



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:59 PM UTC

PDB ID : 6M0Z / pdb_00006m0z
Title : X-ray structure of Drosophila dopamine transporter with NET-like mutations (D121G/S426M/F471L) in L-norepinephrine bound form
Authors : Shabareesh, P.; Mallela, A.K.; Joseph, D.; Penmatsa, A.
Deposited on : 2020-02-24
Resolution : 2.88 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

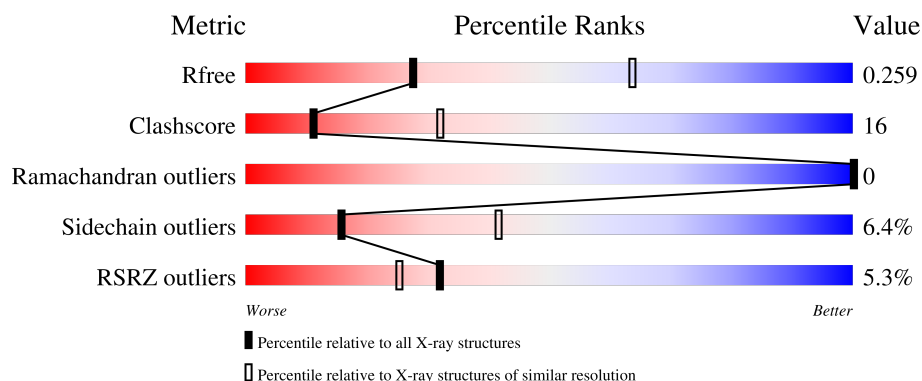
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	4% 63% 33% .
2	L	214	6% 73% 23% .
3	H	219	6% 69% 29% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7665 atoms, of which 11 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium-dependent dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	1	0
			4244	2844	662	718	20			

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

Continued on next page...

Continued from previous page...

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

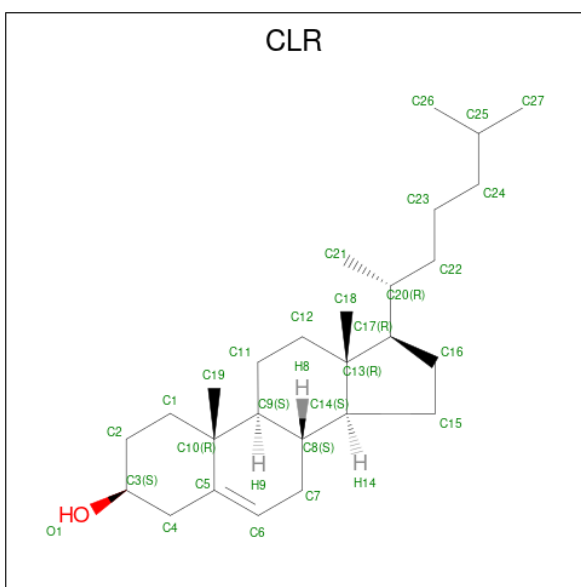
- Molecule 2 is a protein called Antibody fragment (Fab) 9D5 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1620	1008	268	336	8			

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

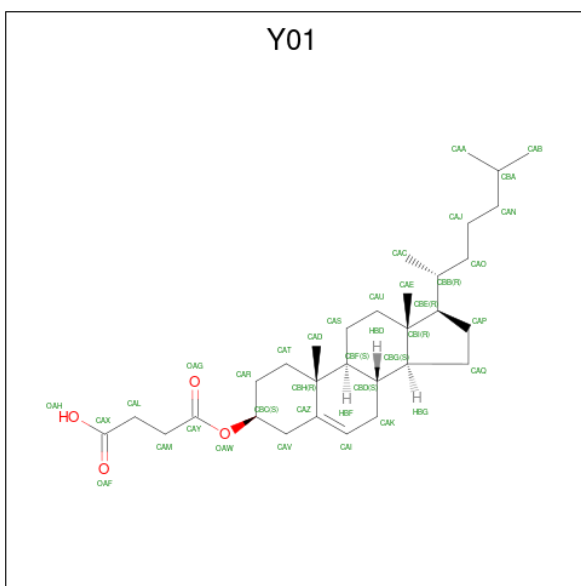
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1643	1034	278	323	8			

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



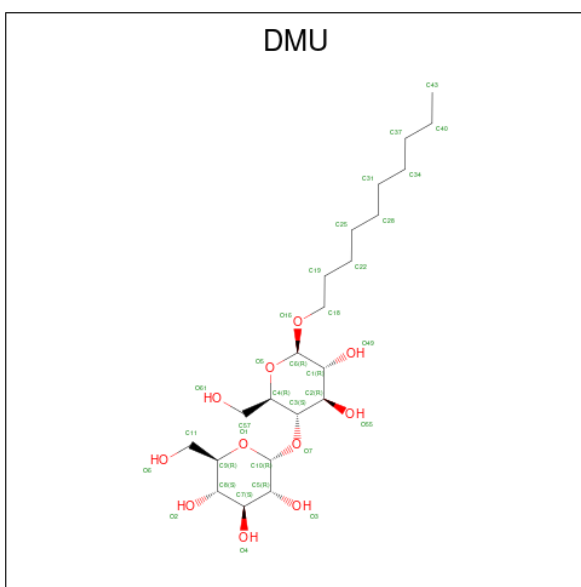
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		

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



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

- Molecule 6 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

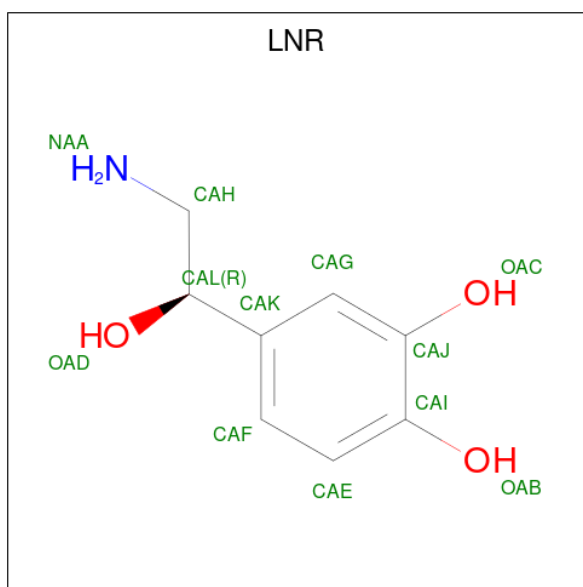
- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is L-NOREPINEPHRINE (CCD ID: LNR) (formula: C₈H₁₁NO₃) (labeled as "Ligand of Interest" by depositor).



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

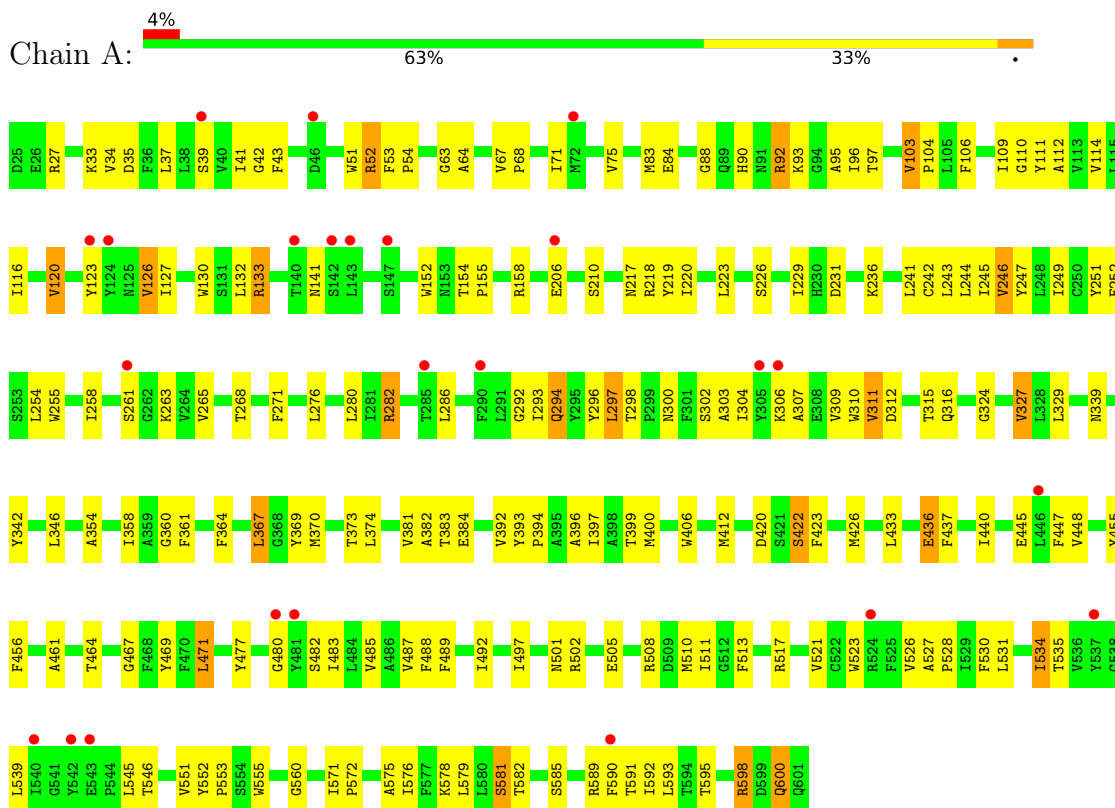
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	6	Total	O	0	0
			6	6		
10	L	11	Total	O	0	0
			11	11		
10	H	19	Total	O	0	0
			19	19		

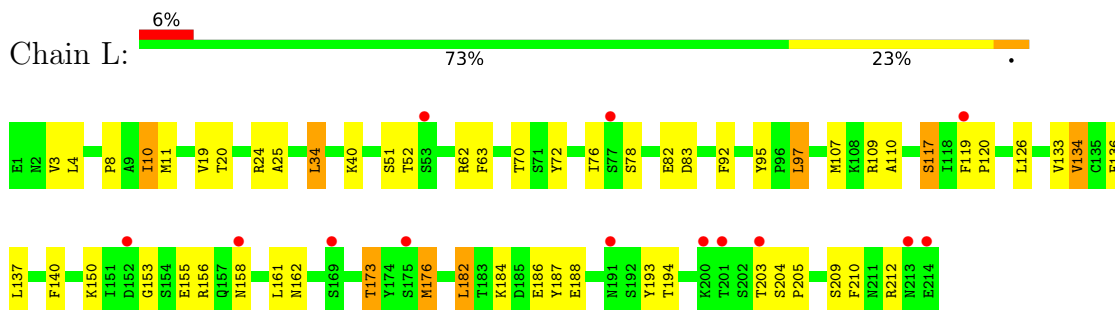
3 Residue-property plots

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.

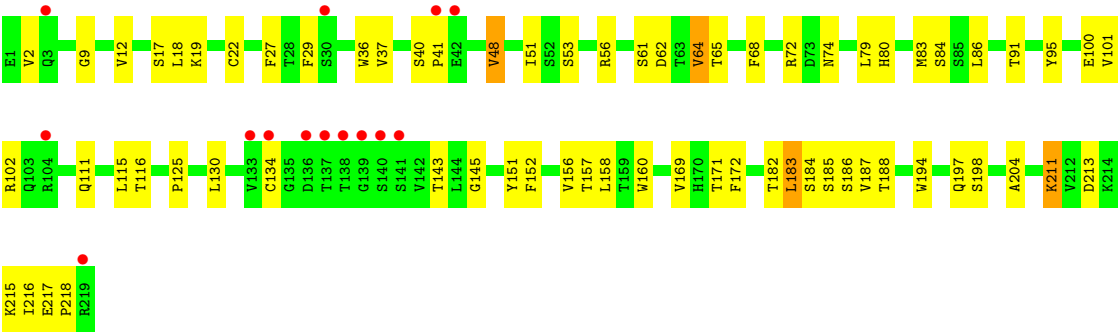
- Molecule 1: Sodium-dependent dopamine transporter



- Molecule 2: Antibody fragment (Fab) 9D5 Light chain



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.29Å 142.80Å 168.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.88 48.61 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.61-2.88) 99.9 (48.61-2.88)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.213 , 0.243 0.225 , 0.259	Depositor DCC
R_{free} test set	2687 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	93.6	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7665	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: NA, Y01, CL, DMU, CLR, LNR

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	0.10	0/4388	0.28	1/5991 (0.0%)
2	L	0.10	0/1658	0.31	0/2255
3	H	0.11	0/1682	0.33	0/2292
All	All	0.10	0/7728	0.30	1/10538 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	GLY	N-CA-C	5.06	125.18	113.18

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	4244	0	4186	149	0
2	L	1620	0	1525	42	0
3	H	1643	0	1590	59	0
4	A	28	0	46	3	0
5	A	35	0	49	0	0
6	A	33	0	42	3	0
7	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
9	A	12	11	11	0	0
10	A	6	0	0	0	0
10	H	19	0	0	3	0
10	L	11	0	0	0	0
All	All	7654	11	7449	246	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 16.

All (246) 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:9:GLY:HA2	3:H:18:LEU:HD21	1.21	1.13
3:H:169:VAL:HG12	3:H:187:VAL:HG12	1.35	1.04
1:A:75:VAL:CG1	1:A:526:VAL:HG11	2.00	0.91
3:H:9:GLY:HA2	3:H:18:LEU:CD2	2.07	0.84
1:A:396:ALA:O	1:A:399:THR:HG22	1.81	0.81
1:A:27:ARG:NH1	1:A:92:ARG:O	2.14	0.81
1:A:369:TYR:O	1:A:373:THR:HG22	1.82	0.80
1:A:589:ARG:HA	1:A:592:ILE:HG22	1.65	0.79
2:L:162:ASN:HB3	2:L:176:MET:HE2	1.62	0.79
1:A:370:MET:HE1	1:A:392:VAL:HG13	1.65	0.78
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.19	0.77
1:A:75:VAL:HG12	1:A:526:VAL:HG11	1.65	0.77
1:A:303:ALA:HA	1:A:306:LYS:HE3	1.65	0.76
1:A:369:TYR:CE1	1:A:373:THR:HG21	2.23	0.74
1:A:282:ARG:O	1:A:282:ARG:HD3	1.88	0.74
1:A:27:ARG:HH12	1:A:93:LYS:HA	1.53	0.73
1:A:477:TYR:CD2	1:A:560:GLY:HA3	2.23	0.73
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.71	0.72
1:A:123:TYR:HB2	1:A:471:LEU:HD13	1.72	0.71
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.73	0.70
1:A:294:GLN:O	1:A:298:THR:HG23	1.91	0.70
1:A:437:PHE:HB2	1:A:440:ILE:HD13	1.74	0.69
6:A:703:DMU:O55	6:A:703:DMU:O3	2.10	0.69
1:A:68:PRO:HD3	1:A:304:ILE:HD12	1.74	0.69
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.74	0.69
1:A:258:ILE:HA	1:A:261:SER:HB3	1.75	0.69
3:H:183:LEU:HD12	3:H:184:SER:N	2.08	0.68
1:A:370:MET:HE1	1:A:392:VAL:CG1	2.22	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.30	0.67
1:A:152:TRP:O	1:A:218:ARG:HD3	1.94	0.67
1:A:219:TYR:HD2	1:A:220:ILE:HD12	1.59	0.67
1:A:535:THR:O	1:A:539:LEU:HD13	1.95	0.67
1:A:591:THR:O	1:A:595:THR:HG23	1.95	0.67
2:L:194:THR:HG23	2:L:209:SER:OG	1.95	0.67
1:A:575:ALA:O	1:A:579:LEU:HB2	1.95	0.67
1:A:33:LYS:HE3	1:A:339:ASN:HD21	1.59	0.66
3:H:29:PHE:O	3:H:72:ARG:NH2	2.30	0.65
1:A:546:THR:HG22	1:A:551:VAL:HA	1.78	0.65
3:H:197:GLN:NE2	10:H:302:HOH:O	2.29	0.65
1:A:220:ILE:O	1:A:236:LYS:HE2	1.97	0.65
1:A:303:ALA:HA	1:A:306:LYS:CE	2.27	0.64
3:H:171:THR:HG22	3:H:185:SER:OG	1.96	0.64
1:A:133:ARG:NH2	6:A:703:DMU:H30	2.12	0.64
2:L:194:THR:HG23	2:L:209:SER:HG	1.62	0.63
1:A:578:LYS:HA	1:A:581:SER:HB2	1.80	0.63
3:H:83:MET:HE1	3:H:115:LEU:HD22	1.81	0.63
1:A:219:TYR:CD2	1:A:220:ILE:HD12	2.33	0.63
3:H:17:SER:HB3	3:H:84:SER:HA	1.80	0.63
1:A:369:TYR:OH	1:A:399:THR:HG23	1.99	0.62
3:H:169:VAL:CG1	3:H:187:VAL:HG12	2.21	0.62
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.82	0.62
1:A:268:THR:OG1	1:A:420:ASP:OD1	2.14	0.62
3:H:91:THR:HG23	3:H:116:THR:HA	1.81	0.62
1:A:123:TYR:HB2	1:A:471:LEU:CD1	2.31	0.61
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.35	0.61
2:L:136:PHE:C	2:L:137:LEU:HD12	2.25	0.61
3:H:172:PHE:O	3:H:183:LEU:HD13	2.00	0.61
1:A:282:ARG:HD3	1:A:282:ARG:C	2.23	0.60
2:L:120:PRO:HB3	2:L:210:PHE:CE1	2.38	0.59
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.37	0.59
2:L:126:LEU:O	2:L:184:LYS:HD2	2.01	0.59
1:A:52:ARG:HG2	1:A:316:GLN:OE1	2.01	0.59
1:A:84:GLU:OE1	1:A:324:GLY:N	2.32	0.59
3:H:64:VAL:HG13	3:H:68:PHE:HB2	1.83	0.59
1:A:300:ASN:OD1	1:A:302:SER:HB3	2.03	0.58
2:L:134:VAL:HG21	3:H:130:LEU:HD13	1.85	0.58
3:H:36:TRP:O	3:H:48:VAL:HG13	2.03	0.58
1:A:93:LYS:HD2	1:A:97:THR:HG21	1.85	0.58
1:A:461:ALA:O	1:A:464:THR:HG22	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ARG:HD2	1:A:508:ARG:O	2.04	0.57
1:A:123:TYR:O	1:A:126:VAL:HG13	2.04	0.57
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.86	0.57
1:A:545:LEU:HG	1:A:552:TYR:CD1	2.40	0.57
1:A:585:SER:O	1:A:589:ARG:HG3	2.04	0.56
1:A:97:THR:OG1	1:A:436:GLU:HG2	2.06	0.56
1:A:64:ALA:O	1:A:304:ILE:HD11	2.06	0.56
1:A:245:ILE:O	1:A:249:ILE:HG13	2.07	0.55
1:A:109:ILE:HD11	1:A:489:PHE:HB3	1.89	0.55
1:A:226:SER:OG	1:A:231:ASP:O	2.17	0.55
1:A:43:PHE:CD1	1:A:327:VAL:HG21	2.41	0.55
2:L:156:ARG:NH1	2:L:158:ASN:HB3	2.22	0.55
1:A:307:ALA:O	1:A:311:VAL:HG12	2.07	0.55
3:H:143:THR:HG22	3:H:188:THR:CG2	2.37	0.55
4:A:701:CLR:H121	4:A:701:CLR:H212	1.88	0.54
1:A:393:TYR:CE2	1:A:397:ILE:HD11	2.41	0.54
1:A:303:ALA:O	1:A:306:LYS:HG3	2.08	0.54
1:A:582:THR:OG1	1:A:589:ARG:HD2	2.07	0.54
2:L:62:ARG:NH1	2:L:83:ASP:OD2	2.41	0.54
1:A:106:PHE:HE2	1:A:497:ILE:CD1	2.20	0.54
3:H:143:THR:HG22	3:H:188:THR:HB	1.90	0.54
2:L:140:PHE:O	2:L:173:THR:HG22	2.07	0.54
1:A:242:CYS:O	1:A:246:VAL:HG13	2.08	0.53
1:A:292:GLY:HA3	1:A:364:PHE:O	2.09	0.53
1:A:37:LEU:O	1:A:41:ILE:HG12	2.08	0.53
2:L:156:ARG:HH12	2:L:158:ASN:HB3	1.73	0.53
1:A:508:ARG:NE	3:H:100:GLU:O	2.32	0.53
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.90	0.52
1:A:116:ILE:O	1:A:120:VAL:HG13	2.09	0.52
3:H:151:TYR:CE2	3:H:156:VAL:HG13	2.45	0.52
1:A:75:VAL:HG13	1:A:526:VAL:HG11	1.87	0.52
1:A:103:VAL:HG22	1:A:106:PHE:HB2	1.91	0.52
2:L:184:LYS:HE2	2:L:188:GLU:OE2	2.09	0.52
3:H:188:THR:HG23	10:H:307:HOH:O	2.09	0.52
1:A:110:GLY:O	1:A:114:VAL:HG23	2.10	0.52
1:A:303:ALA:CA	1:A:306:LYS:HE3	2.38	0.52
2:L:63:PHE:CE1	2:L:76:ILE:HG12	2.45	0.51
1:A:571:ILE:HB	1:A:572:PRO:CD	2.40	0.51
1:A:501:ASN:OD1	1:A:502:ARG:N	2.43	0.51
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.92	0.51
2:L:161:LEU:CD1	3:H:182:THR:HB	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HB2	1:A:456:PHE:CE2	2.45	0.51
1:A:487:VAL:HG12	1:A:531:LEU:HD11	1.93	0.51
1:A:464:THR:HG23	1:A:467:GLY:N	2.26	0.51
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.92	0.51
1:A:35:ASP:OD2	1:A:263:LYS:HE3	2.10	0.51
1:A:95:ALA:HA	1:A:329:LEU:CD2	2.41	0.51
3:H:12:VAL:HG11	3:H:86:LEU:HD12	1.93	0.51
3:H:188:THR:O	10:H:301:HOH:O	2.19	0.50
1:A:223:LEU:HD11	1:A:469:TYR:CE2	2.46	0.50
3:H:215:LYS:HE2	3:H:217:GLU:CD	2.37	0.50
1:A:96:ILE:HD13	1:A:111:TYR:CE1	2.46	0.50
1:A:276:LEU:O	1:A:280:LEU:HB2	2.11	0.50
1:A:354:ALA:O	1:A:358:ILE:HG12	2.12	0.50
1:A:39:SER:HA	1:A:265:VAL:HG11	1.94	0.50
1:A:271:PHE:CE2	1:A:412:MET:HG3	2.46	0.50
1:A:367:LEU:HD21	1:A:382:ALA:HA	1.93	0.50
1:A:219:TYR:HD2	1:A:220:ILE:CD1	2.25	0.50
1:A:63:GLY:N	1:A:297:LEU:O	2.30	0.50
1:A:433:LEU:HD12	1:A:447:PHE:CZ	2.47	0.50
1:A:104:PRO:HD2	1:A:593:LEU:O	2.11	0.50
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.77	0.50
1:A:154:THR:HB	1:A:155:PRO:HD2	1.94	0.49
1:A:511:ILE:HD12	1:A:513:PHE:CZ	2.47	0.49
2:L:95:TYR:OH	3:H:102:ARG:NH2	2.44	0.49
3:H:19:LYS:HE2	3:H:80:HIS:ND1	2.26	0.49
1:A:296:TYR:CD1	1:A:297:LEU:HD13	2.48	0.49
1:A:572:PRO:O	1:A:576:ILE:HG12	2.11	0.49
3:H:9:GLY:CA	3:H:18:LEU:HD21	2.15	0.49
2:L:120:PRO:HB3	2:L:210:PHE:CZ	2.47	0.49
2:L:187:TYR:O	2:L:193:TYR:OH	2.30	0.49
1:A:293:ILE:HD12	1:A:361:PHE:CD1	2.48	0.49
2:L:119:PHE:HB2	2:L:134:VAL:HG22	1.94	0.49
3:H:143:THR:HG22	3:H:188:THR:HG22	1.95	0.49
1:A:252:PHE:HA	1:A:255:TRP:HB2	1.94	0.49
1:A:286:LEU:HD11	1:A:400:MET:HE1	1.94	0.49
3:H:211:LYS:NZ	3:H:213:ASP:OD1	2.46	0.48
1:A:296:TYR:CG	1:A:297:LEU:HD13	2.48	0.48
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.95	0.48
3:H:40:SER:HB2	3:H:41:PRO:HD2	1.93	0.48
1:A:103:VAL:CG2	1:A:106:PHE:HB2	2.44	0.48
1:A:96:ILE:CG2	1:A:436:GLU:HG3	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:SER:C	1:A:426:MET:HE2	2.38	0.48
2:L:137:LEU:HD12	2:L:137:LEU:N	2.28	0.48
1:A:598:ARG:C	1:A:600:GLN:H	2.22	0.48
1:A:83:MET:HE3	1:A:523:TRP:CD1	2.49	0.47
1:A:251:TYR:O	1:A:255:TRP:HB2	2.14	0.47
2:L:187:TYR:CZ	2:L:212:ARG:HD3	2.48	0.47
3:H:130:LEU:HB2	3:H:145:GLY:CA	2.44	0.47
1:A:27:ARG:NH1	1:A:93:LYS:HA	2.25	0.47
2:L:40:LYS:NZ	2:L:82:GLU:O	2.42	0.47
3:H:158:LEU:C	3:H:158:LEU:HD23	2.40	0.47
1:A:370:MET:HE1	1:A:381:VAL:HB	1.97	0.47
1:A:505:GLU:OE1	3:H:56:ARG:HD3	2.15	0.47
4:A:701:CLR:H212	4:A:701:CLR:H183	1.96	0.47
1:A:132:LEU:CD1	1:A:246:VAL:HG12	2.45	0.46
1:A:370:MET:O	1:A:374:LEU:HB2	2.14	0.46
2:L:4:LEU:HD22	2:L:25:ALA:HB2	1.98	0.46
1:A:383:THR:OG1	1:A:384:GLU:N	2.48	0.46
2:L:109:ARG:HG3	2:L:110:ALA:O	2.15	0.46
2:L:161:LEU:C	2:L:161:LEU:HD23	2.40	0.46
1:A:502:ARG:HG3	3:H:56:ARG:NH1	2.31	0.46
2:L:182:LEU:HB3	2:L:186:GLU:HG2	1.97	0.46
1:A:67:VAL:HB	1:A:68:PRO:HD3	1.98	0.46
3:H:18:LEU:HD12	3:H:19:LYS:H	1.80	0.45
1:A:545:LEU:HG	1:A:552:TYR:CE1	2.51	0.45
1:A:254:LEU:HD21	1:A:423:PHE:CD1	2.51	0.45
2:L:92:PHE:CE1	2:L:97:LEU:HD21	2.52	0.45
2:L:117:SER:HB2	2:L:119:PHE:HE1	1.82	0.45
3:H:72:ARG:NE	3:H:74:ASN:OD1	2.42	0.45
3:H:143:THR:HG22	3:H:188:THR:CB	2.47	0.45
1:A:90:HIS:HB2	1:A:510:MET:SD	2.56	0.45
2:L:188:GLU:O	2:L:212:ARG:NH2	2.50	0.45
3:H:143:THR:HA	3:H:187:VAL:O	2.16	0.45
1:A:51:TRP:CD1	1:A:51:TRP:C	2.95	0.45
1:A:370:MET:CE	1:A:381:VAL:HB	2.47	0.45
2:L:11:MET:CE	2:L:19:VAL:HG13	2.47	0.44
1:A:530:PHE:O	1:A:534:ILE:HG13	2.16	0.44
1:A:132:LEU:HD12	1:A:246:VAL:HG12	1.99	0.44
1:A:488:PHE:O	1:A:492:ILE:HG12	2.17	0.44
3:H:37:VAL:O	3:H:95:TYR:HB2	2.17	0.44
1:A:67:VAL:HB	1:A:68:PRO:CD	2.48	0.44
1:A:103:VAL:CG2	1:A:103:VAL:O	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HD2	1:A:133:ARG:HA	1.49	0.44
1:A:342:TYR:CZ	1:A:346:LEU:HD11	2.53	0.44
1:A:120:VAL:HA	1:A:123:TYR:CE2	2.53	0.44
1:A:517:ARG:O	1:A:521:VAL:HG23	2.18	0.43
2:L:161:LEU:HD13	3:H:182:THR:HB	2.00	0.43
1:A:158:ARG:O	1:A:210:SER:HA	2.18	0.43
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.52	0.43
1:A:553:PRO:HB2	1:A:555:TRP:CD1	2.53	0.43
2:L:150:LYS:HG2	2:L:155:GLU:HA	1.99	0.43
3:H:27:PHE:CE2	3:H:29:PHE:HA	2.54	0.43
3:H:130:LEU:HB2	3:H:145:GLY:C	2.43	0.43
1:A:42:GLY:C	1:A:420:ASP:HB3	2.43	0.43
3:H:143:THR:CG2	3:H:188:THR:HG22	2.48	0.43
2:L:150:LYS:HD2	2:L:153:GLY:O	2.19	0.43
3:H:156:VAL:CG2	3:H:183:LEU:HD23	2.49	0.43
1:A:241:LEU:CD2	6:A:703:DMU:H12	2.49	0.42
1:A:445:GLU:H	1:A:445:GLU:CD	2.25	0.42
3:H:151:TYR:O	3:H:152:PHE:HB2	2.19	0.42
3:H:157:THR:OG1	3:H:204:ALA:HB3	2.19	0.42
3:H:62:ASP:O	3:H:65:THR:HG22	2.19	0.42
1:A:440:ILE:N	1:A:440:ILE:HD12	2.34	0.42
1:A:247:TYR:CZ	1:A:455:TYR:HB3	2.55	0.42
1:A:312:ASP:O	1:A:315:THR:HG22	2.19	0.42
1:A:367:LEU:HD12	1:A:370:MET:HE2	2.01	0.42
1:A:393:TYR:HB3	1:A:394:PRO:HD3	2.02	0.42
2:L:10:ILE:N	2:L:10:ILE:HD12	2.35	0.42
3:H:194:TRP:CH2	3:H:218:PRO:HG3	2.54	0.42
1:A:88:GLY:CA	1:A:329:LEU:HD12	2.50	0.41
3:H:22:CYS:HB3	3:H:79:LEU:HB3	2.02	0.41
3:H:169:VAL:HA	3:H:186:SER:O	2.20	0.41
1:A:243:LEU:O	1:A:246:VAL:HG22	2.19	0.41
1:A:71:ILE:HD12	1:A:310:TRP:HH2	1.85	0.41
3:H:51:ILE:HD13	3:H:72:ARG:HB2	2.01	0.41
1:A:112:ALA:O	1:A:116:ILE:HG13	2.20	0.41
1:A:315:THR:HA	1:A:534:ILE:HD13	2.01	0.41
4:A:701:CLR:H121	4:A:701:CLR:C21	2.51	0.41
3:H:216:ILE:N	3:H:216:ILE:HD12	2.35	0.41
2:L:24:ARG:NH2	2:L:70:THR:OG1	2.53	0.41
1:A:370:MET:SD	1:A:396:ALA:HB2	2.60	0.41
1:A:236:LYS:HB3	1:A:236:LYS:HE3	1.84	0.41
2:L:8:PRO:HG2	2:L:11:MET:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:107:MET:HE2	2:L:107:MET:HA	2.03	0.41
1:A:127:ILE:HD13	1:A:130:TRP:CZ3	2.56	0.41
1:A:43:PHE:CE1	1:A:327:VAL:HG21	2.56	0.40
1:A:483:ILE:HD12	1:A:483:ILE:HA	1.90	0.40
2:L:140:PHE:C	2:L:173:THR:HG22	2.47	0.40
3:H:160:TRP:CE2	3:H:187:VAL:HG13	2.55	0.40
2:L:204:SER:HB2	2:L:205:PRO:HD2	2.02	0.40
3:H:64:VAL:CG1	3:H:68:PHE:HB2	2.48	0.40
1:A:280:LEU:HD23	1:A:280:LEU:O	2.21	0.40
2:L:51:SER:O	2:L:52:THR:HB	2.20	0.40
2:L:162:ASN:CB	2:L:176:MET:HE2	2.42	0.40
1:A:297:LEU:O	1:A:298:THR:C	2.64	0.40
3:H:130:LEU:HB2	3:H:145:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/536 (100%)	512 (96%)	23 (4%)	0	100	100
2	L	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
3	H	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
All	All	964/969 (100%)	912 (95%)	52 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/440 (99%)	407 (93%)	29 (7%)	15	39
2	L	182/187 (97%)	169 (93%)	13 (7%)	13	37
3	H	181/187 (97%)	172 (95%)	9 (5%)	22	51
All	All	799/814 (98%)	748 (94%)	51 (6%)	16	42

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	52	ARG
1	A	92	ARG
1	A	103	VAL
1	A	120	VAL
1	A	126	VAL
1	A	133	ARG
1	A	141	ASN
1	A	206	GLU
1	A	217	ASN
1	A	229	ILE
1	A	246	VAL
1	A	282	ARG
1	A	294	GLN
1	A	297	LEU
1	A	309	VAL
1	A	311	VAL
1	A	327	VAL
1	A	367	LEU
1	A	422	SER
1	A	436	GLU
1	A	471	LEU
1	A	482	SER
1	A	485	VAL
1	A	534	ILE
1	A	581	SER
1	A	590	PHE
1	A	598	ARG
1	A	600	GLN
2	L	3	VAL
2	L	10	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	20	THR
2	L	34	LEU
2	L	78	SER
2	L	97	LEU
2	L	117	SER
2	L	133	VAL
2	L	134	VAL
2	L	173	THR
2	L	176	MET
2	L	182	LEU
2	L	203	THR
3	H	48	VAL
3	H	53	SER
3	H	61	SER
3	H	64	VAL
3	H	111	GLN
3	H	134	CYS
3	H	183	LEU
3	H	198	SER
3	H	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
2	L	54	ASN
2	L	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
6	DMU	A	703	-	34,34,34	0.58	1 (2%)	45,45,45	0.68	0
4	CLR	A	701	-	31,31,31	0.65	1 (3%)	48,48,48	1.71	12 (25%)
5	Y01	A	702	-	38,38,38	0.74	1 (2%)	57,57,57	1.62	11 (19%)
9	LNR	A	707	-	12,12,12	2.67	7 (58%)	16,16,16	0.62	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
6	DMU	A	703	-	-	7/19/59/59	0/2/2/2
4	CLR	A	701	-	-	2/10/68/68	0/4/4/4
5	Y01	A	702	-	-	11/19/77/77	0/4/4/4
9	LNR	A	707	-	-	1/6/6/6	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	707	LNR	CAG-CAJ	4.68	1.45	1.38
9	A	707	LNR	OAC-CAJ	4.42	1.45	1.36
9	A	707	LNR	CAH-CAL	3.48	1.62	1.51
9	A	707	LNR	CAF-CAE	2.98	1.43	1.38
9	A	707	LNR	OAB-CAI	2.81	1.42	1.36
9	A	707	LNR	CAI-CAJ	-2.64	1.35	1.40
5	A	702	Y01	CBH-CBF	-2.46	1.52	1.56
9	A	707	LNR	OAD-CAL	-2.30	1.37	1.42
6	A	703	DMU	O16-C6	2.16	1.43	1.40
4	A	701	CLR	C10-C9	-2.07	1.52	1.56

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	Y01	CBI-CBE-CBB	-4.59	112.40	119.50
4	A	701	CLR	C19-C10-C9	-4.23	106.91	111.66
5	A	702	Y01	OAW-CAY-CAM	4.04	120.21	111.48
4	A	701	CLR	C4-C5-C10	3.47	120.87	116.42
4	A	701	CLR	C13-C17-C20	-3.46	114.15	119.50
4	A	701	CLR	C15-C14-C13	-2.94	100.38	103.84
5	A	702	Y01	CAS-CAU-CBI	-2.86	107.92	112.74
4	A	701	CLR	C13-C14-C8	-2.82	110.42	114.41
5	A	702	Y01	CBI-CBG-CBD	-2.80	110.44	114.41
5	A	702	Y01	CAD-CBH-CBF	-2.80	108.52	111.66
5	A	702	Y01	CAQ-CBG-CBI	-2.72	100.64	103.84
5	A	702	Y01	CAK-CBD-CBG	-2.71	107.09	110.93
4	A	701	CLR	C4-C5-C6	-2.67	116.95	120.57
4	A	701	CLR	C2-C3-C4	-2.52	106.75	110.29
4	A	701	CLR	C7-C8-C14	-2.41	107.52	110.93
4	A	701	CLR	C15-C14-C8	-2.26	115.49	119.10
5	A	702	Y01	CAC-CBB-CBE	-2.23	109.53	112.88
5	A	702	Y01	CAQ-CBG-CBD	-2.21	115.58	119.10
4	A	701	CLR	C3-C4-C5	-2.13	108.66	112.05
5	A	702	Y01	CAS-CBF-CBH	-2.13	110.46	113.08
4	A	701	CLR	C18-C13-C14	-2.07	107.92	111.68
5	A	702	Y01	CAV-CAZ-CAI	-2.02	117.83	120.57
4	A	701	CLR	C1-C10-C5	2.00	112.20	108.74

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	Y01	OAG-CAY-OAW-CBC
6	A	703	DMU	C19-C18-O16-C6
5	A	702	Y01	CAM-CAY-OAW-CBC
5	A	702	Y01	CAJ-CAO-CBB-CAC
6	A	703	DMU	C3-C4-C57-O61
6	A	703	DMU	O5-C4-C57-O61
4	A	701	CLR	C22-C23-C24-C25
6	A	703	DMU	C25-C28-C31-C34
6	A	703	DMU	C19-C22-C25-C28
6	A	703	DMU	C31-C34-C37-C40
5	A	702	Y01	CAJ-CAO-CBB-CBE
5	A	702	Y01	CAC-CBB-CBE-CBI
5	A	702	Y01	CAJ-CAN-CBA-CAB

Continued on next page...

Continued from previous page...

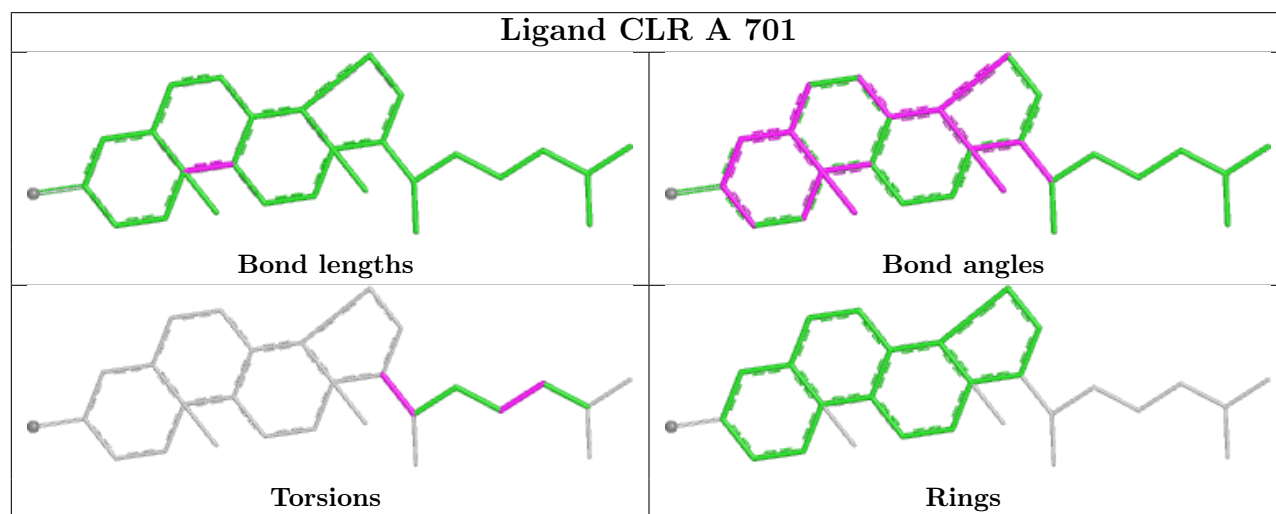
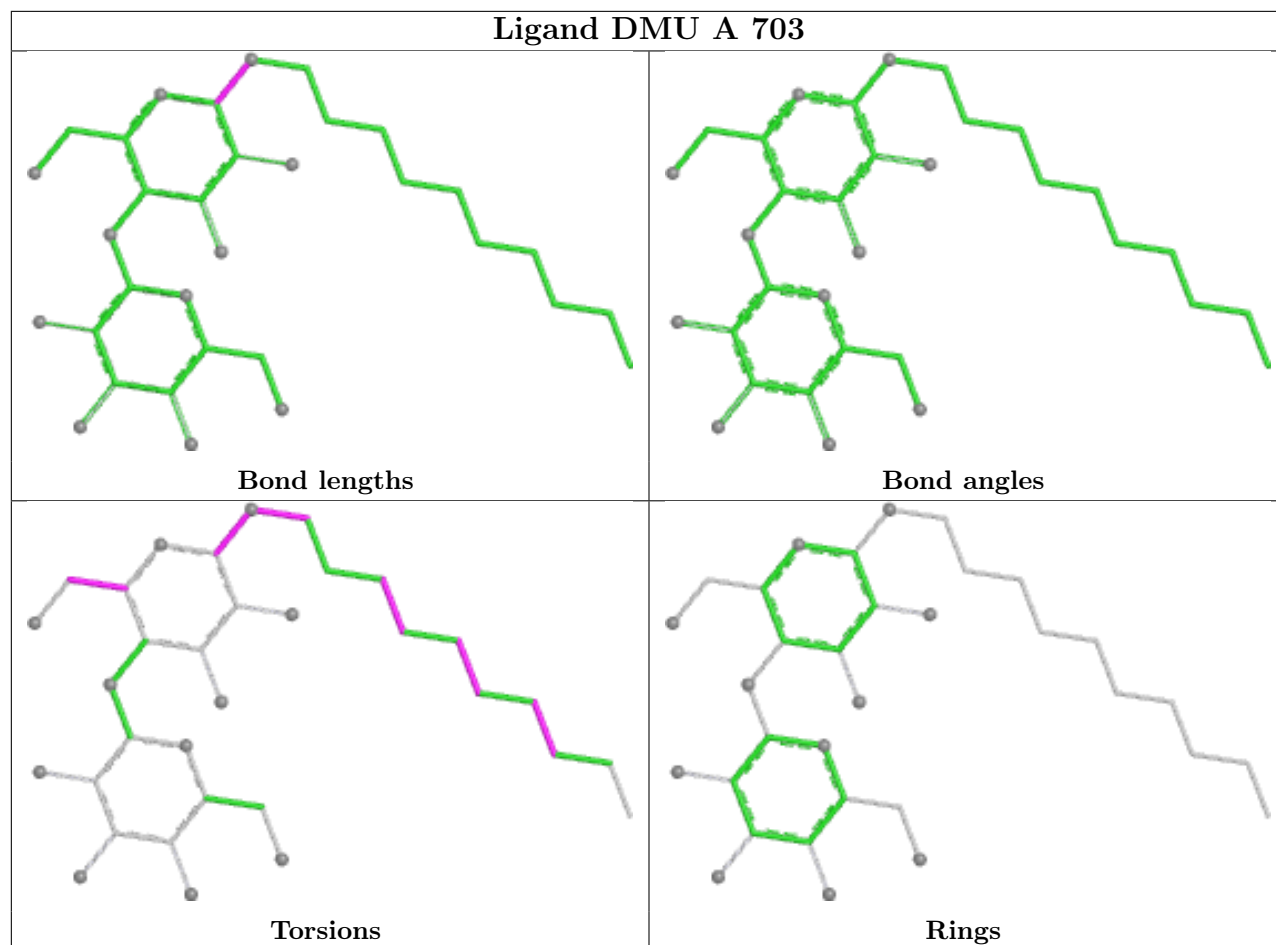
Mol	Chain	Res	Type	Atoms
5	A	702	Y01	CAO-CBB-CBE-CBI
5	A	702	Y01	CAJ-CAN-CBA-CAA
6	A	703	DMU	O5-C6-O16-C18
5	A	702	Y01	CAM-CAL-CAX-OAF
5	A	702	Y01	CAM-CAL-CAX-OAH
4	A	701	CLR	C16-C17-C20-C22
9	A	707	LNR	NAA-CAH-CAL-OAD
5	A	702	Y01	CAC-CBB-CBE-CAP

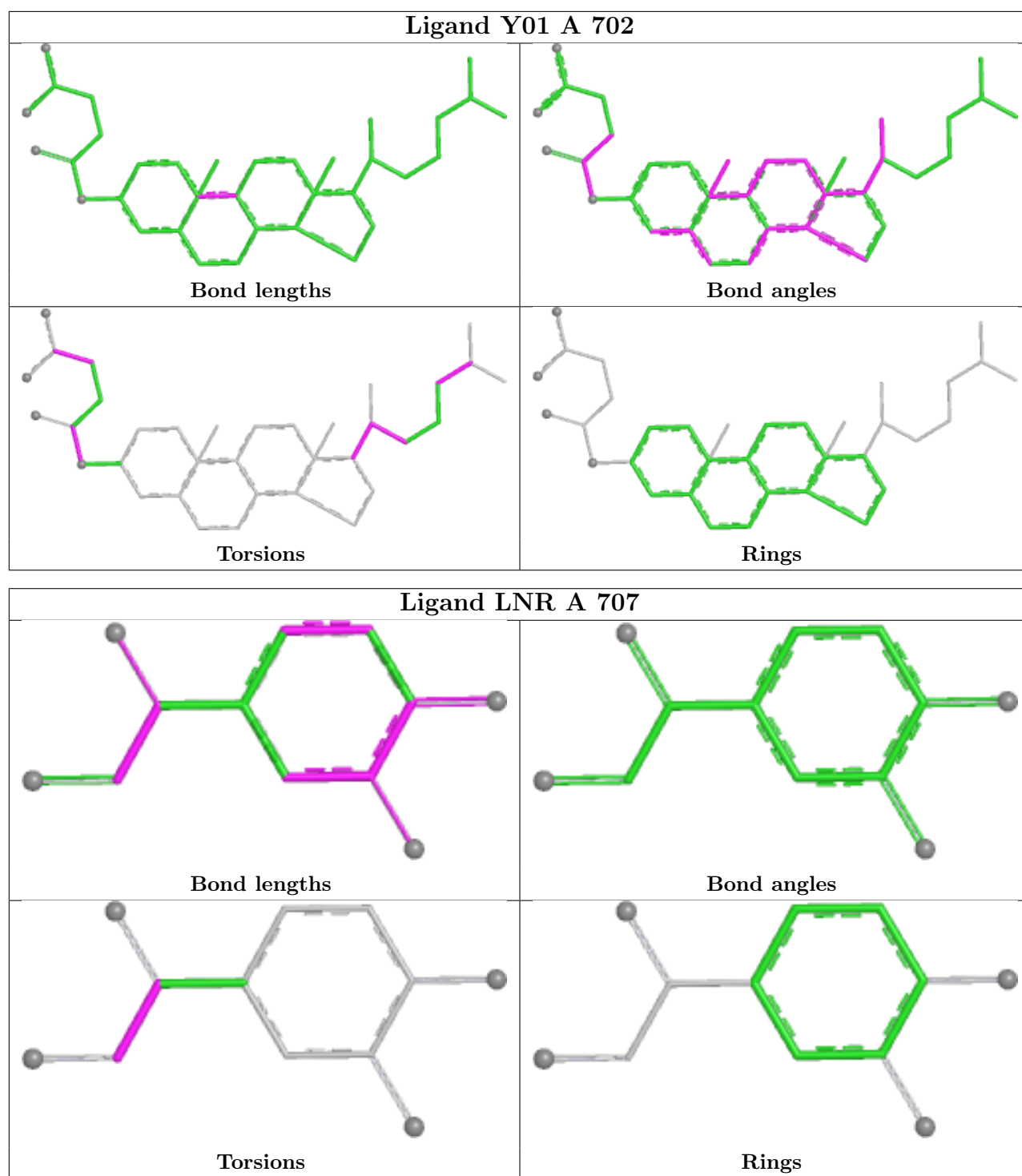
There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

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





5.7 Other polymers ⓘ

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, 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%)	0.38	24 (4%)	38	30	53, 88, 111, 149	1 (0%)
2	L	214/214 (100%)	0.29	13 (6%)	27	21	65, 84, 113, 148	0
3	H	219/219 (100%)	0.27	14 (6%)	25	20	71, 85, 119, 177	0
All	All	969/969 (100%)	0.33	51 (5%)	32	25	53, 86, 113, 177	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	THR	7.3
1	A	290	PHE	5.7
3	H	137	THR	4.4
1	A	142	SER	4.2
2	L	53	SER	4.0
2	L	152	ASP	3.9
1	A	481	TYR	3.6
1	A	480	GLY	3.5
3	H	136	ASP	3.4
1	A	285	THR	3.3
3	H	140	SER	3.3
1	A	206	GLU	3.2
3	H	30	SER	3.2
1	A	537	TYR	3.1
1	A	306	LYS	3.1
1	A	540	ILE	3.1
1	A	524	ARG	3.1
2	L	214	GLU	3.1
2	L	213	ASN	3.0
3	H	104	ARG	3.0
2	L	158	ASN	3.0
1	A	261	SER	2.9
3	H	3	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	543	GLU	2.9
1	A	305	TYR	2.8
1	A	446	LEU	2.8
1	A	123	TYR	2.7
2	L	201	THR	2.7
3	H	219	ARG	2.7
2	L	169	SER	2.7
3	H	133	VAL	2.6
1	A	39	SER	2.5
1	A	72[A]	MET	2.5
1	A	124	TYR	2.4
3	H	134	CYS	2.4
1	A	140	THR	2.4
2	L	203	THR	2.4
1	A	143	LEU	2.3
2	L	200	LYS	2.3
1	A	147	SER	2.3
2	L	175	SER	2.3
1	A	46	ASP	2.2
1	A	590	PHE	2.2
3	H	139	GLY	2.2
3	H	42	GLU	2.2
2	L	191	ASN	2.2
3	H	141	SER	2.1
2	L	119	PHE	2.1
2	L	77	SER	2.1
3	H	41	PRO	2.0
1	A	542	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

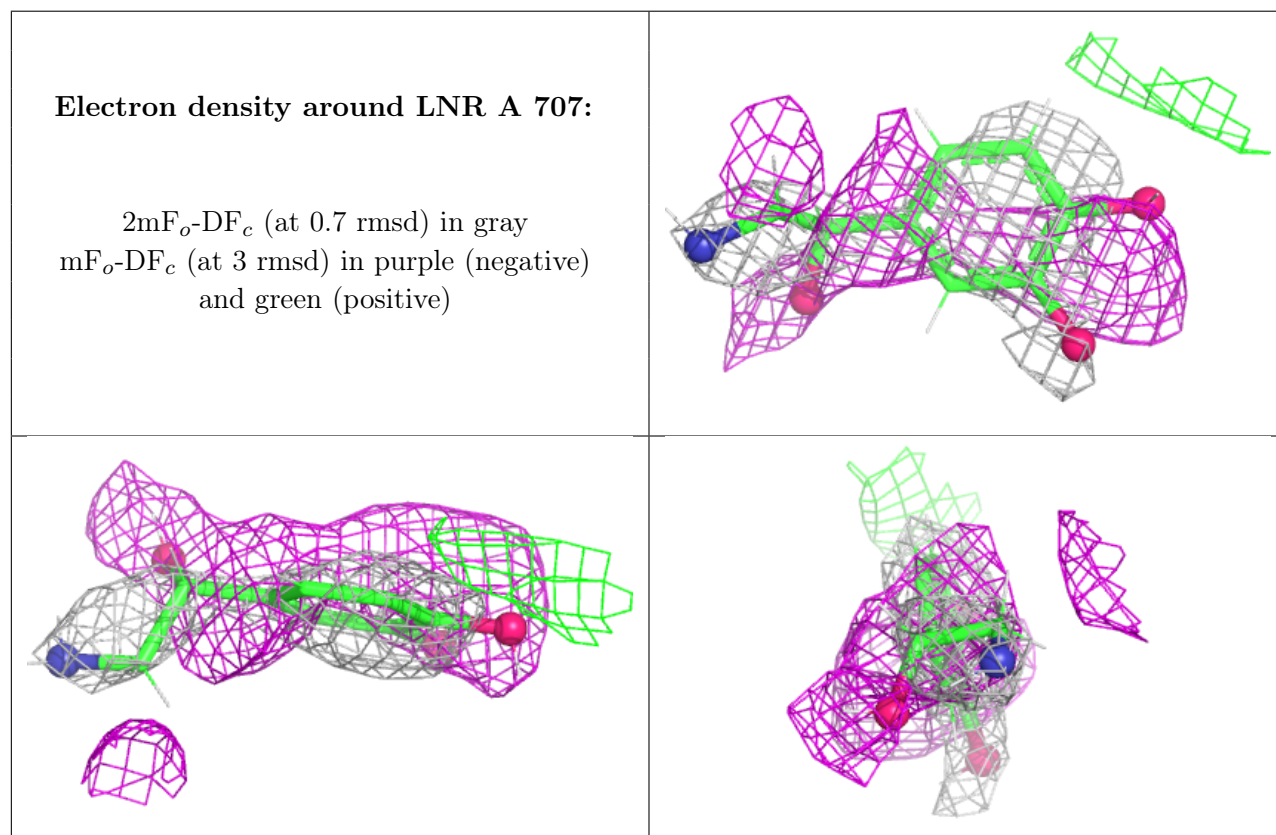
6.4 Ligands [i](#)

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, 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.

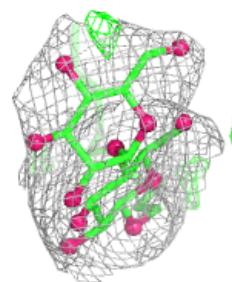
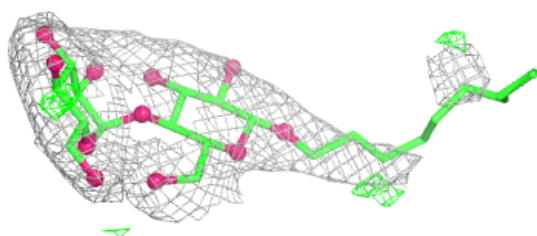
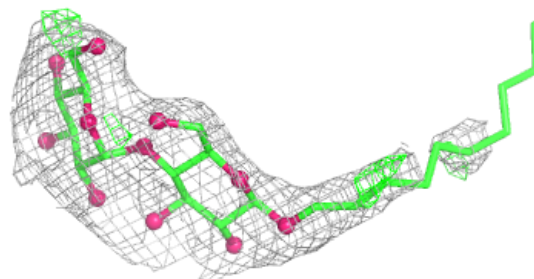
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	LNR	A	707	12/12	0.78	0.25	95,114,126,148	0
6	DMU	A	703	33/33	0.86	0.18	105,126,135,137	0
5	Y01	A	702	35/35	0.90	0.18	93,104,127,130	0
4	CLR	A	701	28/28	0.95	0.13	82,92,99,103	0
7	NA	A	704	1/1	0.96	0.07	88,88,88,88	0
7	NA	A	705	1/1	0.97	0.05	80,80,80,80	0
8	CL	A	706	1/1	0.99	0.10	83,83,83,83	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.

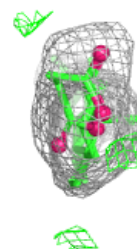
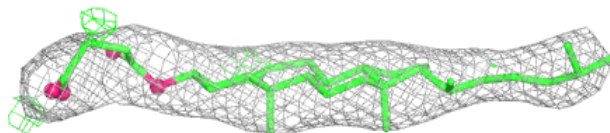
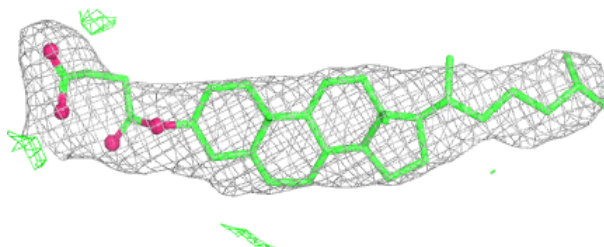


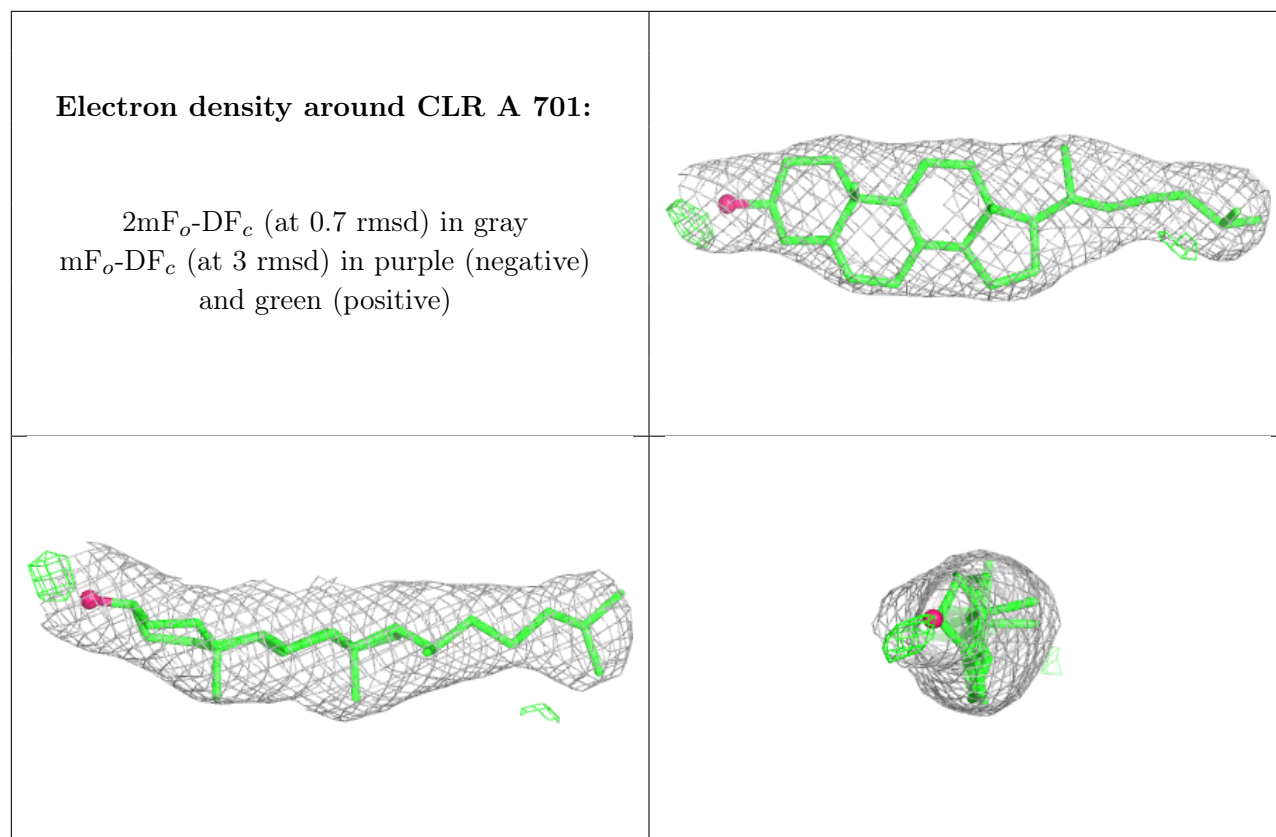
Electron density around DMU A 703:

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

**Electron density around Y01 A 702:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.