



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2021 – 06:12 PM JST

PDB ID : 6M3Z
Title : X-ray structure of a Drosophila dopamine transporter with NET-like mutations (D121G/S426M/F471L) in milnacipran bound form
Authors : Shabareesh, P.; Mallela, A.K.; Joseph, D.; Penmatsa, A.
Deposited on : 2020-03-04
Resolution : 3.11 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.16
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) : 2.16

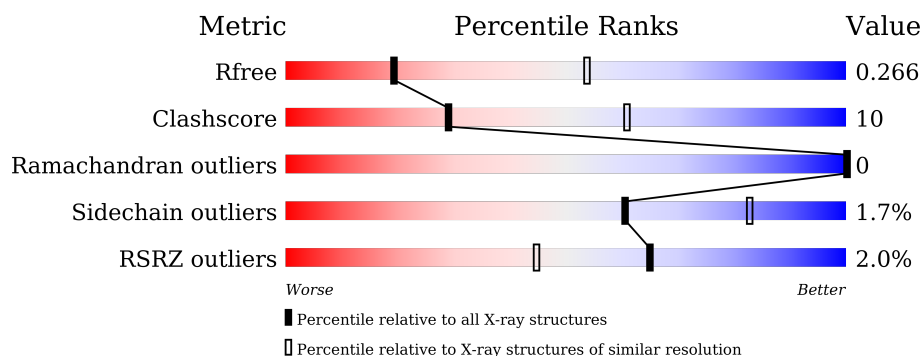
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	536	 79% 21%
2	L	214	 7% 75% 24%
3	H	219	 0% 76% 22%
4	B	2	 100%
4	C	2	 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7670 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
			4237	2840	658	720	19			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	121	GLY	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
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
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	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	426	MET	SER	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
2	L	214	Total	C	N	O	S	0	0	0
			1634	1015	272	339	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1633	1026	278	321	8			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



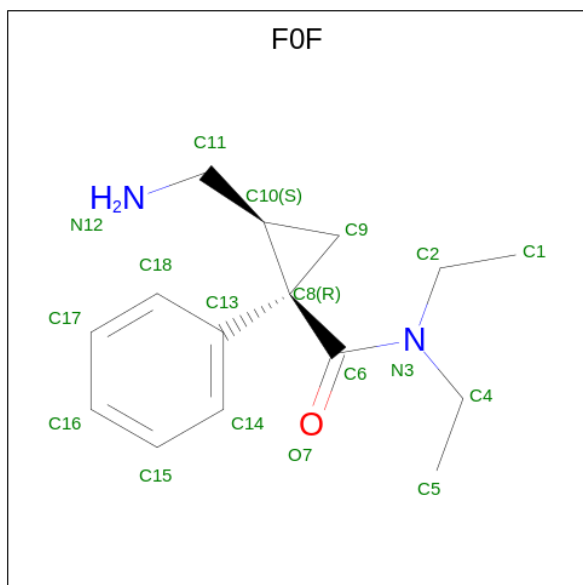
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	B	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is (1R,2S)-2-(aminomethyl)-N,N-diethyl-1-phenyl-cyclopropane-1-carboxamide (three-letter code: F0F) (formula: C₁₅H₂₂N₂O) (labeled as "Ligand of Interest" by depositor).



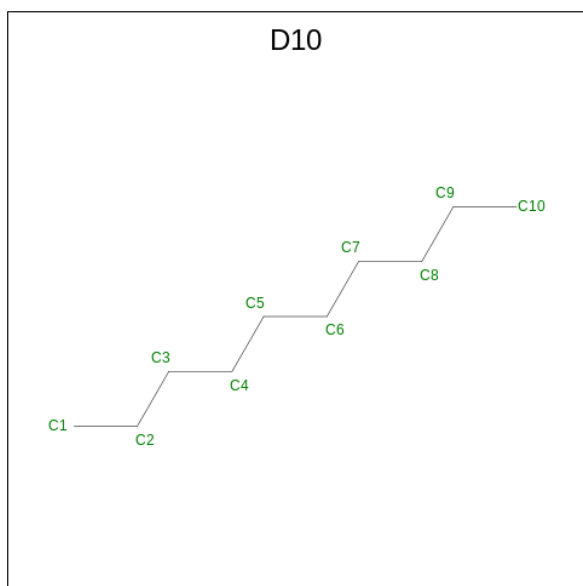
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	15	2	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



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

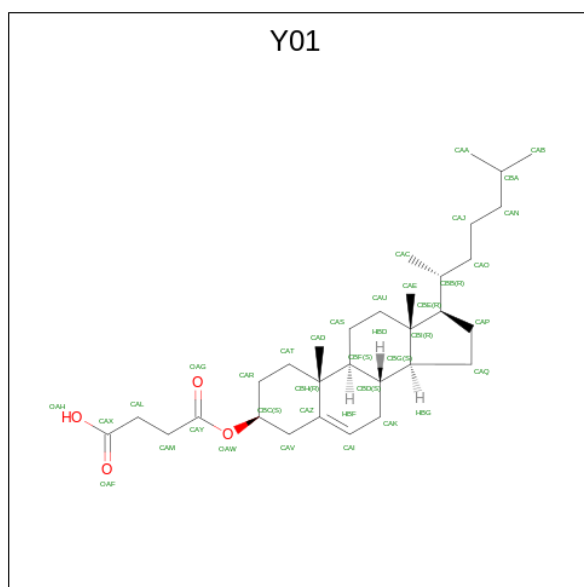
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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).

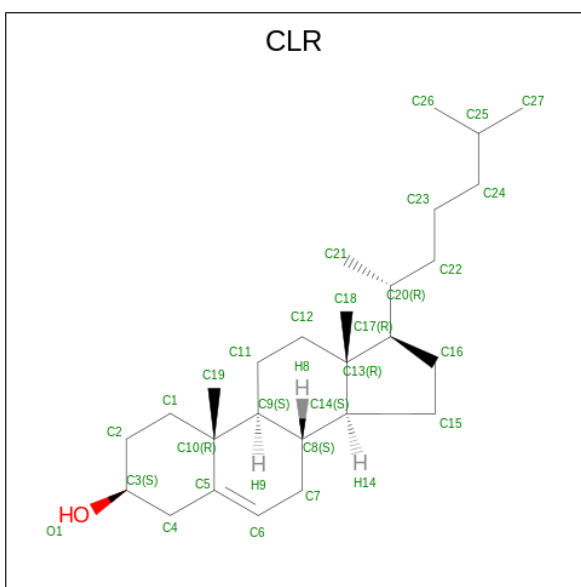
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Na 2 2	0	0

- Molecule 10 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



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

- Molecule 11 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

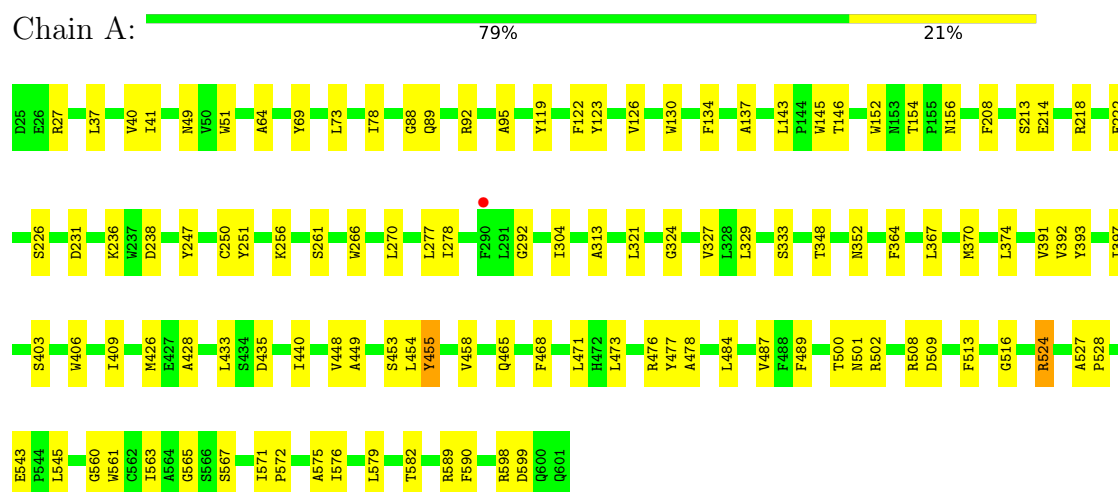
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	O	0	0
			8	8		
12	L	8	Total	O	0	0
			8	8		
12	H	4	Total	O	0	0
			4	4		

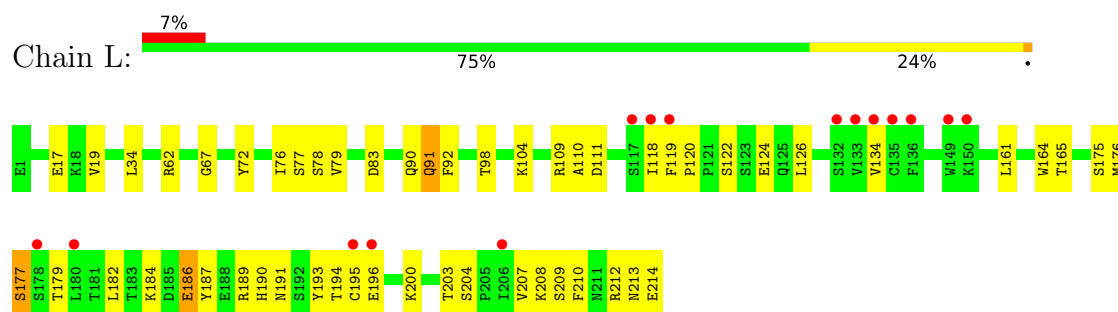
3 Residue-property plots

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.

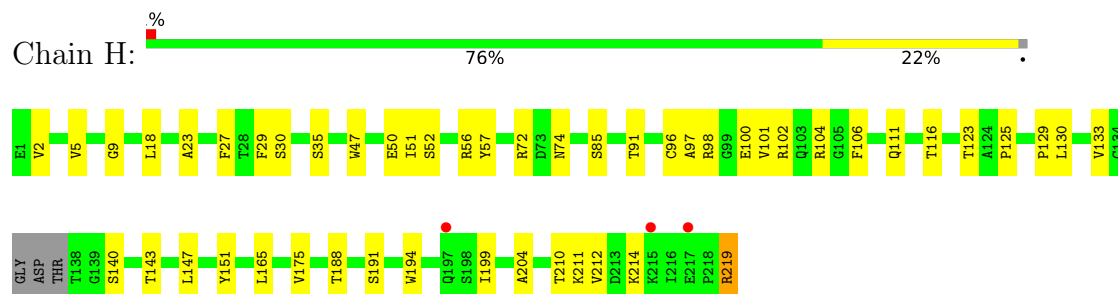
• Molecule 1: Sodium-dependent dopamine transporter



• Molecule 2: Antibody fragment 9D5 Light chain



• Molecule 3: Antibody fragment 9D5 heavy chain



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain B:  100%

GLC1
GLC2

- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.00Å 141.60Å 168.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.55 – 3.11 48.55 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.55-3.11) 99.5 (48.55-3.11)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.222 , 0.264 0.223 , 0.266	Depositor DCC
R_{free} test set	2066 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	94.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7670	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, F0F, D10, CL, NA, GLC, Y01, CLR

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	0.53	0/4379	0.64	0/5981
2	L	0.53	0/1672	0.69	0/2271
3	H	0.56	1/1671 (0.1%)	0.69	0/2273
All	All	0.54	1/7722 (0.0%)	0.66	0/10525

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	123	THR	C-N	7.07	1.50	1.34

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	4237	0	4163	80	0
2	L	1634	0	1552	38	0
3	H	1633	0	1587	35	0
4	B	23	0	21	0	0
4	C	23	0	21	2	0
5	A	18	0	0	0	0
6	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	10	0	22	0	0
8	A	1	0	0	0	0
9	A	2	0	0	0	0
10	A	35	0	50	3	0
11	A	28	0	46	1	0
12	A	8	0	0	1	0
12	H	4	0	0	0	0
12	L	8	0	0	1	0
All	All	7670	0	7470	145	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 10.

All (145) 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)
3:H:140:SER:O	3:H:191:SER:HB2	1.44	1.15
3:H:140:SER:O	3:H:191:SER:CB	2.01	1.07
4:C:1:GLC:O3	4:C:2:GLC:O2	1.78	0.97
2:L:134:VAL:HG12	2:L:179:THR:HG23	1.58	0.82
2:L:109:ARG:NH1	2:L:110:ALA:O	2.14	0.81
1:A:321:LEU:HD23	1:A:352:ASN:HD22	1.47	0.80
2:L:111:ASP:OD2	2:L:200:LYS:NZ	2.20	0.74
3:H:91:THR:HG23	3:H:116:THR:HA	1.68	0.74
1:A:261:SER:OG	12:A:801:HOH:O	2.07	0.71
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.72	0.71
1:A:73:LEU:HD23	10:A:707:Y01:HAC2	1.75	0.69
1:A:152:TRP:O	1:A:218:ARG:HD3	1.93	0.68
3:H:140:SER:O	3:H:191:SER:HB3	1.92	0.66
1:A:502:ARG:NH1	1:A:599:ASP:OD2	2.30	0.65
2:L:124:GLU:HG2	3:H:214:LYS:NZ	2.13	0.64
2:L:191:ASN:ND2	2:L:213:ASN:OD1	2.28	0.64
2:L:196:GLU:HG2	2:L:207:VAL:HG23	1.81	0.62
2:L:186:GLU:HG2	2:L:189:ARG:HH21	1.65	0.61
1:A:579:LEU:HD21	1:A:590:PHE:HE1	1.64	0.60
2:L:118:ILE:HD11	2:L:195:CYS:HB3	1.83	0.60
1:A:27:ARG:NH2	1:A:435:ASP:OD2	2.35	0.60
2:L:120:PRO:HB3	2:L:210:PHE:CZ	2.38	0.59
1:A:370:MET:HG2	1:A:374:LEU:HD12	1.83	0.59
3:H:52:SER:HB3	3:H:57:TYR:HB2	1.84	0.59
1:A:393:TYR:CE1	1:A:397:ILE:HD11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.38	0.58
3:H:5:VAL:HG23	3:H:23:ALA:HB3	1.85	0.58
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.85	0.58
1:A:582:THR:O	1:A:589:ARG:NH2	2.36	0.58
2:L:119:PHE:HB2	2:L:134:VAL:HG22	1.84	0.58
2:L:90:GLN:HG2	2:L:91:GLN:N	2.19	0.57
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.40	0.57
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.87	0.57
1:A:477:TYR:CD2	1:A:560:GLY:HA3	2.41	0.56
2:L:187:TYR:CE2	2:L:212:ARG:HD2	2.41	0.56
1:A:292:GLY:HA3	1:A:364:PHE:O	2.06	0.55
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.41	0.55
1:A:489:PHE:HD2	1:A:571:ILE:HG21	1.71	0.55
1:A:277:LEU:HB2	11:A:710:CLR:H263	1.87	0.55
3:H:9:GLY:HA2	3:H:18:LEU:HD13	1.88	0.55
1:A:516:GLY:HA3	10:A:707:Y01:OAF	2.07	0.55
2:L:118:ILE:HG12	2:L:208:LYS:HB3	1.89	0.55
1:A:582:THR:O	1:A:589:ARG:HD2	2.07	0.54
2:L:210:PHE:HB2	3:H:133:VAL:HG11	1.90	0.54
1:A:69:TYR:HA	1:A:313:ALA:HB1	1.90	0.54
1:A:433:LEU:HB3	1:A:440:ILE:HD11	1.90	0.53
2:L:190:HIS:O	2:L:212:ARG:NH1	2.41	0.53
2:L:67:GLY:HA3	2:L:72:TYR:HA	1.90	0.53
1:A:37:LEU:O	1:A:41:ILE:HG12	2.09	0.53
1:A:156:ASN:HB3	1:A:208:PHE:CD2	2.44	0.53
1:A:278:ILE:HD11	1:A:409:ILE:HD13	1.89	0.52
3:H:129:PRO:HD3	3:H:214:LYS:HE2	1.90	0.52
3:H:29:PHE:O	3:H:72:ARG:NH2	2.42	0.52
2:L:91:GLN:NE2	2:L:98:THR:OG1	2.43	0.52
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.91	0.52
1:A:143:LEU:HD13	1:A:145:TRP:CZ2	2.44	0.52
3:H:9:GLY:HA2	3:H:18:LEU:CD1	2.40	0.52
1:A:123:TYR:O	1:A:126:VAL:HG12	2.09	0.51
1:A:370:MET:O	1:A:374:LEU:HB2	2.10	0.51
1:A:500:THR:OG1	1:A:524:ARG:NH1	2.43	0.51
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.92	0.51
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.46	0.51
1:A:473:LEU:HD12	1:A:545:LEU:HD23	1.93	0.51
2:L:194:THR:HG23	2:L:209:SER:HB2	1.92	0.51
2:L:122:SER:OG	3:H:129:PRO:HD2	2.11	0.51
3:H:130:LEU:HD21	3:H:147:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:203:THR:OG1	2:L:204:SER:N	2.43	0.50
1:A:433:LEU:CB	1:A:440:ILE:HD11	2.42	0.50
1:A:49:ASN:ND2	1:A:352:ASN:OD1	2.45	0.50
1:A:73:LEU:O	1:A:78:ILE:HG12	2.12	0.49
2:L:126:LEU:O	2:L:184:LYS:HE2	2.12	0.49
1:A:476:ARG:HD3	1:A:545:LEU:HD13	1.93	0.49
1:A:89:GLN:O	1:A:92:ARG:HD2	2.13	0.49
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.48	0.49
1:A:143:LEU:O	1:A:146:THR:HG22	2.13	0.48
3:H:2:VAL:HG23	3:H:27:PHE:CD1	2.48	0.48
1:A:501:ASN:OD1	1:A:502:ARG:N	2.46	0.48
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.48	0.48
1:A:327:VAL:HG22	1:A:428:ALA:HB2	1.95	0.48
1:A:222:GLU:OE1	1:A:465:GLN:NE2	2.44	0.48
1:A:508:ARG:NH2	3:H:50:GLU:OE2	2.32	0.48
4:C:1:GLC:H4	4:C:2:GLC:H2	1.76	0.47
1:A:324:GLY:HA3	1:A:487:VAL:HG22	1.96	0.47
1:A:214:GLU:O	1:A:218:ARG:HB2	2.13	0.47
1:A:572:PRO:O	1:A:576:ILE:HG12	2.14	0.47
2:L:19:VAL:HG22	2:L:76:ILE:HB	1.96	0.47
1:A:370:MET:HE1	1:A:392:VAL:CG1	2.45	0.47
1:A:393:TYR:HE1	1:A:397:ILE:HD11	1.80	0.47
1:A:154:THR:OG1	1:A:214:GLU:OE2	2.29	0.47
3:H:143:THR:HG23	3:H:188:THR:HG22	1.97	0.47
2:L:120:PRO:HG2	3:H:219:ARG:CZ	2.45	0.47
1:A:454:LEU:O	1:A:458:VAL:HG12	2.15	0.46
2:L:213:ASN:HB2	2:L:214:GLU:OE1	2.16	0.46
2:L:182:LEU:CD1	2:L:187:TYR:HB2	2.46	0.45
1:A:251:TYR:HE1	1:A:448:VAL:HG23	1.82	0.45
1:A:95:ALA:HA	1:A:329:LEU:CD2	2.47	0.45
1:A:250:CYS:HB3	1:A:426:MET:HE3	1.99	0.45
3:H:194:TRP:HD1	3:H:199:ILE:HG12	1.81	0.45
1:A:575:ALA:O	1:A:579:LEU:HB2	2.17	0.44
2:L:118:ILE:HG23	2:L:118:ILE:HD12	1.65	0.44
2:L:176:MET:HG2	2:L:177:SER:N	2.31	0.44
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.99	0.44
1:A:64:ALA:O	1:A:304:ILE:HD11	2.17	0.44
3:H:204:ALA:HB1	3:H:211:LYS:HZ3	1.83	0.44
1:A:508:ARG:NE	3:H:100:GLU:O	2.41	0.44
3:H:30:SER:HB3	3:H:74:ASN:HB3	2.00	0.44
1:A:40:VAL:HG12	1:A:348:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:TRP:C	1:A:563:ILE:H	2.21	0.43
1:A:509:ASP:O	3:H:102:ARG:NH1	2.51	0.43
3:H:35:SER:OG	3:H:47:TRP:NE1	2.51	0.43
1:A:397:ILE:CG2	1:A:406:TRP:HB2	2.48	0.43
2:L:161:LEU:HD21	3:H:175:VAL:HB	2.00	0.43
2:L:104:LYS:NZ	12:L:304:HOH:O	2.50	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.87	0.43
1:A:256:LYS:HA	1:A:256:LYS:HD3	1.88	0.42
3:H:204:ALA:HB1	3:H:211:LYS:NZ	2.33	0.42
1:A:40:VAL:CG1	1:A:348:THR:HG21	2.50	0.42
1:A:476:ARG:NH2	1:A:543:GLU:O	2.51	0.42
3:H:97:ALA:HB1	3:H:106:PHE:HB3	2.01	0.42
1:A:122:PHE:CE1	1:A:458:VAL:HG11	2.55	0.42
1:A:130:TRP:HH2	1:A:468:PHE:HD1	1.68	0.42
1:A:226:SER:OG	1:A:231:ASP:O	2.28	0.42
10:A:707:Y01:HAP1	10:A:707:Y01:HAC1	1.80	0.42
3:H:27:PHE:CE2	3:H:98:ARG:HD2	2.55	0.41
1:A:236:LYS:HE3	1:A:238:ASP:OD1	2.20	0.41
2:L:17:GLU:O	2:L:79:VAL:HG23	2.19	0.41
3:H:165:LEU:HD12	3:H:165:LEU:HA	1.88	0.41
1:A:278:ILE:HD13	1:A:278:ILE:HG21	1.75	0.41
1:A:88:GLY:O	1:A:333:SER:HA	2.20	0.41
1:A:565:GLY:C	1:A:567:SER:H	2.23	0.41
1:A:449:ALA:O	1:A:453:SER:OG	2.30	0.41
1:A:403:SER:HA	1:A:406:TRP:HD1	1.85	0.41
1:A:502:ARG:HG3	3:H:56:ARG:CZ	2.51	0.41
1:A:247:TYR:CZ	1:A:455:TYR:HB3	2.56	0.41
3:H:210:THR:HG22	3:H:212:VAL:HG13	2.03	0.41
2:L:62:ARG:NH1	2:L:83:ASP:OD2	2.53	0.41
1:A:266:TRP:O	1:A:270:LEU:HB2	2.22	0.40
1:A:513:PHE:HB3	3:H:101:VAL:HG13	2.02	0.40
1:A:134:PHE:HA	1:A:137:ALA:HB3	2.04	0.40
1:A:213:SER:N	1:A:391:VAL:HG13	2.37	0.40
1:A:468:PHE:HA	1:A:471:LEU:HD12	2.02	0.40
2:L:124:GLU:HG2	3:H:214:LYS:HZ3	1.82	0.40
2:L:165:THR:HG23	2:L:175:SER:O	2.21	0.40
1:A:119:TYR:HB3	1:A:478:ALA:HB1	2.04	0.40
2:L:77:SER:OG	2:L:78:SER:N	2.55	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	534/536 (100%)	504 (94%)	30 (6%)	0	100	100
2	L	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	H	212/219 (97%)	202 (95%)	10 (5%)	0	100	100
All	All	958/969 (99%)	908 (95%)	50 (5%)	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	434/440 (99%)	430 (99%)	4 (1%)	78	91
2	L	186/187 (100%)	181 (97%)	5 (3%)	44	73
3	H	182/187 (97%)	177 (97%)	5 (3%)	44	73
All	All	802/814 (98%)	788 (98%)	14 (2%)	60	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TRP
1	A	455	TYR
1	A	524	ARG
1	A	598	ARG
2	L	91	GLN

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Mol	Chain	Res	Type
2	L	92	PHE
2	L	164	TRP
2	L	177	SER
2	L	186	GLU
3	H	85	SER
3	H	96	CYS
3	H	104	ARG
3	H	111	GLN
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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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	$\# Z > 2$
4	GLC	B	1	4	12,12,12	0.50	0	17,17,17	0.97	1 (5%)
4	GLC	B	2	4	11,11,12	0.38	0	15,15,17	1.10	1 (6%)
4	GLC	C	1	4	12,12,12	0.49	0	17,17,17	0.99	1 (5%)
4	GLC	C	2	4	11,11,12	0.43	0	15,15,17	1.03	1 (6%)

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
4	GLC	B	1	4	-	0/2/22/22	0/1/1/1
4	GLC	B	2	4	-	0/2/19/22	0/1/1/1
4	GLC	C	1	4	-	1/2/22/22	0/1/1/1
4	GLC	C	2	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	GLC	C1-O5-C5	-3.18	107.89	112.19
4	C	1	GLC	C1-O5-C5	-3.04	107.93	113.66
4	B	1	GLC	C1-O5-C5	-2.88	108.23	113.66
4	C	2	GLC	C1-O5-C5	-2.81	108.39	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	GLC	2	0
4	C	2	GLC	2	0

5.6 Ligand geometry

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
5	F0F	A	701	-	19,19,19	1.77	2 (10%)	23,27,27	2.19	2 (8%)
10	Y01	A	707	-	35,38,38	1.19	4 (11%)	54,57,57	1.92	17 (31%)
11	CLR	A	710	-	31,31,31	0.93	0	48,48,48	1.56	9 (18%)
7	D10	A	703	-	9,9,9	0.59	0	8,8,8	0.26	0
6	GOL	A	702	-	5,5,5	0.56	0	5,5,5	0.91	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
5	F0F	A	701	-	-	9/22/30/30	0/2/2/2
10	Y01	A	707	-	-	7/17/77/77	0/4/4/4
11	CLR	A	710	-	-	2/10/68/68	0/4/4/4
7	D10	A	703	-	-	2/7/7/7	-
6	GOL	A	702	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	F0F	C6-N3	5.90	1.45	1.35
5	A	701	F0F	O7-C6	2.79	1.26	1.22
10	A	707	Y01	CAT-CBH	2.43	1.58	1.54
10	A	707	Y01	OAW-CAY	2.18	1.40	1.34
10	A	707	Y01	CBB-CBE	2.13	1.58	1.54
10	A	707	Y01	CBH-CBF	2.03	1.59	1.56

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	F0F	C9-C10-C11	-8.36	103.71	121.00
10	A	707	Y01	CBI-CBE-CBB	5.59	128.25	119.49
5	A	701	F0F	O7-C6-C8	-5.04	114.04	120.33
11	A	710	CLR	C4-C5-C10	4.91	122.95	116.42
11	A	710	CLR	C1-C2-C3	4.61	116.38	110.47
10	A	707	Y01	CAT-CBH-CBF	3.85	114.10	108.73
10	A	707	Y01	CAM-CAL-CAX	-3.73	106.42	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	707	Y01	CBG-CBI-CBE	-3.59	95.82	100.07
10	A	707	Y01	CBC-CAV-CAZ	-3.51	106.06	111.52
10	A	707	Y01	OAW-CAY-CAM	3.43	118.90	111.50
11	A	710	CLR	C10-C5-C6	-3.21	117.99	122.90
11	A	710	CLR	C4-C5-C6	-3.04	116.23	120.61
10	A	707	Y01	CAK-CBD-CBG	-2.98	106.59	110.91
11	A	710	CLR	C11-C9-C10	2.71	116.65	113.08
11	A	710	CLR	C8-C7-C6	2.63	116.51	112.73
11	A	710	CLR	C11-C9-C8	-2.49	108.17	111.75
10	A	707	Y01	CAQ-CBG-CBI	2.43	106.77	103.84
10	A	707	Y01	CAV-CAZ-CAI	-2.35	117.22	120.61
10	A	707	Y01	CBH-CBF-CBD	-2.33	109.24	112.73
10	A	707	Y01	CAS-CBF-CBH	2.29	116.10	113.08
10	A	707	Y01	CAC-CBB-CBE	2.27	116.40	112.92
10	A	707	Y01	CAP-CBE-CBB	-2.27	108.64	112.15
10	A	707	Y01	CAO-CBB-CBE	2.25	114.94	110.28
11	A	710	CLR	C23-C22-C20	-2.18	108.77	115.03
10	A	707	Y01	CAK-CAI-CAZ	-2.14	121.11	125.06
10	A	707	Y01	CAL-CAM-CAY	-2.12	107.94	113.82
11	A	710	CLR	C2-C1-C10	2.10	117.28	112.74
10	A	707	Y01	CAQ-CBG-CBD	-2.03	115.74	119.08

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	F0F	C8-C10-C11-N12
5	A	701	F0F	C9-C10-C11-N12
5	A	701	F0F	N3-C6-C8-C10
6	A	702	GOL	O1-C1-C2-C3
10	A	707	Y01	CAO-CBB-CBE-CBI
10	A	707	Y01	CAO-CBB-CBE-CAP
10	A	707	Y01	CAC-CBB-CBE-CAP
11	A	710	CLR	C22-C23-C24-C25
10	A	707	Y01	CAN-CAJ-CAO-CBB
6	A	702	GOL	O1-C1-C2-O2
6	A	702	GOL	O2-C2-C3-O3
10	A	707	Y01	CAC-CBB-CBE-CBI
5	A	701	F0F	C14-C13-C8-C10
5	A	701	F0F	C14-C13-C8-C6
5	A	701	F0F	C18-C13-C8-C6
7	A	703	D10	C7-C8-C9-C10

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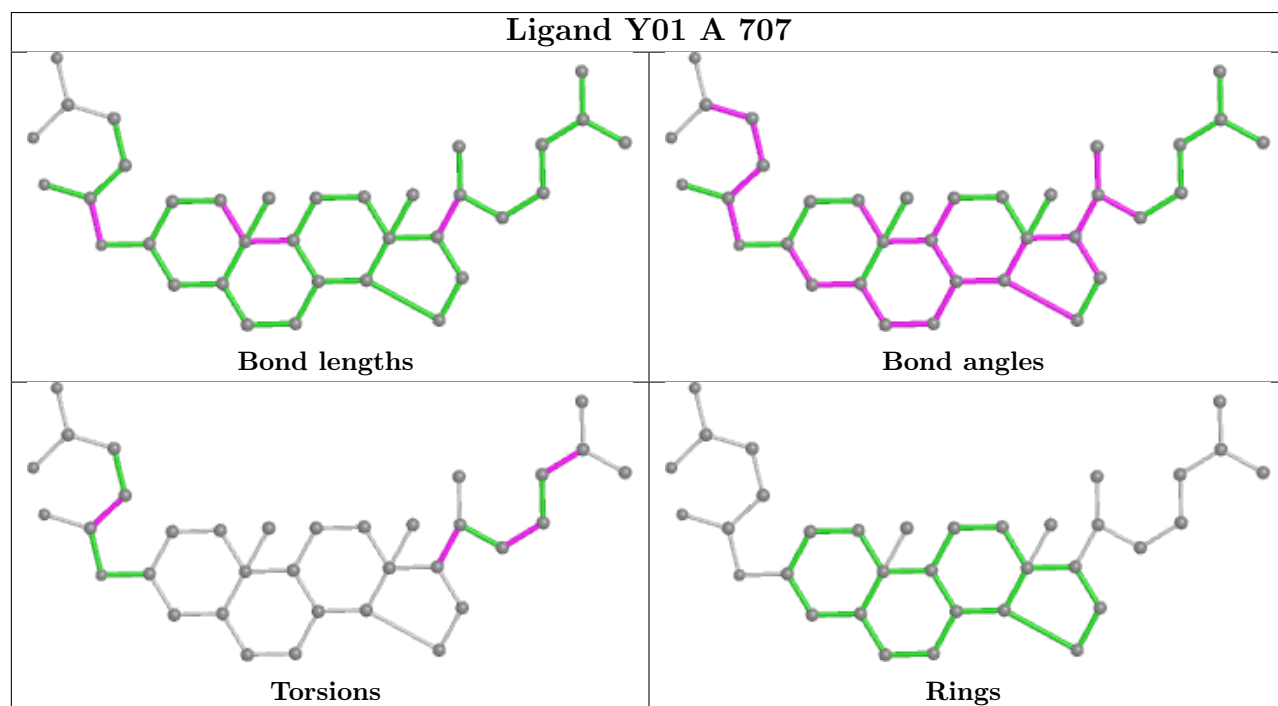
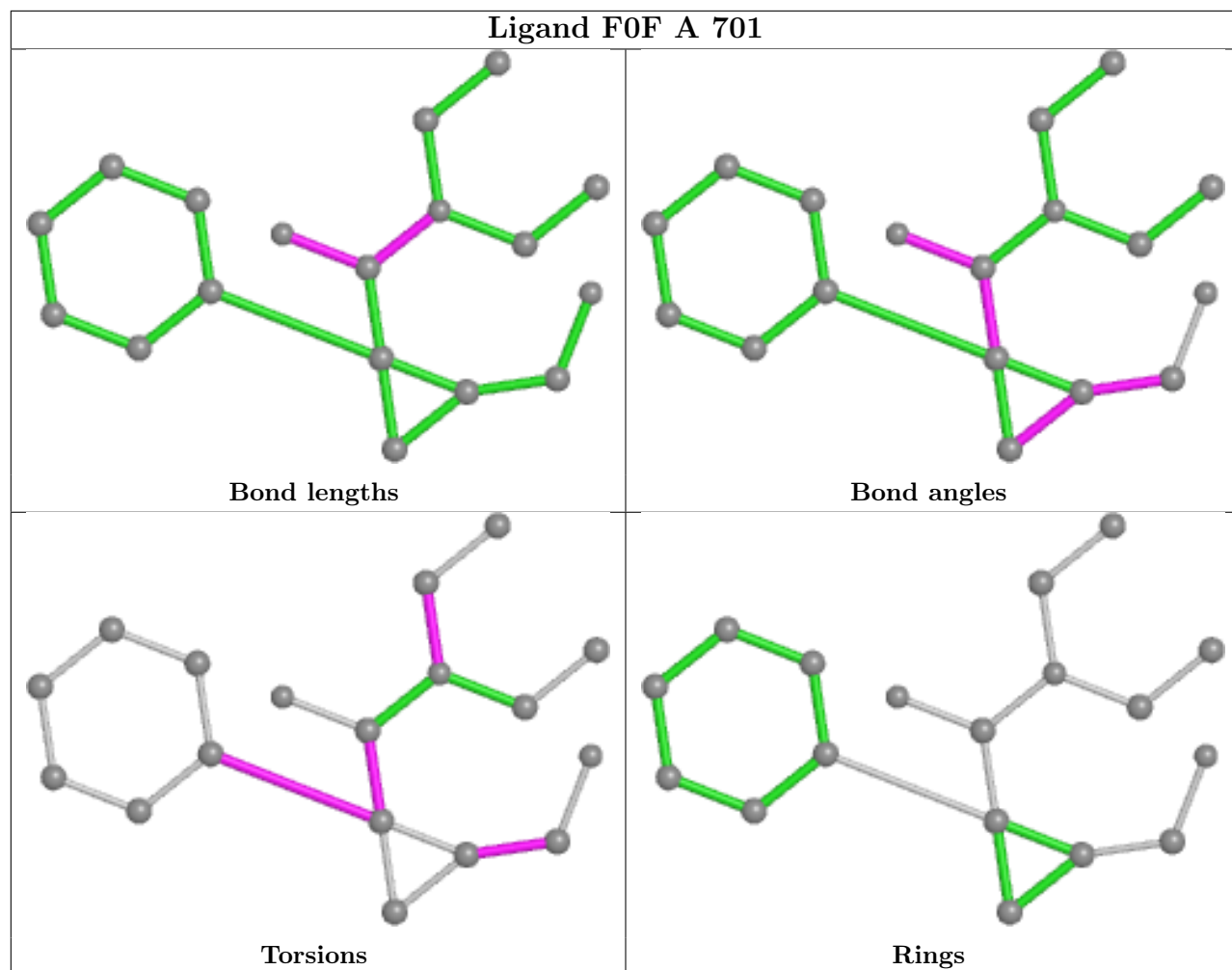
Mol	Chain	Res	Type	Atoms
5	A	701	F0F	O7-C6-C8-C10
5	A	701	F0F	C5-C4-N3-C6
11	A	710	CLR	C20-C22-C23-C24
5	A	701	F0F	C18-C13-C8-C10
7	A	703	D10	C1-C2-C3-C4
10	A	707	Y01	CAJ-CAN-CBA-CAB
10	A	707	Y01	CAL-CAM-CAY-OAW

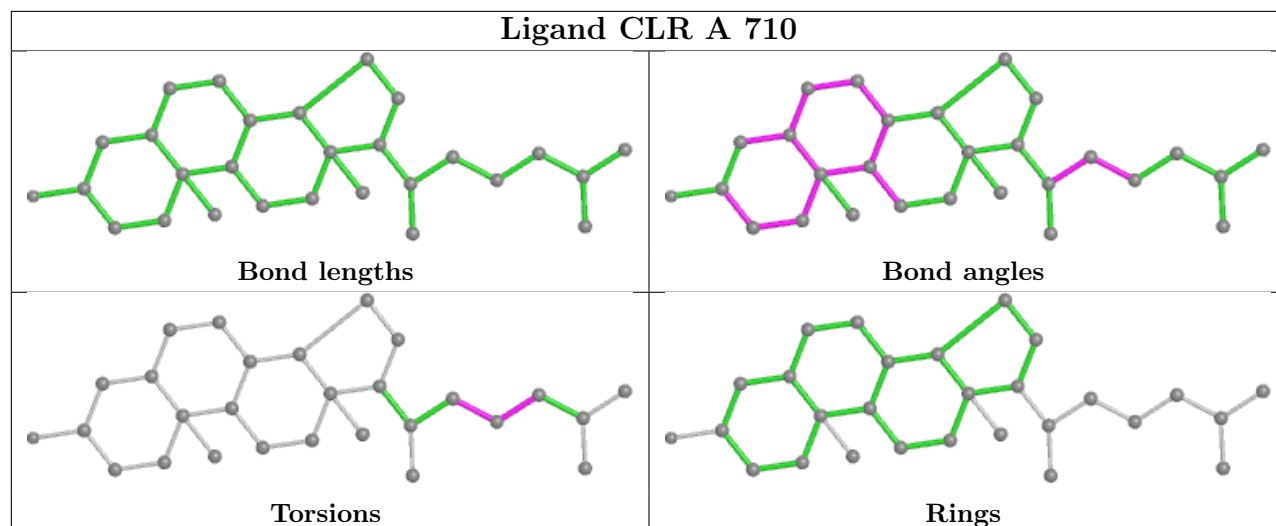
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	707	Y01	3	0
11	A	710	CLR	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	536/536 (100%)	-0.34	1 (0%) 95 91	65, 84, 108, 130	0
2	L	214/214 (100%)	0.34	15 (7%) 16 7	63, 81, 105, 118	0
3	H	216/219 (98%)	-0.04	3 (1%) 75 58	63, 79, 104, 125	0
All	All	966/969 (99%)	-0.12	19 (1%) 65 45	63, 82, 106, 130	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	134	VAL	4.2
2	L	206	ILE	3.5
2	L	136	PHE	3.4
2	L	119	PHE	3.1
2	L	133	VAL	2.8
2	L	195	CYS	2.6
2	L	135	CYS	2.4
3	H	197	GLN	2.3
2	L	149	TRP	2.2
2	L	196	GLU	2.2
2	L	117	SER	2.2
2	L	132	SER	2.2
2	L	178	SER	2.2
1	A	290	PHE	2.2
2	L	150	LYS	2.1
3	H	215	LYS	2.1
2	L	180	LEU	2.1
2	L	118	ILE	2.0
3	H	217	GLU	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GLC	C	1	12/12	0.76	0.25	101,107,110,116	0
4	GLC	B	2	11/12	0.85	0.20	102,114,120,122	0
4	GLC	B	1	12/12	0.88	0.15	105,117,121,129	0
4	GLC	C	2	11/12	0.91	0.28	97,106,111,112	0

6.4 Ligands [i](#)

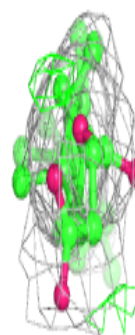
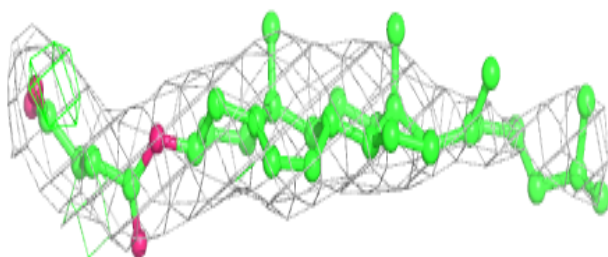
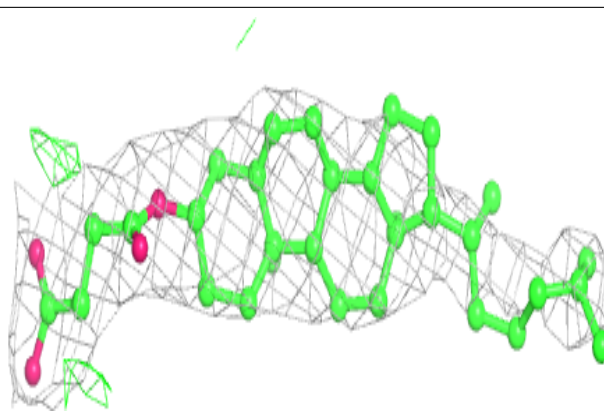
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	702	6/6	0.81	0.47	92,94,107,108	0
7	D10	A	703	10/10	0.83	0.25	74,92,95,98	0
10	Y01	A	707	35/35	0.91	0.32	77,101,109,113	0
9	NA	A	706	1/1	0.92	0.21	73,73,73,73	0
5	F0F	A	701	18/18	0.93	0.36	71,79,83,87	0
11	CLR	A	710	28/28	0.94	0.34	73,86,91,93	0
9	NA	A	705	1/1	0.95	0.24	83,83,83,83	0
8	CL	A	704	1/1	0.99	0.20	78,78,78,78	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.

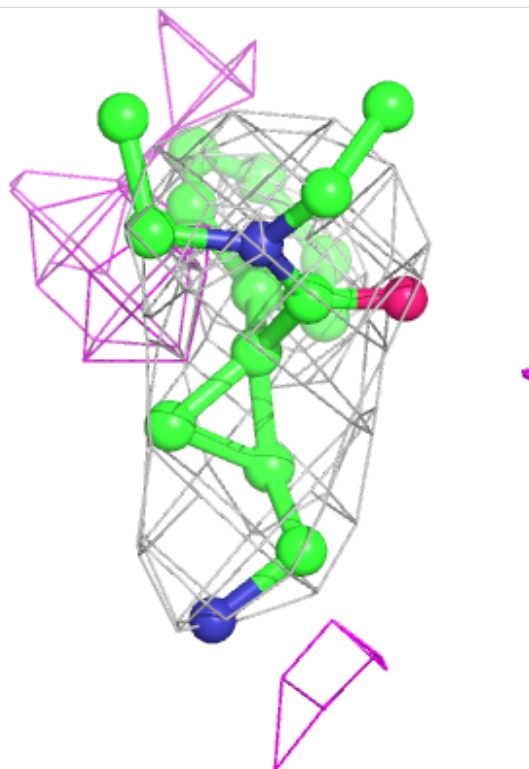
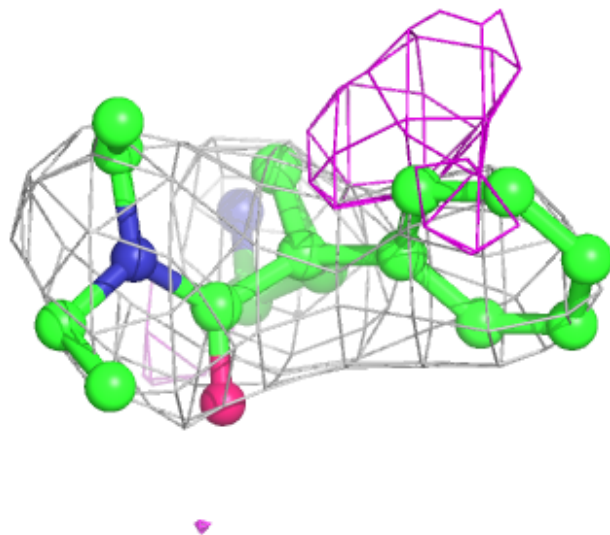
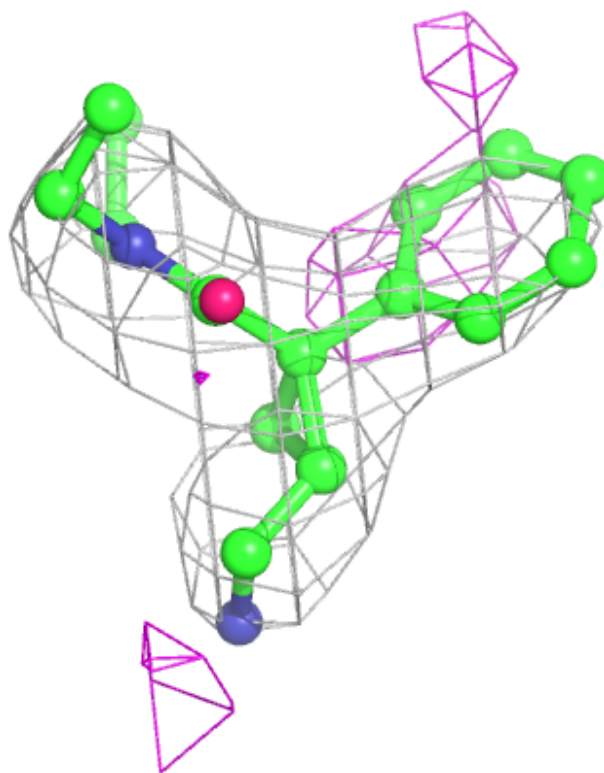
Electron density around Y01 A 707:

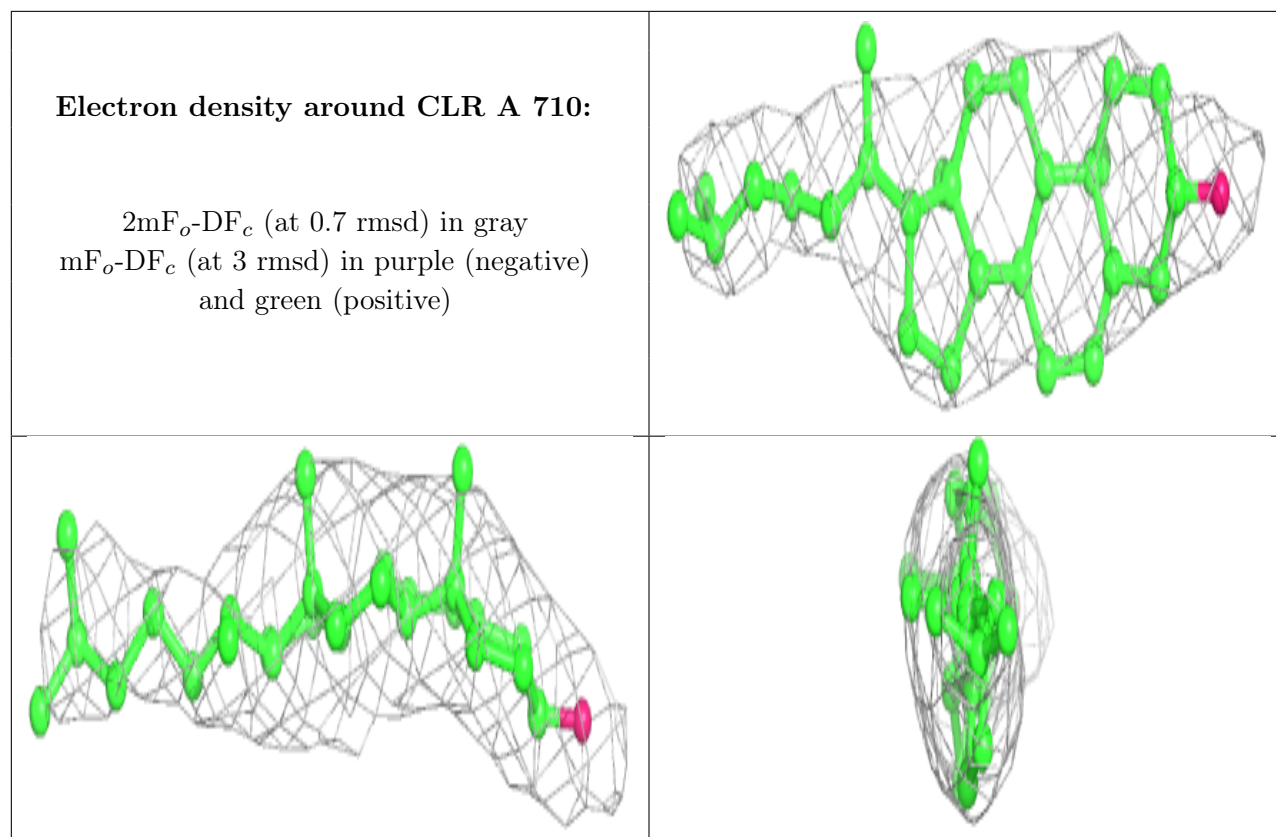
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around F0F 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.