



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:50 AM UTC

PDB ID : 7NF1 / pdb_00007nf1
Title : Structure of T. atroviride variant TaFdcV in complex with prFMN-butynoic acid adduct
Authors : Saaret, A.; Leys, D.
Deposited on : 2021-02-05
Resolution : 1.77 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

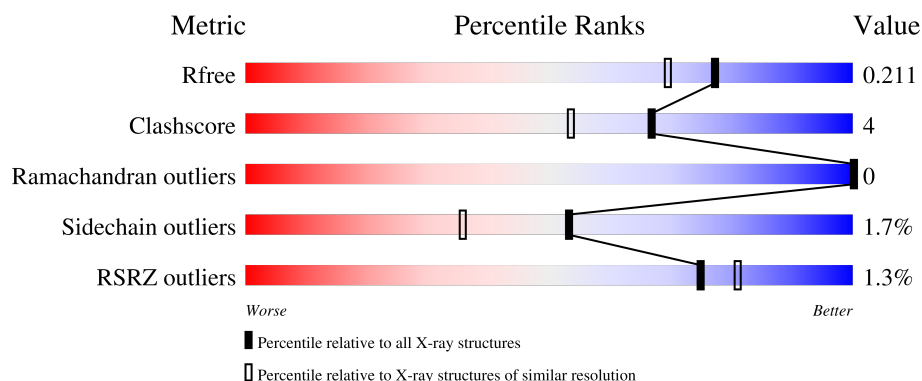
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	519	
1	B	519	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8322 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 Ferulic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3820	2431	654	715	20			
1	B	497	Total	C	N	O	S	0	1	0
			3830	2436	658	716	20			

There are 36 discrepancies between the modelled and reference sequences:

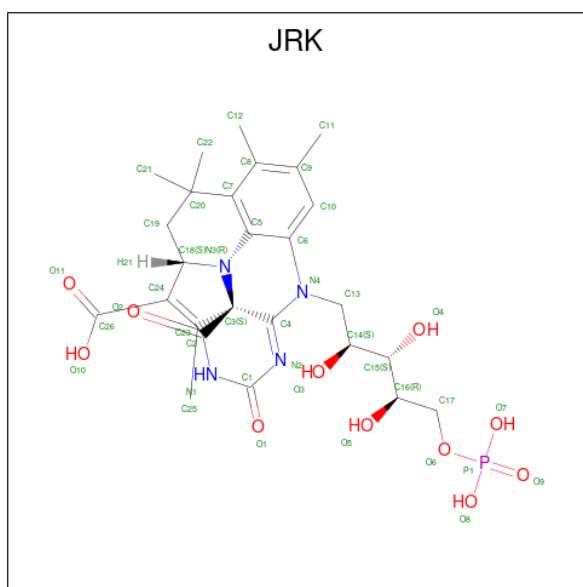
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP G9NLP8
A	-5	HIS	-	expression tag	UNP G9NLP8
A	-4	HIS	-	expression tag	UNP G9NLP8
A	-3	HIS	-	expression tag	UNP G9NLP8
A	-2	HIS	-	expression tag	UNP G9NLP8
A	-1	HIS	-	expression tag	UNP G9NLP8
A	0	HIS	-	expression tag	UNP G9NLP8
A	25	ASN	GLU	engineered mutation	UNP G9NLP8
A	31	GLY	ASN	engineered mutation	UNP G9NLP8
A	305	ALA	GLY	engineered mutation	UNP G9NLP8
A	351	ARG	ASP	engineered mutation	UNP G9NLP8
A	377	HIS	LYS	engineered mutation	UNP G9NLP8
A	402	VAL	PRO	engineered mutation	UNP G9NLP8
A	404	TYR	PHE	engineered mutation	UNP G9NLP8
A	405	MET	THR	engineered mutation	UNP G9NLP8
A	429	ALA	THR	engineered mutation	UNP G9NLP8
A	445	PRO	VAL	engineered mutation	UNP G9NLP8
A	448	TRP	GLN	engineered mutation	UNP G9NLP8
B	-6	MET	-	initiating methionine	UNP G9NLP8
B	-5	HIS	-	expression tag	UNP G9NLP8
B	-4	HIS	-	expression tag	UNP G9NLP8
B	-3	HIS	-	expression tag	UNP G9NLP8
B	-2	HIS	-	expression tag	UNP G9NLP8
B	-1	HIS	-	expression tag	UNP G9NLP8
B	0	HIS	-	expression tag	UNP G9NLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASN	GLU	engineered mutation	UNP G9NLP8
B	31	GLY	ASN	engineered mutation	UNP G9NLP8
B	305	ALA	GLY	engineered mutation	UNP G9NLP8
B	351	ARG	ASP	engineered mutation	UNP G9NLP8
B	377	HIS	LYS	engineered mutation	UNP G9NLP8
B	402	VAL	PRO	engineered mutation	UNP G9NLP8
B	404	TYR	PHE	engineered mutation	UNP G9NLP8
B	405	MET	THR	engineered mutation	UNP G9NLP8
B	429	ALA	THR	engineered mutation	UNP G9NLP8
B	445	PRO	VAL	engineered mutation	UNP G9NLP8
B	448	TRP	GLN	engineered mutation	UNP G9NLP8

- Molecule 2 is prFMN cofactor and butynoic acid adduct (CCD ID: JRK) (formula: $C_{26}H_{33}N_4O_{11}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			42	26	4	11	1	
2	B	1	Total	C	N	O	P	0
			42	26	4	11	1	

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	K	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	K	0	0
			4	4		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		

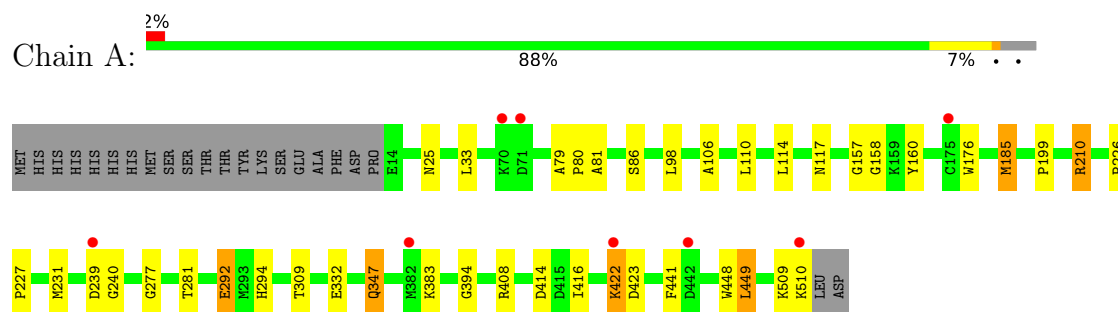
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total	O	0	0
			314	314		
5	B	265	Total	O	0	0
			265	265		

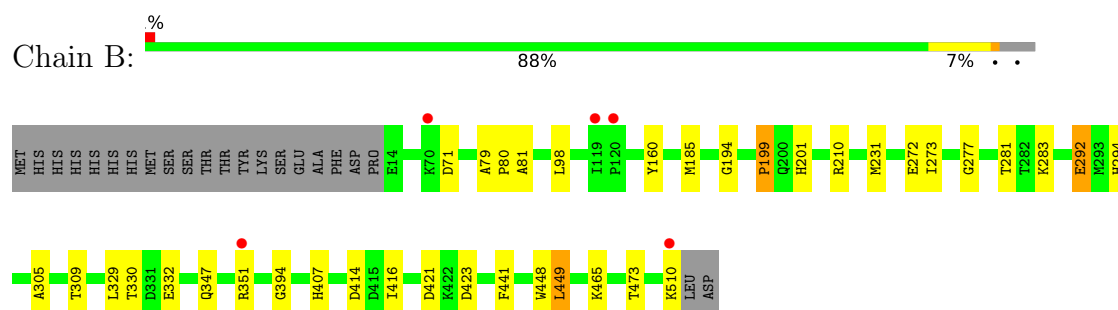
3 Residue-property plots

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: Ferulic acid decarboxylase 1



• Molecule 1: Ferulic acid decarboxylase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.65Å 74.65Å 345.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.65 – 1.77 64.65 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.65-1.77) 100.0 (64.65-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.175 , 0.206 0.184 , 0.211	Depositor DCC
R_{free} test set	5472 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8322	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, JRK, K

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	1.06	0/3915	1.23	4/5332 (0.1%)
1	B	1.07	1/3925 (0.0%)	1.27	6/5345 (0.1%)
All	All	1.06	1/7840 (0.0%)	1.25	10/10677 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	HIS	CE1-NE2	5.46	1.38	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	LYS	CA-C-O	-8.04	107.13	120.80
1	A	510	LYS	CA-C-O	-6.32	110.06	120.80
1	B	421	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	25	ASN	CA-CB-CG	-5.49	107.11	112.60
1	B	473	THR	CA-CB-OG1	-5.43	101.46	109.60
1	A	414	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	414	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	199	PRO	N-CA-CB	-5.18	96.91	102.60
1	B	71	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	210	ARG	NE-CZ-NH1	-5.03	116.47	121.50

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	3820	0	3793	28	0
1	B	3830	0	3803	26	0
2	A	42	0	0	1	0
2	B	42	0	0	1	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	314	0	0	3	0
5	B	265	0	0	2	0
All	All	8322	0	7596	56	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 (56) 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:160:TYR:CE1	1:A:185:MET:HE3	1.79	1.16
1:B:160:TYR:CE1	1:B:185:MET:HE3	1.91	1.04
1:B:160:TYR:CE1	1:B:185:MET:CE	2.52	0.91
1:B:160:TYR:CZ	1:B:185:MET:HE3	2.07	0.89
1:A:158:GLY:N	1:A:185:MET:HE1	1.88	0.87
1:A:114:LEU:HD22	1:A:347:GLN:HG3	1.62	0.80
1:A:160:TYR:HE1	1:A:185:MET:HE3	1.47	0.78
1:B:210:ARG:NH1	1:B:281:THR:O	2.24	0.70
1:A:157:GLY:C	1:A:185:MET:HE1	2.17	0.68
1:B:160:TYR:OH	1:B:185:MET:HE3	1.92	0.68
1:A:158:GLY:N	1:A:185:MET:CE	2.56	0.68
1:B:347:GLN:HG2	1:B:351[A]:ARG:NH2	2.12	0.65
1:B:160:TYR:CE1	1:B:185:MET:HE2	2.34	0.62
1:A:158:GLY:CA	1:A:185:MET:HE2	2.29	0.62
1:B:160:TYR:HE1	1:B:185:MET:CE	2.09	0.60
1:A:292:GLU:OE2	1:A:294:HIS:HD2	1.83	0.60
2:B:601:JRK:C12	2:B:601:JRK:C22	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:HB2	5:A:845:HOH:O	2.03	0.57
1:B:292:GLU:OE2	1:B:294:HIS:HD2	1.87	0.57
2:A:601:JRK:C12	2:A:601:JRK:C22	2.83	0.56
1:A:210:ARG:NH1	1:A:281:THR:O	2.36	0.56
1:B:160:TYR:HE1	1:B:185:MET:HE3	1.59	0.55
1:B:292:GLU:OE2	1:B:294:HIS:CD2	2.61	0.53
1:A:98:LEU:HD11	1:A:231:MET:HE2	1.89	0.53
1:A:294:HIS:HE1	5:A:823:HOH:O	1.92	0.52
1:A:158:GLY:CA	1:A:185:MET:CE	2.89	0.50
1:B:351[A]:ARG:NH1	5:B:705:HOH:O	2.44	0.50
1:B:277:GLY:HA3	1:B:309:THR:O	2.12	0.50
1:A:158:GLY:HA3	1:A:185:MET:HE2	1.94	0.49
1:A:106:ALA:O	1:A:110:LEU:HD13	2.12	0.49
1:B:98:LEU:HD11	1:B:231:MET:HE2	1.95	0.49
1:A:292:GLU:OE2	1:A:294:HIS:CD2	2.65	0.48
1:A:422:LYS:H	1:A:422:LYS:HE3	1.78	0.48
1:A:416:ILE:HG23	1:A:423:ASP:HB3	1.96	0.47
1:B:416:ILE:HG23	1:B:423:ASP:HB3	1.97	0.47
1:B:394:GLY:HA3	1:B:441:PHE:CZ	2.50	0.46
1:A:176:TRP:CD2	1:A:240:GLY:HA2	2.50	0.46
1:B:448:TRP:CZ3	1:B:449:LEU:HD13	2.50	0.46
1:A:81:ALA:HB3	1:A:332:GLU:HG3	1.97	0.46
1:B:294:HIS:HE1	5:B:800:HOH:O	1.98	0.46
1:A:277:GLY:HA3	1:A:309:THR:O	2.15	0.45
1:A:210:ARG:HH11	1:A:210:ARG:HG3	1.82	0.44
1:B:347:GLN:HG2	1:B:351[A]:ARG:HH21	1.83	0.44
1:A:448:TRP:CZ3	1:A:449:LEU:HD13	2.52	0.44
1:A:79:ALA:N	1:A:80:PRO:CD	2.81	0.44
1:A:394:GLY:HA3	1:A:441:PHE:CZ	2.52	0.43
1:B:449:LEU:HD12	1:B:449:LEU:HA	1.89	0.43
1:B:79:ALA:N	1:B:80:PRO:CD	2.81	0.43
1:B:329:LEU:HA	1:B:330:THR:HA	1.76	0.43
1:B:407:HIS:CD2	1:B:465:LYS:HE2	2.54	0.42
1:A:408:ARG:NH2	5:A:713:HOH:O	2.52	0.42
1:B:272:GLU:C	1:B:273:ILE:HG13	2.44	0.42
1:B:194:GLY:O	1:B:305:ALA:HB1	2.20	0.41
1:A:117:ASN:HD21	1:A:347:GLN:CD	2.29	0.41
1:B:81:ALA:HB3	1:B:332:GLU:HG3	2.02	0.41
1:A:226:PRO:HA	1:A:227:PRO:HD3	1.96	0.41

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	495/519 (95%)	484 (98%)	11 (2%)	0	100	100
1	B	496/519 (96%)	487 (98%)	9 (2%)	0	100	100
All	All	991/1038 (96%)	971 (98%)	20 (2%)	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	408/430 (95%)	398 (98%)	10 (2%)	42	22
1	B	409/430 (95%)	405 (99%)	4 (1%)	68	55
All	All	817/860 (95%)	803 (98%)	14 (2%)	53	36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	86	SER
1	A	185	MET
1	A	199	PRO
1	A	292	GLU
1	A	347	GLN
1	A	383	LYS
1	A	422	LYS

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Mol	Chain	Res	Type
1	A	449	LEU
1	A	509	LYS
1	B	199	PRO
1	B	283	LYS
1	B	292	GLU
1	B	449	LEU

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

Mol	Chain	Res	Type
1	A	117	ASN
1	A	154	GLN
1	A	208	GLN
1	A	294	HIS
1	A	347	GLN
1	A	455	HIS
1	A	457	ASN
1	A	489	ASN
1	B	25	ASN
1	B	29	GLN
1	B	154	GLN
1	B	294	HIS
1	B	303	HIS
1	B	377	HIS
1	B	457	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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
2	JRK	A	601	3,4	43,46,46	1.06	4 (9%)	53,76,76	1.50	5 (9%)
2	JRK	B	601	3,4	43,46,46	1.20	5 (11%)	53,76,76	1.53	8 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JRK	A	601	3,4	-	4/22/89/89	0/4/5/5
2	JRK	B	601	3,4	-	5/22/89/89	0/4/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	JRK	C26-C24	-4.19	1.40	1.48
2	A	601	JRK	C26-C24	-3.15	1.42	1.48
2	A	601	JRK	C3-N3	-2.99	1.43	1.47
2	B	601	JRK	C5-C6	2.36	1.44	1.40
2	A	601	JRK	P1-O7	-2.17	1.46	1.54
2	A	601	JRK	C2-N1	-2.15	1.33	1.37
2	B	601	JRK	C1-N2	-2.09	1.31	1.36
2	B	601	JRK	C2-N1	-2.02	1.34	1.37
2	B	601	JRK	C3-N3	-2.01	1.44	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	JRK	C20-C7-C5	-5.45	115.53	121.48
2	B	601	JRK	C18-C24-C23	-5.29	106.90	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	JRK	C20-C7-C5	-5.27	115.72	121.48
2	A	601	JRK	C18-C24-C23	-5.06	107.09	111.36
2	B	601	JRK	O8-P1-O6	-2.94	99.00	106.67
2	B	601	JRK	C2-N1-C1	-2.79	121.22	125.42
2	B	601	JRK	C5-N3-C18	2.70	121.08	114.95
2	B	601	JRK	C19-C20-C7	-2.46	105.62	111.13
2	A	601	JRK	C5-N3-C18	2.34	120.27	114.95
2	A	601	JRK	C1-N2-C4	-2.34	116.42	119.43
2	B	601	JRK	O8-P1-O7	2.14	115.82	107.80
2	B	601	JRK	C10-C9-C8	2.07	121.19	119.10
2	A	601	JRK	C6-C5-N3	-2.06	118.51	120.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	JRK	C18-C24-C26-O10
2	A	601	JRK	C23-C24-C26-O10
2	A	601	JRK	C23-C24-C26-O11
2	B	601	JRK	C18-C24-C26-O10
2	B	601	JRK	C23-C24-C26-O10
2	B	601	JRK	C23-C24-C26-O11
2	B	601	JRK	C18-C24-C26-O11
2	B	601	JRK	C17-O6-P1-O9
2	A	601	JRK	C18-C24-C26-O11

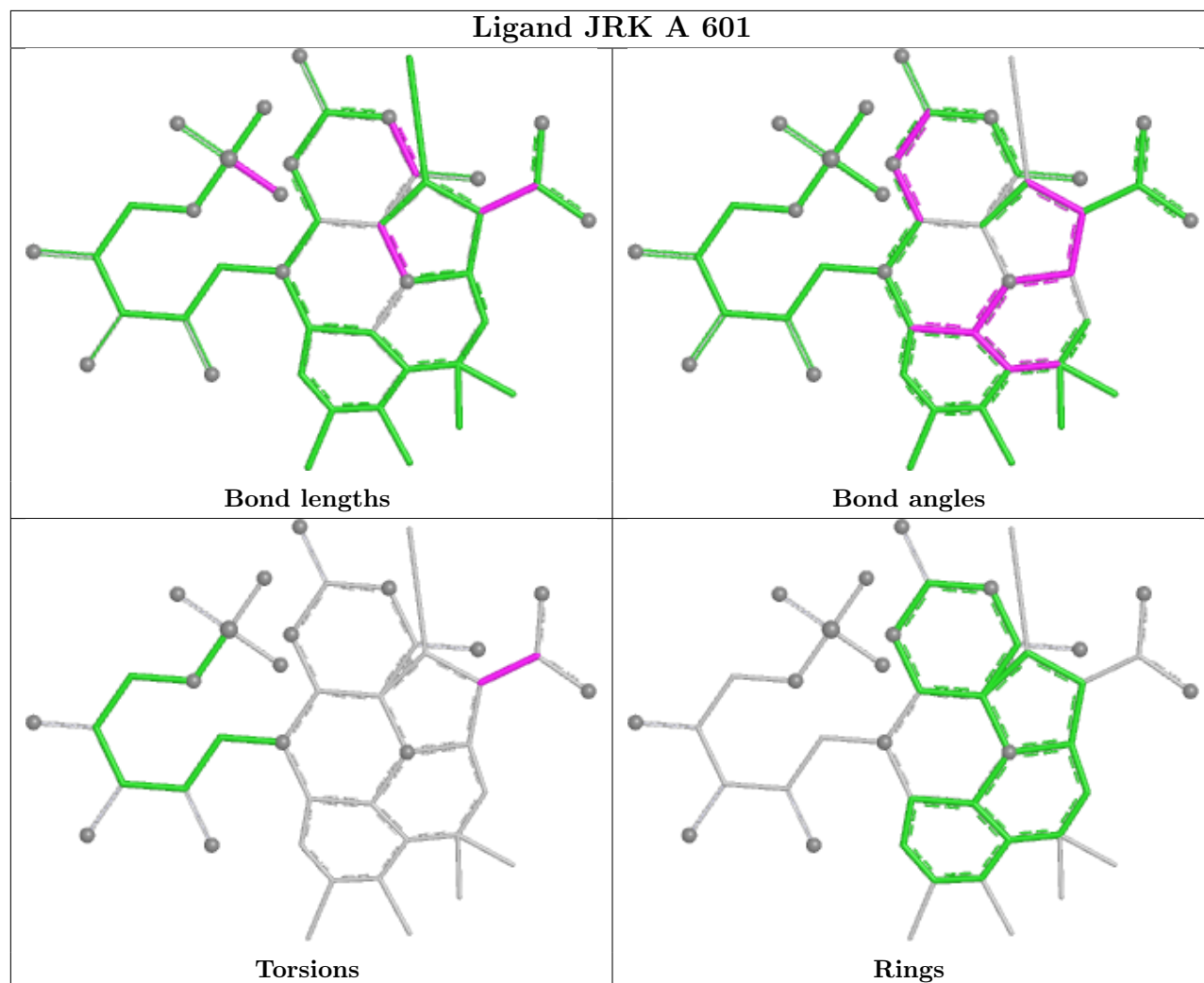
There are no ring outliers.

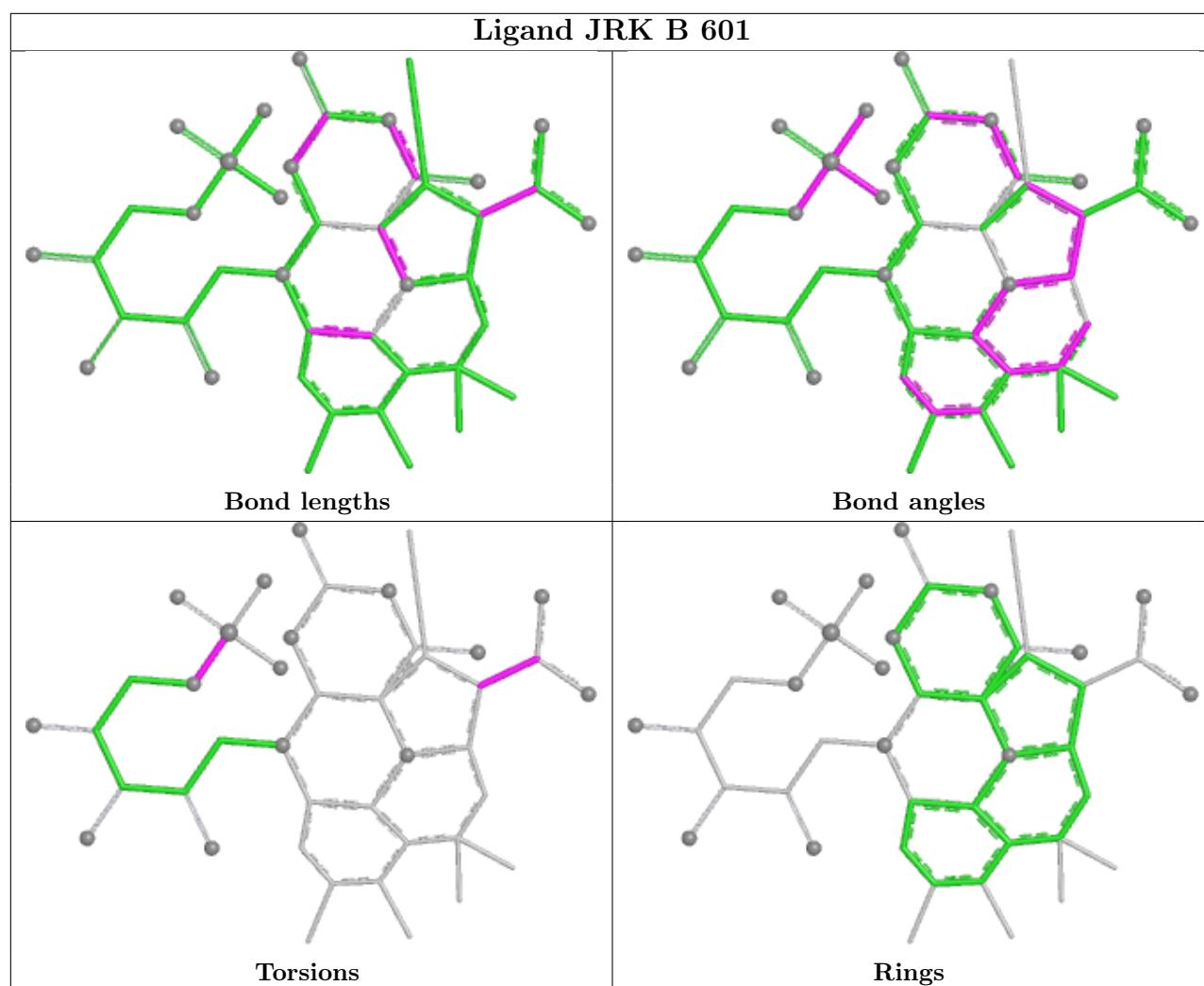
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	JRK	1	0
2	B	601	JRK	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.





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	497/519 (95%)	-0.04	8 (1%) 70 77	14, 20, 34, 49	0
1	B	497/519 (95%)	0.13	5 (1%) 79 85	11, 24, 40, 51	1 (0%)
All	All	994/1038 (95%)	0.05	13 (1%) 75 81	11, 22, 36, 51	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	LYS	3.2
1	A	382	MET	2.7
1	A	71	ASP	2.4
1	A	175	CYS	2.3
1	A	239	ASP	2.3
1	A	70	LYS	2.3
1	A	422	LYS	2.3
1	B	351[A]	ARG	2.2
1	B	510	LYS	2.2
1	A	510	LYS	2.2
1	B	120	PRO	2.1
1	B	119	ILE	2.1
1	A	442	ASP	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

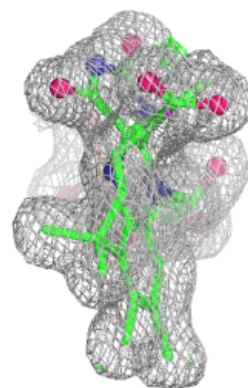
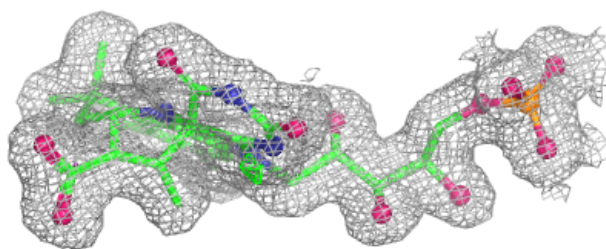
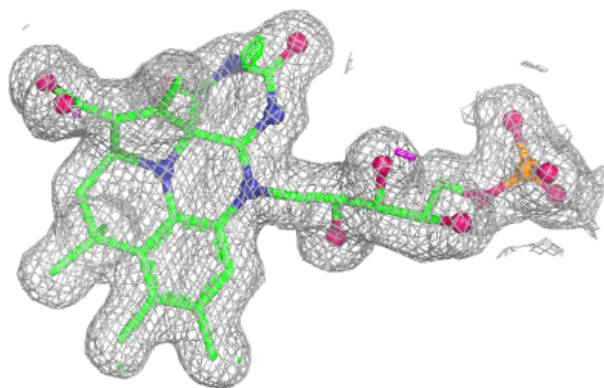
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	K	B	603	1/1	0.84	0.14	54,54,54,54	0
3	K	A	604	1/1	0.95	0.07	40,40,40,40	0
2	JRK	A	601	42/42	0.97	0.05	14,17,25,30	0
3	K	B	602	1/1	0.97	0.06	39,39,39,39	0
2	JRK	B	601	42/42	0.97	0.06	16,19,25,37	0
3	K	A	603	1/1	0.99	0.02	15,15,15,15	0
3	K	B	604	1/1	0.99	0.04	19,19,19,19	0
4	MN	B	606	1/1	0.99	0.05	24,24,24,24	0
3	K	B	605	1/1	1.00	0.02	20,20,20,20	0
4	MN	A	605	1/1	1.00	0.03	21,21,21,21	0
3	K	A	602	1/1	1.00	0.04	18,18,18,18	0

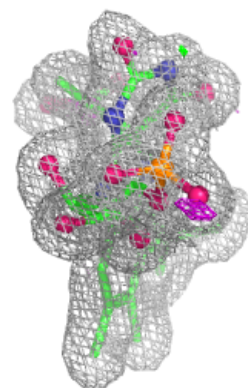
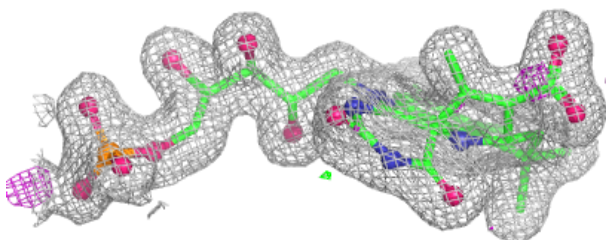
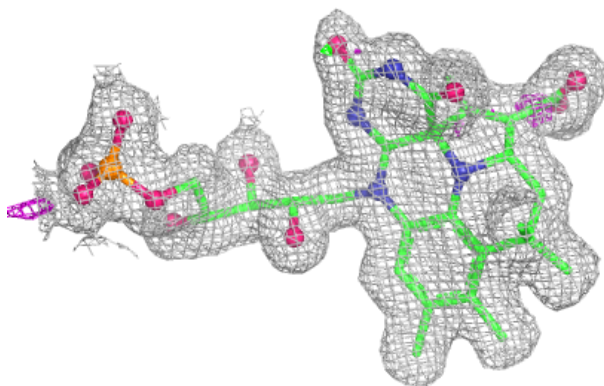
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JRK A 601:

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

**Electron density around JRK B 601:**

$2mF_o-DF_c$ (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.