



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:34 pm BST

PDB ID : 4NTJ  
Title : Structure of the human P2Y12 receptor in complex with an antithrombotic drug  
Authors : Zhang, K.; Zhang, J.; Gao, Z.-G.; Zhang, D.; Zhu, L.; Han, G.W.; Moss, S.M.; Paoletta, S.; Kiselev, E.; Lu, W.; Fenalti, G.; 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 : 2013-12-02  
Resolution : 2.62 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 : 2.11  
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) : 2.11

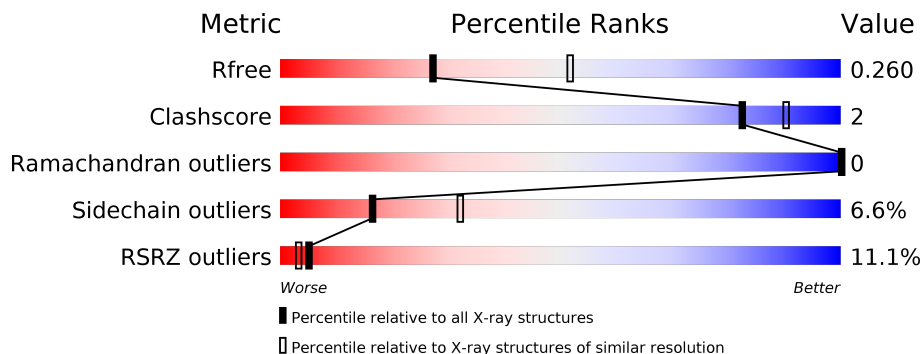
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	466	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLC	A	1204	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3025 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.

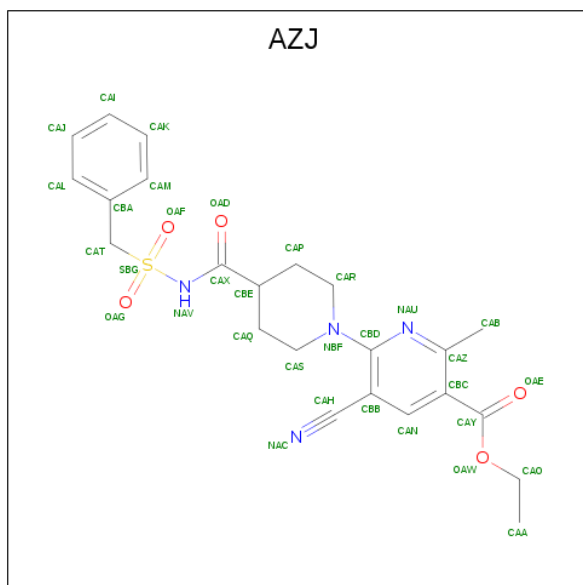
- Molecule 1 is a protein called P2Y purinoceptor 12,Soluble cytochrome b562,P2Y purinoceptor 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	369	2886	1908	459	505	14	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

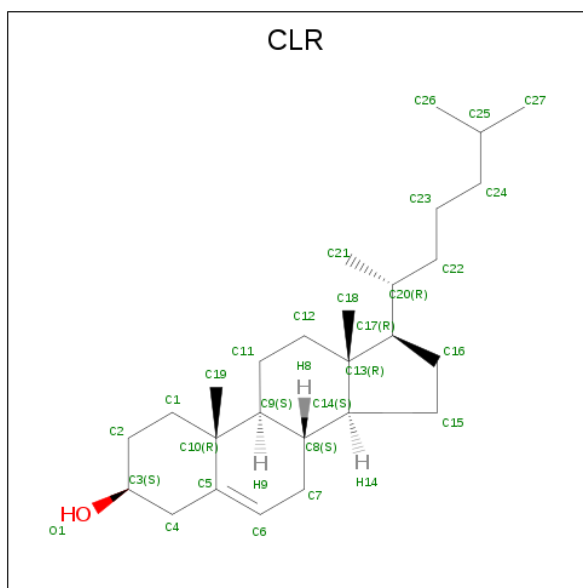
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q9H244
A	-7	TYR	-	expression tag	UNP Q9H244
A	-6	LYS	-	expression tag	UNP Q9H244
A	-5	ASP	-	expression tag	UNP Q9H244
A	-4	ASP	-	expression tag	UNP Q9H244
A	-3	ASP	-	expression tag	UNP Q9H244
A	-2	ASP	-	expression tag	UNP Q9H244
A	-1	GLY	-	expression tag	UNP Q9H244
A	0	ALA	-	expression tag	UNP Q9H244
A	1	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 ethyl 6-{4-[(benzylsulfonyl)carbamoyl]piperidin-1-yl}-5-cyano-2-methylpyridin e-3-carboxylate (three-letter code: AZJ) (formula: C<sub>23</sub>H<sub>26</sub>N<sub>4</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	33	23	4	5	1	0	0

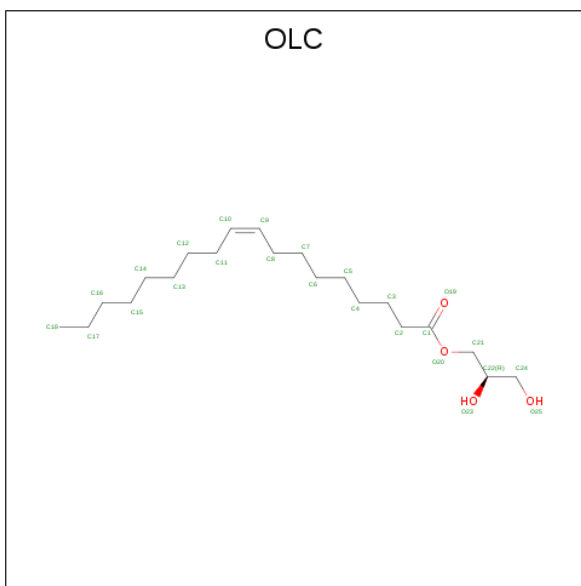
- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



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

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC)

(formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 17 13 4	0	0
4	A	1	Total C O 21 17 4	0	0

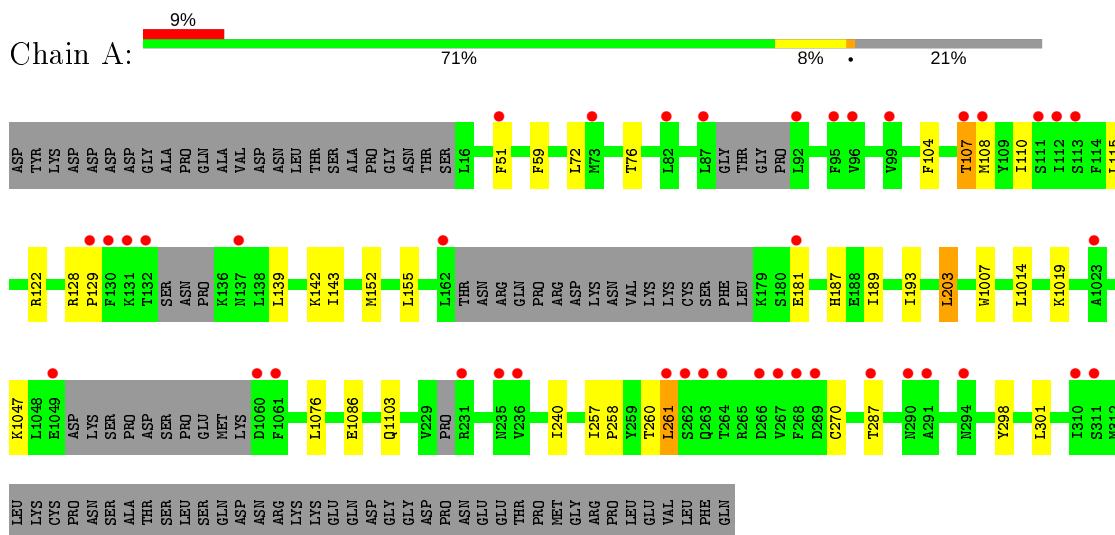
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: P2Y purinoceptor 12,Soluble cytochrome b562,P2Y purinoceptor 12



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.65Å 156.43Å 47.77Å 90.00° 111.08° 90.00°	Depositor
Resolution (Å)	26.44 – 2.62 26.10 – 2.62	Depositor EDS
% Data completeness (in resolution range)	94.2 (26.44-2.62) 94.2 (26.10-2.62)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.60Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.220 , 0.246 0.234 , 0.260	Depositor DCC
$R_{free}$ test set	990 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 91.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k+1,3/2*h-1/2*k+1,-1 0.000 for 1/2*h-1/2*k+1,-3/2*h-1/2*k-1,-1	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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: AZJ, OLC, 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	0.47	0/2946	0.59	0/4005

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	2886	0	2852	12	0
2	A	33	0	26	2	0
3	A	56	0	92	2	0
4	A	38	0	51	1	0
5	A	12	0	0	0	0
All	All	3025	0	3021	15	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 2.

All (15) 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
2:A:1201:AZJ:H4	2:A:1201:AZJ:OAE	2.07	0.55
3:A:1203:CLR:H212	4:A:1205:OLC:H8	1.96	0.46
1:A:1007:TRP:CZ3	1:A:1103:GLN:HG3	2.51	0.46
1:A:128:ARG:HG2	1:A:129:PRO:HD2	1.98	0.44
1:A:104:PHE:O	1:A:107:THR:HG22	2.18	0.44
1:A:110:ILE:HG13	1:A:152:MET:HG3	1.99	0.44
2:A:1201:AZJ:H21	2:A:1201:AZJ:CAH	2.48	0.43
1:A:257:ILE:HB	1:A:258:PRO:HD3	2.01	0.42
1:A:59:PHE:HZ	1:A:301:LEU:HB3	1.84	0.41
1:A:189:ILE:O	1:A:193:ILE:HG12	2.20	0.41
1:A:104:PHE:HZ	1:A:287:THR:HG22	1.85	0.41
1:A:203:LEU:HB3	3:A:1203:CLR:H161	2.03	0.41
1:A:260:THR:HG23	1:A:261:LEU:HD13	2.03	0.40
1:A:139:LEU:O	1:A:143:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	357/466 (77%)	344 (96%)	13 (4%)	0	<b>100</b> <b>100</b>

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	301/420 (72%)	281 (93%)	20 (7%)	16 32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	72	LEU
1	A	107	THR
1	A	108	MET
1	A	115	LEU
1	A	122	ARG
1	A	142	LYS
1	A	155	LEU
1	A	181	GLU
1	A	187	HIS
1	A	203	LEU
1	A	1014	LEU
1	A	1019	LYS
1	A	1047	LYS
1	A	1076	LEU
1	A	1086	GLU
1	A	240	ILE
1	A	261	LEU
1	A	270	CYS
1	A	298	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	1204	-	16,16,24	1.23	1 (6%)	17,17,25	0.98	1 (5%)
2	AZJ	A	1201	-	33,35,35	2.72	7 (21%)	44,49,49	1.70	6 (13%)
4	OLC	A	1205	-	20,20,24	1.07	1 (5%)	21,21,25	0.95	2 (9%)
3	CLR	A	1203	-	31,31,31	0.61	0	48,48,48	1.82	14 (29%)
3	CLR	A	1202	-	31,31,31	0.61	0	48,48,48	1.78	13 (27%)

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	1204	-	-	4/16/16/24	-
2	AZJ	A	1201	-	-	2/26/37/37	0/3/3/3
4	OLC	A	1205	-	-	7/20/20/24	-
3	CLR	A	1203	-	-	5/10/68/68	0/4/4/4
3	CLR	A	1202	-	-	8/10/68/68	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	AZJ	OAF-SBG	7.54	1.54	1.43
2	A	1201	AZJ	OAG-SBG	7.46	1.54	1.43
2	A	1201	AZJ	CAB-CAZ	-5.77	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	AZJ	CAT-CBA	-5.49	1.41	1.50
2	A	1201	AZJ	CBD-NBF	4.83	1.49	1.37
4	A	1204	OLC	O20-C1	4.66	1.47	1.33
4	A	1205	OLC	O20-C1	4.52	1.46	1.33
2	A	1201	AZJ	CBC-CAY	-3.69	1.42	1.50
2	A	1201	AZJ	CAR-NBF	2.36	1.50	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	AZJ	OAG-SBG-OAF	-7.02	109.17	119.35
2	A	1201	AZJ	CBD-NAU-CAZ	5.31	123.56	117.23
3	A	1203	CLR	C16-C17-C20	4.70	119.42	112.15
3	A	1202	CLR	C16-C17-C20	4.50	119.12	112.15
3	A	1202	CLR	C4-C5-C10	4.22	122.02	116.42
3	A	1202	CLR	C22-C20-C17	4.22	118.99	110.28
3	A	1203	CLR	C4-C5-C10	3.73	121.37	116.42
3	A	1203	CLR	C1-C2-C3	3.63	115.13	110.47
3	A	1203	CLR	C15-C14-C13	3.54	108.11	103.84
3	A	1202	CLR	C15-C14-C13	3.30	107.82	103.84
3	A	1203	CLR	C16-C17-C13	3.20	107.70	103.84
3	A	1202	CLR	C16-C17-C13	3.15	107.64	103.84
3	A	1203	CLR	C4-C5-C6	-3.13	116.10	120.61
3	A	1202	CLR	C21-C20-C22	3.10	115.22	110.36
3	A	1203	CLR	C12-C11-C9	3.09	118.47	113.11
3	A	1202	CLR	C4-C5-C6	-2.82	116.54	120.61
4	A	1205	OLC	O20-C1-C2	2.82	120.76	111.91
3	A	1202	CLR	C11-C9-C10	2.75	116.70	113.08
2	A	1201	AZJ	CAT-SBG-NAV	2.58	112.19	105.07
3	A	1203	CLR	C22-C20-C17	2.54	115.53	110.28
4	A	1204	OLC	O20-C1-C2	2.52	119.83	111.91
3	A	1202	CLR	C10-C9-C8	2.39	116.32	112.73
3	A	1203	CLR	C12-C13-C17	-2.28	113.17	116.57
2	A	1201	AZJ	CBA-CAT-SBG	2.27	117.19	112.34
3	A	1202	CLR	C1-C2-C3	2.25	113.35	110.47
3	A	1203	CLR	C11-C9-C10	2.24	116.03	113.08
3	A	1203	CLR	C11-C9-C8	2.23	114.97	111.75
3	A	1203	CLR	C8-C7-C6	-2.22	109.54	112.73
3	A	1203	CLR	C21-C20-C17	-2.17	109.59	112.92
3	A	1202	CLR	C8-C7-C6	-2.17	109.61	112.73
2	A	1201	AZJ	CAX-NAV-SBG	-2.15	120.84	124.49
4	A	1205	OLC	O20-C1-O19	-2.09	118.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	AZJ	CAZ-CBC-CAY	2.08	125.47	122.75
3	A	1202	CLR	C7-C6-C5	-2.08	121.23	125.06
3	A	1202	CLR	C12-C11-C9	2.05	116.67	113.11
3	A	1203	CLR	C11-C12-C13	2.04	116.28	112.78

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1203	CLR	C13-C17-C20-C21
3	A	1202	CLR	C13-C17-C20-C22
2	A	1201	AZJ	CBC-CAY-OAW-CAO
2	A	1201	AZJ	OAE-CAY-OAW-CAO
3	A	1203	CLR	C16-C17-C20-C21
3	A	1202	CLR	C16-C17-C20-C21
3	A	1202	CLR	C13-C17-C20-C21
3	A	1203	CLR	C13-C17-C20-C22
4	A	1205	OLC	C2-C1-O20-C21
3	A	1203	CLR	C16-C17-C20-C22
3	A	1202	CLR	C16-C17-C20-C22
4	A	1205	OLC	O19-C1-O20-C21
3	A	1202	CLR	C17-C20-C22-C23
4	A	1205	OLC	C1-C2-C3-C4
3	A	1203	CLR	C22-C23-C24-C25
4	A	1204	OLC	C2-C3-C4-C5
4	A	1205	OLC	C4-C5-C6-C7
4	A	1205	OLC	C2-C3-C4-C5
4	A	1204	OLC	C3-C4-C5-C6
4	A	1204	OLC	C6-C7-C8-C9
3	A	1202	CLR	C22-C23-C24-C25
3	A	1202	CLR	C21-C20-C22-C23
4	A	1205	OLC	C9-C10-C11-C12
4	A	1205	OLC	C7-C8-C9-C10
3	A	1202	CLR	C23-C24-C25-C27
4	A	1204	OLC	O20-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

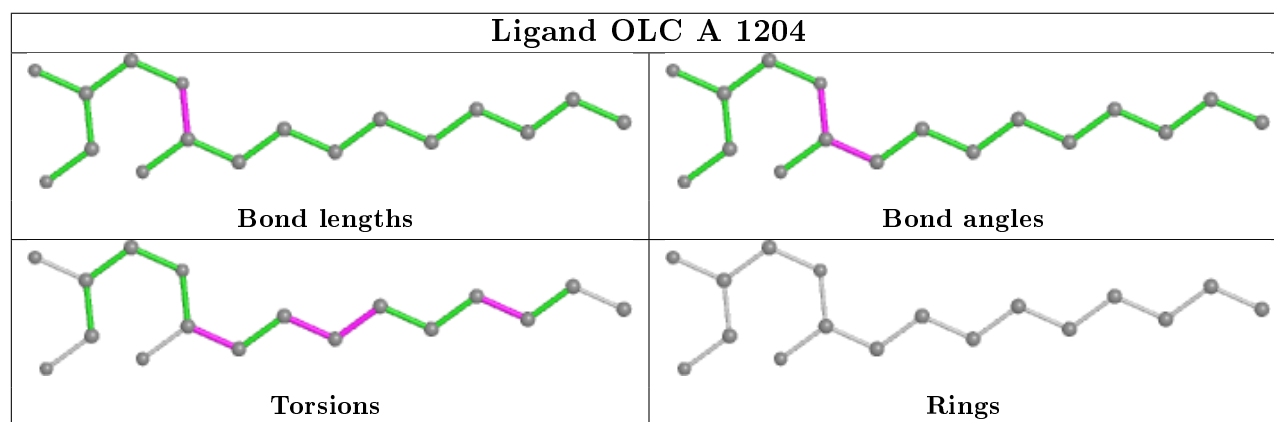
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	AZJ	2	0

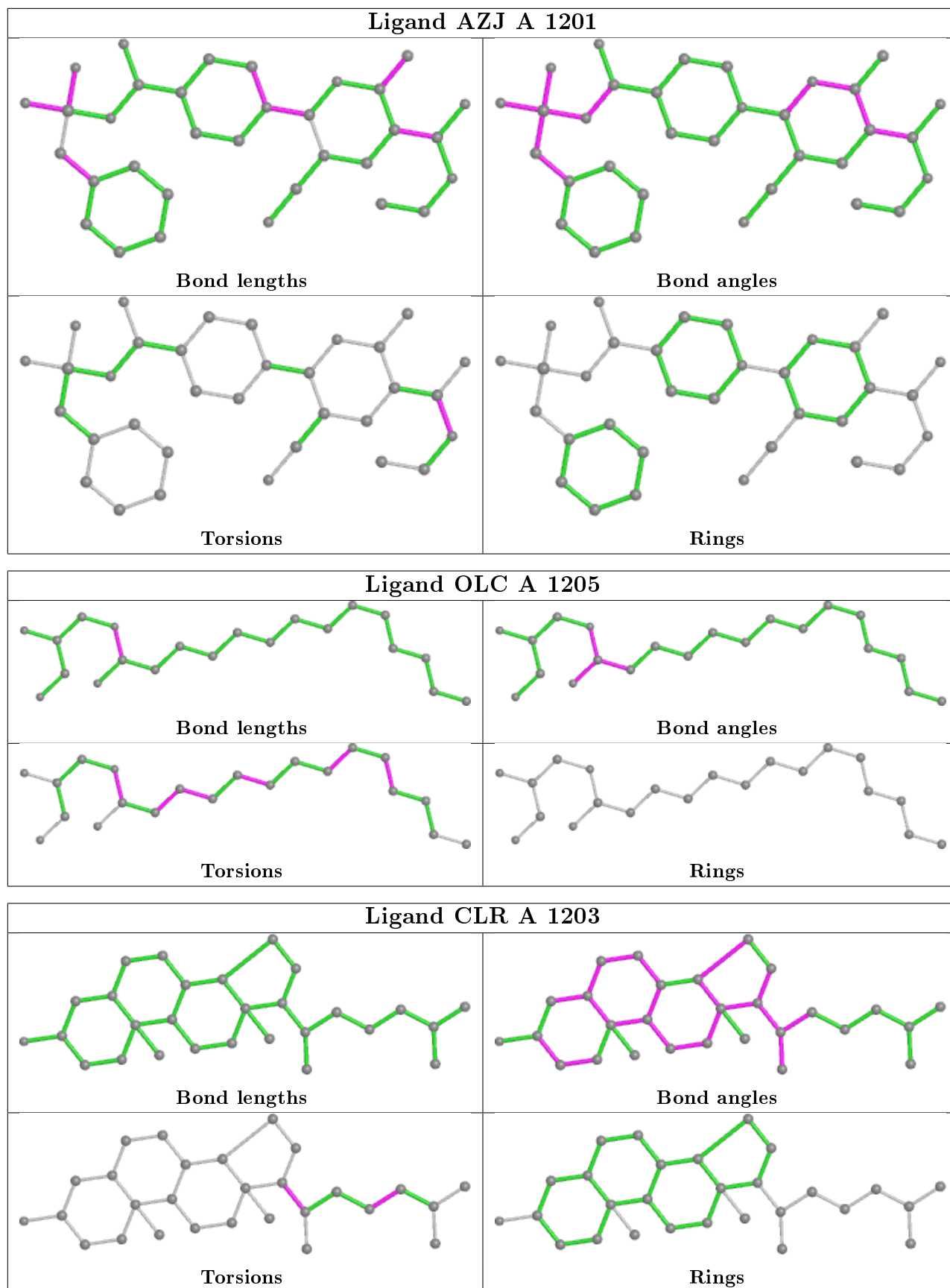
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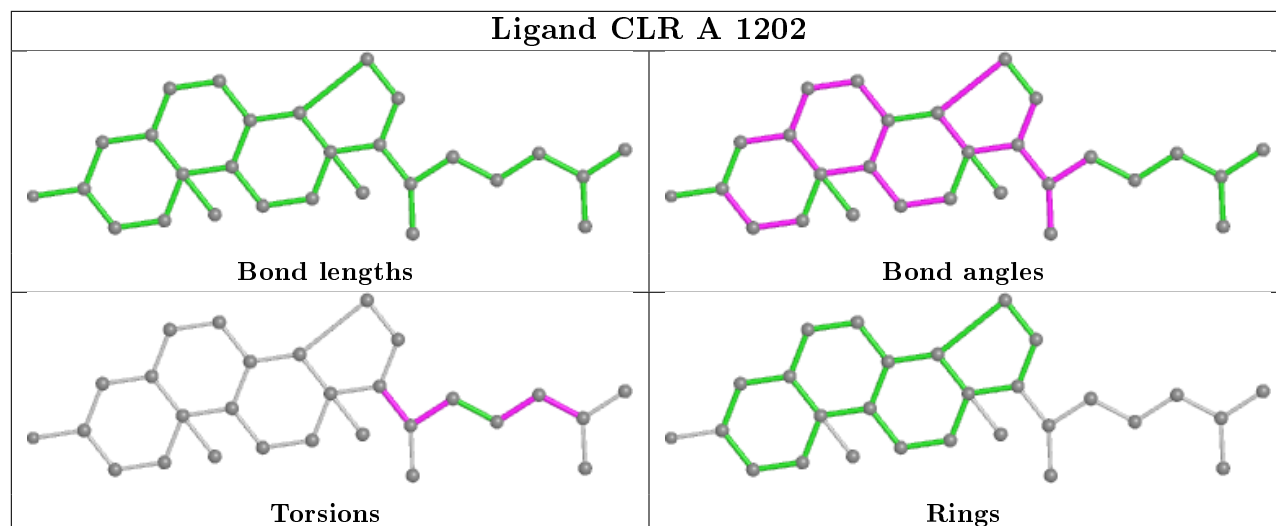
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1205	OLC	1	0
3	A	1203	CLR	2	0

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 [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	369/466 (79%)	0.55	41 (11%) <b>5</b> <b>3</b>	68, 101, 156, 212	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ARG	10.0
1	A	236	VAL	6.9
1	A	264	THR	6.2
1	A	130	PHE	4.6
1	A	51	PHE	4.4
1	A	267	VAL	4.3
1	A	162	LEU	4.0
1	A	262	SER	4.0
1	A	235	ASN	4.0
1	A	311	SER	3.7
1	A	132	THR	3.6
1	A	263	GLN	3.6
1	A	108	MET	3.3
1	A	112	ILE	3.1
1	A	92	LEU	3.0
1	A	290	ASN	3.0
1	A	95	PHE	2.9
1	A	87	LEU	2.8
1	A	111	SER	2.6
1	A	1060	ASP	2.5
1	A	99	VAL	2.4
1	A	113	SER	2.4
1	A	73	MET	2.4
1	A	82	LEU	2.4
1	A	261	LEU	2.4
1	A	291	ALA	2.4
1	A	266	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	294	ASN	2.4
1	A	268	PHE	2.3
1	A	131	LYS	2.2
1	A	269	ASP	2.2
1	A	96	VAL	2.2
1	A	1061	PHE	2.2
1	A	107	THR	2.2
1	A	287	THR	2.2
1	A	137	ASN	2.1
1	A	129	PRO	2.1
1	A	310	ILE	2.1
1	A	181	GLU	2.1
1	A	1049	GLU	2.1
1	A	1023	ALA	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 carbohydrates in this entry.

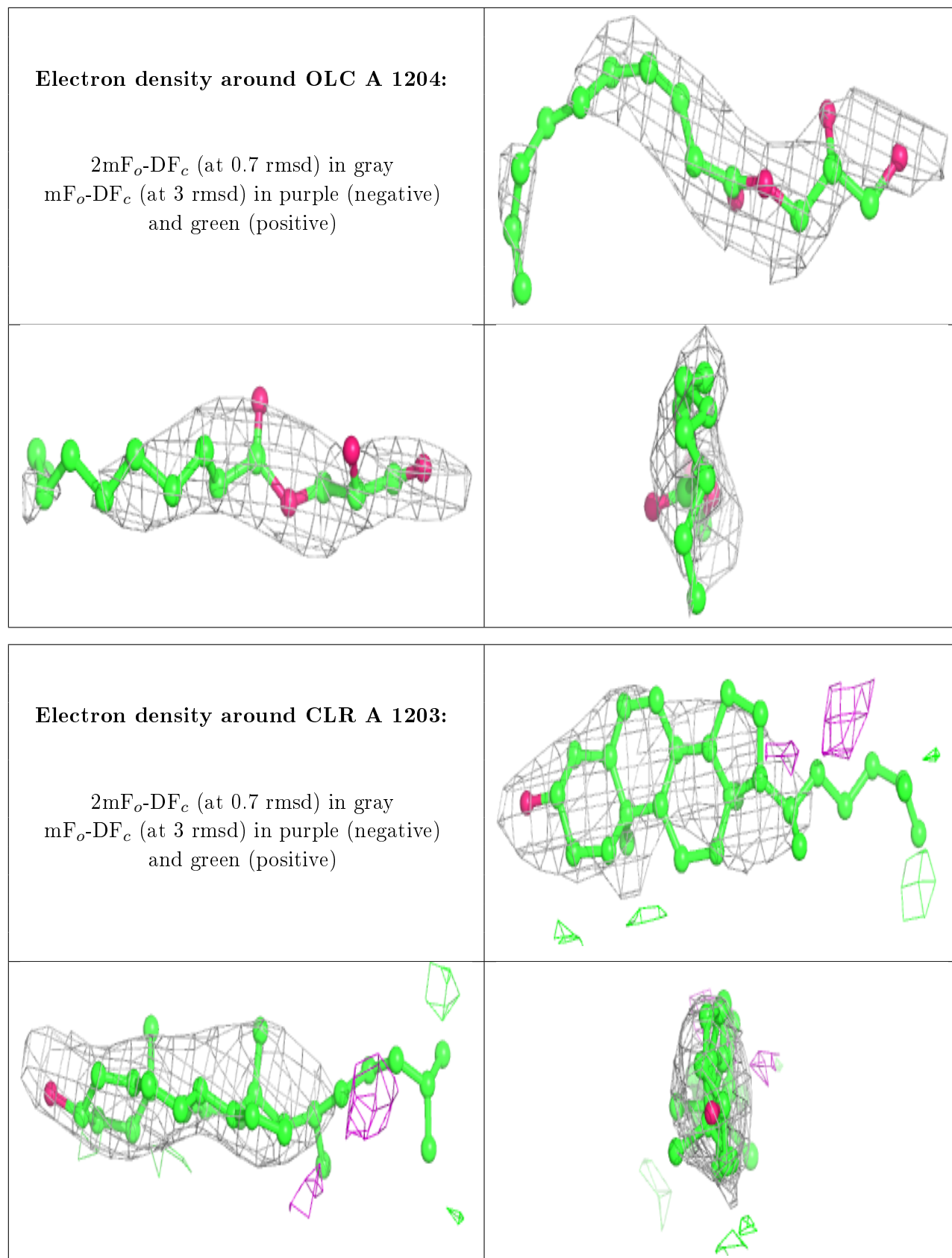
## 6.4 Ligands [i](#)

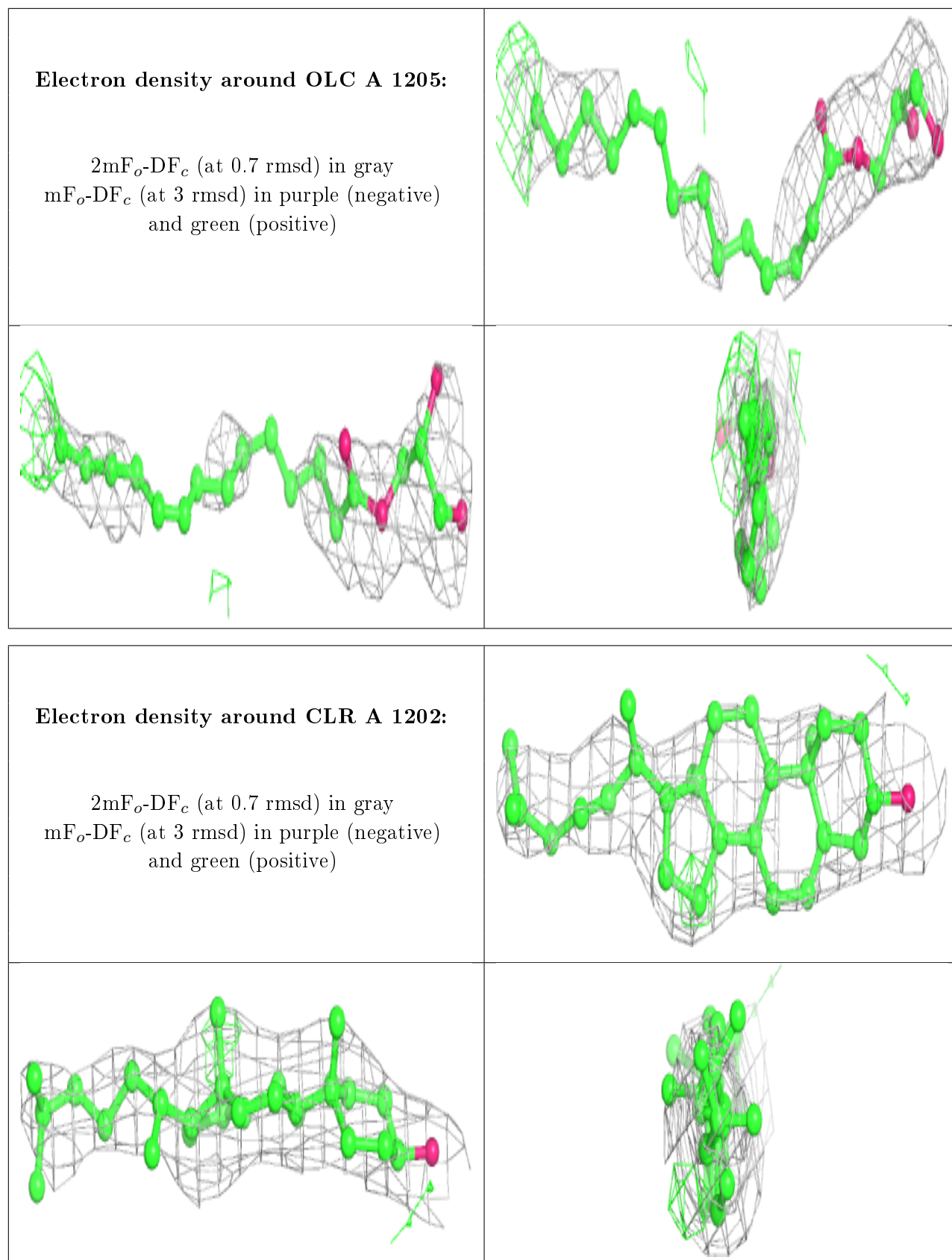
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

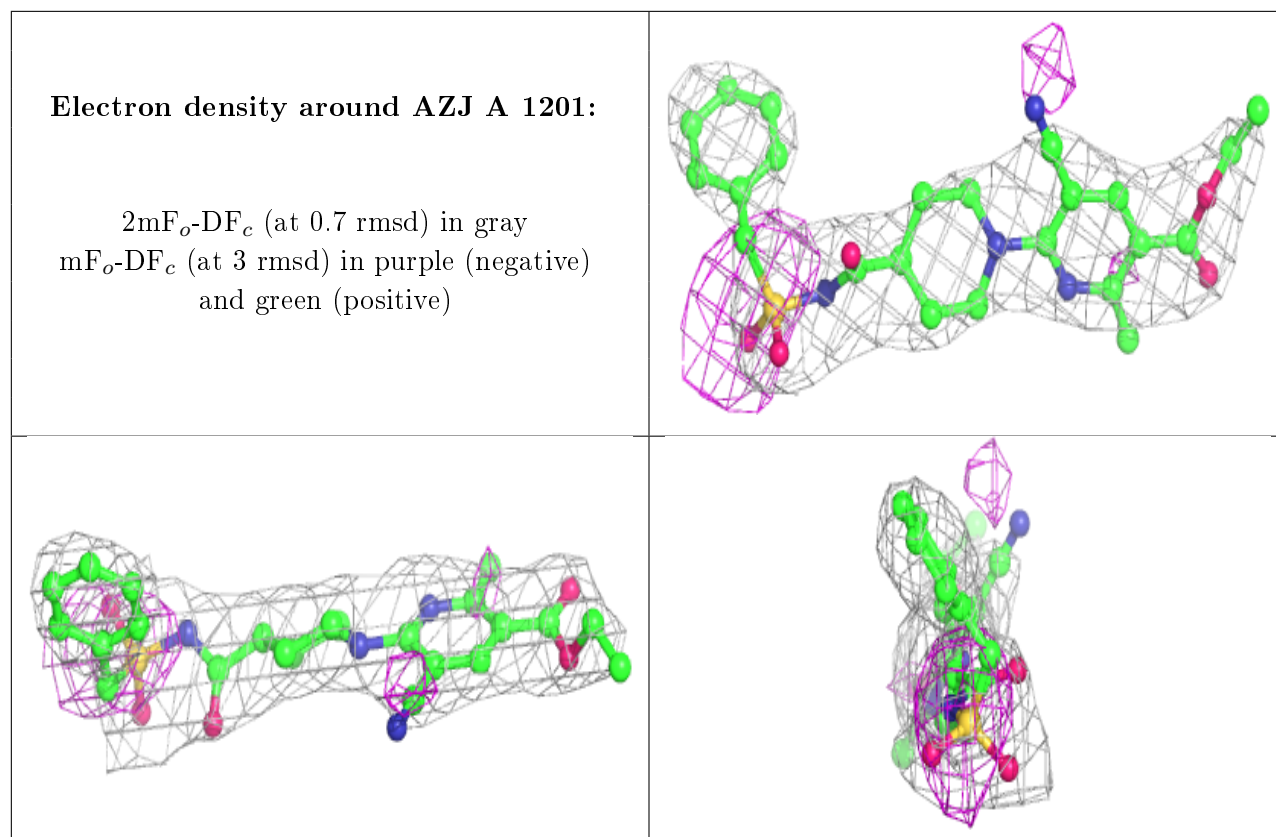
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	OLC	A	1204	17/25	0.76	0.54	120,121,130,131	0
3	CLR	A	1203	28/28	0.81	0.38	136,138,140,140	0
4	OLC	A	1205	21/25	0.82	0.32	126,131,132,135	0
3	CLR	A	1202	28/28	0.84	0.29	124,126,131,131	0
2	AZJ	A	1201	33/33	0.87	0.23	84,92,111,112	0

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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.