



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:54 AM UTC

PDB ID : 5KAJ / pdb_00005kaj
Title : Crystal structure of a dioxygenase in the Crotonase superfamily in P21, A319C mutant
Authors : Li, K.; Fielding, E.N.; Condurso, H.L.; Bruner, S.D.
Deposited on : 2016-06-01
Resolution : 2.68 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

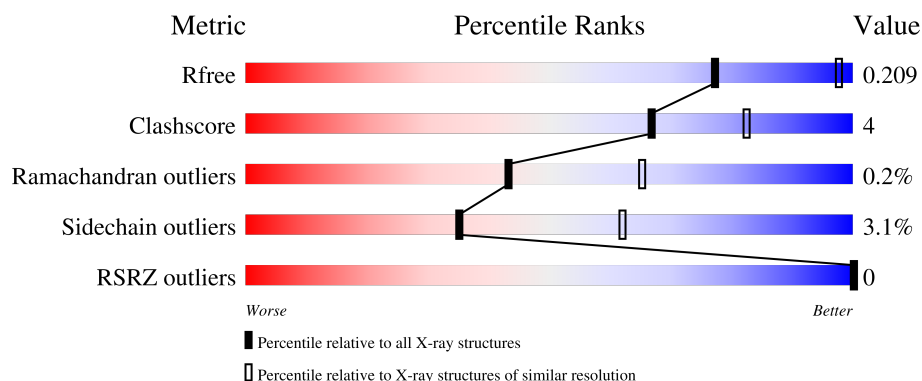
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	438	 84% 9% 5%
1	B	438	 87% 8% 5%
1	C	438	 84% 10% 5%
1	D	438	 86% 8% 5%
1	E	438	 86% 8% 5%

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Mol	Chain	Length	Quality of chain
1	F	438	 87%7% • 5%
1	G	438	 87%7% • 5%
1	H	438	 85%9% • 5%
1	I	438	 85%8% • 5%
1	J	438	 87%7% • 5%
1	K	438	 87%7% • 5%
1	L	438	 87%8% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 40477 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 (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3215	2017	600	587	11			
1	B	416	Total	C	N	O	S	0	0	0
			3230	2028	602	589	11			
1	C	416	Total	C	N	O	S	0	0	0
			3231	2028	602	590	11			
1	D	416	Total	C	N	O	S	0	0	0
			3230	2028	602	589	11			
1	E	417	Total	C	N	O	S	0	0	0
			3238	2032	603	592	11			
1	F	416	Total	C	N	O	S	0	0	0
			3231	2028	602	590	11			
1	G	417	Total	C	N	O	S	0	0	0
			3238	2032	603	592	11			
1	H	417	Total	C	N	O	S	0	0	0
			3238	2032	603	592	11			
1	I	415	Total	C	N	O	S	0	0	0
			3223	2024	601	587	11			
1	J	415	Total	C	N	O	S	0	0	0
			3223	2024	601	587	11			
1	K	416	Total	C	N	O	S	0	0	0
			3230	2028	602	589	11			
1	L	416	Total	C	N	O	S	0	0	0
			3231	2028	602	590	11			

There are 12 discrepancies between the modelled and reference sequences:

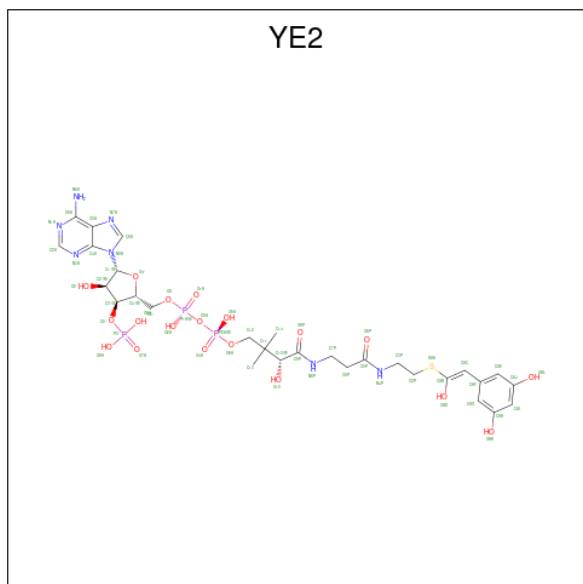
Chain	Residue	Modelled	Actual	Comment	Reference
A	319	CYS	ALA	engineered mutation	UNP Q8KLK7
B	319	CYS	ALA	engineered mutation	UNP Q8KLK7
C	319	CYS	ALA	engineered mutation	UNP Q8KLK7
D	319	CYS	ALA	engineered mutation	UNP Q8KLK7
E	319	CYS	ALA	engineered mutation	UNP Q8KLK7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	319	CYS	ALA	engineered mutation	UNP Q8KLK7
G	319	CYS	ALA	engineered mutation	UNP Q8KLK7
H	319	CYS	ALA	engineered mutation	UNP Q8KLK7
I	319	CYS	ALA	engineered mutation	UNP Q8KLK7
J	319	CYS	ALA	engineered mutation	UNP Q8KLK7
K	319	CYS	ALA	engineered mutation	UNP Q8KLK7
L	319	CYS	ALA	engineered mutation	UNP Q8KLK7

- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphono oxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(3 {R})-4-[[3-[2-[({E})-2-[3,5-bis(oxida nyl)phenyl]-1-oxidanyl-ethenyl]sulfanylethylamino]-3-oxidanylidene-propyl]amino]-2,2-d imethyl-3-oxidanyl-4-oxidanylidene-butyl] hydrogen phosphate (CCD ID: YE2) (formula: C₂₉H₄₂N₇O₁₉P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			59	29	7	19	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			59	29	7	19	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			59	29	7	19	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			59	29	7	19	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			59	29	7	19	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			59	29	7	19	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	G	1	Total 59	C 29	N 7	O 19	P 3	S 1	0	0
2	H	1	Total 59	C 29	N 7	O 19	P 3	S 1	0	0
2	I	1	Total 59	C 29	N 7	O 19	P 3	S 1	0	0
2	J	1	Total 59	C 29	N 7	O 19	P 3	S 1	0	0
2	K	1	Total 59	C 29	N 7	O 19	P 3	S 1	0	0
2	L	1	Total 59	C 29	N 7	O 19	P 3	S 1	0	0

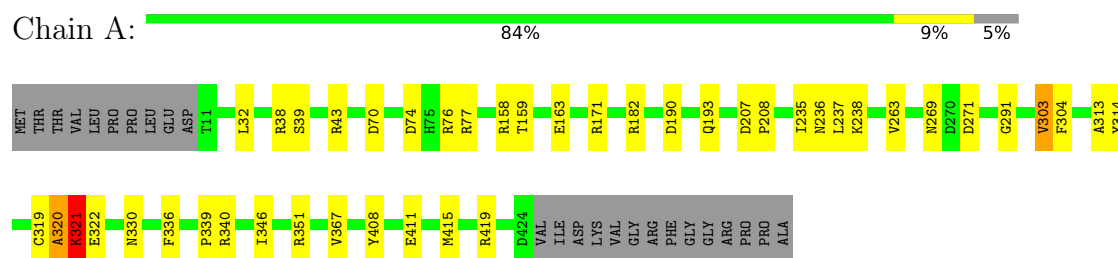
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	116	Total	O	0	0
			116	116		
3	C	69	Total	O	0	0
			69	69		
3	D	82	Total	O	0	0
			82	82		
3	E	81	Total	O	0	0
			81	81		
3	F	83	Total	O	0	0
			83	83		
3	G	86	Total	O	0	0
			86	86		
3	H	91	Total	O	0	0
			91	91		
3	I	81	Total	O	0	0
			81	81		
3	J	85	Total	O	0	0
			85	85		
3	K	91	Total	O	0	0
			91	91		
3	L	72	Total	O	0	0
			72	72		

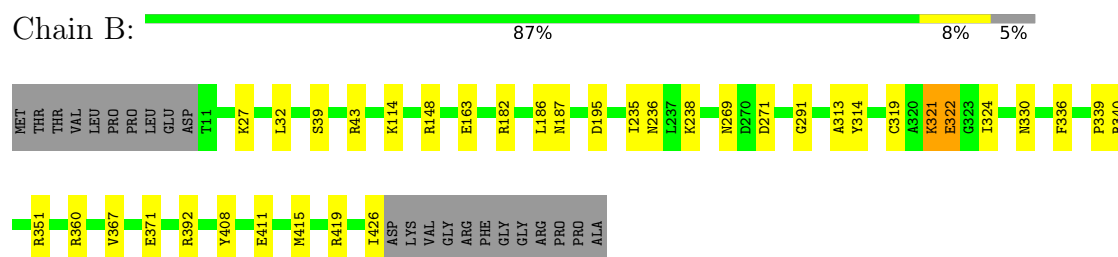
3 Residue-property plots

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.

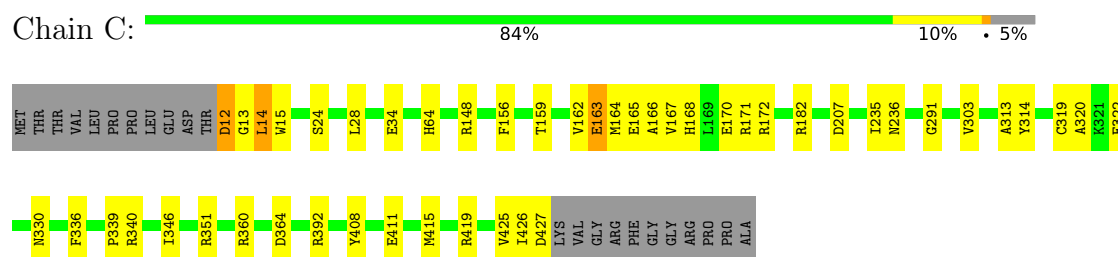
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase



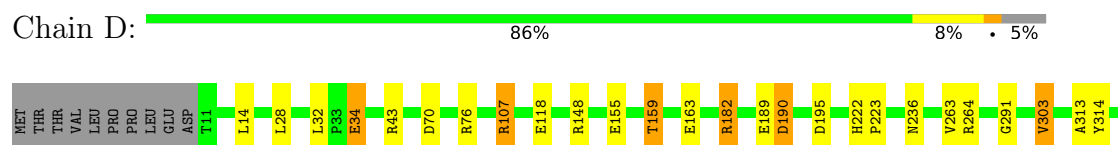
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase



- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

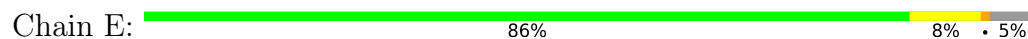


- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

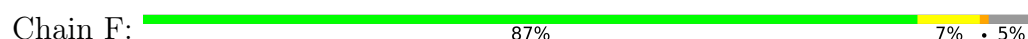




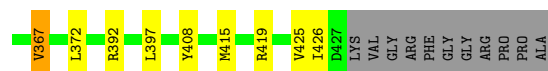
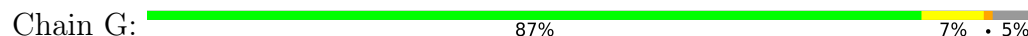
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase



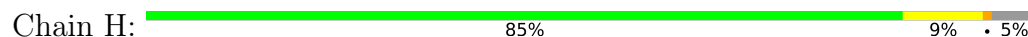
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase



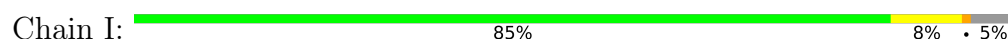
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase



- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase



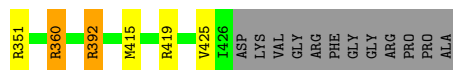
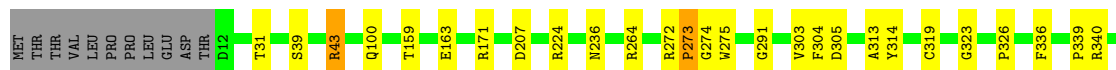
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase





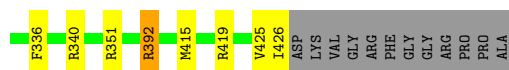
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain J: 87% 7% • 5%



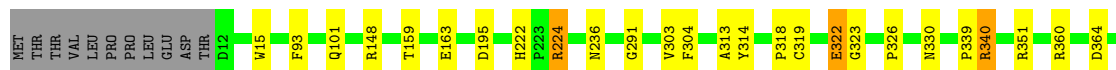
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain K: 87% 7% • 5%



- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain L: 87% 8% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.72Å 170.66Å 155.76Å 90.00° 89.89° 90.00°	Depositor
Resolution (Å)	39.56 – 2.68 39.56 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.56-2.68) 99.4 (39.56-2.68)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.193 , 0.215 0.186 , 0.209	Depositor DCC
R_{free} test set	10234 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 16.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	40477	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2379e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YE2

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	0.21	0/3275	0.53	0/4438
1	B	0.20	0/3290	0.54	0/4459
1	C	0.22	0/3291	0.53	0/4460
1	D	0.22	0/3290	0.55	0/4459
1	E	0.20	0/3298	0.55	0/4470
1	F	0.20	0/3291	0.54	0/4460
1	G	0.21	0/3298	0.54	0/4470
1	H	0.22	0/3298	0.69	4/4470 (0.1%)
1	I	0.23	0/3283	0.58	1/4449 (0.0%)
1	J	0.22	0/3283	0.56	0/4449
1	K	0.22	0/3290	0.56	3/4459 (0.1%)
1	L	0.20	0/3291	0.53	0/4460
All	All	0.21	0/39478	0.56	8/53503 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	155	GLU	N-CA-C	-19.54	77.13	109.96
1	H	156	PHE	N-CA-CB	18.31	141.44	110.49
1	H	322	GLU	N-CA-C	-5.96	105.86	113.01
1	K	321	LYS	CA-C-N	5.89	132.79	121.54
1	K	321	LYS	C-N-CA	5.89	132.79	121.54

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	3215	0	3231	34	0
1	B	3230	0	3251	22	0
1	C	3231	0	3248	38	0
1	D	3230	0	3251	23	0
1	E	3238	0	3255	33	0
1	F	3231	0	3248	24	0
1	G	3238	0	3255	20	0
1	H	3238	0	3255	26	0
1	I	3223	0	3244	32	0
1	J	3223	0	3244	21	0
1	K	3230	0	3251	18	0
1	L	3231	0	3248	21	0
2	A	59	0	0	7	0
2	B	59	0	0	7	0
2	C	59	0	0	6	0
2	D	59	0	0	3	0
2	E	59	0	0	4	0
2	F	59	0	0	1	0
2	G	59	0	0	5	0
2	H	59	0	0	4	0
2	I	59	0	0	2	0
2	J	59	0	0	2	0
2	K	59	0	0	2	0
2	L	59	0	0	2	0
3	A	74	0	0	0	0
3	B	116	0	0	2	0
3	C	69	0	0	2	0
3	D	82	0	0	0	0
3	E	81	0	0	0	0
3	F	83	0	0	2	0
3	G	86	0	0	0	0
3	H	91	0	0	1	0
3	I	81	0	0	4	0
3	J	85	0	0	0	0
3	K	91	0	0	0	0
3	L	72	0	0	0	0
All	All	40477	0	38981	288	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.

The worst 5 of 288 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:CD2	1:C:64:HIS:HE1	1.53	1.22
1:C:14:LEU:HD22	1:C:64:HIS:CE1	1.87	1.10
1:C:14:LEU:CD2	1:C:64:HIS:CE1	2.39	1.04
1:E:319:CYS:SG	2:E:501:YE2:CAC	2.51	0.99
1:A:319:CYS:SG	2:A:501:YE2:CAC	2.50	0.98

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	412/438 (94%)	403 (98%)	7 (2%)	2 (0%)	24	45
1	B	414/438 (94%)	408 (99%)	6 (1%)	0	100	100
1	C	414/438 (94%)	405 (98%)	9 (2%)	0	100	100
1	D	414/438 (94%)	407 (98%)	7 (2%)	0	100	100
1	E	415/438 (95%)	401 (97%)	11 (3%)	3 (1%)	18	37
1	F	414/438 (94%)	407 (98%)	6 (1%)	1 (0%)	43	65
1	G	415/438 (95%)	409 (99%)	6 (1%)	0	100	100
1	H	415/438 (95%)	405 (98%)	9 (2%)	1 (0%)	43	65
1	I	413/438 (94%)	405 (98%)	6 (2%)	2 (0%)	24	45
1	J	413/438 (94%)	402 (97%)	9 (2%)	2 (0%)	24	45
1	K	414/438 (94%)	406 (98%)	7 (2%)	1 (0%)	43	65
1	L	414/438 (94%)	407 (98%)	7 (2%)	0	100	100
All	All	4967/5256 (94%)	4865 (98%)	90 (2%)	12 (0%)	43	65

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	ALA
1	E	324	ILE
1	H	156	PHE
1	E	320	ALA
1	I	111	GLN

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	326/346 (94%)	317 (97%)	9 (3%)	38	65
1	B	328/346 (95%)	317 (97%)	11 (3%)	32	59
1	C	328/346 (95%)	318 (97%)	10 (3%)	36	63
1	D	328/346 (95%)	315 (96%)	13 (4%)	28	53
1	E	329/346 (95%)	323 (98%)	6 (2%)	51	76
1	F	328/346 (95%)	319 (97%)	9 (3%)	39	67
1	G	329/346 (95%)	315 (96%)	14 (4%)	26	51
1	H	329/346 (95%)	320 (97%)	9 (3%)	39	67
1	I	327/346 (94%)	314 (96%)	13 (4%)	28	53
1	J	327/346 (94%)	317 (97%)	10 (3%)	35	62
1	K	328/346 (95%)	321 (98%)	7 (2%)	47	73
1	L	328/346 (95%)	317 (97%)	11 (3%)	32	59
All	All	3935/4152 (95%)	3813 (97%)	122 (3%)	35	62

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	427	ASP
1	K	426	ILE
1	G	426	ILE
1	K	392	ARG

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Mol	Chain	Res	Type
1	L	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	79	HIS
1	L	192	GLN
1	L	222	HIS
1	K	222	HIS
1	D	117	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
2	YE2	E	501	-	59,62,62	4.09	21 (35%)	85,92,92	2.16	12 (14%)
2	YE2	L	501	-	59,62,62	4.09	19 (32%)	85,92,92	1.79	10 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	YE2	B	501	-	59,62,62	4.40	17 (28%)	85,92,92	1.82	13 (15%)
2	YE2	J	501	-	59,62,62	4.27	17 (28%)	85,92,92	1.86	10 (11%)
2	YE2	K	501	-	59,62,62	4.42	17 (28%)	85,92,92	1.80	12 (14%)
2	YE2	F	501	-	59,62,62	4.36	14 (23%)	85,92,92	1.81	12 (14%)
2	YE2	H	501	-	59,62,62	4.12	18 (30%)	85,92,92	1.89	18 (21%)
2	YE2	A	501	-	59,62,62	4.13	18 (30%)	85,92,92	1.89	18 (21%)
2	YE2	C	501	-	59,62,62	4.14	15 (25%)	85,92,92	1.78	12 (14%)
2	YE2	D	501	-	59,62,62	4.28	15 (25%)	85,92,92	1.70	8 (9%)
2	YE2	I	501	-	59,62,62	4.33	15 (25%)	85,92,92	1.84	10 (11%)
2	YE2	G	501	-	59,62,62	4.21	14 (23%)	85,92,92	1.73	9 (10%)

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	YE2	E	501	-	-	13/51/71/71	0/4/4/4
2	YE2	L	501	-	-	6/51/71/71	0/4/4/4
2	YE2	B	501	-	-	17/51/71/71	0/4/4/4
2	YE2	J	501	-	-	8/51/71/71	0/4/4/4
2	YE2	K	501	-	-	17/51/71/71	0/4/4/4
2	YE2	F	501	-	-	12/51/71/71	0/4/4/4
2	YE2	H	501	-	-	11/51/71/71	0/4/4/4
2	YE2	A	501	-	-	11/51/71/71	0/4/4/4
2	YE2	C	501	-	-	6/51/71/71	0/4/4/4
2	YE2	D	501	-	-	6/51/71/71	0/4/4/4
2	YE2	I	501	-	-	7/51/71/71	0/4/4/4
2	YE2	G	501	-	-	10/51/71/71	0/4/4/4

The worst 5 of 200 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	YE2	CAB-SAA	-27.23	1.38	1.74
2	I	501	YE2	CAB-SAA	-27.19	1.38	1.74
2	F	501	YE2	CAB-SAA	-26.91	1.38	1.74
2	K	501	YE2	CAB-SAA	-26.40	1.39	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	YE2	CAB-SAA	-26.13	1.39	1.74

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	YE2	C2P-SAA-CAB	14.12	132.20	101.66
2	J	501	YE2	C2P-SAA-CAB	11.20	125.89	101.66
2	I	501	YE2	C2P-SAA-CAB	11.14	125.75	101.66
2	B	501	YE2	C2P-SAA-CAB	10.86	125.15	101.66
2	L	501	YE2	C2P-SAA-CAB	10.81	125.03	101.66

There are no chirality outliers.

5 of 124 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	YE2	C5'-O5'-P1A-O3A
2	A	501	YE2	C9P-C10-C11-C12
2	A	501	YE2	C9P-C10-C11-C13
2	A	501	YE2	C9P-C10-C11-C14
2	A	501	YE2	O10-C10-C11-C13

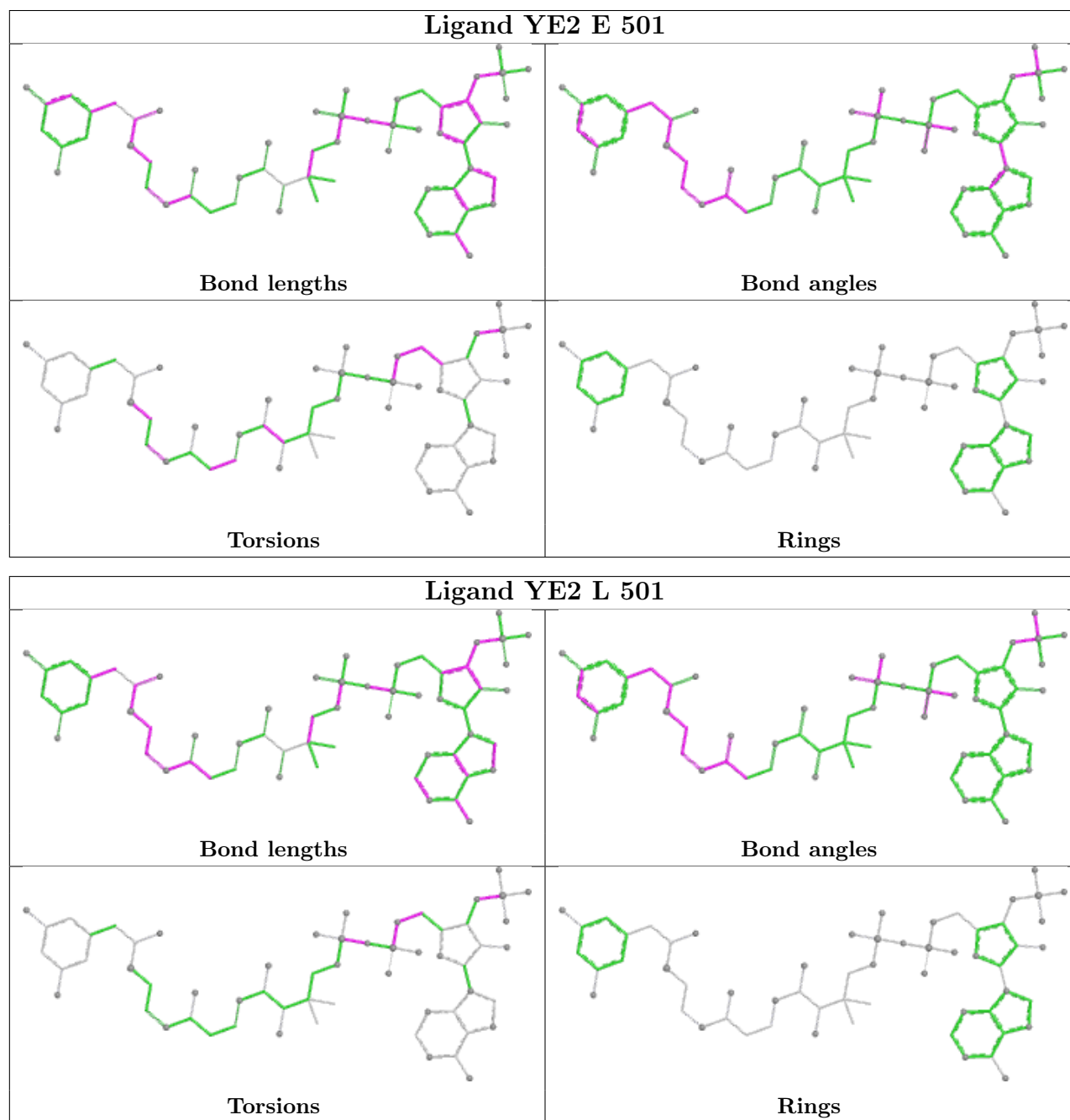
There are no ring outliers.

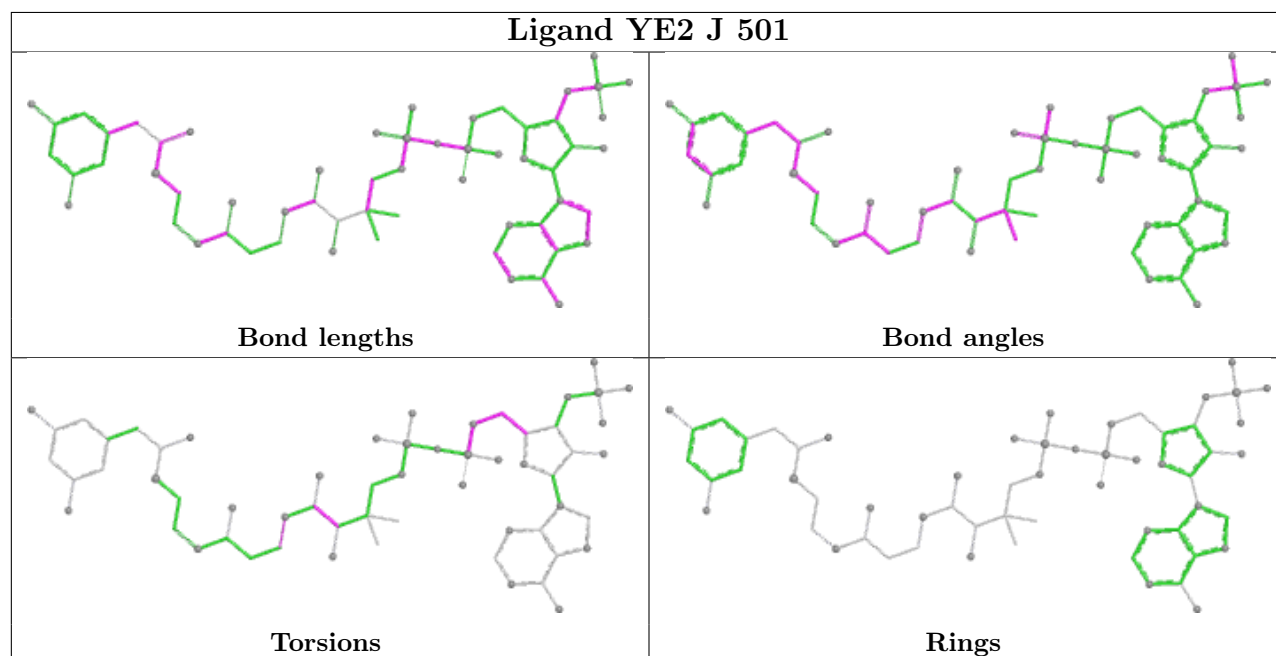
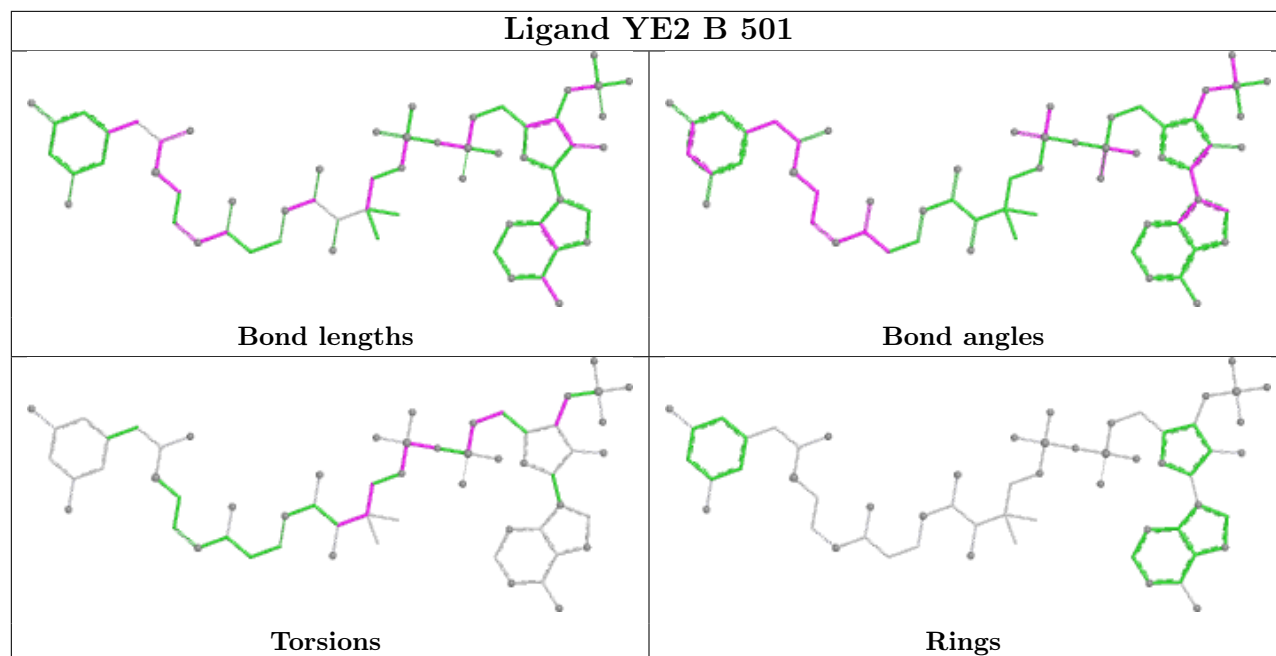
12 monomers are involved in 45 short contacts:

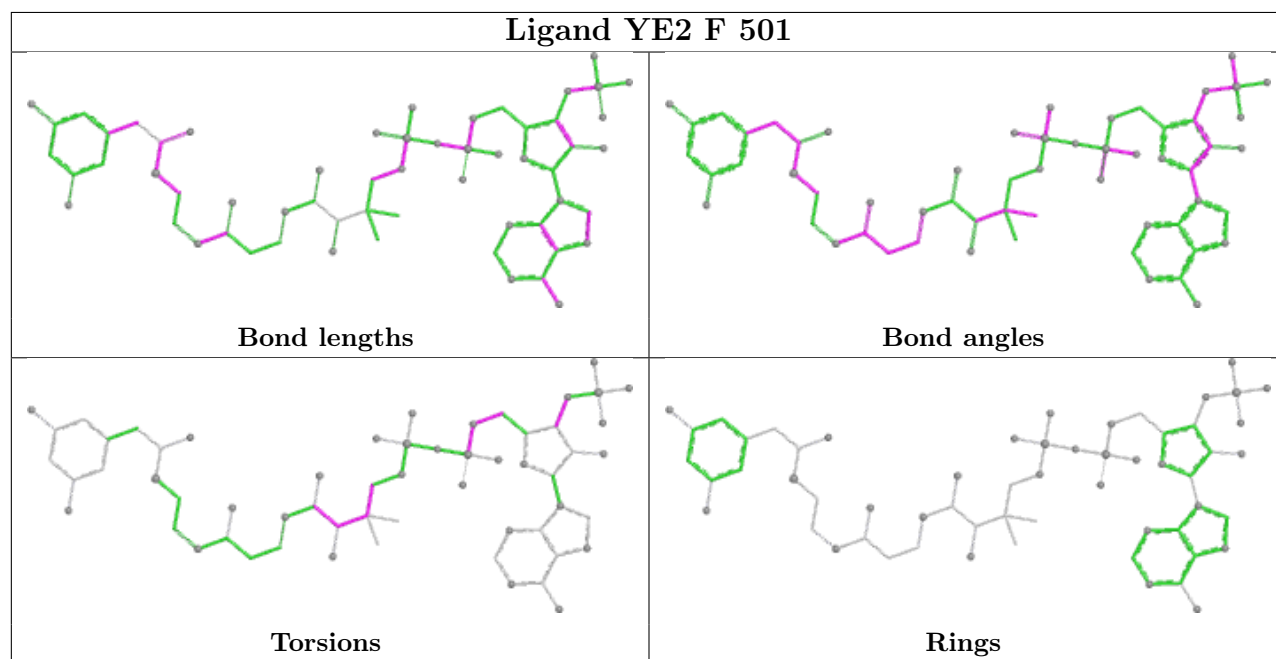
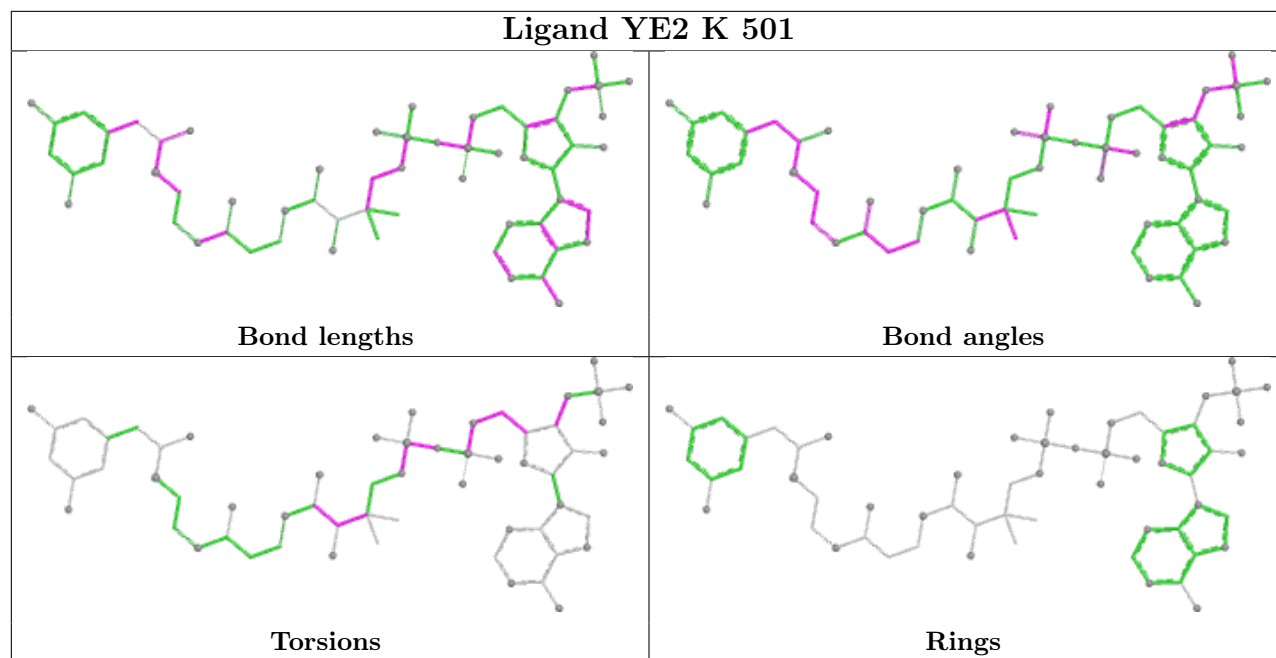
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	YE2	4	0
2	L	501	YE2	2	0
2	B	501	YE2	7	0
2	J	501	YE2	2	0
2	K	501	YE2	2	0
2	F	501	YE2	1	0
2	H	501	YE2	4	0
2	A	501	YE2	7	0
2	C	501	YE2	6	0
2	D	501	YE2	3	0
2	I	501	YE2	2	0
2	G	501	YE2	5	0

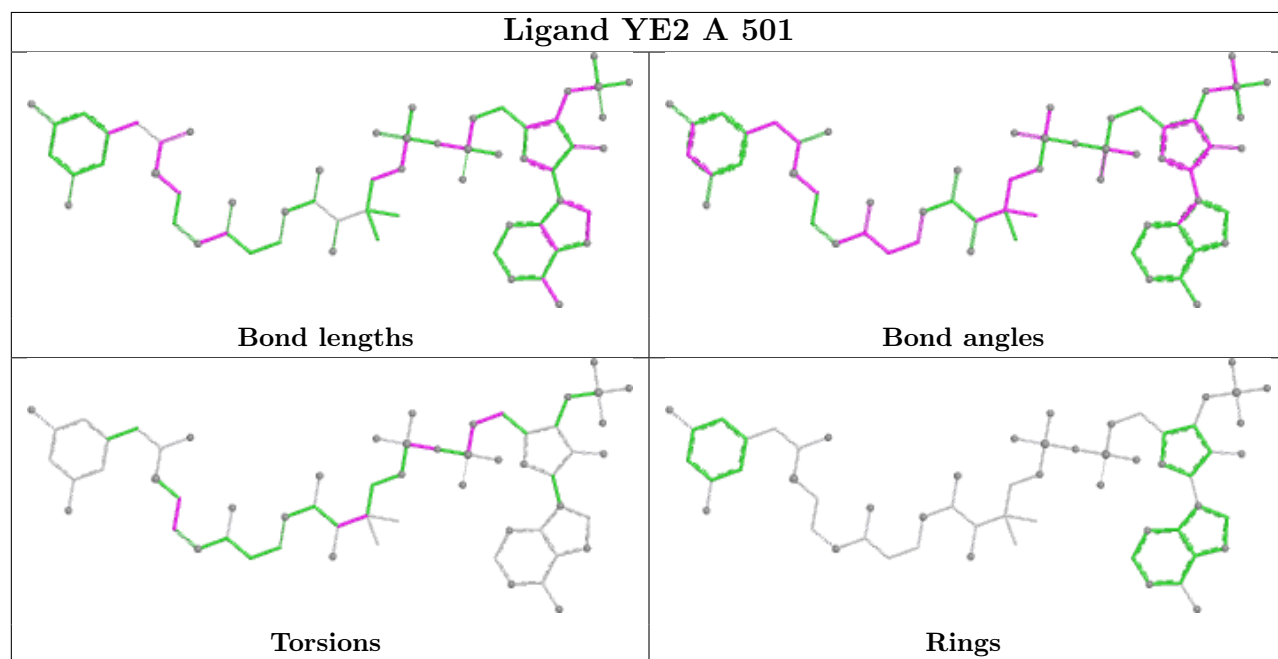
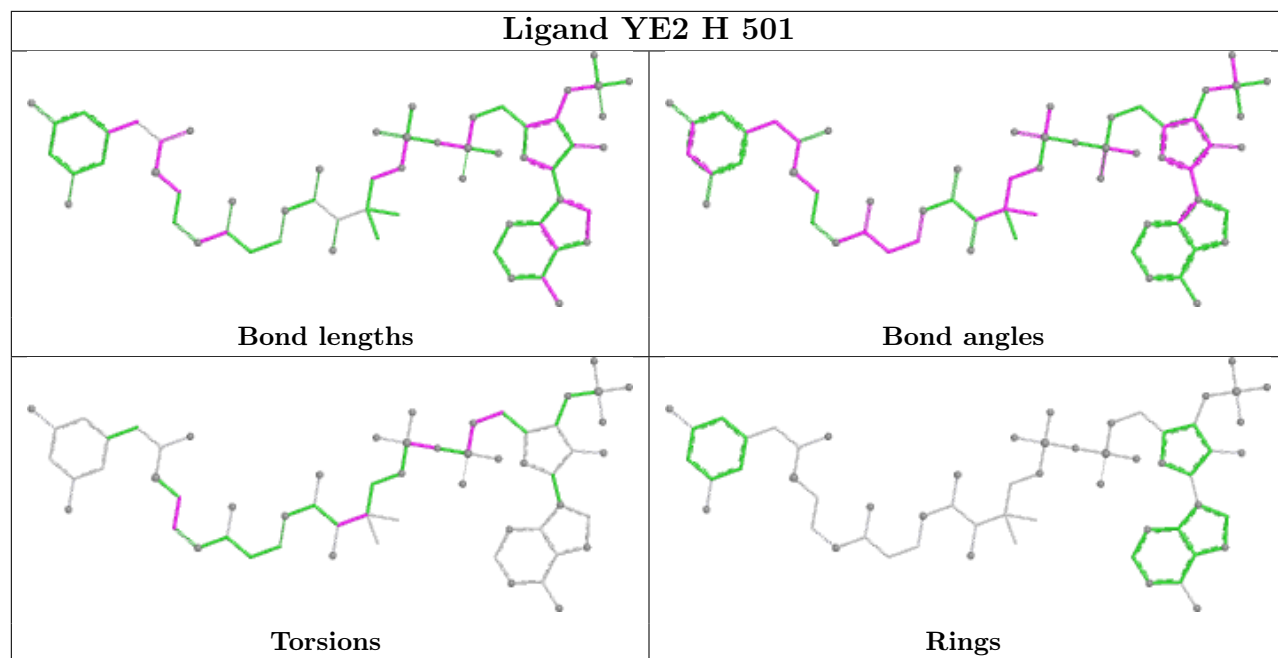
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

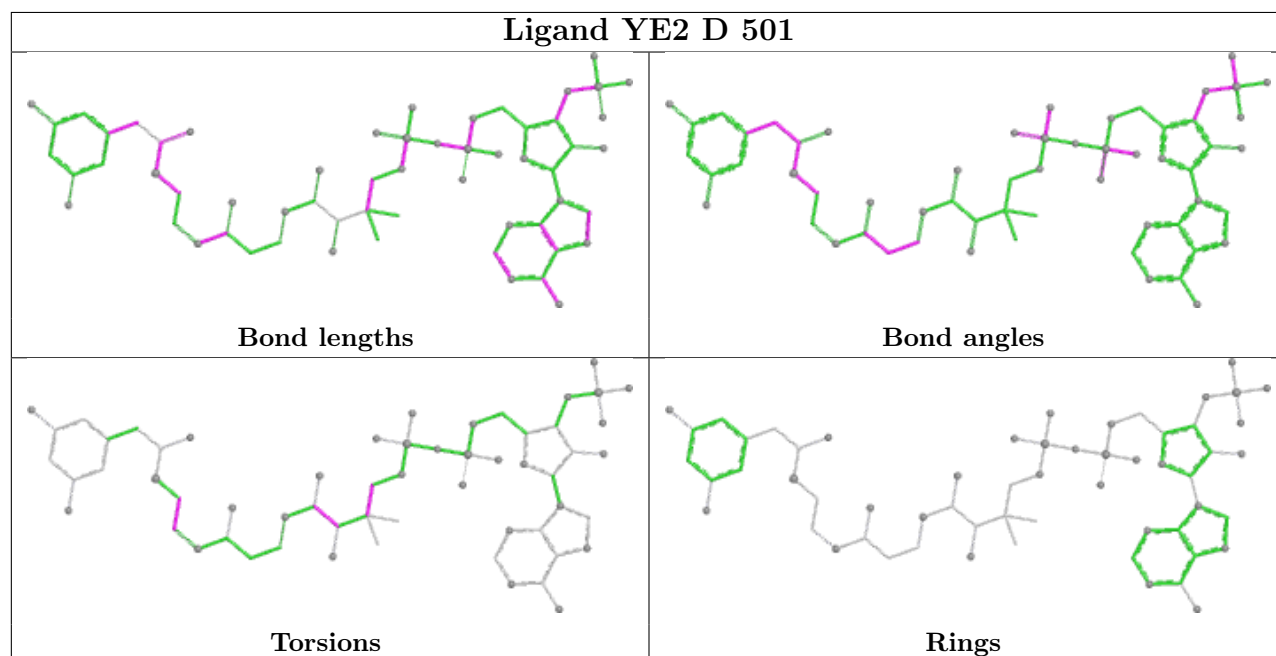
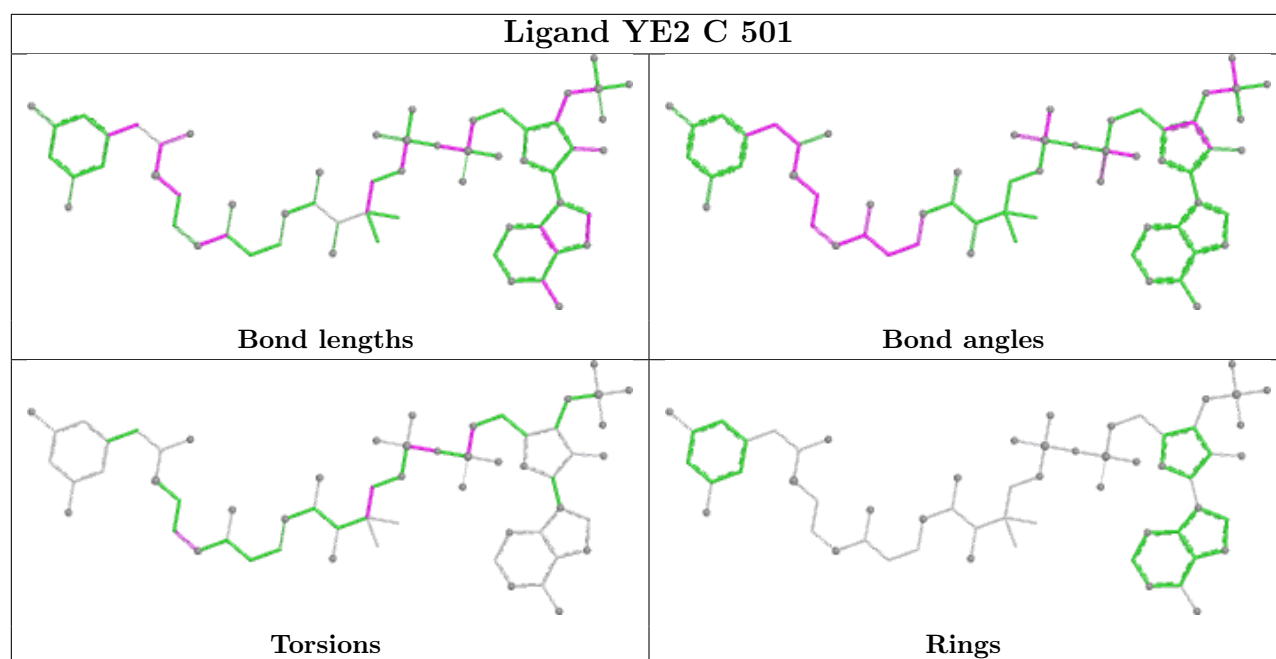
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

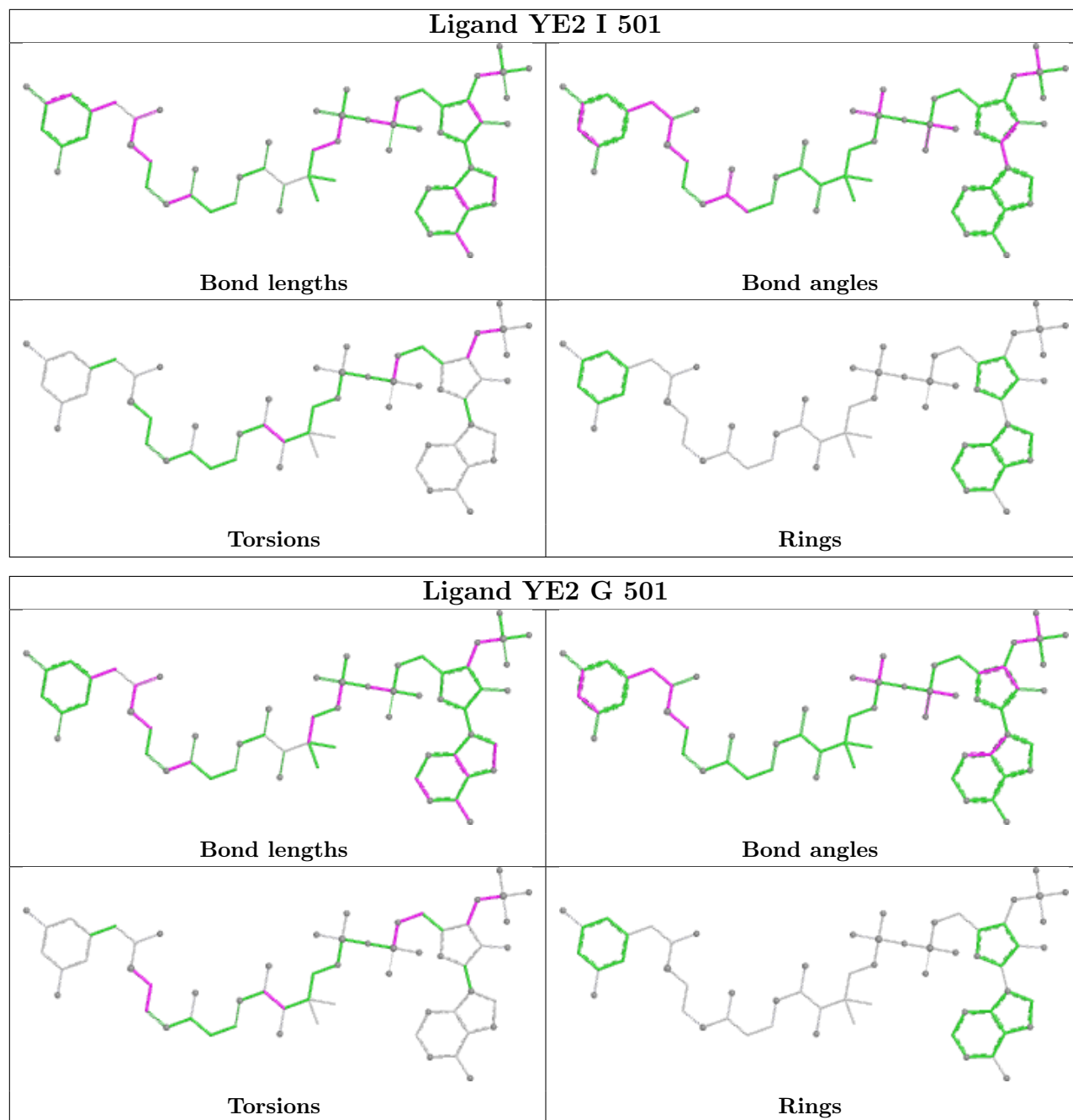












5.7 Other polymers [i](#)

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	414/438 (94%)	-1.48	0 100 100	27, 45, 89, 108	0
1	B	416/438 (94%)	-1.57	0 100 100	26, 39, 65, 90	0
1	C	416/438 (94%)	-1.49	0 100 100	25, 43, 82, 96	0
1	D	416/438 (94%)	-1.55	0 100 100	21, 35, 69, 89	0
1	E	417/438 (95%)	-1.55	0 100 100	24, 40, 64, 86	0
1	F	416/438 (94%)	-1.56	0 100 100	24, 39, 64, 77	0
1	G	417/438 (95%)	-1.59	0 100 100	22, 35, 59, 78	0
1	H	417/438 (95%)	-1.57	0 100 100	25, 39, 64, 81	0
1	I	415/438 (94%)	-1.55	0 100 100	26, 39, 71, 98	0
1	J	415/438 (94%)	-1.50	0 100 100	26, 42, 80, 105	0
1	K	416/438 (94%)	-1.58	0 100 100	25, 37, 62, 88	0
1	L	416/438 (94%)	-1.50	0 100 100	23, 41, 77, 94	0
All	All	4991/5256 (94%)	-1.54	0 100 100	21, 39, 72, 108	0

There are no RSRZ outliers to report.

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

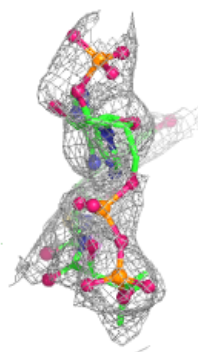
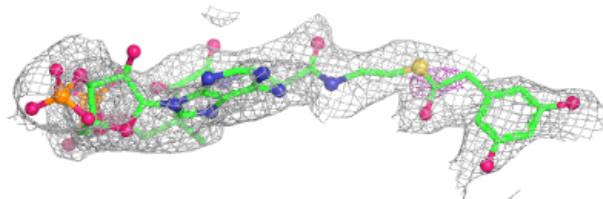
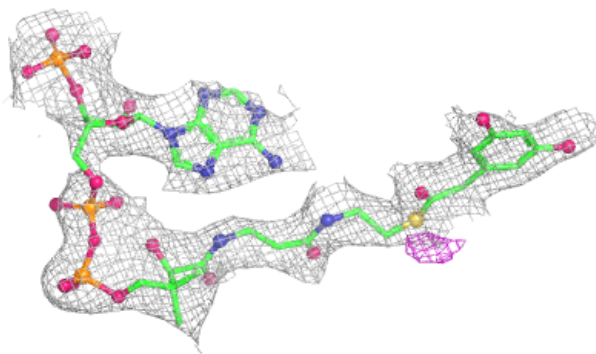
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	YE2	K	501	59/59	0.98	0.05	37,64,88,93	0
2	YE2	B	501	59/59	0.99	0.04	41,62,90,96	0
2	YE2	C	501	59/59	0.99	0.04	40,61,80,83	0
2	YE2	D	501	59/59	0.99	0.03	41,53,69,70	0
2	YE2	E	501	59/59	0.99	0.04	30,69,82,84	0
2	YE2	F	501	59/59	0.99	0.04	39,57,73,76	0
2	YE2	G	501	59/59	0.99	0.03	41,54,76,83	0
2	YE2	H	501	59/59	0.99	0.05	42,74,86,88	0
2	YE2	I	501	59/59	0.99	0.04	38,57,70,78	0
2	YE2	J	501	59/59	0.99	0.04	46,66,81,84	0
2	YE2	A	501	59/59	0.99	0.04	44,76,88,90	0
2	YE2	L	501	59/59	0.99	0.03	39,64,82,92	0

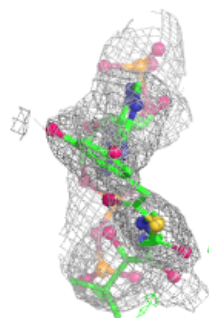
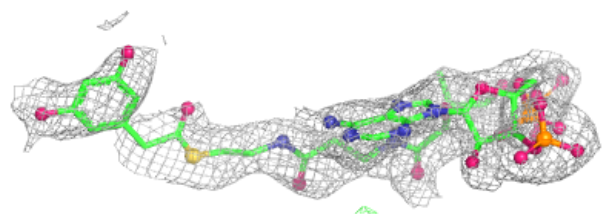
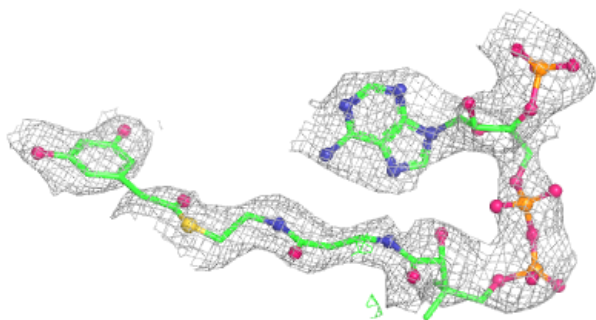
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YE2 K 501:

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

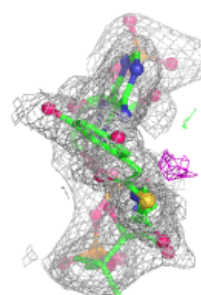
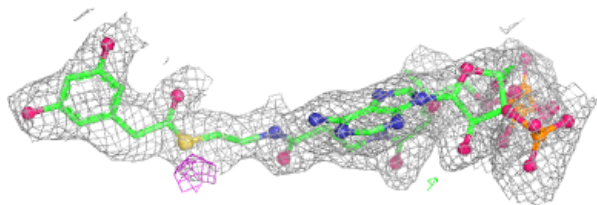
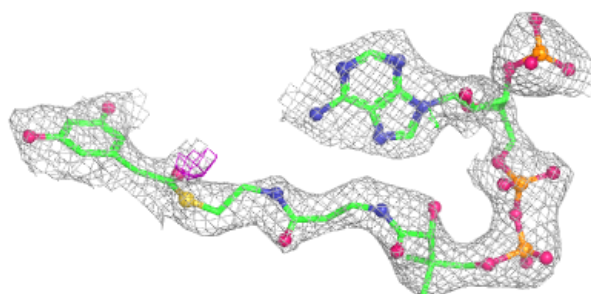
**Electron density around YE2 B 501:**

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and green (positive)

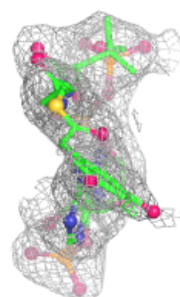
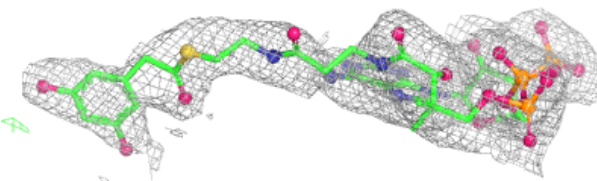
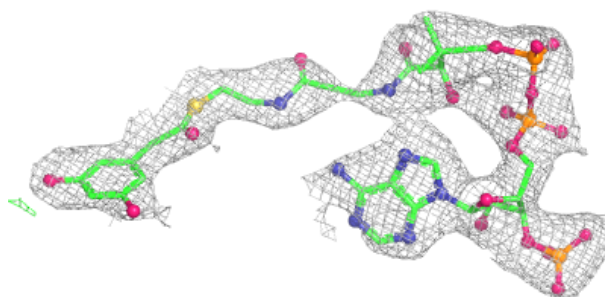


Electron density around YE2 C 501:

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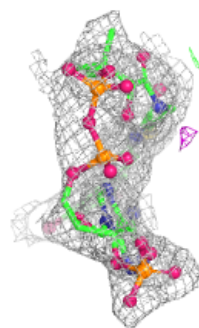
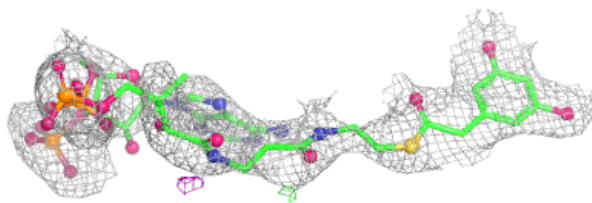
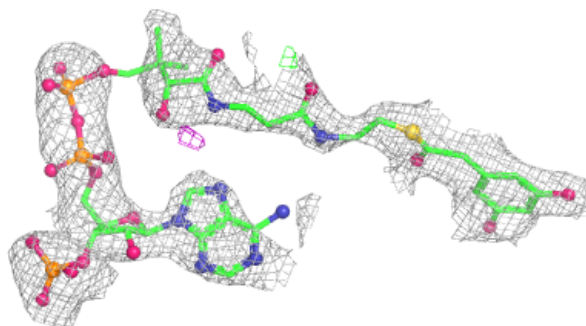
**Electron density around YE2 D 501:**

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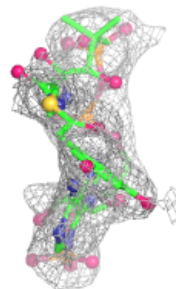
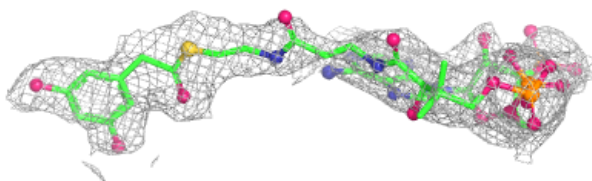
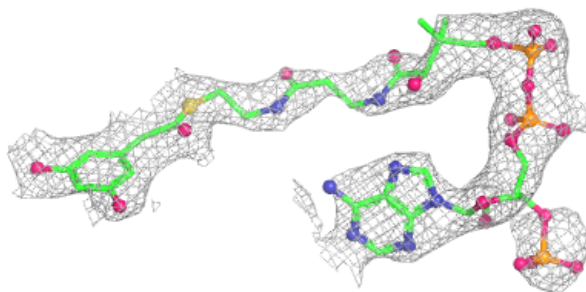


Electron density around YE2 E 501:

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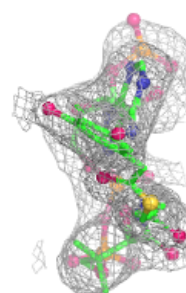
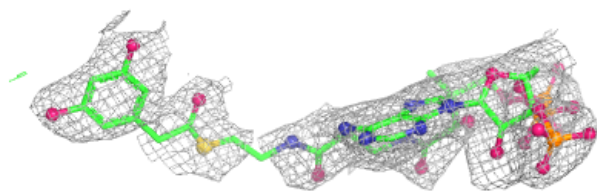
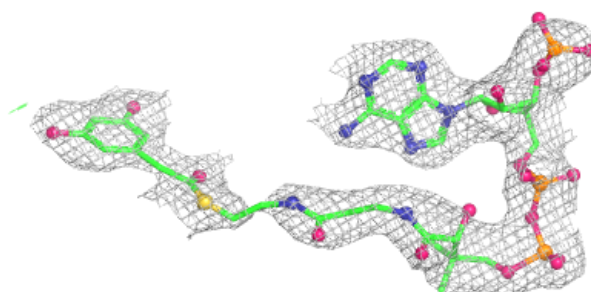
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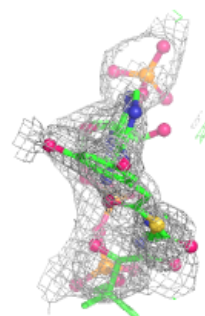
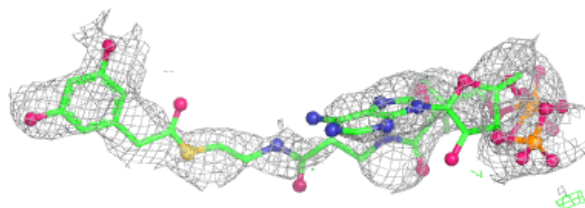
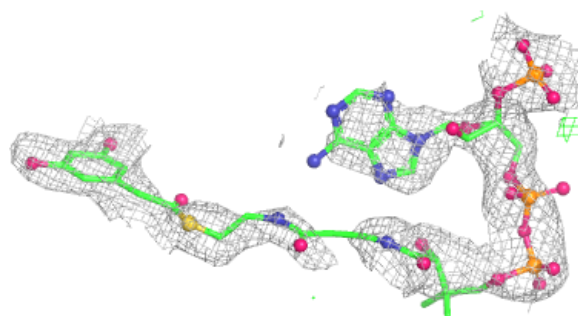


Electron density around YE2 G 501:

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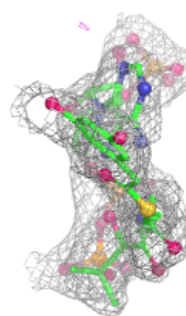
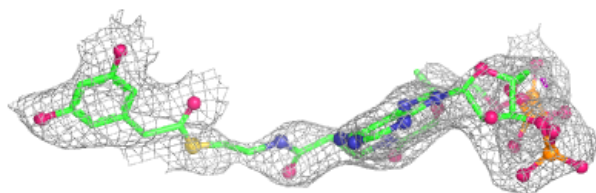
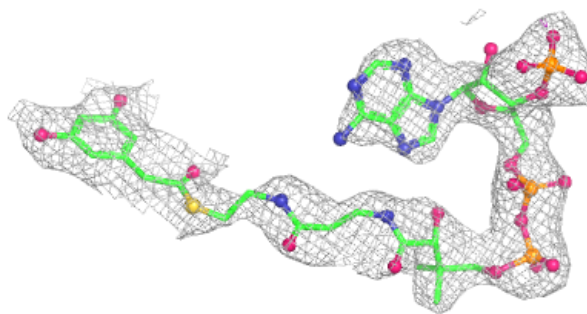
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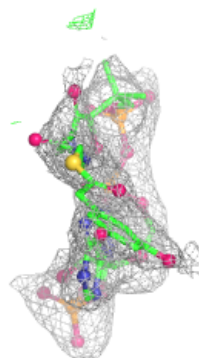
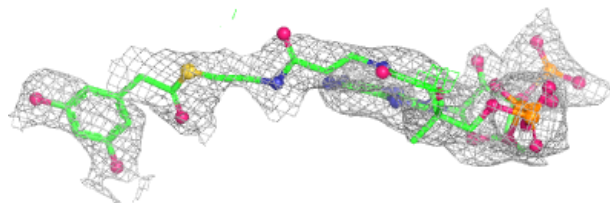
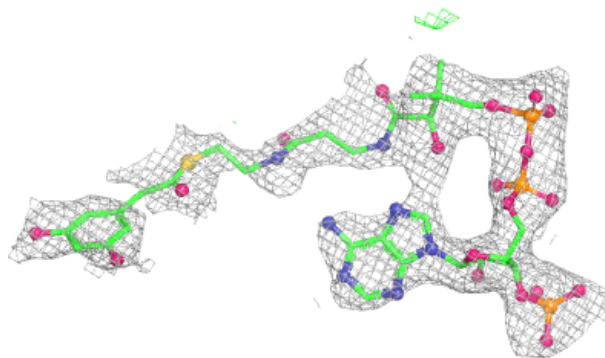


Electron density around YE2 I 501:

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and green (positive)

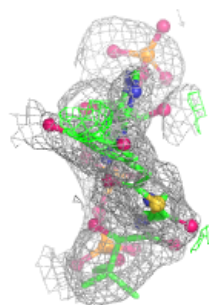
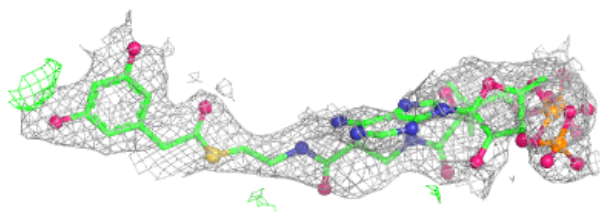
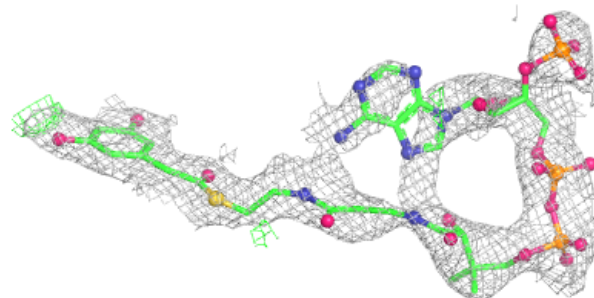
**Electron density around YE2 J 501:**

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and green (positive)

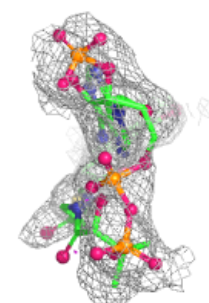
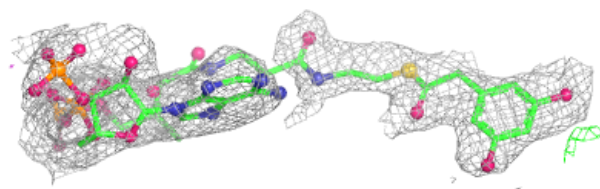
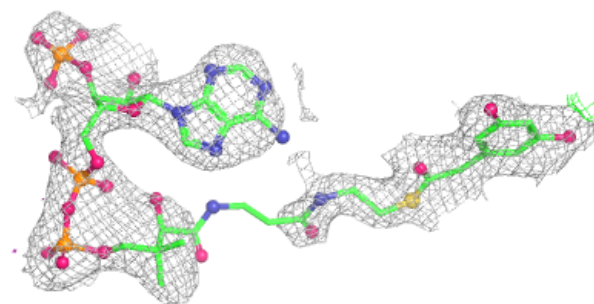


Electron density around YE2 A 501:

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

**Electron density around YE2 L 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.