



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2021 – 10:17 PM EDT

PDB ID : 4KVM
Title : The NatA (Naa10p/Naa15p) amino-terminal acetyltransferase complex bound to a bisubstrate analog
Authors : Liszczak, G.P.; Marmorstein, R.Q.
Deposited on : 2013-05-22
Resolution : 2.60 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 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 : 2.23.1
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) : 2.23.1

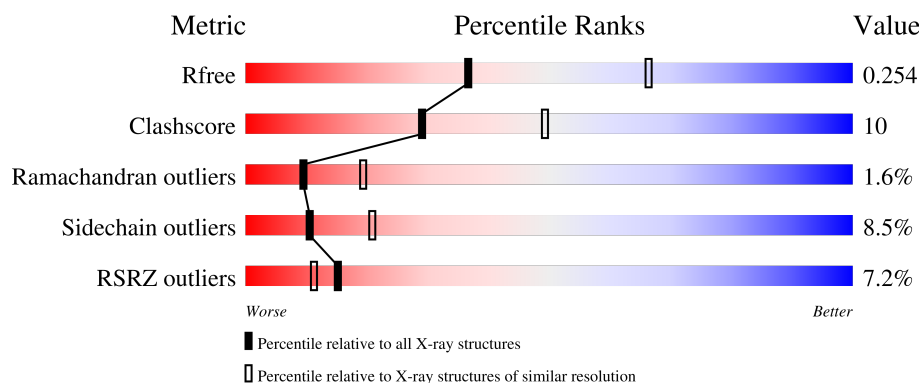
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	734	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>..</div> </div> </div>
1	B	734	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>..</div> </div> </div>
1	C	734	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>..</div> </div> </div>
1	D	734	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>...</div> </div> </div>
2	E	156	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	156	
2	G	156	
2	H	156	
3	I	4	
3	J	4	
3	K	4	
3	L	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	810	-	-	X	-
4	CL	A	814	-	-	X	-
4	CL	B	806	-	-	-	X
4	CL	B	807	-	-	-	X
4	CL	B	813	-	-	-	X
4	CL	C	807	-	-	-	X
4	CL	C	810	-	-	X	-
4	CL	D	803	-	-	-	X
4	CL	D	805	-	-	-	X
4	CL	D	806	-	-	-	X
4	CL	D	811	-	-	X	-
4	CL	D	813	-	-	-	X
4	CL	F	201	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28749 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 N-terminal acetyltransferase A complex subunit nat1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	3	0
			5782	3689	976	1099	18			
1	B	722	Total	C	N	O	S	0	1	0
			5777	3686	971	1102	18			
1	C	717	Total	C	N	O	S	0	1	0
			5753	3671	968	1096	18			
1	D	718	Total	C	N	O	S	0	1	0
			5766	3681	970	1097	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	ALA	-	expression tag	UNP O74985
A	731	ALA	-	expression tag	UNP O74985
A	732	ALA	-	expression tag	UNP O74985
A	733	ALA	-	expression tag	UNP O74985
A	734	ALA	-	expression tag	UNP O74985
B	730	ALA	-	expression tag	UNP O74985
B	731	ALA	-	expression tag	UNP O74985
B	732	ALA	-	expression tag	UNP O74985
B	733	ALA	-	expression tag	UNP O74985
B	734	ALA	-	expression tag	UNP O74985
C	730	ALA	-	expression tag	UNP O74985
C	731	ALA	-	expression tag	UNP O74985
C	732	ALA	-	expression tag	UNP O74985
C	733	ALA	-	expression tag	UNP O74985
C	734	ALA	-	expression tag	UNP O74985
D	730	ALA	-	expression tag	UNP O74985
D	731	ALA	-	expression tag	UNP O74985
D	732	ALA	-	expression tag	UNP O74985
D	733	ALA	-	expression tag	UNP O74985
D	734	ALA	-	expression tag	UNP O74985

- Molecule 2 is a protein called N-terminal acetyltransferase A complex catalytic subunit ard1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	153	Total	C	N	O	S	0	1	0
			1247	790	221	225	11			
2	F	153	Total	C	N	O	S	0	0	0
			1239	785	220	224	10			
2	G	153	Total	C	N	O	S	0	0	0
			1239	785	220	224	10			
2	H	153	Total	C	N	O	S	0	0	0
			1239	785	220	224	10			

- Molecule 3 is a protein called bisubstrate analog inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			26	14	4	8			
3	J	4	Total	C	N	O	0	0	0
			26	14	4	8			
3	K	4	Total	C	N	O	0	0	0
			26	14	4	8			
3	L	4	Total	C	N	O	0	0	0
			26	14	4	8			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

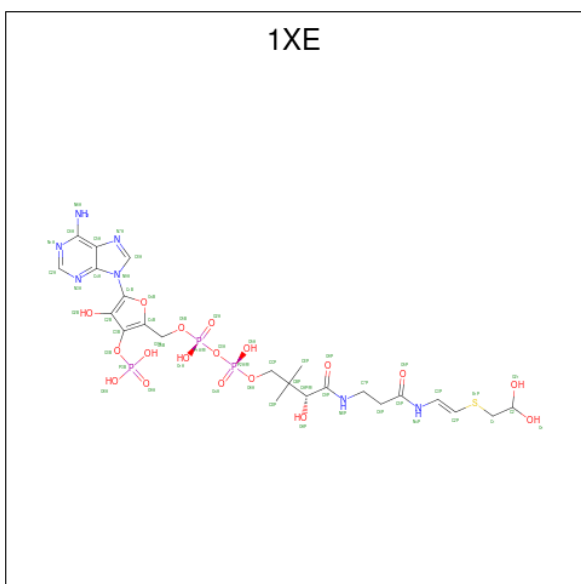
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	Cl	0	0
			14	14		
4	B	16	Total	Cl	0	0
			16	16		
4	C	13	Total	Cl	0	0
			13	13		
4	D	15	Total	Cl	0	0
			15	15		
4	E	3	Total	Cl	0	0
			3	3		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is [5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)furan-2-yl]methyl (3R)-4-{[3-({(E)-2-[(2,2-dihydroxyethyl)sulfanyl]ethenyl}amino)-3-oxopropyl]amino}-3-hydroxy-2,2-dimethyl-4-oxobutyl dihydrogen diphosphate (three-letter code: 1XE) (formula: C₂₃H₃₄N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
6	J	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
6	K	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
6	L	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

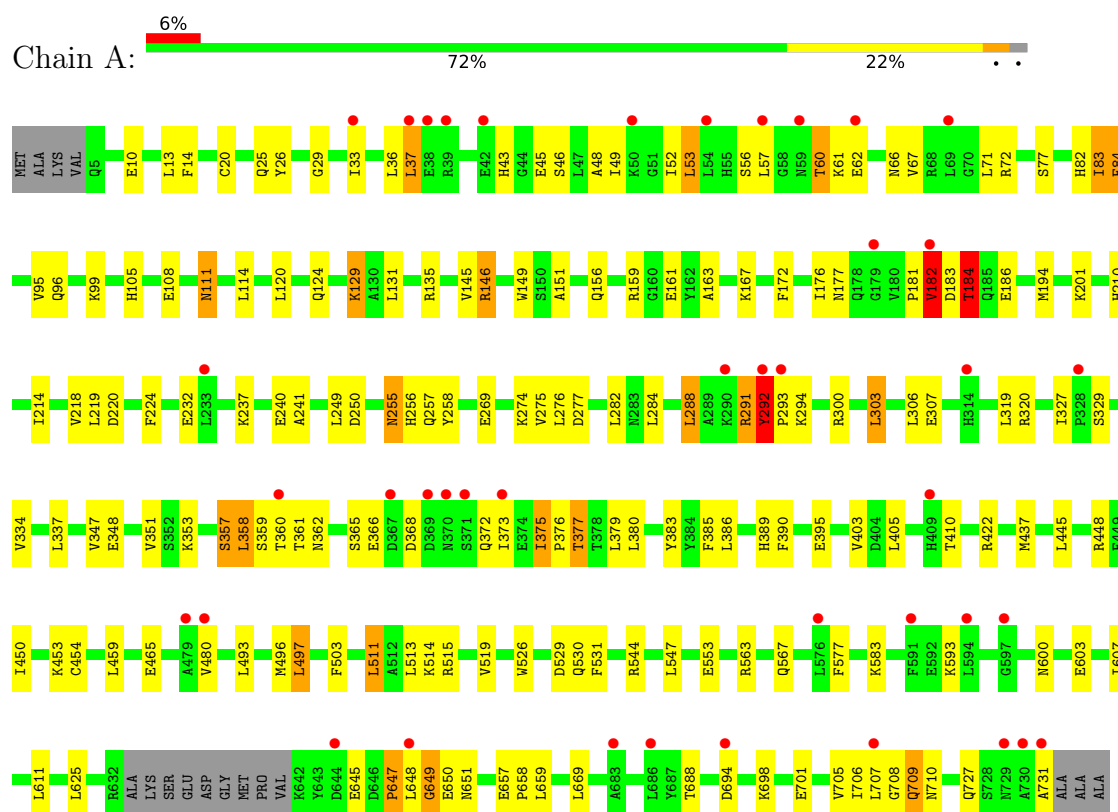
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	79	Total	O	0	0
			79	79		
7	B	50	Total	O	0	0
			50	50		
7	C	80	Total	O	0	0
			80	80		
7	D	64	Total	O	0	0
			64	64		
7	E	20	Total	O	0	0
			20	20		
7	F	6	Total	O	0	0
			6	6		
7	G	5	Total	O	0	0
			5	5		
7	H	18	Total	O	0	0
			18	18		
7	I	1	Total	O	0	0
			1	1		
7	J	1	Total	O	0	0
			1	1		
7	L	1	Total	O	0	0
			1	1		

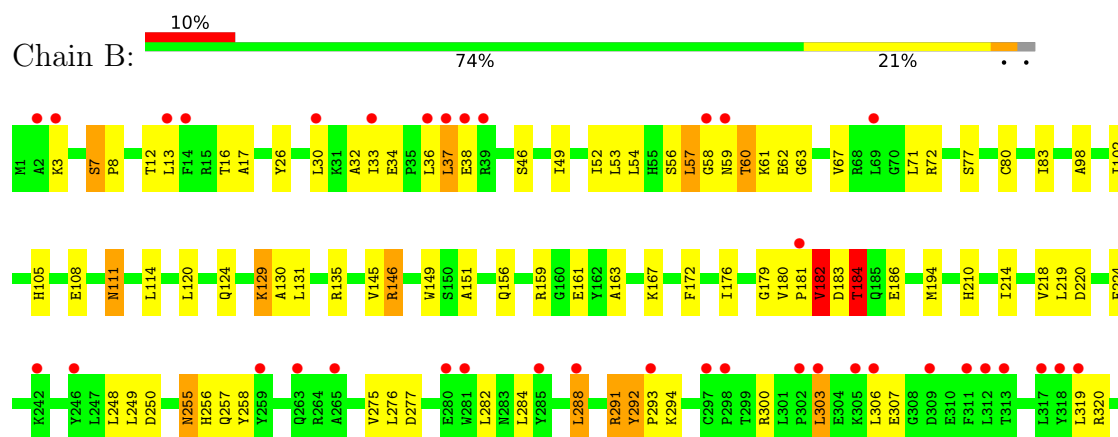
3 Residue-property plots

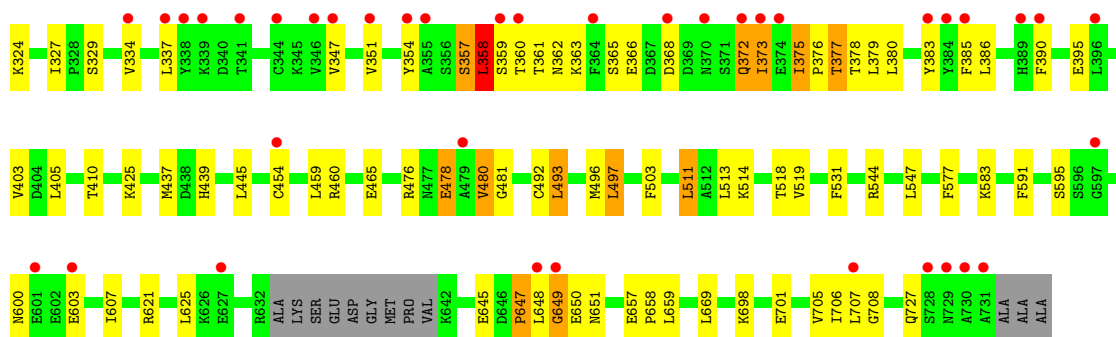
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: N-terminal acetyltransferase A complex subunit nat1



- Molecule 1: N-terminal acetyltransferase A complex subunit nat1

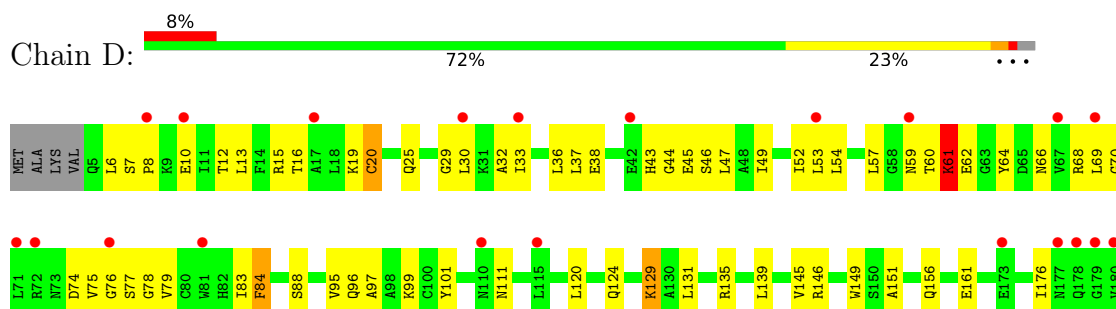


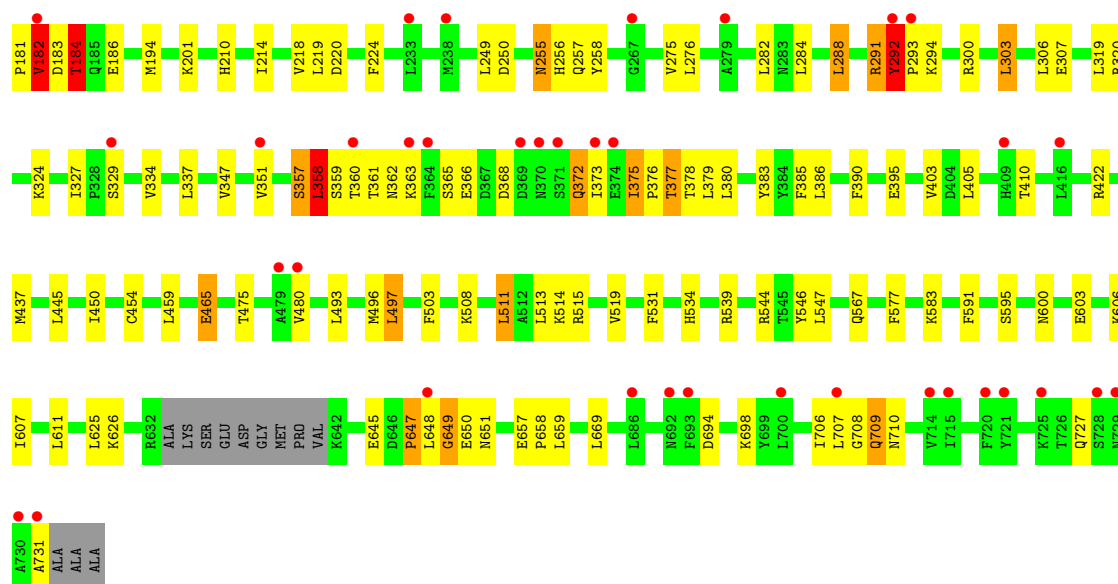


• Molecule 1: N-terminal acetyltransferase A complex subunit nat1

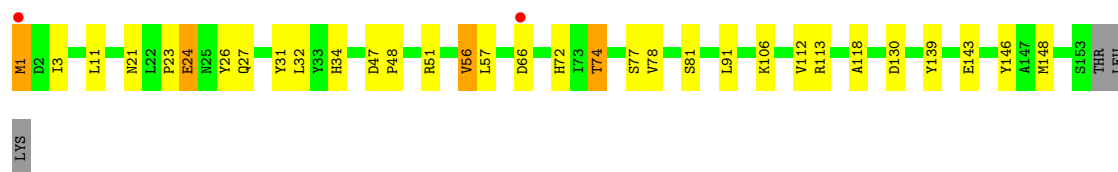
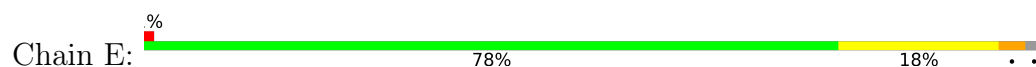


• Molecule 1: N-terminal acetyltransferase A complex subunit nat1

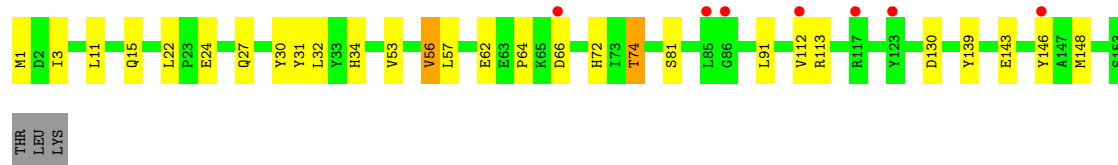
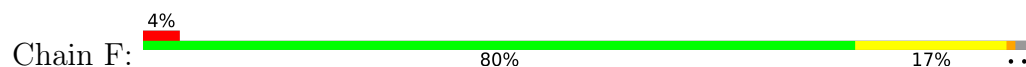




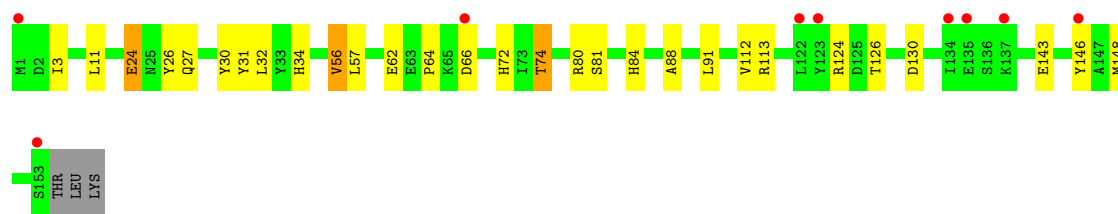
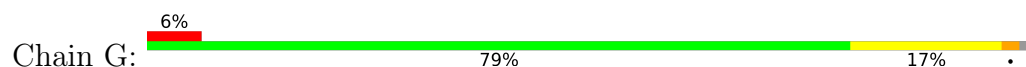
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



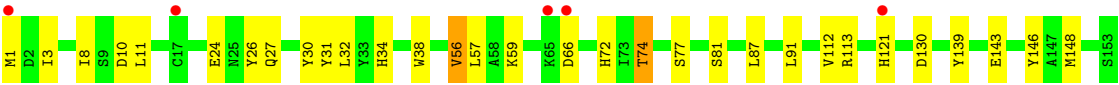
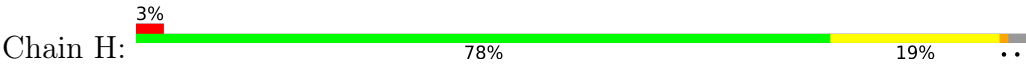
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



THR
LEU
LYS

- Molecule 3: bisubstrate analog inhibitor



There are no outlier residues recorded for this chain.

- Molecule 3: bisubstrate analog inhibitor



S5122
E5125

- Molecule 3: bisubstrate analog inhibitor



S5122
E5125

- Molecule 3: bisubstrate analog inhibitor



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 119.38Å 134.06Å 80.20° 76.60° 70.42°	Depositor
Resolution (Å)	49.59 – 2.60 49.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.59-2.60) 89.8 (49.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.222 , 0.260 0.214 , 0.254	Depositor DCC
R_{free} test set	6916 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28749	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 1XE, SO4

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	0.45	0/5896	0.59	1/7952 (0.0%)
1	B	0.40	0/5891	0.56	0/7948
1	C	0.41	0/5867	0.55	0/7915
1	D	0.43	0/5881	0.56	0/7934
2	E	0.52	0/1277	0.63	0/1722
2	F	0.40	0/1269	0.56	0/1712
2	G	0.41	0/1269	0.56	0/1712
2	H	0.48	0/1269	0.62	0/1712
3	I	0.71	0/25	0.74	0/32
3	J	0.50	0/25	0.58	0/32
3	K	0.34	0/25	0.43	0/32
3	L	0.63	0/25	0.65	0/32
All	All	0.43	0/28719	0.57	1/38735 (0.0%)

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
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	THR	N-CA-C	-5.16	97.08	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	SER	Peptide
1	A	649	GLY	Peptide
1	B	357	SER	Peptide
1	B	649	GLY	Peptide
1	C	357	SER	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	5782	0	5705	124	1
1	B	5777	0	5697	114	0
1	C	5753	0	5675	123	0
1	D	5766	0	5691	115	0
2	E	1247	0	1233	21	0
2	F	1239	0	1223	13	0
2	G	1239	0	1223	19	0
2	H	1239	0	1223	15	0
3	I	26	0	20	0	0
3	J	26	0	20	2	0
3	K	26	0	20	1	0
3	L	26	0	20	0	0
4	A	14	0	0	10	0
4	B	16	0	0	3	0
4	C	13	0	0	4	0
4	D	15	0	0	7	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	1	0
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	51	0	29	5	0
6	J	51	0	30	2	0
6	K	51	0	30	7	0
6	L	51	0	29	3	0
7	A	79	0	0	19	0
7	B	50	0	0	6	0
7	C	80	0	0	22	0
7	D	64	0	0	10	0
7	E	20	0	0	3	0
7	F	6	0	0	1	0
7	G	5	0	0	0	1
7	H	18	0	0	1	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	L	1	0	0	0	0
All	All	28749	0	27868	542	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 10.

The worst 5 of 542 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:237:LYS:O	7:A:957:HOH:O	1.83	0.96
1:C:211:LEU:O	7:C:942:HOH:O	1.86	0.92
1:A:291:ARG:NH2	4:A:813:CL:CL	2.39	0.92
1:A:129[B]:LYS:NZ	4:A:805:CL:CL	2.41	0.91
1:C:463:GLU:O	7:C:915:HOH:O	1.90	0.90

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)
1:A:731:ALA:O	7:G:304:HOH:O[1_556]	2.08	0.12

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	717/734 (98%)	658 (92%)	46 (6%)	13 (2%)	8	16
1	B	719/734 (98%)	660 (92%)	45 (6%)	14 (2%)	8	15
1	C	714/734 (97%)	660 (92%)	42 (6%)	12 (2%)	9	18
1	D	715/734 (97%)	657 (92%)	43 (6%)	15 (2%)	7	13
2	E	151/156 (97%)	144 (95%)	7 (5%)	0	100	100
2	F	151/156 (97%)	147 (97%)	4 (3%)	0	100	100
2	G	151/156 (97%)	146 (97%)	5 (3%)	0	100	100
2	H	151/156 (97%)	145 (96%)	6 (4%)	0	100	100
3	I	2/4 (50%)	2 (100%)	0	0	100	100
3	J	2/4 (50%)	2 (100%)	0	0	100	100
3	K	2/4 (50%)	2 (100%)	0	0	100	100
3	L	2/4 (50%)	2 (100%)	0	0	100	100
All	All	3477/3576 (97%)	3225 (93%)	198 (6%)	54 (2%)	9	19

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	VAL
1	A	184	THR
1	A	256	HIS
1	A	293	PRO
1	A	358	LEU

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	611/638 (96%)	558 (91%)	53 (9%)	10	20
1	B	610/638 (96%)	559 (92%)	51 (8%)	11	21
1	C	609/638 (96%)	561 (92%)	48 (8%)	12	24
1	D	610/638 (96%)	562 (92%)	48 (8%)	12	24
2	E	133/135 (98%)	118 (89%)	15 (11%)	6	10
2	F	132/135 (98%)	118 (89%)	14 (11%)	6	12
2	G	132/135 (98%)	119 (90%)	13 (10%)	8	15
2	H	132/135 (98%)	117 (89%)	15 (11%)	5	10
3	I	3/3 (100%)	3 (100%)	0	100	100
3	J	3/3 (100%)	2 (67%)	1 (33%)	0	0
3	K	3/3 (100%)	3 (100%)	0	100	100
3	L	3/3 (100%)	3 (100%)	0	100	100
All	All	2981/3104 (96%)	2723 (91%)	258 (9%)	10	20

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	26	TYR
2	G	74	THR
1	B	547	LEU
1	B	497	LEU
2	H	3	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	255	ASN
2	E	27	GLN
2	H	27	GLN
2	G	27	GLN
1	B	255	ASN

5.3.3 RNA ⓘ

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](#)

Of 70 ligands modelled in this entry, 64 are monoatomic - leaving 6 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	$\# Z > 2$
5	SO4	A	815	-	4,4,4	0.20	0	6,6,6	0.17	0
6	1XE	I	5201	3	43,53,54	2.49	13 (30%)	45,78,80	2.82	16 (35%)
5	SO4	D	816	-	4,4,4	0.18	0	6,6,6	0.22	0
6	1XE	K	5201	3	43,53,54	2.49	11 (25%)	45,78,80	2.47	14 (31%)
6	1XE	J	5201	3	43,53,54	2.51	12 (27%)	45,78,80	2.14	15 (33%)
6	1XE	L	5201	3	43,53,54	2.42	11 (25%)	45,78,80	2.39	14 (31%)

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
6	1XE	I	5201	3	-	17/42/51/52	0/3/3/3
6	1XE	L	5201	3	-	17/42/51/52	0/3/3/3
6	1XE	K	5201	3	-	16/42/51/52	0/3/3/3
6	1XE	J	5201	3	-	17/42/51/52	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	5201	1XE	C3P-C2P	8.20	1.50	1.31
6	K	5201	1XE	C3P-C2P	8.00	1.50	1.31
6	I	5201	1XE	C3P-C2P	7.86	1.50	1.31
6	J	5201	1XE	C3P-C2P	7.48	1.49	1.31
6	L	5201	1XE	C9P-N8P	6.83	1.48	1.33

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	5201	1XE	O5B-C5B-C4B	8.59	125.26	109.44
6	I	5201	1XE	C7P-C6P-C5P	8.02	125.72	112.36
6	I	5201	1XE	C7P-N8P-C9P	-7.83	108.62	122.59
6	L	5201	1XE	C1-S1P-C2P	7.25	112.24	100.33
6	K	5201	1XE	C1-S1P-C2P	7.17	112.11	100.33

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	5201	1XE	C4B-C5B-O5B-P1A
6	I	5201	1XE	C5B-O5B-P1A-O1A
6	I	5201	1XE	C5B-O5B-P1A-O2A
6	I	5201	1XE	CCP-O6A-P2A-O3A
6	I	5201	1XE	CAP-CBP-CCP-O6A

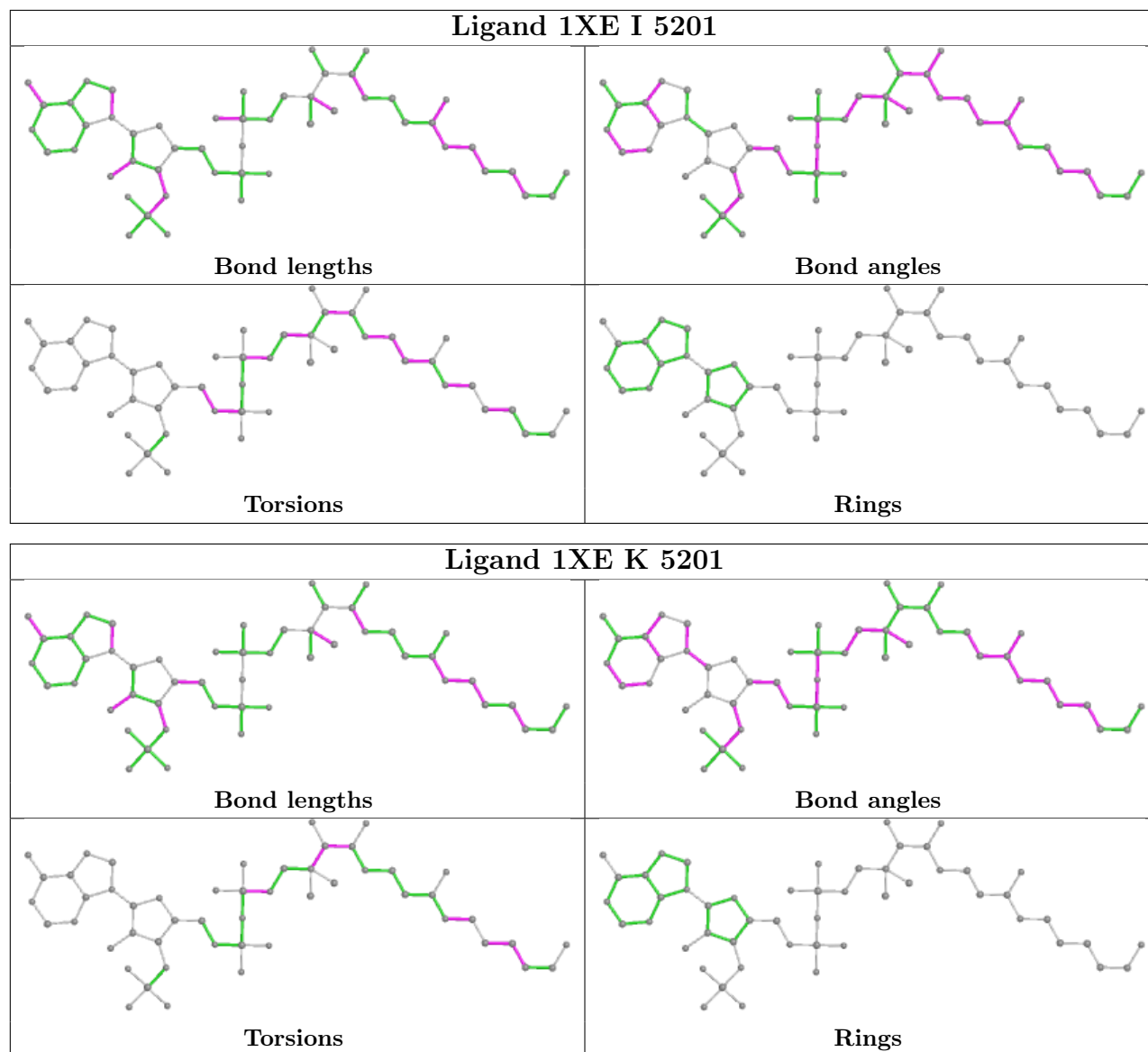
There are no ring outliers.

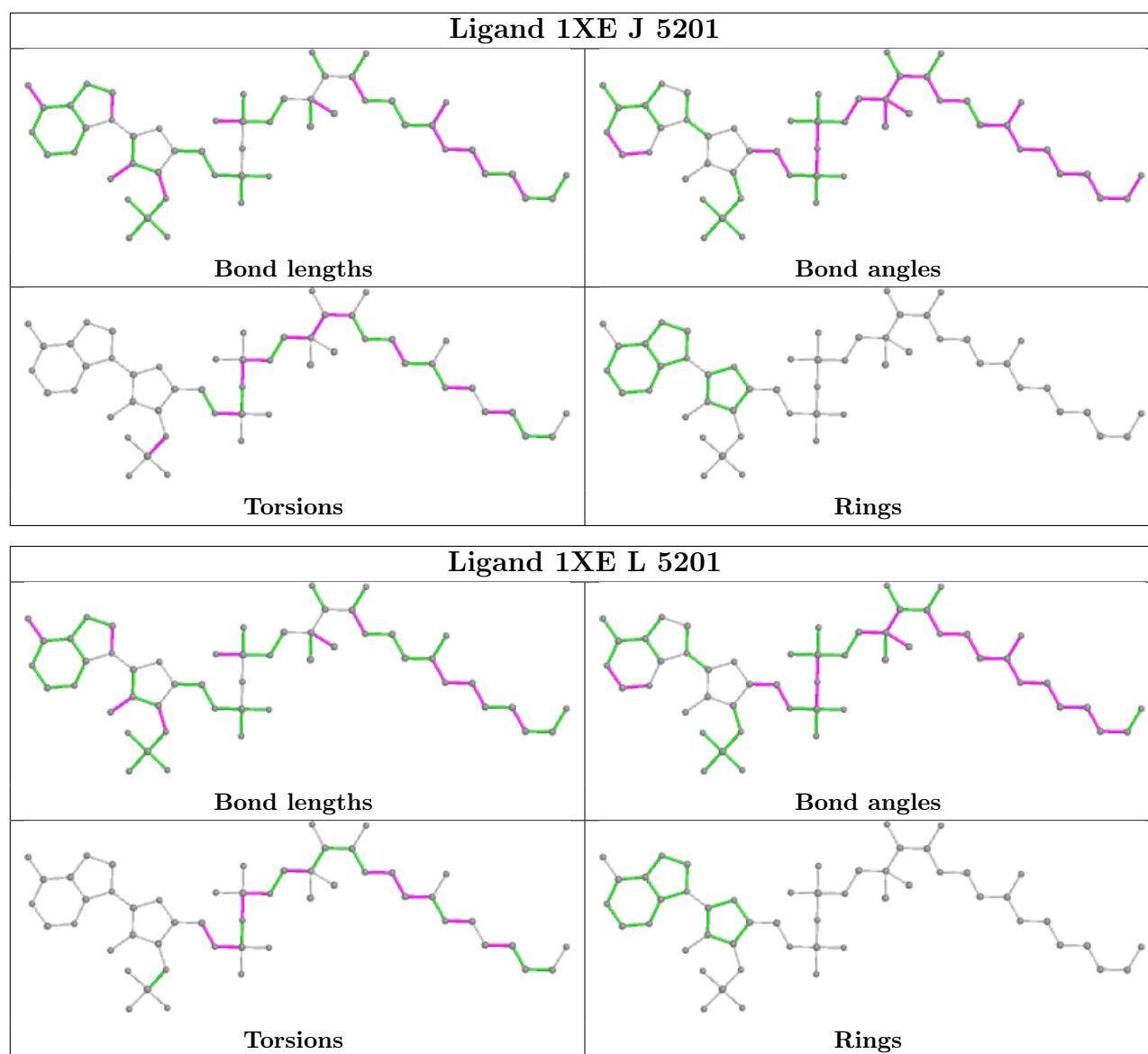
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	5201	1XE	5	0
6	K	5201	1XE	7	0
6	J	5201	1XE	2	0
6	L	5201	1XE	3	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	718/734 (97%)	0.35	41 (5%) 23 18	55, 89, 162, 258	0
1	B	722/734 (98%)	0.64	75 (10%) 6 4	52, 109, 199, 296	0
1	C	717/734 (97%)	0.56	56 (7%) 13 9	52, 104, 191, 257	0
1	D	718/734 (97%)	0.41	57 (7%) 12 9	56, 95, 180, 280	0
2	E	153/156 (98%)	0.36	2 (1%) 77 73	51, 72, 139, 167	0
2	F	153/156 (98%)	0.57	7 (4%) 32 26	58, 104, 168, 207	0
2	G	153/156 (98%)	0.72	9 (5%) 22 17	59, 110, 179, 215	0
2	H	153/156 (98%)	0.36	5 (3%) 46 39	52, 78, 137, 182	0
3	I	4/4 (100%)	0.09	0 100 100	60, 65, 80, 111	0
3	J	4/4 (100%)	0.25	0 100 100	80, 92, 100, 125	0
3	K	4/4 (100%)	0.25	0 100 100	90, 93, 130, 151	0
3	L	4/4 (100%)	0.03	0 100 100	65, 66, 88, 108	0
All	All	3503/3576 (97%)	0.49	252 (7%) 15 11	51, 96, 181, 296	0

The worst 5 of 252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	ALA	17.1
1	C	730	ALA	16.0
1	B	730	ALA	10.4
1	C	370	ASN	9.9
1	A	38	GLU	8.5

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 ⓘ

There are no monosaccharides 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
4	CL	B	808	1/1	-0.35	0.18	161,161,161,161	0
4	CL	D	805	1/1	0.08	1.56	288,288,288,288	0
4	CL	C	813	1/1	0.09	0.24	137,137,137,137	0
4	CL	A	812	1/1	0.10	0.27	141,141,141,141	0
4	CL	D	803	1/1	0.30	0.43	118,118,118,118	0
4	CL	C	803	1/1	0.48	0.17	129,129,129,129	0
4	CL	B	806	1/1	0.54	0.63	151,151,151,151	0
4	CL	F	201	1/1	0.56	0.92	148,148,148,148	0
4	CL	A	804	1/1	0.57	0.09	143,143,143,143	0
4	CL	B	807	1/1	0.58	0.66	140,140,140,140	0
4	CL	B	813	1/1	0.59	0.88	145,145,145,145	0
4	CL	E	202	1/1	0.59	0.31	102,102,102,102	0
4	CL	A	807	1/1	0.59	0.30	148,148,148,148	0
4	CL	D	806	1/1	0.64	0.48	139,139,139,139	0
4	CL	C	807	1/1	0.67	0.41	125,125,125,125	0
4	CL	D	804	1/1	0.67	0.20	132,132,132,132	0
4	CL	D	802	1/1	0.70	0.17	149,149,149,149	0
4	CL	D	807	1/1	0.71	0.30	173,173,173,173	0
4	CL	D	810	1/1	0.71	0.30	157,157,157,157	0
4	CL	B	815	1/1	0.74	0.27	192,192,192,192	0
4	CL	D	812	1/1	0.74	0.21	138,138,138,138	0
4	CL	D	809	1/1	0.75	0.24	127,127,127,127	0
4	CL	C	804	1/1	0.76	0.22	118,118,118,118	0
4	CL	G	201	1/1	0.76	0.14	133,133,133,133	0
4	CL	D	813	1/1	0.79	0.41	130,130,130,130	0
4	CL	A	809	1/1	0.79	0.15	125,125,125,125	0
4	CL	A	808	1/1	0.79	0.36	113,113,113,113	0
4	CL	B	801	1/1	0.79	0.14	127,127,127,127	0
4	CL	A	811	1/1	0.80	0.67	188,188,188,188	0
4	CL	C	801	1/1	0.81	0.09	111,111,111,111	0
4	CL	C	812	1/1	0.81	0.75	126,126,126,126	0
4	CL	B	804	1/1	0.81	0.41	107,107,107,107	0

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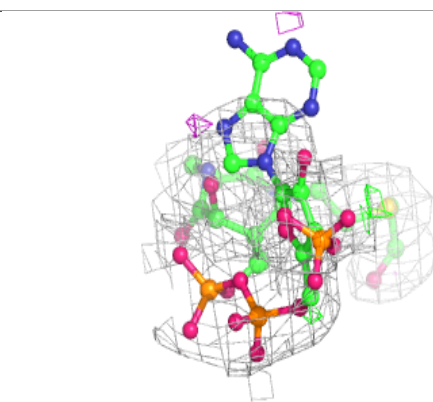
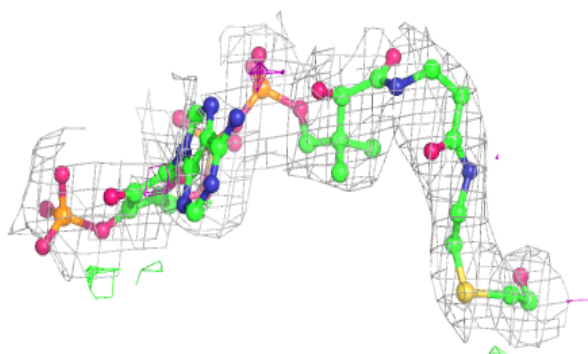
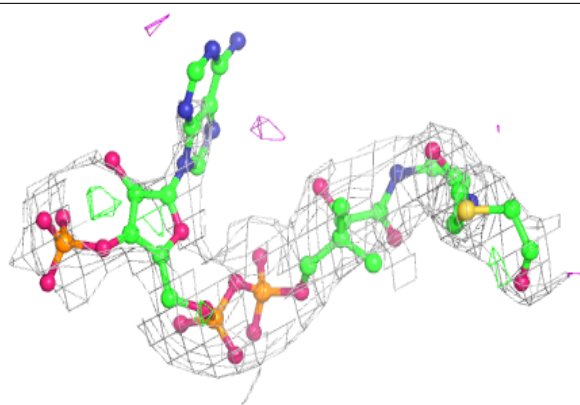
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	B	816	1/1	0.81	0.11	107,107,107,107	0
4	CL	C	808	1/1	0.83	0.26	110,110,110,110	0
4	CL	B	805	1/1	0.83	0.23	108,108,108,108	0
4	CL	C	809	1/1	0.85	0.11	151,151,151,151	0
4	CL	C	806	1/1	0.85	0.13	117,117,117,117	0
4	CL	B	814	1/1	0.85	0.17	141,141,141,141	0
4	CL	C	805	1/1	0.85	0.11	119,119,119,119	0
4	CL	A	806	1/1	0.87	0.17	145,145,145,145	0
4	CL	E	203	1/1	0.87	0.14	110,110,110,110	0
4	CL	B	809	1/1	0.87	0.19	109,109,109,109	0
4	CL	D	815	1/1	0.87	0.26	105,105,105,105	0
4	CL	A	810	1/1	0.88	0.41	86,86,86,86	0
4	CL	D	808	1/1	0.89	0.39	131,131,131,131	0
4	CL	B	812	1/1	0.89	0.34	112,112,112,112	0
6	1XE	J	5201	51/52	0.89	0.20	67,142,228,241	0
6	1XE	K	5201	51/52	0.89	0.21	53,128,279,303	0
4	CL	A	814	1/1	0.90	0.10	120,120,120,120	0
4	CL	B	803	1/1	0.91	0.12	99,99,99,99	0
4	CL	A	805	1/1	0.91	0.24	138,138,138,138	0
4	CL	B	810	1/1	0.92	0.30	99,99,99,99	0
5	SO4	D	816	5/5	0.92	0.14	80,110,119,124	0
4	CL	A	803	1/1	0.92	0.08	99,99,99,99	0
4	CL	D	801	1/1	0.92	0.11	93,93,93,93	0
4	CL	C	802	1/1	0.93	0.33	106,106,106,106	0
6	1XE	I	5201	51/52	0.93	0.22	49,92,190,217	0
4	CL	C	811	1/1	0.94	0.19	94,94,94,94	0
4	CL	H	201	1/1	0.94	0.27	84,84,84,84	0
6	1XE	L	5201	51/52	0.94	0.21	49,92,179,181	0
4	CL	D	814	1/1	0.95	0.54	110,110,110,110	0
4	CL	C	810	1/1	0.95	0.35	97,97,97,97	0
4	CL	A	801	1/1	0.95	0.49	96,96,96,96	0
4	CL	A	813	1/1	0.96	0.18	124,124,124,124	0
4	CL	A	802	1/1	0.97	0.19	93,93,93,93	0
4	CL	E	201	1/1	0.97	0.26	79,79,79,79	0
5	SO4	A	815	5/5	0.98	0.12	88,104,110,121	0
4	CL	B	811	1/1	0.98	0.37	99,99,99,99	0
4	CL	D	811	1/1	0.98	0.23	73,73,73,73	0
4	CL	B	802	1/1	0.99	0.33	96,96,96,96	0

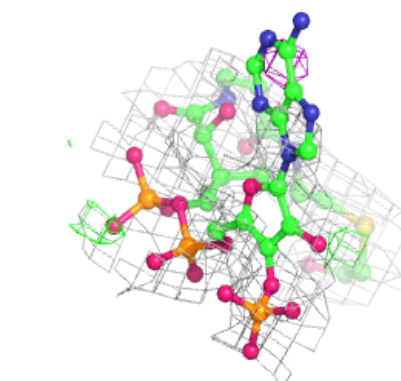
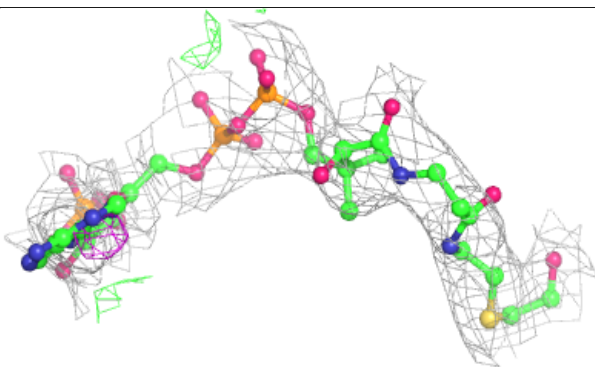
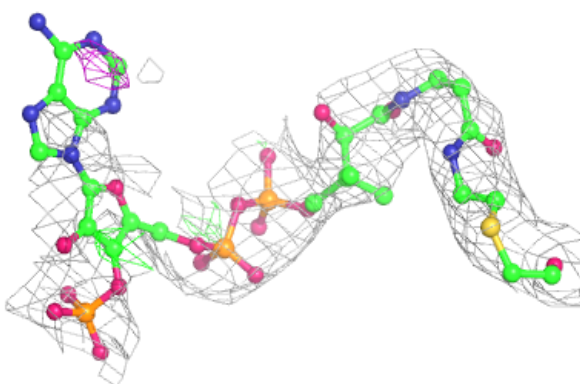
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1XE J 5201:

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

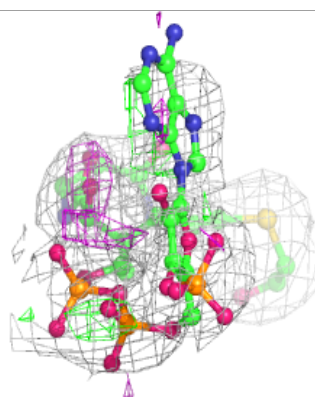
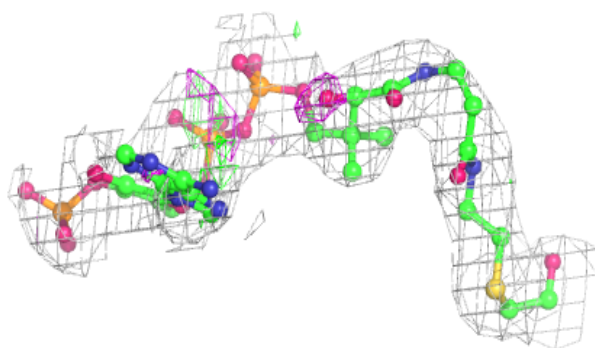
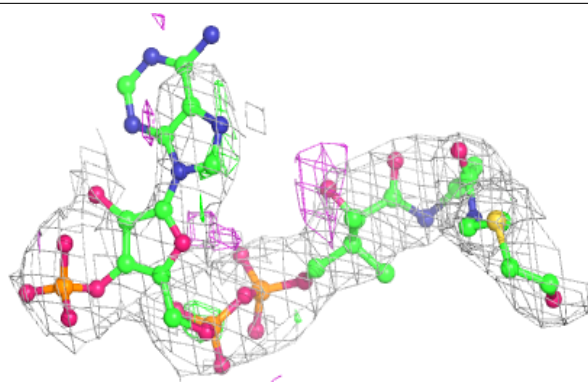
**Electron density around 1XE K 5201:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

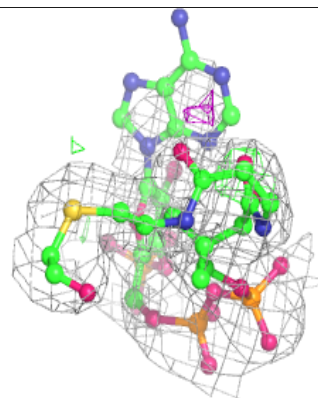
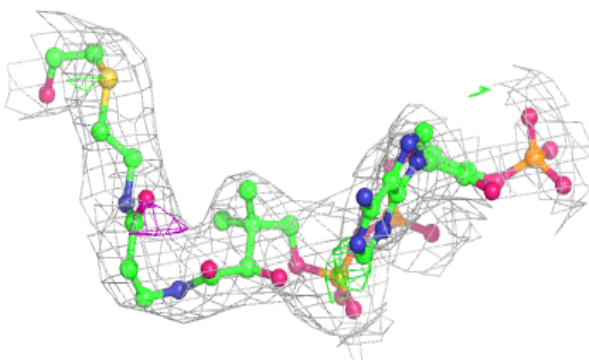
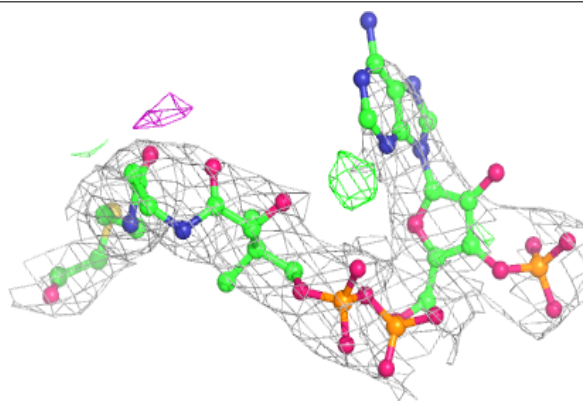


Electron density around 1XE I 5201:

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

**Electron density around 1XE L 5201:**

$2mF_o-DF_c$ (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.