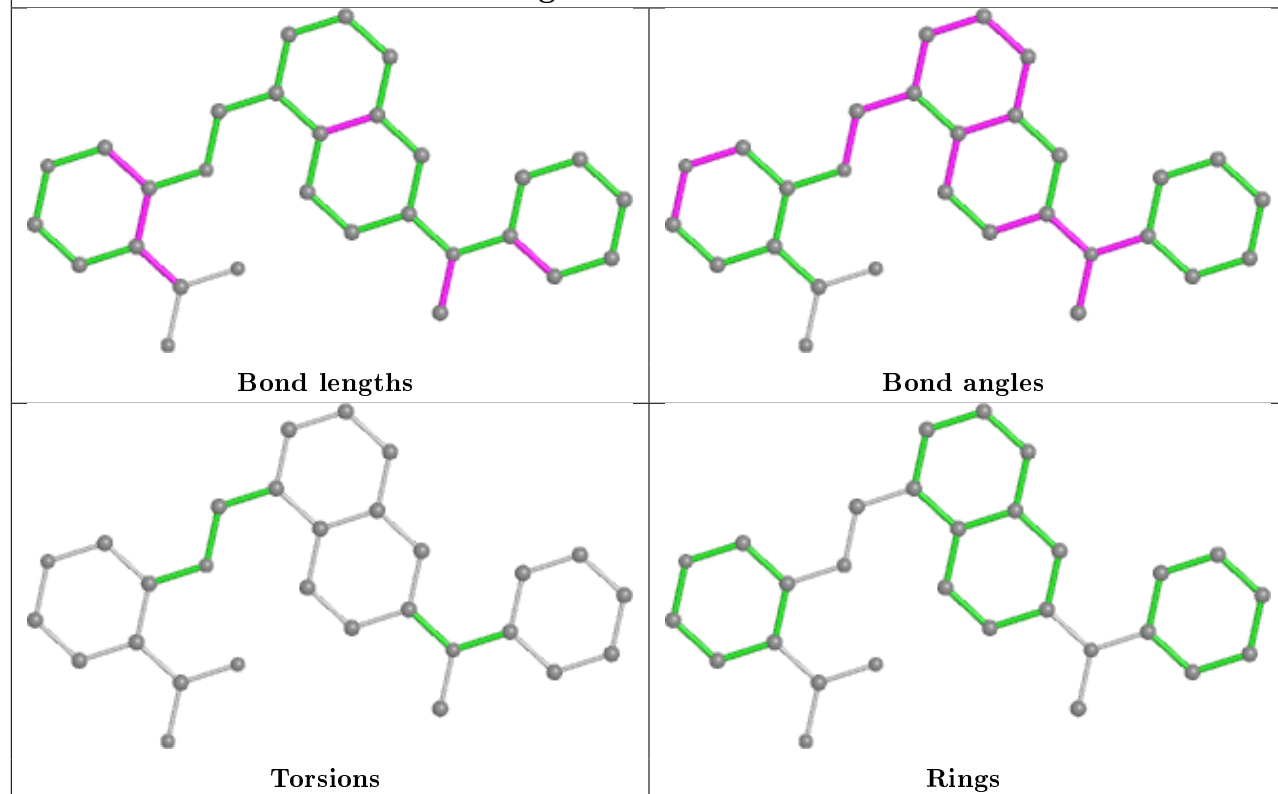
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	9DJ	1	0

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.

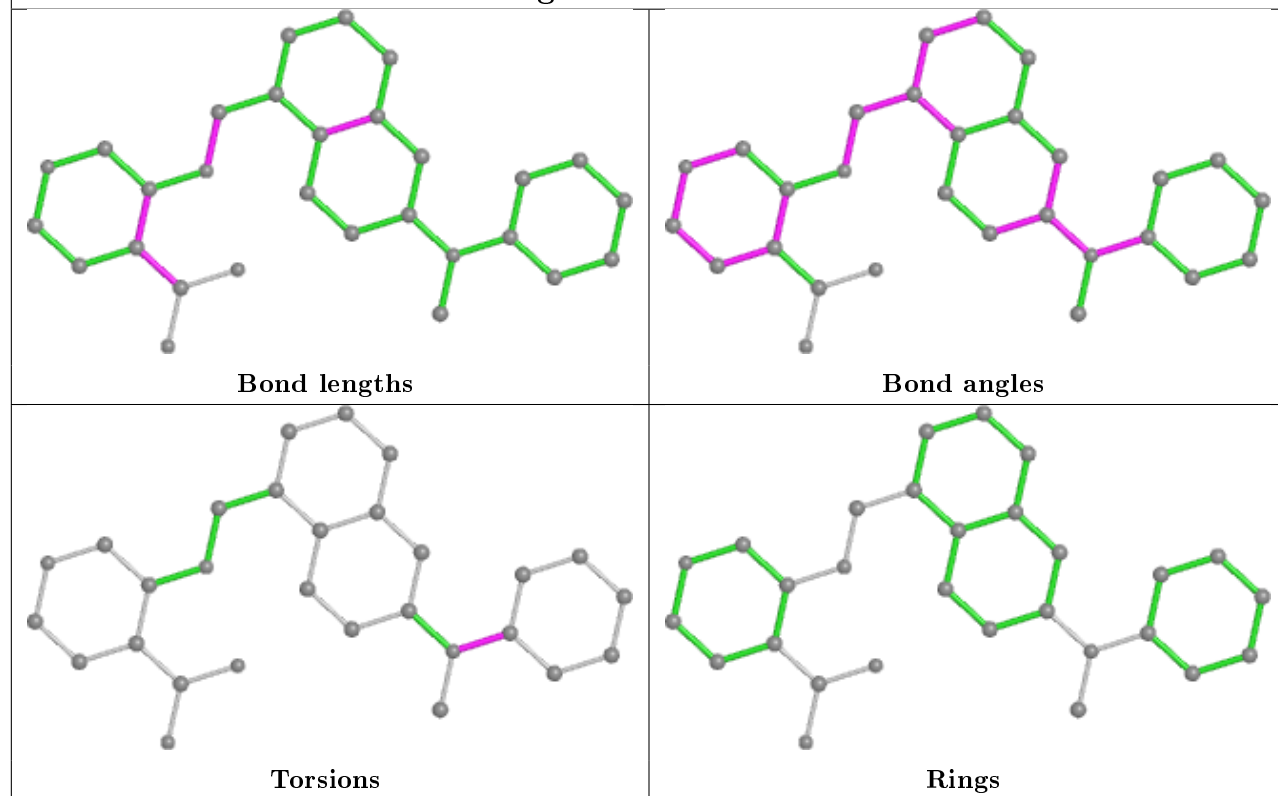
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

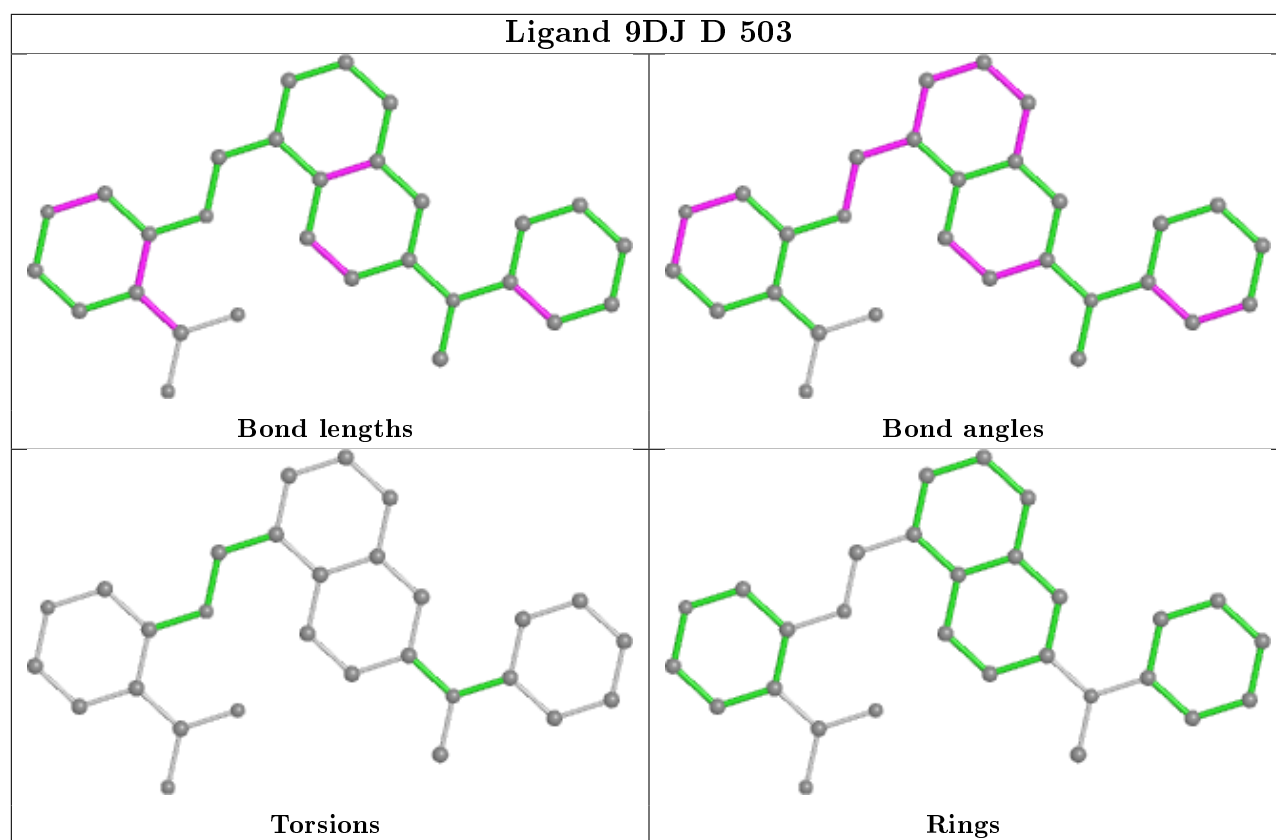


Ligand 9DJ B 503



Ligand 9DJ C 503





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	345/370 (93%)	0.11	7 (2%) 65 67	22, 35, 62, 77	1 (0%)
1	B	345/370 (93%)	0.03	9 (2%) 56 59	20, 35, 68, 92	1 (0%)
1	C	337/370 (91%)	-0.06	5 (1%) 73 75	20, 29, 52, 76	2 (0%)
1	D	345/370 (93%)	0.04	9 (2%) 56 59	20, 35, 70, 85	1 (0%)
All	All	1372/1480 (92%)	0.03	30 (2%) 62 64	20, 33, 64, 92	5 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	PHE	3.8
1	D	351	ALA	3.4
1	C	353	PHE	3.2
1	A	334	ALA	3.2
1	D	334	ALA	3.1
1	D	353	PHE	3.1
1	B	351	ALA	3.0
1	D	166	ILE	2.9
1	B	331	LEU	2.9
1	D	335	GLY	2.9
1	B	350	ALA	2.8
1	C	170	GLY	2.8
1	B	162	LYS	2.7
1	C	351	ALA	2.6
1	A	331	LEU	2.6
1	C	114	PHE	2.6
1	D	338	ASN	2.6
1	B	310	LYS	2.5
1	A	329	TYR	2.5
1	A	339	THR	2.4
1	B	326	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	330	LYS	2.4
1	B	114	PHE	2.3
1	A	351	ALA	2.2
1	A	144	HIS	2.2
1	D	154	ARG	2.2
1	A	22	GLU	2.2
1	D	326	PRO	2.2
1	C	312	MET	2.1
1	B	328	ARG	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 carbohydrates 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.

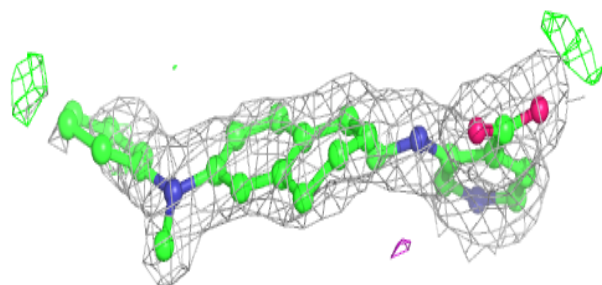
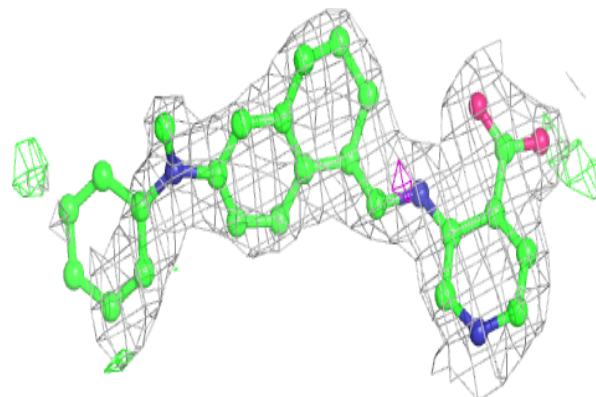
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	9DJ	A	503	29/29	0.93	0.14	30,42,78,82	0
4	9DJ	D	503	29/29	0.93	0.15	29,42,71,74	0
4	9DJ	B	503	29/29	0.93	0.14	32,40,65,72	0
4	9DJ	C	503	29/29	0.95	0.13	28,43,70,72	0
3	ZN	D	502	1/1	0.99	0.09	42,42,42,42	0
3	ZN	B	502	1/1	0.99	0.12	42,42,42,42	0
3	ZN	A	502	1/1	0.99	0.13	38,38,38,38	0
2	NI	C	501	1/1	1.00	0.11	26,26,26,26	0
3	ZN	C	502	1/1	1.00	0.14	29,29,29,29	0
2	NI	A	501	1/1	1.00	0.10	28,28,28,28	0
2	NI	B	501	1/1	1.00	0.11	35,35,35,35	0
2	NI	D	501	1/1	1.00	0.10	30,30,30,30	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.

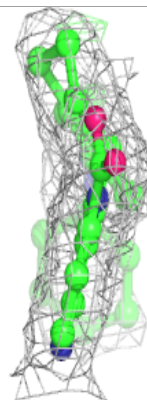
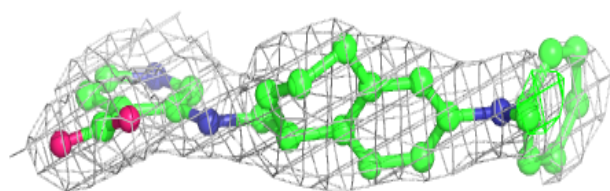
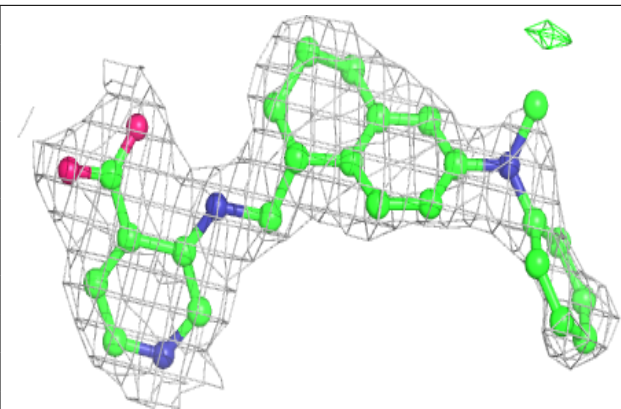
Electron density around 9DJ A 503:

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

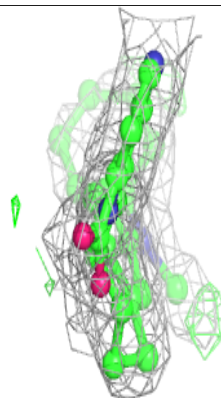
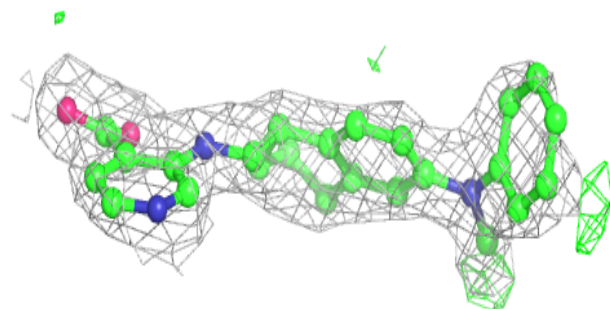
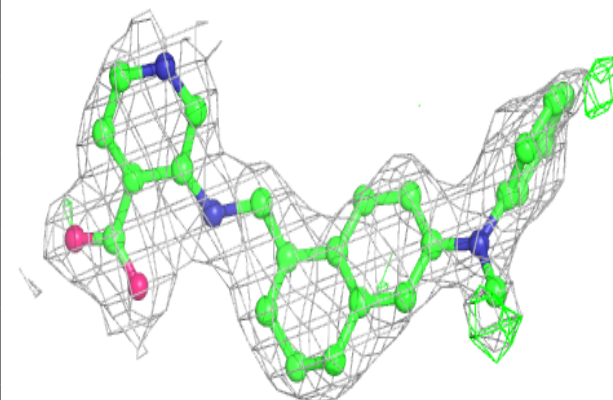


Electron density around 9DJ D 503:

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

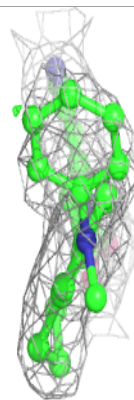
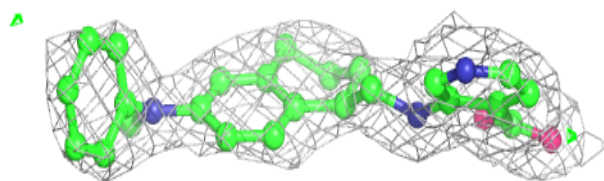
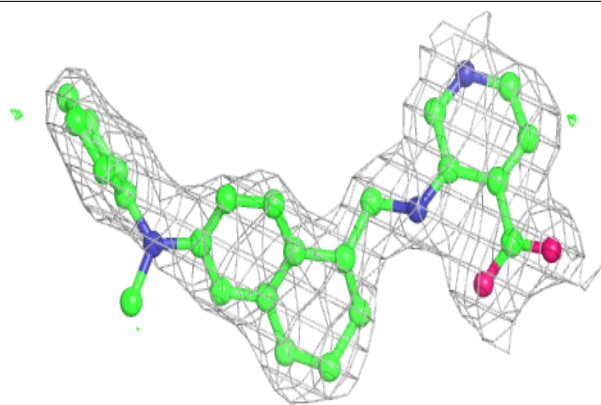
**Electron density around 9DJ B 503:**

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



Electron density around 9DJ C 503:

$2mF_o-DF_c$ (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.