



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:51 PM UTC

PDB ID : 4PXZ / pdb_00004pxz
Title : Crystal structure of P2Y12 receptor in complex with 2MeSADP
Authors : Zhang, J.; Zhang, K.; Gao, Z.G.; Paoletta, S.; Zhang, D.; Han, G.W.; Li, T.;
Ma, L.; Zhang, W.; Muller, C.E.; Yang, H.; Jiang, H.; Cherezov, V.; Katritch,
V.; Jacobson, K.A.; Stevens, R.C.; Wu, B.; Zhao, Q.; GPCR Network (GPCR)
Deposited on : 2014-03-25
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

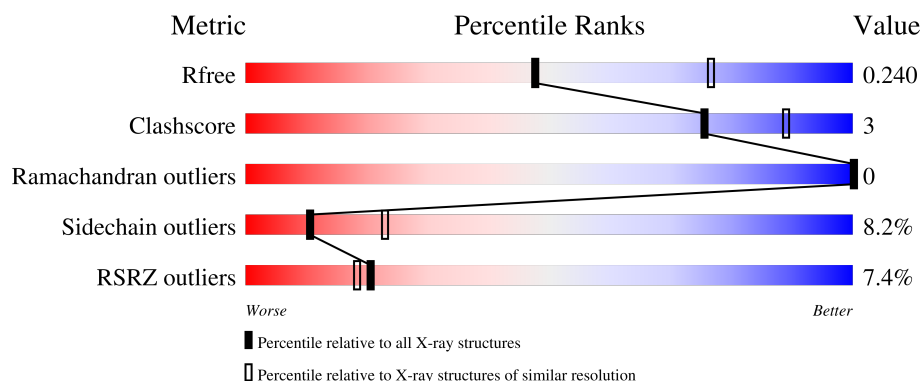
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	466	6% 71% 11% 16%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3302 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.

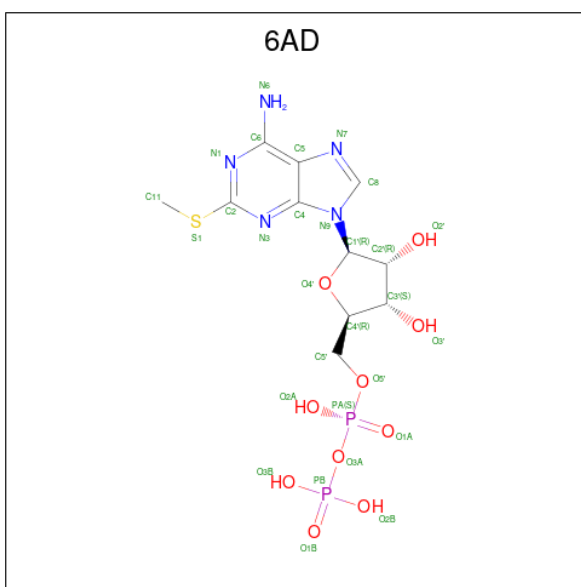
- Molecule 1 is a protein called P2Y purinoceptor 12, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	1	0
			3140	2071	509	545	15			

There are 23 discrepancies between the modelled and reference sequences:

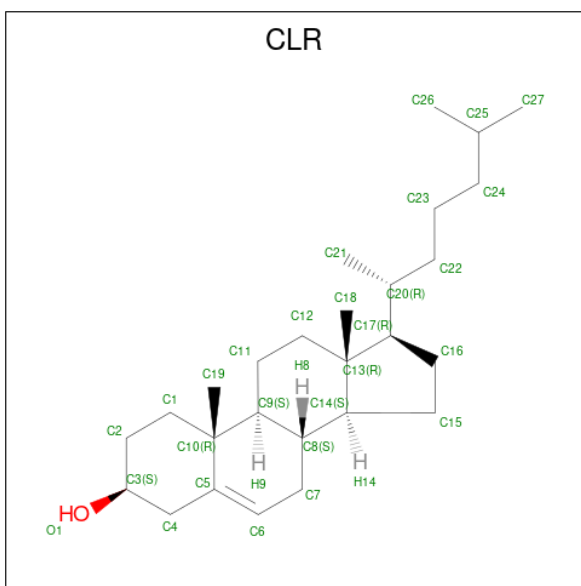
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ASP	-	expression tag	UNP Q9H244
A	-8	TYR	-	expression tag	UNP Q9H244
A	-7	LYS	-	expression tag	UNP Q9H244
A	-6	ASP	-	expression tag	UNP Q9H244
A	-5	ASP	-	expression tag	UNP Q9H244
A	-4	ASP	-	expression tag	UNP Q9H244
A	-3	ASP	-	expression tag	UNP Q9H244
A	-2	GLY	-	expression tag	UNP Q9H244
A	-1	ALA	-	expression tag	UNP Q9H244
A	0	PRO	-	expression tag	UNP Q9H244
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	294	ASN	ASP	engineered mutation	UNP Q9H244
A	343	GLY	-	expression tag	UNP Q9H244
A	344	ARG	-	expression tag	UNP Q9H244
A	345	PRO	-	expression tag	UNP Q9H244
A	346	LEU	-	expression tag	UNP Q9H244
A	347	GLU	-	expression tag	UNP Q9H244
A	348	VAL	-	expression tag	UNP Q9H244
A	349	LEU	-	expression tag	UNP Q9H244
A	350	PHE	-	expression tag	UNP Q9H244
A	351	GLN	-	expression tag	UNP Q9H244

- Molecule 2 is 2-(methylsulfanyl)adenosine 5'-(trihydrogen diphosphate) (CCD ID: 6AD) (formula: C₁₁H₁₇N₅O₁₀P₂S).



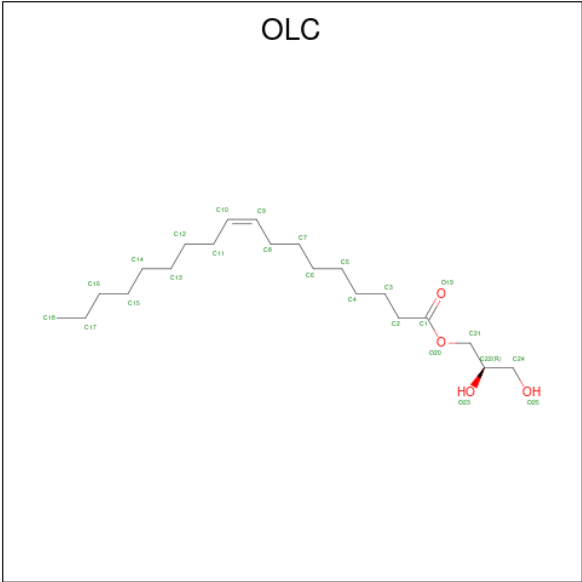
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			29	11	5	10	2	1		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



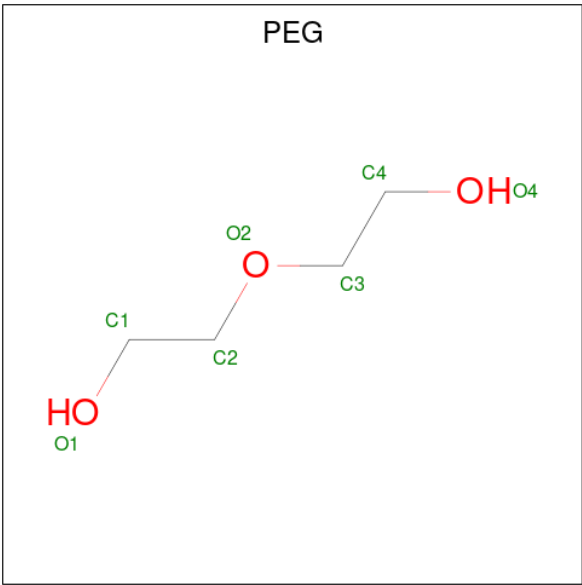
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			28	27 1		

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	13	4		
4	A	1	Total	C	O	0	0
			17	13	4		
4	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.11Å 104.17Å 169.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.88 – 2.50 28.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.88-2.50) 99.9 (28.88-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.201 , 0.230 0.208 , 0.240	Depositor DCC
R_{free} test set	1041 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	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	0.95	EDS
Total number of atoms	3302	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% 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: OLC, CLR, 6AD, PEG

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	0.84	0/3213	1.42	10/4359 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ILE	N-CA-CB	7.75	115.71	110.52
1	A	106	PHE	CA-CB-CG	7.43	121.23	113.80
1	A	70	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	286	LEU	CA-C-N	5.48	127.63	120.28
1	A	286	LEU	C-N-CA	5.48	127.63	120.28
1	A	153	PHE	CA-C-N	5.41	127.47	120.44
1	A	153	PHE	C-N-CA	5.41	127.47	120.44
1	A	256	ARG	N-CA-C	5.12	116.72	111.03
1	A	272	ALA	CA-C-N	5.04	126.99	120.44
1	A	272	ALA	C-N-CA	5.04	126.99	120.44

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	3140	0	3218	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	17	0	0
3	A	28	0	46	2	0
4	A	49	0	63	2	0
5	A	7	0	10	0	0
6	A	49	0	0	0	0
All	All	3302	0	3354	20	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 3.

All (20) 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:76:THR:HG21	1:A:104:PHE:HB2	1.75	0.67
1:A:98:GLN:HE22	4:A:1203:OLC:H21A	1.63	0.62
1:A:122:ARG:HH21	1:A:122:ARG:HA	1.69	0.58
1:A:1004:GLU:O	1:A:1008:GLU:HG2	2.05	0.56
1:A:152:MET:HE1	1:A:197:ILE:HD13	1.86	0.56
1:A:53:ILE:HD11	1:A:60:ILE:HG12	1.87	0.55
1:A:68:ILE:HG12	3:A:1202:CLR:H151	1.88	0.54
1:A:296:PHE:HA	1:A:299:PHE:HB2	1.92	0.51
1:A:122:ARG:HD2	1:A:237:LYS:HD2	1.95	0.49
1:A:21:TYR:HD1	1:A:24:THR:HG21	1.77	0.49
1:A:142:LYS:O	1:A:146:VAL:HG23	2.13	0.48
1:A:1012:ASP:HA	1:A:1015:LYS:HE3	1.95	0.47
1:A:110:ILE:HG13	1:A:152:MET:HG3	1.97	0.46
1:A:64:LYS:HB3	3:A:1202:CLR:H6	1.98	0.46
4:A:1204:OLC:H21	4:A:1205:OLC:H24A	1.98	0.45
1:A:35:LEU:HD11	1:A:289:LEU:HD12	2.00	0.44
1:A:59:PHE:HB2	1:A:121:ASP:OD2	2.17	0.43
1:A:108:MET:HE2	1:A:112:ILE:HD11	2.01	0.42
1:A:43:ASN:HB3	1:A:71:LEU:HD12	2.02	0.42
1:A:119:THR:HG21	1:A:205:VAL:HA	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	389/466 (84%)	384 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	343/420 (82%)	315 (92%)	28 (8%)	10	23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	18	THR
1	A	24	THR
1	A	30	LEU
1	A	41	ILE
1	A	53	ILE
1	A	60	ILE
1	A	66	THR
1	A	68	ILE
1	A	71	LEU
1	A	72	LEU
1	A	76	THR
1	A	106	PHE

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Mol	Chain	Res	Type
1	A	143	ILE
1	A	156	SER
1	A	157	LEU
1	A	174	LYS
1	A	184	LEU
1	A	203	LEU
1	A	1014	LEU
1	A	1062	ARG
1	A	231	ARG
1	A	233	LYS
1	A	256	ARG
1	A	267	VAL
1	A	280	LYS
1	A	287	THR
1	A	301	LEU

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

Mol	Chain	Res	Type
1	A	43	ASN
1	A	52	GLN
1	A	98	GLN
1	A	137	ASN
1	A	159	ASN
1	A	1006	ASN
1	A	1025	GLN
1	A	235	ASN
1	A	290	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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
4	OLC	A	1205	-	14,14,24	0.62	0	15,15,25	0.68	0
2	6AD	A	1201	-	30,31,31	1.41	7 (23%)	45,48,48	1.93	11 (24%)
3	CLR	A	1202	-	31,31,31	1.41	4 (12%)	48,48,48	1.48	8 (16%)
5	PEG	A	1206	-	6,6,6	0.67	0	5,5,5	0.49	0
4	OLC	A	1203	-	16,16,24	1.11	1 (6%)	17,17,25	0.87	0
4	OLC	A	1204	-	16,16,24	1.17	1 (6%)	17,17,25	0.75	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
4	OLC	A	1205	-	-	3/14/14/24	-
2	6AD	A	1201	-	-	2/18/34/34	0/3/3/3
3	CLR	A	1202	-	-	2/10/68/68	0/4/4/4
5	PEG	A	1206	-	-	2/4/4/4	-
4	OLC	A	1203	-	-	8/16/16/24	-
4	OLC	A	1204	-	-	9/16/16/24	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1204	OLC	C10-C9	3.81	1.53	1.29
4	A	1203	OLC	C10-C9	3.79	1.53	1.29
2	A	1201	6AD	PA-O3A	3.16	1.62	1.59
3	A	1202	CLR	C18-C13	3.01	1.59	1.54
3	A	1202	CLR	C8-C9	2.76	1.58	1.53
2	A	1201	6AD	C5-N7	-2.73	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	6AD	O4'-C1'	2.16	1.47	1.42
3	A	1202	CLR	C4-C3	2.15	1.56	1.52
2	A	1201	6AD	PB-O2B	2.13	1.62	1.54
2	A	1201	6AD	C8-N9	-2.12	1.33	1.37
2	A	1201	6AD	C4-N9	-2.11	1.33	1.37
2	A	1201	6AD	C5-C4	-2.05	1.35	1.39
3	A	1202	CLR	C13-C14	2.02	1.58	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	6AD	C5-C4-N3	-6.60	120.23	127.18
2	A	1201	6AD	N1-C2-N3	-3.97	119.75	127.00
2	A	1201	6AD	N9-C8-N7	-3.55	108.90	113.94
2	A	1201	6AD	N3-C4-N9	3.38	131.28	126.99
3	A	1202	CLR	C11-C9-C8	3.27	116.34	111.78
3	A	1202	CLR	O1-C3-C2	-3.12	102.01	110.17
3	A	1202	CLR	C21-C20-C22	-3.12	105.52	110.34
2	A	1201	6AD	C2-N3-C4	3.06	120.31	112.29
2	A	1201	6AD	C4-C5-N7	-3.01	107.14	110.58
2	A	1201	6AD	N6-C6-N1	2.95	121.01	117.03
2	A	1201	6AD	C5-N7-C8	2.92	108.04	103.45
3	A	1202	CLR	C12-C13-C17	-2.65	112.69	116.60
2	A	1201	6AD	C11-S1-C2	2.59	104.19	102.25
3	A	1202	CLR	C18-C13-C14	2.54	116.28	111.68
3	A	1202	CLR	C23-C22-C20	-2.45	108.22	115.08
2	A	1201	6AD	C5-C4-N9	2.41	108.43	105.81
2	A	1201	6AD	O4'-C1'-N9	2.33	112.56	108.09
3	A	1202	CLR	C1-C2-C3	2.24	113.45	110.48
3	A	1202	CLR	C12-C13-C14	-2.22	103.92	107.25

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	6AD	N3-C2-S1-C11
2	A	1201	6AD	N1-C2-S1-C11
4	A	1205	OLC	C2-C1-O20-C21
4	A	1204	OLC	C2-C1-O20-C21
4	A	1205	OLC	O19-C1-O20-C21
5	A	1206	PEG	O1-C1-C2-O2
4	A	1204	OLC	O19-C1-O20-C21

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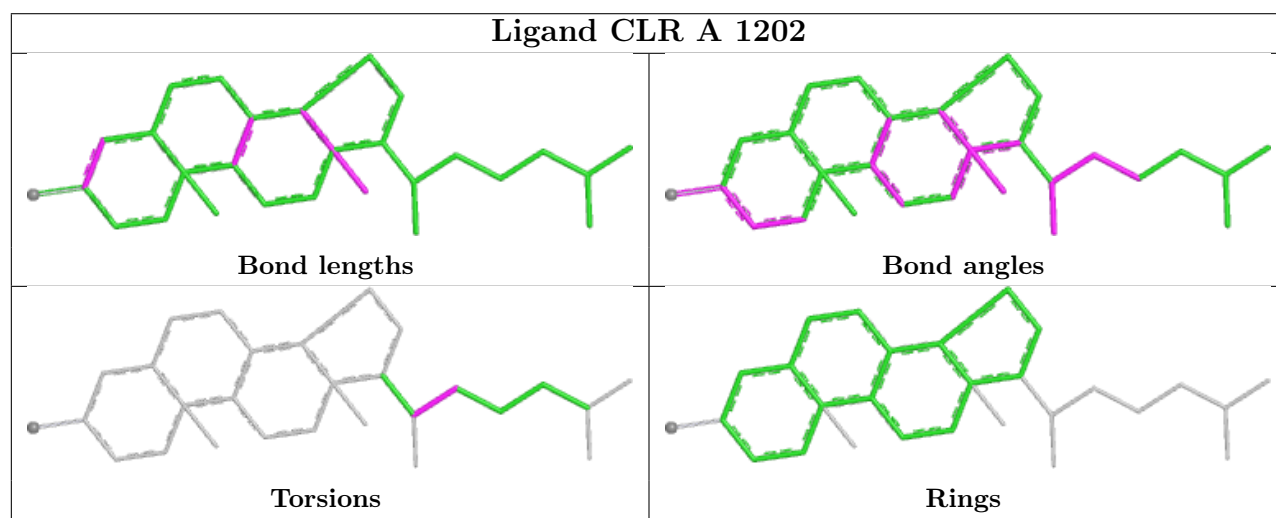
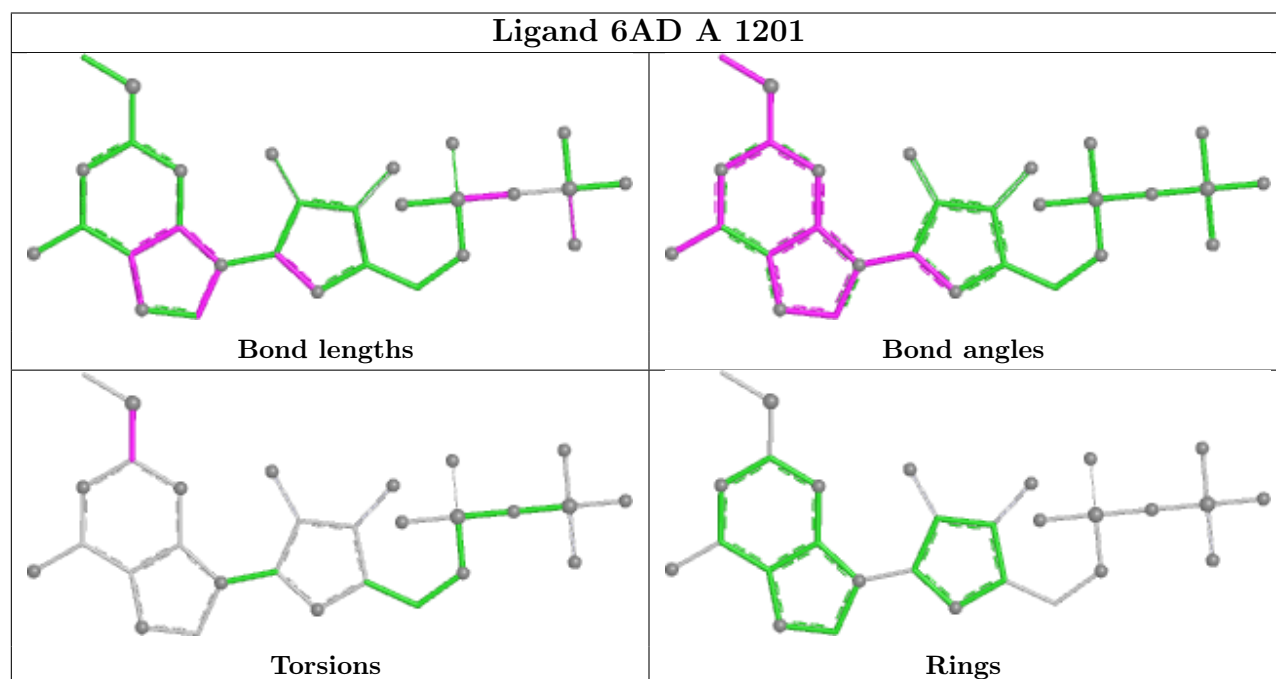
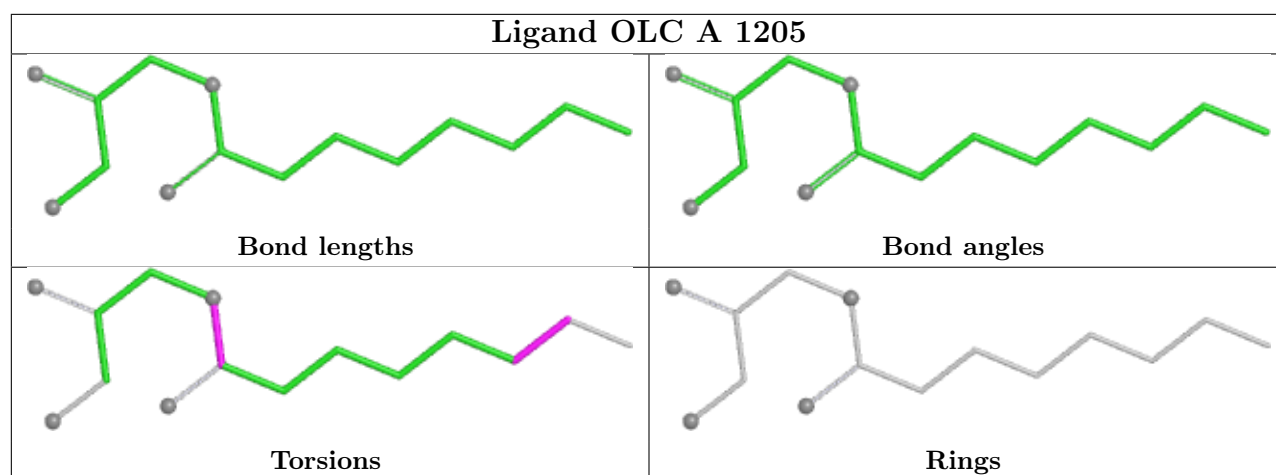
Mol	Chain	Res	Type	Atoms
4	A	1203	OLC	C21-C22-C24-O25
3	A	1202	CLR	C17-C20-C22-C23
4	A	1204	OLC	C5-C6-C7-C8
4	A	1204	OLC	C3-C4-C5-C6
4	A	1204	OLC	C2-C3-C4-C5
3	A	1202	CLR	C21-C20-C22-C23
4	A	1204	OLC	C4-C5-C6-C7
4	A	1203	OLC	O19-C1-O20-C21
4	A	1204	OLC	C1-C2-C3-C4
4	A	1203	OLC	C2-C1-O20-C21
4	A	1205	OLC	C5-C6-C7-C8
4	A	1203	OLC	O23-C22-C24-O25
4	A	1204	OLC	C21-C22-C24-O25
4	A	1203	OLC	C4-C5-C6-C7
4	A	1204	OLC	C7-C8-C9-C10
4	A	1203	OLC	C1-C2-C3-C4
5	A	1206	PEG	O2-C3-C4-O4
4	A	1203	OLC	O20-C1-C2-C3
4	A	1203	OLC	O19-C1-C2-C3

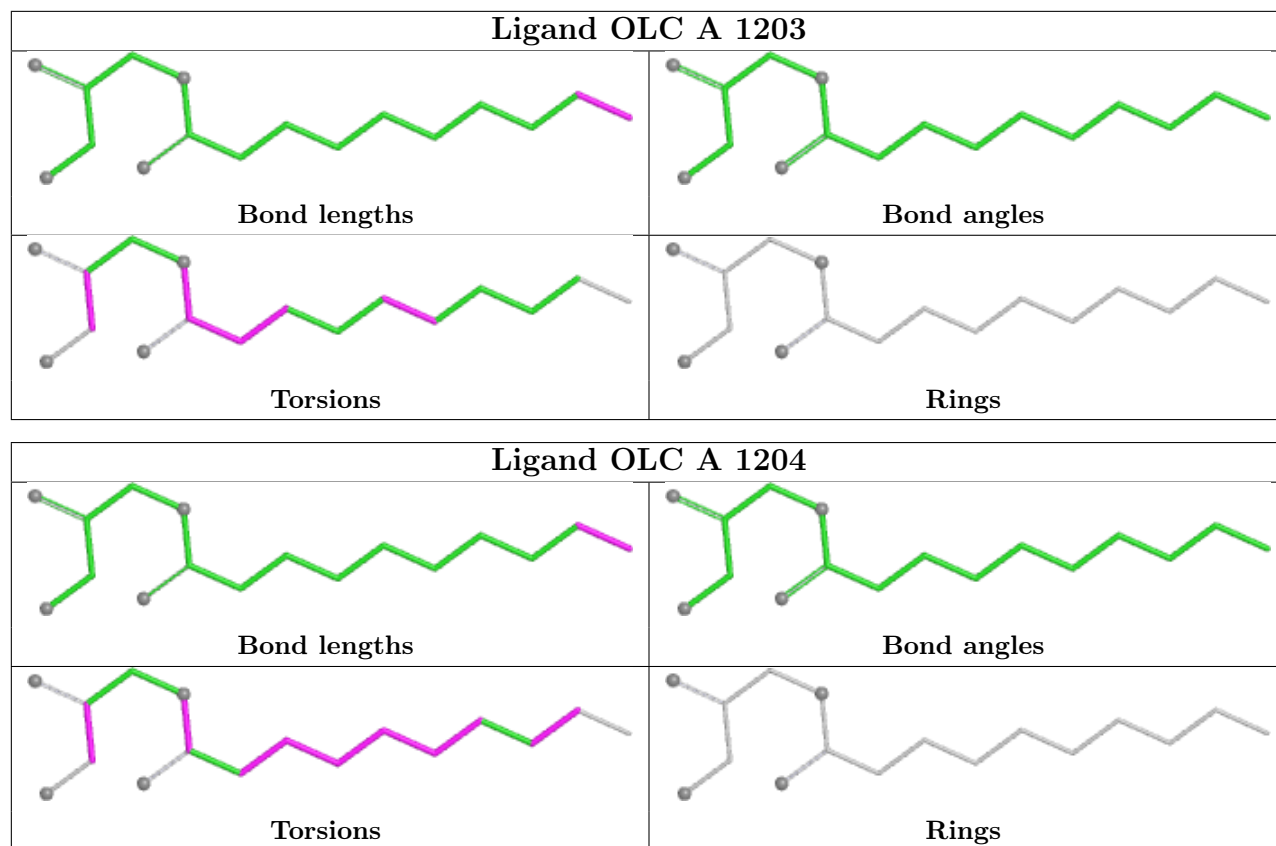
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1205	OLC	1	0
3	A	1202	CLR	2	0
4	A	1203	OLC	1	0
4	A	1204	OLC	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, 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	392/466 (84%)	0.38	29 (7%) 20 18	34, 60, 105, 164	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	PHE	5.3
1	A	301	LEU	5.3
1	A	15	SER	5.0
1	A	300	PHE	5.0
1	A	129	PRO	4.7
1	A	302	CYS	4.5
1	A	17	CYS	3.4
1	A	297	ILE	3.3
1	A	135	PRO	2.9
1	A	167	PRO	2.9
1	A	293	LEU	2.9
1	A	136	LYS	2.6
1	A	50	PHE	2.6
1	A	106	PHE	2.6
1	A	299	PHE	2.5
1	A	166	GLN	2.4
1	A	304	SER	2.4
1	A	45	LEU	2.4
1	A	128	ARG	2.4
1	A	21	TYR	2.4
1	A	296	PHE	2.3
1	A	270	CYS	2.3
1	A	41	ILE	2.2
1	A	18	THR	2.2
1	A	177	PHE	2.2
1	A	16	LEU	2.1
1	A	24	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	67	VAL	2.0
1	A	40	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

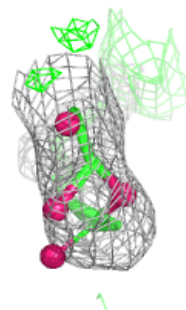
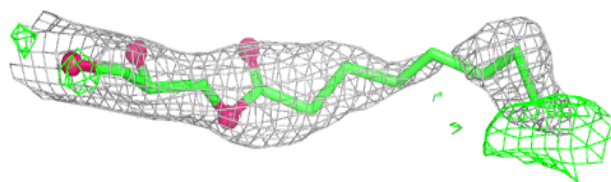
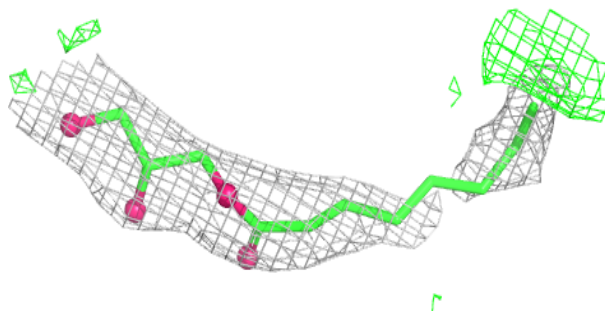
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OLC	A	1205	15/25	0.72	0.23	90,95,95,97	0
4	OLC	A	1203	17/25	0.85	0.15	69,80,95,96	0
5	PEG	A	1206	7/7	0.87	0.15	59,62,65,65	0
3	CLR	A	1202	28/28	0.88	0.20	82,87,91,92	0
4	OLC	A	1204	17/25	0.88	0.16	66,73,86,86	0
2	6AD	A	1201	29/29	0.98	0.06	36,43,51,51	0

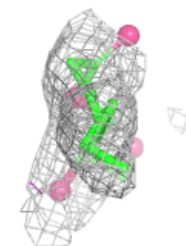
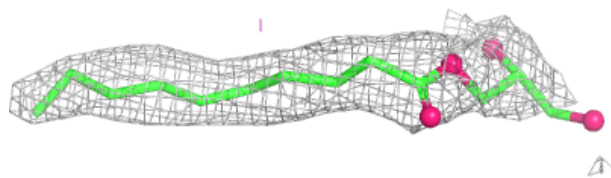
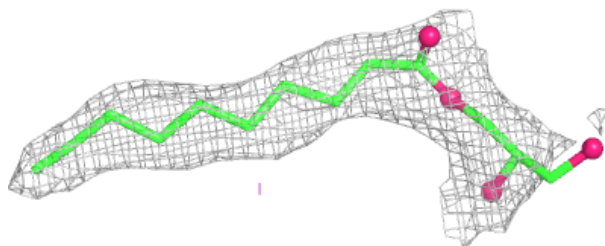
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 1205:

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

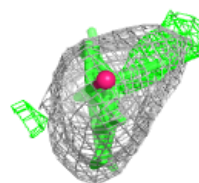
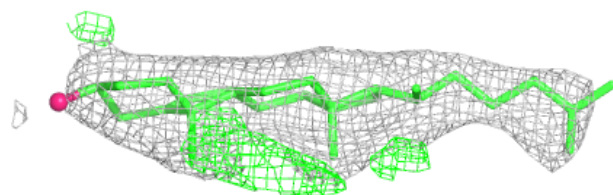
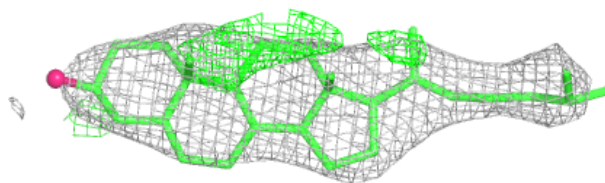
**Electron density around OLC A 1203:**

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

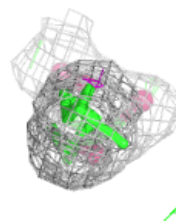
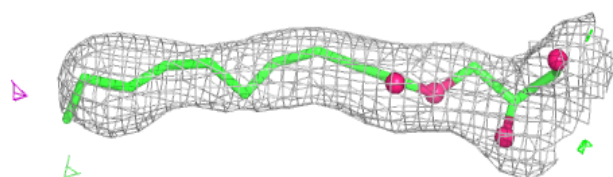
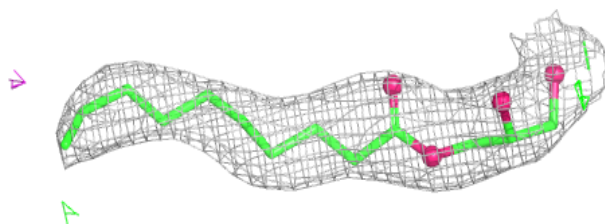


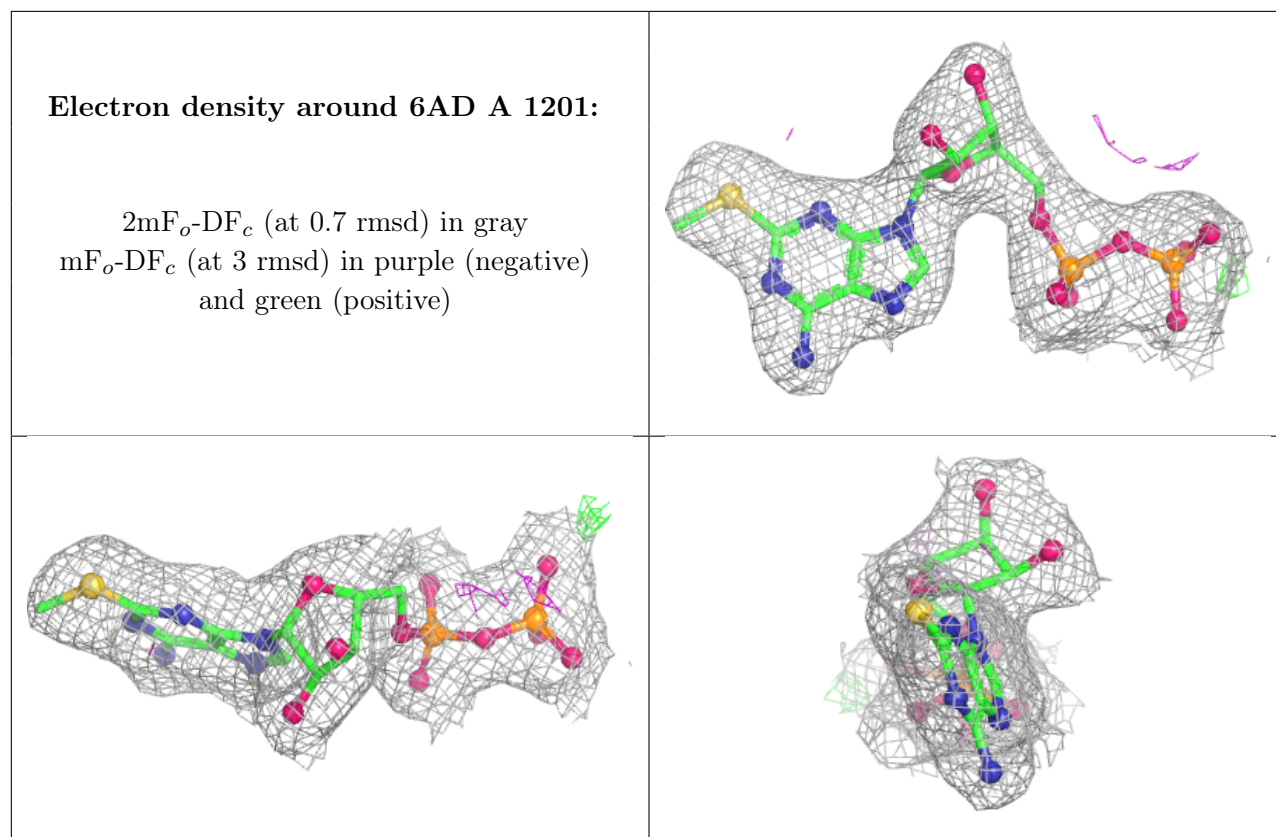
Electron density around CLR A 1202:

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

**Electron density around OLC A 1204:**

$2mF_o-DF_c$ (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.