



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:46 PM UTC

PDB ID : 4XNU / pdb_00004xnu
Title : X-ray structure of Drosophila dopamine transporter in complex with nisoxetine
Authors : Aravind, P.; Wang, K.; Gouaux, E.
Deposited on : 2015-01-16
Resolution : 2.98 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

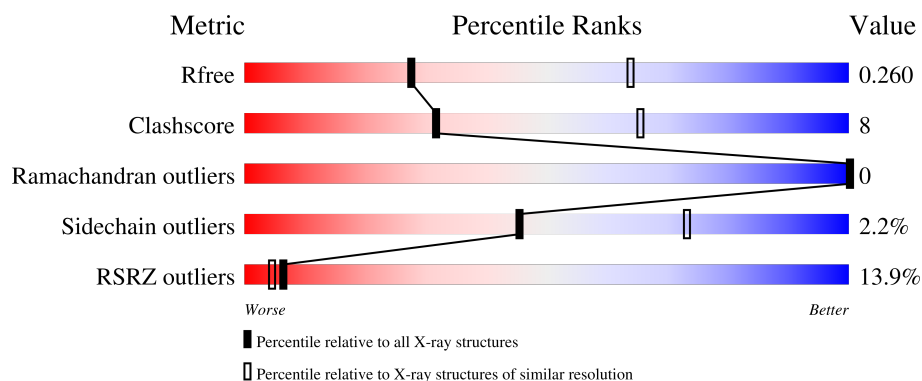
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	532	14% 82% 17% .
2	L	214	11% 83% 17%
3	H	240	15% 72% 17% 10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7470 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 Integral membrane protein-dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	2	0
			4192	2814	647	713	18			

- 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	0	0
			1621	1007	270	336	8			

- Molecule 3 is a protein called antibody fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1598	1009	270	312	7			

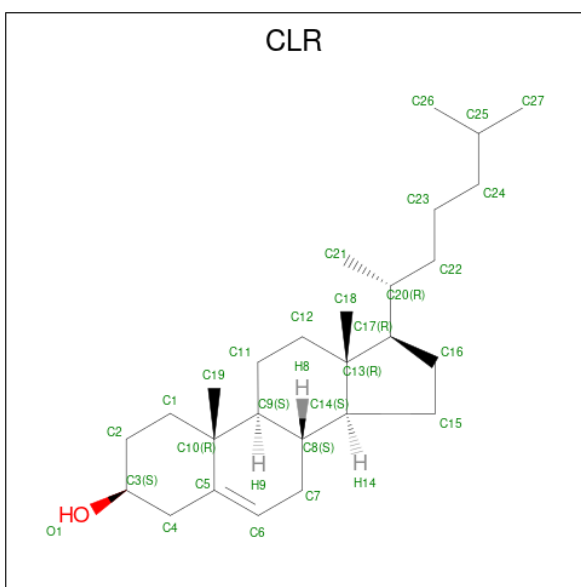
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

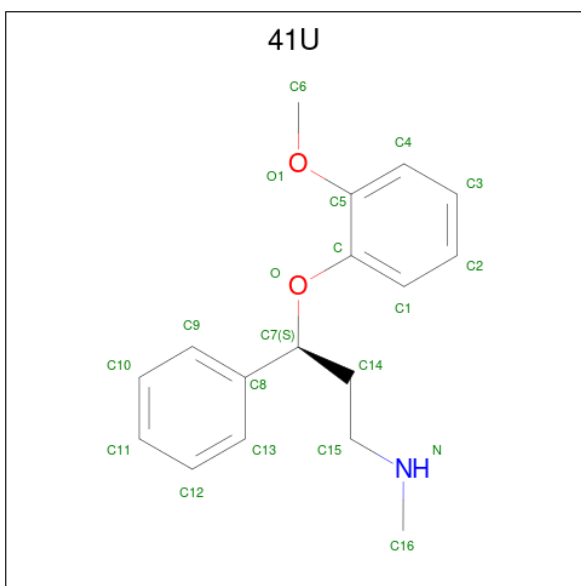
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 7 is nisoxetine (CCD ID: 41U) (formula: $C_{17}H_{21}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			20	17	1	2		

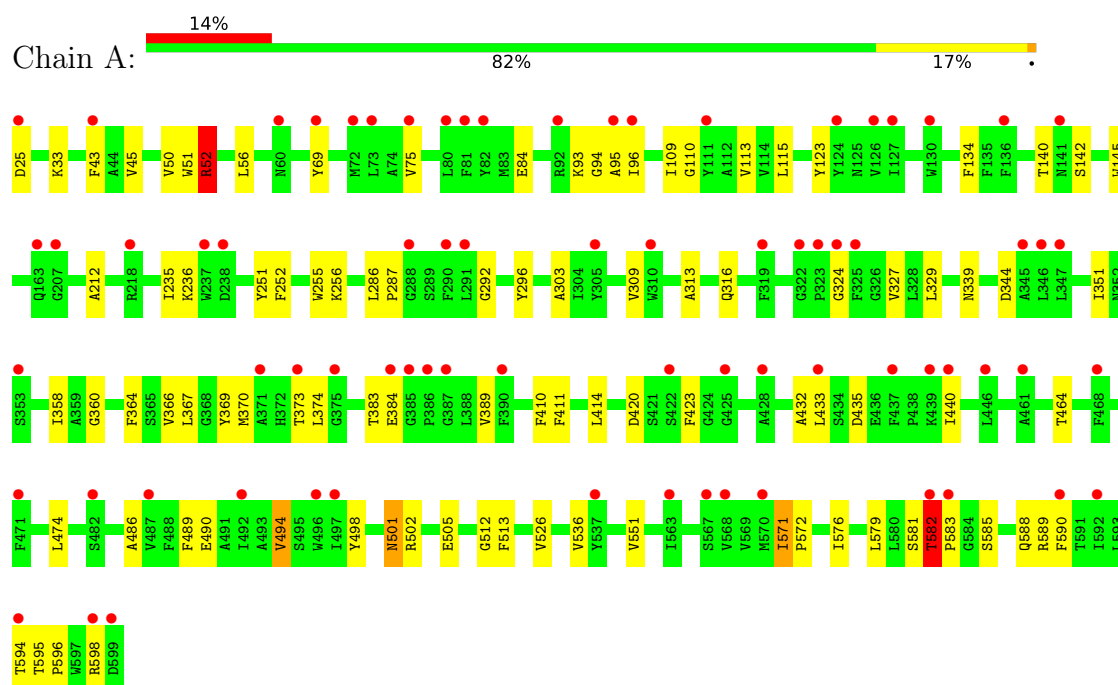
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total 8	O 8	0	0

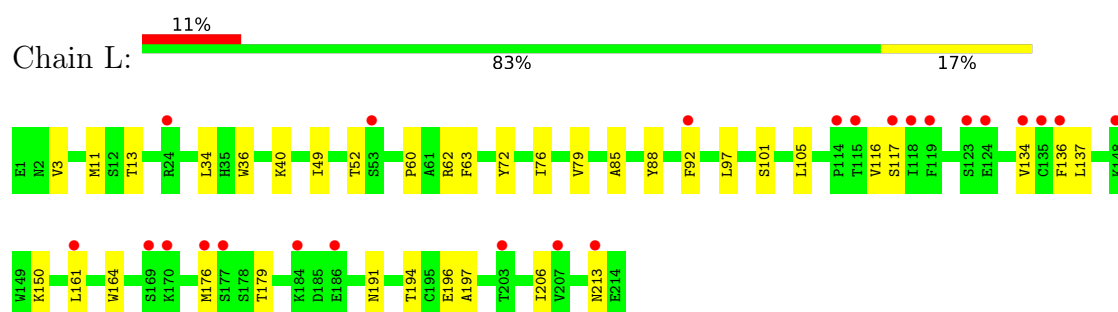
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Integral membrane protein-dopamine transporter

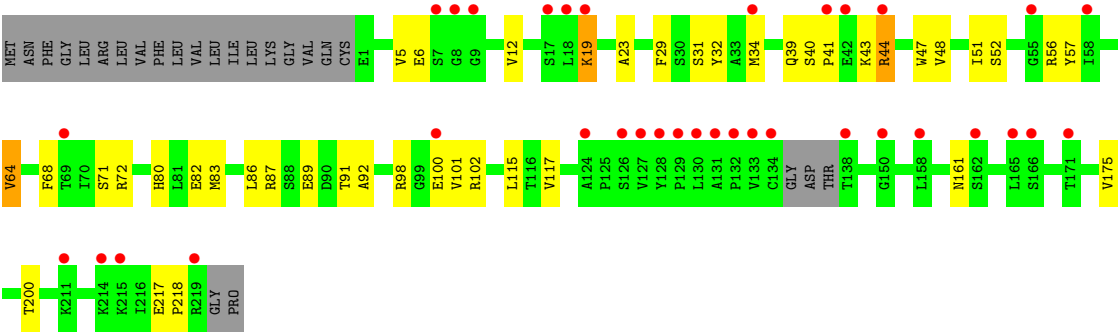


- Molecule 2: antibody fragment light chain



- 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, α , β , γ	96.90Å 133.67Å 161.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 2.98 47.10 – 2.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.10-2.98) 93.9 (47.10-2.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.251 0.236 , 0.260	Depositor DCC
R_{free} test set	1973 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7470	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 41U, NA, CLR, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	2/4340 (0.0%)	0.77	8/5932 (0.1%)
2	L	0.30	0/1659	0.72	0/2257
3	H	0.34	0/1636	0.77	0/2230
All	All	0.35	2/7635 (0.0%)	0.76	8/10419 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	THR	C-N	5.81	1.41	1.33
1	A	583	PRO	N-CD	5.06	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	VAL	N-CA-C	6.79	116.91	110.53
1	A	582	THR	CA-C-N	-6.38	113.41	119.85
1	A	582	THR	C-N-CA	-6.38	113.41	119.85
1	A	52	ARG	N-CA-C	5.63	120.16	113.12
1	A	25	ASP	CA-C-N	-5.51	115.28	123.11
1	A	25	ASP	C-N-CA	-5.51	115.28	123.11
1	A	571	ILE	CA-C-N	-5.13	113.42	119.84
1	A	571	ILE	C-N-CA	-5.13	113.42	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4192	0	4087	65	0
2	L	1621	0	1523	24	0
3	H	1598	0	1524	38	0
4	A	2	0	0	0	0
5	A	1	0	0	1	0
6	A	28	0	46	3	0
7	A	20	0	21	1	0
8	A	8	0	0	4	0
All	All	7470	0	7201	118	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 8.

All (118) 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:40:SER:HB3	3:H:41:PRO:HD2	1.53	0.91
3:H:91:THR:HG22	3:H:117:VAL:H	1.46	0.78
3:H:31:SER:O	3:H:100:GLU:OE1	2.08	0.72
1:A:585:SER:H	1:A:588:GLN:HB2	1.55	0.71
3:H:89:GLU:N	3:H:89:GLU:OE1	2.24	0.71
2:L:197:ALA:HB3	2:L:206:ILE:HD11	1.72	0.70
3:H:34:MET:SD	3:H:98:ARG:HB2	2.32	0.70
1:A:598:ARG:O	8:A:707:HOH:O	2.09	0.69
1:A:252:PHE:HA	1:A:255:TRP:CD1	2.30	0.67
1:A:502[A]:ARG:NH2	8:A:707:HOH:O	2.22	0.66
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.78	0.66
3:H:39:GLN:O	3:H:92:ALA:HB1	1.95	0.66
1:A:33:LYS:NZ	1:A:339:ASN:OD1	2.30	0.65
3:H:48:VAL:HG13	3:H:64:VAL:HG21	1.79	0.65
1:A:502[B]:ARG:NH2	8:A:707:HOH:O	2.22	0.64
1:A:512:GLY:HA2	3:H:102:ARG:HG3	1.79	0.64
1:A:585:SER:O	1:A:589:ARG:HG2	1.97	0.64
3:H:40:SER:CB	3:H:41:PRO:HD2	2.27	0.62
3:H:83:MET:HE1	3:H:115:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.83	0.60
1:A:94:GLY:HA3	1:A:432:ALA:HA	1.83	0.60
1:A:43:PHE:CZ	1:A:327:VAL:HG11	2.37	0.60
2:L:134:VAL:HG22	2:L:179:THR:HG23	1.85	0.59
2:L:40:LYS:HD3	2:L:85:ALA:HB2	1.83	0.59
1:A:93:LYS:HE3	1:A:435:ASP:HB3	1.84	0.59
2:L:62:ARG:HG3	2:L:76:ILE:HG23	1.84	0.58
3:H:71:SER:HB2	3:H:80:HIS:HB2	1.85	0.58
1:A:94:GLY:N	1:A:435:ASP:OD2	2.36	0.58
1:A:52:ARG:HH11	1:A:52:ARG:HG3	1.69	0.57
1:A:84:GLU:OE1	1:A:324:GLY:N	2.34	0.57
1:A:255:TRP:CZ3	1:A:256:LYS:HE2	2.40	0.56
2:L:101:SER:O	3:H:44:ARG:HD2	2.04	0.56
3:H:64:VAL:HG13	3:H:68:PHE:HB2	1.87	0.56
1:A:303:ALA:HB1	1:A:309:VAL:HG21	1.87	0.56
1:A:33:LYS:NZ	1:A:344:ASP:OD2	2.38	0.55
2:L:13:THR:HG21	2:L:79:VAL:HG21	1.89	0.55
3:H:39:GLN:O	3:H:92:ALA:CB	2.56	0.54
1:A:96:ILE:HA	1:A:110:GLY:HA3	1.89	0.54
1:A:287:PRO:HG2	1:A:373:THR:HG21	1.90	0.54
3:H:87:ARG:HB3	3:H:89:GLU:OE1	2.07	0.54
2:L:150:LYS:HB2	2:L:194:THR:HB	1.90	0.53
1:A:590:PHE:O	1:A:594:THR:N	2.43	0.52
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.91	0.52
1:A:235:ILE:HG12	1:A:464:THR:HG22	1.92	0.51
1:A:51:TRP:C	1:A:51:TRP:CD1	2.88	0.51
1:A:123:TYR:HB3	1:A:474:LEU:HD12	1.91	0.51
2:L:88:TYR:OH	3:H:43:LYS:O	2.26	0.51
1:A:286:LEU:HD13	1:A:369:TYR:CG	2.46	0.51
1:A:582:THR:O	1:A:589:ARG:NH1	2.44	0.50
2:L:164:TRP:CE2	2:L:176:MET:HG3	2.46	0.50
1:A:433:LEU:HB3	1:A:440:ILE:HD11	1.92	0.50
1:A:358:ILE:HD13	6:A:604:CLR:H263	1.94	0.50
1:A:109:ILE:HG21	1:A:490:GLU:HG2	1.93	0.50
2:L:191:ASN:ND2	2:L:213:ASN:OD1	2.45	0.49
1:A:512:GLY:CA	3:H:102:ARG:HG3	2.42	0.49
2:L:52:THR:HG21	2:L:72:TYR:CD2	2.47	0.49
3:H:32:TYR:CB	3:H:98:ARG:HD2	2.43	0.48
3:H:52:SER:HB3	3:H:57:TYR:HB2	1.95	0.48
1:A:255:TRP:CD1	1:A:255:TRP:H	2.31	0.48
2:L:34:LEU:HD13	2:L:72:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:92:PHE:CE1	2:L:97:LEU:HD11	2.49	0.47
1:A:52:ARG:HH11	1:A:52:ARG:CG	2.28	0.47
3:H:83:MET:HE2	3:H:86:LEU:HD21	1.96	0.47
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.50	0.46
2:L:97:LEU:HB2	3:H:47:TRP:CD2	2.51	0.46
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.97	0.46
3:H:6:GLU:N	3:H:6:GLU:OE1	2.49	0.46
1:A:582:THR:OG1	1:A:589:ARG:HD3	2.17	0.45
1:A:383:THR:OG1	1:A:384:GLU:N	2.50	0.45
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.52	0.45
1:A:494:VAL:HA	1:A:498:TYR:HB3	1.98	0.45
1:A:590:PHE:O	1:A:594:THR:OG1	2.21	0.45
1:A:351:ILE:HD13	6:A:604:CLR:H71	1.99	0.44
1:A:389:VAL:HB	1:A:414:LEU:HD21	1.98	0.44
2:L:92:PHE:CD1	3:H:102:ARG:HD3	2.52	0.44
1:A:292:GLY:HA3	1:A:364:PHE:O	2.17	0.44
1:A:582:THR:OG1	1:A:589:ARG:CD	2.66	0.44
2:L:92:PHE:CE2	2:L:97:LEU:HD21	2.53	0.43
1:A:69:TYR:HA	1:A:313:ALA:HB1	2.00	0.43
2:L:161:LEU:HD21	3:H:175:VAL:HB	2.01	0.43
3:H:12:VAL:O	3:H:117:VAL:HA	2.18	0.43
1:A:502[B]:ARG:HH21	3:H:56:ARG:HH11	1.66	0.43
1:A:370:MET:HG2	1:A:374:LEU:HD22	2.01	0.43
1:A:51:TRP:HD1	1:A:52:ARG:N	2.16	0.42
2:L:52:THR:HG21	2:L:72:TYR:CE2	2.54	0.42
3:H:29:PHE:O	3:H:72:ARG:NH2	2.52	0.42
1:A:501:ASN:OD1	1:A:501:ASN:N	2.53	0.42
1:A:505:GLU:OE2	3:H:52:SER:OG	2.35	0.42
1:A:410:PHE:CZ	1:A:414:LEU:HD11	2.55	0.42
2:L:11:MET:HE3	2:L:105:LEU:HD21	2.02	0.42
3:H:44:ARG:NH1	3:H:44:ARG:HG2	2.34	0.42
1:A:140:THR:HG22	1:A:142:SER:H	1.85	0.42
1:A:572:PRO:O	1:A:576:ILE:HG12	2.20	0.42
2:L:60:PRO:HG2	2:L:63:PHE:CD2	2.55	0.42
1:A:367:LEU:HA	1:A:370:MET:HE2	2.01	0.41
3:H:19:LYS:HG3	3:H:82:GLU:HG3	2.01	0.41
3:H:217:GLU:HA	3:H:218:PRO:HD3	1.93	0.41
2:L:92:PHE:CE1	3:H:102:ARG:HD3	2.56	0.41
3:H:5:VAL:HG23	3:H:23:ALA:HB3	2.02	0.41
3:H:31:SER:O	3:H:100:GLU:CD	2.63	0.41
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:HA	1:A:596:PRO:HD3	1.89	0.41
1:A:134:PHE:HB3	1:A:411:PHE:CE2	2.56	0.41
7:A:605:41U:H8	7:A:605:41U:H7	1.86	0.41
2:L:116:VAL:HG21	2:L:206:ILE:HD13	2.03	0.41
1:A:95:ALA:HA	1:A:329:LEU:HD23	2.02	0.41
1:A:115:LEU:HB3	8:A:706:HOH:O	2.20	0.41
1:A:145:TRP:HB2	1:A:212:ALA:HA	2.03	0.41
3:H:19:LYS:NZ	3:H:82:GLU:HB2	2.34	0.41
6:A:604:CLR:H232	6:A:604:CLR:H211	1.78	0.41
3:H:161:ASN:OD1	3:H:200:THR:N	2.33	0.41
1:A:316:GLN:NE2	5:A:603:CL:CL	2.84	0.41
1:A:486:ALA:O	1:A:490:GLU:HG3	2.20	0.41
2:L:36:TRP:HB2	2:L:49:ILE:HB	2.01	0.40
2:L:136:PHE:C	2:L:137:LEU:HD12	2.46	0.40
1:A:579:LEU:O	1:A:582:THR:OG1	2.39	0.40
1:A:420:ASP:HA	1:A:423:PHE:CD2	2.57	0.40
1:A:251:TYR:O	1:A:255:TRP:HD1	2.04	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	532/532 (100%)	516 (97%)	16 (3%)	0	100	100
2	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
3	H	212/240 (88%)	203 (96%)	9 (4%)	0	100	100
All	All	956/986 (97%)	924 (97%)	32 (3%)	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	425/437 (97%)	414 (97%)	11 (3%)	40	70
2	L	182/187 (97%)	179 (98%)	3 (2%)	55	78
3	H	171/205 (83%)	168 (98%)	3 (2%)	51	76
All	All	778/829 (94%)	761 (98%)	17 (2%)	45	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	52	ARG
1	A	113	VAL
1	A	236	LYS
1	A	366	VAL
1	A	494	VAL
1	A	501	ASN
1	A	536	VAL
1	A	551	VAL
1	A	581	SER
1	A	582	THR
2	L	3	VAL
2	L	117	SER
2	L	196	GLU
3	H	19	LYS
3	H	44	ARG
3	H	64	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
2	L	38	GLN
2	L	138	ASN
2	L	158	ASN

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Mol	Chain	Res	Type
2	L	162	ASN
2	L	190	HIS
3	H	170	HIS
3	H	197	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	CLR	A	604	-	31,31,31	0.67	0	48,48,48	1.19	4 (8%)
7	41U	A	605	-	21,21,21	0.57	0	25,26,26	1.79	5 (20%)

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	CLR	A	604	-	-	0/10/68/68	0/4/4/4
7	41U	A	605	-	-	13/14/14/14	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	605	41U	C-O-C7	6.81	125.33	118.26
6	A	604	CLR	C7-C8-C9	3.24	113.46	109.72
6	A	604	CLR	C4-C5-C10	3.09	120.38	116.42
7	A	605	41U	C16-N-C15	2.88	120.02	112.01
7	A	605	41U	O1-C5-C	2.52	118.83	115.40
6	A	604	CLR	C14-C8-C9	-2.42	105.93	109.09
6	A	604	CLR	C3-C4-C5	-2.09	108.72	112.05
7	A	605	41U	O1-C5-C4	-2.06	120.83	124.30
7	A	605	41U	O-C7-C14	2.04	110.88	105.60

There are no chirality outliers.

All (13) torsion outliers are listed below:

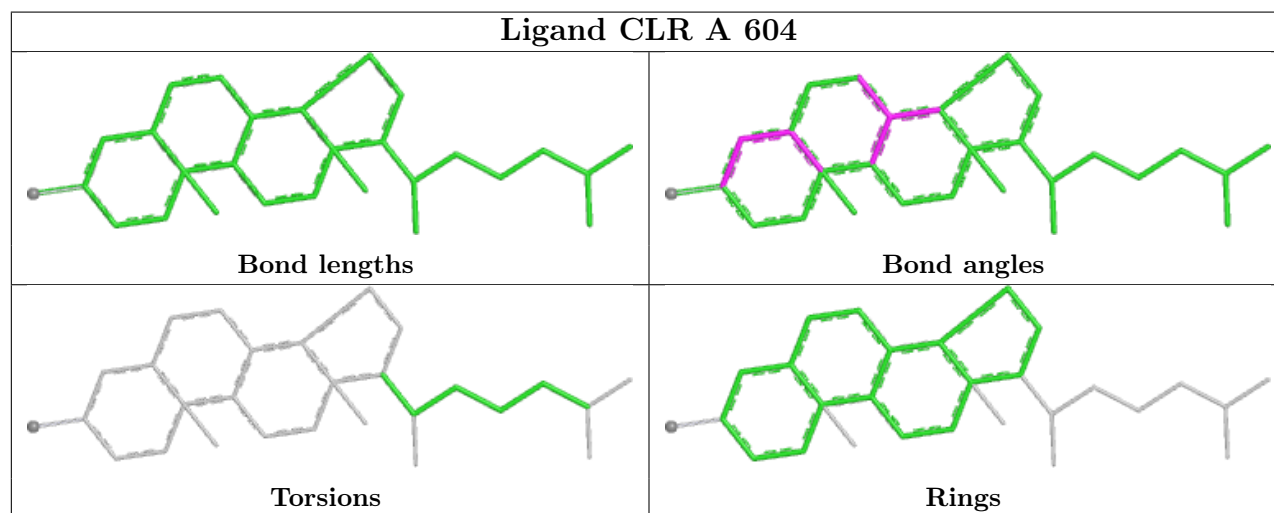
Mol	Chain	Res	Type	Atoms
7	A	605	41U	C7-C14-C15-N
7	A	605	41U	C14-C15-N-C16
7	A	605	41U	C15-C14-C7-O
7	A	605	41U	C15-C14-C7-C8
7	A	605	41U	C-C5-O1-C6
7	A	605	41U	C4-C5-O1-C6
7	A	605	41U	O-C7-C8-C9
7	A	605	41U	O-C7-C8-C13
7	A	605	41U	C8-C7-O-C
7	A	605	41U	C14-C7-C8-C13
7	A	605	41U	C1-C-O-C7
7	A	605	41U	C14-C7-C8-C9
7	A	605	41U	C14-C7-O-C

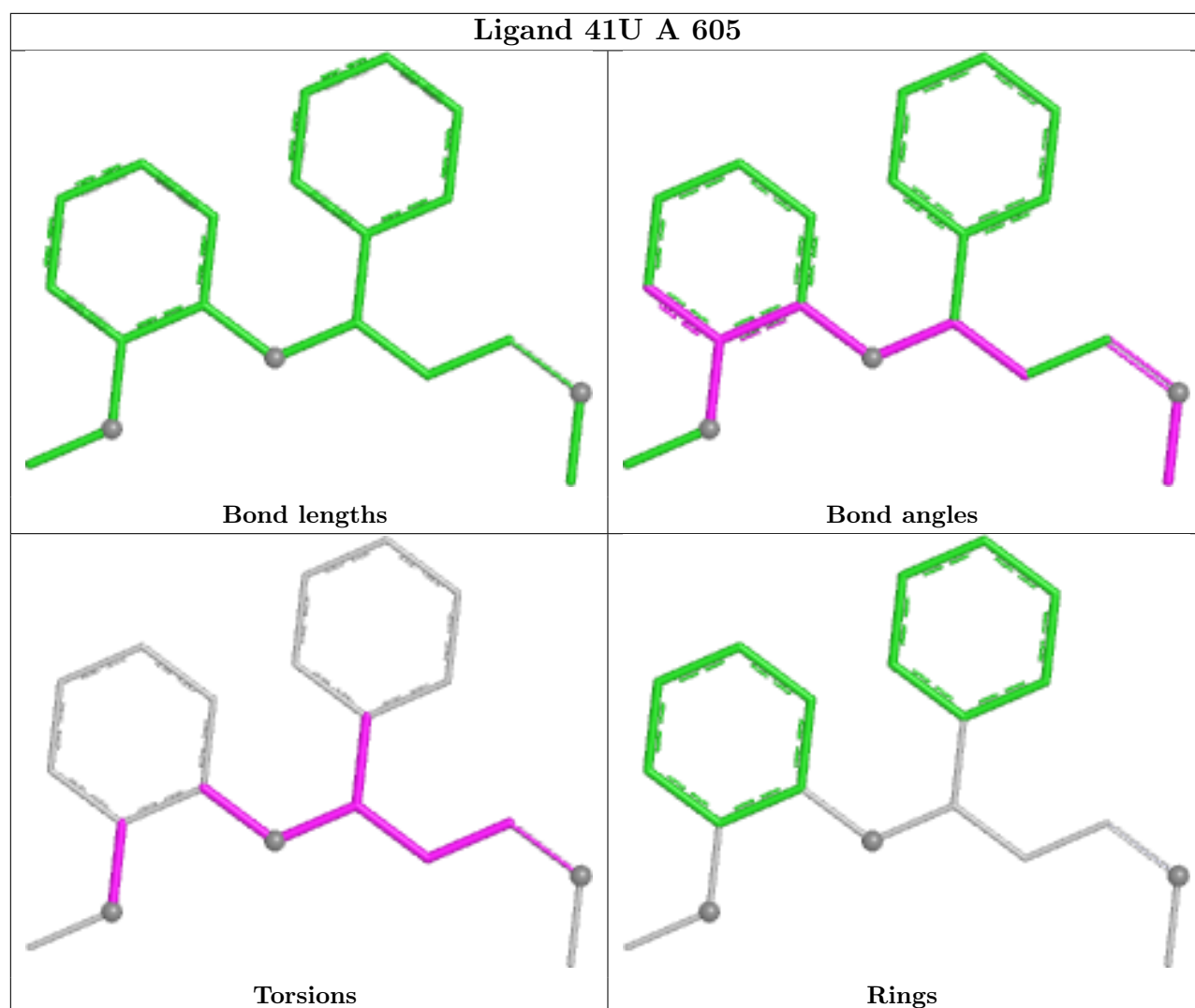
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	604	CLR	3	0
7	A	605	41U	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	532/532 (100%)	0.87	75 (14%) 6 4	58, 85, 109, 145	2 (0%)
2	L	214/214 (100%)	0.70	24 (11%) 10 7	57, 77, 110, 146	0
3	H	216/240 (90%)	0.93	35 (16%) 4 3	61, 85, 114, 134	0
All	All	962/986 (97%)	0.85	134 (13%) 6 4	57, 84, 111, 146	2 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290[A]	PHE	7.8
1	A	384	GLU	6.5
3	H	138	THR	6.2
2	L	117	SER	5.9
1	A	437	PHE	5.9
2	L	119	PHE	5.9
2	L	136	PHE	5.8
1	A	375	GLY	5.3
1	A	461	ALA	5.1
1	A	111	TYR	5.0
3	H	42	GLU	5.0
3	H	100	GLU	5.0
1	A	323	PRO	5.0
1	A	207	GLY	4.9
1	A	346	LEU	4.8
1	A	96	ILE	4.6
1	A	291	LEU	4.6
3	H	134	CYS	4.5
3	H	129	PRO	4.4
3	H	131	ALA	4.3
1	A	468	PHE	4.3
2	L	213	ASN	4.3
2	L	115	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	124	TYR	4.2
2	L	203	THR	4.1
1	A	130	TRP	4.0
1	A	322	GLY	4.0
1	A	446	LEU	4.0
2	L	134	VAL	3.9
2	L	135	CYS	3.8
1	A	324	GLY	3.8
3	H	165	LEU	3.7
3	H	128	TYR	3.7
1	A	75	VAL	3.7
3	H	55	GLY	3.6
3	H	130	LEU	3.6
3	H	126	SER	3.6
1	A	497	ILE	3.6
1	A	492	ILE	3.6
1	A	163	GLN	3.6
2	L	170	LYS	3.5
1	A	583	PRO	3.5
2	L	148	LYS	3.4
3	H	44	ARG	3.4
3	H	211	LYS	3.3
3	H	58	ILE	3.3
2	L	92	PHE	3.3
2	L	24	ARG	3.2
3	H	127	VAL	3.2
1	A	126	VAL	3.1
1	A	439	LYS	3.1
3	H	219	ARG	3.1
1	A	567	SER	3.0
1	A	425	GLY	3.0
2	L	114	PRO	3.0
2	L	169	SER	3.0
1	A	345	ALA	3.0
2	L	207	VAL	3.0
1	A	590	PHE	3.0
1	A	73	LEU	2.9
1	A	72	MET	2.9
1	A	25	ASP	2.9
1	A	141	ASN	2.9
1	A	319	PHE	2.9
3	H	7	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	594	THR	2.9
3	H	69	THR	2.9
1	A	288	GLY	2.8
3	H	132	PRO	2.8
2	L	118	ILE	2.8
3	H	133	VAL	2.8
2	L	123	SER	2.7
1	A	433	LEU	2.7
1	A	82	TYR	2.7
1	A	537	TYR	2.7
3	H	17	SER	2.7
1	A	592	ILE	2.6
3	H	215	LYS	2.6
1	A	496	TRP	2.6
2	L	177	SER	2.6
1	A	582	THR	2.6
3	H	124	ALA	2.6
3	H	8	GLY	2.6
1	A	353	SER	2.6
3	H	171	THR	2.5
1	A	422	SER	2.5
1	A	387	GLY	2.5
2	L	176	MET	2.5
2	L	53	SER	2.5
1	A	570	MET	2.5
1	A	305	TYR	2.5
1	A	428	ALA	2.5
1	A	81	PHE	2.5
3	H	18	LEU	2.4
3	H	162	SER	2.4
1	A	43	PHE	2.4
1	A	598	ARG	2.4
2	L	184	LYS	2.4
3	H	214	LYS	2.4
1	A	440	ILE	2.4
1	A	136	PHE	2.4
1	A	310	TRP	2.4
3	H	41	PRO	2.4
1	A	127	ILE	2.4
1	A	563	ILE	2.4
1	A	60	ASN	2.3
1	A	371	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	H	158	LEU	2.3
1	A	237	TRP	2.3
1	A	69	TYR	2.3
1	A	325	PHE	2.3
1	A	471	PHE	2.3
2	L	124	GLU	2.3
1	A	482	SER	2.3
1	A	390	PHE	2.2
1	A	347	LEU	2.2
1	A	80	LEU	2.2
1	A	568	VAL	2.2
1	A	599	ASP	2.2
1	A	218	ARG	2.1
1	A	487	VAL	2.1
1	A	386	PRO	2.1
1	A	373	THR	2.1
2	L	186	GLU	2.1
1	A	385	GLY	2.1
1	A	92	ARG	2.1
2	L	161	LEU	2.1
1	A	238	ASP	2.1
3	H	19	LYS	2.0
3	H	34	MET	2.0
3	H	166	SER	2.0
3	H	9	GLY	2.0
3	H	150	GLY	2.0
1	A	95	ALA	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.

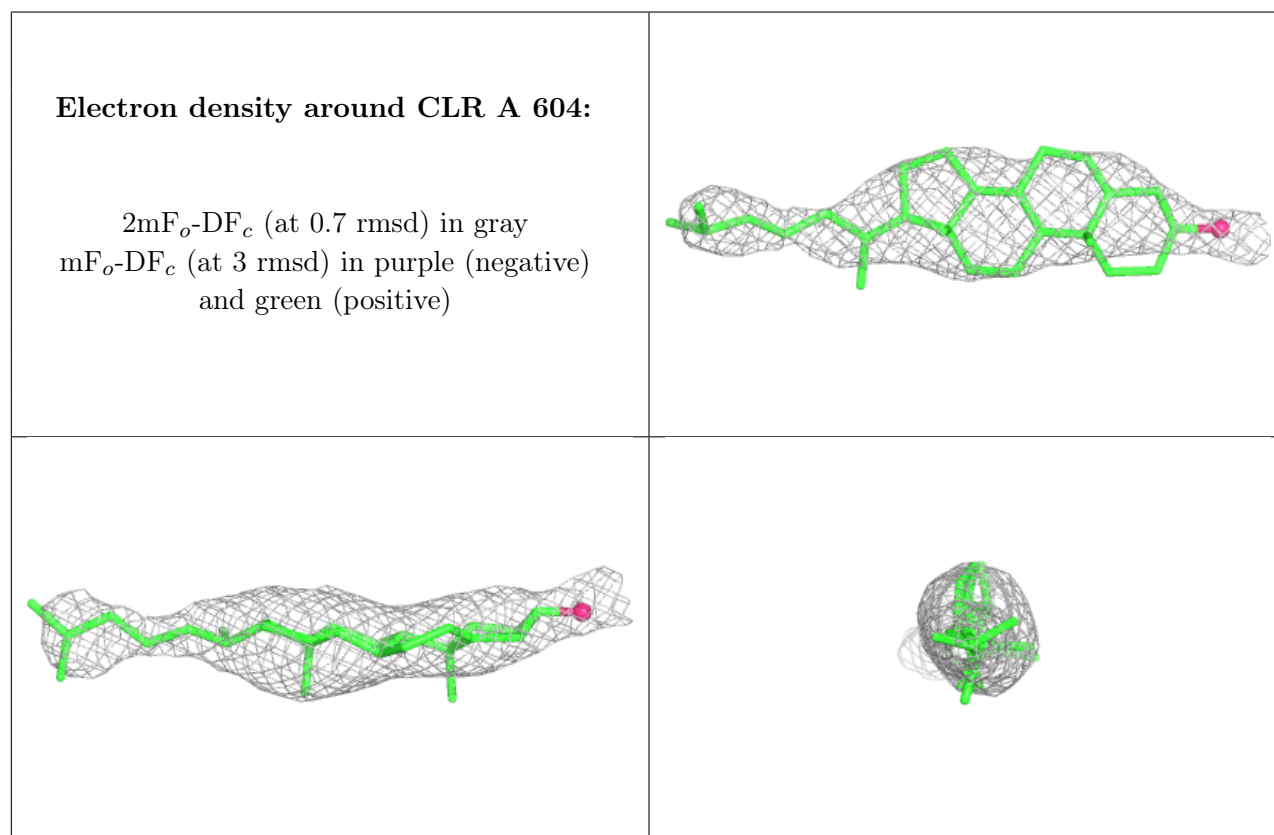
6.4 Ligands [i](#)

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.

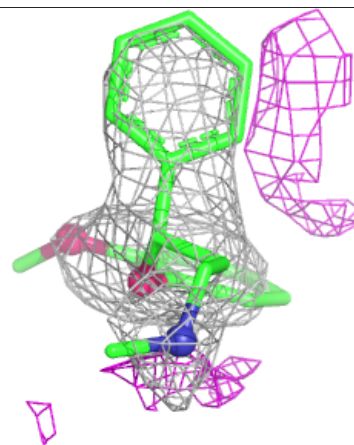
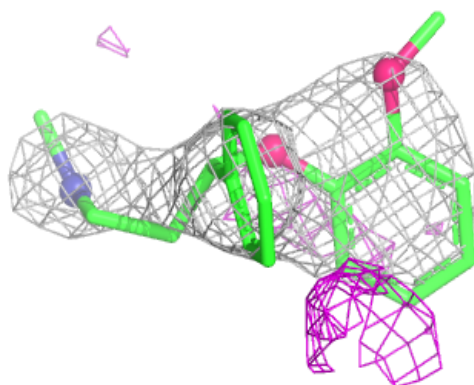
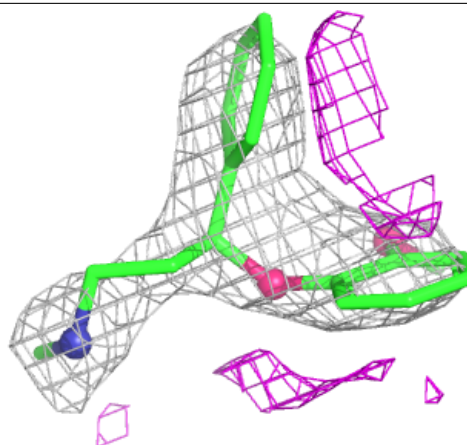
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CLR	A	604	28/28	0.92	0.17	84,97,109,113	0
4	NA	A	602	1/1	0.93	0.13	70,70,70,70	0
4	NA	A	601	1/1	0.94	0.08	84,84,84,84	0
5	CL	A	603	1/1	0.95	0.12	74,74,74,74	0
7	41U	A	605	20/20	0.95	0.18	88,94,111,113	0

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 41U A 605:

$2mF_o-DF_c$ (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.