



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2022 – 06:09 PM JST

PDB ID : 7WGT  
Title : X-ray structure of thermostabilized *Drosophila* dopamine transporter with GABA transporter1-like substitutions in the binding site, in complex with NO711.  
Authors : Joseph, D.; Penmatsa, A.  
Deposited on : 2021-12-28  
Resolution : 2.75 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	:	2.29
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

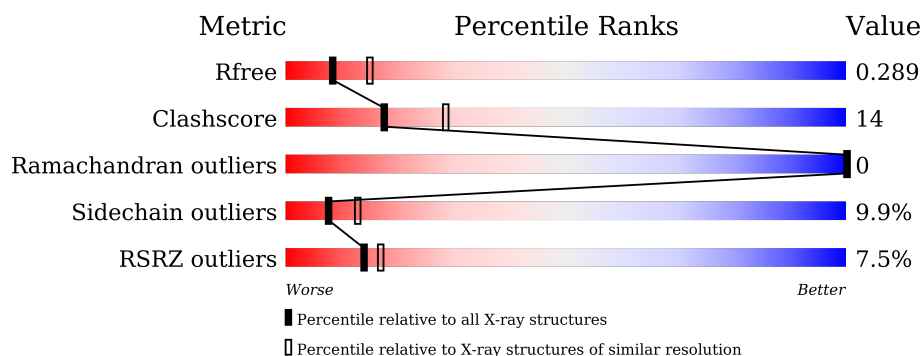
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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>6%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>.</div> </div> </div>
2	L	214	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>.</div> </div> </div>
3	H	219	<div> <div>12%</div> <div> <div></div> <div>63%</div> <div>33%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7608 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
1	A	536	Total	C	N	O	S	0	0	0
			4221	2829	653	721	18			

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

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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

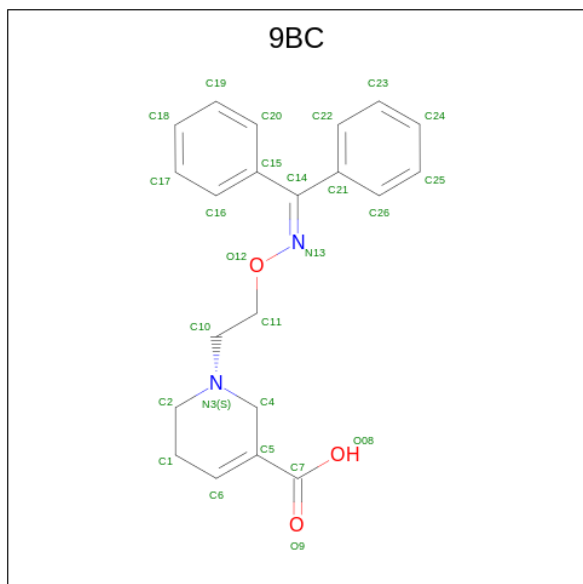
- Molecule 2 is a protein called Antibody fragment (9D5) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1623	1008	269	338	8			

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

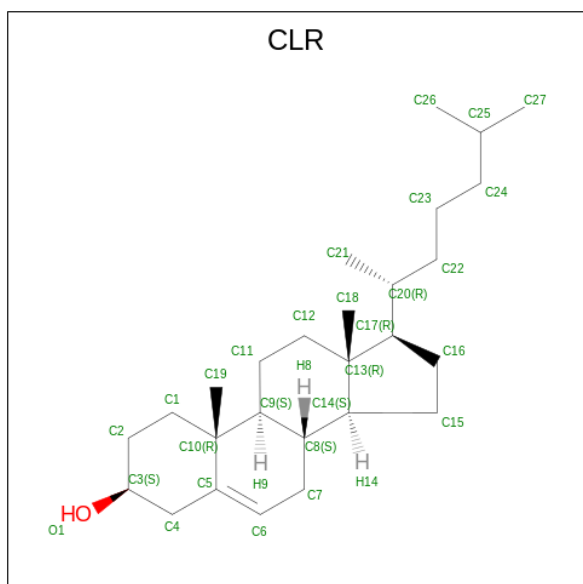
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1644	1033	278	325	8			

- Molecule 4 is 1-(2-{[(diphenylmethylidene)amino]oxy}ethyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (three-letter code: 9BC) (formula:  $C_{21}H_{22}N_2O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	21	2	3		

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



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

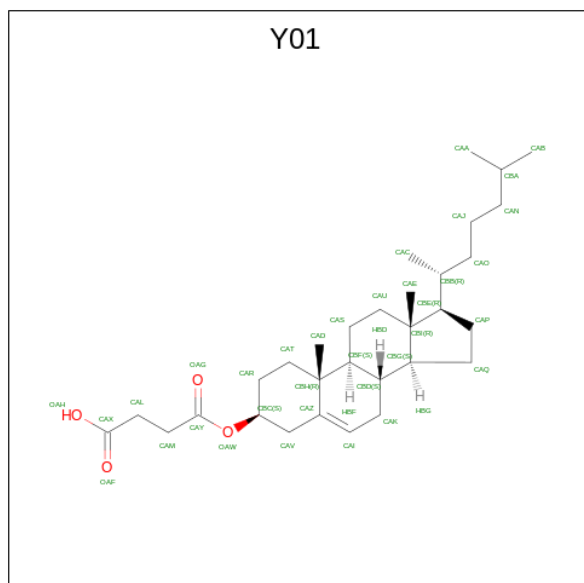
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



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

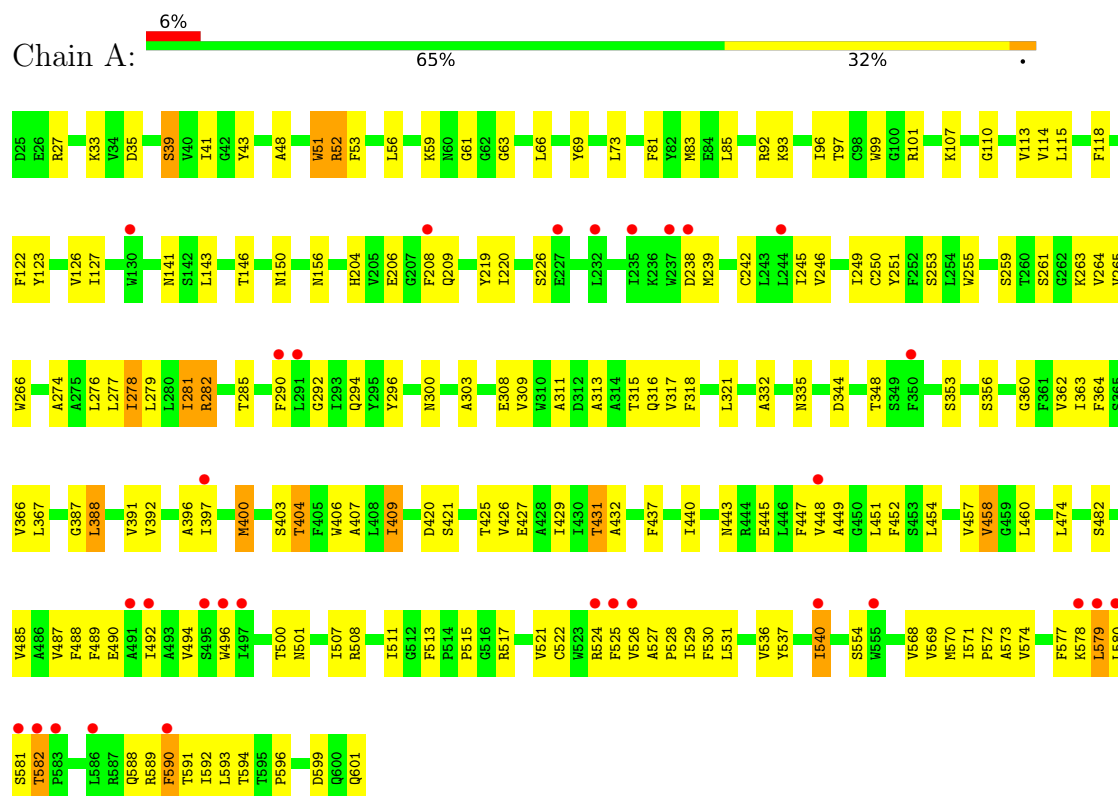
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	15	Total O 15 15	0	0
9	L	7	Total O 7 7	0	0
9	H	6	Total O 6 6	0	0

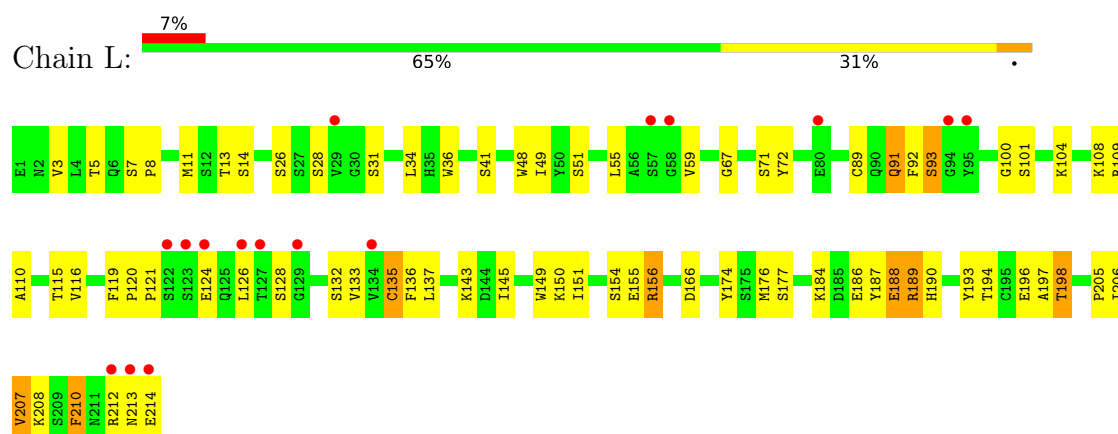
### 3 Residue-property plots

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.

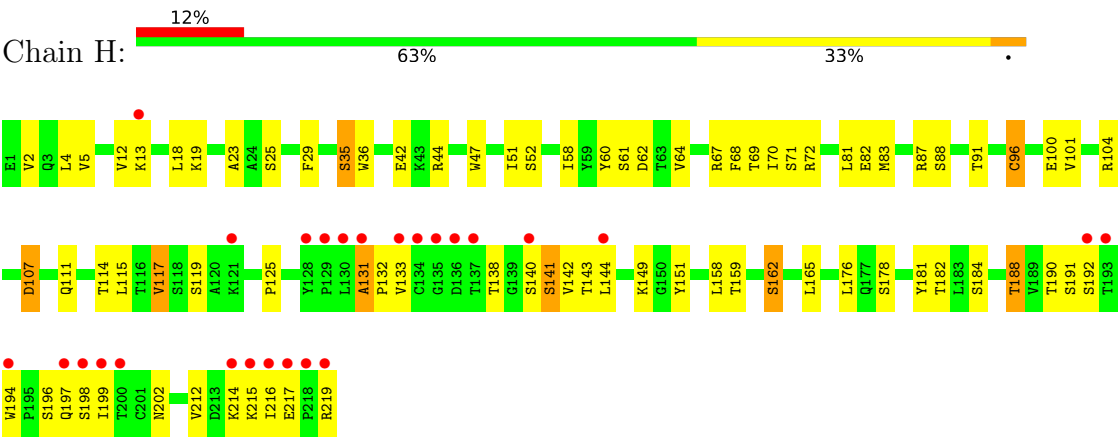
#### • Molecule 1: Sodium-dependent dopamine transporter



#### • 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, $\alpha$ , $\beta$ , $\gamma$	98.01Å 135.03Å 162.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 2.75 47.42 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.42-2.75) 99.6 (47.42-2.75)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20rc4_4425	Depositor
R, $R_{free}$	0.248 , 0.295 0.246 , 0.289	Depositor DCC
$R_{free}$ test set	2846 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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, 9BC, Y01, CLR, CL

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	0.29	0/4362	0.50	0/5963
2	L	0.29	0/1661	0.55	0/2259
3	H	0.30	0/1683	0.62	1/2294 (0.0%)
All	All	0.29	0/7706	0.54	1/10516 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	131	ALA	CB-CA-C	10.40	125.70	110.10

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	4221	0	4137	112	0
2	L	1623	0	1526	42	0
3	H	1644	0	1591	54	0
4	A	26	0	0	0	0
5	A	28	0	46	3	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	35	0	48	2	0
9	A	15	0	0	0	0
9	H	6	0	0	0	0
9	L	7	0	0	0	0
All	All	7608	0	7348	205	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 (205) 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:119:PHE:HD2	3:H:131:ALA:O	1.47	0.98
2:L:119:PHE:CD2	3:H:131:ALA:O	2.32	0.82
3:H:36:TRP:HD1	3:H:70:ILE:HD12	1.45	0.81
1:A:290:PHE:HE2	1:A:294:GLN:HE21	1.25	0.81
1:A:574:VAL:HG13	1:A:578:LYS:HE2	1.64	0.79
1:A:582:THR:HG21	1:A:593:LEU:HD21	1.68	0.76
1:A:279:LEU:HG	1:A:409:ILE:HD11	1.68	0.74
1:A:143:LEU:H	1:A:143:LEU:HD12	1.53	0.73
3:H:162:SER:H	3:H:202:ASN:HD21	1.35	0.73
1:A:277:LEU:HB2	5:A:702:CLR:H271	1.73	0.71
3:H:4:LEU:HD23	3:H:96:CYS:SG	2.31	0.70
1:A:250:CYS:HB2	1:A:452:PHE:HE2	1.58	0.67
1:A:437:PHE:HB2	1:A:440:ILE:HG22	1.76	0.67
1:A:513:PHE:HB3	3:H:101:VAL:HG23	1.78	0.66
1:A:397:ILE:HG21	1:A:407:ALA:HB2	1.78	0.65
1:A:485:VAL:HG23	1:A:568:VAL:HG21	1.78	0.65
2:L:196:GLU:HG2	2:L:207:VAL:HG12	1.76	0.65
1:A:500:THR:HG23	1:A:524:ARG:HH21	1.61	0.65
2:L:198:THR:HG22	2:L:205:PRO:HB3	1.79	0.64
1:A:588:GLN:O	1:A:592:ILE:HD13	1.98	0.63
3:H:5:VAL:HG22	3:H:23:ALA:HB3	1.80	0.62
1:A:487:VAL:HA	1:A:490:GLU:HB2	1.80	0.62
2:L:3:VAL:HG12	2:L:26:SER:HB3	1.82	0.62
1:A:508:ARG:NE	3:H:100:GLU:O	2.32	0.62
2:L:109:ARG:NH1	2:L:110:ALA:O	2.30	0.62
1:A:426:VAL:O	1:A:429:ILE:N	2.32	0.62
3:H:101:VAL:HG13	3:H:104:ARG:HB2	1.81	0.61
3:H:42:GLU:N	3:H:42:GLU:OE1	2.34	0.61
3:H:62:ASP:OD2	3:H:62:ASP:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:137:LEU:HD23	2:L:145:ILE:HG21	1.83	0.61
2:L:186:GLU:HA	2:L:189:ARG:HE	1.66	0.61
1:A:63:GLY:HA2	1:A:66:LEU:HD12	1.81	0.60
3:H:51:ILE:HD12	3:H:58:ILE:HD11	1.82	0.60
1:A:579:LEU:O	1:A:582:THR:HG23	2.02	0.59
1:A:311:ALA:O	1:A:315:THR:HG22	2.02	0.59
2:L:184:LYS:NZ	2:L:188:GLU:OE2	2.31	0.59
2:L:187:TYR:O	2:L:193:TYR:OH	2.21	0.59
1:A:35:ASP:O	1:A:39:SER:OG	2.20	0.59
2:L:116:VAL:HG13	2:L:208:LYS:HG3	1.83	0.58
2:L:14:SER:HB3	2:L:108:LYS:HG2	1.85	0.58
3:H:133:VAL:HG22	3:H:133:VAL:O	2.03	0.58
3:H:197:GLN:OE1	3:H:198:SER:N	2.36	0.58
2:L:150:LYS:HA	2:L:155:GLU:HA	1.86	0.58
3:H:67:ARG:HE	3:H:87:ARG:HH21	1.50	0.58
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.86	0.57
1:A:249:ILE:O	1:A:253:SER:OG	2.21	0.57
1:A:308:GLU:N	1:A:308:GLU:OE2	2.38	0.57
3:H:132:PRO:O	3:H:219:ARG:HD2	2.04	0.57
1:A:250:CYS:HB2	1:A:452:PHE:CE2	2.39	0.57
2:L:150:LYS:HB2	2:L:194:THR:OG1	2.05	0.57
1:A:282:ARG:HD2	1:A:406:TRP:CE2	2.40	0.57
3:H:149:LYS:HA	3:H:182:THR:HG23	1.87	0.57
1:A:245:ILE:O	1:A:249:ILE:HG13	2.04	0.56
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.86	0.56
1:A:118:PHE:HZ	1:A:454:LEU:HD23	1.71	0.56
1:A:39:SER:HA	1:A:265:VAL:HG21	1.86	0.55
1:A:522:CYS:HA	1:A:526:VAL:HG22	1.88	0.55
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.41	0.55
2:L:213:ASN:O	2:L:214:GLU:C	2.45	0.55
3:H:88:SER:O	3:H:91:THR:HG22	2.07	0.55
1:A:27:ARG:NH1	1:A:92:ARG:O	2.40	0.55
1:A:570:MET:HA	1:A:573:ALA:HB3	1.87	0.55
1:A:445:GLU:OE2	1:A:445:GLU:N	2.28	0.54
1:A:253:SER:HB3	1:A:264:VAL:HG21	1.88	0.54
2:L:104:LYS:NZ	2:L:166:ASP:OD2	2.40	0.54
1:A:579:LEU:O	1:A:589:ARG:HD2	2.08	0.53
2:L:213:ASN:C	2:L:214:GLU:HG2	2.28	0.53
3:H:18:LEU:HD23	3:H:115:LEU:HD12	1.90	0.53
1:A:83:MET:SD	1:A:494:VAL:HG11	2.47	0.53
3:H:29:PHE:O	3:H:72:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:162:SER:N	3:H:202:ASN:HD21	2.05	0.53
1:A:93:LYS:HE3	1:A:101:ARG:NH2	2.23	0.53
1:A:206:GLU:O	1:A:209:GLN:NE2	2.32	0.53
1:A:427:GLU:O	1:A:431:THR:HG23	2.09	0.53
1:A:276:LEU:HD22	1:A:362:VAL:HG11	1.91	0.52
1:A:507:ILE:HD11	1:A:515:PRO:HG3	1.90	0.52
3:H:141:SER:HA	3:H:190:THR:HA	1.91	0.52
3:H:199:ILE:HG22	3:H:216:ILE:HD13	1.91	0.52
2:L:143:LYS:HD2	2:L:174:TYR:CE1	2.45	0.52
1:A:69:TYR:HA	1:A:313:ALA:HB1	1.91	0.52
2:L:8:PRO:HG2	2:L:11:MET:HB2	1.92	0.52
1:A:387:GLY:O	1:A:391:VAL:HG22	2.10	0.52
1:A:123:TYR:O	1:A:126:VAL:HG12	2.10	0.51
1:A:580:LEU:HD12	1:A:581:SER:N	2.25	0.51
1:A:596:PRO:HD2	1:A:599:ASP:HB2	1.93	0.51
1:A:251:TYR:CE1	1:A:448:VAL:HG13	2.45	0.51
1:A:99:TRP:CZ2	1:A:490:GLU:HG2	2.46	0.51
1:A:156:ASN:HB3	1:A:208:PHE:HA	1.93	0.50
2:L:67:GLY:HA3	2:L:72:TYR:HA	1.94	0.50
1:A:569:VAL:O	1:A:572:PRO:HD2	2.12	0.50
1:A:437:PHE:HB2	1:A:440:ILE:CG2	2.40	0.50
1:A:536:VAL:O	1:A:540:ILE:HG23	2.12	0.49
3:H:36:TRP:CD1	3:H:70:ILE:HD12	2.36	0.49
2:L:121:PRO:HD3	2:L:133:VAL:HG12	1.94	0.49
3:H:19:LYS:HG3	3:H:82:GLU:CB	2.43	0.49
1:A:396:ALA:O	1:A:400:MET:HG2	2.13	0.49
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.47	0.49
1:A:489:PHE:HA	1:A:492:ILE:HD11	1.94	0.49
2:L:91:GLN:OE1	2:L:93:SER:N	2.42	0.48
3:H:83:MET:HE1	3:H:115:LEU:HD13	1.96	0.48
2:L:186:GLU:HA	2:L:189:ARG:NE	2.28	0.48
1:A:388:LEU:HA	1:A:392:VAL:HG13	1.96	0.48
3:H:13:LYS:HD3	3:H:119:SER:HA	1.96	0.48
3:H:144:LEU:HD12	3:H:199:ILE:HG21	1.96	0.48
1:A:73:LEU:HA	1:A:317:VAL:HG11	1.96	0.48
3:H:58:ILE:HD12	3:H:70:ILE:HG23	1.97	0.47
1:A:251:TYR:OH	1:A:449:ALA:HB2	2.14	0.47
3:H:215:LYS:HD3	3:H:217:GLU:OE1	2.15	0.47
1:A:591:THR:HA	1:A:594:THR:HB	1.96	0.47
2:L:210:PHE:HB2	3:H:133:VAL:HG21	1.95	0.47
3:H:143:THR:HG22	3:H:188:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ALA:HA	1:A:51:TRP:CD1	2.50	0.47
1:A:59:LYS:O	1:A:59:LYS:HG2	2.14	0.47
1:A:353:SER:HB3	8:A:706:Y01:HAB1	1.97	0.47
3:H:35:SER:HG	3:H:47:TRP:HE1	1.61	0.47
3:H:88:SER:HA	3:H:117:VAL:HG22	1.96	0.47
2:L:14:SER:HB3	2:L:108:LYS:CG	2.45	0.47
1:A:521:VAL:HG23	1:A:525:PHE:HD2	1.79	0.46
1:A:457:VAL:O	1:A:460:LEU:HD12	2.15	0.46
1:A:525:PHE:O	1:A:529:ILE:HG12	2.15	0.46
1:A:487:VAL:HG12	1:A:531:LEU:HD11	1.97	0.46
3:H:60:TYR:OH	3:H:69:THR:HA	2.15	0.46
3:H:67:ARG:CZ	3:H:87:ARG:HE	2.28	0.46
1:A:440:ILE:HD11	1:A:447:PHE:CE2	2.51	0.46
1:A:123:TYR:HB3	1:A:474:LEU:HD23	1.98	0.46
2:L:126:LEU:HB3	2:L:184:LYS:HD2	1.97	0.46
3:H:158:LEU:HD23	3:H:159:THR:N	2.30	0.46
1:A:52:ARG:CZ	1:A:56:LEU:HD11	2.46	0.45
1:A:579:LEU:HD11	1:A:590:PHE:HE1	1.81	0.45
1:A:292:GLY:HA3	1:A:364:PHE:O	2.16	0.45
5:A:702:CLR:H162	5:A:702:CLR:H221	1.56	0.45
1:A:41:ILE:HG13	1:A:348:THR:HG22	1.96	0.45
1:A:219:TYR:HD2	1:A:220:ILE:HD12	1.82	0.45
1:A:531:LEU:HD23	1:A:531:LEU:HA	1.85	0.45
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.52	0.45
1:A:582:THR:O	1:A:589:ARG:NH1	2.37	0.45
1:A:52:ARG:HG3	1:A:56:LEU:HD13	1.99	0.45
8:A:706:Y01:HAE2	8:A:706:Y01:HBB	1.74	0.45
1:A:93:LYS:HD2	1:A:97:THR:HG21	1.99	0.45
2:L:135:CYS:HB2	2:L:149:TRP:CZ2	2.52	0.45
3:H:68:PHE:CE1	3:H:83:MET:HB3	2.52	0.45
1:A:311:ALA:HB1	1:A:537:TYR:CD1	2.52	0.45
1:A:110:GLY:O	1:A:114:VAL:HG22	2.17	0.44
2:L:36:TRP:HB2	2:L:49:ILE:HB	1.98	0.44
3:H:194:TRP:HA	3:H:196:SER:H	1.82	0.44
1:A:363:ILE:HD12	1:A:388:LEU:HD21	2.00	0.44
2:L:13:THR:O	2:L:108:LYS:N	2.41	0.44
2:L:151:ILE:N	2:L:154:SER:O	2.50	0.44
1:A:96:ILE:HG13	1:A:432:ALA:HB1	1.99	0.44
1:A:517:ARG:O	1:A:521:VAL:HG12	2.18	0.44
1:A:52:ARG:HG2	1:A:316:GLN:OE1	2.18	0.44
1:A:143:LEU:O	1:A:146:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:HB1	1:A:309:VAL:HG11	1.99	0.44
1:A:421:SER:O	1:A:425:THR:HG23	2.18	0.44
2:L:190:HIS:O	2:L:212:ARG:NH1	2.50	0.44
3:H:19:LYS:HG3	3:H:82:GLU:HB3	1.98	0.44
1:A:53:PHE:CD2	1:A:356:SER:HB3	2.53	0.44
1:A:526:VAL:O	1:A:530:PHE:HB3	2.17	0.44
2:L:120:PRO:HB3	2:L:210:PHE:CZ	2.53	0.44
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.84	0.43
1:A:274:ALA:O	1:A:278:ILE:HG23	2.18	0.43
1:A:507:ILE:O	1:A:511:ILE:HG12	2.19	0.43
3:H:178:SER:O	3:H:178:SER:OG	2.29	0.43
1:A:122:PHE:CD1	1:A:458:VAL:HG11	2.54	0.43
3:H:67:ARG:NH2	3:H:87:ARG:HE	2.16	0.43
2:L:126:LEU:HD12	2:L:126:LEU:H	1.84	0.43
1:A:492:ILE:HG22	1:A:496:TRP:CD1	2.53	0.43
2:L:89:CYS:O	2:L:100:GLY:N	2.52	0.43
3:H:104:ARG:NH1	3:H:107:ASP:OD2	2.51	0.43
2:L:151:ILE:HG12	2:L:156:ARG:HB3	2.00	0.42
3:H:140:SER:O	3:H:191:SER:N	2.51	0.42
3:H:36:TRP:CD1	3:H:81:LEU:HB2	2.54	0.42
1:A:51:TRP:HH2	1:A:127:ILE:HD13	1.84	0.42
1:A:282:ARG:HB2	1:A:406:TRP:CH2	2.54	0.42
3:H:64:VAL:HG22	3:H:68:PHE:CG	2.55	0.42
2:L:48:TRP:CE2	2:L:59:VAL:HG13	2.54	0.42
3:H:61:SER:O	3:H:64:VAL:HG12	2.19	0.42
2:L:197:ALA:HB3	2:L:206:ILE:HG23	2.01	0.42
1:A:281:ILE:O	1:A:285:THR:HG23	2.20	0.42
3:H:12:VAL:O	3:H:117:VAL:HA	2.20	0.42
3:H:52:SER:O	3:H:72:ARG:NH1	2.52	0.42
1:A:43:TYR:HA	1:A:421:SER:HA	2.02	0.41
1:A:143:LEU:H	1:A:143:LEU:CD1	2.29	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.95	0.41
2:L:116:VAL:HA	2:L:136:PHE:O	2.20	0.41
1:A:33:LYS:NZ	1:A:344:ASP:OD2	2.52	0.41
1:A:332:ALA:O	1:A:335:ASN:HB2	2.21	0.41
1:A:403:SER:OG	1:A:404:THR:N	2.53	0.41
3:H:176:LEU:HB2	3:H:181:TYR:CE1	2.54	0.41
1:A:61:GLY:HA2	1:A:300:ASN:HB3	2.02	0.41
1:A:242:CYS:O	1:A:246:VAL:HG13	2.21	0.41
1:A:488:PHE:O	1:A:492:ILE:HG13	2.20	0.41
1:A:445:GLU:H	1:A:445:GLU:CD	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:121:PRO:HB2	2:L:126:LEU:HD11	2.02	0.41
1:A:318:PHE:HB2	1:A:530:PHE:HZ	1.86	0.41
1:A:524:ARG:HE	1:A:524:ARG:HB2	1.72	0.41
5:A:702:CLR:H121	5:A:702:CLR:H212	2.03	0.41
3:H:36:TRP:NE1	3:H:81:LEU:HB2	2.36	0.41
3:H:165:LEU:HD12	3:H:165:LEU:HA	1.86	0.41
1:A:263:LYS:O	1:A:266:TRP:HB2	2.20	0.40
2:L:109:ARG:HG2	2:L:110:ALA:N	2.36	0.40
1:A:107:LYS:HD3	1:A:578:LYS:HE3	2.03	0.40
2:L:120:PRO:HG2	3:H:219:ARG:CZ	2.52	0.40
1:A:81:PHE:CD1	1:A:321:LEU:HD22	2.57	0.40
1:A:527:ALA:HB3	1:A:528:PRO:HD3	2.03	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	534/536 (100%)	508 (95%)	26 (5%)	0	100	100
2	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
3	H	217/219 (99%)	197 (91%)	20 (9%)	0	100	100
All	All	963/969 (99%)	905 (94%)	58 (6%)	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	432/441 (98%)	397 (92%)	35 (8%)	11	21
2	L	183/187 (98%)	158 (86%)	25 (14%)	3	5
3	H	182/187 (97%)	163 (90%)	19 (10%)	7	11
All	All	797/815 (98%)	718 (90%)	79 (10%)	8	13

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	51	TRP
1	A	52	ARG
1	A	113	VAL
1	A	141	ASN
1	A	150	ASN
1	A	204	HIS
1	A	226	SER
1	A	238	ASP
1	A	239	MET
1	A	255	TRP
1	A	259	SER
1	A	261	SER
1	A	278	ILE
1	A	281	ILE
1	A	282	ARG
1	A	366	VAL
1	A	388	LEU
1	A	400	MET
1	A	404	THR
1	A	409	ILE
1	A	420	ASP
1	A	431	THR
1	A	443	ASN
1	A	451	LEU
1	A	458	VAL
1	A	482	SER
1	A	501	ASN
1	A	540	ILE
1	A	554	SER
1	A	577	PHE

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Mol	Chain	Res	Type
1	A	579	LEU
1	A	582	THR
1	A	590	PHE
1	A	601	GLN
2	L	5	THR
2	L	7	SER
2	L	28	SER
2	L	31	SER
2	L	41	SER
2	L	51	SER
2	L	55	LEU
2	L	71	SER
2	L	91	GLN
2	L	92	PHE
2	L	93	SER
2	L	101	SER
2	L	115	THR
2	L	124	GLU
2	L	128	SER
2	L	132	SER
2	L	135	CYS
2	L	156	ARG
2	L	176	MET
2	L	177	SER
2	L	188	GLU
2	L	189	ARG
2	L	198	THR
2	L	207	VAL
2	L	210	PHE
3	H	2	VAL
3	H	25	SER
3	H	35	SER
3	H	44	ARG
3	H	71	SER
3	H	96	CYS
3	H	107	ASP
3	H	111	GLN
3	H	114	THR
3	H	117	VAL
3	H	138	THR
3	H	141	SER
3	H	142	VAL

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Mol	Chain	Res	Type
3	H	162	SER
3	H	184	SER
3	H	188	THR
3	H	192	SER
3	H	212	VAL
3	H	214	LYS

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

Mol	Chain	Res	Type
3	H	161	ASN

### 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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
5	CLR	A	702	-	31,31,31	3.56	14 (45%)	48,48,48	1.88	16 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	Y01	A	706	-	38,38,38	4.37	21 (55%)	57,57,57	1.98	15 (26%)
4	9BC	A	701	6	28,28,28	4.04	8 (28%)	33,36,36	1.84	4 (12%)

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
5	CLR	A	702	-	-	9/10/68/68	0/4/4/4
8	Y01	A	706	-	-	13/19/77/77	0/4/4/4
4	9BC	A	701	6	-	7/19/29/29	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	9BC	C4-N3	15.80	1.61	1.46
8	A	706	Y01	CAS-CBF	-10.02	1.37	1.53
8	A	706	Y01	CBH-CAZ	-9.64	1.33	1.52
5	A	702	CLR	C11-C9	8.61	1.68	1.53
5	A	702	CLR	C12-C11	8.14	1.70	1.53
8	A	706	Y01	CAK-CAI	-8.14	1.32	1.50
8	A	706	Y01	CAV-CAZ	7.87	1.68	1.51
8	A	706	Y01	CBD-CBG	-7.72	1.38	1.53
8	A	706	Y01	CAI-CAZ	-7.66	1.16	1.33
8	A	706	Y01	CAK-CBD	7.58	1.66	1.53
4	A	701	9BC	C6-C5	7.35	1.55	1.34
4	A	701	9BC	C2-C1	7.16	1.64	1.51
5	A	702	CLR	C12-C13	-6.86	1.41	1.54
8	A	706	Y01	CAU-CBI	6.21	1.65	1.54
8	A	706	Y01	CBH-CBF	5.79	1.65	1.56
4	A	701	9BC	C2-N3	-5.63	1.31	1.46
5	A	702	CLR	C1-C2	5.25	1.64	1.53
5	A	702	CLR	C6-C5	-5.16	1.21	1.33
5	A	702	CLR	C16-C15	5.15	1.68	1.54
8	A	706	Y01	CAU-CAS	5.14	1.64	1.53
8	A	706	Y01	CBI-CBE	-4.55	1.46	1.55
5	A	702	CLR	C7-C6	-4.54	1.40	1.50
5	A	702	CLR	C10-C9	-4.45	1.48	1.56
8	A	706	Y01	CAV-CBC	4.44	1.62	1.52
5	A	702	CLR	C8-C14	-4.25	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	9BC	C15-C14	4.11	1.55	1.49
4	A	701	9BC	C4-C5	-3.88	1.44	1.50
4	A	701	9BC	C1-C6	-3.71	1.40	1.50
8	A	706	Y01	CBD-CBF	3.64	1.60	1.53
5	A	702	CLR	C13-C14	-3.53	1.48	1.55
8	A	706	Y01	OAW-CBC	-3.44	1.38	1.46
4	A	701	9BC	C21-C14	3.34	1.54	1.49
8	A	706	Y01	CAT-CAR	-3.03	1.47	1.53
8	A	706	Y01	CAQ-CAP	3.00	1.62	1.54
5	A	702	CLR	C1-C10	3.00	1.59	1.54
5	A	702	CLR	C2-C3	2.93	1.58	1.51
8	A	706	Y01	CAP-CBE	2.90	1.60	1.54
8	A	706	Y01	OAW-CAY	2.89	1.42	1.34
5	A	702	CLR	C8-C9	2.79	1.58	1.53
5	A	702	CLR	C15-C14	2.76	1.60	1.54
8	A	706	Y01	CAL-CAX	2.72	1.56	1.50
8	A	706	Y01	CAQ-CBG	2.15	1.58	1.54
8	A	706	Y01	OAF-CAX	2.15	1.29	1.22

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	9BC	C11-O12-N13	8.12	115.30	108.36
8	A	706	Y01	CAV-CAZ-CAI	-5.91	112.09	120.61
8	A	706	Y01	CBH-CBF-CBD	-4.87	105.44	112.73
8	A	706	Y01	CAK-CAI-CAZ	4.67	133.68	125.06
5	A	702	CLR	C13-C17-C20	-4.27	112.80	119.49
8	A	706	Y01	CAV-CAZ-CBH	4.15	121.93	116.42
5	A	702	CLR	C15-C14-C8	-4.10	112.33	119.08
8	A	706	Y01	CBI-CBE-CBB	-4.08	113.10	119.49
4	A	701	9BC	C5-C4-N3	3.97	116.21	110.80
8	A	706	Y01	OAW-CAY-CAM	3.86	119.83	111.50
5	A	702	CLR	C17-C13-C14	3.70	104.45	100.07
8	A	706	Y01	CAS-CAU-CBI	-3.48	106.82	112.78
5	A	702	CLR	C12-C13-C17	-3.47	111.38	116.57
5	A	702	CLR	C3-C4-C5	-3.34	106.36	112.03
4	A	701	9BC	C4-N3-C2	3.06	113.91	109.95
8	A	706	Y01	CAC-CBB-CBE	-3.02	108.30	112.92
5	A	702	CLR	C11-C9-C8	-3.01	107.42	111.75
8	A	706	Y01	CAK-CBD-CBF	-2.97	106.11	109.71
8	A	706	Y01	CBI-CBG-CBD	-2.76	110.30	114.38
8	A	706	Y01	CAP-CAQ-CBG	-2.75	99.69	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	CLR	C10-C9-C8	-2.73	108.64	112.73
5	A	702	CLR	C12-C11-C9	-2.61	108.59	113.11
5	A	702	CLR	C4-C5-C6	-2.60	116.86	120.61
5	A	702	CLR	C16-C15-C14	-2.51	100.15	105.13
5	A	702	CLR	C4-C5-C10	2.47	119.70	116.42
5	A	702	CLR	C1-C10-C5	2.44	113.21	108.75
5	A	702	CLR	C19-C10-C9	-2.40	108.81	111.68
8	A	706	Y01	CAQ-CBG-CBD	-2.38	115.16	119.08
5	A	702	CLR	C12-C13-C14	2.31	110.85	107.27
4	A	701	9BC	C1-C6-C5	-2.28	116.99	123.27
8	A	706	Y01	CAD-CBH-CBF	-2.12	109.15	111.68
5	A	702	CLR	C2-C3-C4	-2.12	107.40	110.31
5	A	702	CLR	C7-C8-C9	-2.09	107.18	109.71
8	A	706	Y01	OAH-CAX-CAL	2.03	120.56	114.03
8	A	706	Y01	CBH-CAZ-CAI	2.00	125.97	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	9BC	N3-C10-C11-O12
8	A	706	Y01	CAC-CBB-CBE-CBI
8	A	706	Y01	OAG-CAY-OAW-CBC
8	A	706	Y01	CAM-CAY-OAW-CBC
8	A	706	Y01	CAJ-CAO-CBB-CAC
8	A	706	Y01	CAC-CBB-CBE-CAP
8	A	706	Y01	CAO-CBB-CBE-CBI
8	A	706	Y01	CAO-CBB-CBE-CAP
5	A	702	CLR	C21-C20-C22-C23
5	A	702	CLR	C17-C20-C22-C23
8	A	706	Y01	CAJ-CAO-CBB-CBE
8	A	706	Y01	CAX-CAL-CAM-CAY
5	A	702	CLR	C13-C17-C20-C21
5	A	702	CLR	C13-C17-C20-C22
5	A	702	CLR	C23-C24-C25-C26
8	A	706	Y01	CAJ-CAN-CBA-CAA
5	A	702	CLR	C16-C17-C20-C21
5	A	702	CLR	C22-C23-C24-C25
4	A	701	9BC	C11-C10-N3-C4
8	A	706	Y01	CAJ-CAN-CBA-CAB
5	A	702	CLR	C23-C24-C25-C27
5	A	702	CLR	C16-C17-C20-C22

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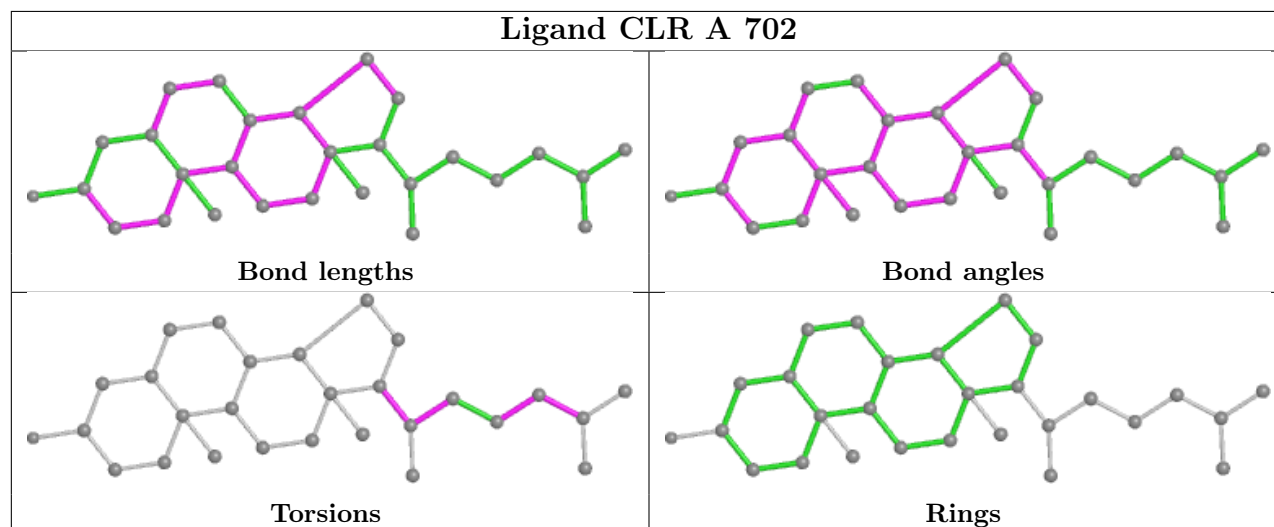
Mol	Chain	Res	Type	Atoms
4	A	701	9BC	C4-C5-C7-O08
4	A	701	9BC	C4-C5-C7-O9
4	A	701	9BC	C6-C5-C7-O08
4	A	701	9BC	C6-C5-C7-O9
4	A	701	9BC	C11-C10-N3-C2
8	A	706	Y01	CAM-CAL-CAX-OAH
8	A	706	Y01	CAM-CAL-CAX-OAF

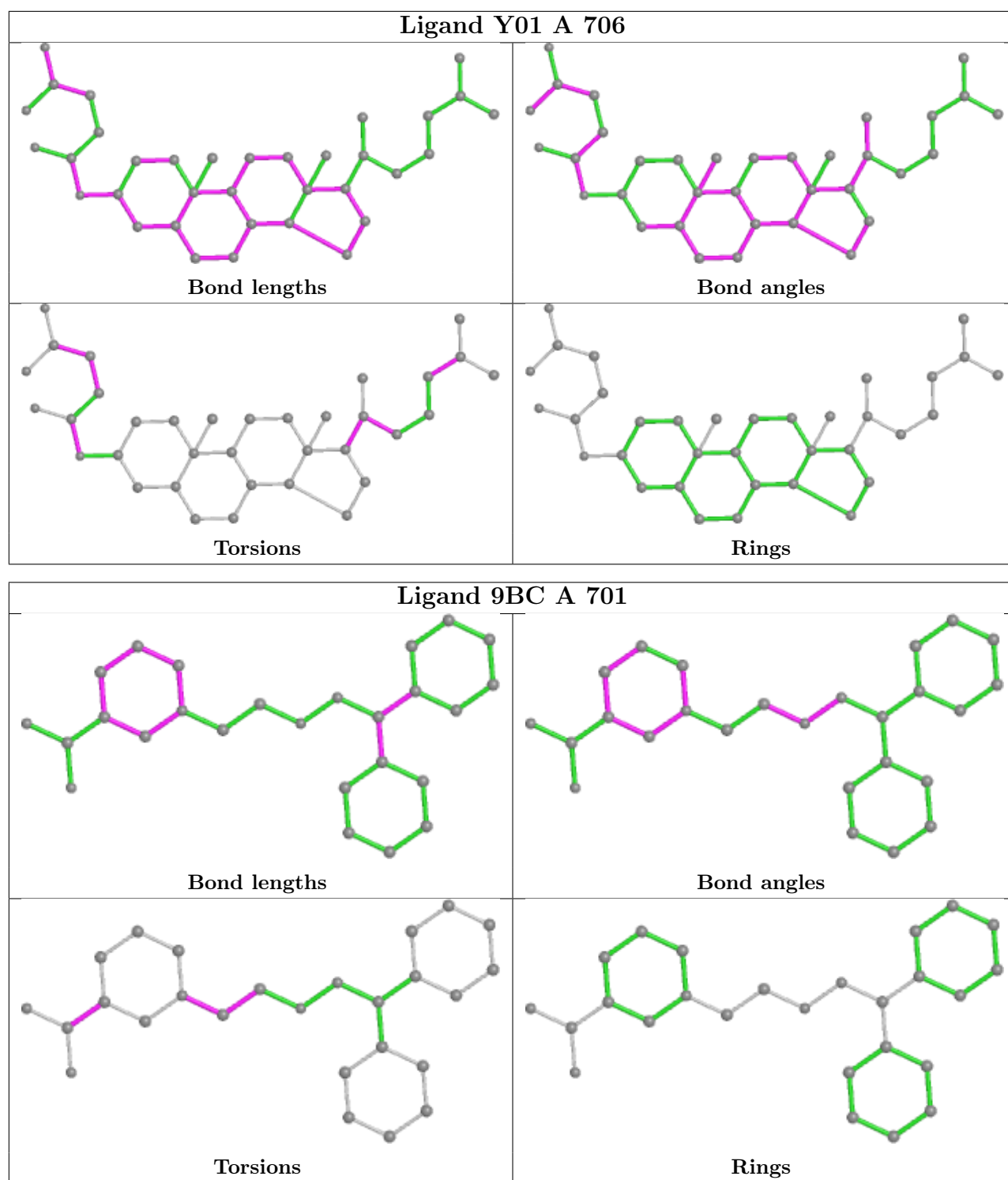
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	CLR	3	0
8	A	706	Y01	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

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	536/536 (100%)	0.53	31 (5%)	23 28	74, 96, 118, 144	0
2	L	214/214 (100%)	0.31	16 (7%)	14 17	63, 86, 118, 154	0
3	H	219/219 (100%)	0.37	26 (11%)	4 5	72, 92, 127, 149	0
All	All	969/969 (100%)	0.45	73 (7%)	14 17	63, 93, 120, 154	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	213	ASN	7.1
1	A	586	LEU	6.2
1	A	580	LEU	5.2
1	A	590	PHE	4.9
1	A	582	THR	4.9
1	A	581	SER	4.8
1	A	578	LYS	4.7
1	A	583	PRO	4.7
2	L	214	GLU	4.5
3	H	133	VAL	4.3
3	H	198	SER	4.1
3	H	219	ARG	4.0
1	A	237	TRP	3.9
3	H	193	THR	3.9
3	H	199	ILE	3.8
3	H	134	CYS	3.7
2	L	123	SER	3.7
3	H	131	ALA	3.6
1	A	525	PHE	3.4
2	L	58	GLY	3.3
1	A	496	TRP	3.3
2	L	94	GLY	3.2
1	A	227	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	524	ARG	3.1
3	H	216	ILE	3.1
1	A	448	VAL	3.0
3	H	197	GLN	3.0
2	L	127	THR	2.9
3	H	192	SER	2.9
3	H	13	LYS	2.9
1	A	290	PHE	2.8
3	H	136	ASP	2.8
2	L	129	GLY	2.8
2	L	122	SER	2.8
3	H	217	GLU	2.8
3	H	129	PRO	2.7
1	A	208	PHE	2.7
2	L	57	SER	2.6
3	H	214	LYS	2.6
3	H	130	LEU	2.6
1	A	555	TRP	2.6
1	A	238	ASP	2.6
1	A	497	ILE	2.5
3	H	140	SER	2.5
2	L	124	GLU	2.4
1	A	492	ILE	2.4
3	H	121	LYS	2.4
1	A	491	ALA	2.3
1	A	579	LEU	2.3
3	H	135	GLY	2.3
3	H	200	THR	2.3
1	A	526	VAL	2.3
2	L	95	TYR	2.3
3	H	128	TYR	2.3
3	H	194	TRP	2.2
1	A	130	TRP	2.2
3	H	144	LEU	2.2
1	A	495	SER	2.1
2	L	126	LEU	2.1
2	L	80	GLU	2.1
2	L	134	VAL	2.1
3	H	218	PRO	2.1
3	H	215	LYS	2.1
1	A	235	ILE	2.1
1	A	540	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	212	ARG	2.1
1	A	291	LEU	2.1
3	H	137	THR	2.1
1	A	244	LEU	2.0
2	L	29	VAL	2.0
1	A	397	ILE	2.0
1	A	350	PHE	2.0
1	A	232	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

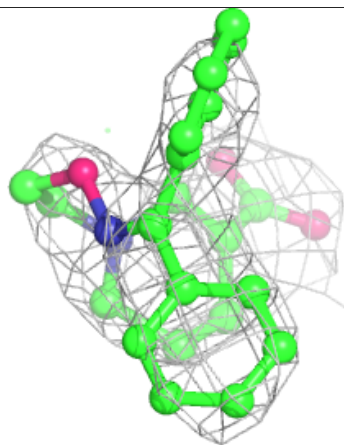
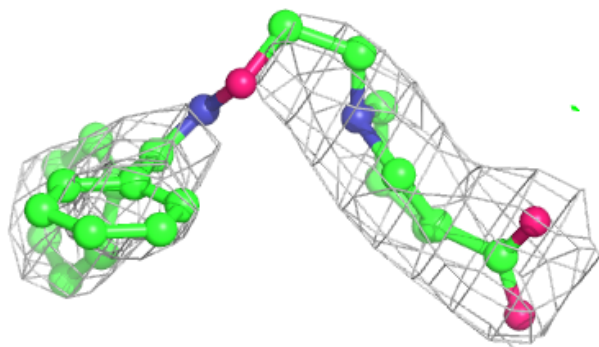
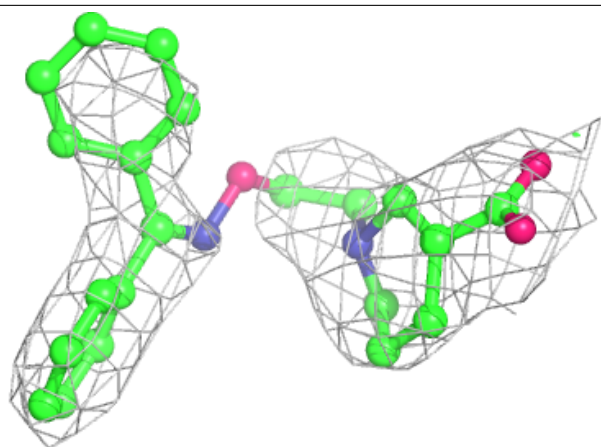
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NA	A	704	1/1	0.86	0.29	78,78,78,78	0
4	9BC	A	701	26/26	0.88	0.39	86,94,107,114	26
5	CLR	A	702	28/28	0.89	0.39	87,97,100,102	0
8	Y01	A	706	35/35	0.89	0.35	90,109,118,118	0
6	NA	A	703	1/1	0.94	0.29	88,88,88,88	0
7	CL	A	705	1/1	0.96	0.14	81,81,81,81	0

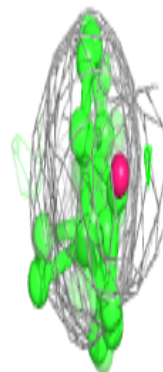
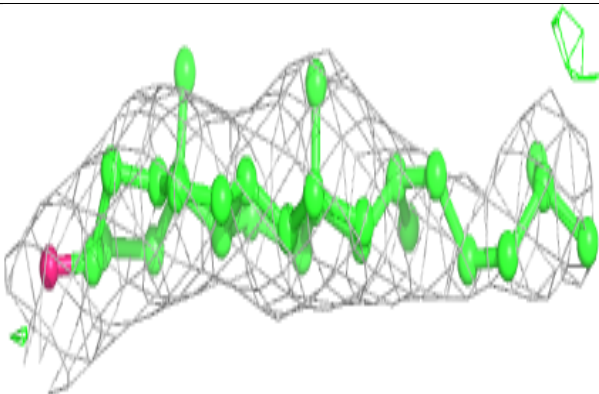
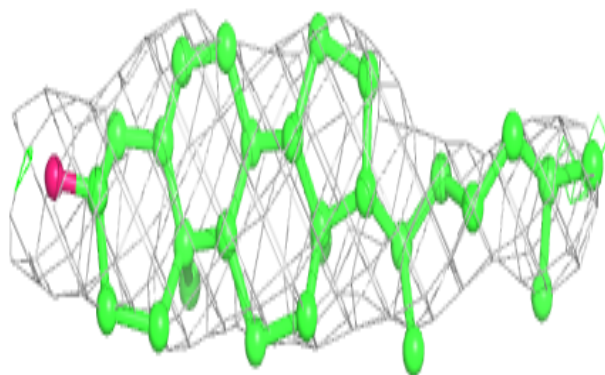
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 9BC 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)

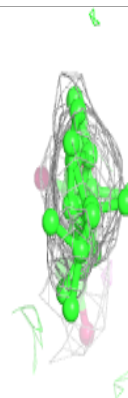
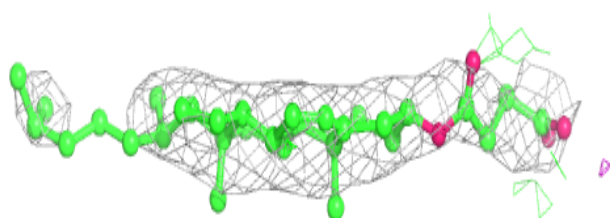
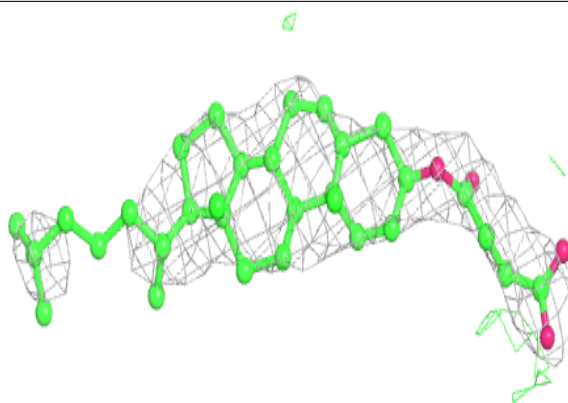
**Electron density around CLR A 702:**

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



**Electron density around Y01 A 706:**

$2mF_o - DF_c$  (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.