



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2022 – 06:05 PM JST

PDB ID : 7WLW  
Title : X-ray structure of thermostabilized *Drosophila* dopamine transporter with GABA transporter1-like substitutions in the binding site, in complex with SKF89976a  
Authors : Penmatsa, A.; Joseph, D.  
Deposited on : 2022-01-13  
Resolution : 2.90 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

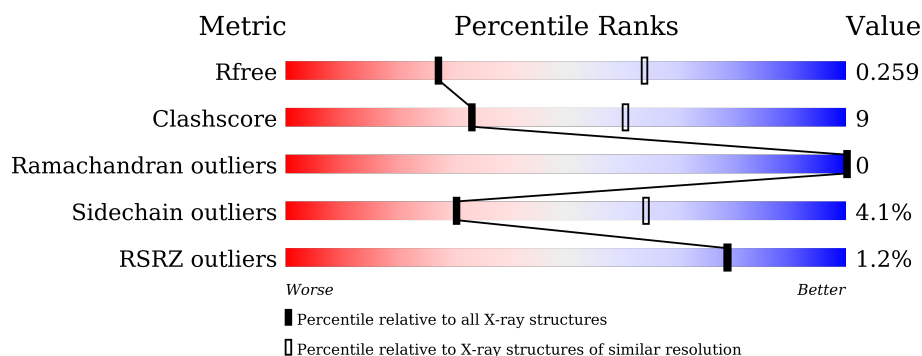
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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>76%</div> <div>23%</div> <div>.</div> </div>
2	L	214	<div> <div>3%</div> <div>79%</div> <div>21%</div> <div>.</div> </div>
3	H	219	<div> <div></div> <div>81%</div> <div>19%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7736 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	1	0
			4259	2854	664	723	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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	1	0
			1631	1013	268	342	8			

- Molecule 3 is a protein called Antibody Fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1658	1040	281	329	8			

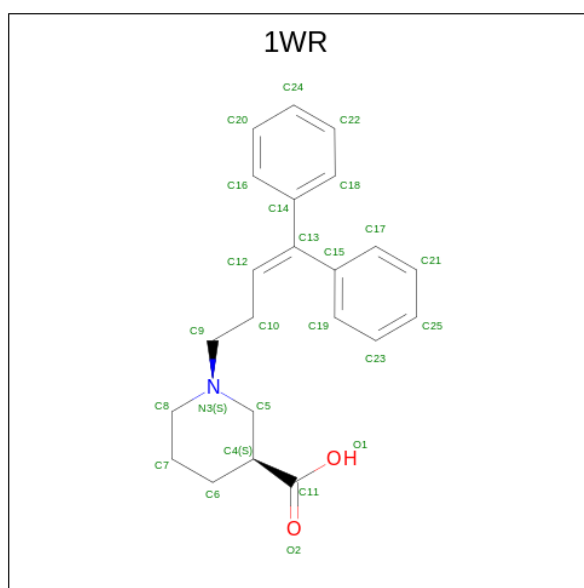
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

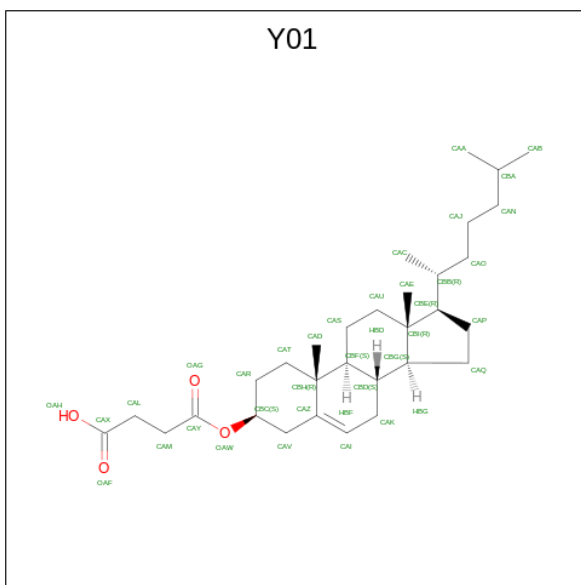
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is (3S)-1-(4,4-diphenylbut-3-enyl)piperidine-3-carboxylic acid (three-letter code: 1WR) (formula: C<sub>22</sub>H<sub>25</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



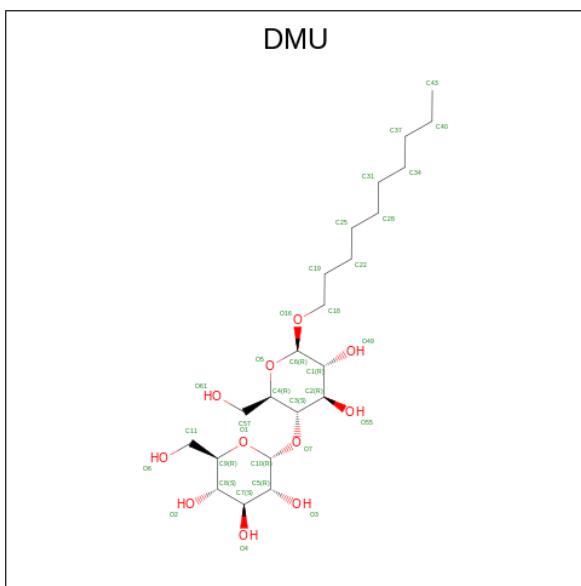
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			25	22	1	2		
6	A	1	Total	C	N	O	0	0
			25	22	1	2		

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



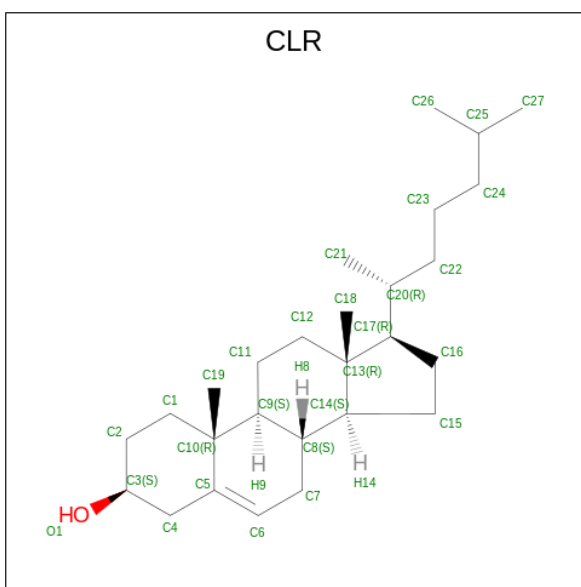
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			35	31	4		

- Molecule 8 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



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

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



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

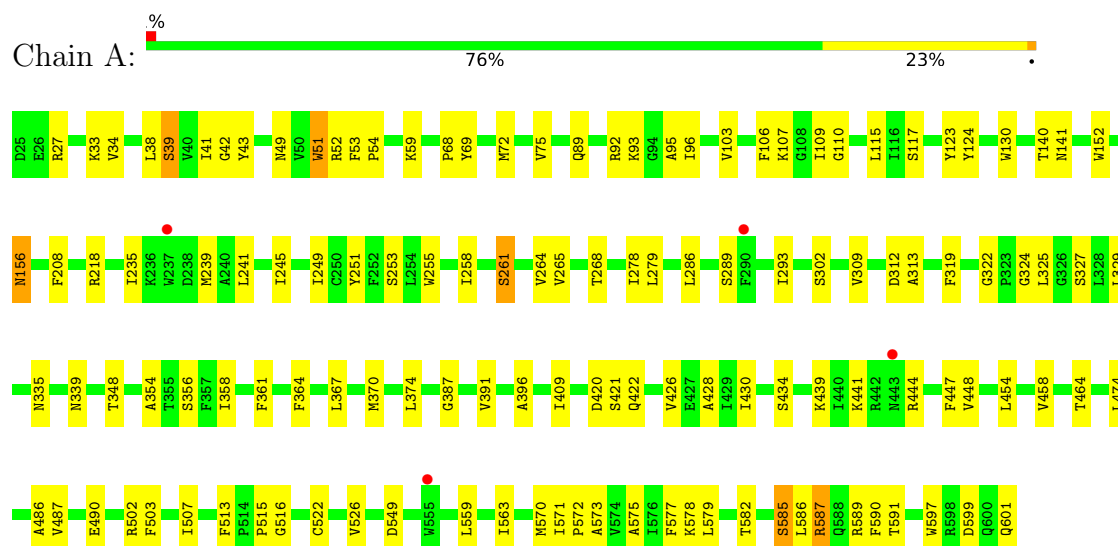
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	20	Total	O	0	0
			20	20		
10	L	9	Total	O	0	0
			9	9		
10	H	10	Total	O	0	0
			10	10		

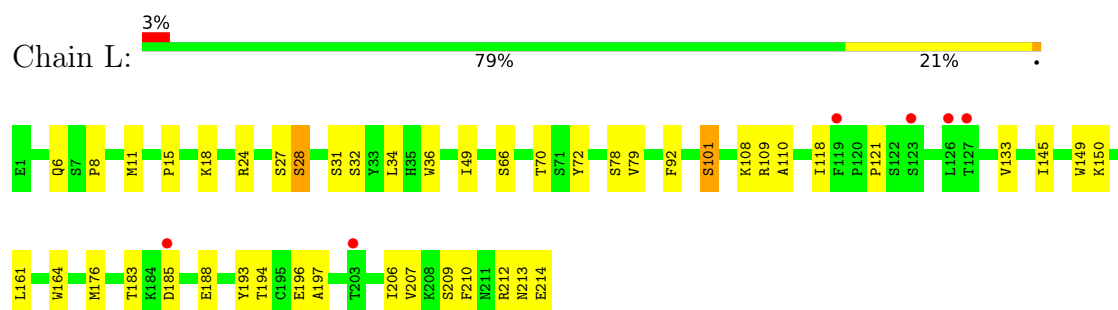
### 3 Residue-property plots

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.

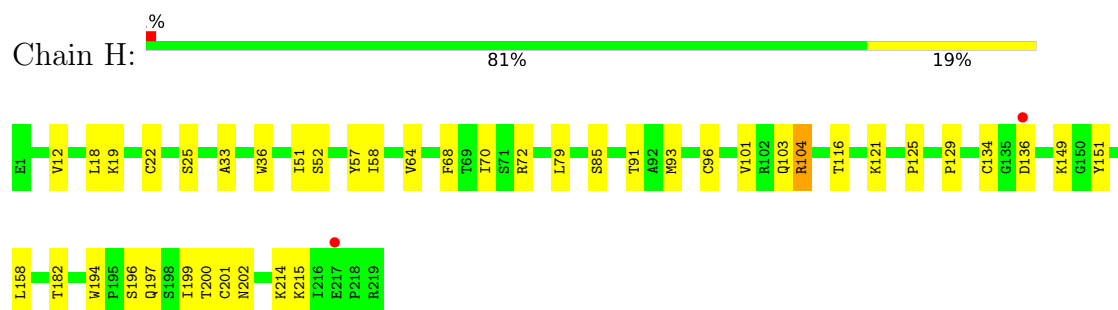
- Molecule 1: Sodium-dependent dopamine transporter



- Molecule 2: Antibody fragment light chain



- Molecule 3: Antibody Fragment heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.78Å 141.75Å 168.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.96 – 2.90 45.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.96-2.90) 99.5 (45.80-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20rc4_4425	Depositor
R, $R_{free}$	0.235 , 0.264 0.232 , 0.259	Depositor DCC
$R_{free}$ test set	2523 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.8	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: CL, 1WR, NA, Y01, CLR, DMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/4404	0.46	0/6015
2	L	0.26	0/1672	0.50	0/2273
3	H	0.27	0/1697	0.56	1/2311 (0.0%)
All	All	0.27	0/7773	0.50	1/10599 (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	33	ALA	CB-CA-C	7.67	121.61	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	4259	0	4205	80	0
2	L	1631	0	1539	24	0
3	H	1658	0	1619	26	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	50	0	0	2	0
7	A	35	0	49	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	33	0	42	4	0
9	A	28	0	46	0	0
10	A	20	0	0	1	0
10	H	10	0	0	2	0
10	L	9	0	0	1	0
All	All	7736	0	7500	131	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 9.

All (131) 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:194:THR:HG22	2:L:209:SER:HB2	1.64	0.79
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.67	0.75
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.75	0.67
2:L:213:ASN:OD1	2:L:214:GLU:N	2.28	0.67
1:A:258:ILE:HA	1:A:261:SER:HB3	1.77	0.66
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.77	0.66
3:H:51:ILE:HG13	3:H:58:ILE:HG12	1.79	0.64
1:A:245:ILE:HD11	8:A:707:DMU:H15	1.79	0.64
2:L:197:ALA:HB3	2:L:206:ILE:HG22	1.80	0.62
1:A:39:SER:HA	1:A:265:VAL:HG21	1.81	0.62
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.65	0.61
2:L:196:GLU:HG2	2:L:207:VAL:HG13	1.81	0.61
1:A:579:LEU:HD11	1:A:590:PHE:HE1	1.65	0.60
1:A:507:ILE:HD12	1:A:515:PRO:HG3	1.83	0.60
1:A:130:TRP:CD1	1:A:239:MET:HE1	2.37	0.60
1:A:582:THR:O	1:A:589:ARG:NE	2.35	0.59
3:H:36:TRP:HD1	3:H:70:ILE:HD12	1.68	0.59
1:A:309:VAL:HA	1:A:312:ASP:HB2	1.85	0.58
1:A:502:ARG:NH1	1:A:599:ASP:OD2	2.36	0.58
2:L:150:LYS:HB2	2:L:194:THR:OG1	2.04	0.57
3:H:129:PRO:HD3	3:H:214:LYS:HG2	1.87	0.56
2:L:121:PRO:HD3	2:L:133:VAL:HG22	1.88	0.56
1:A:235:ILE:CG1	1:A:464:THR:HG22	2.36	0.56
1:A:279:LEU:HG	1:A:409:ILE:HD11	1.88	0.55
3:H:101:VAL:HG11	3:H:104:ARG:HE	1.71	0.55
1:A:68:PRO:O	1:A:72:MET:HG2	2.07	0.55
1:A:152:TRP:O	1:A:218:ARG:HD3	2.07	0.55
1:A:43:TYR:HA	1:A:421:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:SER:HB3	1:A:264:VAL:HG21	1.92	0.52
1:A:444:ARG:O	1:A:447:PHE:N	2.43	0.52
3:H:200:THR:HG22	3:H:215:LYS:HB2	1.92	0.52
3:H:194:TRP:CD1	3:H:199:ILE:HD12	2.45	0.51
3:H:149:LYS:NZ	10:H:302:HOH:O	2.44	0.51
1:A:582:THR:HG23	1:A:589:ARG:HG2	1.93	0.50
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.46	0.50
1:A:59:LYS:NZ	1:A:312:ASP:OD2	2.41	0.50
1:A:103:VAL:HG12	1:A:106:PHE:H	1.77	0.50
1:A:597:TRP:O	1:A:601:GLN:HG2	2.12	0.50
3:H:51:ILE:HB	3:H:70:ILE:HG12	1.94	0.50
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.94	0.49
3:H:18:LEU:HD23	3:H:19:LYS:H	1.77	0.49
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.94	0.49
1:A:235:ILE:HG12	1:A:464:THR:HG22	1.94	0.49
1:A:387:GLY:O	1:A:391:VAL:HG22	2.12	0.49
2:L:161:LEU:HD13	3:H:182:THR:HB	1.95	0.49
1:A:42:GLY:C	1:A:420:ASP:HB3	2.33	0.48
1:A:454:LEU:O	1:A:458:VAL:HG12	2.13	0.48
1:A:426:VAL:O	1:A:430:ILE:HG13	2.14	0.48
1:A:503:PHE:O	1:A:507:ILE:HG13	2.13	0.48
1:A:370:MET:SD	1:A:396:ALA:HB2	2.53	0.48
3:H:91:THR:HG23	3:H:116:THR:HA	1.95	0.48
1:A:156:ASN:HB3	1:A:208:PHE:CD2	2.48	0.48
2:L:28:SER:HA	2:L:70:THR:HG22	1.96	0.48
2:L:188:GLU:HG2	2:L:212:ARG:NH1	2.29	0.48
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.95	0.47
3:H:18:LEU:HD23	3:H:19:LYS:N	2.29	0.47
1:A:587:ARG:O	1:A:591:THR:HG23	2.14	0.47
1:A:27:ARG:NH2	1:A:93:LYS:HA	2.28	0.47
1:A:123:TYR:HB3	1:A:474:LEU:HD12	1.96	0.47
1:A:486:ALA:O	1:A:490:GLU:HG3	2.15	0.47
1:A:249:ILE:O	1:A:253:SER:OG	2.28	0.47
3:H:101:VAL:HG12	3:H:103:GLN:H	1.81	0.46
3:H:12:VAL:CG2	3:H:18:LEU:HD12	2.46	0.46
8:A:707:DMU:H17	8:A:707:DMU:H23	1.61	0.46
2:L:8:PRO:HG2	2:L:11:MET:HB2	1.97	0.46
2:L:214:GLU:HB3	3:H:134:CYS:HB2	1.98	0.46
2:L:6:GLN:H	2:L:101:SER:HB3	1.80	0.46
1:A:319:PHE:HB2	6:A:705:1WR:C23	2.45	0.45
1:A:33:LYS:HE3	1:A:339:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HG12	1:A:464:THR:CG2	2.46	0.45
1:A:570:MET:HA	1:A:573:ALA:HB3	1.98	0.45
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.52	0.45
1:A:327:SER:HB3	1:A:428:ALA:HB2	1.98	0.45
1:A:516:GLY:HA3	7:A:706:Y01:OAH	2.16	0.45
1:A:107:LYS:HD2	1:A:578:LYS:HE2	1.99	0.45
1:A:422:GLN:HB3	10:A:816:HOH:O	2.17	0.45
3:H:51:ILE:HD13	3:H:72:ARG:CG	2.44	0.45
1:A:96:ILE:HG22	1:A:110:GLY:C	2.37	0.45
1:A:117:SER:HB3	1:A:325:LEU:HD11	1.98	0.45
2:L:15:PRO:HA	2:L:79:VAL:HG13	1.99	0.45
7:A:706:Y01:HAO1	7:A:706:Y01:HAP1	1.82	0.45
3:H:22:CYS:HB3	3:H:79:LEU:HB3	2.00	0.44
7:A:706:Y01:HAA1	7:A:706:Y01:HAJ2	1.72	0.44
1:A:89:GLN:HG3	1:A:335:ASN:HB2	2.00	0.44
2:L:6:GLN:HB3	10:L:301:HOH:O	2.17	0.44
2:L:133:VAL:HG12	2:L:149:TRP:CH2	2.53	0.44
1:A:95:ALA:HA	1:A:329:LEU:CD2	2.47	0.44
1:A:69:TYR:HA	1:A:313:ALA:HB1	2.00	0.44
1:A:96:ILE:HA	1:A:110:GLY:HA3	1.99	0.44
1:A:239:MET:HE3	1:A:239:MET:HB3	1.88	0.43
1:A:575:ALA:O	1:A:579:LEU:HB2	2.18	0.43
1:A:41:ILE:HG13	1:A:348:THR:HG22	2.00	0.43
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.87	0.43
1:A:571:ILE:HB	1:A:572:PRO:HD3	2.00	0.43
2:L:145:ILE:HG22	2:L:164:TRP:CZ2	2.52	0.43
1:A:559:LEU:O	1:A:563:ILE:HG13	2.19	0.43
3:H:194:TRP:HD1	3:H:199:ILE:HD12	1.82	0.43
2:L:15:PRO:HA	2:L:79:VAL:CG1	2.48	0.43
1:A:434:SER:O	1:A:441:LYS:HB2	2.18	0.43
1:A:278:ILE:HD11	1:A:409:ILE:HD13	2.00	0.42
1:A:585:SER:OG	1:A:586:LEU:N	2.51	0.42
2:L:109:ARG:HG2	2:L:110:ALA:N	2.35	0.42
3:H:196:SER:OG	3:H:197:GLN:N	2.51	0.42
1:A:324:GLY:HA3	1:A:487:VAL:HG22	2.02	0.42
8:A:707:DMU:O7	8:A:707:DMU:O61	2.35	0.42
2:L:118:ILE:HG12	2:L:210:PHE:HD1	1.84	0.42
3:H:52:SER:HB3	3:H:57:TYR:HB2	2.02	0.42
1:A:49:ASN:ND2	1:A:356:SER:OG	2.52	0.42
1:A:522:CYS:HA	1:A:526:VAL:HB	2.02	0.42
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.55	0.42
1:A:286:LEU:O	1:A:289:SER:HB2	2.20	0.42
2:L:36:TRP:HB2	2:L:49:ILE:HB	2.02	0.42
1:A:109:ILE:HG21	1:A:490:GLU:HG2	2.01	0.42
3:H:18:LEU:HD21	10:H:307:HOH:O	2.20	0.41
1:A:241:LEU:HD21	8:A:707:DMU:H14	2.01	0.41
1:A:265:VAL:HA	1:A:268:THR:OG1	2.20	0.41
2:L:183:THR:HG22	2:L:185:ASP:H	1.86	0.41
1:A:140:THR:OG1	1:A:141:ASN:N	2.53	0.41
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.86	0.41
1:A:370:MET:O	1:A:374:LEU:HB2	2.21	0.41
3:H:64:VAL:HG13	3:H:68:PHE:CG	2.55	0.41
1:A:95:ALA:HA	1:A:329:LEU:HD21	2.02	0.41
1:A:115:LEU:HD12	1:A:570:MET:HE1	2.03	0.41
1:A:354:ALA:O	1:A:358:ILE:HD13	2.21	0.41
1:A:322:GLY:HA2	6:A:704:1WR:C24	2.51	0.41
1:A:507:ILE:HB	1:A:515:PRO:HD3	2.03	0.40
3:H:158:LEU:HD21	3:H:201:CYS:HB2	2.02	0.40
1:A:241:LEU:O	1:A:245:ILE:HG13	2.21	0.40
1:A:34:VAL:HG12	1:A:38:LEU:HG	2.03	0.40
1:A:51:TRP:CD1	1:A:51:TRP:C	2.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	518 (97%)	17 (3%)	0	100	100
2	L	213/214 (100%)	205 (96%)	8 (4%)	0	100	100
3	H	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
All	All	965/969 (100%)	931 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	439/441 (100%)	426 (97%)	13 (3%)	41	75
2	L	186/187 (100%)	174 (94%)	12 (6%)	17	45
3	H	187/187 (100%)	179 (96%)	8 (4%)	29	62
All	All	812/815 (100%)	779 (96%)	33 (4%)	30	64

All (33) 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	124	TYR
1	A	156	ASN
1	A	255	TRP
1	A	261	SER
1	A	302	SER
1	A	439	LYS
1	A	549	ASP
1	A	577	PHE
1	A	585	SER
1	A	587	ARG
2	L	18	LYS
2	L	24	ARG
2	L	27	SER
2	L	28	SER
2	L	31	SER
2	L	32	SER
2	L	66	SER
2	L	78	SER
2	L	92	PHE
2	L	101	SER

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Mol	Chain	Res	Type
2	L	108	LYS
2	L	176	MET
3	H	25	SER
3	H	85	SER
3	H	93	MET
3	H	96	CYS
3	H	104	ARG
3	H	121	LYS
3	H	136	ASP
3	H	202	ASN

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

Mol	Chain	Res	Type
1	A	209	GLN
2	L	191	ASN
2	L	211	ASN
3	H	111	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	Y01	A	706	-	38,38,38	1.36	2 (5%)	57,57,57	1.53	9 (15%)
6	1WR	A	705	-	27,27,27	1.29	2 (7%)	33,35,35	1.13	2 (6%)
8	DMU	A	707	-	34,34,34	1.91	9 (26%)	45,45,45	0.97	3 (6%)
6	1WR	A	704	-	27,27,27	1.20	2 (7%)	33,35,35	1.79	6 (18%)
9	CLR	A	708	-	31,31,31	0.67	0	48,48,48	1.76	14 (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	Y01	A	706	-	-	5/19/77/77	0/4/4/4
6	1WR	A	705	-	-	3/18/28/28	0/3/3/3
8	DMU	A	707	-	-	15/19/59/59	0/2/2/2
6	1WR	A	704	-	-	7/18/28/28	0/3/3/3
9	CLR	A	708	-	-	2/10/68/68	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	706	Y01	OAF-CAX	6.11	1.42	1.22
8	A	707	DMU	O5-C4	4.97	1.56	1.44
8	A	707	DMU	O1-C9	4.94	1.56	1.44
6	A	705	1WR	C15-C13	4.09	1.55	1.49
6	A	704	1WR	C14-C13	3.93	1.55	1.49
6	A	705	1WR	C14-C13	3.48	1.54	1.49
8	A	707	DMU	O1-C10	3.14	1.49	1.41
6	A	704	1WR	C15-C13	3.13	1.53	1.49
8	A	707	DMU	C57-C4	-2.85	1.42	1.51
8	A	707	DMU	C11-C9	-2.73	1.42	1.51
8	A	707	DMU	O5-C6	2.49	1.48	1.41
8	A	707	DMU	O3-C5	2.19	1.48	1.43
7	A	706	Y01	OAW-CBC	-2.10	1.41	1.46
8	A	707	DMU	O49-C1	2.03	1.47	1.43
8	A	707	DMU	O55-C2	2.02	1.47	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	704	1WR	C15-C13-C12	-5.25	114.72	121.78
9	A	708	CLR	C19-C10-C9	-4.71	106.06	111.68
6	A	704	1WR	C4-C5-N3	-4.13	105.40	110.06
7	A	706	Y01	CBF-CBD-CBG	-3.90	103.86	109.09
7	A	706	Y01	CBC-OAW-CAY	3.87	127.32	117.79
6	A	704	1WR	C8-N3-C5	3.85	115.41	109.52
9	A	708	CLR	C2-C3-C4	-3.85	105.02	110.31
7	A	706	Y01	CAM-CAL-CAX	-3.65	105.76	113.60
9	A	708	CLR	C4-C5-C10	3.26	120.75	116.42
7	A	706	Y01	CAV-CAZ-CAI	-3.26	115.92	120.61
7	A	706	Y01	CBI-CBG-CBD	-3.05	109.86	114.38
9	A	708	CLR	C16-C17-C20	-2.93	107.61	112.15
8	A	707	DMU	O7-C3-C2	2.83	114.80	107.28
9	A	708	CLR	C15-C14-C13	-2.76	100.51	103.84
6	A	705	1WR	C15-C13-C12	-2.75	118.09	121.78
9	A	708	CLR	C15-C14-C8	-2.74	114.57	119.08
6	A	705	1WR	O1-C11-C4	2.70	121.26	114.21
9	A	708	CLR	C22-C20-C17	-2.69	104.72	110.28
6	A	704	1WR	C9-C10-C12	-2.65	107.21	111.12
9	A	708	CLR	C11-C12-C13	-2.64	108.25	112.78
6	A	704	1WR	C14-C13-C12	2.59	125.27	121.78
7	A	706	Y01	CAK-CBD-CBF	2.53	112.78	109.71
8	A	707	DMU	O5-C6-C1	2.45	115.54	110.35
6	A	704	1WR	C15-C13-C14	2.44	120.01	116.92
9	A	708	CLR	C11-C9-C8	-2.41	108.29	111.75
7	A	706	Y01	CAK-CBD-CBG	-2.31	107.56	110.91
9	A	708	CLR	C1-C10-C9	2.26	111.88	108.73
7	A	706	Y01	CBI-CBE-CBB	-2.21	116.03	119.49
8	A	707	DMU	C6-O5-C4	2.20	118.00	113.69
9	A	708	CLR	C10-C5-C6	-2.18	119.57	122.90
7	A	706	Y01	CAC-CBB-CBE	-2.09	109.71	112.92
9	A	708	CLR	C12-C11-C9	-2.09	109.49	113.11
9	A	708	CLR	C13-C14-C8	-2.06	111.32	114.38
9	A	708	CLR	C7-C8-C14	-2.01	108.00	110.91

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	704	1WR	O1-C11-C4-C5
6	A	704	1WR	O2-C11-C4-C5

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Mol	Chain	Res	Type	Atoms
6	A	704	1WR	C12-C10-C9-N3
8	A	707	DMU	C1-C6-O16-C18
8	A	707	DMU	O5-C6-O16-C18
8	A	707	DMU	C19-C18-O16-C6
8	A	707	DMU	C2-C3-O7-C10
6	A	704	1WR	C10-C9-N3-C8
8	A	707	DMU	O5-C4-C57-O61
8	A	707	DMU	C25-C28-C31-C34
8	A	707	DMU	C31-C34-C37-C40
6	A	704	1WR	C10-C9-N3-C5
8	A	707	DMU	O16-C18-C19-C22
7	A	706	Y01	CAX-CAL-CAM-CAY
7	A	706	Y01	CAN-CAJ-CAO-CBB
9	A	708	CLR	C23-C24-C25-C26
9	A	708	CLR	C23-C24-C25-C27
8	A	707	DMU	O6-C11-C9-O1
8	A	707	DMU	C18-C19-C22-C25
8	A	707	DMU	C3-C4-C57-O61
8	A	707	DMU	C4-C3-O7-C10
7	A	706	Y01	CAJ-CAN-CBA-CAA
8	A	707	DMU	C28-C31-C34-C37
7	A	706	Y01	CAO-CAJ-CAN-CBA
6	A	704	1WR	O2-C11-C4-C6
8	A	707	DMU	C22-C25-C28-C31
6	A	705	1WR	C10-C9-N3-C5
6	A	704	1WR	O1-C11-C4-C6
6	A	705	1WR	C10-C9-N3-C8
6	A	705	1WR	O2-C11-C4-C5
8	A	707	DMU	C34-C37-C40-C43
7	A	706	Y01	CAO-CBB-CBE-CAP

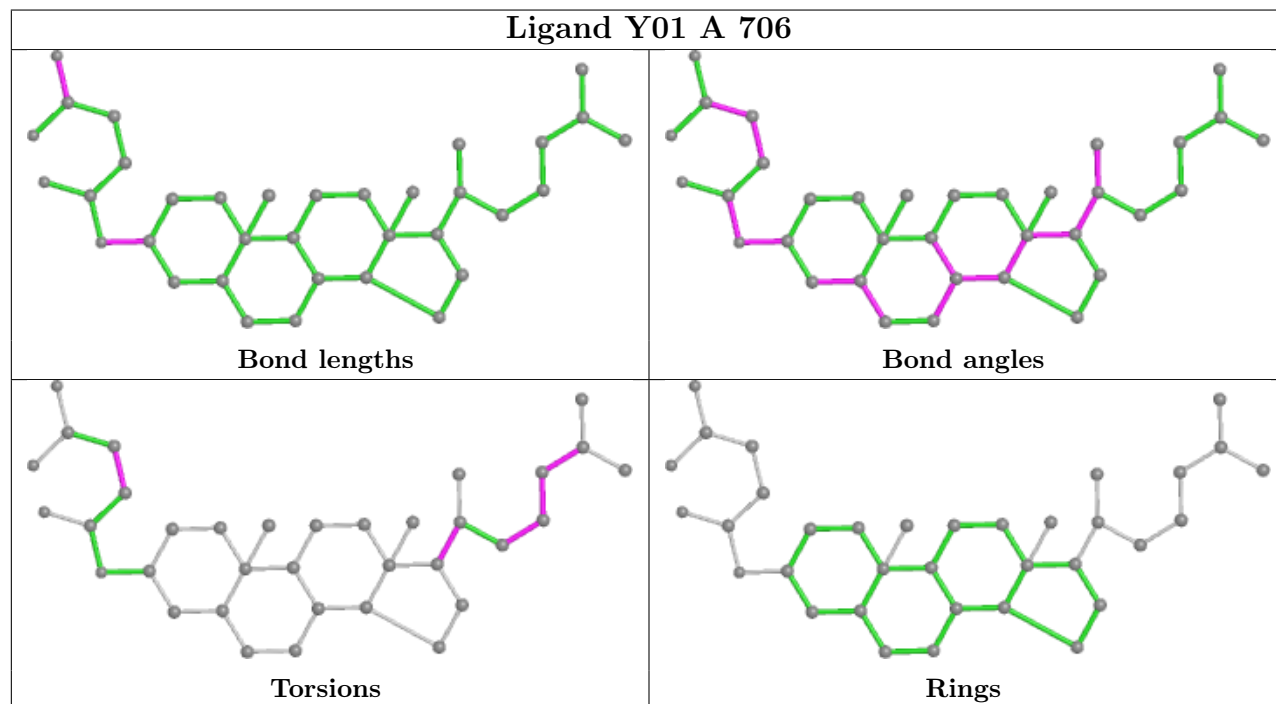
There are no ring outliers.

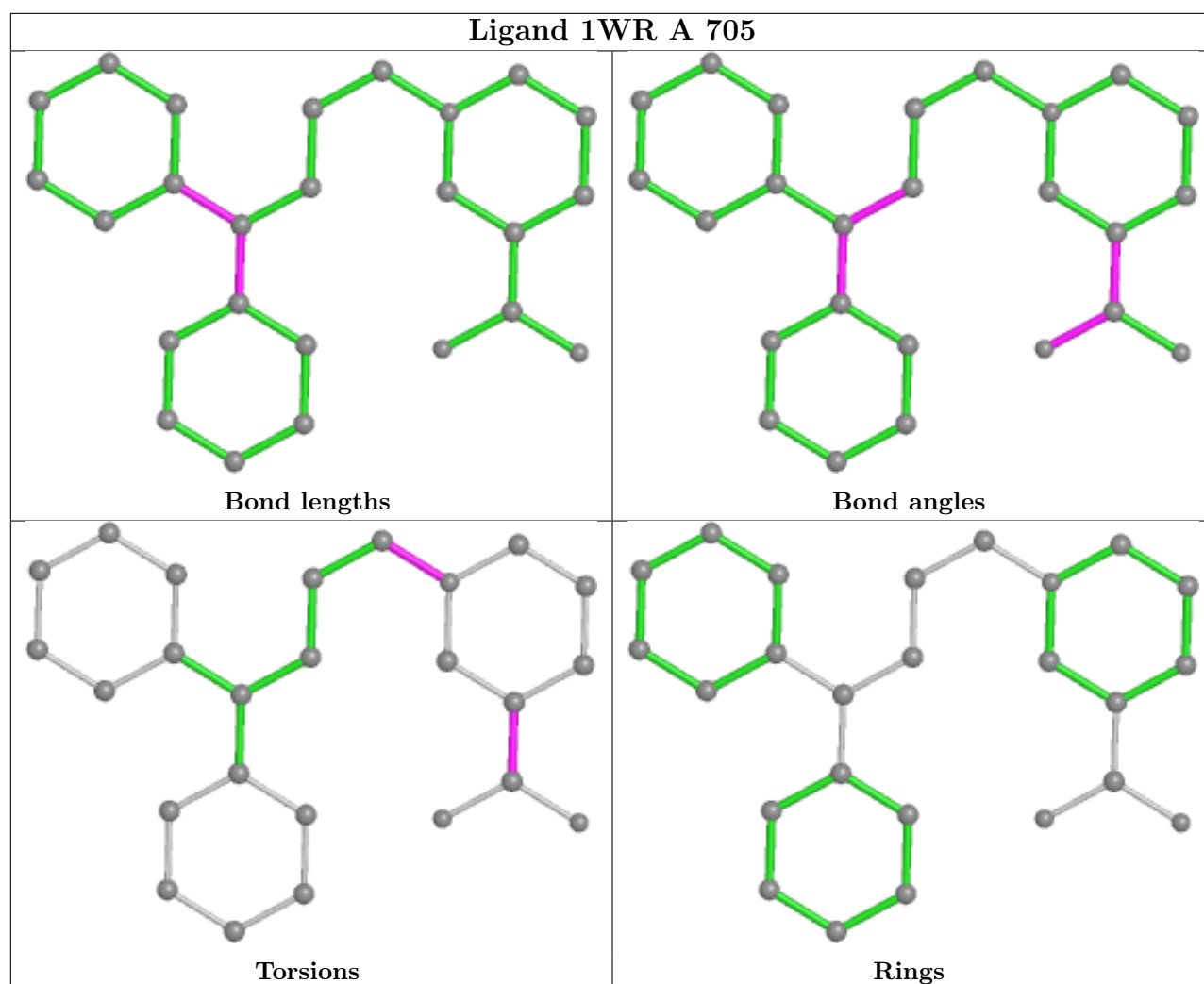
4 monomers are involved in 9 short contacts:

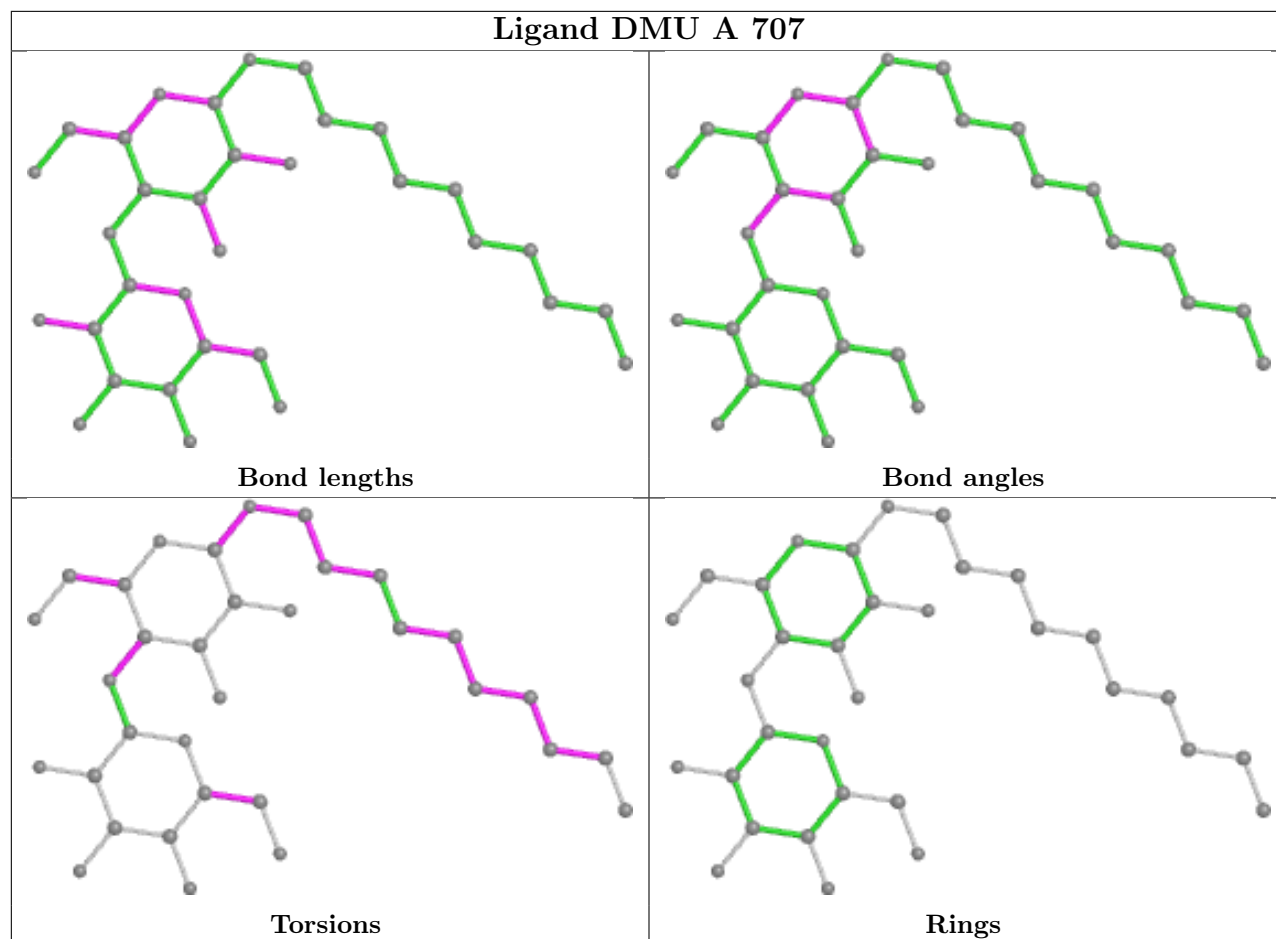
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	706	Y01	3	0
6	A	705	1WR	1	0
8	A	707	DMU	4	0
6	A	704	1WR	1	0

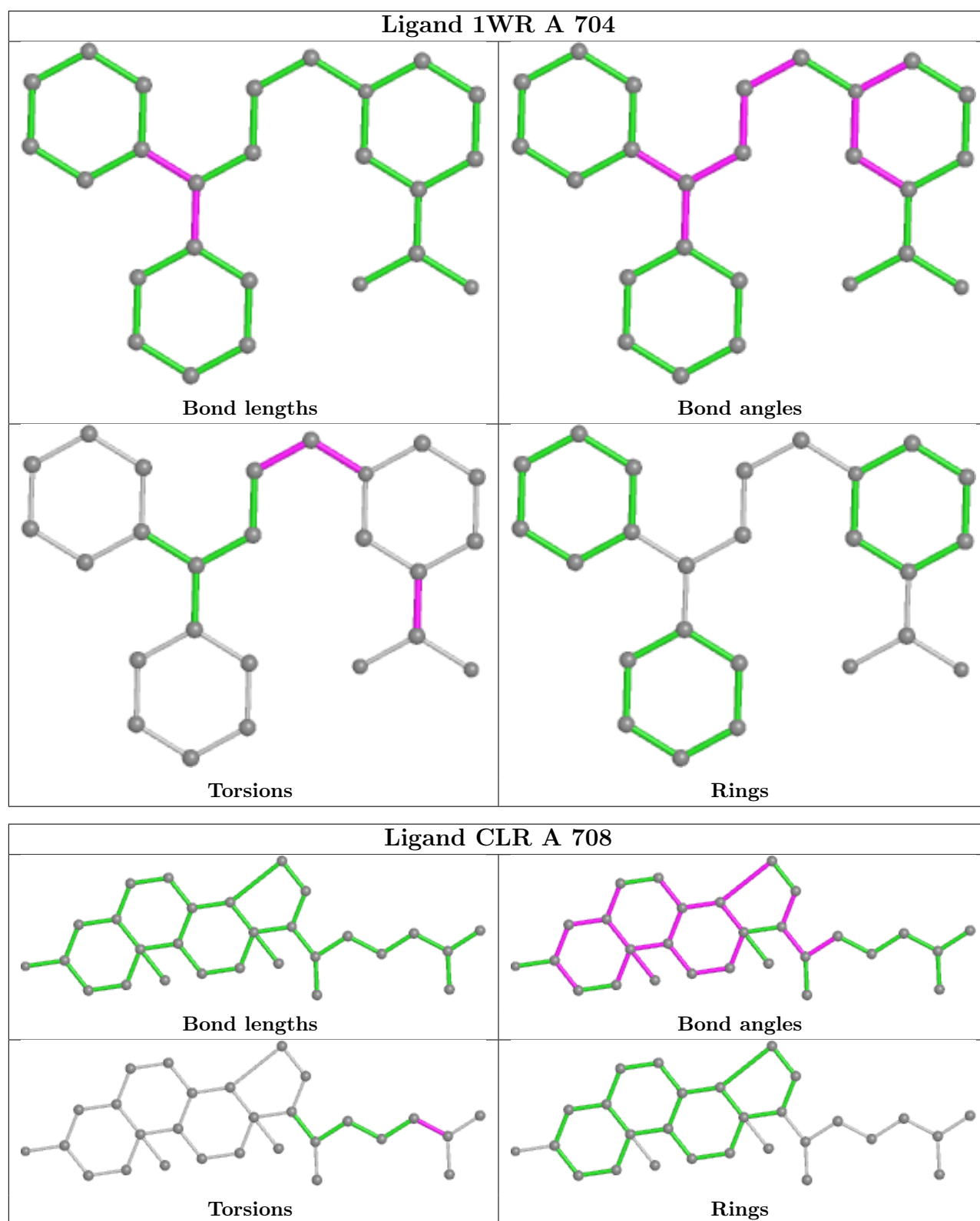
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	-0.07	4 (0%) 87 87	52, 68, 87, 125	0
2	L	214/214 (100%)	0.12	6 (2%) 53 49	48, 62, 87, 123	0
3	H	219/219 (100%)	-0.02	2 (0%) 84 84	49, 64, 86, 140	0
All	All	969/969 (100%)	-0.01	12 (1%) 79 79	48, 66, 87, 140	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	136	ASP	4.4
1	A	443	ASN	3.2
1	A	290	PHE	3.2
3	H	217	GLU	3.2
2	L	126	LEU	2.9
1	A	555	TRP	2.5
1	A	237	TRP	2.5
2	L	127	THR	2.4
2	L	123	SER	2.2
2	L	203	THR	2.1
2	L	185	ASP	2.1
2	L	119	PHE	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](#)

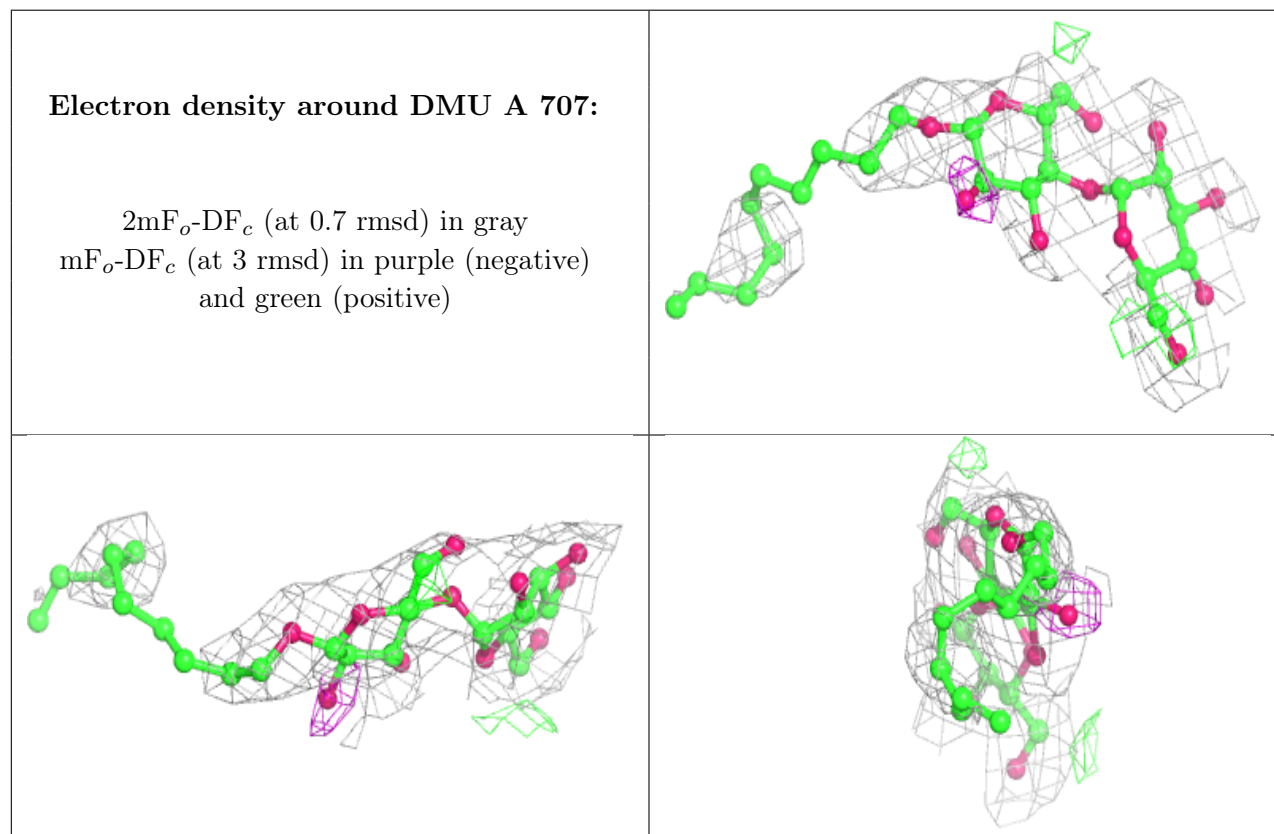
There are no monosaccharides in this entry.

## 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.

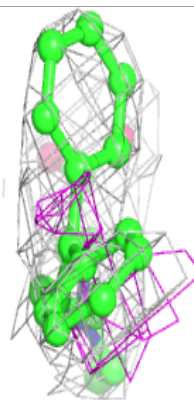
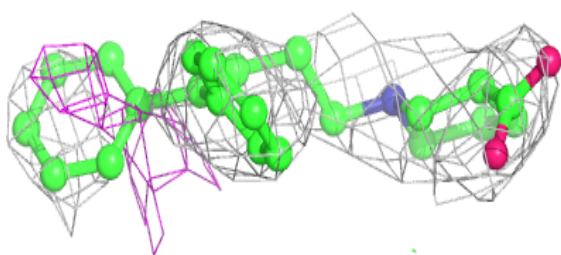
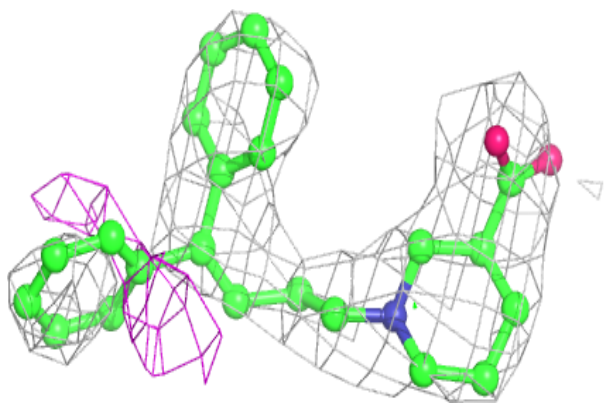
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	A	703	1/1	0.79	0.25	67,67,67,67	0
8	DMU	A	707	33/33	0.82	0.29	76,96,105,110	0
6	1WR	A	705	25/25	0.87	0.33	74,84,91,97	25
7	Y01	A	706	35/35	0.92	0.27	76,87,91,96	0
9	CLR	A	708	28/28	0.92	0.20	59,74,80,84	0
5	NA	A	702	1/1	0.94	0.34	74,74,74,74	0
6	1WR	A	704	25/25	0.94	0.30	65,74,87,93	25
4	CL	A	701	1/1	0.98	0.16	67,67,67,67	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.

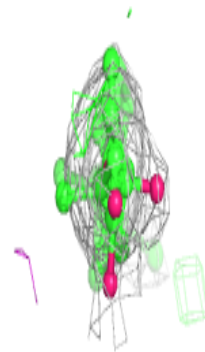
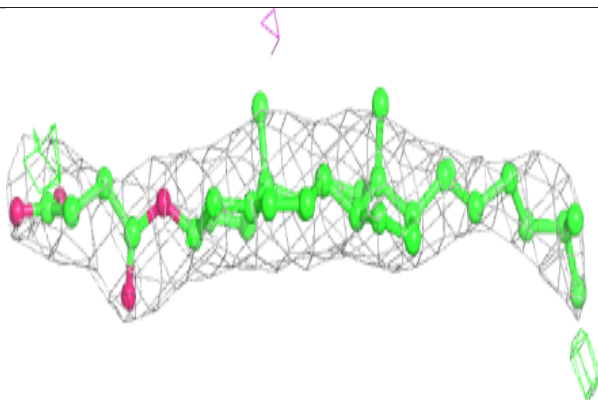
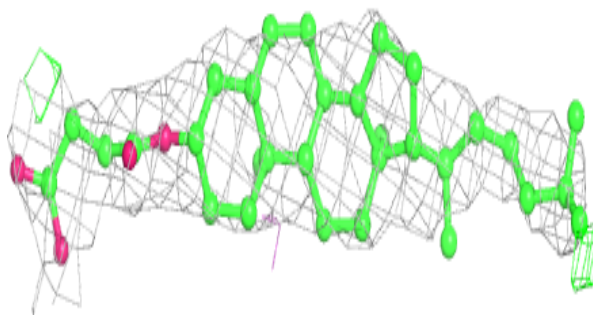


**Electron density around 1WR A 705:**

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

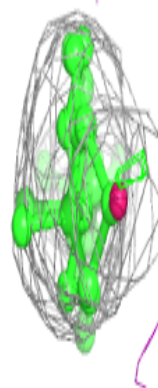
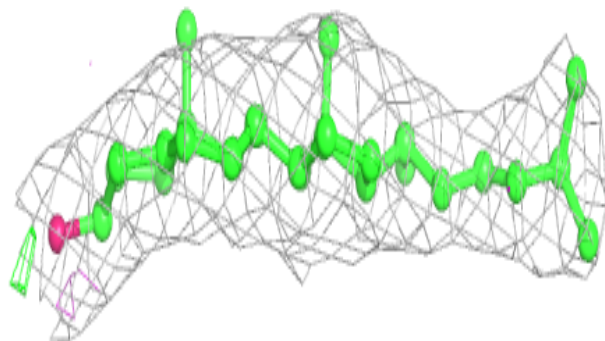
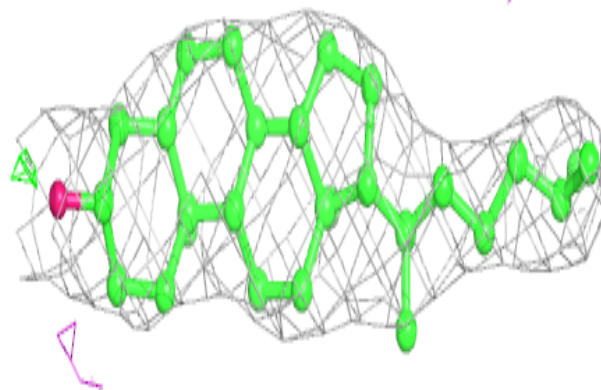
**Electron density around Y01 A 706:**

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



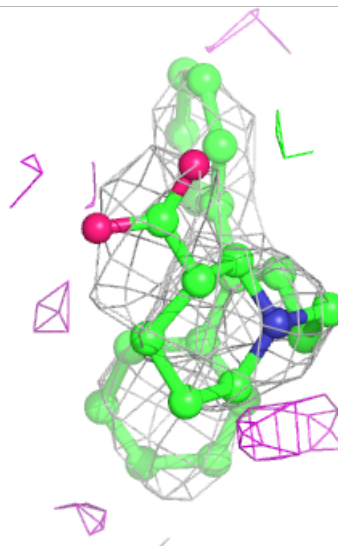
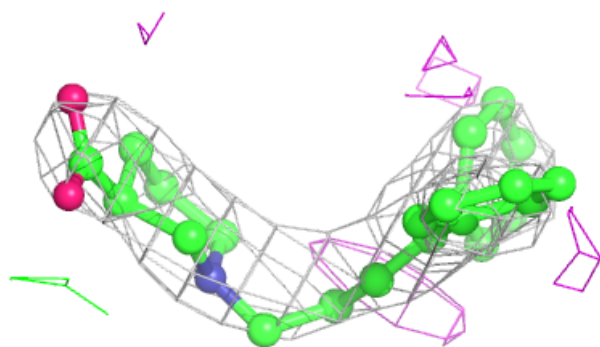
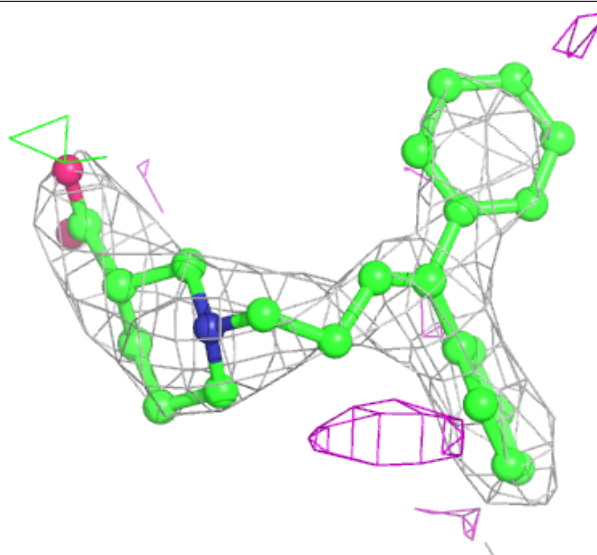
**Electron density around CLR A 708:**

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



**Electron density around 1WR A 704:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.