



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2020 – 10:18 PM JST

PDB ID : 6LPK
Title : A2AR crystallized in EROCO17+4, LCP-SFX at 293 K
Authors : Ihara, K.; Hato, M.; Nakane, T.; Yamashita, K.; Kimura-Someya, T.; Hosaka, T.; Ishizuka-Katsura, Y.; Tanaka, R.; Tanaka, T.; Sugahara, M.; Hirata, K.; Yamamoto, M.; Nureki, O.; Tono, K.; Nango, E.; Iwata, S.; Shirouzu, M.
Deposited on : 2020-01-10
Resolution : 1.80 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 : 2.14.6
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) : 2.14.6

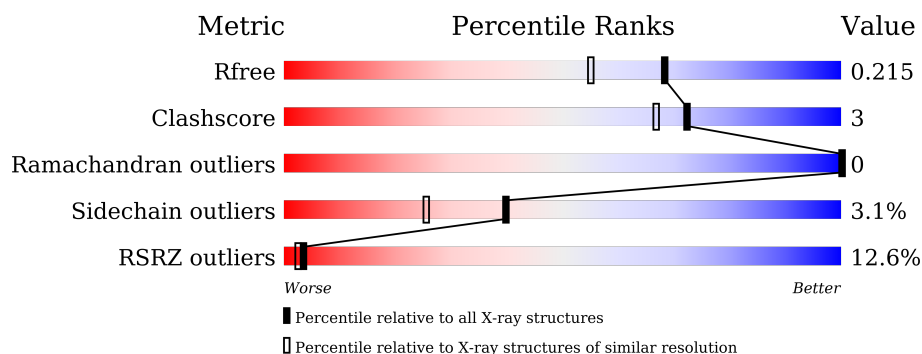
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	447	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 3583 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 Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3036	1977	515	522	22			

There are 39 discrepancies between the modelled and reference sequences:

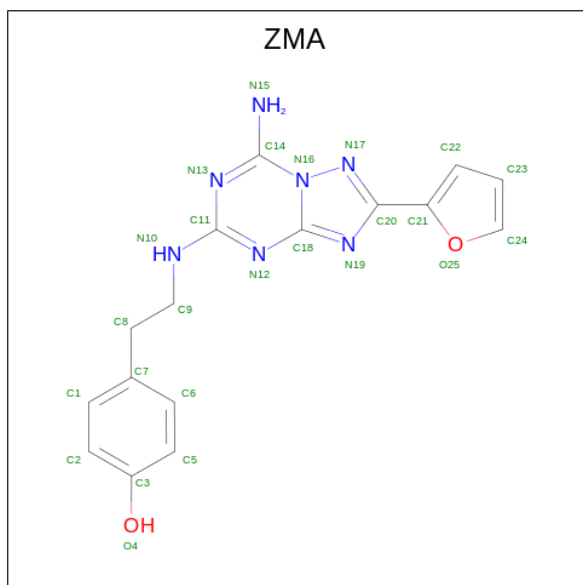
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl)[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl} phenol (three-letter code: ZMA) (formula: C₁₆H₁₅N₇O₂).

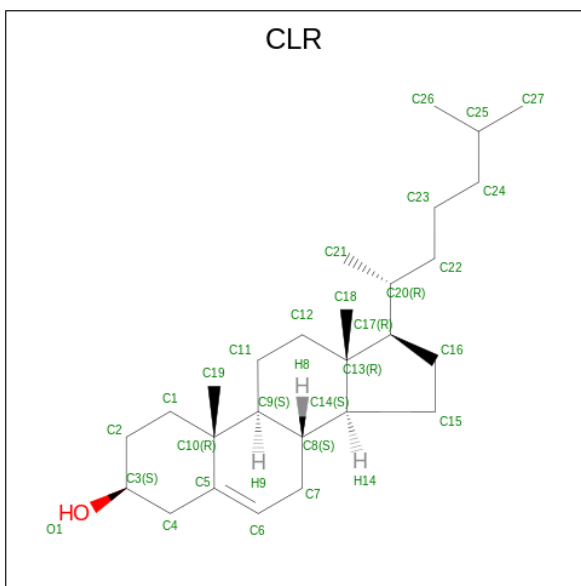


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

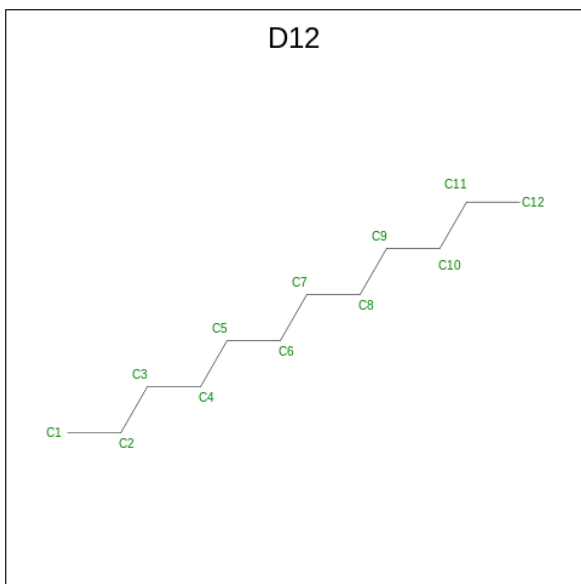
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



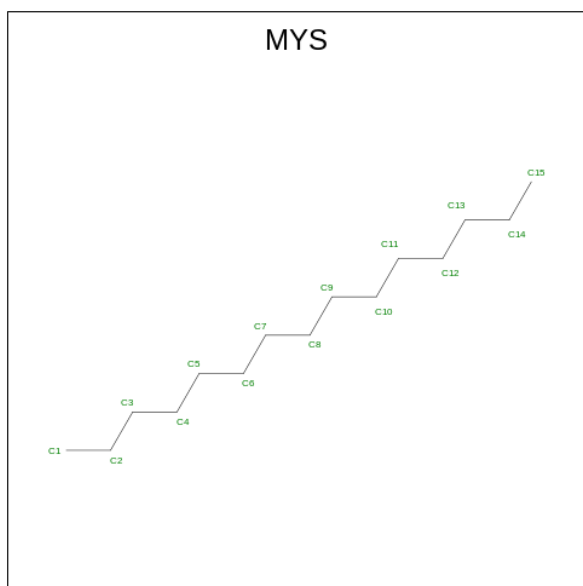
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



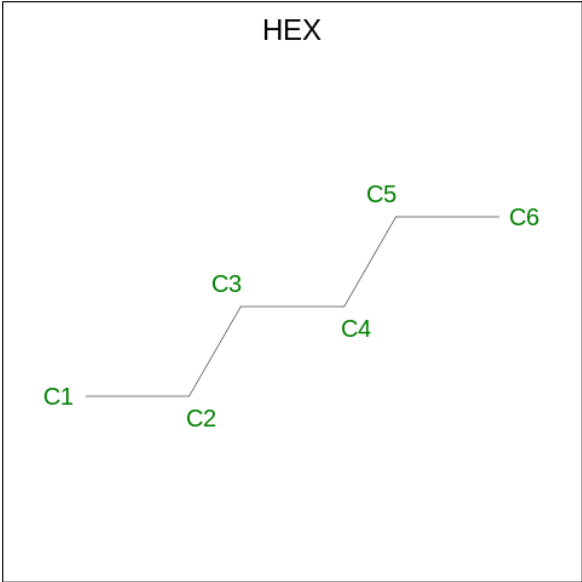
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 12 12	0	0

- Molecule 6 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).



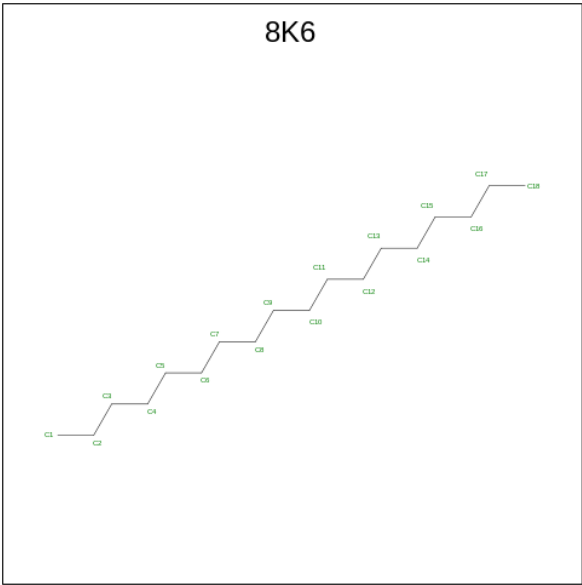
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0

- Molecule 7 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



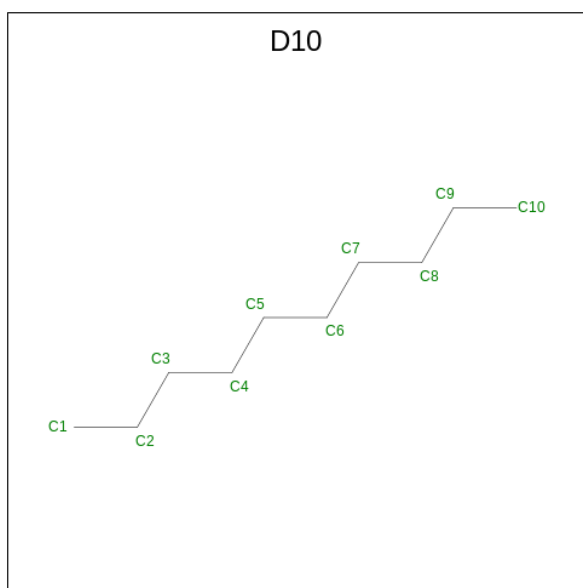
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 6 6	0	0

- Molecule 8 is Octadecane (three-letter code: 8K6) (formula: C₁₈H₃₈).



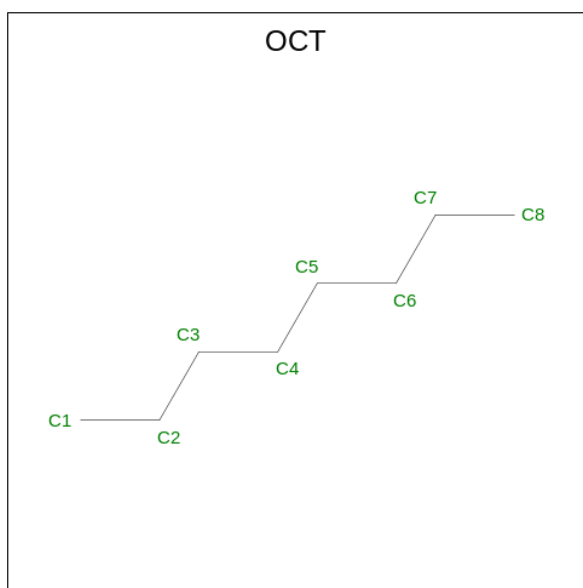
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 18 18	0	0
8	A	1	Total C 18 18	0	0
8	A	1	Total C 18 18	0	0

- Molecule 9 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C 10 10	0	0

- Molecule 10 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



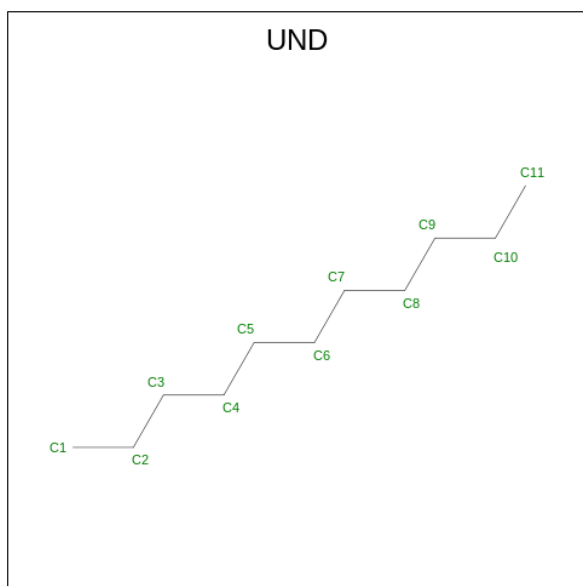
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 8 8	0	0
10	A	1	Total C 8 8	0	0

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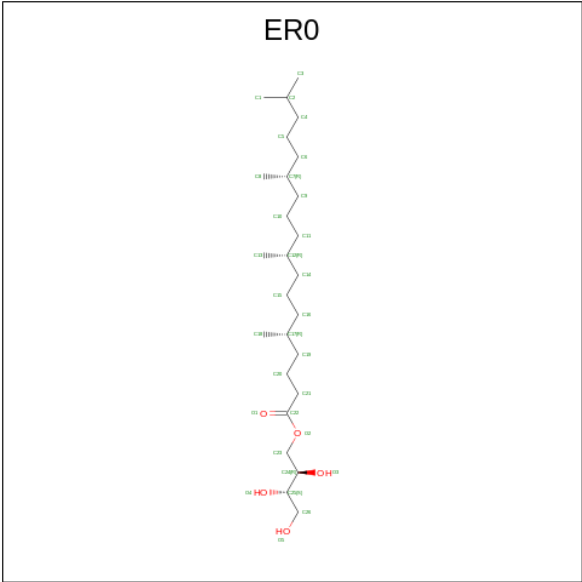
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 8 8	0	0

- Molecule 11 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



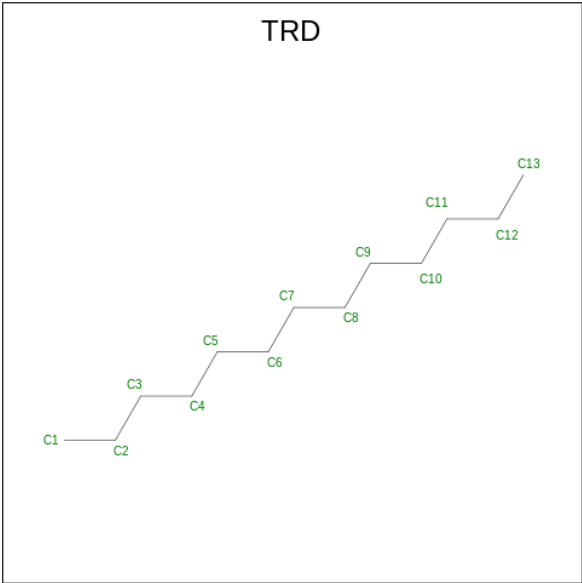
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C 11 11	0	0

- Molecule 12 is [(2 {R},3 {S})-2,3,4-tris(oxidanyl)butyl] (5 {R},9 {R},13 {R})-5,9,13,17-tetramethyloctadecanoate (three-letter code: ER0) (formula: $C_{26}H_{52}O_5$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			31	26	5		
12	A	1	Total	C	O	0	0
			31	26	5		

- Molecule 13 is TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	C	0	0
			13	13		
13	A	1	Total	C	0	0
			13	13		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C 13 13	0	0
13	A	1	Total C 13 13	0	0

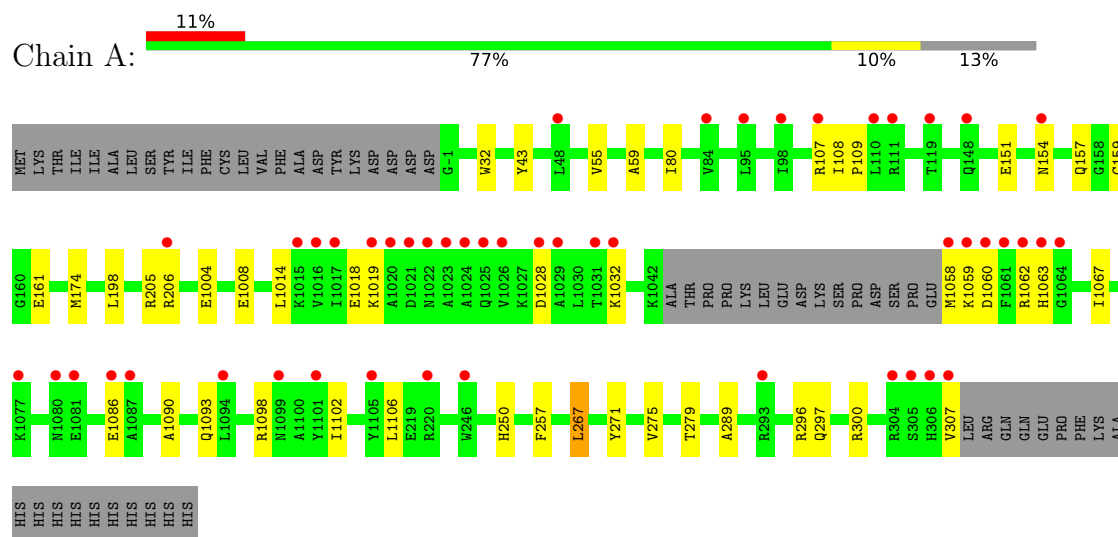
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	116	Total O 116 116	0	0

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: Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	40.50Å 179.20Å 142.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.40 – 1.80 30.35 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.40-1.80) 100.0 (30.35-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.177 , 0.209 0.188 , 0.215	Depositor DCC
R_{free} test set	2453 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3583	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: D10, D12, NA, MYS, ZMA, HEX, TRD, UND, ER0, 8K6, OCT, CLR

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	0.68	0/3101	0.82	0/4215

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3036	0	3112	23	1
2	A	25	0	14	1	0
3	A	1	0	0	0	0
4	A	84	0	138	2	0
5	A	12	0	26	0	0
6	A	90	0	192	1	0
7	A	6	0	14	0	0
8	A	54	0	114	2	0
9	A	10	0	22	0	0
10	A	24	0	54	0	0
11	A	11	0	24	0	0
12	A	62	0	0	0	0
13	A	52	0	112	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	116	0	0	2	0
All	All	3583	0	3822	25	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 3.

The worst 5 of 25 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:154:ASN:OD1	1:A:159:CYS:HB2	1.90	0.72
6:A:2414:MYS:H91	8:A:2419:8K6:H13C	1.79	0.64
1:A:275:VAL:O	1:A:279:THR:HG23	1.97	0.64
1:A:80:ILE:HD11	4:A:2403:CLR:H182	1.81	0.61
1:A:80:ILE:HD11	4:A:2403:CLR:C18	2.32	0.59

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:32:TRP:O	1:A:205:ARG:NH2[1_455]	2.09	0.11

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	386/447 (86%)	380 (98%)	6 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	321/374 (86%)	311 (97%)	10 (3%)	40 25

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	A	1019	LYS
1	A	1058	MET
1	A	198	LEU
1	A	1028	ASP

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

Mol	Chain	Res	Type
1	A	1063	HIS
1	A	297	GLN
1	A	1071	GLN
1	A	1006	ASN
1	A	226	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

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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
8	8K6	A	2418	-	17,17,17	0.28	0	16,16,16	0.05	0
4	CLR	A	2405	-	31,31,31	0.52	0	48,48,48	0.77	1 (2%)
6	MYS	A	2414	-	14,14,14	0.34	0	13,13,13	0.37	0
6	MYS	A	2426	-	14,14,14	0.22	0	13,13,13	0.65	0
13	TRD	A	2427	-	12,12,12	0.13	0	11,11,11	0.24	0
10	OCT	A	2413	-	7,7,7	0.15	0	6,6,6	0.10	0
6	MYS	A	2424	-	14,14,14	0.38	0	13,13,13	0.39	0
12	ER0	A	2416	-	30,30,30	0.34	0	35,36,36	0.36	0
2	ZMA	A	2401	-	21,28,28	1.09	2 (9%)	22,39,39	2.50	4 (18%)
8	8K6	A	2410	-	17,17,17	0.21	0	16,16,16	0.06	0
13	TRD	A	2425	-	12,12,12	0.14	0	11,11,11	0.09	0
4	CLR	A	2404	-	31,31,31	0.34	0	48,48,48	0.75	0
6	MYS	A	2409	-	14,14,14	0.25	0	13,13,13	0.50	0
9	D10	A	2411	-	9,9,9	0.18	0	8,8,8	0.22	0
10	OCT	A	2421	-	7,7,7	0.13	0	6,6,6	0.13	0
10	OCT	A	2412	-	7,7,7	0.14	0	6,6,6	0.09	0
13	TRD	A	2420	-	12,12,12	0.11	0	11,11,11	0.08	0
6	MYS	A	2417	-	14,14,14	0.34	0	13,13,13	0.48	0
8	8K6	A	2419	-	17,17,17	0.25	0	16,16,16	0.06	0
5	D12	A	2406	-	11,11,11	0.24	0	10,10,10	0.58	0
6	MYS	A	2407	-	14,14,14	0.20	0	13,13,13	0.62	0
7	HEX	A	2408	-	5,5,5	0.14	0	4,4,4	0.10	0
13	TRD	A	2422	-	12,12,12	0.14	0	11,11,11	0.14	0
4	CLR	A	2403	-	31,31,31	0.38	0	48,48,48	0.57	0
12	ER0	A	2423	-	30,30,30	0.42	0	35,36,36	0.37	0
11	UND	A	2415	-	10,10,10	0.18	0	9,9,9	0.11	0

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
8	8K6	A	2418	-	-	7/15/15/15	-
4	CLR	A	2405	-	-	1/10/68/68	0/4/4/4
6	MYS	A	2414	-	-	4/12/12/12	-
6	MYS	A	2426	-	-	3/12/12/12	-
13	TRD	A	2427	-	-	5/10/10/10	-
10	OCT	A	2413	-	-	4/5/5/5	-
6	MYS	A	2424	-	-	7/12/12/12	-
12	ER0	A	2416	-	-	15/35/35/35	-
2	ZMA	A	2401	-	-	0/6/10/10	0/4/4/4
8	8K6	A	2410	-	-	10/15/15/15	-
13	TRD	A	2425	-	-	2/10/10/10	-
4	CLR	A	2404	-	-	2/10/68/68	0/4/4/4
6	MYS	A	2409	-	-	4/12/12/12	-
9	D10	A	2411	-	-	5/7/7/7	-
10	OCT	A	2421	-	-	2/5/5/5	-
10	OCT	A	2412	-	-	2/5/5/5	-
13	TRD	A	2420	-	-	5/10/10/10	-
6	MYS	A	2417	-	-	5/12/12/12	-
8	8K6	A	2419	-	-	9/15/15/15	-
5	D12	A	2406	-	-	5/9/9/9	-
6	MYS	A	2407	-	-	7/12/12/12	-
7	HEX	A	2408	-	-	1/3/3/3	-
13	TRD	A	2422	-	-	8/10/10/10	-
4	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
12	ER0	A	2423	-	-	10/35/35/35	-
11	UND	A	2415	-	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	ZMA	C18-N19	-2.83	1.31	1.35
2	A	2401	ZMA	C20-N19	2.23	1.38	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	ZMA	N15-C14-N16	10.34	124.94	117.97
2	A	2401	ZMA	C9-C8-C7	-3.29	105.24	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	2401	ZMA	C21-C20-N17	-2.66	118.81	123.44
4	A	2405	CLR	C11-C9-C8	2.18	114.90	111.75
2	A	2401	ZMA	C21-C20-N19	2.04	126.22	123.61

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

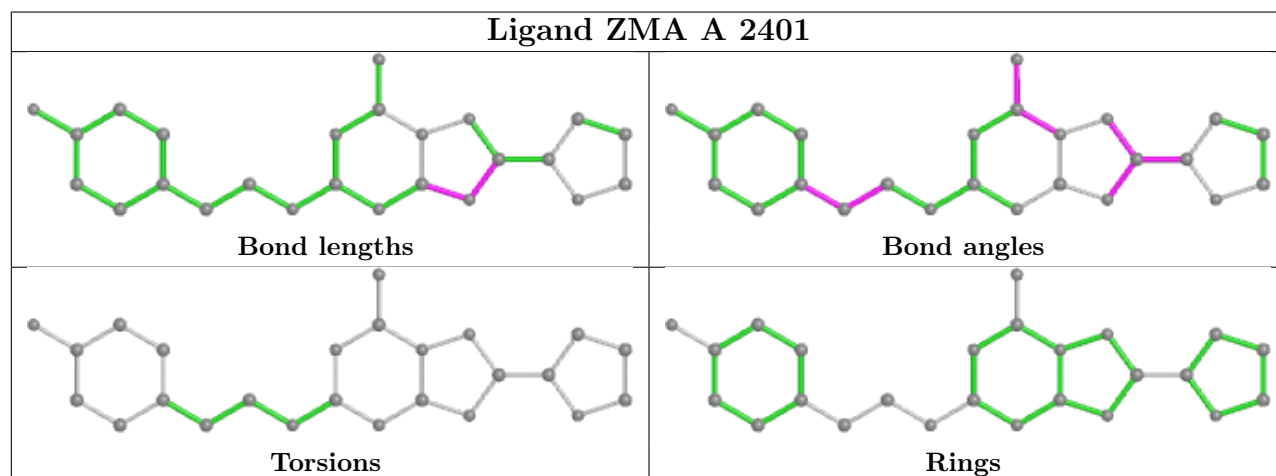
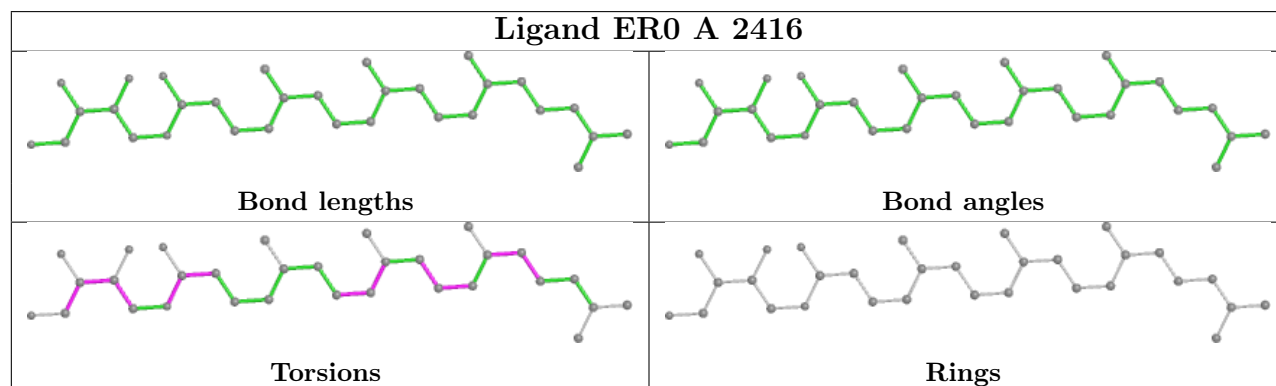
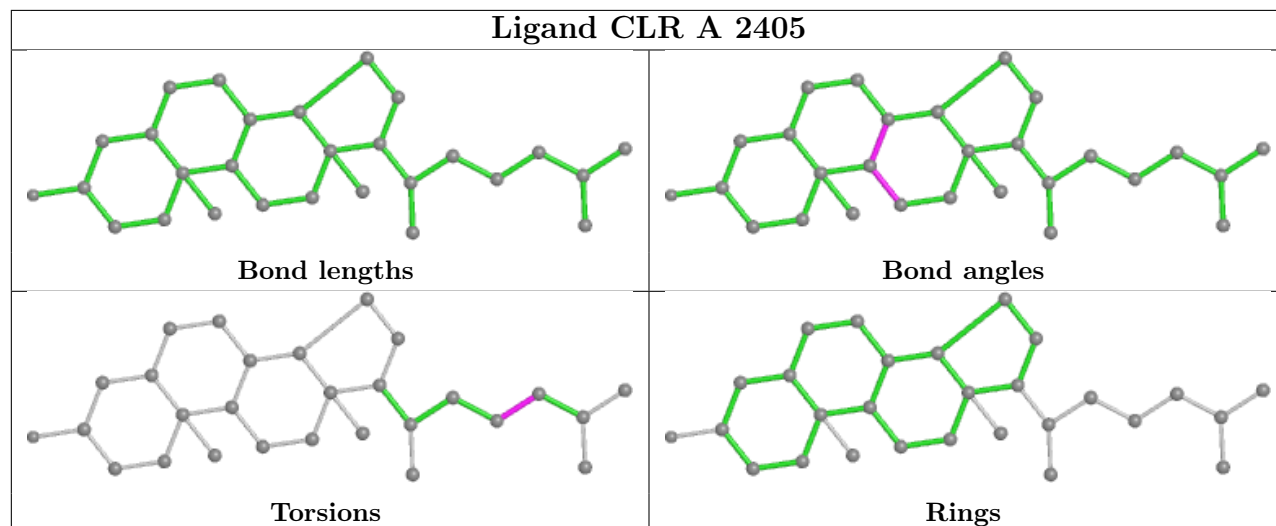
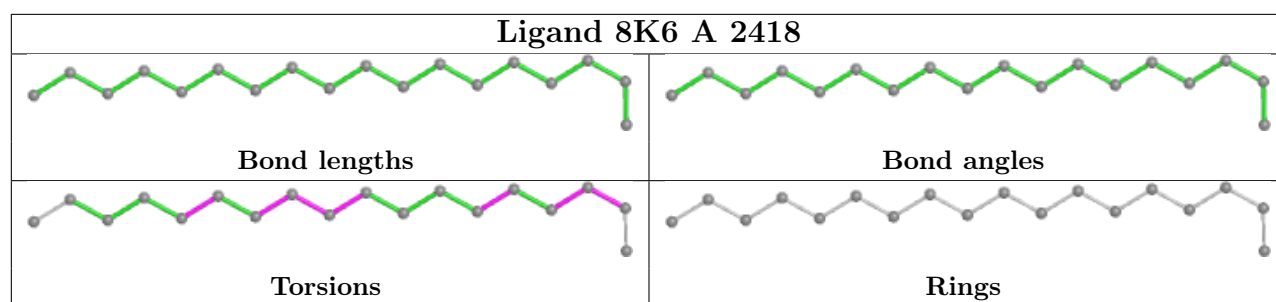
Mol	Chain	Res	Type	Atoms
12	A	2416	ER0	O2-C23-C24-O3
12	A	2416	ER0	O2-C23-C24-C25
12	A	2416	ER0	C23-C24-C25-C26
12	A	2423	ER0	O2-C23-C24-O3
12	A	2423	ER0	O2-C23-C24-C25

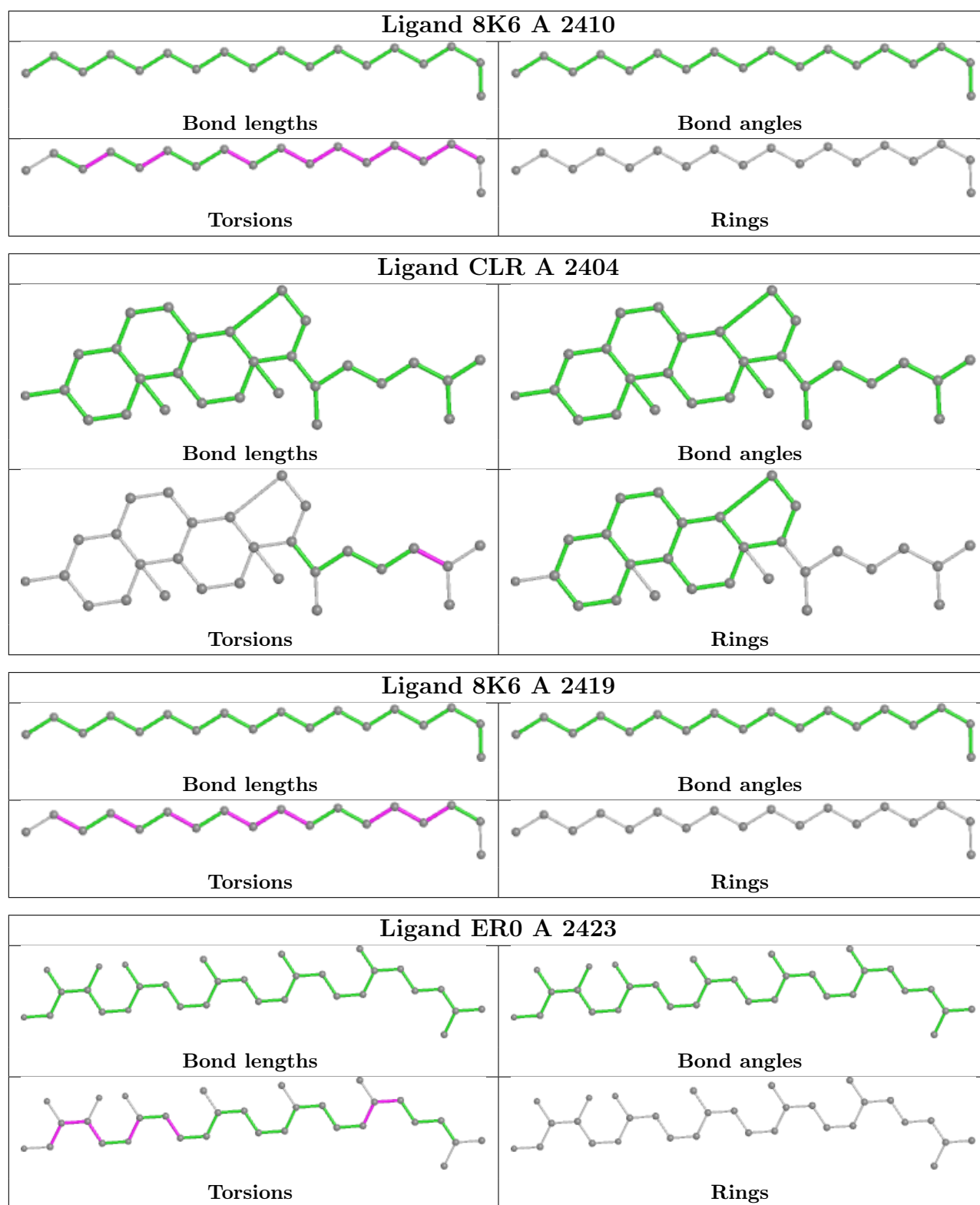
There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2414	MYS	1	0
13	A	2427	TRD	1	0
2	A	2401	ZMA	1	0
8	A	2410	8K6	1	0
8	A	2419	8K6	1	0
4	A	2403	CLR	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/447 (87%)	0.67	49 (12%) 3 2	26, 43, 95, 123	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1059	LYS	7.0
1	A	1020	ALA	6.9
1	A	1062	ARG	6.3
1	A	1061	PHE	6.2
1	A	1024	ALA	5.6

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(Å ²)	Q<0.9
6	MYS	A	2417	15/15	0.39	0.31	73,84,99,105	0
8	8K6	A	2419	18/18	0.42	0.21	85,93,110,114	0

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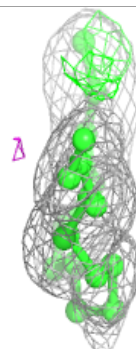
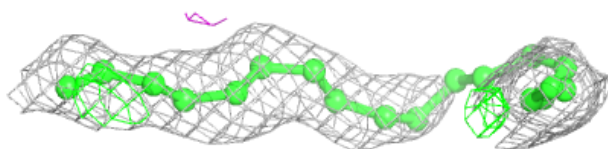
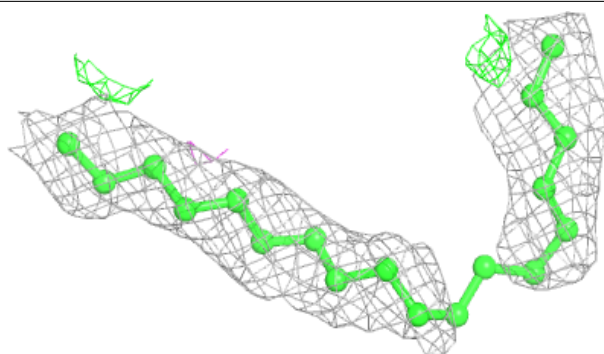
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	8K6	A	2418	18/18	0.49	0.27	84,102,108,109	0
6	MYS	A	2424	15/15	0.54	0.20	68,76,88,88	0
13	TRD	A	2420	13/13	0.54	0.17	91,97,106,106	0
9	D10	A	2411	10/10	0.59	0.38	69,71,81,87	0
13	TRD	A	2427	13/13	0.66	0.18	80,84,89,90	0
13	TRD	A	2425	13/13	0.67	0.27	82,90,93,94	0
6	MYS	A	2414	15/15	0.67	0.29	69,82,92,92	0
10	OCT	A	2412	8/8	0.67	0.17	82,87,98,101	0
6	MYS	A	2407	15/15	0.70	0.14	76,80,85,89	0
8	8K6	A	2410	18/18	0.71	0.23	70,86,98,99	0
11	UND	A	2415	11/11	0.71	0.19	59,77,93,96	0
10	OCT	A	2413	8/8	0.72	0.32	72,77,83,86	0
7	HEX	A	2408	6/6	0.73	0.16	87,94,95,97	0
12	ER0	A	2416	31/31	0.79	0.21	68,92,103,115	0
4	CLR	A	2404	28/28	0.82	0.14	44,50,67,76	0
10	OCT	A	2421	8/8	0.83	0.19	78,89,92,93	0
12	ER0	A	2423	31/31	0.85	0.18	50,82,101,109	0
13	TRD	A	2422	13/13	0.85	0.14	79,86,99,105	0
5	D12	A	2406	12/12	0.86	0.22	72,81,91,93	0
4	CLR	A	2403	28/28	0.87	0.14	51,58,82,86	0
6	MYS	A	2426	15/15	0.88	0.15	58,66,84,90	0
6	MYS	A	2409	15/15	0.90	0.13	62,67,85,85	0
4	CLR	A	2405	28/28	0.93	0.09	42,46,75,83	0
2	ZMA	A	2401	25/25	0.97	0.15	24,28,47,55	0
3	NA	A	2402	1/1	0.99	0.19	31,31,31,31	0

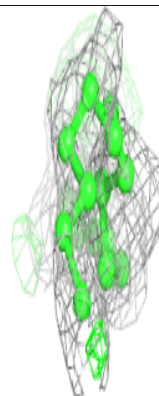
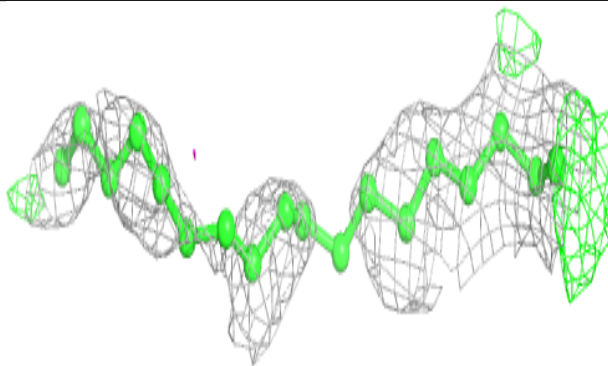
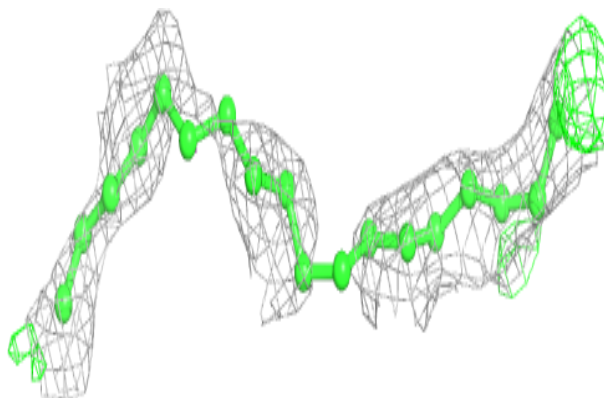
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8K6 A 2419:

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

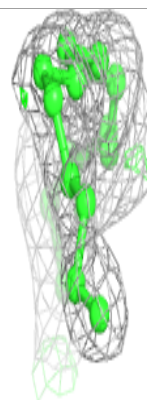
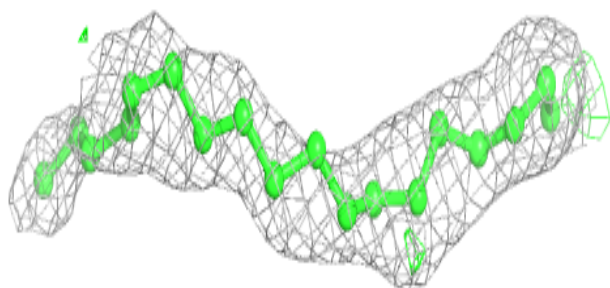
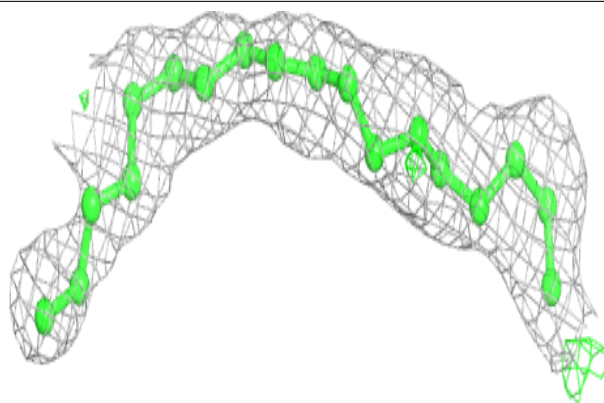
**Electron density around 8K6 A 2418:**

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

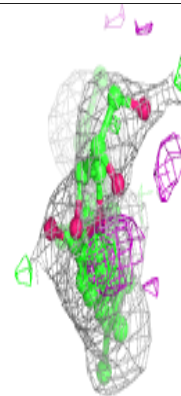
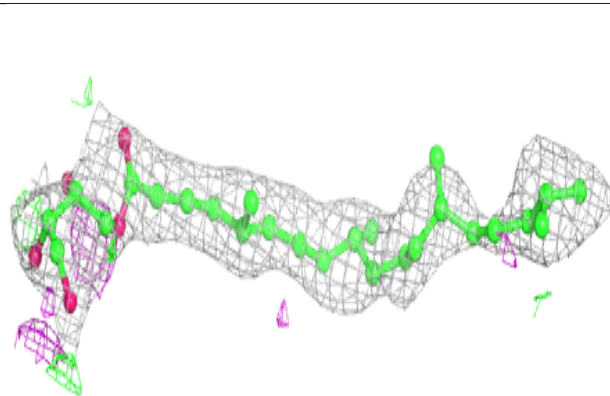
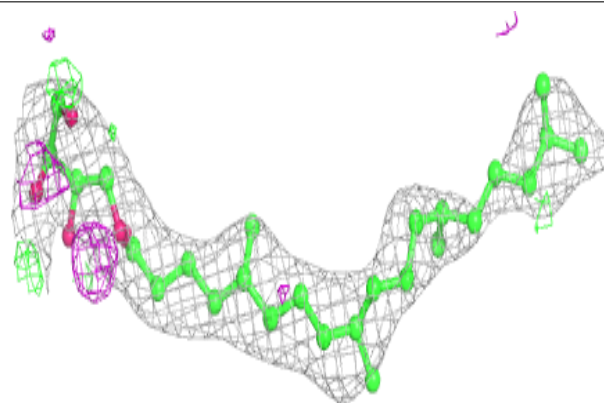


Electron density around 8K6 A 2410:

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

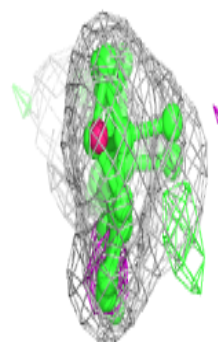
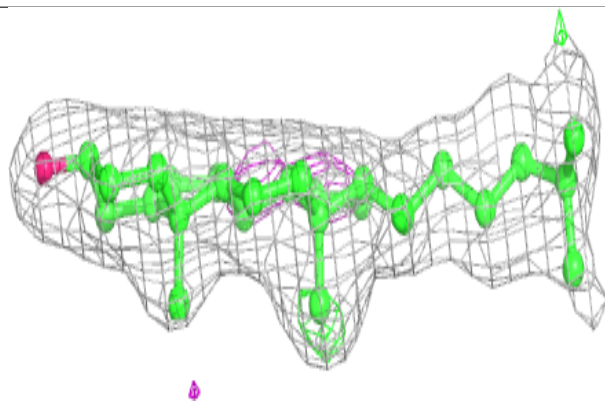
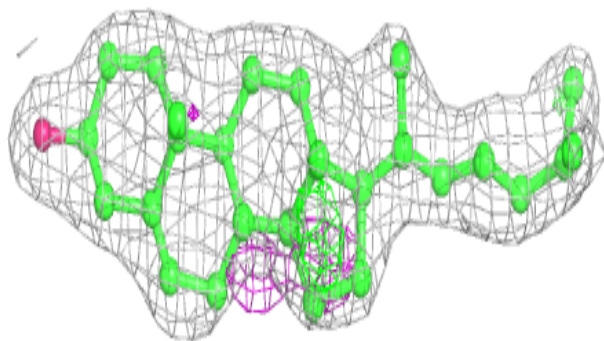
**Electron density around ER0 A 2416:**

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

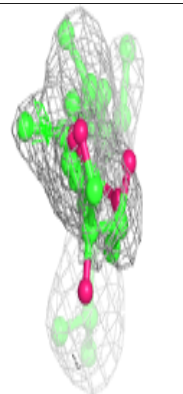
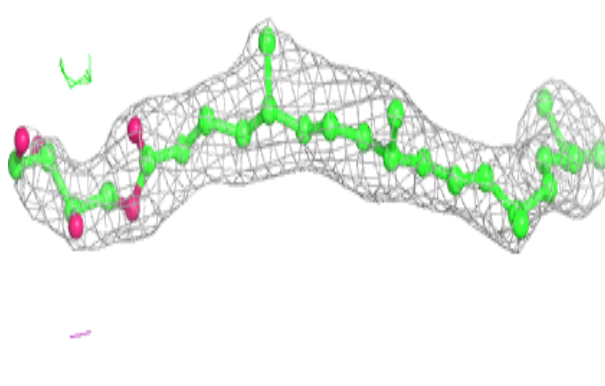
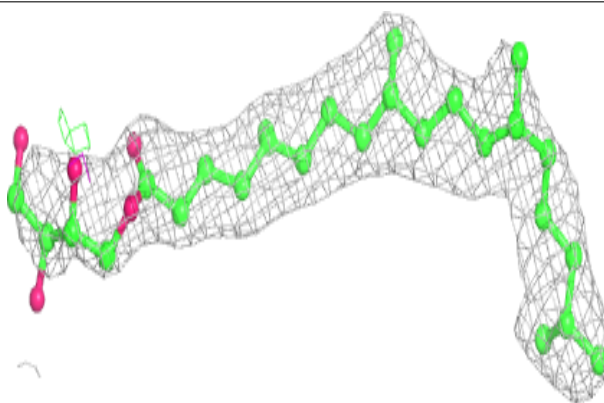


Electron density around CLR A 2404:

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

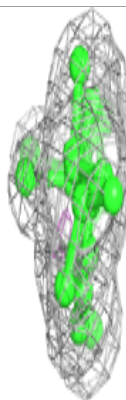
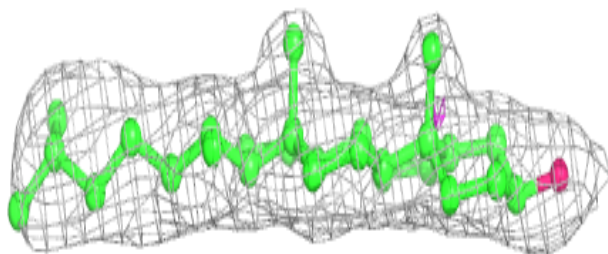
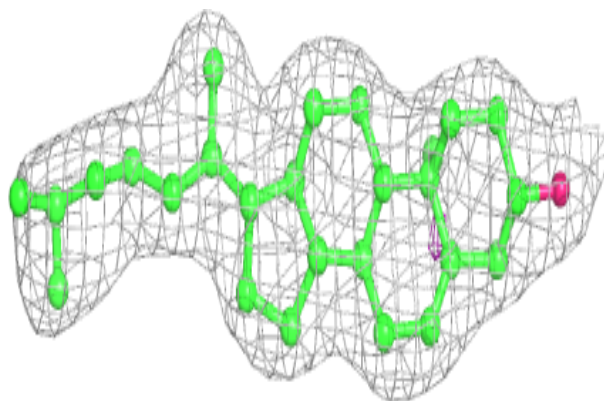
**Electron density around ER0 A 2423:**

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and green (positive)

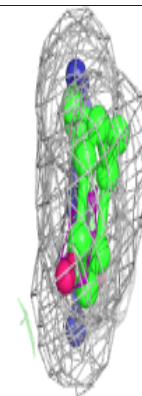
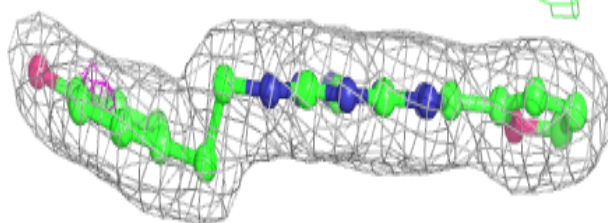
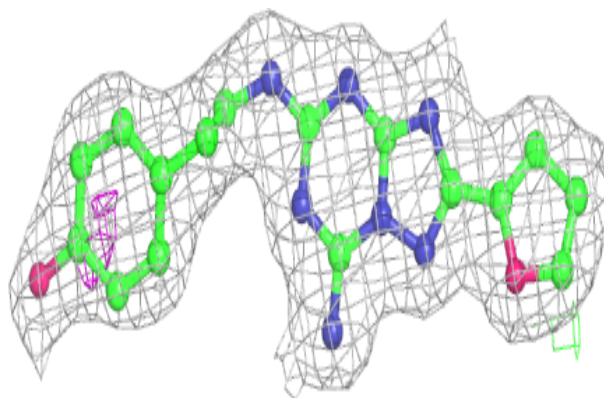


Electron density around CLR A 2405:

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

**Electron density around ZMA A 2401:**

$2mF_o-DF_c$ (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.