



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2022 – 06:05 PM JST

PDB ID : 7WGD  
Title : X-ray structure of thermostabilized *Drosophila* dopamine transporter with GABA transporter1-like substitutions in the binding site, in substrate-free form.  
Authors : Joseph, D.; Penmatsa, A.  
Deposited on : 2021-12-28  
Resolution : 3.20 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.

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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

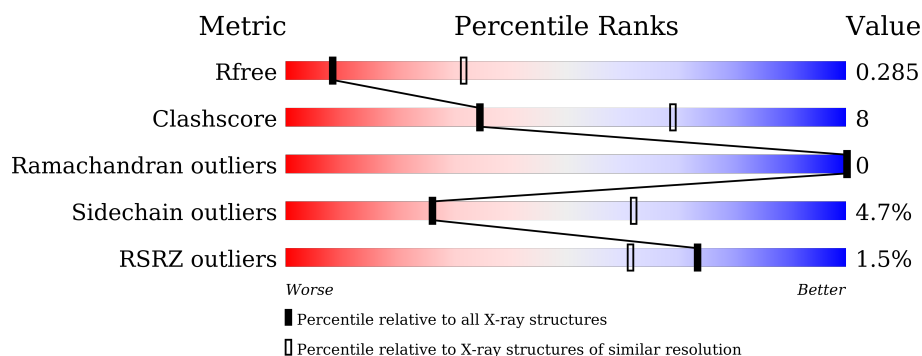
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	536	<div> <div> <div></div> <div>77%</div> <div>21%</div> <div></div> </div> </div>
2	L	214	<div> <div> <div></div> <div>78%</div> <div>22%</div> <div></div> </div> </div>
3	H	219	<div> <div> <div></div> <div>77%</div> <div>21%</div> <div></div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7574 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 Sodium-dependent dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4228	2833	657	720	18	0	1	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	TYR	PHE	engineered mutation	UNP Q7K4Y6
A	46	GLY	ASP	engineered mutation	UNP Q7K4Y6
A	74	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	117	SER	ALA	engineered mutation	UNP Q7K4Y6
A	120	LEU	VAL	engineered mutation	UNP Q7K4Y6
A	121	ASN	ASP	engineered mutation	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ARG	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	PRO	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	ILE	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLU	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	275	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	311	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	325	LEU	PHE	engineered mutation	UNP Q7K4Y6
A	327	SER	VAL	engineered mutation	UNP Q7K4Y6
A	384	SER	GLU	engineered mutation	UNP Q7K4Y6
A	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	422	GLN	SER	engineered mutation	UNP Q7K4Y6
A	425	THR	GLY	engineered mutation	UNP Q7K4Y6
A	426	VAL	SER	engineered mutation	UNP Q7K4Y6
A	538	LEU	GLY	engineered mutation	UNP Q7K4Y6

- Molecule 2 is a protein called Antibody fragment (9D5) Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1618	1005	266	339	8			

- Molecule 3 is a protein called Antibody fragment (9D5) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1643	1032	278	325	8			

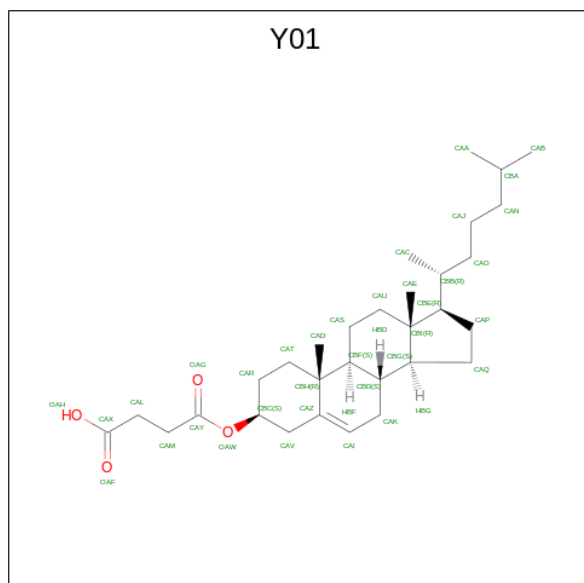
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			35	31 4		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

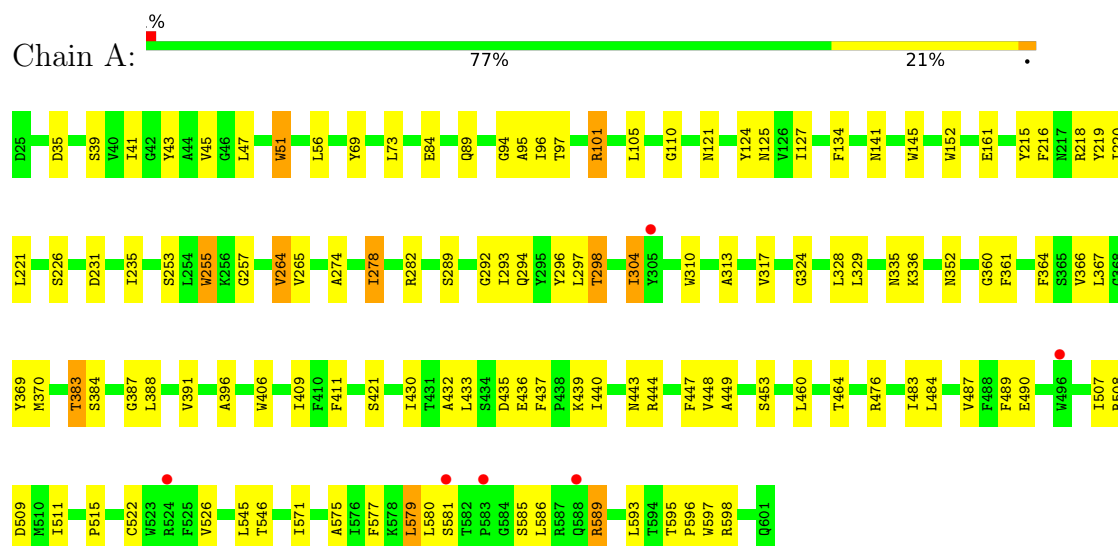
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total	O	0	0
			16	16		
8	L	3	Total	O	0	0
			3	3		

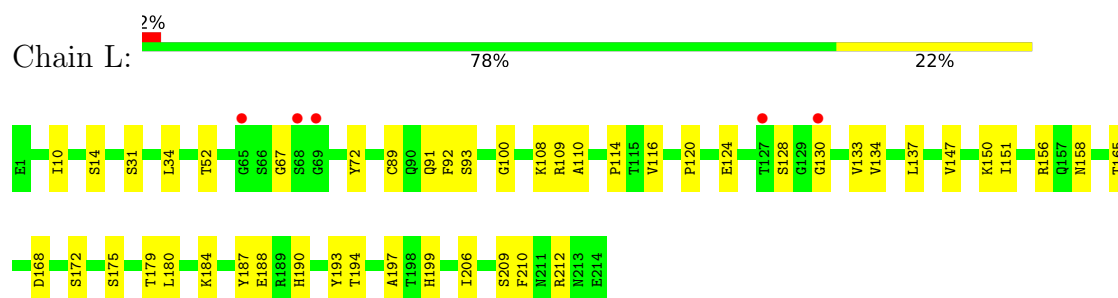
### 3 Residue-property plots [i](#)

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.

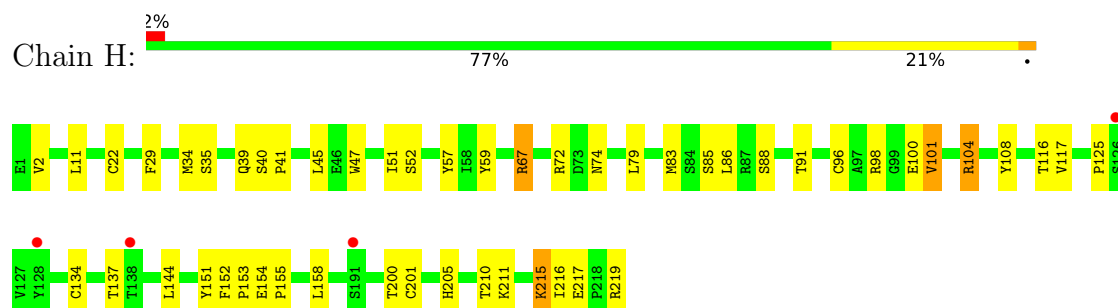
- Molecule 1: Sodium-dependent dopamine transporter



- Molecule 2: Antibody fragment (9D5) Light Chain



- Molecule 3: Antibody fragment (9D5) heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.39Å 140.71Å 168.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 3.20 48.43 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.43-3.20) 99.8 (48.43-3.20)	Depositor EDS
$R_{merge}$	0.72	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 3.19Å)	Xtriage
Refinement program	PHENIX v1.20rc4-4425	Depositor
R, $R_{free}$	0.244 , 0.286 0.244 , 0.285	Depositor DCC
$R_{free}$ test set	1921 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.8	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: NA, CL, CLR, Y01

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	0.26	0/4373	0.43	0/5980
2	L	0.25	0/1656	0.49	0/2253
3	H	0.25	0/1682	0.51	0/2292
All	All	0.26	0/7711	0.46	0/10525

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	4228	0	4135	71	0
2	L	1618	0	1518	31	0
3	H	1643	0	1589	24	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	35	0	48	0	0
7	A	28	0	46	0	0
8	A	16	0	0	0	0
8	L	3	0	0	0	0
All	All	7574	0	7336	124	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 8.

All (124) 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)
2:L:150:LYS:HB2	2:L:194:THR:HB	1.73	0.70
3:H:158:LEU:HD11	3:H:201:CYS:HB2	1.73	0.70
3:H:29:PHE:O	3:H:72:ARG:NH2	2.28	0.67
2:L:190:HIS:O	2:L:212:ARG:NH1	2.29	0.66
1:A:324:GLY:HA3	1:A:487:VAL:HG22	1.79	0.65
3:H:39:GLN:HB3	3:H:45:LEU:HD23	1.81	0.63
1:A:489:PHE:HD2	1:A:571:ILE:HG21	1.64	0.62
1:A:39:SER:HA	1:A:265:VAL:HG21	1.81	0.62
1:A:219:TYR:HD2	1:A:220:ILE:HD12	1.64	0.62
1:A:433:LEU:HB3	1:A:440:ILE:HD11	1.82	0.61
1:A:487:VAL:HA	1:A:490:GLU:HB2	1.82	0.60
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.82	0.60
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.83	0.60
2:L:124:GLU:N	2:L:124:GLU:OE1	2.35	0.60
1:A:101:ARG:HG3	1:A:597:TRP:HB3	1.85	0.59
2:L:109:ARG:NH1	2:L:110:ALA:O	2.34	0.57
1:A:43:TYR:HA	1:A:421:SER:HA	1.85	0.57
1:A:94:GLY:N	1:A:435:ASP:OD2	2.37	0.57
3:H:67:ARG:HG2	3:H:85:SER:HB3	1.87	0.56
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.87	0.56
2:L:197:ALA:HB3	2:L:206:ILE:HG23	1.89	0.55
2:L:156:ARG:NH1	2:L:158:ASN:O	2.39	0.55
1:A:522:CYS:HA	1:A:526:VAL:HG12	1.88	0.55
1:A:121:ASN:O	1:A:125:ASN:ND2	2.39	0.55
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.88	0.54
3:H:205:HIS:HB3	3:H:210:THR:HB	1.89	0.54
1:A:255:TRP:HA	1:A:448:VAL:HG11	1.90	0.54
1:A:366:VAL:HA	1:A:369:TYR:HB3	1.90	0.53
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.90	0.53
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.43	0.53
2:L:91:GLN:HG2	2:L:93:SER:H	1.74	0.53
1:A:507:ILE:HD11	1:A:515:PRO:HG3	1.90	0.52
1:A:253:SER:HB2	1:A:264:VAL:HG11	1.90	0.52
1:A:89:GLN:NE2	1:A:336:LYS:O	2.43	0.51
1:A:145:TRP:HB3	1:A:215:TYR:CD2	2.45	0.51
3:H:52:SER:HB3	3:H:57:TYR:HB2	1.92	0.51
3:H:200:THR:HG22	3:H:215:LYS:HA	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:133:VAL:HG23	2:L:180:LEU:HB3	1.93	0.51
1:A:89:GLN:HG3	1:A:335:ASN:HB2	1.93	0.50
1:A:387:GLY:O	1:A:391:VAL:HG22	2.11	0.50
1:A:51:TRP:HH2	1:A:127:ILE:HD13	1.77	0.50
2:L:187:TYR:O	2:L:193:TYR:OH	2.30	0.50
1:A:579:LEU:HD13	1:A:593:LEU:HD12	1.94	0.49
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.47	0.49
2:L:184:LYS:NZ	2:L:188:GLU:OE1	2.44	0.49
2:L:114:PRO:HD3	2:L:199:HIS:CD2	2.48	0.49
3:H:35:SER:HG	3:H:47:TRP:HE1	1.58	0.49
1:A:69:TYR:HA	1:A:313:ALA:HB1	1.93	0.49
3:H:88:SER:O	3:H:91:THR:HG22	2.13	0.49
1:A:73:LEU:HA	1:A:317:VAL:HG11	1.94	0.49
3:H:35:SER:OG	3:H:47:TRP:NE1	2.42	0.49
1:A:96:ILE:HA	1:A:110:GLY:HA3	1.95	0.48
1:A:585:SER:O	1:A:589:ARG:HB2	2.13	0.48
3:H:154:GLU:HG3	3:H:155:PRO:HA	1.95	0.48
1:A:508:ARG:NE	3:H:100:GLU:O	2.46	0.48
1:A:292:GLY:HA3	1:A:364:PHE:O	2.14	0.48
1:A:304:ILE:O	1:A:310:TRP:NE1	2.44	0.48
1:A:84:GLU:HG2	1:A:328:LEU:HB2	1.95	0.47
2:L:194:THR:HG23	2:L:209:SER:HB2	1.96	0.47
2:L:151:ILE:HD12	2:L:156:ARG:HD2	1.95	0.47
1:A:383:THR:HG22	1:A:384:SER:H	1.80	0.47
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.78	0.47
1:A:430:ILE:HG22	1:A:447:PHE:CE1	2.49	0.47
2:L:151:ILE:HD11	2:L:180:LEU:HD21	1.96	0.47
1:A:437:PHE:O	1:A:440:ILE:HG12	2.16	0.46
2:L:31:SER:O	2:L:52:THR:HG23	2.15	0.46
3:H:2:VAL:HG11	3:H:108:TYR:CE1	2.51	0.46
1:A:507:ILE:O	1:A:511:ILE:HG12	2.16	0.46
1:A:257:GLY:HA2	1:A:444:ARG:NH2	2.31	0.46
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.98	0.46
1:A:282:ARG:HD2	1:A:406:TRP:CZ2	2.51	0.45
2:L:165:THR:HG22	2:L:175:SER:H	1.81	0.45
1:A:278:ILE:HG13	1:A:409:ILE:HD12	1.98	0.45
2:L:116:VAL:HG22	2:L:137:LEU:HD22	1.98	0.45
2:L:134:VAL:HG22	2:L:179:THR:HG23	1.97	0.45
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.99	0.45
1:A:51:TRP:HA	1:A:388:LEU:HD23	1.99	0.45
2:L:52:THR:HG22	2:L:72:TYR:HE2	1.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ILE:HG22	1:A:447:PHE:HE1	1.82	0.44
1:A:577:PHE:O	1:A:581:SER:HB2	2.17	0.44
1:A:294:GLN:O	1:A:298:THR:OG1	2.32	0.44
2:L:187:TYR:CE2	2:L:212:ARG:HD2	2.53	0.44
1:A:274:ALA:O	1:A:278:ILE:HG12	2.18	0.44
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.53	0.44
1:A:45:VAL:HG12	1:A:352:ASN:HA	2.00	0.43
2:L:34:LEU:HD13	2:L:72:TYR:CD1	2.53	0.43
3:H:11:LEU:HA	3:H:116:THR:O	2.18	0.43
1:A:152:TRP:O	1:A:218:ARG:HD3	2.19	0.43
1:A:97:THR:OG1	1:A:436:GLU:OE1	2.28	0.43
1:A:134:PHE:HB3	1:A:411:PHE:CE2	2.54	0.43
1:A:226:SER:OG	1:A:231:ASP:O	2.28	0.43
1:A:483:ILE:O	1:A:487:VAL:HG23	2.19	0.43
1:A:105:LEU:HB2	1:A:593:LEU:HB3	2.01	0.42
2:L:89:CYS:O	2:L:100:GLY:N	2.44	0.42
1:A:509:ASP:OD1	3:H:59:TYR:OH	2.34	0.42
1:A:95:ALA:H	1:A:432:ALA:HB2	1.85	0.42
1:A:235:ILE:HA	1:A:464:THR:HA	2.02	0.42
1:A:449:ALA:O	1:A:453:SER:OG	2.35	0.42
2:L:137:LEU:HD11	2:L:147:VAL:HG12	2.02	0.42
1:A:235:ILE:HD11	1:A:460:LEU:HD22	2.02	0.42
1:A:585:SER:OG	1:A:586:LEU:N	2.52	0.42
2:L:114:PRO:HD3	2:L:199:HIS:HD2	1.84	0.42
1:A:439:LYS:O	1:A:443:ASN:ND2	2.53	0.42
1:A:575:ALA:O	1:A:579:LEU:HB2	2.20	0.42
1:A:219:TYR:CD2	1:A:220:ILE:HD12	2.49	0.41
2:L:14:SER:N	2:L:108:LYS:HB2	2.35	0.41
2:L:67:GLY:HA3	2:L:72:TYR:HA	2.02	0.41
1:A:406:TRP:HE3	1:A:409:ILE:HD11	1.85	0.41
1:A:476:ARG:HA	1:A:476:ARG:HD2	1.70	0.41
1:A:507:ILE:HG13	1:A:515:PRO:HD3	2.02	0.41
3:H:40:SER:HB2	3:H:41:PRO:HD2	2.01	0.41
1:A:41:ILE:O	1:A:45:VAL:HG22	2.20	0.41
3:H:101:VAL:HG13	3:H:104:ARG:HB2	2.03	0.41
1:A:47:LEU:HD13	1:A:127:ILE:HG21	2.02	0.41
1:A:370:MET:SD	1:A:396:ALA:HB2	2.61	0.41
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.56	0.41
2:L:128:SER:O	2:L:130:GLY:N	2.54	0.41
2:L:168:ASP:O	2:L:172:SER:HA	2.20	0.41
2:L:52:THR:HG22	2:L:72:TYR:CE2	2.56	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PHE:O	1:A:221:LEU:HB2	2.19	0.40
3:H:152:PHE:HA	3:H:153:PRO:HA	1.87	0.40
3:H:144:LEU:HB3	3:H:216:ILE:HG21	2.02	0.40
1:A:296:TYR:HB2	1:A:364:PHE:CG	2.56	0.40
1:A:595:THR:HA	1:A:596:PRO:HD3	1.94	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	535/536 (100%)	510 (95%)	25 (5%)	0	100	100
2	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	H	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
All	All	964/969 (100%)	914 (95%)	50 (5%)	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	431/441 (98%)	409 (95%)	22 (5%)	24	60
2	L	183/187 (98%)	181 (99%)	2 (1%)	73	88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	182/187 (97%)	169 (93%)	13 (7%)	14	47
All	All	796/815 (98%)	759 (95%)	37 (5%)	26	63

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	51	TRP
1	A	56	LEU
1	A	101	ARG
1	A	124	TYR
1	A	141	ASN
1	A	161	GLU
1	A	255	TRP
1	A	264	VAL
1	A	278	ILE
1	A	289	SER
1	A	297	LEU
1	A	298	THR
1	A	304	ILE
1	A	383	THR
1	A	484	LEU
1	A	545	LEU
1	A	546	THR
1	A	579	LEU
1	A	580	LEU
1	A	589	ARG
1	A	598	ARG
2	L	10	ILE
2	L	92	PHE
3	H	67	ARG
3	H	74	ASN
3	H	96	CYS
3	H	98	ARG
3	H	101	VAL
3	H	104	ARG
3	H	117	VAL
3	H	134	CYS
3	H	137	THR
3	H	211	LYS
3	H	215	LYS
3	H	217	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	H	219	ARG

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

Mol	Chain	Res	Type
1	A	89	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	3.56	15 (48%)	48,48,48	1.87	16 (33%)
6	Y01	A	704	-	38,38,38	4.34	21 (55%)	57,57,57	2.06	17 (29%)

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	-	-	2/10/68/68	0/4/4/4
6	Y01	A	704	-	-	8/19/77/77	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	704	Y01	CAS-CBF	-10.06	1.36	1.53
6	A	704	Y01	CBH-CAZ	-9.68	1.33	1.52
7	A	705	CLR	C11-C9	8.51	1.68	1.53
6	A	704	Y01	CAK-CAI	-8.35	1.32	1.50
7	A	705	CLR	C12-C11	8.01	1.70	1.53
6	A	704	Y01	CBD-CBG	-7.87	1.38	1.53
6	A	704	Y01	CAI-CAZ	-7.79	1.15	1.33
6	A	704	Y01	CAV-CAZ	7.54	1.68	1.51
6	A	704	Y01	CAK-CBD	7.32	1.65	1.53
7	A	705	CLR	C12-C13	-7.08	1.41	1.54
6	A	704	Y01	CAU-CBI	6.17	1.65	1.54
6	A	704	Y01	CBH-CBF	5.74	1.65	1.56
7	A	705	CLR	C16-C15	5.14	1.68	1.54
7	A	705	CLR	C6-C5	-5.07	1.21	1.33
7	A	705	CLR	C1-C2	4.98	1.64	1.53
6	A	704	Y01	CAU-CAS	4.95	1.64	1.53
7	A	705	CLR	C7-C6	-4.93	1.39	1.50
6	A	704	Y01	CBI-CBE	-4.41	1.46	1.55
6	A	704	Y01	CAV-CBC	4.35	1.62	1.52
7	A	705	CLR	C10-C9	-4.28	1.48	1.56
7	A	705	CLR	C8-C14	-4.15	1.45	1.53
6	A	704	Y01	OAW-CBC	-3.54	1.37	1.46
7	A	705	CLR	C13-C14	-3.47	1.48	1.55
6	A	704	Y01	CBD-CBF	3.44	1.60	1.53
7	A	705	CLR	C1-C10	3.17	1.60	1.54
6	A	704	Y01	CAT-CAR	-2.97	1.47	1.53
7	A	705	CLR	C2-C3	2.97	1.58	1.51
6	A	704	Y01	CAP-CBE	2.95	1.60	1.54
6	A	704	Y01	CAQ-CAP	2.86	1.61	1.54
6	A	704	Y01	OAW-CAY	2.74	1.42	1.34
7	A	705	CLR	C8-C9	2.73	1.58	1.53
7	A	705	CLR	C15-C14	2.65	1.59	1.54
6	A	704	Y01	CAL-CAX	2.53	1.56	1.50
7	A	705	CLR	C10-C5	-2.21	1.48	1.52
6	A	704	Y01	OAF-CAX	2.15	1.29	1.22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	704	Y01	CAQ-CBG	2.01	1.58	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	704	Y01	CBC-CAV-CAZ	-5.23	103.39	111.52
6	A	704	Y01	CAV-CAZ-CAI	-4.91	113.54	120.61
6	A	704	Y01	CBH-CBF-CBD	-4.07	106.63	112.73
6	A	704	Y01	CAK-CAI-CAZ	4.01	132.45	125.06
6	A	704	Y01	CAK-CBD-CBF	-3.95	104.92	109.71
6	A	704	Y01	OAW-CAY-CAM	3.87	119.84	111.50
7	A	705	CLR	C11-C9-C8	-3.78	106.31	111.75
7	A	705	CLR	C15-C14-C8	-3.67	113.04	119.08
7	A	705	CLR	C12-C13-C17	-3.57	111.22	116.57
7	A	705	CLR	C12-C11-C9	-3.48	107.09	113.11
6	A	704	Y01	CAP-CAQ-CBG	-3.31	98.57	105.13
6	A	704	Y01	CAS-CAU-CBI	-3.30	107.13	112.78
7	A	705	CLR	C16-C15-C14	-3.18	98.83	105.13
6	A	704	Y01	CBI-CBE-CBB	-3.16	114.54	119.49
7	A	705	CLR	C4-C5-C6	-2.97	116.32	120.61
6	A	704	Y01	CBH-CAZ-CAI	2.93	127.39	122.90
6	A	704	Y01	CBI-CBG-CBD	-2.77	110.27	114.38
7	A	705	CLR	C16-C17-C20	-2.74	107.90	112.15
7	A	705	CLR	C14-C8-C9	-2.67	105.51	109.09
7	A	705	CLR	C21-C20-C22	-2.64	106.22	110.36
6	A	704	Y01	CBF-CBH-CAZ	2.59	113.72	109.65
7	A	705	CLR	C12-C13-C14	2.53	111.20	107.27
7	A	705	CLR	C4-C5-C10	2.52	119.76	116.42
7	A	705	CLR	C17-C13-C14	2.51	103.05	100.07
7	A	705	CLR	C1-C10-C5	2.46	113.26	108.75
7	A	705	CLR	C3-C4-C5	-2.40	107.96	112.03
7	A	705	CLR	C1-C2-C3	-2.37	107.42	110.47
6	A	704	Y01	CAQ-CBG-CBD	-2.36	115.19	119.08
6	A	704	Y01	CBF-CBD-CBG	-2.18	106.17	109.09
6	A	704	Y01	CAP-CBE-CBB	-2.11	108.89	112.15
6	A	704	Y01	CAM-CAL-CAX	-2.07	109.15	113.60
6	A	704	Y01	CBG-CBI-CBE	2.03	102.48	100.07
7	A	705	CLR	C23-C22-C20	-2.01	109.26	115.03

There are no chirality outliers.

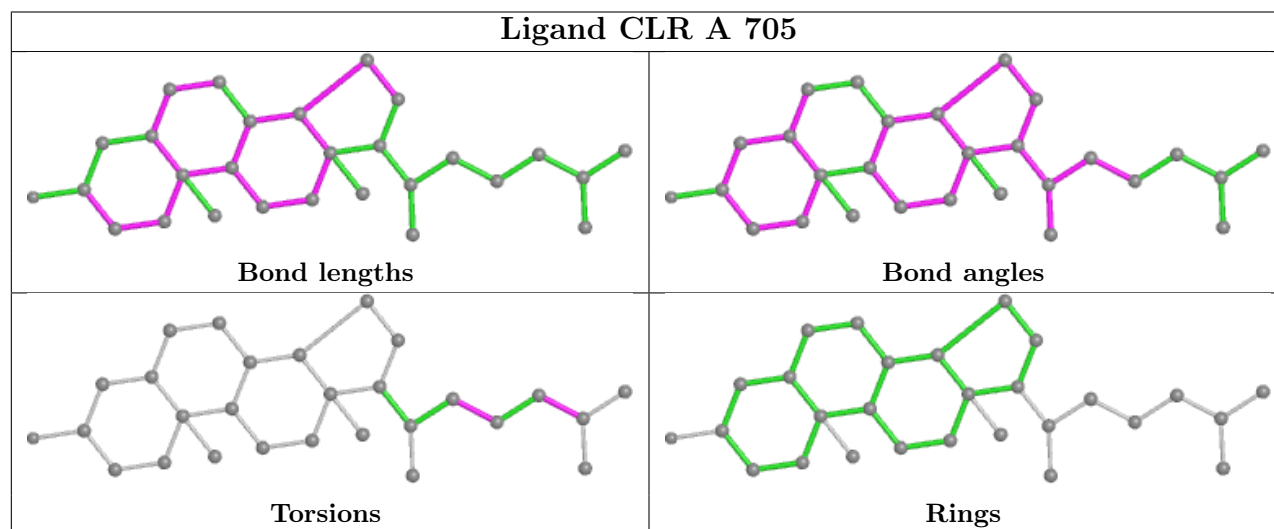
All (10) torsion outliers are listed below:

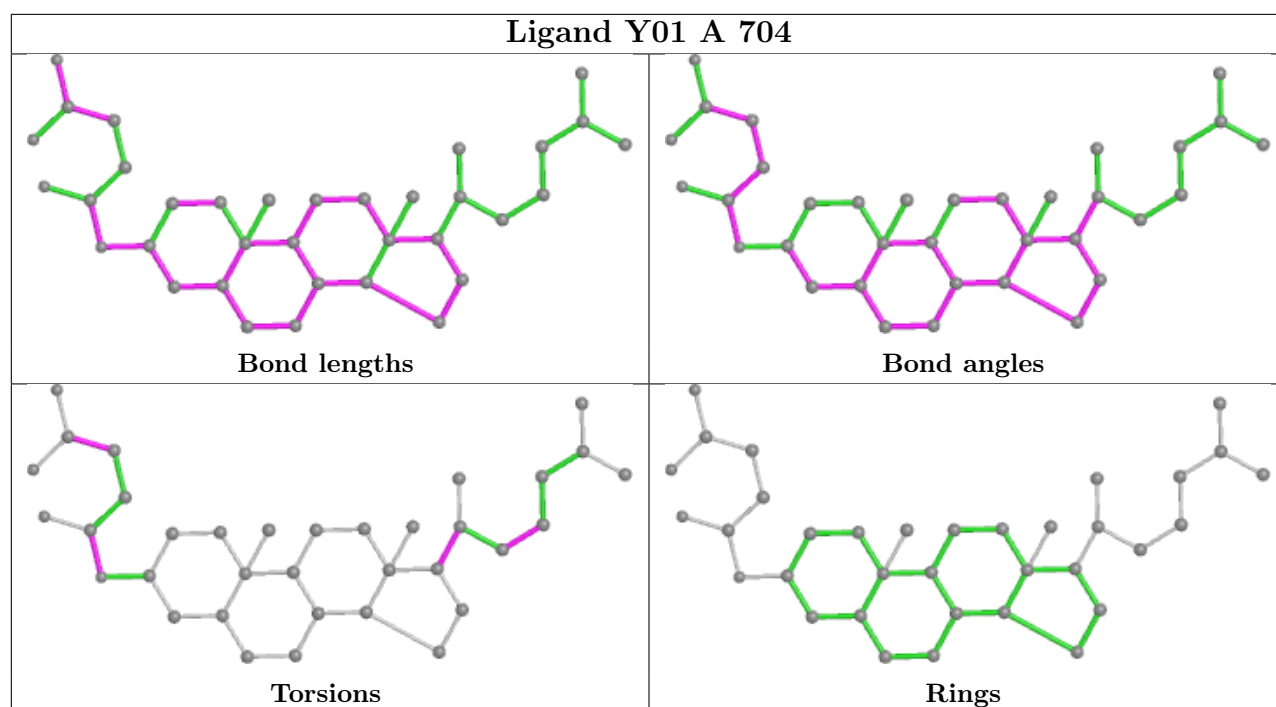
Mol	Chain	Res	Type	Atoms
6	A	704	Y01	CAN-CAJ-CAO-CBB
6	A	704	Y01	CAM-CAY-OAW-CBC
6	A	704	Y01	OAG-CAY-OAW-CBC
7	A	705	CLR	C20-C22-C23-C24
6	A	704	Y01	CAC-CBB-CBE-CBI
6	A	704	Y01	CAM-CAL-CAX-OAH
6	A	704	Y01	CAM-CAL-CAX-OAF
7	A	705	CLR	C23-C24-C25-C26
6	A	704	Y01	CAO-CBB-CBE-CBI
6	A	704	Y01	CAC-CBB-CBE-CAP

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	536/536 (100%)	-0.18	6 (1%) 80 69	69, 85, 106, 133	0
2	L	214/214 (100%)	-0.09	5 (2%) 60 47	60, 80, 104, 128	0
3	H	219/219 (100%)	0.01	4 (1%) 68 55	60, 82, 111, 158	0
All	All	969/969 (100%)	-0.12	15 (1%) 73 61	60, 84, 107, 158	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	PRO	3.2
3	H	126	SER	3.2
2	L	127	THR	3.0
1	A	588	GLN	2.7
1	A	496	TRP	2.6
1	A	524	ARG	2.5
2	L	65	GLY	2.4
3	H	138	THR	2.2
1	A	305	TYR	2.2
1	A	581	SER	2.2
2	L	130	GLY	2.2
2	L	68	SER	2.1
3	H	191	SER	2.1
2	L	69	GLY	2.0
3	H	128	TYR	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](#)

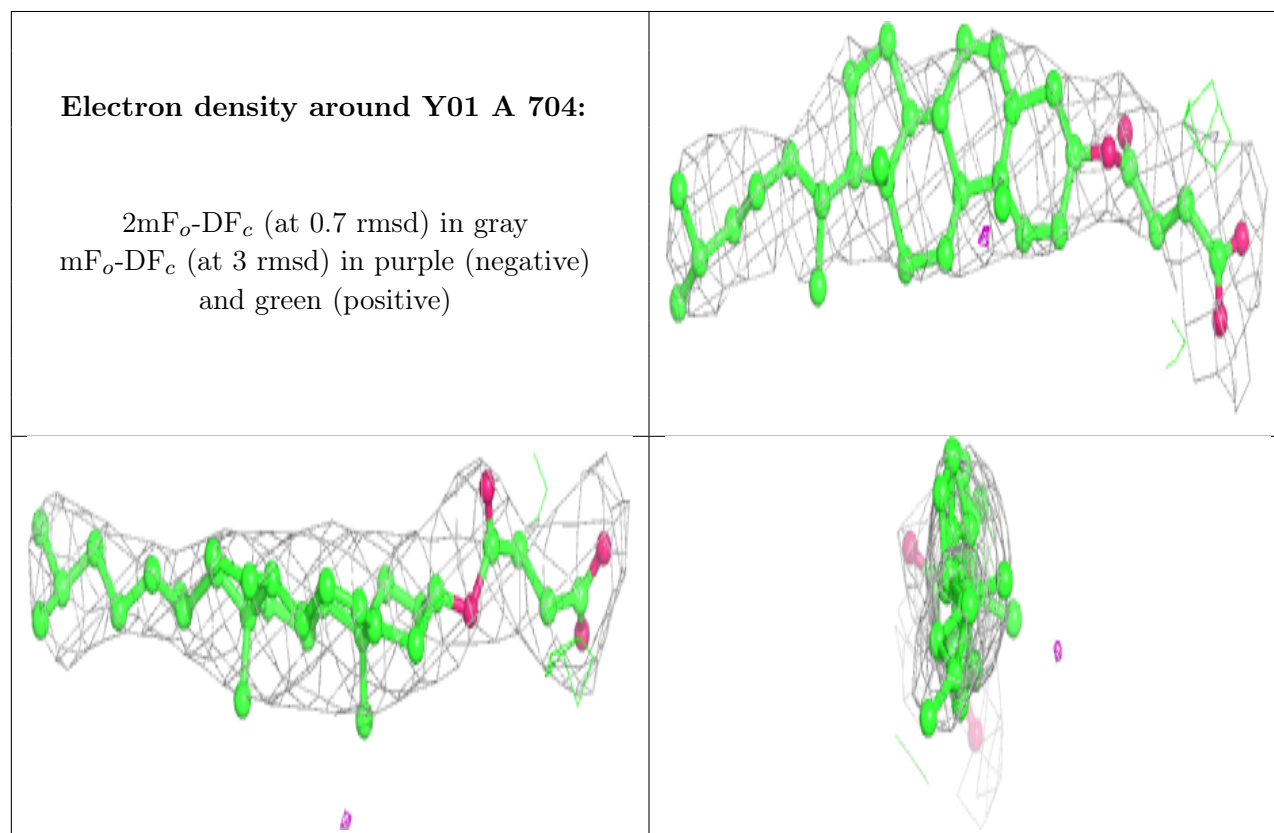
There are no monosaccharides in this entry.

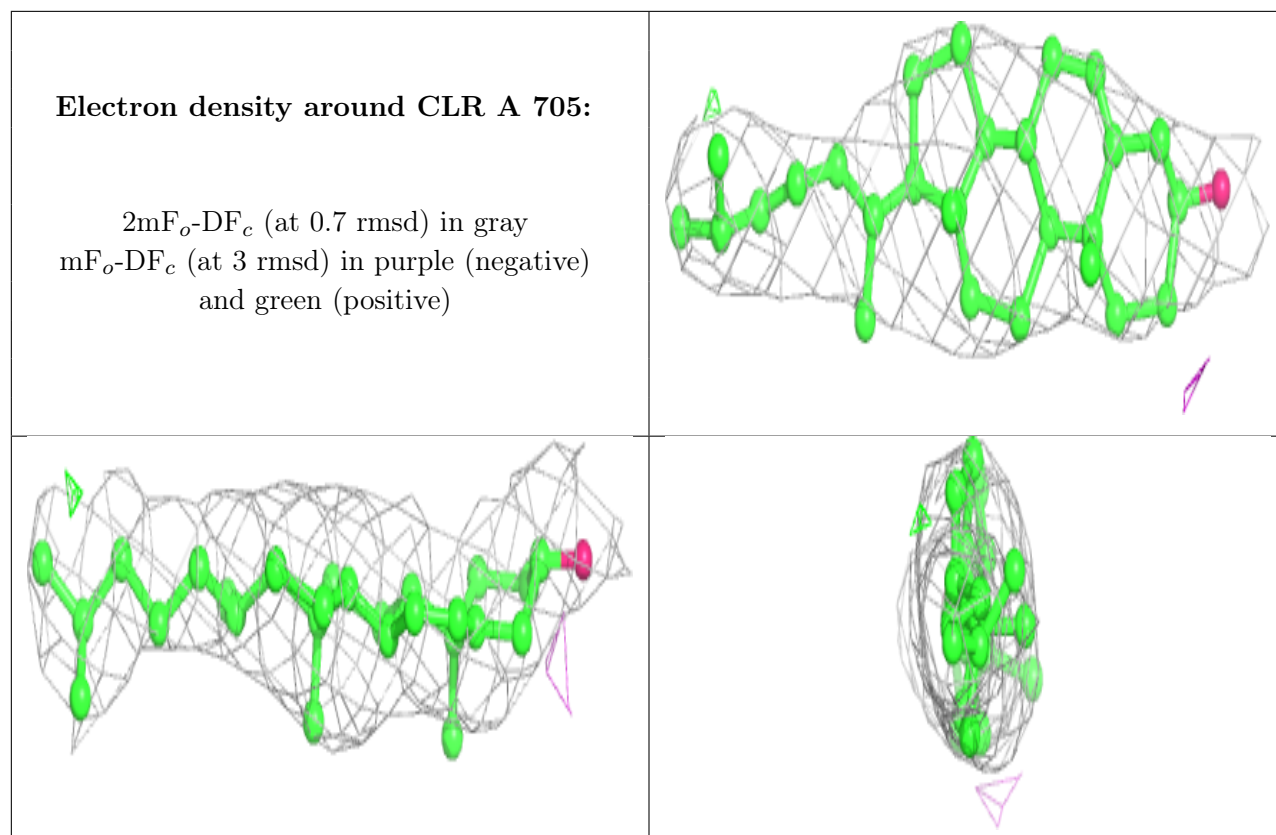
## 6.4 Ligands [i](#)

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
4	NA	A	702	1/1	0.73	0.10	94,94,94,94	0
6	Y01	A	704	35/35	0.88	0.32	83,99,113,115	0
4	NA	A	701	1/1	0.89	0.36	86,86,86,86	0
7	CLR	A	705	28/28	0.89	0.32	67,83,92,94	0
5	CL	A	703	1/1	0.90	0.19	82,82,82,82	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.