



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2020 – 10:18 PM JST

PDB ID : 6LPL  
Title : A2AR crystallized in EROCO17+4, SS-ROX at 100 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 : 2020-01-11  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

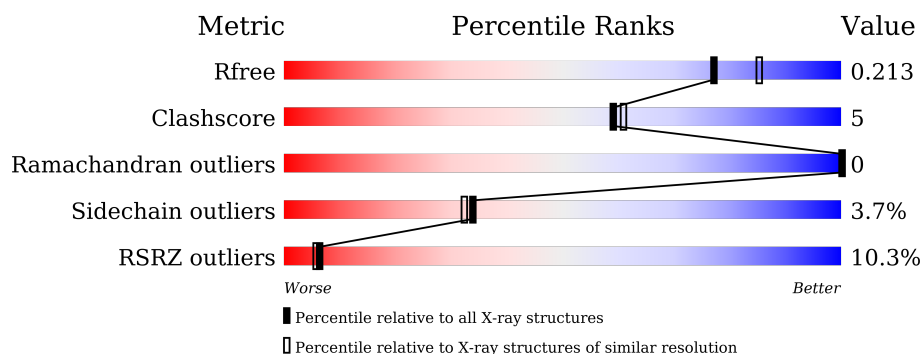
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>9%</div> <div>77%</div> <div>9%</div> <div>13%</div> </div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 3605 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:

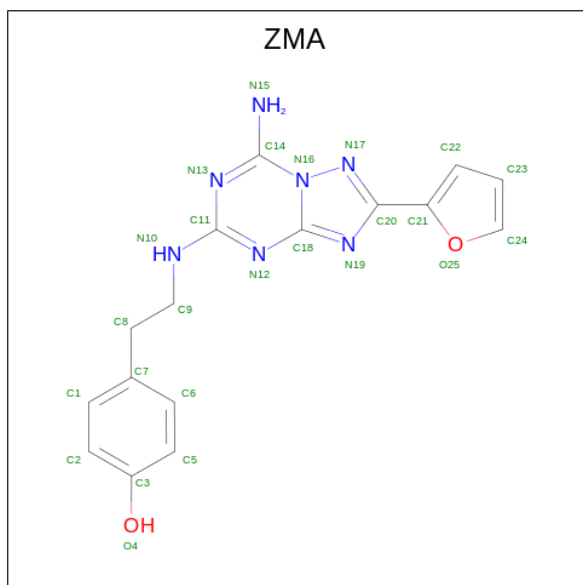
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression 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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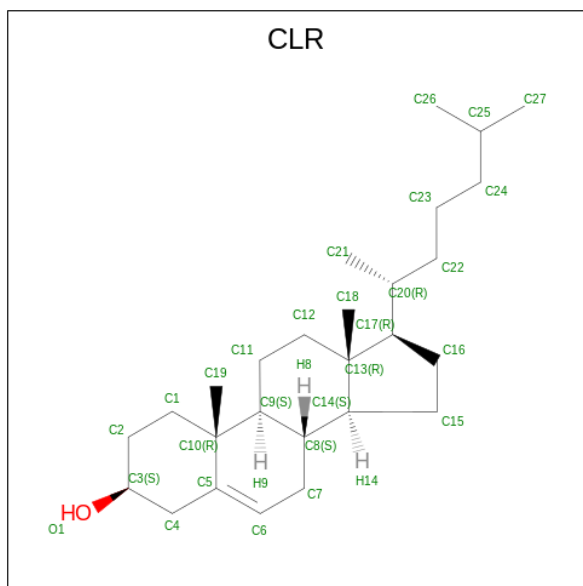
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	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: C<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O<sub>2</sub>).

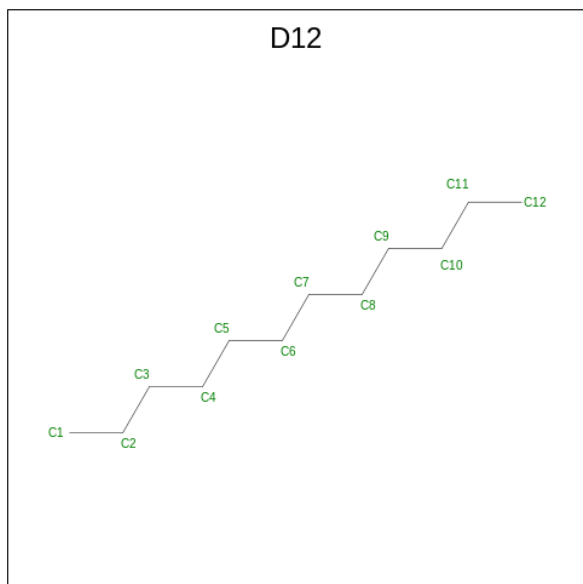


- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



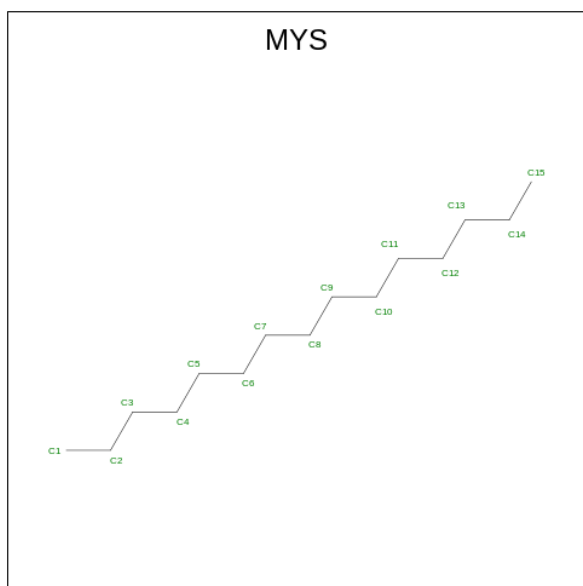
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

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



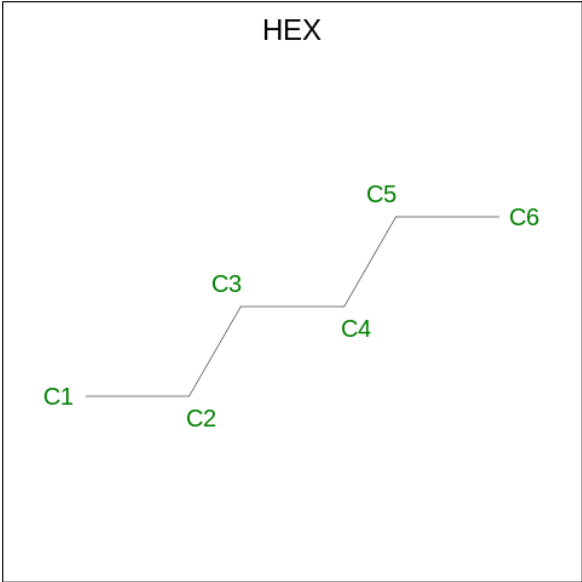
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 12 12	0	0

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



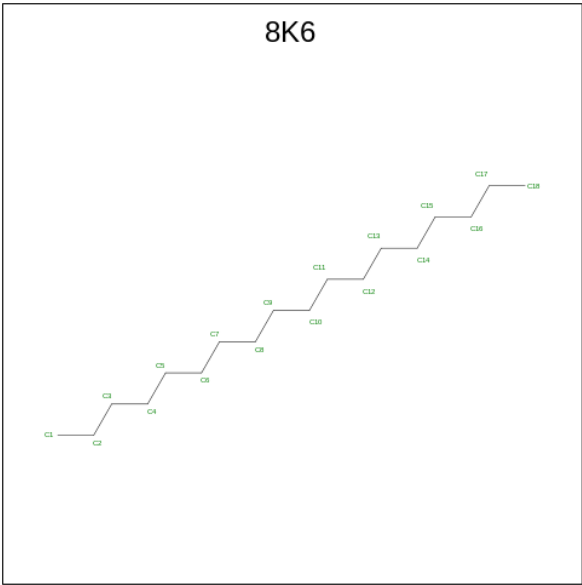
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0
6	A	1	Total C 15 15	0	0

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



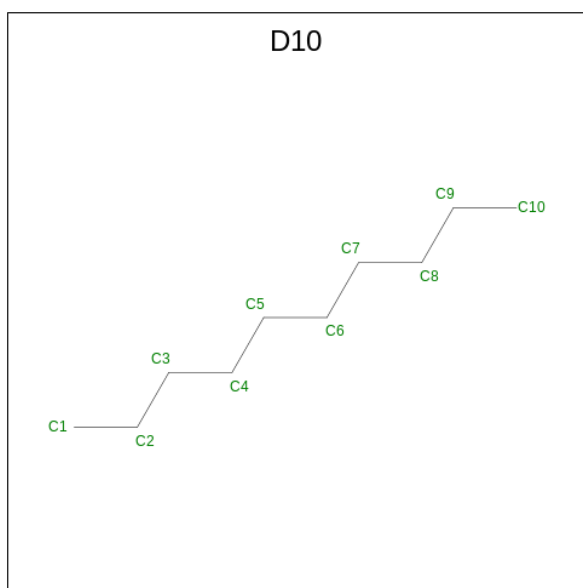
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 6 6	0	0

- Molecule 8 is Octadecane (three-letter code: 8K6) (formula: C<sub>18</sub>H<sub>38</sub>).



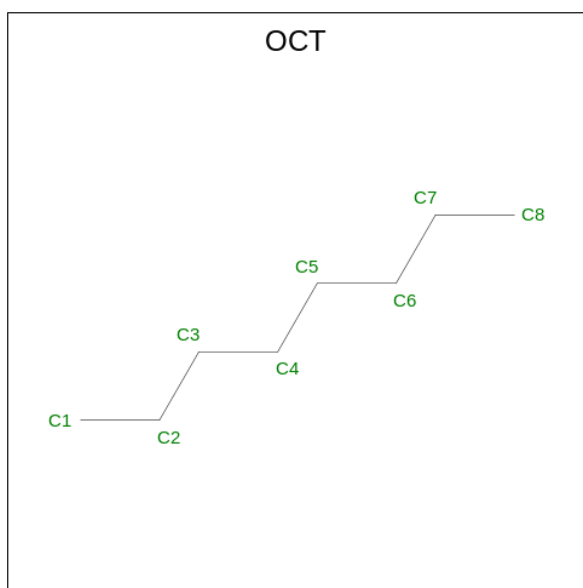
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 18 18	0	0
8	A	1	Total C 18 18	0	0
8	A	1	Total C 18 18	0	0

- 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

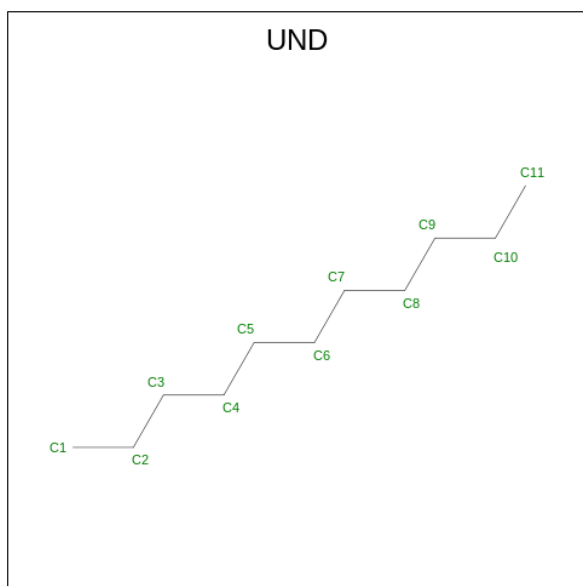
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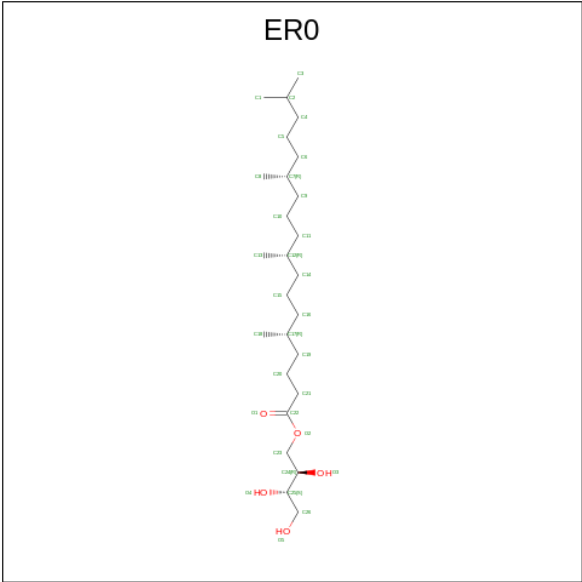
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 8 8	0	0

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



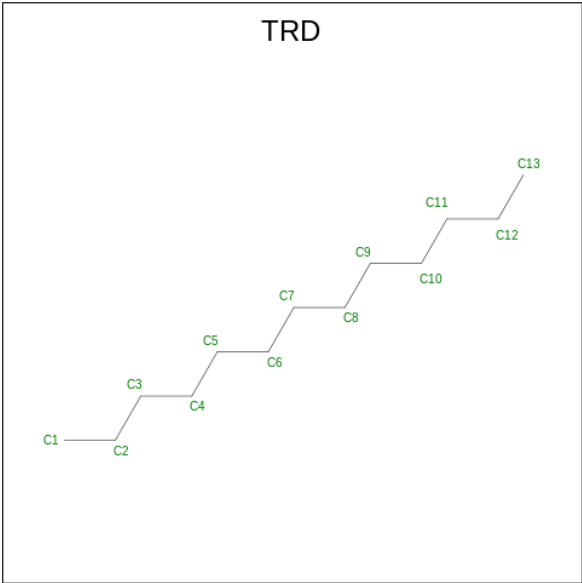
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C 11 11	0	0

- 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: C<sub>13</sub>H<sub>28</sub>).



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

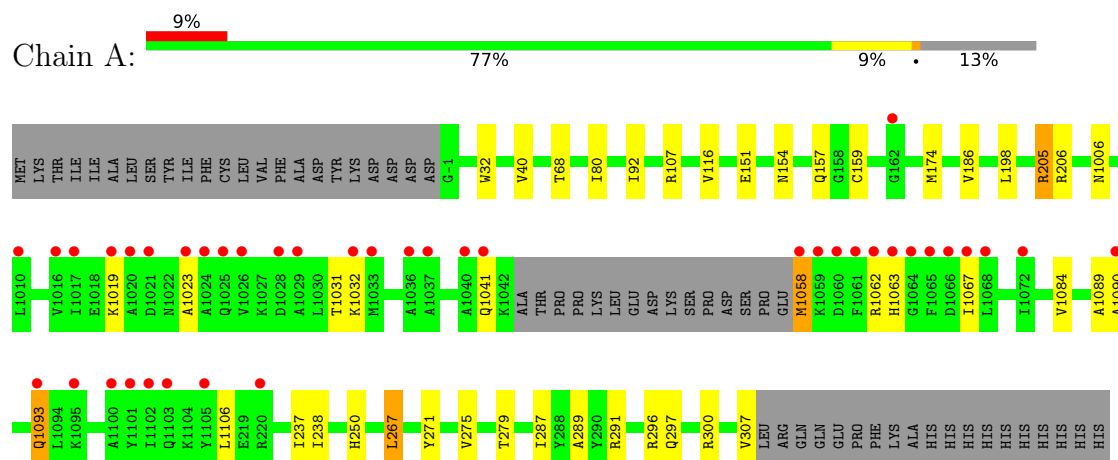
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	138	Total O 138 138	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, $\alpha$ , $\beta$ , $\gamma$	39.89Å 179.28Å 140.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.75 – 2.00 42.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.75-2.00) 99.9 (42.71-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.173 , 0.208 0.185 , 0.213	Depositor DCC
$R_{free}$ test set	1756 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 81.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.74	0/3101	0.85	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	30	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	3	0
7	A	6	0	14	0	0
8	A	54	0	114	4	0
9	A	10	0	22	1	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	138	0	0	2	1
All	All	3605	0	3822	34	2

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 5.

All (34) 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:1031:THR:O	14:A:2501:HOH:O	1.95	0.84
1:A:80:ILE:HD11	4:A:2403:CLR:H182	1.77	0.66
1:A:154:ASN:OD1	1:A:159:CYS:HB2	1.97	0.64
1:A:1032:LYS:N	1:A:1032:LYS:HE2	2.13	0.62
1:A:174:MET:HE1	14:A:2561:HOH:O	2.03	0.58
1:A:1090:ALA:O	1:A:1093:GLN:HB2	2.06	0.56
1:A:1058:MET:O	1:A:1062:ARG:HG2	2.06	0.55
1:A:80:ILE:HD11	4:A:2403:CLR:C18	2.40	0.51
1:A:1063:HIS:CE1	1:A:1067:ILE:HD11	2.46	0.51
1:A:1062:ARG:HH11	1:A:1062:ARG:HA	1.76	0.51
1:A:275:VAL:O	1:A:279:THR:HG23	2.11	0.51
1:A:307:VAL:O	1:A:307:VAL:HG23	2.11	0.50
1:A:1089:ALA:O	1:A:1093:GLN:NE2	2.45	0.49
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.42	0.49
1:A:250:HIS:CE1	2:A:2401:ZMA:H24	2.49	0.47
1:A:289:ALA:O	1:A:296:ARG:HB2	2.15	0.47
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.96	0.46
1:A:1058:MET:HA	1:A:1058:MET:HE2	1.98	0.46
1:A:1041:GLN:HE21	1:A:1062:ARG:NH1	2.14	0.45
1:A:1063:HIS:O	1:A:1067:ILE:HG13	2.16	0.45
6:A:2414:MYS:H91	8:A:2419:8K6:H13C	1.99	0.45
1:A:92:ILE:CD1	1:A:186:VAL:HG22	2.47	0.44
1:A:237:ILE:HD13	8:A:2419:8K6:H82C	2.00	0.43
1:A:238:ILE:HD11	1:A:287:ILE:HB	2.02	0.42
1:A:1032:LYS:CA	1:A:1032:LYS:HE2	2.49	0.42
9:A:2411:D10:H81	9:A:2411:D10:H51	1.76	0.42
8:A:2418:8K6:H142	6:A:2424:MYS:H51	2.00	0.42
1:A:1058:MET:CE	1:A:1058:MET:HA	2.50	0.42
1:A:267:LEU:HD13	1:A:271:TYR:HE2	1.84	0.42
6:A:2417:MYS:H81	6:A:2417:MYS:H51	1.88	0.41
1:A:68:THR:HA	8:A:2410:8K6:H172	2.01	0.41
1:A:297:GLN:HG2	1:A:300:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:ALA:CA	1:A:1084:VAL:HG22	2.50	0.41
1:A:1006:ASN:HA	1:A:1006:ASN:HD22	1.53	0.40

All (2) 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]	1.70	0.50
14:A:2638:HOH:O	14:A:2638:HOH:O[3_455]	2.07	0.13

## 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%)	379 (98%)	7 (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%)	309 (96%)	12 (4%)	34	32

All (12) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	107	ARG
1	A	151	GLU
1	A	157	GLN
1	A	198	LEU
1	A	205	ARG
1	A	206	ARG
1	A	1019	LYS
1	A	1058	MET
1	A	1093	GLN
1	A	1106	LEU
1	A	267	LEU
1	A	291	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	1006	ASN
1	A	1041	GLN
1	A	1063	HIS
1	A	1071	GLN
1	A	226	GLN
1	A	297	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
10	OCT	A	2421	-	7,7,7	0.15	0	6,6,6	0.18	0
4	CLR	A	2405	-	31,31,31	0.48	0	48,48,48	0.60	0
13	TRD	A	2427	-	12,12,12	0.15	0	11,11,11	0.21	0
6	MYS	A	2407	-	14,14,14	0.26	0	13,13,13	0.55	0
6	MYS	A	2417	-	14,14,14	0.39	0	13,13,13	0.56	0
8	8K6	A	2410	-	17,17,17	0.18	0	16,16,16	0.07	0
2	ZMA	A	2401	-	21,28,28	0.72	0	22,39,39	1.64	2 (9%)
13	TRD	A	2422	-	12,12,12	0.17	0	11,11,11	0.21	0
8	8K6	A	2419	-	17,17,17	0.31	0	16,16,16	0.07	0
12	ER0	A	2423	-	30,30,30	0.36	0	35,36,36	0.45	0
4	CLR	A	2403	-	31,31,31	0.41	0	48,48,48	0.63	0
10	OCT	A	2412	-	7,7,7	0.23	0	6,6,6	0.17	0
6	MYS	A	2409	-	14,14,14	0.29	0	13,13,13	0.65	0
9	D10	A	2411	-	9,9,9	0.29	0	8,8,8	0.36	0
4	CLR	A	2404	-	31,31,31	0.35	0	48,48,48	0.72	0
8	8K6	A	2418	-	17,17,17	0.24	0	16,16,16	0.07	0
5	D12	A	2406	-	11,11,11	0.30	0	10,10,10	0.69	0
6	MYS	A	2414	-	14,14,14	0.43	0	13,13,13	0.29	0
6	MYS	A	2424	-	14,14,14	0.44	0	13,13,13	0.41	0
11	UND	A	2415	-	10,10,10	0.19	0	9,9,9	0.19	0
10	OCT	A	2413	-	7,7,7	0.17	0	6,6,6	0.14	0
7	HEX	A	2408	-	5,5,5	0.16	0	4,4,4	0.20	0
6	MYS	A	2426	-	14,14,14	0.18	0	13,13,13	0.70	0
13	TRD	A	2420	-	12,12,12	0.17	0	11,11,11	0.13	0
13	TRD	A	2425	-	12,12,12	0.18	0	11,11,11	0.13	0
12	ER0	A	2416	-	30,30,30	0.40	0	35,36,36	0.47	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
10	OCT	A	2421	-	-	2/5/5/5	-
4	CLR	A	2405	-	-	1/10/68/68	0/4/4/4

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	ZMA	N15-C14-N16	5.58	121.73	117.97
2	A	2401	ZMA	C9-C8-C7	-3.43	104.91	112.87

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	2423	ER0	O2-C23-C24-O3
12	A	2423	ER0	O2-C23-C24-C25
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	O1-C22-O2-C23
8	A	2419	8K6	C4-C5-C6-C7
12	A	2423	ER0	C24-C25-C26-O5
12	A	2423	ER0	C21-C22-O2-C23
6	A	2417	MYS	C5-C6-C7-C8
9	A	2411	D10	C5-C6-C7-C8
12	A	2423	ER0	C8-C7-C9-C10
12	A	2423	ER0	O4-C25-C26-O5
10	A	2412	OCT	C4-C5-C6-C7
12	A	2416	ER0	C12-C14-C15-C16
8	A	2419	8K6	C11-C10-C9-C8
8	A	2419	8K6	C11-C12-C13-C14
13	A	2420	TRD	C11-C10-C9-C8
8	A	2418	8K6	C11-C10-C9-C8
6	A	2407	MYS	C4-C5-C6-C7
5	A	2406	D12	C3-C4-C5-C6
6	A	2407	MYS	C6-C7-C8-C9
9	A	2411	D10	C4-C5-C6-C7
8	A	2410	8K6	C6-C7-C8-C9
8	A	2410	8K6	C3-C4-C5-C6
6	A	2424	MYS	C7-C8-C9-C10
5	A	2406	D12	C2-C3-C4-C5
6	A	2424	MYS	C6-C7-C8-C9
6	A	2426	MYS	C2-C3-C4-C5
13	A	2422	TRD	C4-C5-C6-C7
8	A	2418	8K6	C12-C13-C14-C15
8	A	2410	8K6	C5-C6-C7-C8
8	A	2410	8K6	C7-C8-C9-C10
6	A	2424	MYS	C10-C11-C12-C13
7	A	2408	HEX	C2-C3-C4-C5
12	A	2416	ER0	C9-C10-C11-C12
8	A	2410	8K6	C4-C5-C6-C7
11	A	2415	UND	C4-C5-C6-C7
12	A	2423	ER0	C5-C6-C7-C9
8	A	2419	8K6	C13-C14-C15-C16
4	A	2405	CLR	C22-C23-C24-C25
10	A	2421	OCT	C2-C3-C4-C5
6	A	2407	MYS	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	A	2410	8K6	C2-C3-C4-C5
8	A	2418	8K6	C10-C11-C12-C13
8	A	2410	8K6	C14-C15-C16-C17
13	A	2422	TRD	C3-C4-C5-C6
13	A	2422	TRD	C9-C10-C11-C12
8	A	2410	8K6	C1-C2-C3-C4
8	A	2418	8K6	C1-C2-C3-C4
10	A	2421	OCT	C1-C2-C3-C4
13	A	2420	TRD	C2-C3-C4-C5
6	A	2417	MYS	C11-C12-C13-C14
6	A	2417	MYS	C12-C13-C14-C15
6	A	2424	MYS	C9-C10-C11-C12
13	A	2427	TRD	C10-C11-C12-C13
10	A	2413	OCT	C4-C5-C6-C7
6	A	2407	MYS	C11-C10-C9-C8
6	A	2407	MYS	C12-C13-C14-C15
6	A	2424	MYS	C11-C10-C9-C8
8	A	2419	8K6	C7-C8-C9-C10
10	A	2413	OCT	C1-C2-C3-C4
10	A	2413	OCT	C2-C3-C4-C5
12	A	2416	ER0	O3-C24-C25-C26
6	A	2414	MYS	C7-C8-C9-C10
6	A	2407	MYS	C11-C12-C13-C14
13	A	2422	TRD	C10-C11-C12-C13
6	A	2424	MYS	C1-C2-C3-C4
13	A	2427	TRD	C2-C3-C4-C5
6	A	2417	MYS	C4-C5-C6-C7
11	A	2415	UND	C3-C4-C5-C6
8	A	2419	8K6	C9-C10-C11-C12
12	A	2416	ER0	C5-C6-C7-C9
13	A	2422	TRD	C1-C2-C3-C4
8	A	2418	8K6	C4-C5-C6-C7
6	A	2414	MYS	C2-C3-C4-C5
13	A	2420	TRD	C1-C2-C3-C4
9	A	2411	D10	C1-C2-C3-C4
8	A	2410	8K6	C9-C10-C11-C12
6	A	2426	MYS	C3-C4-C5-C6
12	A	2416	ER0	O1-C22-O2-C23
12	A	2423	ER0	C19-C20-C21-C22
8	A	2418	8K6	C2-C3-C4-C5
4	A	2404	CLR	C23-C24-C25-C27
6	A	2417	MYS	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
11	A	2415	UND	C5-C6-C7-C8
6	A	2426	MYS	C4-C5-C6-C7
12	A	2416	ER0	C4-C5-C6-C7
12	A	2416	ER0	C5-C6-C7-C8
8	A	2418	8K6	C9-C10-C11-C12
6	A	2417	MYS	C1-C2-C3-C4
10	A	2412	OCT	C1-C2-C3-C4
4	A	2404	CLR	C23-C24-C25-C26
11	A	2415	UND	C11-C10-C9-C8
8	A	2419	8K6	C3-C4-C5-C6
13	A	2420	TRD	C6-C7-C8-C9
6	A	2417	MYS	C9-C10-C11-C12
13	A	2425	TRD	C9-C10-C11-C12
8	A	2410	8K6	C12-C13-C14-C15
13	A	2425	TRD	C1-C2-C3-C4
6	A	2409	MYS	C1-C2-C3-C4
13	A	2422	TRD	C2-C3-C4-C5
6	A	2417	MYS	C10-C11-C12-C13
10	A	2413	OCT	C5-C6-C7-C8
13	A	2425	TRD	C7-C8-C9-C10
8	A	2418	8K6	C15-C16-C17-C18
13	A	2427	TRD	C4-C5-C6-C7
8	A	2419	8K6	C2-C3-C4-C5
5	A	2406	D12	C1-C2-C3-C4
13	A	2427	TRD	C7-C8-C9-C10
8	A	2419	8K6	C15-C16-C17-C18
5	A	2406	D12	C9-C10-C11-C12
11	A	2415	UND	C1-C2-C3-C4
13	A	2427	TRD	C11-C10-C9-C8
13	A	2422	TRD	C11-C10-C9-C8
6	A	2409	MYS	C5-C6-C7-C8
12	A	2416	ER0	C21-C22-O2-C23
12	A	2416	ER0	C8-C7-C9-C10
6	A	2409	MYS	C12-C13-C14-C15
12	A	2423	ER0	O3-C24-C25-O4
12	A	2416	ER0	O3-C24-C25-O4
6	A	2409	MYS	C7-C8-C9-C10
12	A	2416	ER0	C20-C21-C22-O2
9	A	2411	D10	C6-C7-C8-C9
6	A	2414	MYS	C5-C6-C7-C8
11	A	2415	UND	C6-C7-C8-C9
12	A	2416	ER0	C6-C7-C9-C10

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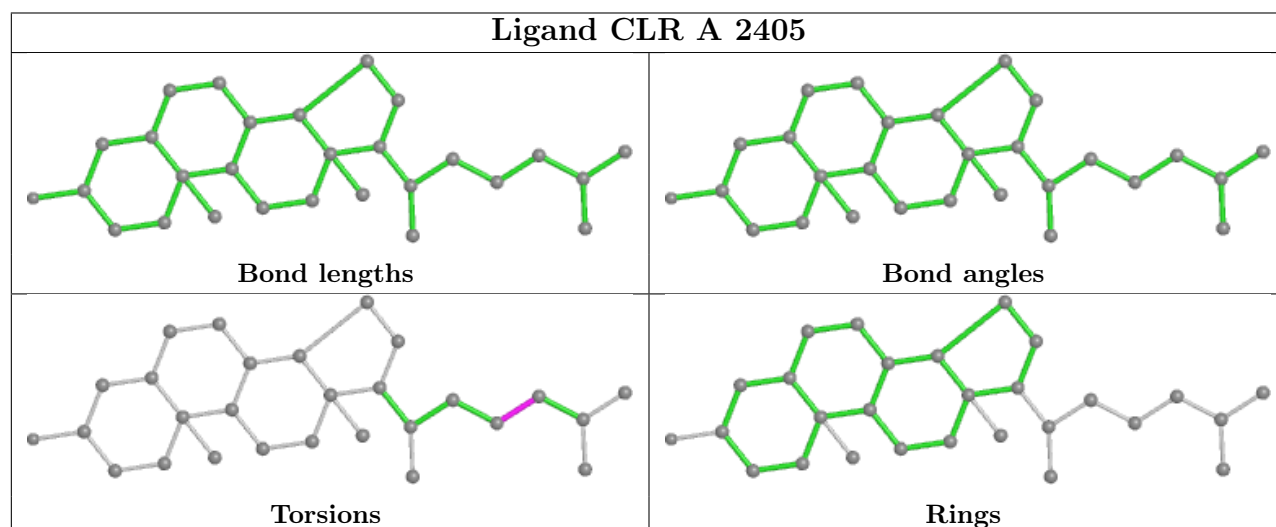
Mol	Chain	Res	Type	Atoms
13	A	2427	TRD	C1-C2-C3-C4

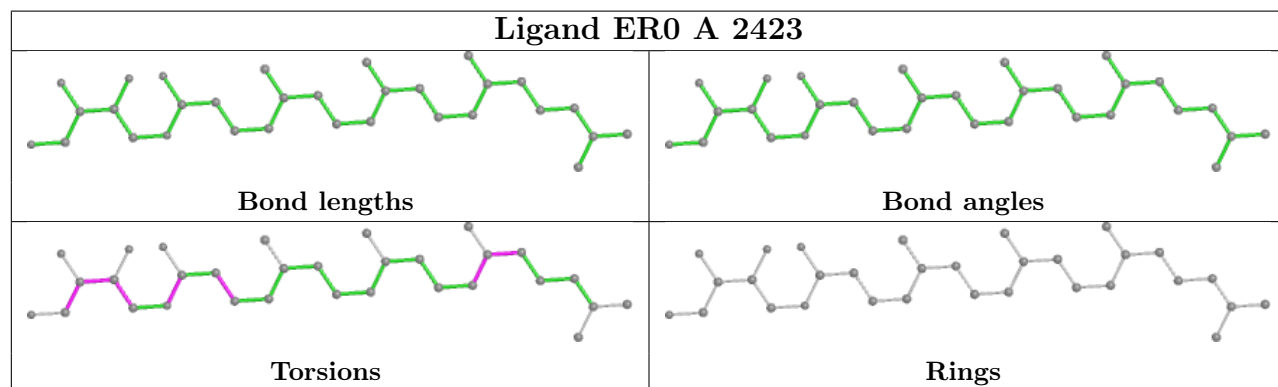
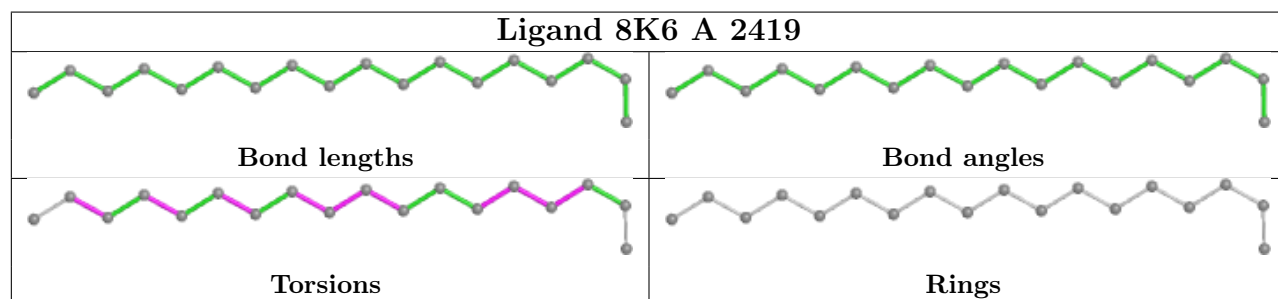
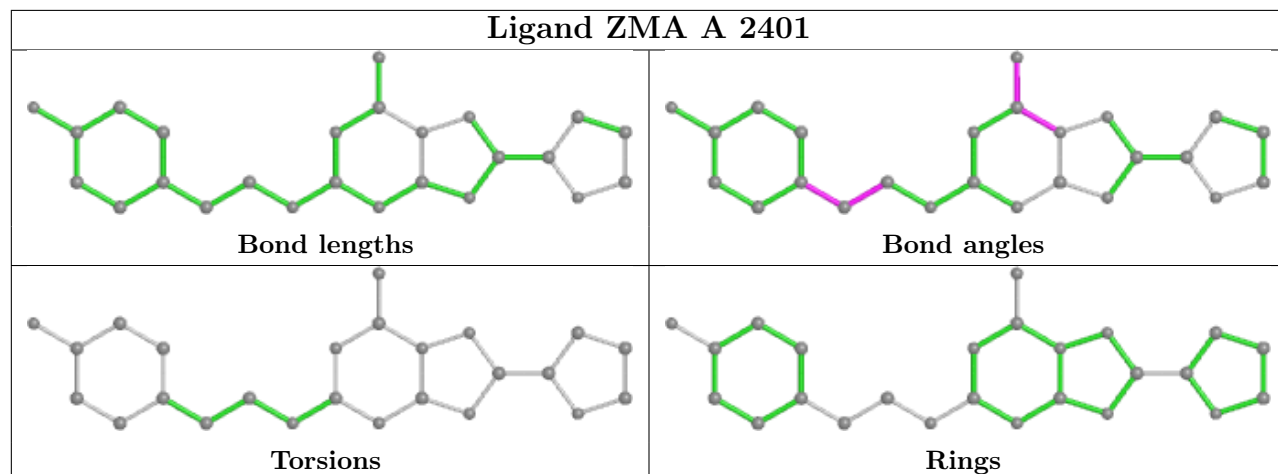
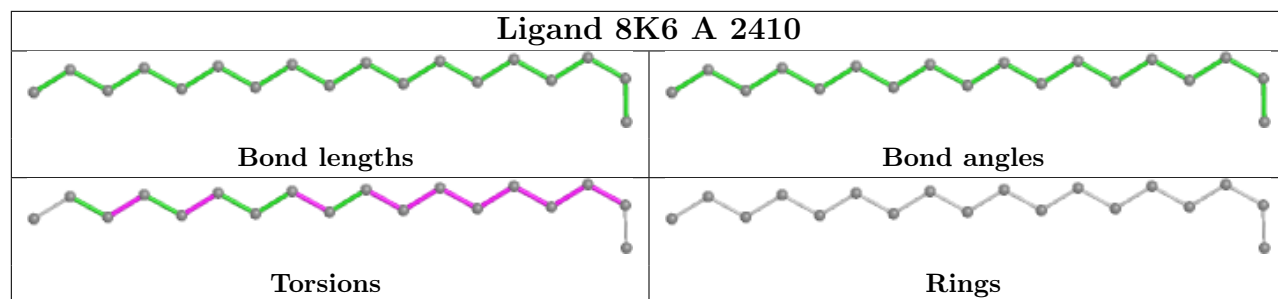
There are no ring outliers.

9 monomers are involved in 9 short contacts:

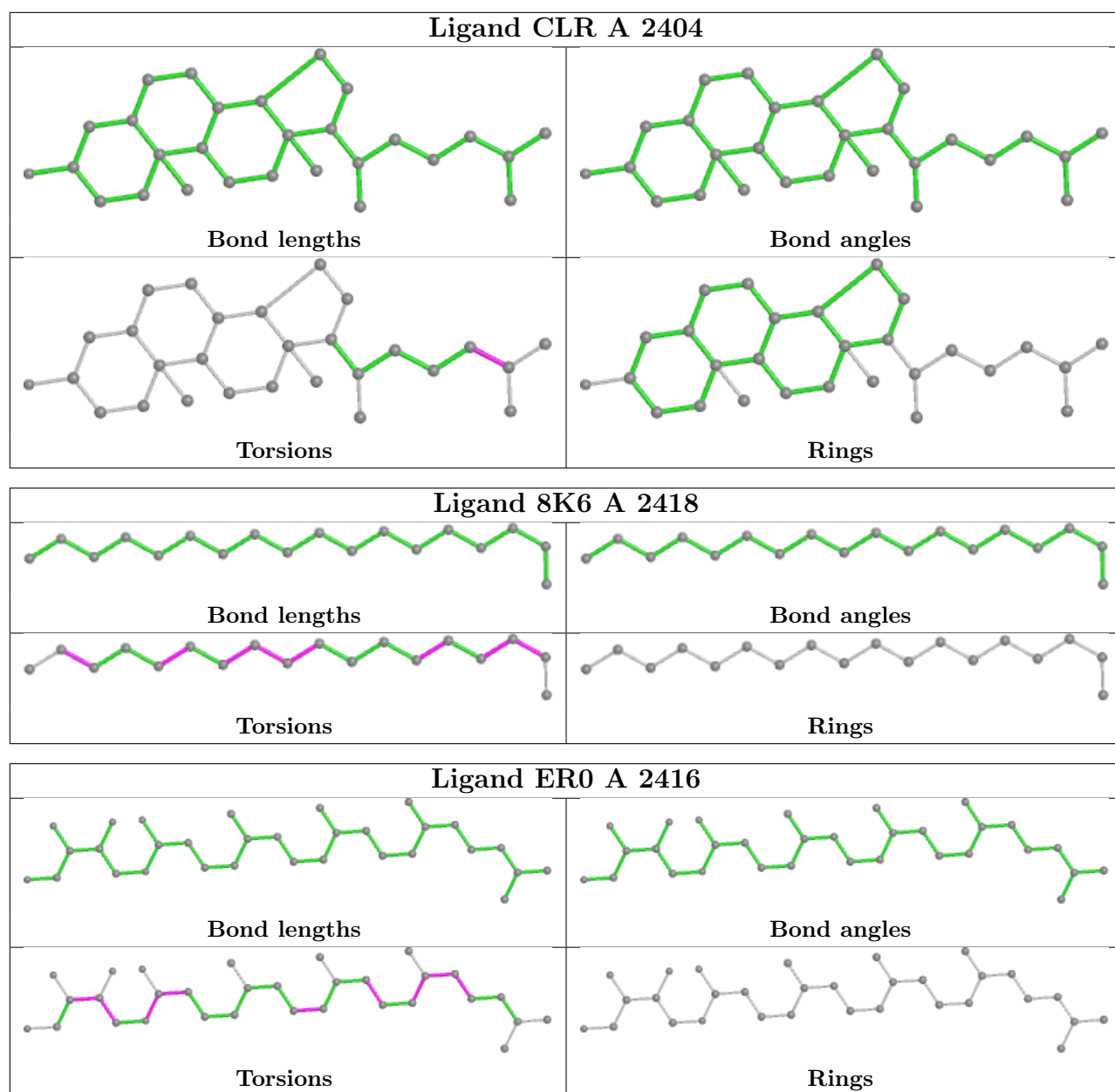
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2417	MYS	1	0
8	A	2410	8K6	1	0
2	A	2401	ZMA	1	0
8	A	2419	8K6	2	0
4	A	2403	CLR	2	0
9	A	2411	D10	1	0
8	A	2418	8K6	1	0
6	A	2414	MYS	1	0
6	A	2424	MYS	1	0

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	390/447 (87%)	0.45	40 (10%) 6 6	24, 37, 83, 122	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1059	LYS	8.9
1	A	1061	PHE	7.5
1	A	1062	ARG	6.8
1	A	1063	HIS	6.7
1	A	1101	TYR	5.8
1	A	1040	ALA	4.7
1	A	1021	ASP	4.1
1	A	1020	ALA	4.1
1	A	1058	MET	4.1
1	A	1017	ILE	4.0
1	A	1023	ALA	4.0
1	A	1060	ASP	3.8
1	A	1029	ALA	3.7
1	A	1019	LYS	3.6
1	A	1037	ALA	3.2
1	A	1066	ASP	3.1
1	A	1105	TYR	3.1
1	A	1026	VAL	3.1
1	A	1041	GLN	3.1
1	A	1100	ALA	3.0
1	A	1033	MET	3.0
1	A	1025	GLN	2.9
1	A	220	ARG	2.9
1	A	1016	VAL	2.9
1	A	1032	LYS	2.7
1	A	1028	ASP	2.7
1	A	1024	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1064	GLY	2.6
1	A	1067	ILE	2.6
1	A	1093	GLN	2.5
1	A	1102	ILE	2.4
1	A	1103	GLN	2.4
1	A	1010	LEU	2.4
1	A	1036	ALA	2.4
1	A	1065	PHE	2.2
1	A	162	GLY	2.2
1	A	1090	ALA	2.2
1	A	1068	LEU	2.0
1	A	1072	ILE	2.0
1	A	1095	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

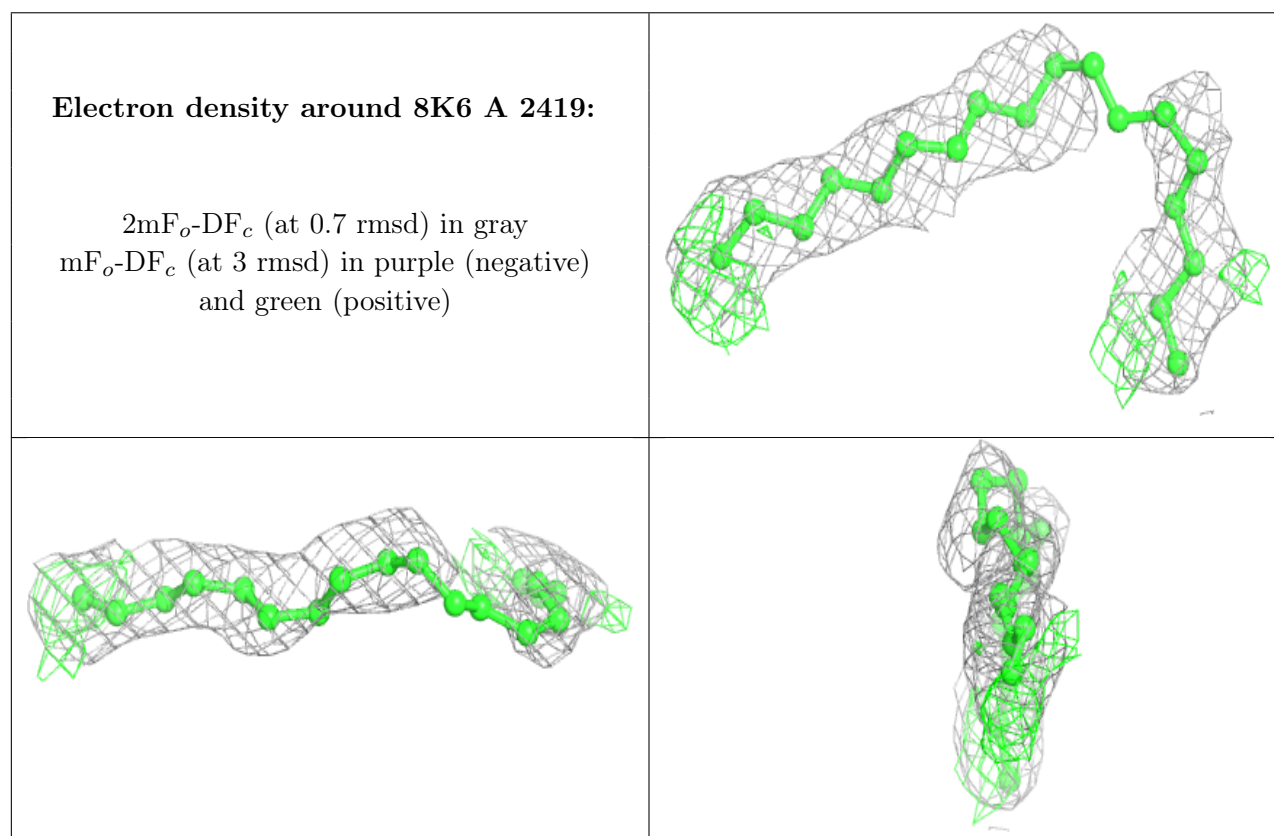
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	8K6	A	2419	18/18	0.51	0.34	75,82,96,97	0
8	8K6	A	2418	18/18	0.63	0.32	64,82,90,90	0
13	TRD	A	2425	13/13	0.66	0.27	73,81,87,91	0
6	MYS	A	2424	15/15	0.72	0.31	53,59,73,73	0
12	ER0	A	2416	31/31	0.73	0.22	55,77,96,104	0
6	MYS	A	2414	15/15	0.74	0.24	60,72,77,79	0
10	OCT	A	2412	8/8	0.74	0.29	63,76,80,81	0
9	D10	A	2411	10/10	0.75	0.23	56,60,71,72	0
6	MYS	A	2407	15/15	0.77	0.27	58,73,88,94	0
10	OCT	A	2421	8/8	0.78	0.29	70,72,74,74	0

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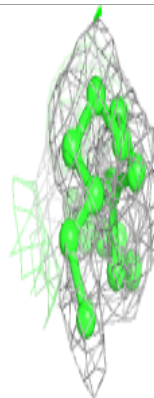
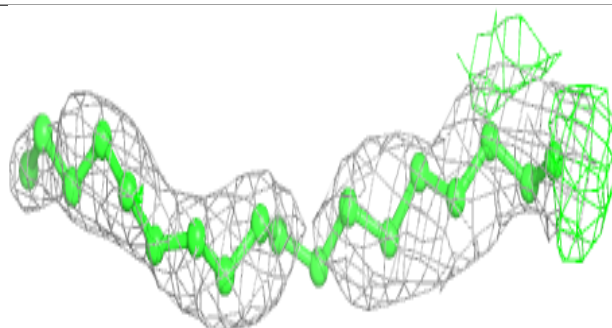
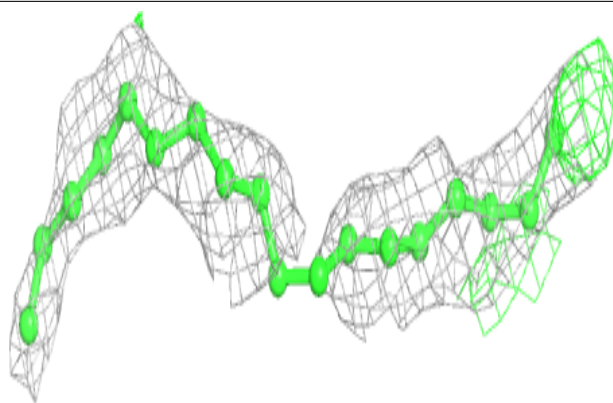
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	OCT	A	2413	8/8	0.79	0.25	65,67,71,75	0
13	TRD	A	2422	13/13	0.80	0.31	66,79,90,92	0
7	HEX	A	2408	6/6	0.81	0.26	77,78,82,86	0
6	MYS	A	2417	15/15	0.82	0.29	57,66,74,76	0
13	TRD	A	2427	13/13	0.82	0.28	60,68,76,79	0
13	TRD	A	2420	13/13	0.83	0.26	63,72,89,90	0
8	8K6	A	2410	18/18	0.84	0.24	61,73,87,89	0
12	ER0	A	2423	31/31	0.85	0.22	40,71,98,99	0
4	CLR	A	2403	28/28	0.86	0.17	34,41,64,74	0
4	CLR	A	2404	28/28	0.88	0.17	45,52,61,71	0
11	UND	A	2415	11/11	0.89	0.22	47,63,83,84	0
6	MYS	A	2426	15/15	0.90	0.25	45,49,66,69	0
5	D12	A	2406	12/12	0.90	0.28	58,68,75,77	0
6	MYS	A	2409	15/15	0.91	0.19	53,57,73,75	0
4	CLR	A	2405	28/28	0.95	0.13	34,37,72,78	0
2	ZMA	A	2401	25/25	0.97	0.12	21,25,43,50	0
3	NA	A	2402	1/1	0.99	0.07	35,35,35,35	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.

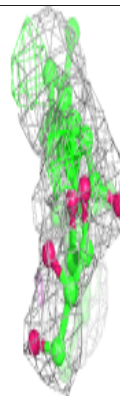
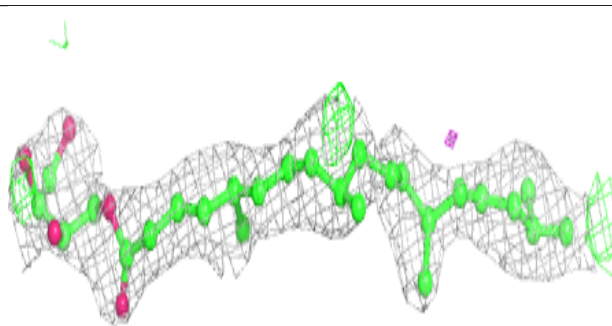
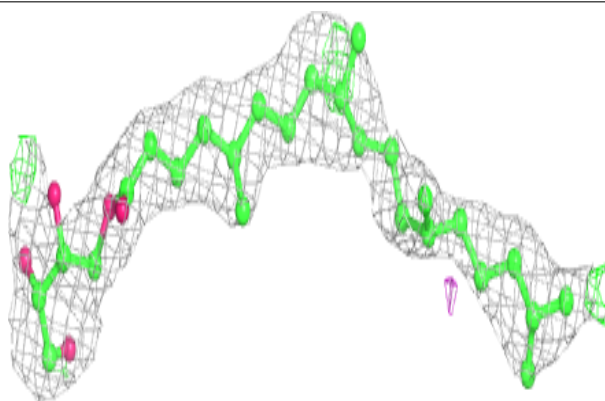


**Electron density around 8K6 A 2418:**

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

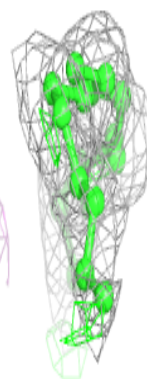
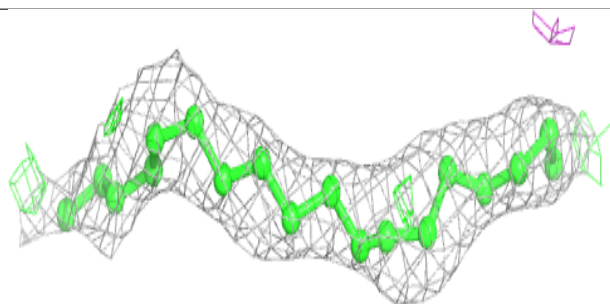
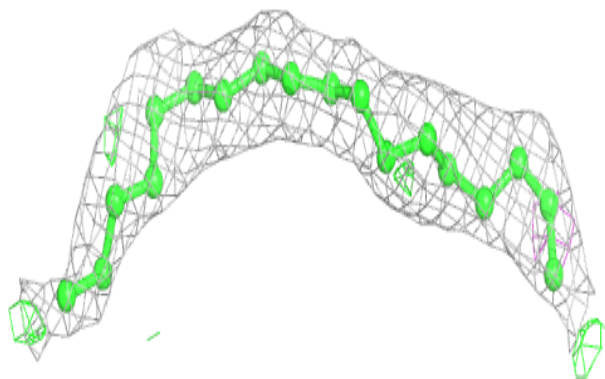
**Electron density around ER0 A 2416:**

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

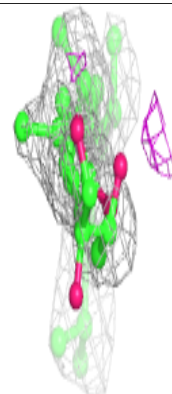
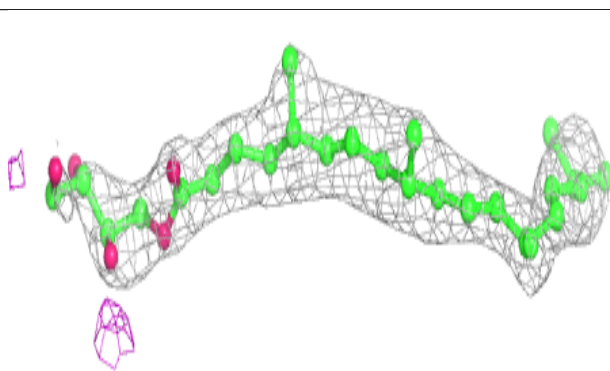
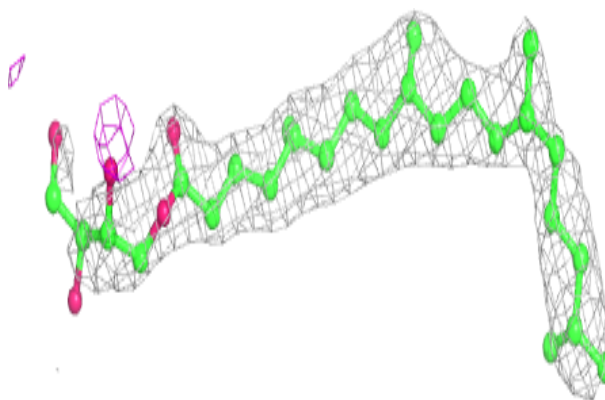


**Electron density around 8K6 A 2410:**

$2mF_o-DF_c$  (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:**

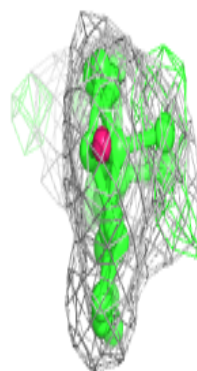
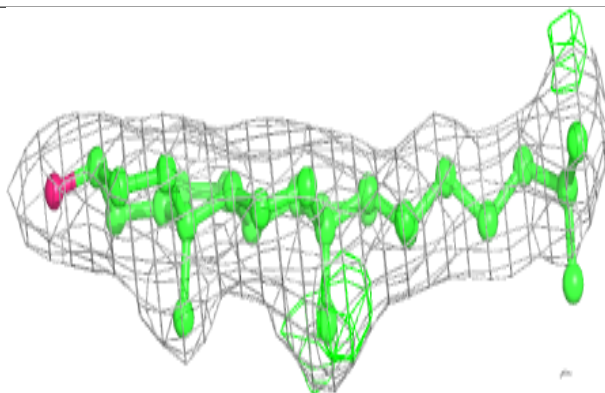
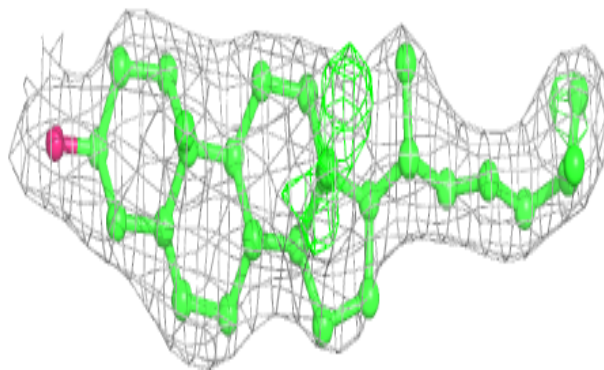
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



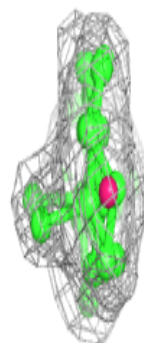
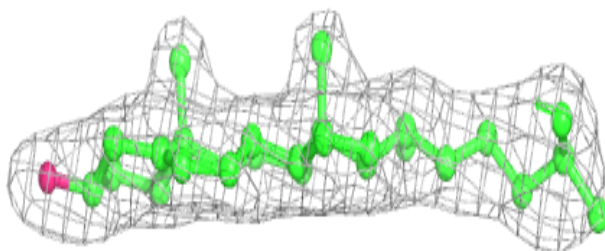
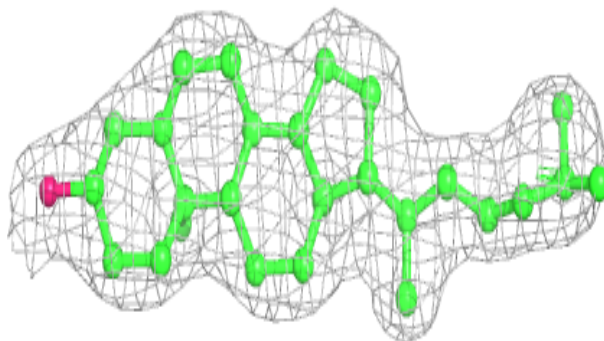


**Electron density around CLR A 2404:**

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

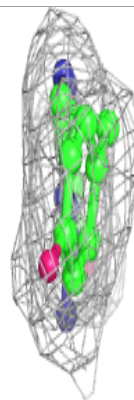
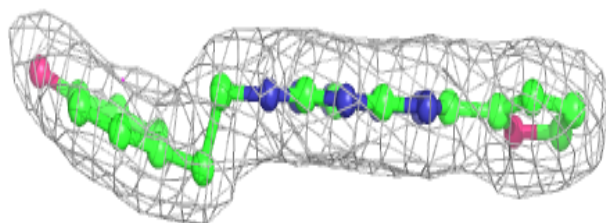
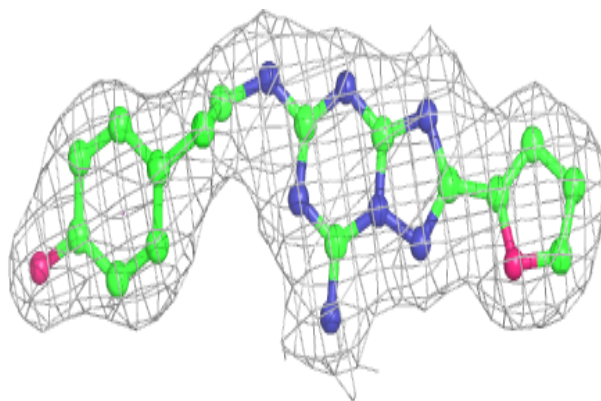
**Electron density around CLR A 2405:**

$2mF_o-DF_c$  (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.