



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2021 – 02:26 PM JST

PDB ID : 7DSY
Title : Crystal Structure of RNase L in complex with KM05073
Authors : Tang, J.; Huang, H.
Deposited on : 2021-01-03
Resolution : 2.65 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 : 2.23.2
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) : 2.23.2

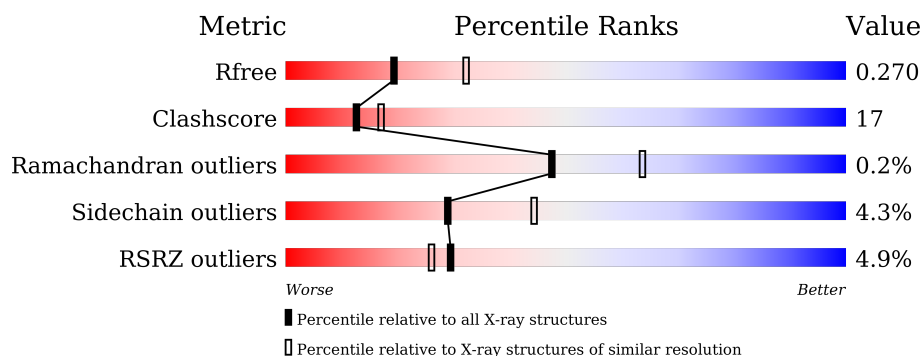
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	717	<div> <div>4%</div> <div>90%</div> <div>6%</div> </div>
1	b	717	<div> <div>5%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10986 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.

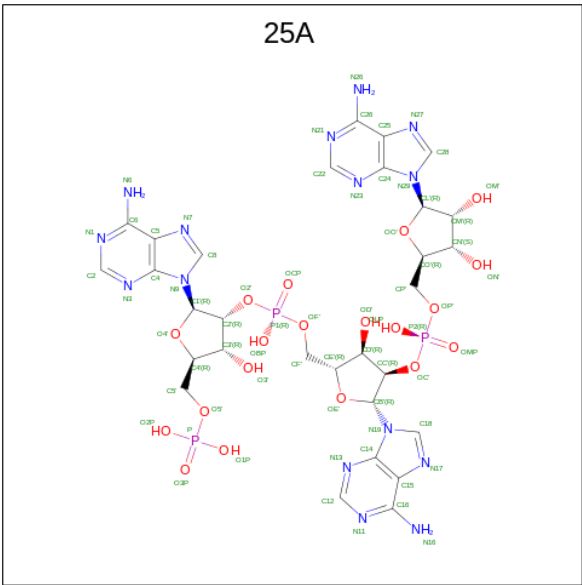
- Molecule 1 is a protein called Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	672	Total	C	N	O	S	0	0	0
			5339	3353	942	1022	22			
1	b	676	Total	C	N	O	S	0	0	0
			5361	3365	947	1027	22			

There are 10 discrepancies between the modelled and reference sequences:

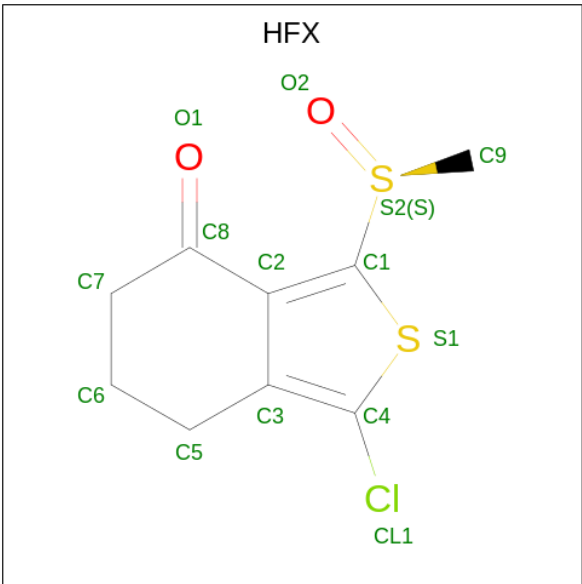
Chain	Residue	Modelled	Actual	Comment	Reference
a	16	GLY	-	expression tag	UNP A5H025
a	17	ALA	-	expression tag	UNP A5H025
a	18	MET	-	expression tag	UNP A5H025
a	19	ASP	-	expression tag	UNP A5H025
a	20	PRO	-	expression tag	UNP A5H025
b	16	GLY	-	expression tag	UNP A5H025
b	17	ALA	-	expression tag	UNP A5H025
b	18	MET	-	expression tag	UNP A5H025
b	19	ASP	-	expression tag	UNP A5H025
b	20	PRO	-	expression tag	UNP A5H025

- Molecule 2 is 5'-O-MONOPHOSPHORYLADENYLYL(2'->5')ADENYLYL(2'->5')ADENOSINE (three-letter code: 25A) (formula: C₃₀H₃₈N₁₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	a	1	Total	C	N	O	P	0	0
			67	30	15	19	3		
2	b	1	Total	C	N	O	P	0	0
			67	30	15	19	3		

- Molecule 3 is 1-chloranyl-3-methylsulfinyl-6,7-dihydro-5H-2-benzothiophen-4-one (three-letter code: HFX) (formula: C₉H₉ClO₂S₂) (labeled as "Ligand of Interest" by depositor).



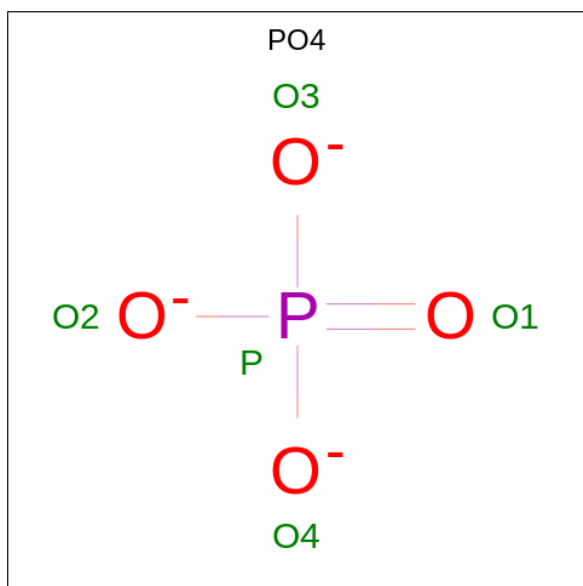
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	a	1	Total	C	Cl	O	S	0	0
			14	9	1	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	b	1	Total	C	Cl	O	S	0	0
			14	9	1	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	O	P	0	0
			5	4	1		

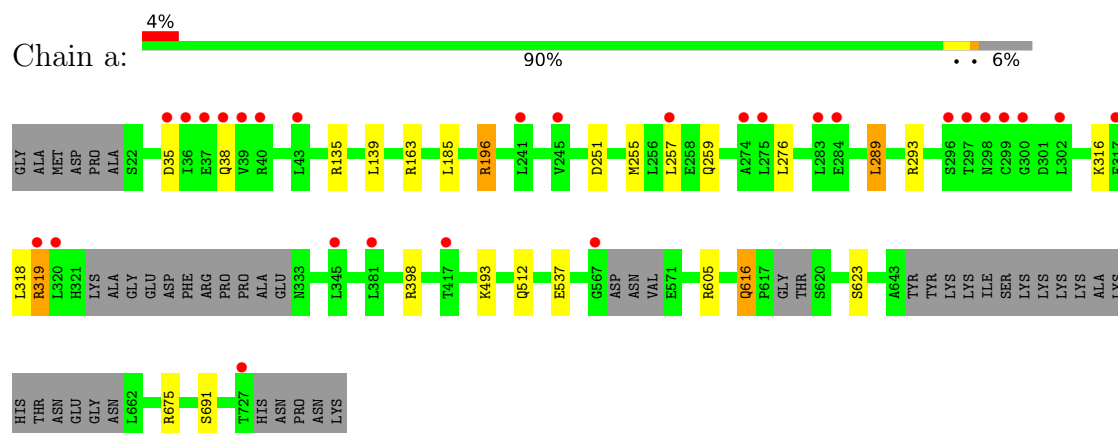
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	a	50	Total	O	0	0
			50	50		
5	b	69	Total	O	0	0
			69	69		

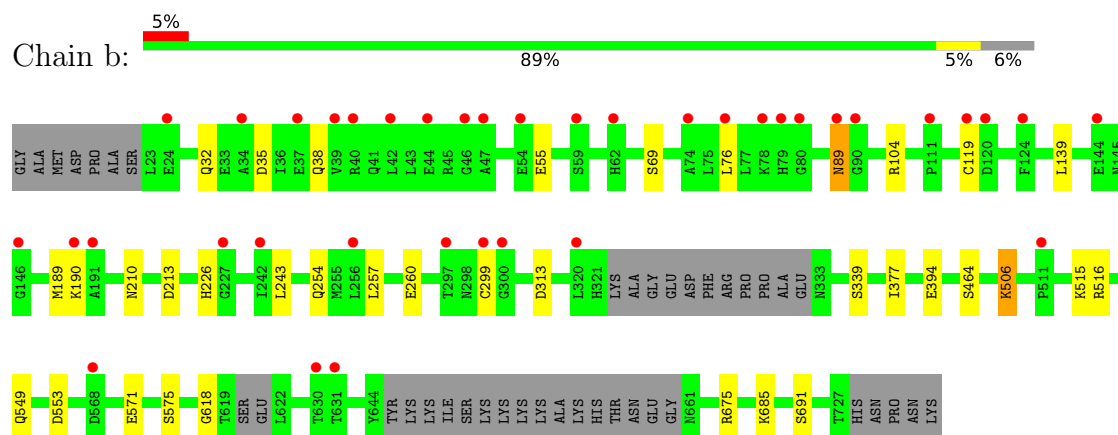
3 Residue-property plots [i](#)

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: Ribonuclease L



• Molecule 1: Ribonuclease L



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.32Å 111.05Å 262.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 2.65 31.50 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.50-2.65) 99.7 (31.50-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.199 , 0.270 0.199 , 0.270	Depositor DCC
R_{free} test set	2568 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10986	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: PO4, HFX, 25A

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	0.48	1/5431 (0.0%)	0.78	15/7330 (0.2%)
1	b	0.46	0/5455	0.72	5/7365 (0.1%)
All	All	0.47	1/10886 (0.0%)	0.75	20/14695 (0.1%)

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	a	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	537	GLU	CB-CG	-5.80	1.41	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	257	LEU	CB-CG-CD1	-12.47	89.81	111.00
1	a	537	GLU	N-CA-CB	-10.30	92.06	110.60
1	a	276	LEU	CB-CG-CD2	-9.58	94.72	111.00
1	a	289	LEU	CB-CG-CD2	-7.99	97.42	111.00
1	a	289	LEU	CA-CB-CG	7.99	133.67	115.30
1	a	276	LEU	CB-CG-CD1	7.78	124.22	111.00
1	a	139	LEU	CA-CB-CG	7.72	133.06	115.30
1	a	537	GLU	CA-CB-CG	7.67	130.26	113.40
1	b	506	LYS	CB-CG-CD	-6.44	94.85	111.60
1	a	257	LEU	CA-CB-CG	6.33	129.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	616	GLN	CA-CB-CG	6.29	127.23	113.40
1	b	76	LEU	CA-CB-CG	-5.92	101.69	115.30
1	a	38	GLN	CA-CB-CG	5.87	126.31	113.40
1	a	537	GLU	CB-CG-CD	-5.82	98.47	114.20
1	b	377	ILE	CG1-CB-CG2	-5.77	98.71	111.40
1	a	512	GLN	CB-CA-C	-5.68	99.05	110.40
1	b	139	LEU	CA-CB-CG	5.47	127.89	115.30
1	b	89	ASN	N-CA-CB	-5.27	101.11	110.60
1	a	196	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	a	537	GLU	CB-CA-C	5.08	120.56	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	318	LEU	Peptide
1	a	616	GLN	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	5339	0	5258	0	0
1	b	5361	0	5261	0	0
2	a	67	0	29	0	0
2	b	67	0	29	0	0
3	a	14	0	0	0	0
3	b	14	0	0	0	0
4	a	5	0	0	0	0
5	a	50	0	0	0	0
5	b	69	0	0	0	0
All	All	10986	0	10577	0	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 17.

There are no clashes within the asymmetric unit.

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	662/717 (92%)	638 (96%)	23 (4%)	1 (0%)	47 64
1	b	668/717 (93%)	639 (96%)	27 (4%)	2 (0%)	41 56
All	All	1330/1434 (93%)	1277 (96%)	50 (4%)	3 (0%)	47 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	319	ARG
1	b	618	GLY
1	b	571	GLU

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	575/617 (93%)	557 (97%)	18 (3%)	40 57
1	b	574/617 (93%)	543 (95%)	31 (5%)	22 34
All	All	1149/1234 (93%)	1100 (96%)	49 (4%)	29 44

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	35	ASP
1	a	135	ARG
1	a	163	ARG
1	a	185	LEU
1	a	196	ARG
1	a	251	ASP
1	a	255	MET
1	a	259	GLN
1	a	289	LEU
1	a	293	ARG
1	a	316	LYS
1	a	319	ARG
1	a	398	ARG
1	a	493	LYS
1	a	605	ARG
1	a	623	SER
1	a	675	ARG
1	a	691	SER
1	b	32	GLN
1	b	35	ASP
1	b	38	GLN
1	b	55	GLU
1	b	69	SER
1	b	89	ASN
1	b	104	ARG
1	b	119	CYS
1	b	189	MET
1	b	190	LYS
1	b	210	ASN
1	b	213	ASP
1	b	226	HIS
1	b	243	LEU
1	b	254	GLN
1	b	257	LEU
1	b	260	GLU
1	b	299	CYS
1	b	313	ASP
1	b	339	SER
1	b	394	GLU
1	b	464	SER
1	b	506	LYS
1	b	515	LYS
1	b	516	ARG

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Mol	Chain	Res	Type
1	b	549	GLN
1	b	553	ASP
1	b	575	SER
1	b	675	ARG
1	b	685	LYS
1	b	691	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	178	HIS
1	a	487	ASN
1	b	32	GLN
1	b	159	GLN
1	b	210	ASN
1	b	259	GLN
1	b	481	GLN
1	b	684	GLN
1	b	716	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	HFX	b	802	-	12,15,15	1.44	1 (8%)	8,22,22	4.88	1 (12%)
4	PO4	a	803	-	4,4,4	0.84	0	6,6,6	0.68	0
3	HFX	a	802	-	12,15,15	1.37	1 (8%)	8,22,22	4.45	1 (12%)
2	25A	a	801	-	64,75,75	4.60	22 (34%)	75,116,116	2.32	12 (16%)
2	25A	b	801	-	64,75,75	4.57	24 (37%)	75,116,116	2.42	14 (18%)

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	HFX	b	802	-	-	0/0/14/14	0/2/2/2
2	25A	a	801	-	-	5/28/88/88	0/9/9/9
3	HFX	a	802	-	-	0/0/14/14	0/2/2/2
2	25A	b	801	-	-	8/28/88/88	0/9/9/9

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	801	25A	OO'-CL'	18.62	1.67	1.41
2	a	801	25A	OO'-CL'	17.81	1.65	1.41
2	a	801	25A	O4'-C1'	16.16	1.63	1.41
2	b	801	25A	O4'-C1'	15.91	1.63	1.41
2	a	801	25A	OE'-CB'	15.73	1.63	1.41
2	b	801	25A	OE'-CB'	14.87	1.61	1.41
2	a	801	25A	CM'-CL'	-13.55	1.33	1.53
2	b	801	25A	CM'-CL'	-13.51	1.33	1.53
2	b	801	25A	O4'-C4'	-6.36	1.30	1.45
2	b	801	25A	OO'-CO'	-6.19	1.31	1.45
2	a	801	25A	O4'-C4'	-6.16	1.31	1.45
2	a	801	25A	OO'-CO'	-5.93	1.31	1.45
2	a	801	25A	OE'-CE'	-5.77	1.32	1.45
2	a	801	25A	P-O3P	5.38	1.67	1.50
2	b	801	25A	OE'-CE'	-5.22	1.33	1.45
2	a	801	25A	OD'-CD'	-5.13	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	801	25A	P-O3P	5.02	1.66	1.50
2	b	801	25A	ON'-CN'	-4.42	1.32	1.43
2	a	801	25A	ON'-CN'	-4.33	1.32	1.43
2	a	801	25A	C16-N16	4.26	1.49	1.34
2	b	801	25A	C16-N16	4.25	1.49	1.34
2	b	801	25A	OD'-CD'	-4.23	1.33	1.43
3	b	802	HFX	C2-C8	-4.15	1.36	1.46
3	a	802	HFX	C2-C8	-4.05	1.37	1.46
2	a	801	25A	C26-N26	3.78	1.47	1.34
2	b	801	25A	C26-N26	3.69	1.47	1.34
2	b	801	25A	O3'-C3'	-3.58	1.34	1.43
2	a	801	25A	O3'-C3'	-3.53	1.34	1.43
2	b	801	25A	P1-O2'	3.31	1.69	1.60
2	b	801	25A	C5-C4	-3.28	1.32	1.40
2	a	801	25A	C12-N13	3.23	1.37	1.32
2	b	801	25A	OM'-CM'	3.00	1.50	1.43
2	a	801	25A	OM'-CM'	2.97	1.50	1.43
2	b	801	25A	C22-N23	2.96	1.36	1.32
2	a	801	25A	C5-C4	-2.94	1.33	1.40
2	a	801	25A	P1-O2'	2.80	1.67	1.60
2	a	801	25A	C2-N3	2.62	1.36	1.32
2	a	801	25A	C22-N23	2.62	1.36	1.32
2	b	801	25A	C6-N6	2.59	1.43	1.34
2	b	801	25A	C12-N13	2.52	1.36	1.32
2	a	801	25A	C15-C14	-2.46	1.34	1.40
2	b	801	25A	C25-C24	-2.32	1.34	1.40
2	b	801	25A	P2-OC'	2.30	1.66	1.60
2	b	801	25A	C2-N3	2.27	1.35	1.32
2	a	801	25A	C3'-C4'	2.23	1.58	1.53
2	a	801	25A	C25-C24	-2.17	1.35	1.40
2	b	801	25A	C3'-C4'	2.12	1.58	1.53
2	b	801	25A	C15-C14	-2.08	1.35	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	802	HFX	C9-S2-C1	13.64	112.68	97.64
3	a	802	HFX	C9-S2-C1	12.38	111.29	97.64
2	b	801	25A	C15-C16-N16	10.24	135.92	120.35
2	a	801	25A	C15-C16-N16	8.62	133.45	120.35
2	b	801	25A	C5-C6-N6	8.41	133.12	120.35
2	a	801	25A	C5-C6-N6	8.40	133.12	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	801	25A	N16-C16-N11	-6.69	104.69	118.57
2	a	801	25A	N16-C16-N11	-5.87	106.40	118.57
2	b	801	25A	C25-C26-N26	5.75	129.09	120.35
2	a	801	25A	N6-C6-N1	-5.65	106.84	118.57
2	b	801	25A	N6-C6-N1	-5.59	106.97	118.57
2	a	801	25A	N3-C2-N1	-5.29	120.41	128.68
2	b	801	25A	N23-C22-N21	-5.28	120.43	128.68
2	a	801	25A	C25-C26-N26	5.10	128.09	120.35
2	a	801	25A	N23-C22-N21	-5.03	120.82	128.68
2	b	801	25A	N3-C2-N1	-4.77	121.22	128.68
2	b	801	25A	N13-C12-N11	-4.68	121.36	128.68
2	a	801	25A	N13-C12-N11	-4.61	121.47	128.68
2	b	801	25A	N26-C26-N21	-4.04	110.19	118.57
2	a	801	25A	CN'-CM'-CL'	3.63	106.45	100.98
2	a	801	25A	O5'-P-O3P	3.41	116.03	106.47
2	a	801	25A	N26-C26-N21	-3.21	111.91	118.57
2	b	801	25A	CP'-CO'-CN'	-2.94	104.16	115.18
2	b	801	25A	C2'-C3'-C4'	2.27	106.93	101.99
2	b	801	25A	CN'-CM'-CL'	2.27	104.39	100.98
2	b	801	25A	C5'-C4'-C3'	-2.25	106.77	115.18
2	b	801	25A	P-O5'-C5'	-2.16	112.35	118.30
2	a	801	25A	OBP-P1-O2'	-2.03	98.77	106.78

There are no chirality outliers.

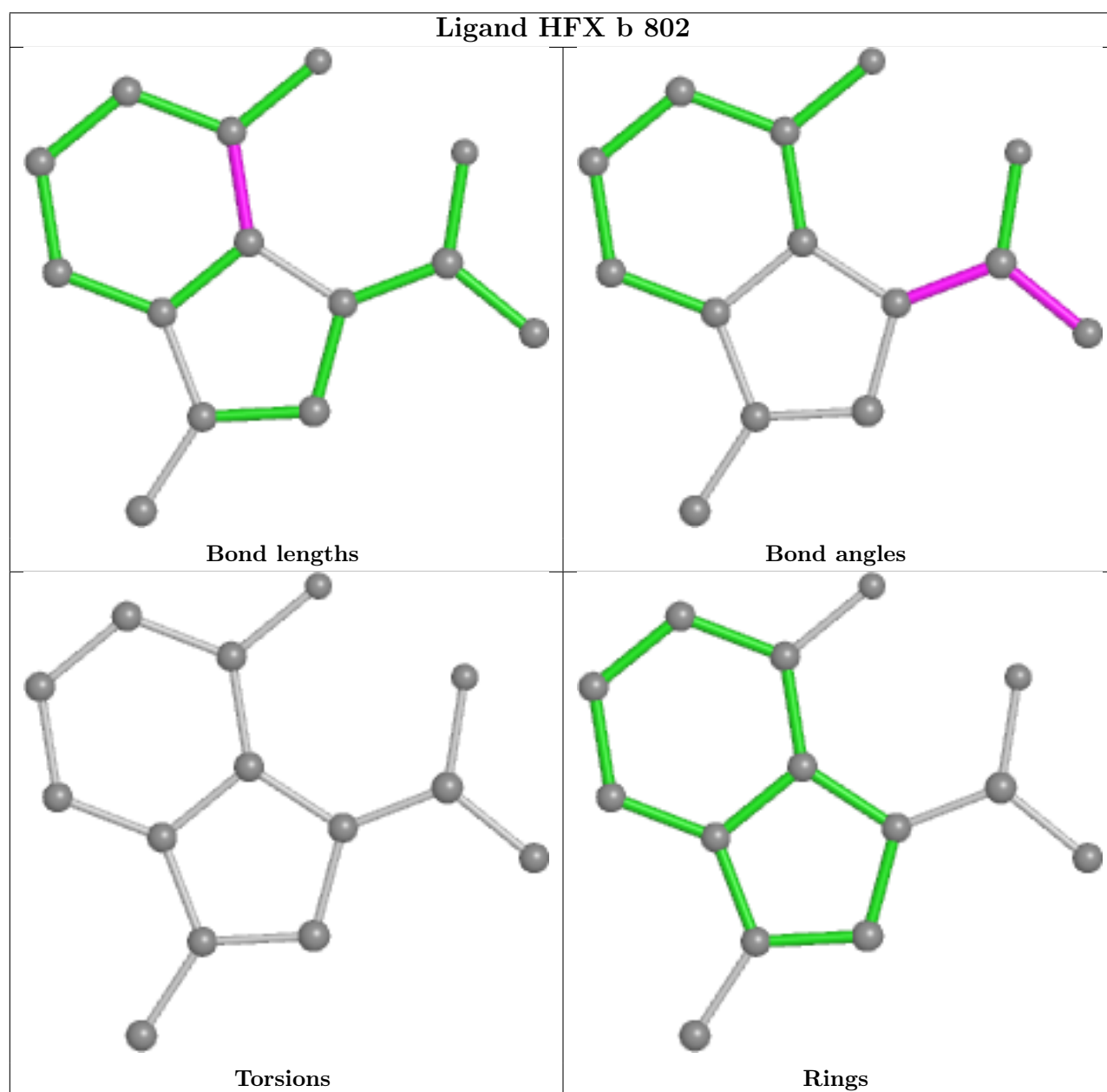
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	801	25A	OO'-CO'-CP'-OP'
2	a	801	25A	CN'-CO'-CP'-OP'
2	b	801	25A	OO'-CO'-CP'-OP'
2	b	801	25A	CN'-CO'-CP'-OP'
2	b	801	25A	OE'-CE'-CF'-OF'
2	b	801	25A	CC'-OC'-P2-OLP
2	b	801	25A	CC'-OC'-P2-OMP
2	b	801	25A	CC'-OC'-P2-OP'
2	a	801	25A	CP'-OP'-P2-OC'
2	a	801	25A	CP'-OP'-P2-OMP
2	b	801	25A	CD'-CE'-CF'-OF'
2	a	801	25A	CC'-OC'-P2-OP'
2	b	801	25A	CP'-OP'-P2-OMP

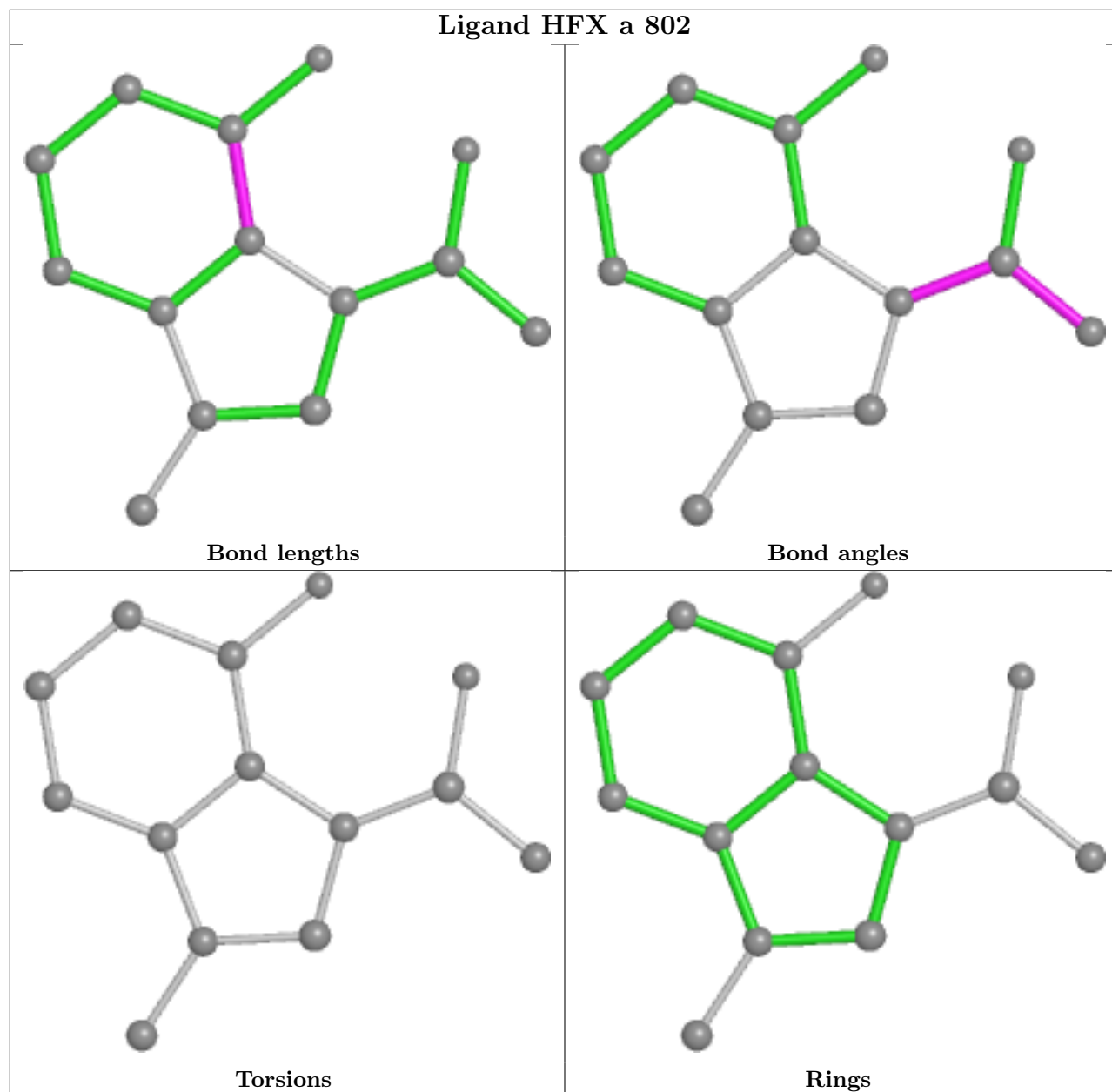
There are no ring outliers.

No monomer is involved in short contacts.

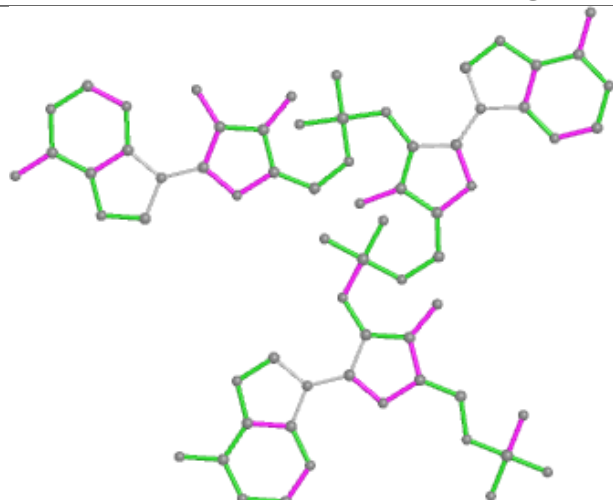
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



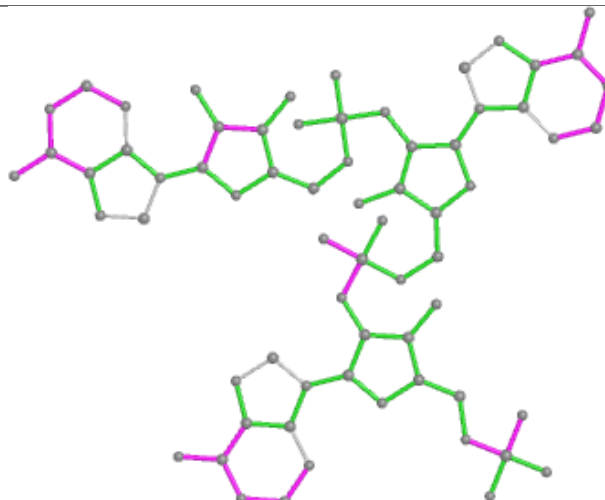
Ligand HFX a 802



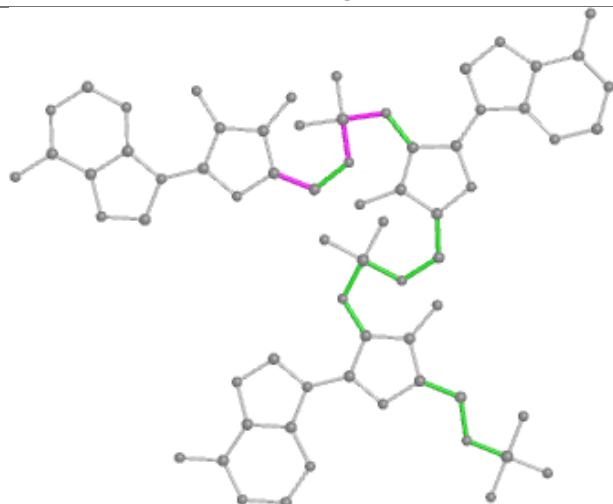
Ligand 25A a 801



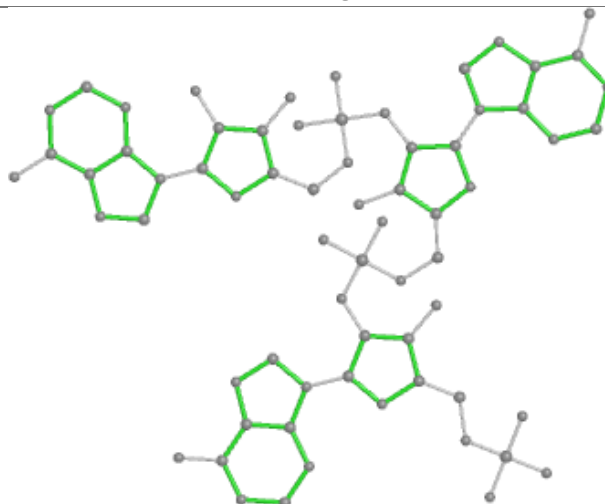
Bond lengths



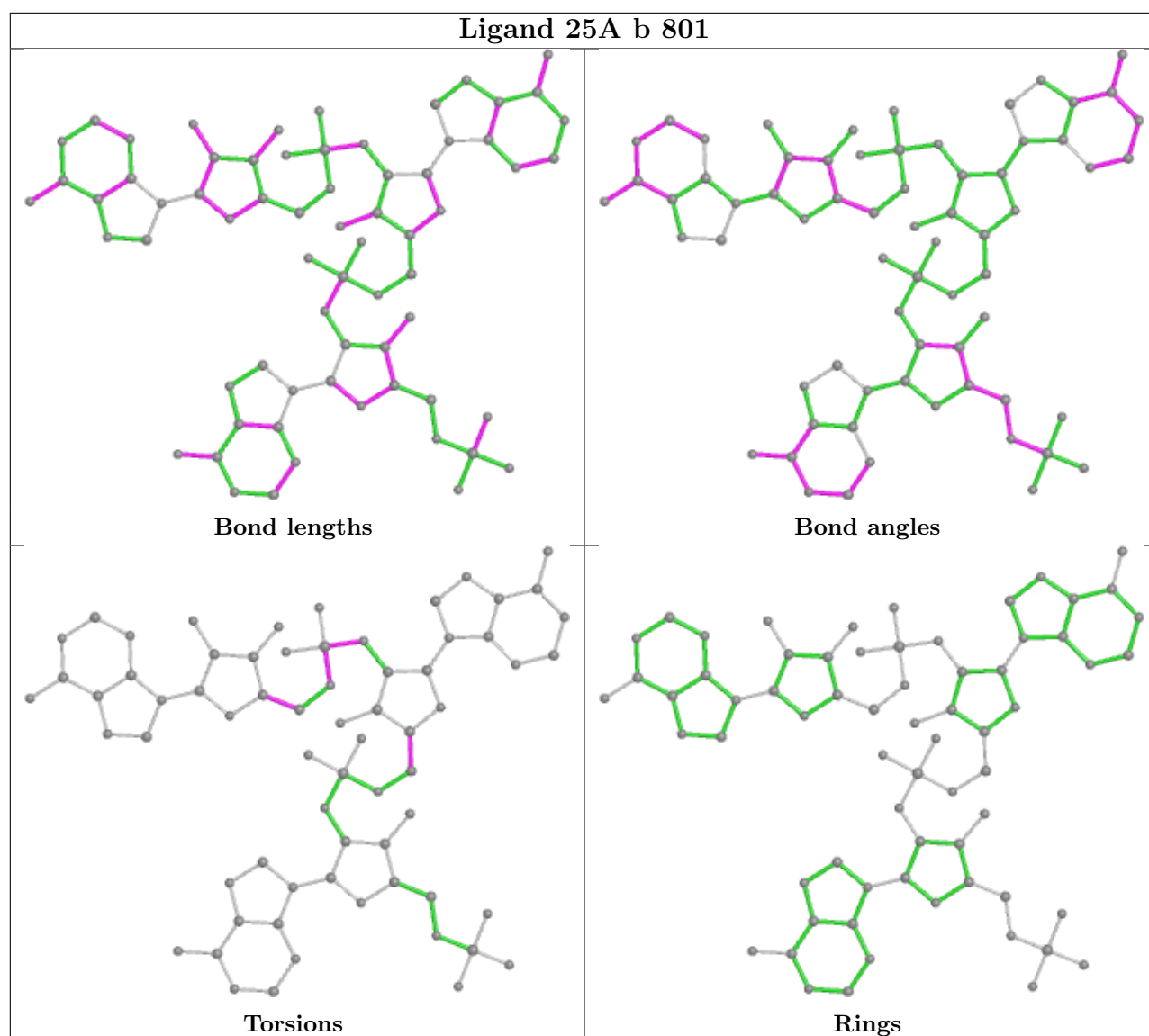
Bond angles



Torsions



Rings



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	672/717 (93%)	0.10	28 (4%) 36 33	59, 98, 146, 195	0
1	b	676/717 (94%)	0.15	38 (5%) 24 21	59, 102, 173, 219	0
All	All	1348/1434 (94%)	0.13	66 (4%) 29 26	59, 100, 161, 219	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	299	CYS	11.7
1	b	300	GLY	11.7
1	a	297	THR	6.1
1	a	245	VAL	5.2
1	b	24	GLU	4.6
1	b	44	GLU	4.5
1	b	42	LEU	4.5
1	a	36	ILE	4.4
1	a	300	GLY	4.3
1	a	283	LEU	4.2
1	b	46	GLY	3.8
1	b	568	ASP	3.8
1	a	298	ASN	3.7
1	b	37	GLU	3.7
1	b	299	CYS	3.7
1	b	90	GLY	3.6
1	b	120	ASP	3.4
1	a	317	PHE	3.4
1	a	275	LEU	3.4
1	b	111	PRO	3.3
1	a	39	VAL	3.2
1	b	144	GLU	3.2
1	b	190	LYS	3.2
1	a	567	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	b	78	LYS	3.2
1	b	631	THR	3.1
1	a	727	THR	3.1
1	b	191	ALA	3.1
1	b	47	ALA	3.0
1	b	89	ASN	3.0
1	b	62	HIS	2.7
1	b	76	LEU	2.7
1	b	74	ALA	2.7
1	b	320	LEU	2.6
1	b	124	PHE	2.5
1	b	297	THR	2.5
1	b	146	GLY	2.5
1	a	35	ASP	2.5
1	a	345	LEU	2.5
1	a	319	ARG	2.5
1	b	227	GLY	2.5
1	a	284	GLU	2.5
1	a	37	GLU	2.5
1	b	39	VAL	2.4
1	a	302	LEU	2.4
1	b	256	LEU	2.4
1	b	59	SER	2.3
1	a	381	LEU	2.3
1	a	43	LEU	2.3
1	a	274	ALA	2.2
1	b	242	ILE	2.2
1	b	80	GLY	2.2
1	a	257	LEU	2.2
1	b	79	HIS	2.2
1	b	511	PRO	2.2
1	a	38	GLN	2.2
1	b	119	CYS	2.2
1	b	34	ALA	2.2
1	a	320	LEU	2.1
1	a	40	ARG	2.1
1	b	54	GLU	2.1
1	b	630	THR	2.1
1	a	417	THR	2.1
1	a	296	SER	2.1
1	b	40	ARG	2.1
1	a	241	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

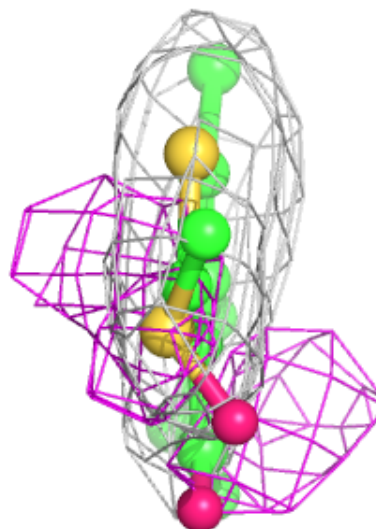
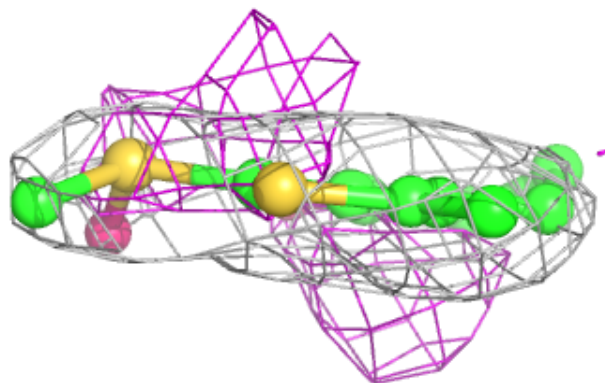
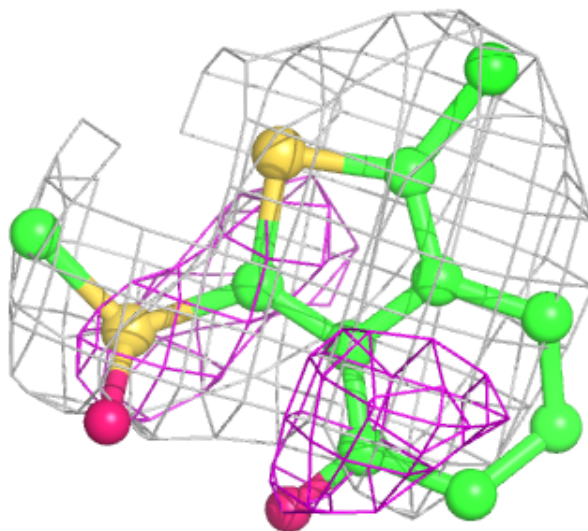
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HFX	a	802	14/14	0.91	0.32	66,108,127,127	0
2	25A	b	801	67/67	0.93	0.32	85,110,127,131	0
3	HFX	b	802	14/14	0.93	0.16	82,98,115,116	0
2	25A	a	801	67/67	0.95	0.21	61,84,102,105	0
4	PO4	a	803	5/5	0.96	0.12	72,73,92,106	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.

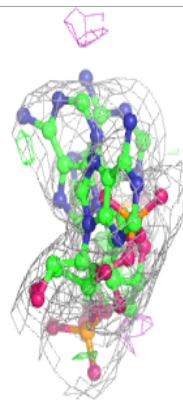
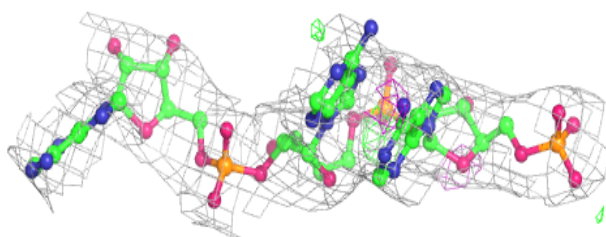
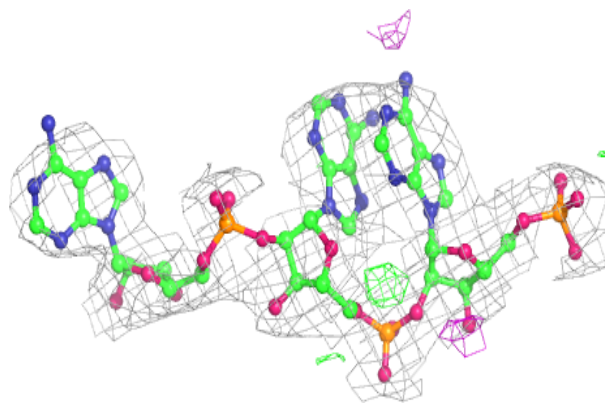
Electron density around HFX a 802:

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



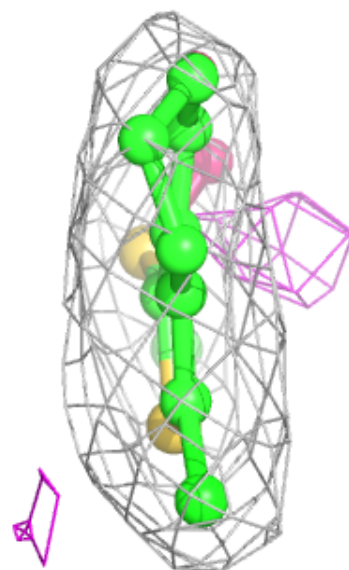
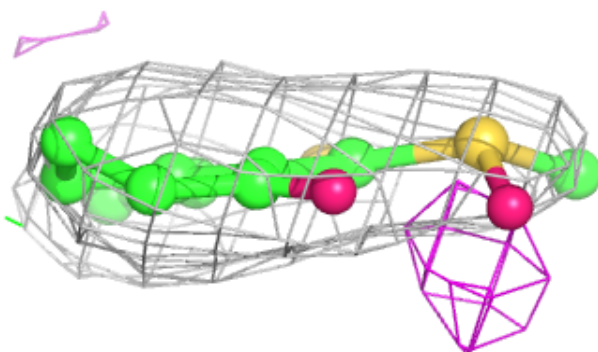
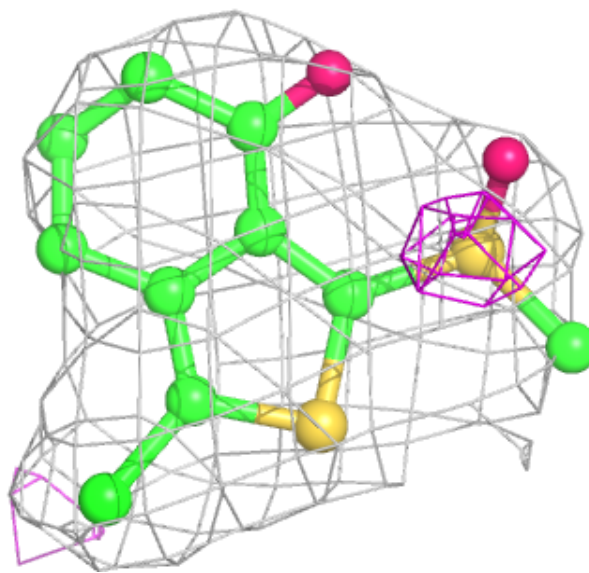
Electron density around 25A b 801:

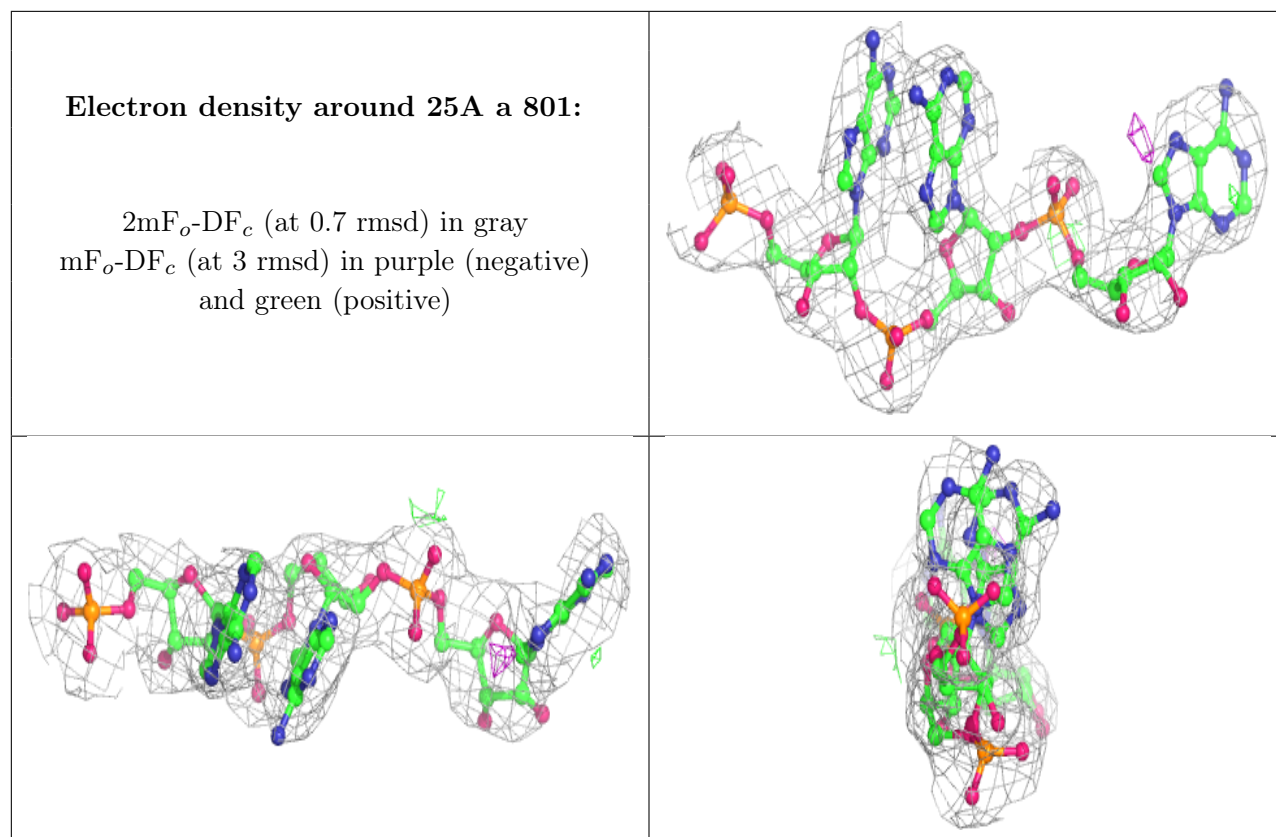
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HFX b 802:

$2mF_o-DF_c$ (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.