



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 07:15 PM JST

PDB ID : 6M2R  
Title : X-ray structure of a functional Drosophila dopamine transporter in L-norepinephrine bound form  
Authors : Shabareesh, P.; Mallela, A.K.; Joseph, D.; Penmatsa, A.  
Deposited on : 2020-02-28  
Resolution : 2.80 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>.

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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 : 2.36  
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) : 2.36

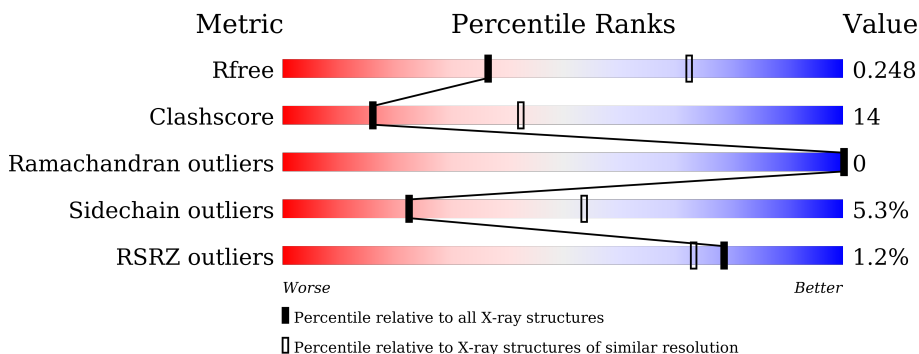
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	
2	L	214	
3	H	219	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7791 atoms, of which 11 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	4250	2846	662	723	19	0	1	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	VAL	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	471	LEU	PHE	engineered mutation	UNP Q7K4Y6

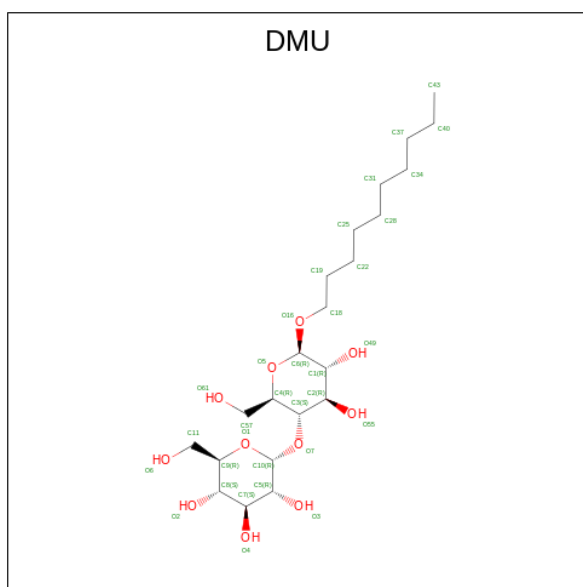
- Molecule 2 is a protein called Antibody fragment 9D5 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1633	1015	272	338	8	0	0	0

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

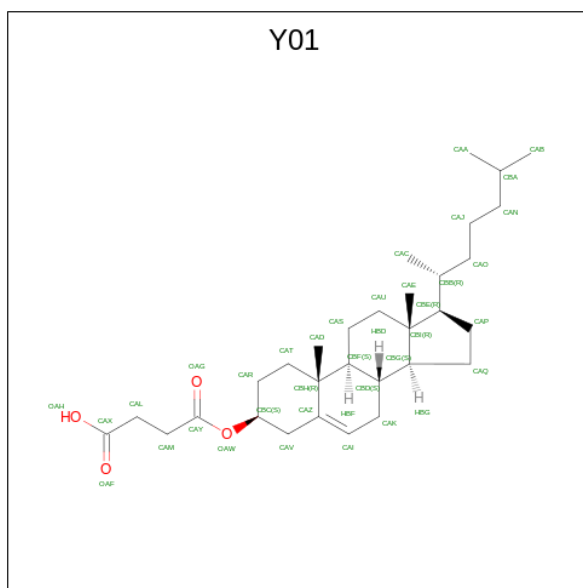
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	219	1655	1039	281	327	8	0	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

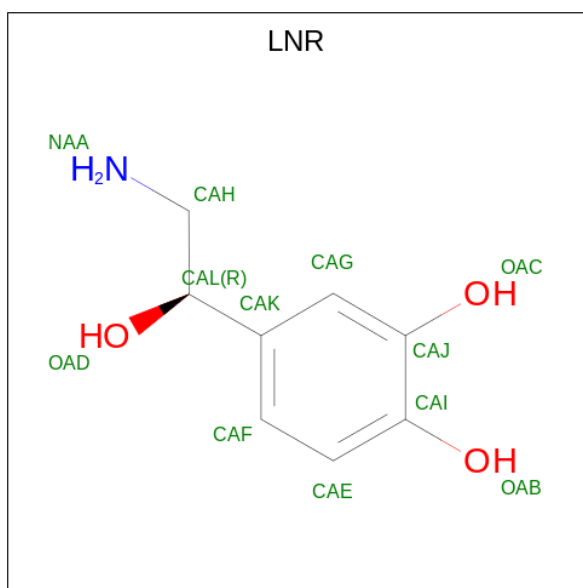
- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).





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

- Molecule 7 is L-NOREPINEPHRINE (three-letter code: LNR) (formula:  $C_8H_{11}NO_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	A	1	Total	C	H	N	O	0	0
			23	8	11	1	3		

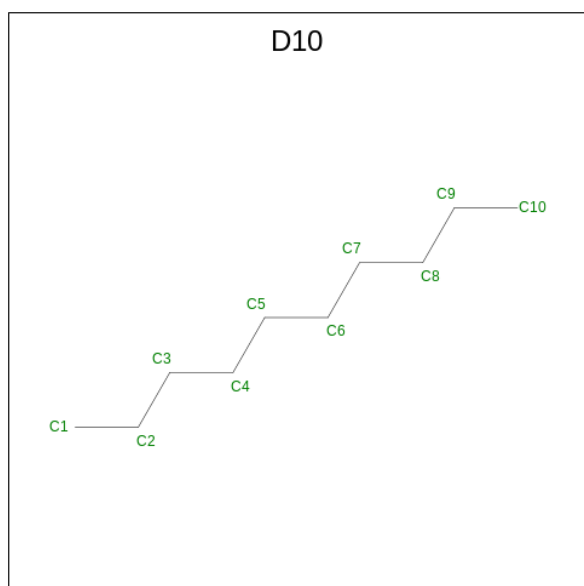
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Na 2 2	0	0
9	L	2	Total Na 2 2	0	0

- Molecule 10 is DECANE (three-letter code: D10) (formula: C<sub>10</sub>H<sub>22</sub>).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	27	Total O 27 27	0	0

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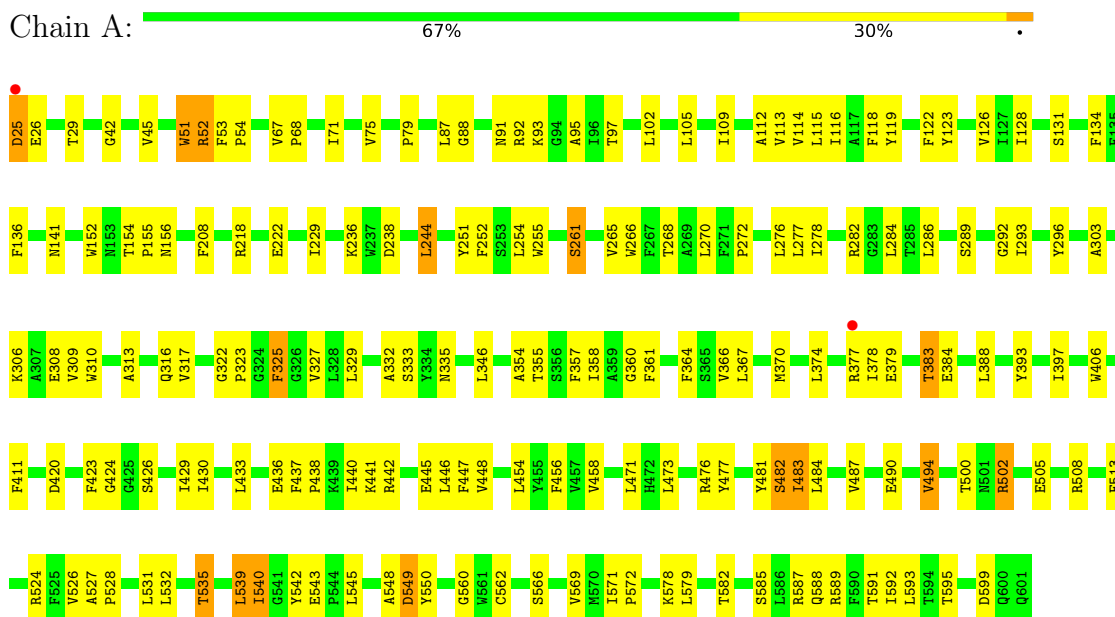
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
11	L	38	Total	O	0	0
			38	38		
11	H	34	Total	O	0	0
			34	34		



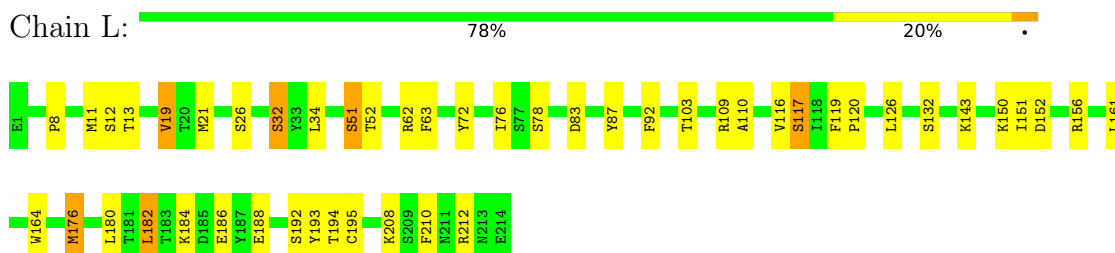
### 3 Residue-property plots [i](#)

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.

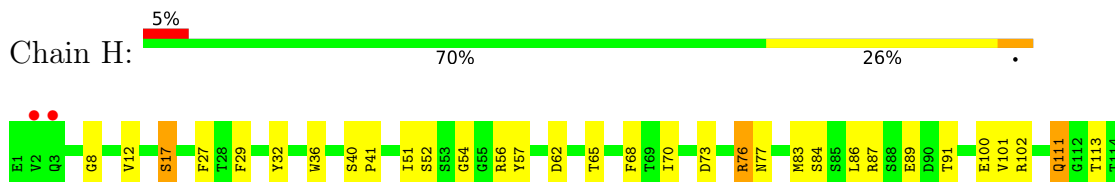
- Molecule 1: Sodium-dependent dopamine transporter

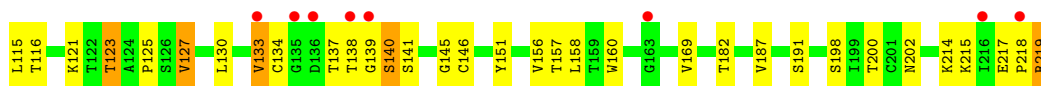


- Molecule 2: Antibody fragment 9D5 Light chain



- 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, $\alpha$ , $\beta$ , $\gamma$	96.80Å 141.27Å 167.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 2.80 48.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.40-2.80) 99.8 (48.41-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.211 , 0.247 0.211 , 0.248	Depositor DCC
$R_{free}$ test set	2787 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.2	Xtrriage
Anisotropy	0.377	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: Y01, CLR, DMU, LNR, NA, CL, D10

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	0.32	0/4394	0.48	0/6000
2	L	0.33	0/1671	0.55	0/2270
3	H	0.36	0/1694	0.55	0/2307
All	All	0.33	0/7759	0.51	0/10577

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	4250	0	4186	134	0
2	L	1633	0	1549	43	0
3	H	1655	0	1617	48	0
4	A	33	0	42	3	0
5	A	35	0	49	1	0
6	A	28	0	46	4	0
7	A	12	11	11	0	0
8	A	1	0	0	0	0
9	A	2	0	0	0	0
9	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	30	0	66	0	0
11	A	27	0	0	2	0
11	H	34	0	0	2	0
11	L	38	0	0	1	0
All	All	7780	11	7566	221	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 14.

All (221) 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:437:PHE:HB2	1:A:440:ILE:HD12	1.59	0.83
2:L:21:MET:CE	2:L:103:THR:HB	2.09	0.83
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.61	0.82
1:A:420:ASP:OD2	11:A:801:HOH:O	1.99	0.80
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.65	0.77
2:L:109:ARG:NH1	2:L:110:ALA:O	2.20	0.75
1:A:123:TYR:O	1:A:126:VAL:HG22	1.86	0.74
3:H:36:TRP:HD1	3:H:70:ILE:HD12	1.52	0.74
3:H:198:SER:HB2	3:H:215:LYS:HE3	1.67	0.74
2:L:21:MET:HE1	2:L:103:THR:HB	1.70	0.74
1:A:123:TYR:HB2	1:A:471:LEU:HD22	1.72	0.72
1:A:477:TYR:CD2	1:A:560:GLY:HA3	2.25	0.71
3:H:111:GLN:NE2	11:H:301:HOH:O	2.23	0.71
2:L:21:MET:CE	2:L:87:TYR:HB2	2.21	0.69
1:A:438:PRO:O	1:A:442:ARG:HG3	1.93	0.69
2:L:164:TRP:CD1	2:L:176:MET:HG3	2.28	0.69
2:L:21:MET:HE2	2:L:87:TYR:HB2	1.74	0.68
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.28	0.68
3:H:68:PHE:CZ	3:H:83:MET:HE2	2.28	0.68
1:A:454:LEU:O	1:A:458:VAL:HG12	1.94	0.67
2:L:164:TRP:HD1	2:L:176:MET:HG3	1.58	0.67
2:L:21:MET:HE3	2:L:103:THR:HB	1.75	0.67
1:A:303:ALA:HB1	1:A:309:VAL:HG21	1.78	0.66
2:L:151:ILE:HD11	2:L:180:LEU:HD21	1.77	0.66
1:A:585:SER:O	1:A:589:ARG:HG3	1.96	0.66
3:H:73:ASP:OD2	3:H:76:ARG:HB2	1.96	0.65
1:A:222:GLU:OE2	1:A:236:LYS:HE2	1.98	0.64
1:A:383:THR:HG22	1:A:384:GLU:H	1.63	0.64
1:A:502:ARG:NH1	1:A:599:ASP:OD2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:102:ARG:NH2	11:H:302:HOH:O	2.28	0.64
1:A:587:ARG:O	1:A:591:THR:HG23	1.98	0.63
1:A:591:THR:O	1:A:595:THR:HG23	1.98	0.63
3:H:91:THR:HG23	3:H:116:THR:HA	1.81	0.63
1:A:441:LYS:NZ	11:A:804:HOH:O	2.31	0.62
3:H:52:SER:HB3	3:H:57:TYR:HB2	1.81	0.62
1:A:42:GLY:C	1:A:420:ASP:HB3	2.20	0.61
1:A:52:ARG:HG2	1:A:316:GLN:OE1	2.01	0.61
2:L:8:PRO:HG2	2:L:11:MET:HB3	1.82	0.61
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.36	0.61
2:L:120:PRO:HG2	3:H:219:ARG:CZ	2.31	0.61
1:A:481:TYR:CE1	1:A:539:LEU:HD13	2.36	0.60
2:L:156:ARG:HD3	2:L:180:LEU:HD21	1.82	0.60
1:A:476:ARG:HD2	1:A:545:LEU:HD13	1.82	0.60
1:A:502:ARG:HG3	3:H:56:ARG:CZ	2.31	0.60
1:A:532:LEU:HA	1:A:535:THR:OG1	2.01	0.60
2:L:13:THR:HG21	2:L:19:VAL:HG11	1.84	0.59
1:A:136:PHE:CD2	4:A:701:DMU:H14	2.38	0.58
1:A:95:ALA:HA	1:A:329:LEU:CD2	2.34	0.58
1:A:156:ASN:HB3	1:A:208:PHE:CD2	2.39	0.58
1:A:508:ARG:O	1:A:508:ARG:HD3	2.03	0.58
1:A:582:THR:O	1:A:589:ARG:NH2	2.29	0.58
1:A:112:ALA:O	1:A:116:ILE:HG13	2.04	0.57
1:A:126:VAL:HG21	1:A:471:LEU:HD21	1.87	0.57
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.39	0.57
2:L:210:PHE:HB2	3:H:133:VAL:HG11	1.87	0.57
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.87	0.56
2:L:117:SER:HB2	2:L:119:PHE:CE1	2.41	0.56
1:A:105:LEU:O	1:A:105:LEU:HG	2.06	0.56
1:A:377:ARG:HB3	1:A:379:GLU:OE2	2.05	0.56
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.88	0.56
1:A:268:THR:OG1	1:A:420:ASP:OD1	2.13	0.55
1:A:505:GLU:OE1	3:H:56:ARG:HD3	2.06	0.55
1:A:284:LEU:HA	1:A:289:SER:OG	2.07	0.55
3:H:12:VAL:HG11	3:H:86:LEU:HD12	1.89	0.55
1:A:71:ILE:O	1:A:75:VAL:HG22	2.06	0.55
6:A:703:CLR:H121	6:A:703:CLR:H212	1.89	0.55
6:A:703:CLR:H212	6:A:703:CLR:H183	1.88	0.55
1:A:266:TRP:O	1:A:270:LEU:HB2	2.07	0.55
1:A:238:ASP:HB2	4:A:701:DMU:H8	1.89	0.54
1:A:42:GLY:O	1:A:420:ASP:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:188:GLU:O	2:L:212:ARG:NH2	2.41	0.54
1:A:45:VAL:HG11	1:A:355:THR:HG21	1.89	0.54
1:A:487:VAL:HA	1:A:490:GLU:HG3	1.90	0.54
1:A:126:VAL:HG21	1:A:471:LEU:HD11	1.89	0.53
1:A:502:ARG:HG3	3:H:56:ARG:NH1	2.23	0.53
1:A:483:ILE:O	1:A:487:VAL:HG13	2.09	0.53
3:H:139:GLY:O	3:H:191:SER:CB	2.56	0.53
1:A:327:VAL:HG22	1:A:424:GLY:O	2.09	0.52
1:A:251:TYR:O	1:A:255:TRP:HB2	2.08	0.52
1:A:393:TYR:CE1	1:A:397:ILE:HD11	2.45	0.52
3:H:36:TRP:CD1	3:H:70:ILE:HD12	2.40	0.52
1:A:265:VAL:HA	1:A:268:THR:OG1	2.09	0.52
1:A:154:THR:HB	1:A:155:PRO:HD2	1.92	0.52
3:H:215:LYS:HD3	3:H:217:GLU:OE2	2.10	0.52
1:A:238:ASP:HB2	4:A:701:DMU:C19	2.39	0.52
2:L:63:PHE:CE1	2:L:76:ILE:HG12	2.45	0.52
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.92	0.51
5:A:702:Y01:HAC1	5:A:702:Y01:HAU2	1.92	0.51
2:L:161:LEU:CD1	3:H:182:THR:HB	2.40	0.51
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.93	0.51
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.47	0.50
2:L:120:PRO:HB3	2:L:210:PHE:CZ	2.46	0.50
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.94	0.50
2:L:126:LEU:HD23	2:L:184:LYS:HG3	1.94	0.50
3:H:139:GLY:O	3:H:191:SER:HB3	2.11	0.50
1:A:437:PHE:CB	1:A:440:ILE:HD12	2.38	0.50
3:H:83:MET:HE1	3:H:115:LEU:CD2	2.41	0.50
1:A:282:ARG:O	1:A:282:ARG:NE	2.41	0.49
2:L:132:SER:HA	2:L:180:LEU:O	2.11	0.49
1:A:490:GLU:O	1:A:494:VAL:HG13	2.12	0.49
6:A:703:CLR:H121	6:A:703:CLR:C21	2.42	0.49
1:A:433:LEU:HD12	1:A:447:PHE:CZ	2.47	0.49
1:A:88:GLY:O	1:A:333:SER:HA	2.12	0.49
1:A:325:PHE:N	1:A:325:PHE:CD1	2.81	0.49
3:H:68:PHE:CZ	3:H:83:MET:CE	2.96	0.49
1:A:25:ASP:HB3	1:A:26:GLU:H	1.50	0.48
1:A:306:LYS:HB3	1:A:308:GLU:OE2	2.13	0.48
3:H:121:LYS:O	3:H:123:THR:HG22	2.12	0.48
1:A:325:PHE:N	1:A:325:PHE:HD1	2.12	0.48
2:L:116:VAL:O	2:L:208:LYS:HG3	2.13	0.48
1:A:282:ARG:HD2	1:A:406:TRP:CZ2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:CE1	1:A:458:VAL:HG11	2.48	0.47
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.49	0.47
3:H:40:SER:HB2	3:H:41:PRO:HD2	1.96	0.47
3:H:17:SER:HB2	3:H:84:SER:HA	1.96	0.47
1:A:500:THR:HG23	1:A:524:ARG:NH1	2.29	0.47
1:A:426:SER:O	1:A:430:ILE:HG13	2.15	0.47
2:L:152:ASP:HA	2:L:192:SER:HB3	1.96	0.47
3:H:27:PHE:CE2	3:H:29:PHE:HA	2.50	0.47
1:A:542:TYR:O	1:A:543:GLU:HG3	2.15	0.47
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.75	0.46
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.97	0.46
2:L:26:SER:HB3	11:L:425:HOH:O	2.16	0.46
2:L:126:LEU:O	2:L:184:LYS:HE2	2.15	0.46
2:L:161:LEU:HD13	3:H:182:THR:HB	1.96	0.46
1:A:67:VAL:HB	1:A:68:PRO:CD	2.46	0.46
1:A:313:ALA:O	1:A:317:VAL:HG13	2.16	0.46
1:A:548:ALA:O	1:A:549:ASP:HB2	2.15	0.46
2:L:164:TRP:HD1	2:L:176:MET:CG	2.26	0.46
1:A:254:LEU:HD11	1:A:423:PHE:HA	1.98	0.46
1:A:277:LEU:HB2	6:A:703:CLR:H273	1.98	0.46
3:H:169:VAL:HG22	3:H:187:VAL:HG23	1.97	0.46
1:A:134:PHE:HB3	1:A:411:PHE:CE2	2.52	0.45
1:A:473:LEU:HA	1:A:545:LEU:HD21	1.98	0.45
1:A:484:LEU:HD13	1:A:535:THR:HG23	1.97	0.45
2:L:143:LYS:HE3	2:L:164:TRP:CE3	2.51	0.45
3:H:51:ILE:HB	3:H:70:ILE:HG12	1.98	0.45
1:A:67:VAL:HB	1:A:68:PRO:HD3	1.98	0.45
1:A:562:CYS:O	1:A:566:SER:HB3	2.17	0.45
2:L:21:MET:HE3	2:L:103:THR:CB	2.44	0.45
1:A:393:TYR:HE1	1:A:397:ILE:HD11	1.80	0.45
1:A:508:ARG:HD3	1:A:508:ARG:C	2.36	0.45
2:L:21:MET:HE1	2:L:87:TYR:HB2	1.98	0.45
1:A:91:ASN:C	1:A:92:ARG:HG2	2.38	0.45
1:A:119:TYR:O	1:A:122:PHE:HB2	2.17	0.45
3:H:127:VAL:O	3:H:127:VAL:CG2	2.65	0.45
3:H:127:VAL:HG23	3:H:214:LYS:HG3	1.98	0.45
1:A:579:LEU:HA	1:A:593:LEU:HD11	1.98	0.45
1:A:105:LEU:HB2	1:A:593:LEU:HB3	2.00	0.44
1:A:582:THR:O	1:A:589:ARG:CD	2.65	0.44
1:A:582:THR:O	1:A:589:ARG:HD3	2.16	0.44
3:H:76:ARG:O	3:H:77:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:PHE:HA	1:A:367:LEU:HB2	2.00	0.44
1:A:588:GLN:O	1:A:592:ILE:HG13	2.17	0.44
2:L:117:SER:HB2	2:L:119:PHE:HE1	1.83	0.44
1:A:92:ARG:O	1:A:93:LYS:HD3	2.18	0.44
3:H:87:ARG:HD2	3:H:89:GLU:OE1	2.18	0.44
1:A:293:ILE:HD12	1:A:361:PHE:CD1	2.52	0.44
2:L:182:LEU:HB3	2:L:186:GLU:HG2	2.00	0.44
1:A:357:PHE:CE2	1:A:361:PHE:HE2	2.36	0.43
1:A:75:VAL:O	1:A:79:PRO:HG2	2.18	0.43
1:A:430:ILE:HD13	1:A:448:VAL:CG2	2.47	0.43
1:A:45:VAL:CG1	1:A:355:THR:HG21	2.48	0.43
1:A:97:THR:OG1	1:A:436:GLU:HG2	2.17	0.43
2:L:51:SER:O	2:L:52:THR:HB	2.18	0.43
1:A:531:LEU:HD23	1:A:531:LEU:HA	1.92	0.43
3:H:130:LEU:HB2	3:H:145:GLY:CA	2.49	0.43
1:A:68:PRO:HB3	1:A:310:TRP:CE2	2.54	0.43
1:A:571:ILE:HB	1:A:572:PRO:CD	2.49	0.43
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.00	0.43
1:A:114:VAL:HG13	1:A:429:ILE:HG12	2.01	0.42
1:A:278:ILE:HG22	1:A:406:TRP:HZ3	1.84	0.42
1:A:483:ILE:HD12	1:A:483:ILE:HA	1.84	0.42
1:A:578:LYS:HB2	1:A:578:LYS:HE3	1.82	0.42
2:L:126:LEU:HD23	2:L:184:LYS:CG	2.49	0.42
2:L:151:ILE:HD13	2:L:156:ARG:HD2	2.00	0.42
3:H:32:TYR:HA	3:H:100:GLU:HB2	2.00	0.42
3:H:127:VAL:HG23	3:H:214:LYS:CG	2.49	0.42
1:A:128:ILE:O	1:A:131:SER:HB2	2.18	0.42
1:A:540:ILE:O	1:A:540:ILE:CG2	2.67	0.42
3:H:217:GLU:HA	3:H:218:PRO:HD3	1.79	0.42
1:A:109:ILE:HG21	1:A:490:GLU:HG2	2.00	0.42
2:L:19:VAL:HG22	2:L:76:ILE:HB	2.01	0.42
1:A:308:GLU:H	1:A:308:GLU:CD	2.23	0.42
1:A:366:VAL:O	1:A:370:MET:HG3	2.19	0.42
3:H:139:GLY:O	3:H:191:SER:HB2	2.19	0.42
3:H:146:CYS:HB2	3:H:160:TRP:CH2	2.54	0.42
1:A:126:VAL:CG2	1:A:471:LEU:HD11	2.50	0.42
1:A:292:GLY:HA3	1:A:364:PHE:O	2.19	0.42
2:L:32:SER:HA	2:L:51:SER:OG	2.20	0.42
1:A:254:LEU:HD23	1:A:261:SER:HB2	2.02	0.42
1:A:272:PRO:O	1:A:276:LEU:HG	2.20	0.42
2:L:150:LYS:HB2	2:L:194:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:OE1	1:A:445:GLU:N	2.48	0.41
1:A:286:LEU:O	1:A:289:SER:HB2	2.20	0.41
3:H:139:GLY:O	3:H:140:SER:C	2.57	0.41
3:H:158:LEU:HA	3:H:202:ASN:O	2.20	0.41
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.92	0.41
1:A:51:TRP:HA	1:A:388:LEU:HD23	2.02	0.41
3:H:8:GLY:O	3:H:113:THR:OG1	2.30	0.41
1:A:370:MET:O	1:A:374:LEU:HB2	2.19	0.41
3:H:151:TYR:CE2	3:H:156:VAL:HG13	2.54	0.41
1:A:244:LEU:HB2	1:A:456:PHE:CE1	2.56	0.41
3:H:54:GLY:O	3:H:56:ARG:HG3	2.21	0.41
1:A:229:ILE:HG22	1:A:550:TYR:OH	2.20	0.41
1:A:322:GLY:N	1:A:323:PRO:HD3	2.35	0.41
1:A:569:VAL:O	1:A:572:PRO:HD2	2.21	0.41
1:A:115:LEU:O	1:A:118:PHE:HB3	2.21	0.41
1:A:152:TRP:O	1:A:218:ARG:HD3	2.21	0.41
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.86	0.40
1:A:354:ALA:O	1:A:358:ILE:HG12	2.21	0.40
2:L:62:ARG:NH1	2:L:83:ASP:OD1	2.54	0.40
1:A:332:ALA:O	1:A:335:ASN:HB2	2.22	0.40
1:A:378:ILE:HG23	1:A:379:GLU:N	2.37	0.40
1:A:252:PHE:HA	1:A:255:TRP:HB2	2.03	0.40
3:H:62:ASP:O	3:H:65:THR:HG22	2.21	0.40
1:A:42:GLY:CA	1:A:420:ASP:HB3	2.51	0.40
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.81	0.40
1:A:116:ILE:CD1	1:A:482:SER:HB2	2.51	0.40
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.84	0.40
3:H:127:VAL:CG2	3:H:214:LYS:HG2	2.51	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%)	507 (95%)	28 (5%)	0	100	100
2	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
3	H	217/219 (99%)	205 (94%)	12 (6%)	0	100	100
All	All	964/969 (100%)	912 (95%)	52 (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	438/441 (99%)	419 (96%)	19 (4%)	29	62
2	L	185/187 (99%)	175 (95%)	10 (5%)	22	53
3	H	186/187 (100%)	172 (92%)	14 (8%)	13	37
All	All	809/815 (99%)	766 (95%)	43 (5%)	22	54

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	29	THR
1	A	51	TRP
1	A	52	ARG
1	A	113	VAL
1	A	141	ASN
1	A	244	LEU
1	A	261	SER
1	A	325	PHE
1	A	383	THR
1	A	446	LEU
1	A	482	SER
1	A	483	ILE
1	A	494	VAL
1	A	502	ARG

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Mol	Chain	Res	Type
1	A	535	THR
1	A	539	LEU
1	A	540	ILE
1	A	549	ASP
2	L	12	SER
2	L	19	VAL
2	L	32	SER
2	L	51	SER
2	L	78	SER
2	L	92	PHE
2	L	117	SER
2	L	176	MET
2	L	182	LEU
2	L	195	CYS
3	H	17	SER
3	H	76	ARG
3	H	111	GLN
3	H	123	THR
3	H	127	VAL
3	H	133	VAL
3	H	134	CYS
3	H	137	THR
3	H	138	THR
3	H	140	SER
3	H	141	SER
3	H	157	THR
3	H	200	THR
3	H	219	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	D10	A	709	-	9,9,9	0.38	0	8,8,8	0.19	0
5	Y01	A	702	-	38,38,38	1.22	1 (2%)	57,57,57	1.19	7 (12%)
6	CLR	A	703	-	31,31,31	0.67	1 (3%)	48,48,48	1.74	11 (22%)
7	LNR	A	704	-	12,12,12	1.11	2 (16%)	15,16,16	0.69	0
10	D10	A	710	-	9,9,9	0.44	0	8,8,8	0.20	0
4	DMU	A	701	-	34,34,34	1.11	2 (5%)	45,45,45	1.04	3 (6%)
10	D10	A	708	-	9,9,9	0.42	0	8,8,8	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	D10	A	709	-	-	4/7/7/7	-
5	Y01	A	702	-	-	7/19/77/77	0/4/4/4
6	CLR	A	703	-	-	4/10/68/68	0/4/4/4
7	LNR	A	704	-	-	2/6/6/6	0/1/1/1
10	D10	A	710	-	-	2/7/7/7	-
4	DMU	A	701	-	-	6/19/59/59	0/2/2/2
10	D10	A	708	-	-	3/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	Y01	OAF-CAX	5.14	1.39	1.22
4	A	701	DMU	O5-C6	3.13	1.49	1.41
4	A	701	DMU	O1-C10	2.89	1.49	1.41
7	A	704	LNR	OAB-CAI	2.35	1.41	1.36
7	A	704	LNR	OAC-CAJ	2.31	1.41	1.36
6	A	703	CLR	C10-C9	-2.02	1.52	1.56

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	CLR	C19-C10-C9	-4.86	105.89	111.68
6	A	703	CLR	C13-C17-C20	-3.28	114.35	119.49
4	A	701	DMU	C10-O7-C3	-3.27	109.86	117.96
6	A	703	CLR	C2-C3-C4	-3.22	105.89	110.31
5	A	702	Y01	OAW-CAY-CAM	3.16	118.31	111.50
5	A	702	Y01	CBC-OAW-CAY	3.03	125.24	117.79
6	A	703	CLR	C15-C14-C13	-2.92	100.33	103.84
6	A	703	CLR	C15-C14-C8	-2.76	114.54	119.08
6	A	703	CLR	C13-C14-C8	-2.73	110.33	114.38
6	A	703	CLR	C4-C5-C10	2.73	120.05	116.42
5	A	702	Y01	CAV-CAZ-CAI	-2.61	116.85	120.61
6	A	703	CLR	C7-C8-C14	-2.54	107.22	110.91
6	A	703	CLR	C16-C17-C20	-2.44	108.37	112.15
5	A	702	Y01	CAC-CBB-CBE	-2.36	109.31	112.92
6	A	703	CLR	C18-C13-C14	-2.33	107.37	111.71
5	A	702	Y01	CBI-CBE-CBB	-2.29	115.90	119.49
4	A	701	DMU	C7-C8-C9	2.19	114.15	110.24
5	A	702	Y01	CAT-CAR-CBC	2.19	114.05	110.33
5	A	702	Y01	CAJ-CAO-CBB	-2.17	108.80	115.03
6	A	703	CLR	C4-C5-C6	-2.06	117.64	120.61
4	A	701	DMU	C11-C9-C8	-2.06	108.19	113.00

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	DMU	C19-C18-O16-C6
7	A	704	LNR	NAA-CAH-CAL-CAK
7	A	704	LNR	NAA-CAH-CAL-OAD
5	A	702	Y01	CAJ-CAO-CBB-CAC
6	A	703	CLR	C16-C17-C20-C22
5	A	702	Y01	CAJ-CAO-CBB-CBE

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Mol	Chain	Res	Type	Atoms
10	A	710	D10	C3-C4-C5-C6
5	A	702	Y01	CAO-CAJ-CAN-CBA
10	A	709	D10	C3-C4-C5-C6
10	A	709	D10	C5-C6-C7-C8
10	A	709	D10	C6-C7-C8-C9
4	A	701	DMU	C25-C28-C31-C34
10	A	708	D10	C5-C6-C7-C8
4	A	701	DMU	C31-C34-C37-C40
4	A	701	DMU	C19-C22-C25-C28
4	A	701	DMU	C34-C37-C40-C43
6	A	703	CLR	C21-C20-C22-C23
6	A	703	CLR	C16-C17-C20-C21
10	A	708	D10	C2-C3-C4-C5
10	A	709	D10	C2-C3-C4-C5
10	A	710	D10	C7-C8-C9-C10
4	A	701	DMU	O16-C18-C19-C22
6	A	703	CLR	C17-C20-C22-C23
5	A	702	Y01	CAM-CAL-CAX-OAH
5	A	702	Y01	CAM-CAL-CAX-OAF
5	A	702	Y01	CAL-CAM-CAY-OAW
5	A	702	Y01	CAL-CAM-CAY-OAG
10	A	708	D10	C4-C5-C6-C7

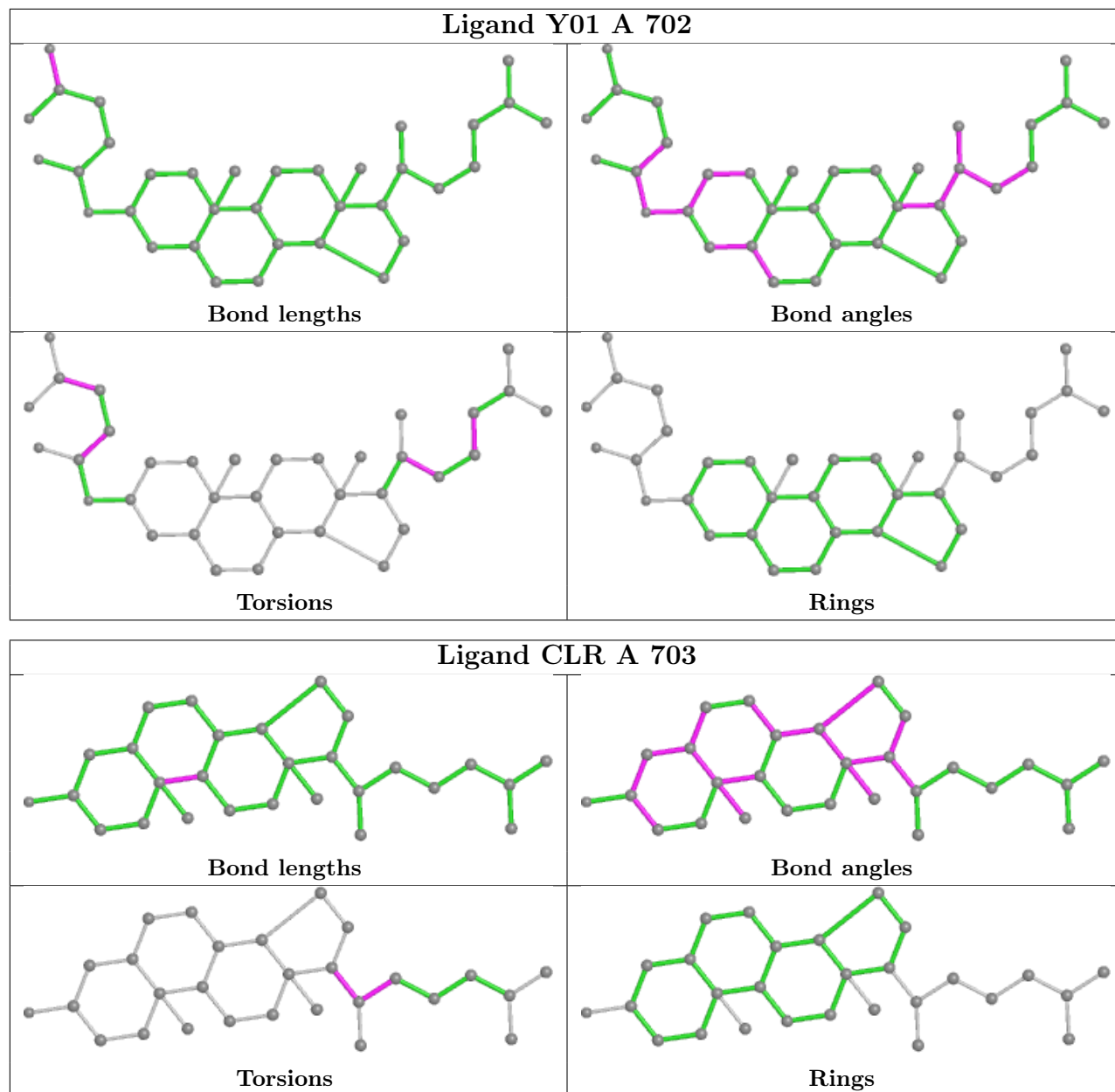
There are no ring outliers.

3 monomers are involved in 8 short contacts:

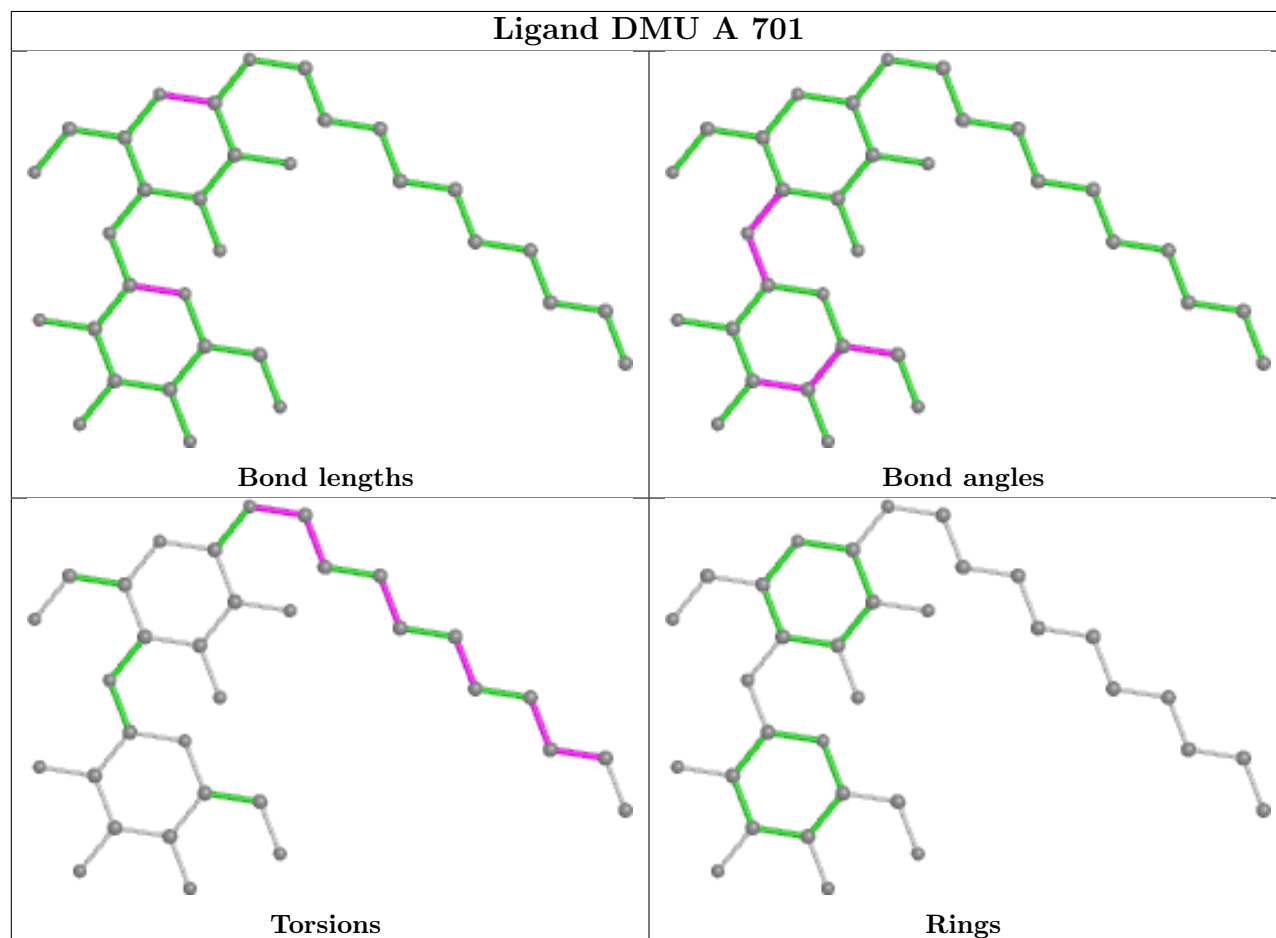
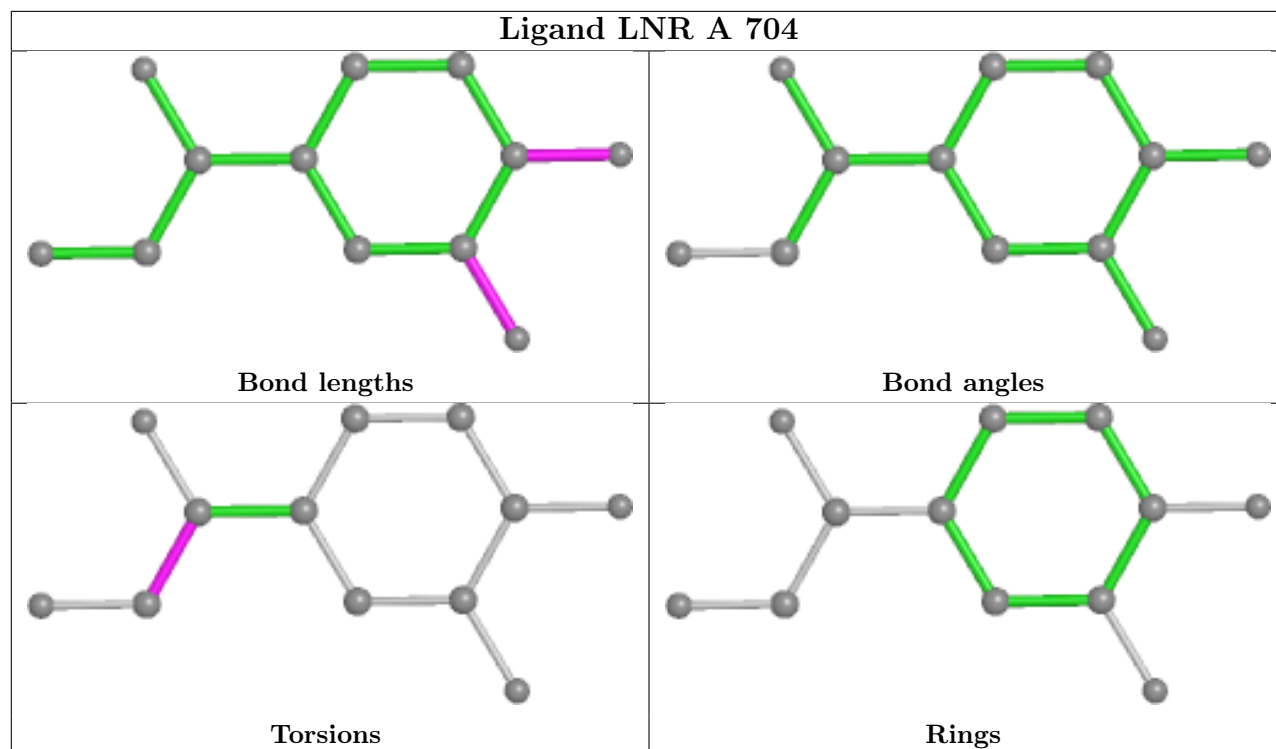
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	Y01	1	0
6	A	703	CLR	4	0
4	A	701	DMU	3	0

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, 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%)	-0.39	2 (0%) 92 91	48, 64, 89, 128	0
2	L	214/214 (100%)	-0.29	0 100 100	42, 57, 82, 106	0
3	H	219/219 (100%)	-0.20	10 (4%) 32 22	46, 57, 89, 136	0
All	All	969/969 (100%)	-0.33	12 (1%) 79 73	42, 61, 88, 136	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	136	ASP	4.9
3	H	138	THR	4.3
1	A	25	ASP	4.2
3	H	135	GLY	3.0
3	H	133	VAL	2.9
3	H	2	VAL	2.7
3	H	163	GLY	2.7
3	H	3	GLN	2.7
3	H	139	GLY	2.4
1	A	377	ARG	2.4
3	H	216	ILE	2.1
3	H	218	PRO	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](#)

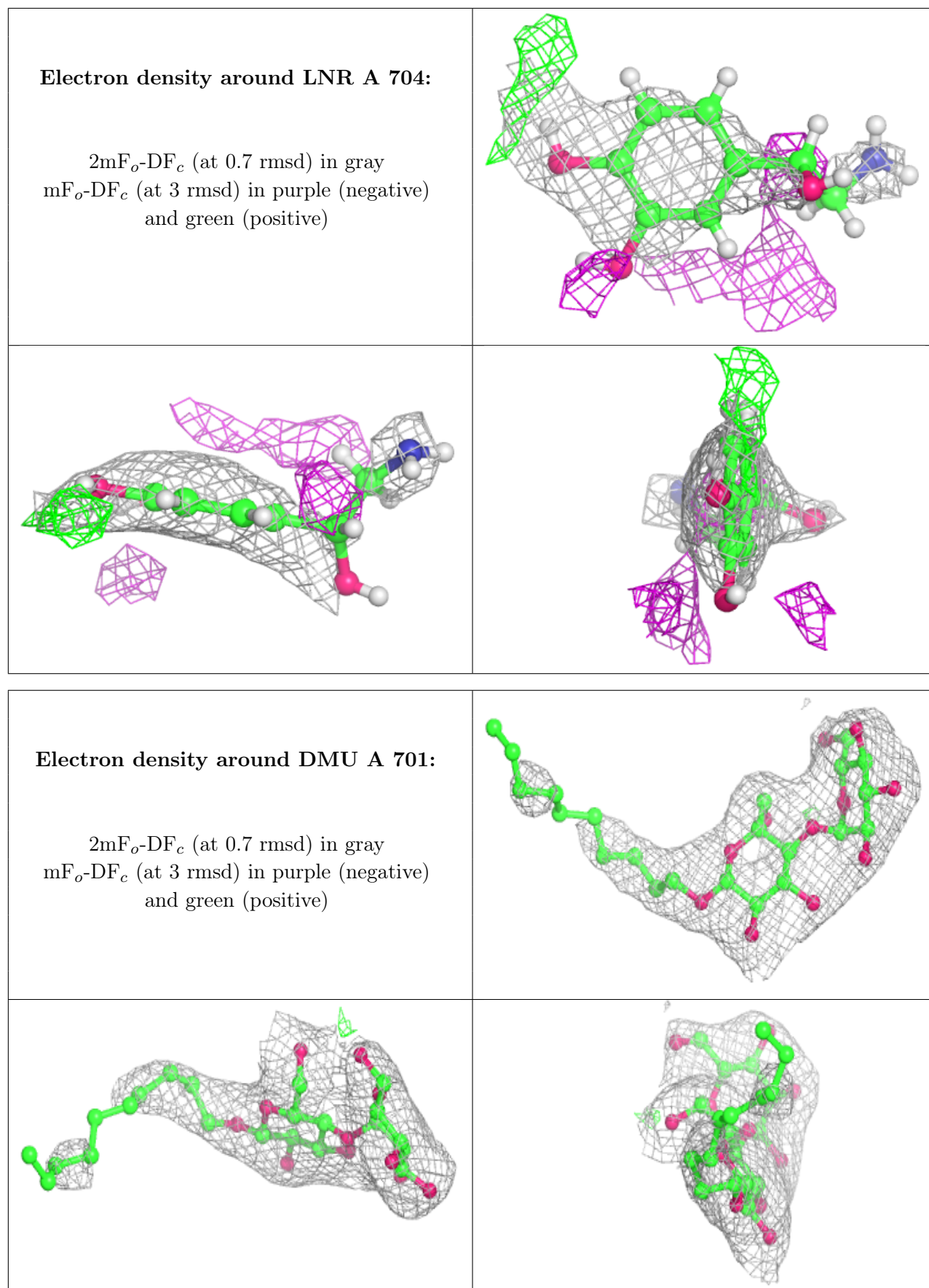
There are no monosaccharides in this entry.

## 6.4 Ligands

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.

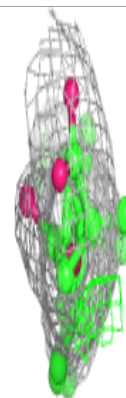
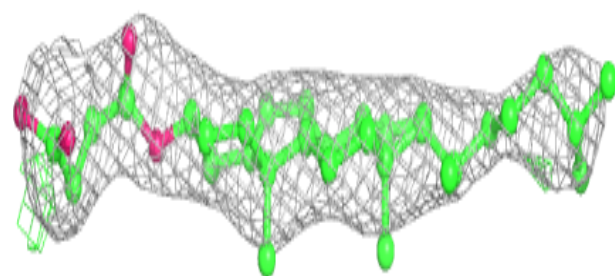
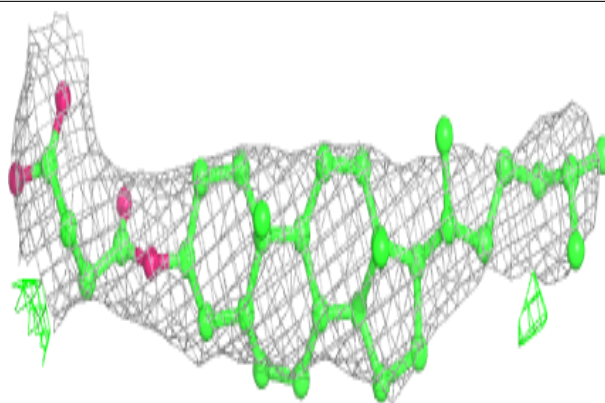
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	D10	A	710	10/10	0.74	0.38	60,81,85,89	0
10	D10	A	709	10/10	0.75	0.24	69,82,87,88	0
7	LNR	A	704	12/12	0.80	0.39	81,96,107,119	0
10	D10	A	708	10/10	0.80	0.29	60,76,84,85	0
9	NA	L	301	1/1	0.87	0.38	60,60,60,60	0
4	DMU	A	701	33/33	0.94	0.19	73,80,86,88	0
9	NA	A	707	1/1	0.94	0.12	56,56,56,56	0
5	Y01	A	702	35/35	0.94	0.32	69,76,92,96	0
9	NA	L	302	1/1	0.95	0.33	56,56,56,56	0
6	CLR	A	703	28/28	0.95	0.21	49,68,76,77	0
9	NA	A	706	1/1	0.97	0.16	65,65,65,65	0
8	CL	A	705	1/1	0.98	0.08	55,55,55,55	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.

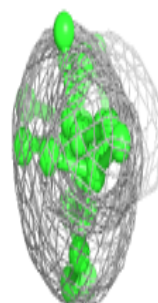
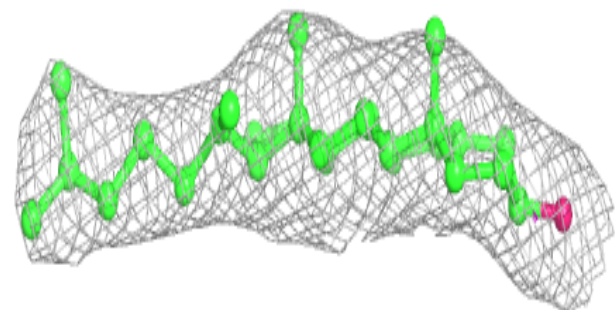
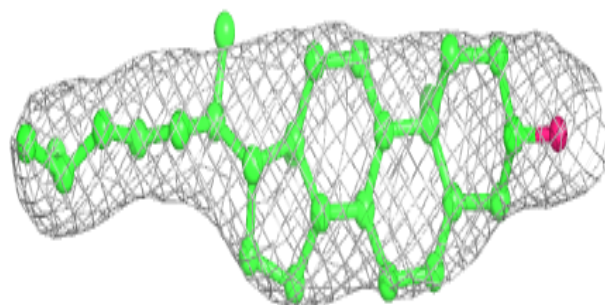


**Electron density around Y01 A 702:**

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

**Electron density around CLR A 703:**

$2mF_o-DF_c$  (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.