



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 01:57 PM EDT

PDB ID : 5JI3 / pdb_00005ji3
Title : HslUV complex
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Deposited on : 2016-04-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

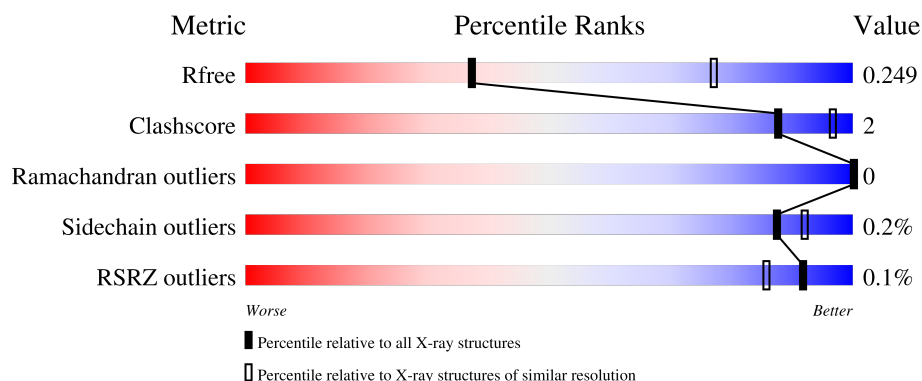
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	176	97% 97% 97% 97% 97% 97%
1	B	176	94% 94% 94% 94% 94% 94%
1	C	176	95% 95% 95% 95% 95% 95%
1	D	176	93% 93% 93% 93% 93% 93%
2	E	443	79% 79% 79% 79% 79% 79%

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Mol	Chain	Length	Quality of chain
2	F	443	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 75%, a yellow segment representing 20%, and a grey segment representing 5%. The green segment is the largest, followed by the yellow segment, and the grey segment is the smallest. The bar is labeled with '75%' and '20%' at the end of the green and yellow segments respectively.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22148 atoms, of which 11121 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.

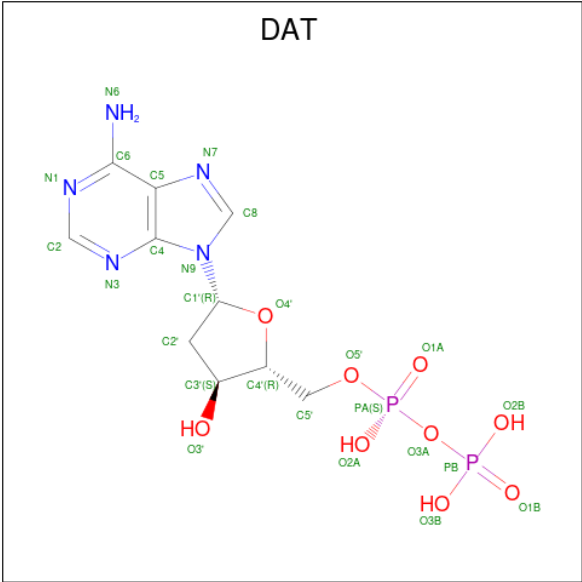
- Molecule 1 is a protein called ATP-dependent protease subunit HslV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	174	Total	C	H	N	O	S	1	0	0
			2640	828	1324	231	253	4			
1	B	174	Total	C	H	N	O	S	1	0	0
			2640	828	1324	231	253	4			
1	C	174	Total	C	H	N	O	S	1	0	0
			2640	828	1324	231	253	4			
1	D	174	Total	C	H	N	O	S	1	0	0
			2640	828	1324	231	253	4			

- Molecule 2 is a protein called ATP-dependent protease ATPase subunit HslU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	375	Total	C	H	N	O	S	0	0	0
			5932	1838	2993	521	570	10			
2	F	353	Total	C	H	N	O	S	0	0	0
			5580	1729	2808	498	536	9			

- Molecule 3 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (CCD ID: DAT) (formula: C₁₀H₁₅N₅O₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	E	1	Total	C	H	N	O	P	0	0
			38	10	12	5	9	2		
3	F	1	Total	C	H	N	O	P	0	0
			38	10	12	5	9	2		

i

- Molecule 1: ATP-dependent protease subunit HslV

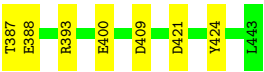
MET
T1
N30
N109
G110
K174
ALA

Diagram illustrating the structure of the T1 domain, showing residues MET, T1, A51, Q114, D118, P127, Y128, A131, E149, H166, K174, and ALA.

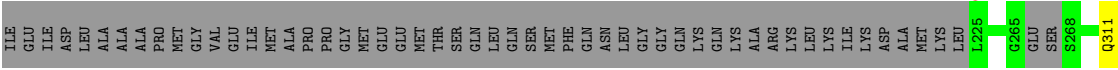
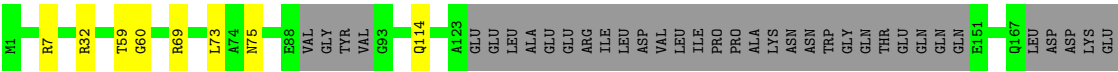
MET	T1	K28	G29	N30	R83	V113	E116	Y128	A131	K174	ALA
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Amino Acid	Relative Abundance (%)
MET	100
T1	85
M27	75
K28	70
G29	65
N30	60
E58	55
R62	50
R83	45
K90	40
L91	35
N109	30
D157	25
H164	20
K174	15
ALA	10

PRO	PRO	PRO	GLY	GLU	MET	GLU	MET	THR	SER	GLN	LEU	GLN	SER	MET	PHE	GLN	ASN	GLY	GLY	GLN	GLN	LYS	ALA	ARG	LYS	K217	K219	K283	GLY	GLY	GLU	SER	S288	L282	P283	S316	Q323	Q333	R342	T343	L344	P347	T352	Y355	E362		
MI	Q20	R36	T59	K63	T64	E58	VAL	GLY	T7R	VAL	G93	K94	E95	E128	A139	LYS	ASN	ASN	TRP	GLY	GLN	THR	GLU	GLN	GLN	E151	R164	Q167	LEU	ASP	LYS	GLU	I1E	GLU	I1E	ASP	LEU	ALA	ALA	PRO	MET	GLY	VAL	GLU	I1E	MET	ALA



● Molecule 2: ATP-dependent protease ATPase subunit HslU



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.00Å 170.00Å 161.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.00 – 3.00 85.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	85.8 (85.00-3.00) 85.7 (85.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.01Å)	Xtriage
Refinement program	CNS (1.10_2155: ???), PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.222 , 0.253 0.219 , 0.249	Depositor DCC
R_{free} test set	4647 reflections (8.56%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.426 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22148	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.33% 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: DAT

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	0.13	0/1333	0.31	0/1803
1	B	0.15	0/1333	0.31	0/1803
1	C	0.14	0/1333	0.32	0/1803
1	D	0.14	0/1333	0.33	0/1803
2	E	0.12	0/2972	0.27	0/4006
2	F	0.12	0/2803	0.26	0/3774
All	All	0.13	0/11107	0.29	0/14992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1316	1324	1326	4	0
1	B	1316	1324	1326	10	0
1	C	1316	1324	1326	10	0
1	D	1316	1324	1326	9	0
2	E	2939	2993	2993	15	1
2	F	2772	2808	2823	11	1
3	E	26	12	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	26	12	12	1	0
All	All	11027	11121	11144	44	1

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 2.

The worst 5 of 44 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)
2:E:59:THR:OG1	2:E:393:ARG:NH2	2.23	0.71
2:E:344:LEU:O	2:E:352:THR:OG1	2.03	0.71
1:C:116:GLU:OE1	1:D:30:ASN:ND2	2.24	0.70
1:D:28:LYS:NZ	1:D:30:ASN:OD1	2.25	0.64
1:D:83:ARG:NH2	1:D:109:ASN:O	2.31	0.63

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:ARG:HH22	2:F:407:SER:O[3_565]	1.59	0.01

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	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
1	B	172/176 (98%)	171 (99%)	1 (1%)	0	100	100
1	C	172/176 (98%)	171 (99%)	1 (1%)	0	100	100
1	D	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	E	365/443 (82%)	361 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	343/443 (77%)	336 (98%)	7 (2%)	0	100	100
All	All	1396/1590 (88%)	1379 (99%)	17 (1%)	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	134/137 (98%)	134 (100%)	0	100	100
1	B	134/137 (98%)	134 (100%)	0	100	100
1	C	134/137 (98%)	134 (100%)	0	100	100
1	D	134/137 (98%)	134 (100%)	0	100	100
2	E	318/377 (84%)	317 (100%)	1 (0%)	86	91
2	F	300/377 (80%)	299 (100%)	1 (0%)	86	91
All	All	1154/1302 (89%)	1152 (100%)	2 (0%)	87	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	355	TYR
2	F	355	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	166	HIS
2	E	235	ASN
2	F	114	GLN
2	F	75	ASN
1	D	139	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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	DAT	F	501	-	27,28,28	1.39	4 (14%)	41,43,43	1.96	10 (24%)
3	DAT	E	501	-	27,28,28	1.39	4 (14%)	41,43,43	1.90	9 (21%)

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	DAT	F	501	-	-	3/16/28/28	0/3/3/3
3	DAT	E	501	-	-	7/16/28/28	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	DAT	C5-C4	4.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	DAT	C5-C4	4.48	1.47	1.39
3	F	501	DAT	C5-C6	2.63	1.48	1.41
3	E	501	DAT	C5-C6	2.60	1.48	1.41
3	E	501	DAT	C5-N7	-2.35	1.34	1.39

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	DAT	C5-C4-N3	-5.86	118.65	126.72
3	E	501	DAT	C5-C4-N3	-5.78	118.76	126.72
3	F	501	DAT	N3-C4-N9	4.90	135.50	127.17
3	E	501	DAT	N3-C4-N9	4.78	135.29	127.17
3	F	501	DAT	C2-N3-C4	3.91	121.39	111.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	501	DAT	C5'-O5'-PA-O1A
3	E	501	DAT	C5'-O5'-PA-O2A
3	E	501	DAT	C5'-O5'-PA-O3A
3	F	501	DAT	C5'-O5'-PA-O2A
3	F	501	DAT	C5'-O5'-PA-O3A

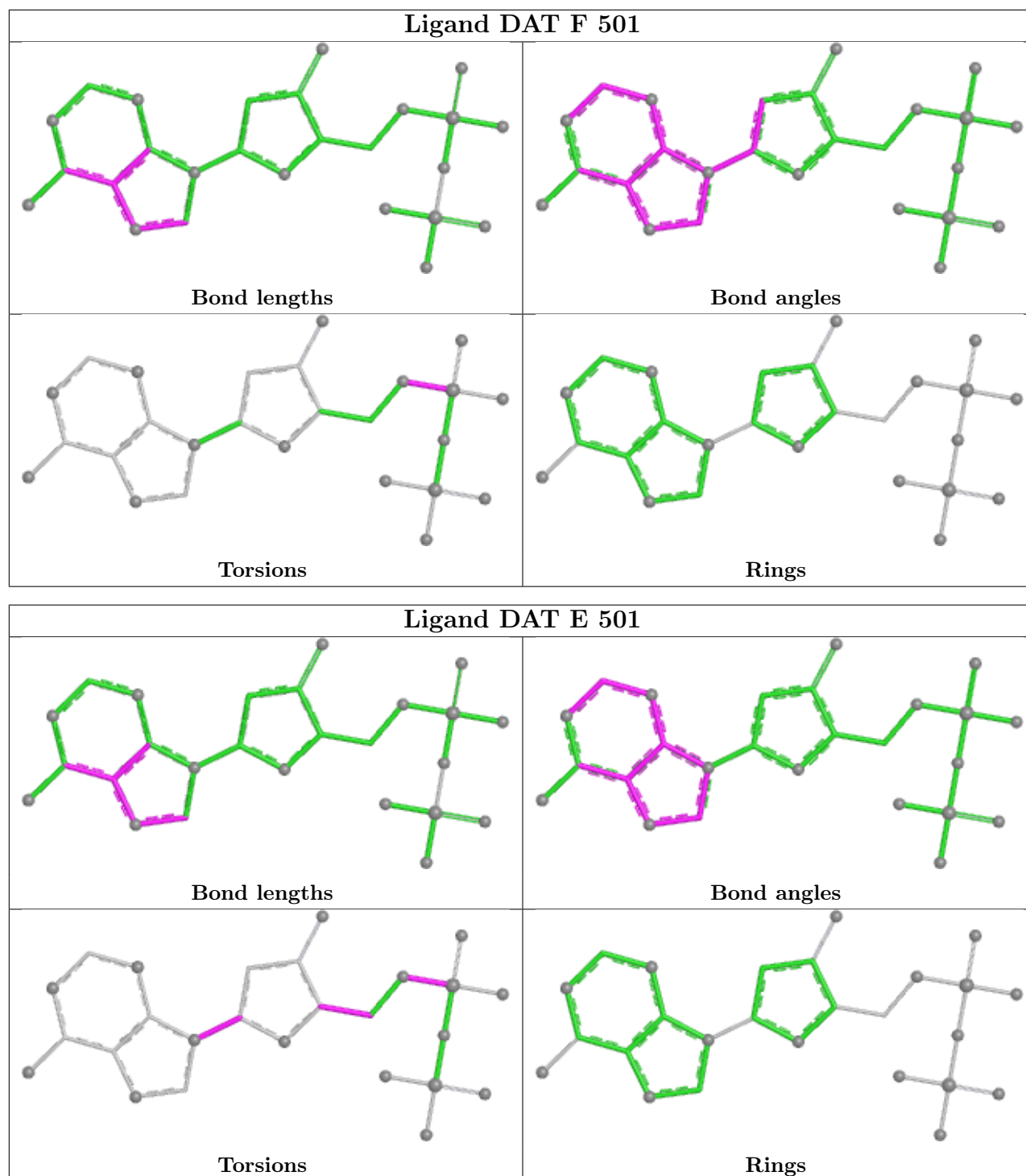
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	DAT	1	0
3	E	501	DAT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9	
1	A	174/176 (98%)	-1.30	0	100	100	50, 83, 113, 128	1 (0%)
1	B	174/176 (98%)	-1.41	0	100	100	53, 69, 89, 106	1 (0%)
1	C	174/176 (98%)	-1.30	0	100	100	52, 80, 103, 113	1 (0%)
1	D	174/176 (98%)	-1.27	0	100	100	54, 82, 110, 117	1 (0%)
2	E	375/443 (84%)	-1.31	1 (0%)	90	79	51, 72, 109, 127	0
2	F	353/443 (79%)	-1.20	1 (0%)	90	79	43, 78, 116, 132	0
All	All	1424/1590 (89%)	-1.29	2 (0%)	92	86	43, 77, 109, 132	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	225	LEU	6.1
2	E	221	ALA	2.3

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](#)

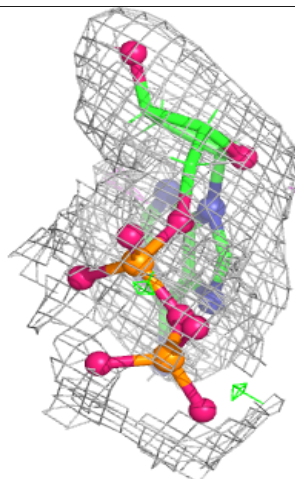
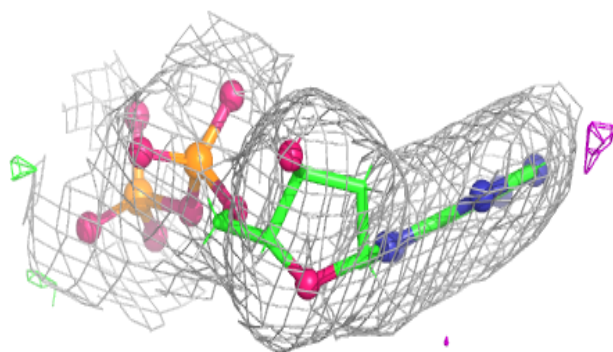
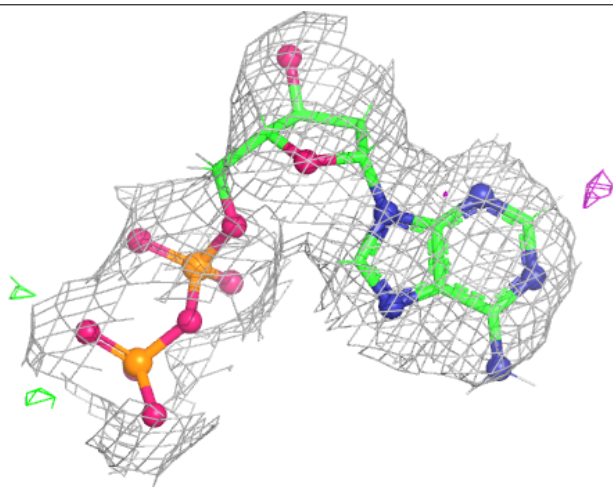
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	DAT	E	501	26/26	1.00	0.03	50,68,87,87	0
3	DAT	F	501	26/26	1.00	0.04	44,66,91,93	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.

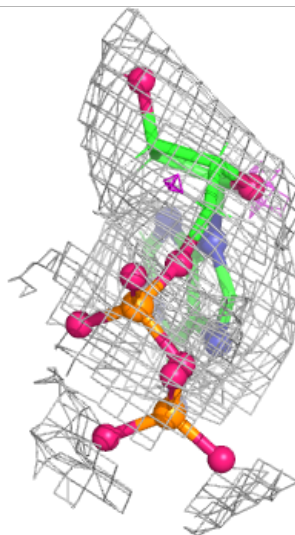
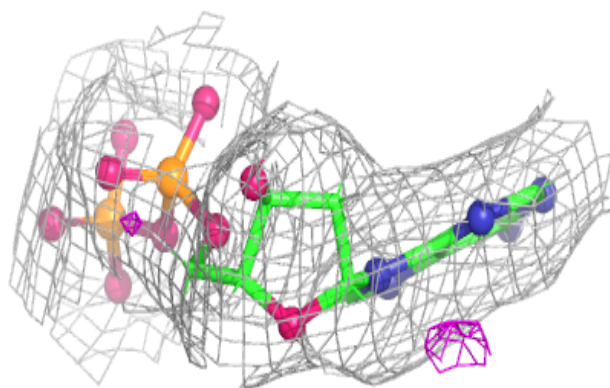
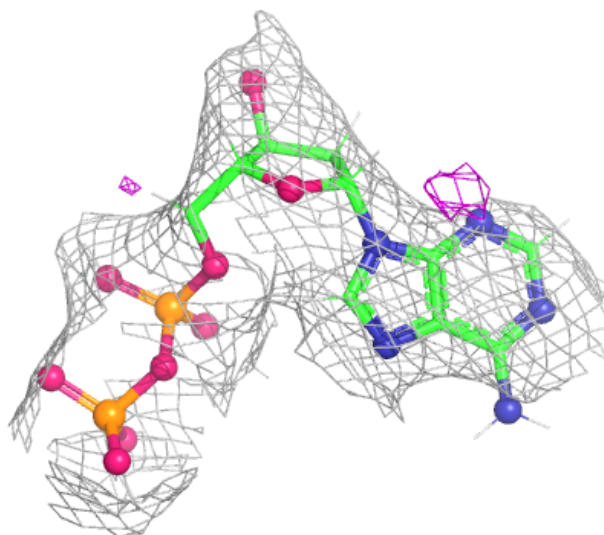
Electron density around DAT E 501:

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 DAT F 501:

$2mF_o-DF_c$ (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.