



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:50 AM UTC

PDB ID : 4XPF / pdb_00004xpf
Title : X-ray structure of Drosophila dopamine transporter with subsiteB mutations (D121G/S426M) bound to RTI-55
Authors : Penmatsa, A.; Wang, K.H.; Gouaux, E.
Deposited on : 2015-01-16
Resolution : 3.27 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

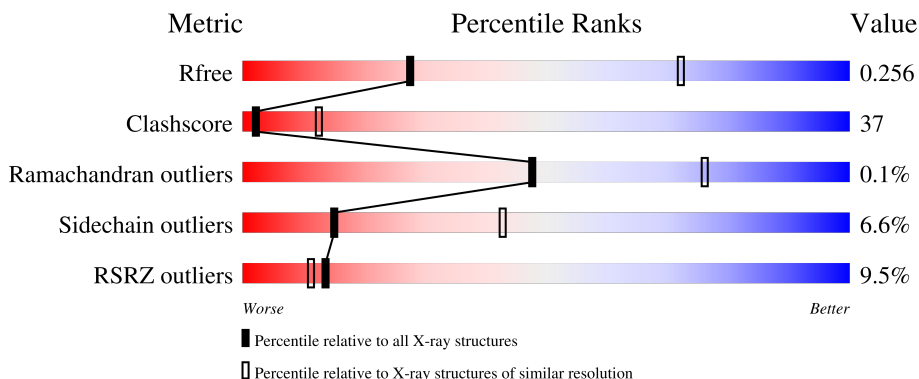
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	543	
2	L	237	
3	H	240	

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
6	42F	A	703	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7532 atoms, of which 18 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 Dopamine transporter-protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4167	2796	642	710	19	0	0	0

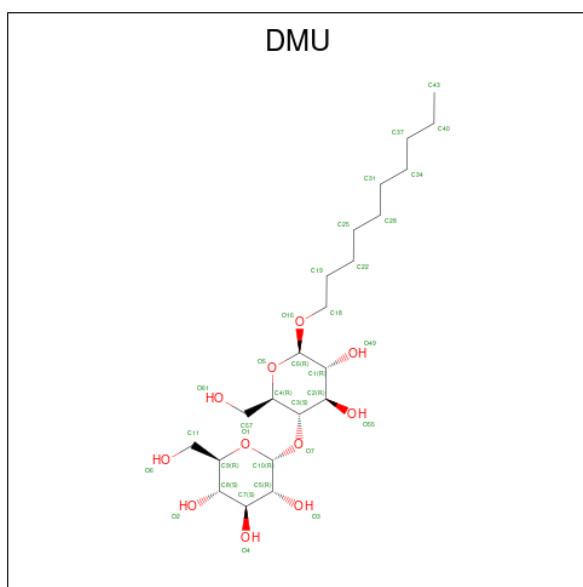
- Molecule 2 is a protein called ANTIBODY FRAGMENT HEAVY CHAIN-PROTEIN, 9D5-HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1616	1004	267	337	8	0	0	0

- Molecule 3 is a protein called ANTIBODY FRAGMENT LIGHT CHAIN-PROTEIN, 9D5-LIGHT CHAIN.

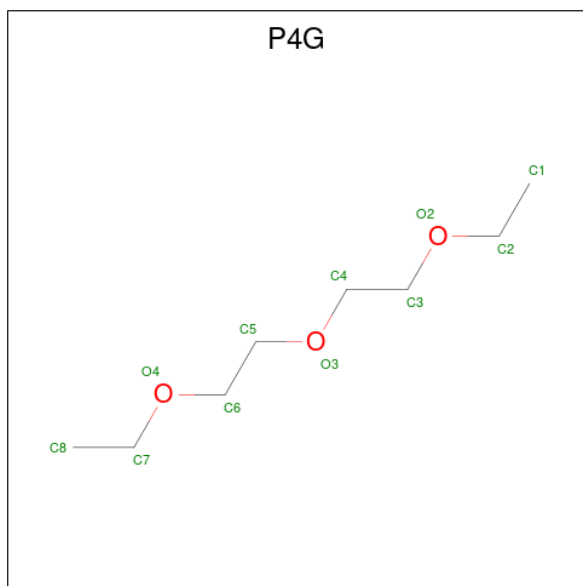
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	215	1602	1011	269	314	8	0	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



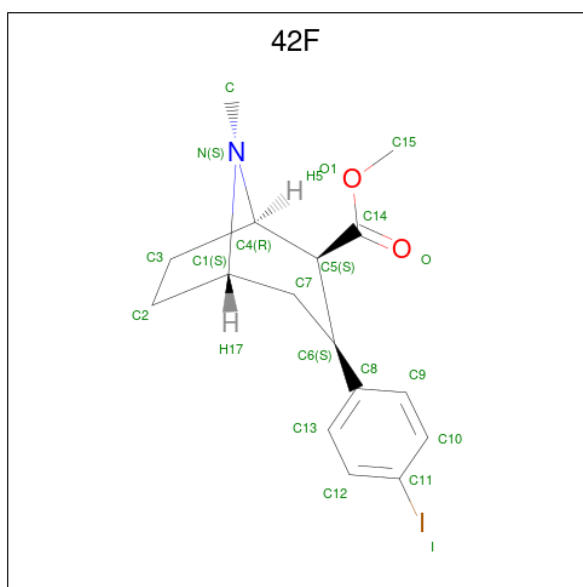
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			33	22	11		

- Molecule 5 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula: $C_8H_{18}O_3$).



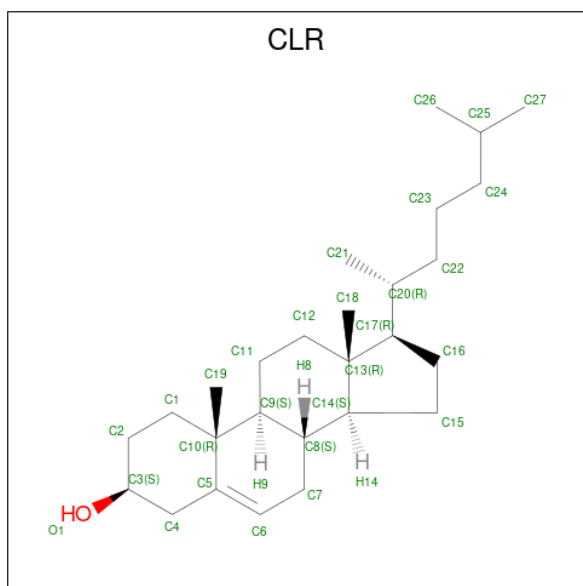
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			29	8	18	3		

- Molecule 6 is methyl (1R,2S,3S,5S)-3-(4-iodophenyl)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylate (CCD ID: 42F) (formula: $C_{16}H_{20}INO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	I	N	O	0	0
			20	16	1	1	2		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

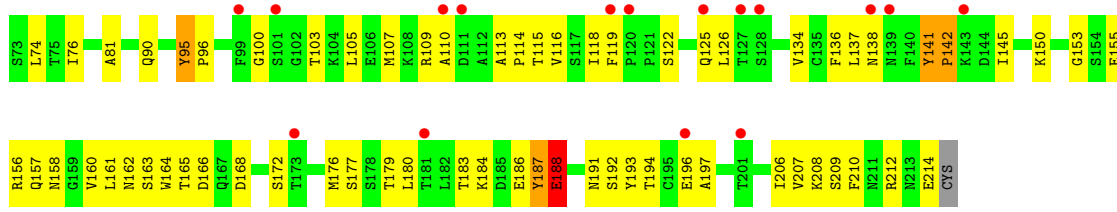
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Na 2 2	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

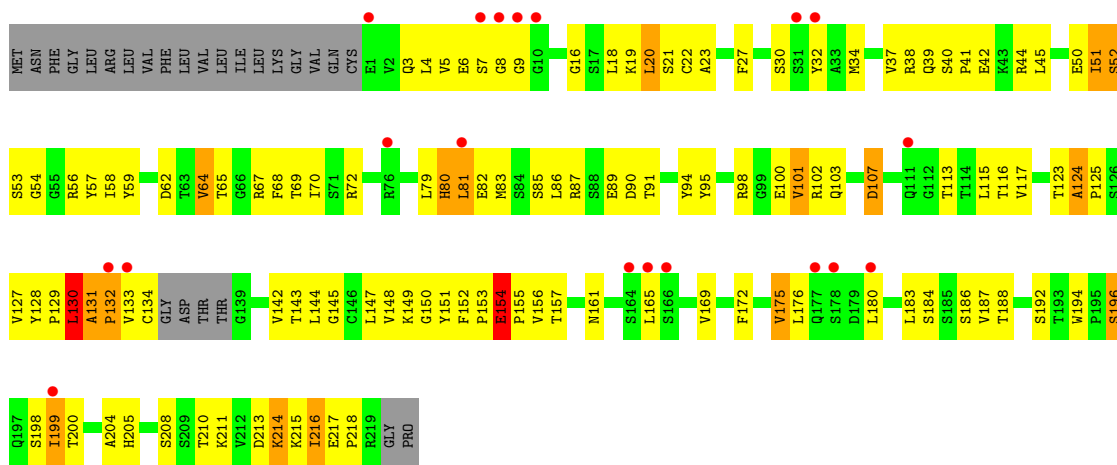
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O 1 1	0	0
10	L	3	Total O 3 3	0	0
10	H	2	Total O 2 2	0	0



● Molecule 3: ANTIBODY FRAGMENT LIGHT CHAIN-PROTEIN, 9D5-LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.42Å 140.31Å 166.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 3.27 48.32 – 3.27	Depositor EDS
% Data completeness (in resolution range)	89.1 (48.32-3.27) 89.2 (48.32-3.27)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.25Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.241 , 0.296 0.255 , 0.256	Depositor DCC
R_{free} test set	1599 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	113.8	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: P4G, 42F, CL, CLR, NA, DMU

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	0.42	2/4308 (0.0%)	0.87	15/5891 (0.3%)
2	L	0.50	2/1654 (0.1%)	0.90	6/2251 (0.3%)
3	H	0.47	0/1640	0.95	8/2235 (0.4%)
All	All	0.45	4/7602 (0.1%)	0.90	29/10377 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	H	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	PHE	C-N	5.84	1.41	1.34
2	L	96	PRO	N-CD	5.67	1.55	1.47
2	L	142	PRO	N-CD	5.56	1.55	1.47
1	A	54	PRO	N-CD	5.20	1.55	1.47

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	154	GLU	C-N-CD	-14.34	89.06	120.60
1	A	595	THR	CA-C-N	9.08	129.13	119.78
1	A	595	THR	C-N-CA	9.08	129.13	119.78
2	L	141	TYR	C-N-CD	8.01	138.23	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	L	95	TYR	C-N-CD	7.95	138.09	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	ARG	Peptide
3	H	98	ARG	Peptide

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	4167	0	4048	315	0
2	L	1616	0	1515	89	0
3	H	1602	0	1541	172	0
4	A	33	0	42	1	0
5	A	11	18	18	0	0
6	A	20	0	20	17	0
7	A	56	0	92	5	0
8	A	2	0	0	0	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
10	H	2	0	0	1	0
10	L	3	0	0	0	0
All	All	7514	18	7276	546	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 37.

The worst 5 of 546 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:A:124:TYR:CD2	6:A:703:42F:H3	1.35	1.56
3:H:194:TRP:CD1	3:H:199:ILE:HD11	1.42	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:CD2	1:A:356:SER:HB3	1.51	1.44
1:A:124:TYR:HD2	6:A:703:42F:C15	1.29	1.42
3:H:194:TRP:CD1	3:H:199:ILE:CD1	2.05	1.38

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	530/543 (98%)	503 (95%)	27 (5%)	0	100	100
2	L	212/237 (90%)	204 (96%)	8 (4%)	0	100	100
3	H	211/240 (88%)	203 (96%)	7 (3%)	1 (0%)	24	55
All	All	953/1020 (93%)	910 (96%)	42 (4%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	132	PRO

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	421/448 (94%)	401 (95%)	20 (5%)	23	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	182/207 (88%)	169 (93%)	13 (7%)	13	40
3	H	175/205 (85%)	157 (90%)	18 (10%)	7	26
All	All	778/860 (90%)	727 (93%)	51 (7%)	15	43

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	158	ASN
3	H	52	SER
3	H	214	LYS
2	L	166	ASP
2	L	210	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	38	GLN
2	L	54	ASN
3	H	77	ASN
3	H	80	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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
7	CLR	A	705	-	31,31,31	0.72	0	48,48,48	1.19	4 (8%)
4	DMU	A	701	-	34,34,34	0.40	0	45,45,45	0.74	1 (2%)
5	P4G	A	702	-	10,10,10	0.68	0	9,9,9	0.25	0
6	42F	A	703	-	22,22,22	1.76	1 (4%)	29,32,32	1.27	5 (17%)
7	CLR	A	704	-	31,31,31	0.69	0	48,48,48	1.38	7 (14%)

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
7	CLR	A	705	-	-	3/10/68/68	0/4/4/4
4	DMU	A	701	-	-	10/19/59/59	0/2/2/2
5	P4G	A	702	-	-	5/8/8/8	-
6	42F	A	703	-	-	2/10/35/35	0/4/3/3
7	CLR	A	704	-	-	2/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	42F	C8-C6	-7.75	1.40	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	704	CLR	C4-C5-C10	5.08	122.93	116.42
7	A	705	CLR	C4-C5-C10	3.71	121.17	116.42
7	A	705	CLR	C11-C12-C13	-3.12	107.48	112.74
7	A	705	CLR	C4-C5-C6	-2.85	116.70	120.57
6	A	703	42F	C15-O1-C14	-2.80	109.56	115.92

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

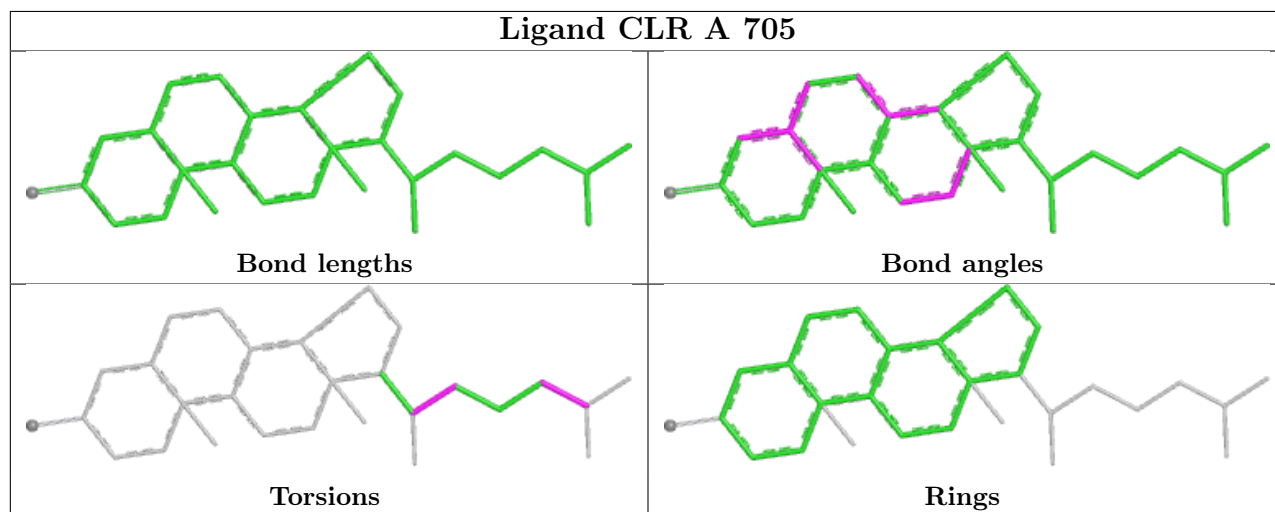
Mol	Chain	Res	Type	Atoms
4	A	701	DMU	C1-C6-O16-C18
4	A	701	DMU	O5-C6-O16-C18
6	A	703	42F	C5-C14-O1-C15
4	A	701	DMU	C4-C3-O7-C10
6	A	703	42F	O-C14-O1-C15

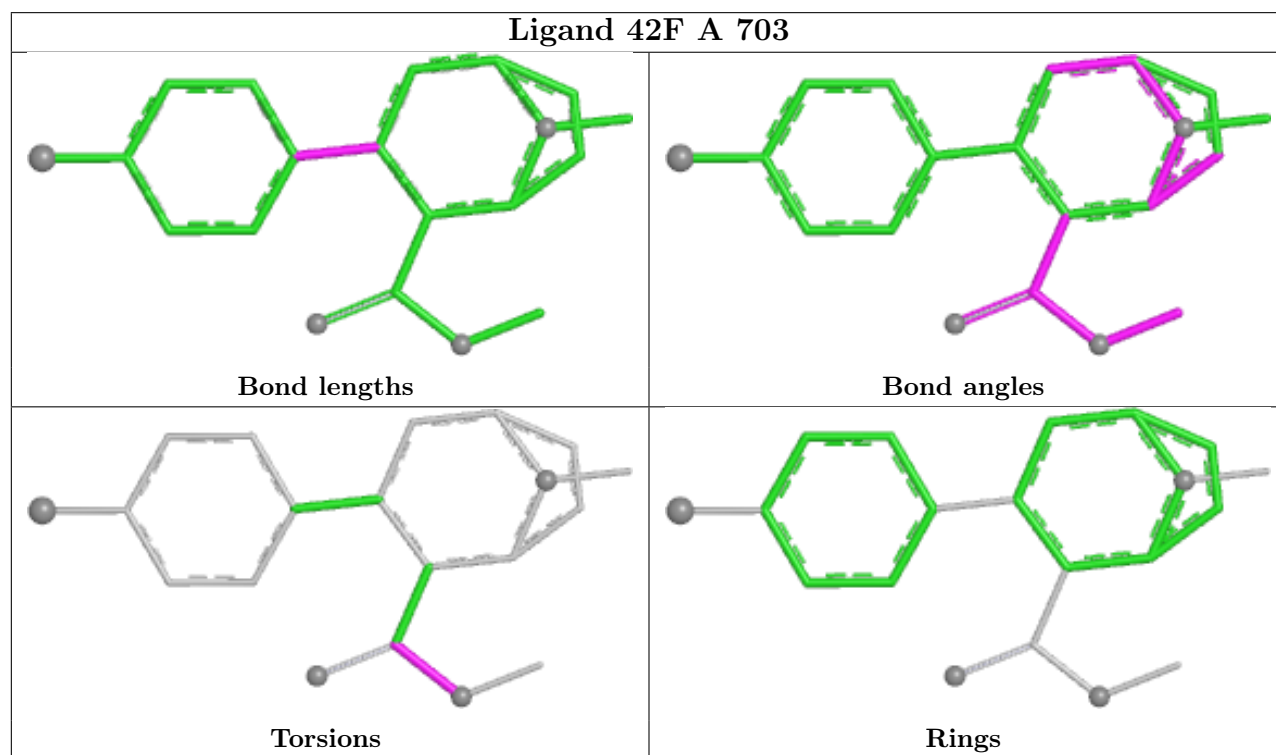
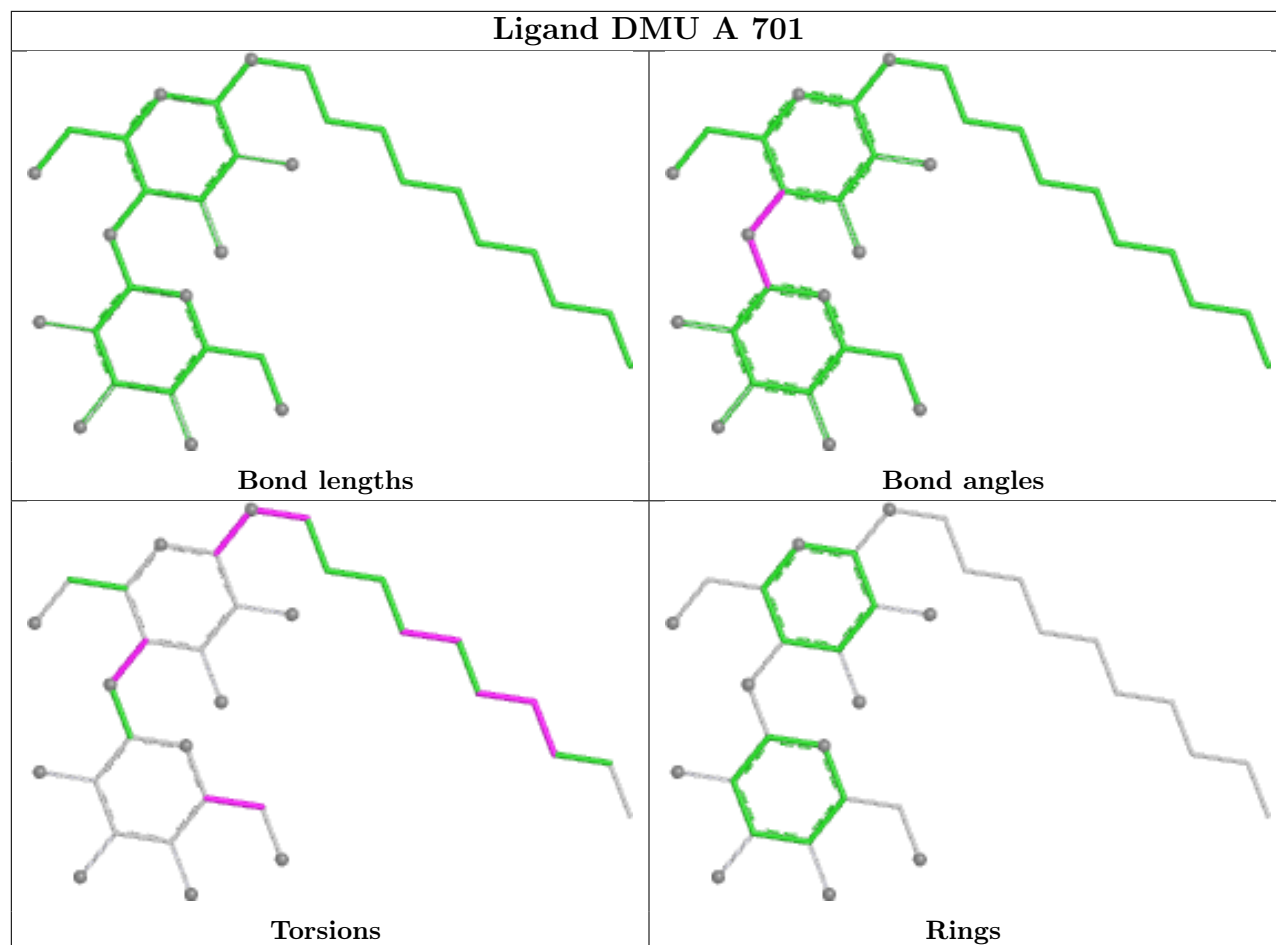
There are no ring outliers.

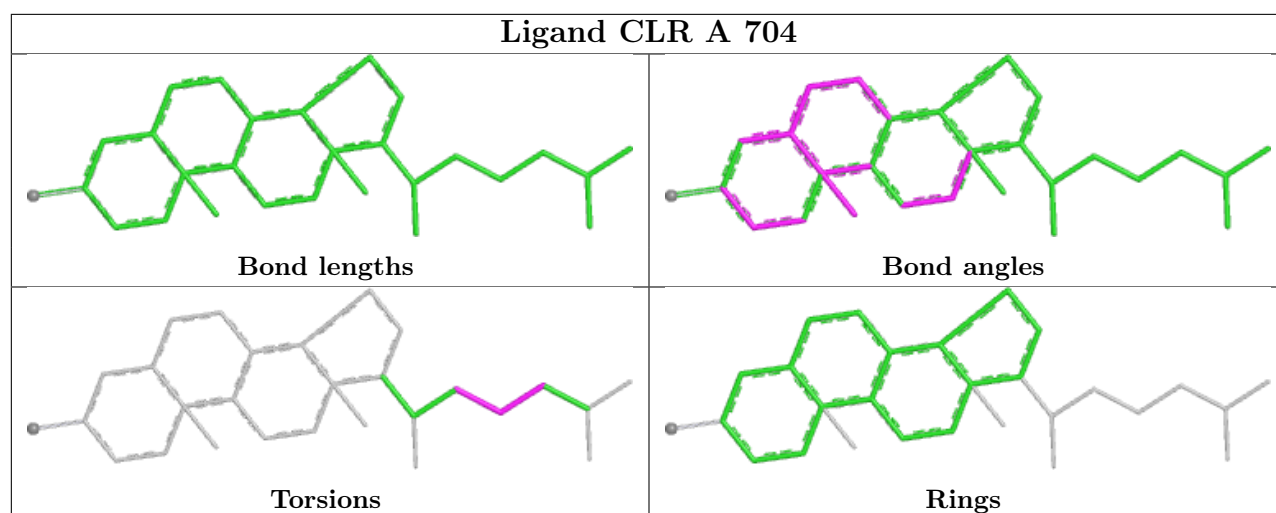
4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	705	CLR	4	0
4	A	701	DMU	1	0
6	A	703	42F	17	0
7	A	704	CLR	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 [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	532/543 (97%)	0.59	53 (9%) 12 10	84, 107, 135, 157	0
2	L	214/237 (90%)	0.46	19 (8%) 15 12	79, 106, 150, 189	0
3	H	215/240 (89%)	0.60	19 (8%) 15 12	81, 106, 149, 191	0
All	All	961/1020 (94%)	0.56	91 (9%) 14 11	79, 107, 144, 191	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	111	ASP	8.3
3	H	178	SER	7.6
1	A	318	PHE	6.7
1	A	124	TYR	5.9
1	A	436	GLU	5.9

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](#)

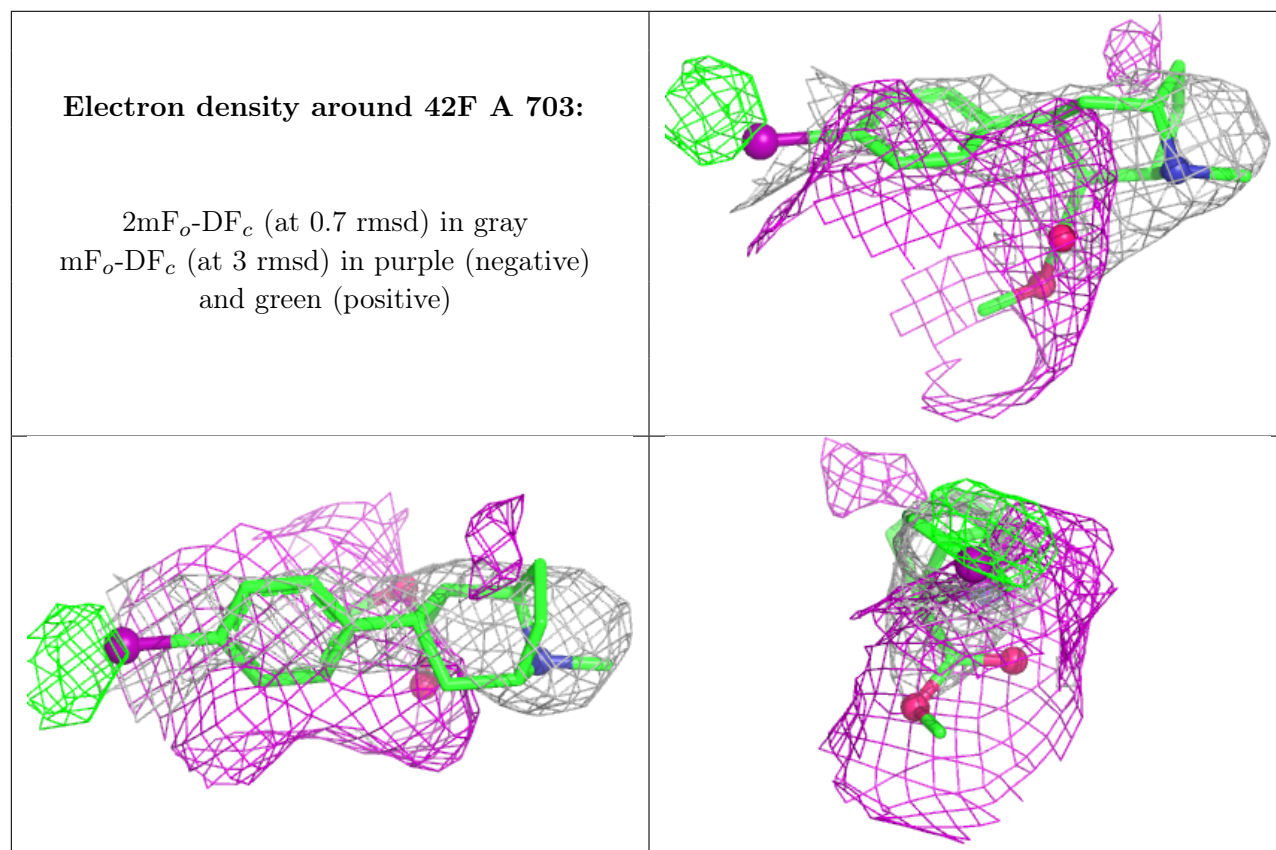
There are no oligosaccharides in this entry.

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.

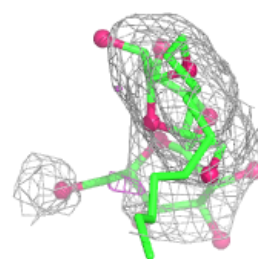
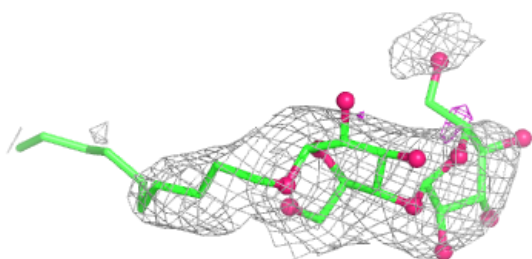
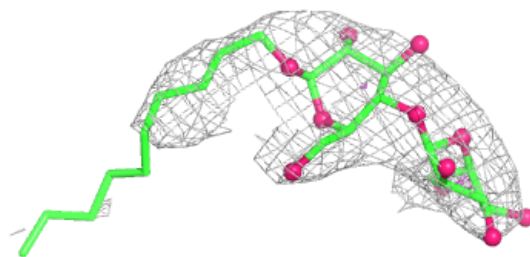
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	42F	A	703	20/20	0.62	0.30	102,121,134,307	0
4	DMU	A	701	33/33	0.64	0.20	105,134,143,152	0
5	P4G	A	702	11/11	0.84	0.22	114,137,155,156	0
7	CLR	A	704	28/28	0.88	0.18	78,111,115,118	0
7	CLR	A	705	28/28	0.91	0.16	87,112,123,126	0
8	NA	A	707	1/1	0.91	0.07	106,106,106,106	0
9	CL	A	708	1/1	0.94	0.19	107,107,107,107	0
8	NA	A	706	1/1	0.96	0.09	106,106,106,106	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.

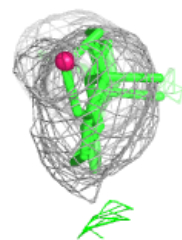
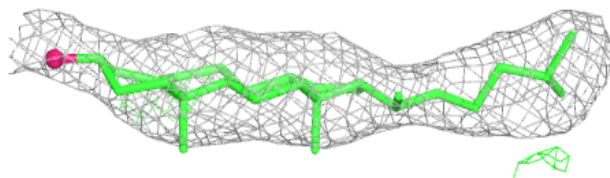
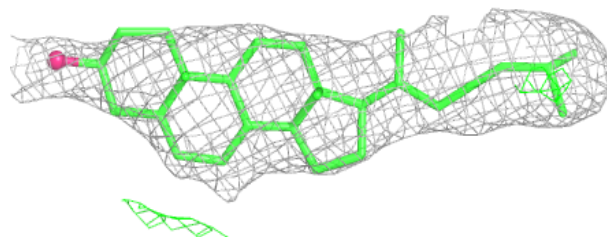


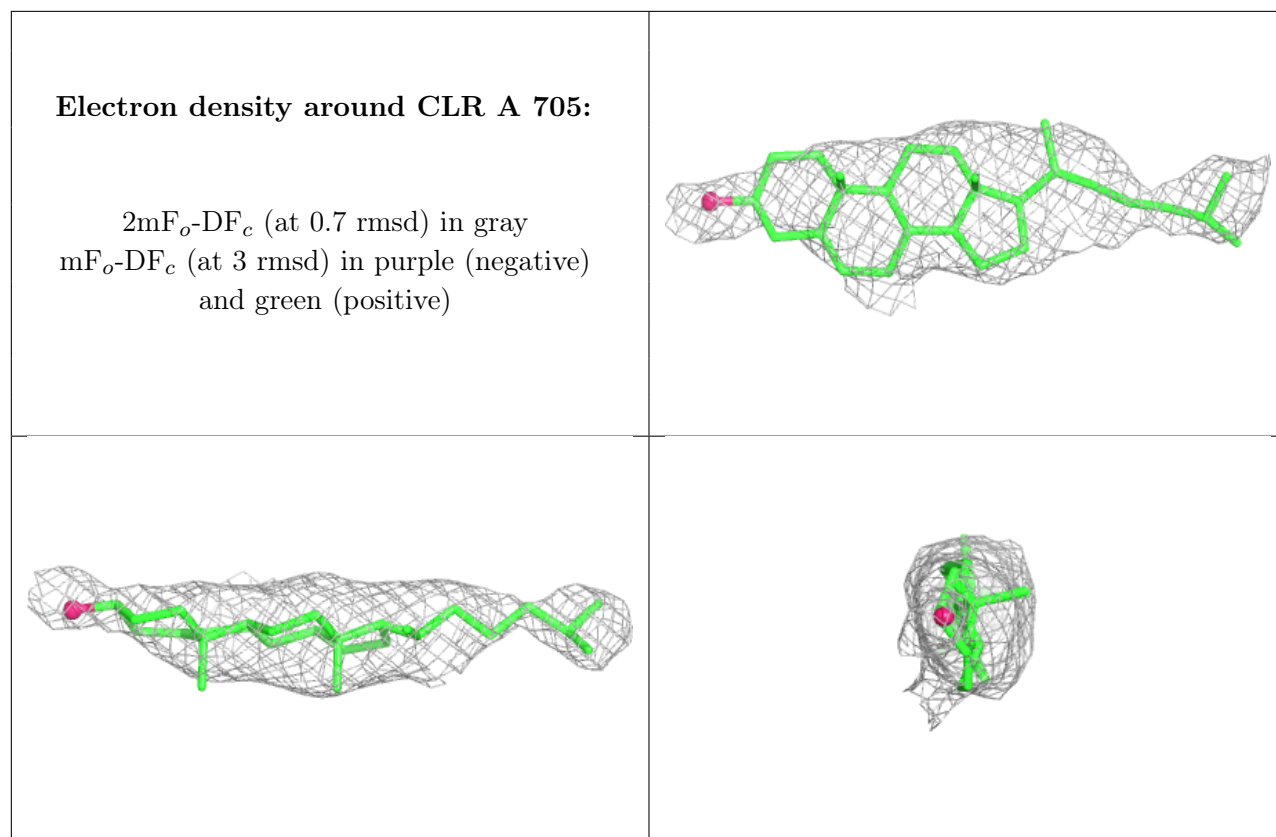
Electron density around DMU A 701:

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

**Electron density around CLR A 704:**

$2mF_o-DF_c$ (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.