



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 07:58 PM EDT

PDB ID : 8DXM
Title : HIV-1 reverse transcriptase/rilpivirine with bound fragment 4-bromophenol at the Knuckles site
Authors : Chopra, A.; Ruiz, F.X.; Bauman, J.D.; Arnold, E.
Deposited on : 2022-08-02
Resolution : 1.99 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

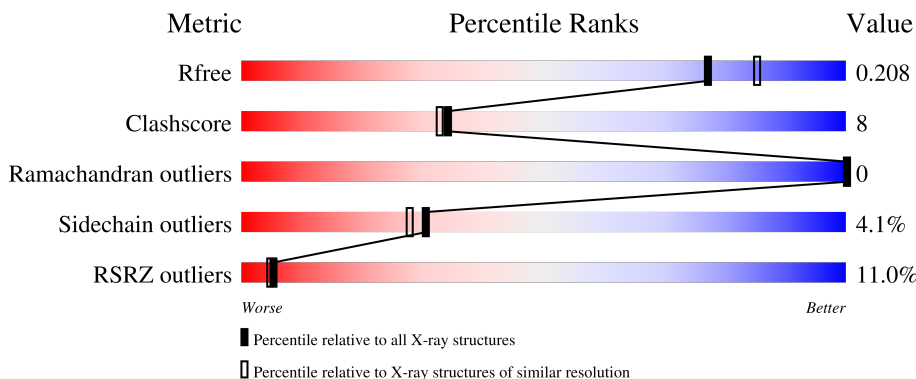
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

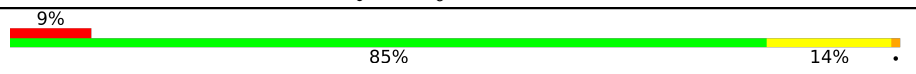
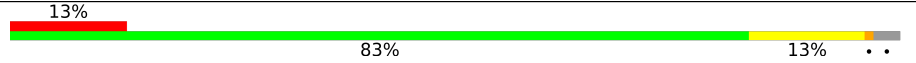
The reported resolution of this entry is 1.99 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	557	
2	B	428	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BML	A	601[A]	-	-	X	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8552 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4516	2923	750	835	8	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

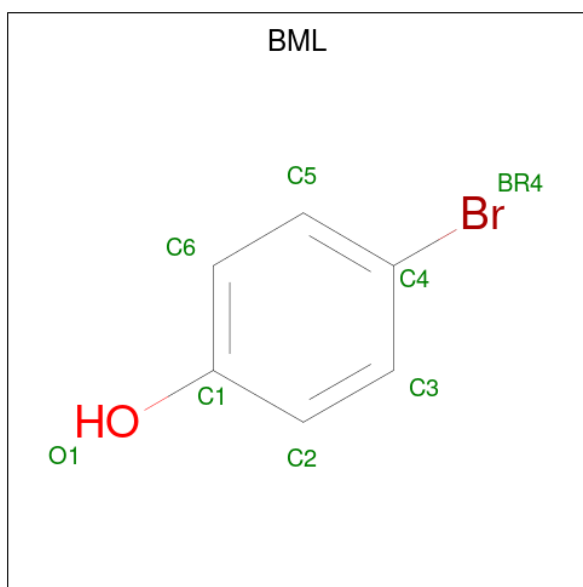
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	415	3459	2259	569	624	7	0	4	0

There is a discrepancy between the modelled and reference sequences:

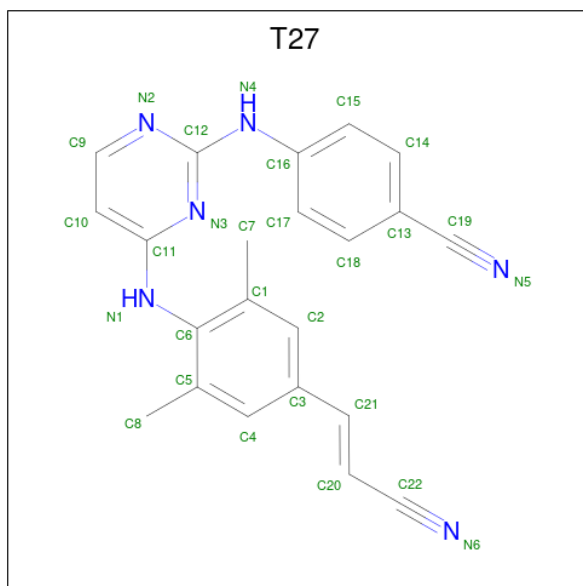
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-BROMOPHENOL (three-letter code: BML) (formula: C₆H₅BrO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
3	A	1	8	1	6	1	0	1

- Molecule 4 is 4-{{4-{{4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl}amino}benzotrile (three-letter code: T27) (formula: C₂₂H₁₈N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	28	22	6	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

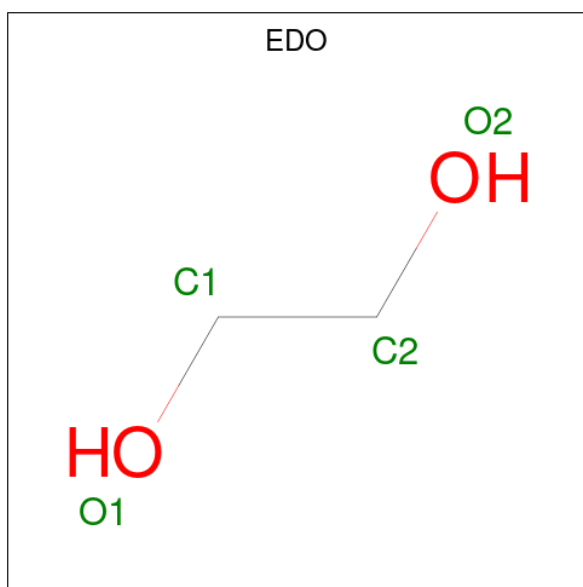
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0

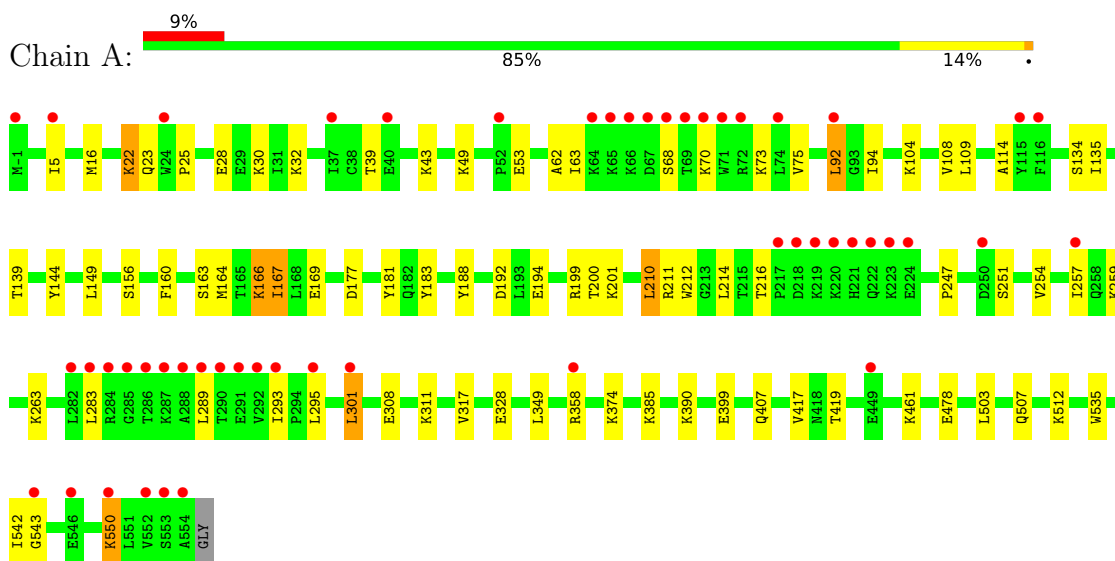
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	287	Total 287	O 287	0	0
9	B	198	Total 198	O 198	0	0

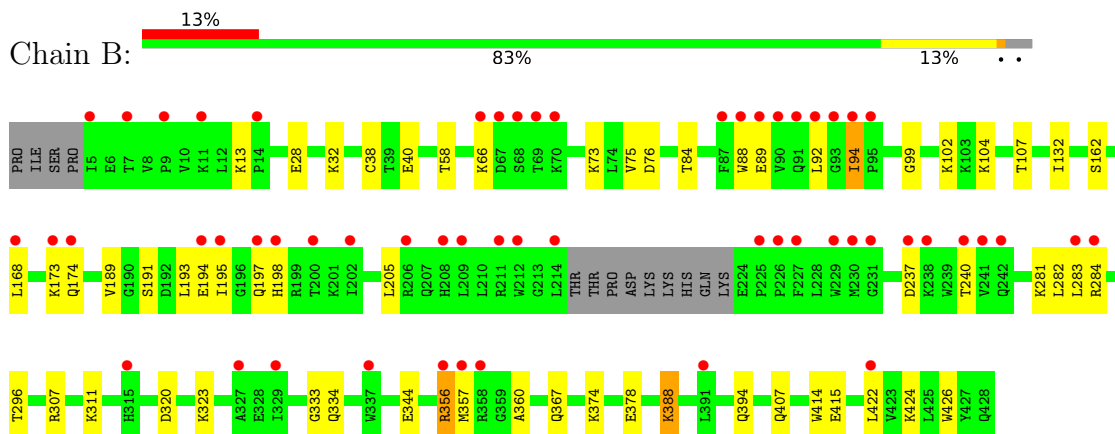
3 Residue-property plots [i](#)

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: Reverse transcriptase/ribonuclease H



- Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.51Å 72.97Å 109.42Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	42.15 – 1.99 42.15 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.0 (42.15-1.99) 94.5 (42.15-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.00Å)	Xtrriage
Refinement program	PHENIX dev_3051	Depositor
R, R_{free}	0.197 , 0.208 0.197 , 0.208	Depositor DCC
R_{free} test set	1982 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8552	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: DMS, EDO, T27, BML, SO4, MG

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	0.41	0/4634	0.60	0/6299
2	B	0.35	0/3570	0.59	0/4852
All	All	0.38	0/8204	0.59	0/11151

There are no bond length outliers.

There are no bond angle outliers.

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	4516	0	4572	91	0
2	B	3459	0	3488	45	0
3	A	8	0	4	27	0
4	A	28	0	18	1	0
5	A	16	0	24	0	0
5	B	20	0	30	2	0
6	A	1	0	0	0	0
7	A	15	0	0	0	0
8	B	4	0	6	0	0
9	A	287	0	0	9	0
9	B	198	0	0	5	0
All	All	8552	0	8142	136	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 (136) 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)
1:A:5:ILE:HD11	3:A:601[A]:BML:C1	1.60	1.28
1:A:5:ILE:CD1	3:A:601[A]:BML:C1	2.41	0.99
1:A:214:LEU:HD11	3:A:601[A]:BML:C1	1.98	0.93
1:A:5:ILE:HD11	3:A:601[A]:BML:C6	2.04	0.87
2:B:13:LYS:HE2	2:B:84:THR:O	1.75	0.87
1:A:503:LEU:CD1	1:A:535:TRP:HB2	2.05	0.86
1:A:160:PHE:CD1	3:A:601[A]:BML:BR4	2.84	0.85
1:A:5:ILE:HD11	3:A:601[A]:BML:O1	1.80	0.81
1:A:257:ILE:CG2	1:A:283:LEU:HD11	2.12	0.80
1:A:385:LYS:HD2	9:A:920:HOH:O	1.82	0.79
1:A:163:SER:HB2	3:A:601[A]:BML:BR4	2.37	0.79
1:A:259:LYS:HE3	1:A:263:LYS:HZ1	1.48	0.78
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.67	0.77
1:A:30:LYS:CD	1:A:62:ALA:HB3	2.17	0.75
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.68	0.73
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.70	0.72
1:A:259:LYS:CE	1:A:263:LYS:NZ	2.53	0.71
1:A:104:LYS:NZ	1:A:104:LYS:HB3	2.05	0.71
1:A:214:LEU:HD21	3:A:601[A]:BML:H6	1.71	0.71
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.71	0.71
1:A:543:GLY:N	9:A:701:HOH:O	2.21	0.70
2:B:92:LEU:HD23	2:B:92:LEU:O	1.92	0.69
2:B:424:LYS:HD2	9:B:634:HOH:O	1.93	0.68
1:A:5:ILE:CD1	3:A:601[A]:BML:C6	2.69	0.68
2:B:422:LEU:HD23	2:B:426[B]:TRP:CH2	2.29	0.67
1:A:114:ALA:HB1	3:A:601[A]:BML:C5	2.23	0.67
9:A:701:HOH:O	2:B:283:LEU:C	2.33	0.67
1:A:503:LEU:O	1:A:507:GLN:HG3	1.97	0.65
1:A:247:PRO:HG3	1:A:259:LYS:NZ	2.12	0.65
2:B:107:THR:HG1	2:B:198:HIS:HE2	1.45	0.64
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.78	0.64
1:A:22:LYS:HD3	9:A:935:HOH:O	1.96	0.64
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.28	0.64
1:A:259:LYS:HE3	1:A:263:LYS:NZ	2.13	0.63
1:A:214:LEU:HD21	3:A:601[A]:BML:O1	1.98	0.63
1:A:503:LEU:HD11	1:A:535:TRP:HB2	1.80	0.63
2:B:281:LYS:O	2:B:281:LYS:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:CD2	3:A:601[A]:BML:H6	2.30	0.61
1:A:214:LEU:HD11	3:A:601[A]:BML:O1	1.99	0.61
1:A:214:LEU:HD21	3:A:601[A]:BML:C6	2.30	0.61
2:B:104:LYS:HD2	2:B:237:ASP:CG	2.21	0.60
1:A:114:ALA:HB1	3:A:601[A]:BML:H5	1.83	0.59
1:A:160:PHE:CE1	3:A:601[A]:BML:BR4	3.11	0.58
2:B:40:GLU:HG2	9:B:635:HOH:O	2.03	0.58
1:A:167:ILE:HG12	3:A:601[A]:BML:H2	1.86	0.57
1:A:167:ILE:CG1	3:A:601[A]:BML:H2	2.34	0.56
1:A:177:ASP:OD2	1:A:201:LYS:HE3	2.05	0.56
1:A:160:PHE:HD1	3:A:601[A]:BML:BR4	2.39	0.56
1:A:257:ILE:HG21	1:A:283:LEU:HD11	1.86	0.56
2:B:194:GLU:HB2	2:B:197:GLN:HG2	1.86	0.56
2:B:193:LEU:HD12	2:B:193:LEU:N	2.21	0.55
9:A:701:HOH:O	2:B:283:LEU:HB2	2.05	0.55
2:B:394:GLN:HB3	9:B:636:HOH:O	2.07	0.55
5:B:501:DMS:H13	9:B:757:HOH:O	2.07	0.55
1:A:53:GLU:H	1:A:53:GLU:CD	2.10	0.54
4:A:602:T27:N3	4:A:602:T27:H17	2.22	0.54
1:A:160:PHE:O	3:A:601[A]:BML:BR4	2.80	0.54
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.89	0.54
1:A:5:ILE:HG12	3:A:601[A]:BML:C2	2.39	0.53
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.44	0.52
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.92	0.52
1:A:503:LEU:HD12	1:A:535:TRP:CD1	2.44	0.52
2:B:168:LEU:HD22	2:B:205:LEU:HD11	1.92	0.51
2:B:104:LYS:HA	2:B:237:ASP:OD1	2.10	0.51
1:A:149:LEU:HD13	1:A:156:SER:HA	1.92	0.51
1:A:134:SER:HB2	1:A:139:THR:OG1	2.10	0.51
1:A:259:LYS:HE2	1:A:263:LYS:CE	2.41	0.50
1:A:503:LEU:HD12	1:A:535:TRP:HD1	1.75	0.50
2:B:422:LEU:HD23	2:B:426[B]:TRP:HH2	1.77	0.50
1:A:478:GLU:HG2	9:A:724:HOH:O	2.10	0.50
1:A:39:THR:HG22	1:A:43:LYS:HE3	1.95	0.49
1:A:512:LYS:HZ2	1:A:512:LYS:HB3	1.77	0.49
1:A:63:ILE:HG13	1:A:63:ILE:O	2.13	0.49
2:B:28:GLU:CG	2:B:32:LYS:HE2	2.42	0.48
1:A:104:LYS:HB3	1:A:104:LYS:HZ1	1.77	0.48
1:A:164:MET:N	3:A:601[A]:BML:BR4	3.02	0.48
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.96	0.48
2:B:422:LEU:CD2	2:B:426[B]:TRP:CH2	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.95	0.48
2:B:193:LEU:N	2:B:193:LEU:CD1	2.77	0.48
2:B:307:ARG:O	2:B:311:LYS:HG3	2.14	0.47
1:A:5:ILE:CD1	3:A:601[A]:BML:C2	2.90	0.47
1:A:49:LYS:HG2	1:A:144:TYR:CE1	2.50	0.47
1:A:22:LYS:C	1:A:22:LYS:HD2	2.34	0.47
1:A:104:LYS:HD3	1:A:192:ASP:O	2.15	0.47
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.43	0.47
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.96	0.47
1:A:212:TRP:HB3	3:A:601[A]:BML:O1	2.15	0.47
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.97	0.46
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.51	0.46
2:B:174:GLN:O	2:B:174:GLN:HG3	2.15	0.46
2:B:281:LYS:HA	2:B:284:ARG:HD2	1.98	0.46
1:A:214:LEU:HD21	3:A:601[A]:BML:C1	2.46	0.45
1:A:22:LYS:HD2	1:A:23:GLN:N	2.30	0.45
2:B:374:LYS:O	2:B:378:GLU:HG3	2.16	0.45
1:A:109:LEU:HD12	1:A:109:LEU:N	2.31	0.45
1:A:30:LYS:HD2	1:A:62:ALA:HB3	1.94	0.45
1:A:210:LEU:HD13	1:A:210:LEU:HA	1.86	0.45
1:A:407:GLN:OE1	2:B:394:GLN:HG2	2.17	0.45
1:A:39:THR:O	1:A:43:LYS:HG3	2.16	0.44
1:A:308:GLU:HA	1:A:311:LYS:HG3	1.99	0.44
2:B:360:ALA:O	2:B:367:GLN:NE2	2.39	0.44
2:B:422:LEU:HD23	5:B:505:DMS:O	2.16	0.44
2:B:94:ILE:H	2:B:94:ILE:HG13	1.40	0.44
1:A:259:LYS:HE2	1:A:263:LYS:NZ	2.32	0.44
1:A:512:LYS:CB	1:A:512:LYS:NZ	2.79	0.43
1:A:167:ILE:HG12	3:A:601[A]:BML:C2	2.48	0.43
2:B:189:VAL:HG21	2:B:205:LEU:HD23	2.00	0.43
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.86	0.43
1:A:28:GLU:HG3	1:A:135:ILE:HD12	2.01	0.43
1:A:22:LYS:NZ	1:A:25:PRO:HD3	2.34	0.43
1:A:30:LYS:HD3	1:A:62:ALA:CB	2.47	0.43
2:B:424:LYS:CD	9:B:634:HOH:O	2.62	0.43
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.72	0.42
1:A:550:LYS:HB2	1:A:550:LYS:HE2	1.70	0.42
1:A:385:LYS:CD	9:A:920:HOH:O	2.55	0.42
2:B:388:LYS:HE2	2:B:415:GLU:HB3	2.01	0.42
1:A:108:VAL:C	1:A:109:LEU:HD12	2.39	0.42
2:B:195:ILE:HA	2:B:198:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HB2	1:A:166:LYS:HE2	1.61	0.42
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.59	0.42
2:B:73:LYS:NZ	2:B:75:VAL:CG2	2.82	0.42
1:A:247:PRO:CG	1:A:259:LYS:NZ	2.83	0.42
1:A:301:LEU:HD13	1:A:301:LEU:HA	1.79	0.42
1:A:543:GLY:CA	9:A:701:HOH:O	2.65	0.42
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.50	0.42
1:A:32:LYS:HB2	1:A:32:LYS:HE3	1.79	0.42
9:A:701:HOH:O	2:B:284:ARG:N	2.53	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.20	0.42
1:A:247:PRO:HG3	1:A:259:LYS:HZ2	1.85	0.41
2:B:333:GLY:O	2:B:334:GLN:HB2	2.20	0.41
1:A:214:LEU:CD2	3:A:601[A]:BML:C6	2.96	0.41
1:A:283:LEU:HD12	1:A:283:LEU:N	2.35	0.41
2:B:356:ARG:H	2:B:356:ARG:CD	2.33	0.41
2:B:356:ARG:H	2:B:356:ARG:HE	1.68	0.41
2:B:320:ASP:HB3	2:B:323:LYS:HD3	2.02	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	554/557 (100%)	541 (98%)	13 (2%)	0	100	100
2	B	415/428 (97%)	399 (96%)	16 (4%)	0	100	100
All	All	969/985 (98%)	940 (97%)	29 (3%)	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	495/495 (100%)	471 (95%)	24 (5%)	25	22
2	B	380/390 (97%)	368 (97%)	12 (3%)	39	38
All	All	875/885 (99%)	839 (96%)	36 (4%)	30	28

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	22	LYS
1	A	68	SER
1	A	70	LYS
1	A	92	LEU
1	A	94	ILE
1	A	166	LYS
1	A	167	ILE
1	A	169	GLU
1	A	194	GLU
1	A	199	ARG
1	A	200	THR
1	A	210	LEU
1	A	211	ARG
1	A	216	THR
1	A	251	SER
1	A	289	LEU
1	A	295	LEU
1	A	301	LEU
1	A	358	ARG
1	A	374	LYS
1	A	399	GLU
1	A	461	LYS
1	A	550	LYS
2	B	66	LYS
2	B	88	TRP
2	B	89	GLU

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Mol	Chain	Res	Type
2	B	94	ILE
2	B	162	SER
2	B	173	LYS
2	B	240	THR
2	B	356	ARG
2	B	357	MET
2	B	388	LYS
2	B	407	GLN
2	B	414	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	207	GLN
2	B	182	GLN
2	B	258	GLN
2	B	428	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	DMS	B	504	-	3,3,3	2.54	1 (33%)	3,3,3	0.45	0
5	DMS	A	604	-	3,3,3	2.54	1 (33%)	3,3,3	0.67	0
5	DMS	B	505	-	3,3,3	2.56	1 (33%)	3,3,3	0.35	0
4	T27	A	602	-	30,30,30	1.12	3 (10%)	39,40,40	1.75	6 (15%)
5	DMS	A	605	-	3,3,3	2.77	1 (33%)	3,3,3	0.79	0
5	DMS	A	603	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
5	DMS	B	502	-	3,3,3	2.56	1 (33%)	3,3,3	0.40	0
7	SO4	A	608	-	4,4,4	0.47	0	6,6,6	0.05	0
3	BML	A	601[A]	-	8,8,8	0.34	0	10,10,10	0.14	0
5	DMS	A	606	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
5	DMS	B	501	-	3,3,3	2.65	1 (33%)	3,3,3	0.44	0
7	SO4	A	609	-	4,4,4	0.44	0	6,6,6	0.06	0
7	SO4	A	610	-	4,4,4	0.45	0	6,6,6	0.06	0
8	EDO	B	506	-	3,3,3	0.20	0	2,2,2	0.23	0
5	DMS	B	503	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	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
3	BML	A	601[A]	-	-	-	0/1/1/1
8	EDO	B	506	-	-	1/1/1/1	-
4	T27	A	602	-	-	2/13/14/14	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	DMS	O-S	4.66	1.81	1.50
5	A	606	DMS	O-S	4.51	1.80	1.50
5	B	503	DMS	O-S	4.47	1.80	1.50
5	A	603	DMS	O-S	4.46	1.80	1.50
5	B	501	DMS	O-S	4.45	1.80	1.50
5	B	502	DMS	O-S	4.35	1.79	1.50
5	B	505	DMS	O-S	4.29	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	DMS	O-S	4.29	1.79	1.50
5	B	504	DMS	O-S	4.27	1.79	1.50
4	A	602	T27	C12-N4	3.84	1.44	1.36
4	A	602	T27	C11-N1	2.90	1.43	1.38
4	A	602	T27	C13-C19	2.13	1.49	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	T27	C9-N2-C12	5.42	120.25	115.45
4	A	602	T27	N2-C12-N3	-4.89	121.91	126.55
4	A	602	T27	C9-C10-C11	4.20	119.51	116.76
4	A	602	T27	C10-C9-N2	-3.93	119.07	123.96
4	A	602	T27	C10-C11-N3	-2.70	118.61	123.16
4	A	602	T27	C12-N3-C11	2.19	120.64	116.28

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	T27	C20-C21-C3-C4
4	A	602	T27	C20-C21-C3-C2
8	B	506	EDO	O1-C1-C2-O2

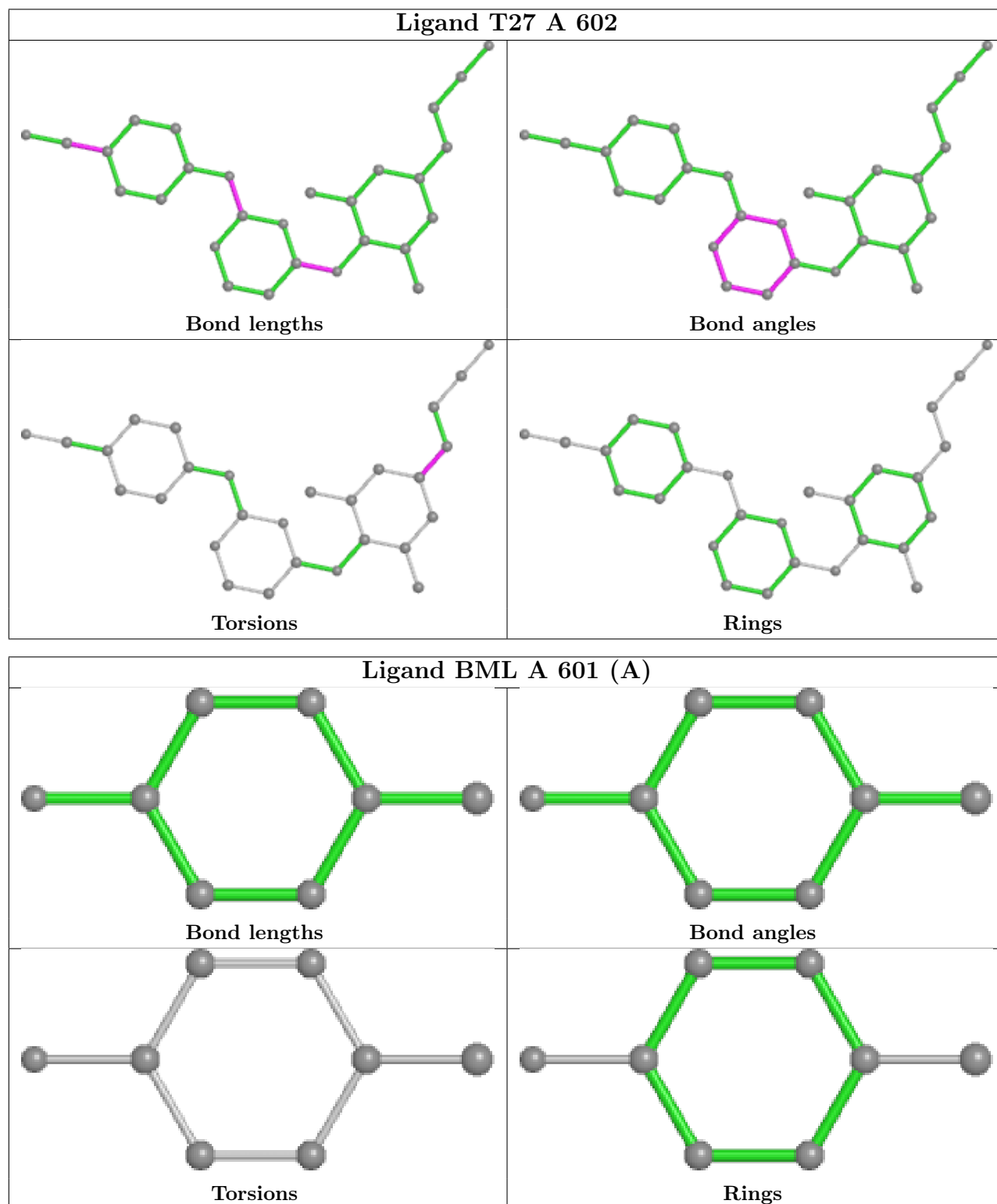
There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	DMS	1	0
4	A	602	T27	1	0
3	A	601[A]	BML	27	0
5	B	501	DMS	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	556/557 (99%)	0.51	51 (9%) 9 8	25, 45, 95, 177	0
2	B	415/428 (96%)	0.94	56 (13%) 3 2	26, 46, 108, 226	0
All	All	971/985 (98%)	0.69	107 (11%) 5 5	25, 46, 104, 226	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	22.8
2	B	89	GLU	12.6
2	B	90	VAL	11.6
1	A	220	LYS	11.4
2	B	93	GLY	9.7
1	A	285	GLY	7.9
2	B	88	TRP	7.4
1	A	218	ASP	7.4
1	A	24	TRP	7.4
1	A	67	ASP	7.2
1	A	221	HIS	7.1
1	A	289	LEU	7.1
1	A	287	LYS	6.8
2	B	229	TRP	6.5
1	A	219	LYS	6.4
1	A	223	LYS	6.3
1	A	286	THR	6.2
2	B	95	PRO	5.9
2	B	91	GLN	5.8
2	B	5	ILE	5.7
2	B	202	ILE	5.7
2	B	356	ARG	5.6
1	A	553	SER	5.3
1	A	69	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLN	4.9
1	A	290	THR	4.6
2	B	212	TRP	4.5
1	A	66	LYS	4.3
2	B	357	MET	4.2
1	A	284	ARG	4.1
1	A	292	VAL	4.1
2	B	315	HIS	4.0
1	A	257	ILE	3.8
2	B	238	LYS	3.8
1	A	293	ILE	3.7
1	A	224	GLU	3.7
2	B	67	ASP	3.7
1	A	301	LEU	3.7
2	B	226	PRO	3.7
1	A	115	TYR	3.6
2	B	237	ASP	3.6
1	A	68	SER	3.6
2	B	209	LEU	3.6
2	B	94	ILE	3.5
2	B	211	ARG	3.4
2	B	173	LYS	3.3
1	A	554	ALA	3.3
1	A	92	LEU	3.3
1	A	282	LEU	3.3
2	B	168	LEU	3.3
1	A	283	LEU	3.2
2	B	70	LYS	3.1
2	B	200	THR	3.1
1	A	116	PHE	3.1
2	B	214	LEU	3.1
1	A	64	LYS	3.1
2	B	225	PRO	3.0
1	A	295	LEU	3.0
2	B	227	PHE	3.0
2	B	194	GLU	3.0
2	B	358	ARG	3.0
1	A	288	ALA	3.0
2	B	87	PHE	2.9
2	B	284	ARG	2.9
1	A	546	GLU	2.9
1	A	71	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	2.8
1	A	65	LYS	2.8
2	B	195	ILE	2.8
1	A	37	ILE	2.7
2	B	7	THR	2.7
2	B	66	LYS	2.7
1	A	5	ILE	2.7
1	A	72	ARG	2.7
1	A	291	GLU	2.6
1	A	70	LYS	2.6
2	B	197	GLN	2.6
2	B	174	GLN	2.6
2	B	242	GLN	2.6
2	B	14	PRO	2.6
2	B	422	LEU	2.5
2	B	68	SER	2.4
2	B	69	THR	2.4
1	A	217	PRO	2.4
2	B	240	THR	2.3
2	B	241	VAL	2.3
1	A	74	LEU	2.3
2	B	391	LEU	2.3
1	A	52	PRO	2.3
2	B	9	PRO	2.3
1	A	250	ASP	2.2
1	A	543	GLY	2.2
2	B	329	ILE	2.1
1	A	-1	MET	2.1
1	A	552	VAL	2.1
1	A	550	LYS	2.1
2	B	337	TRP	2.1
1	A	358	ARG	2.1
2	B	327	ALA	2.0
2	B	283	LEU	2.0
1	A	449	GLU	2.0
2	B	230	MET	2.0
2	B	198	HIS	2.0
1	A	40	GLU	2.0
2	B	11	LYS	2.0
2	B	208	HIS	2.0
2	B	206	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

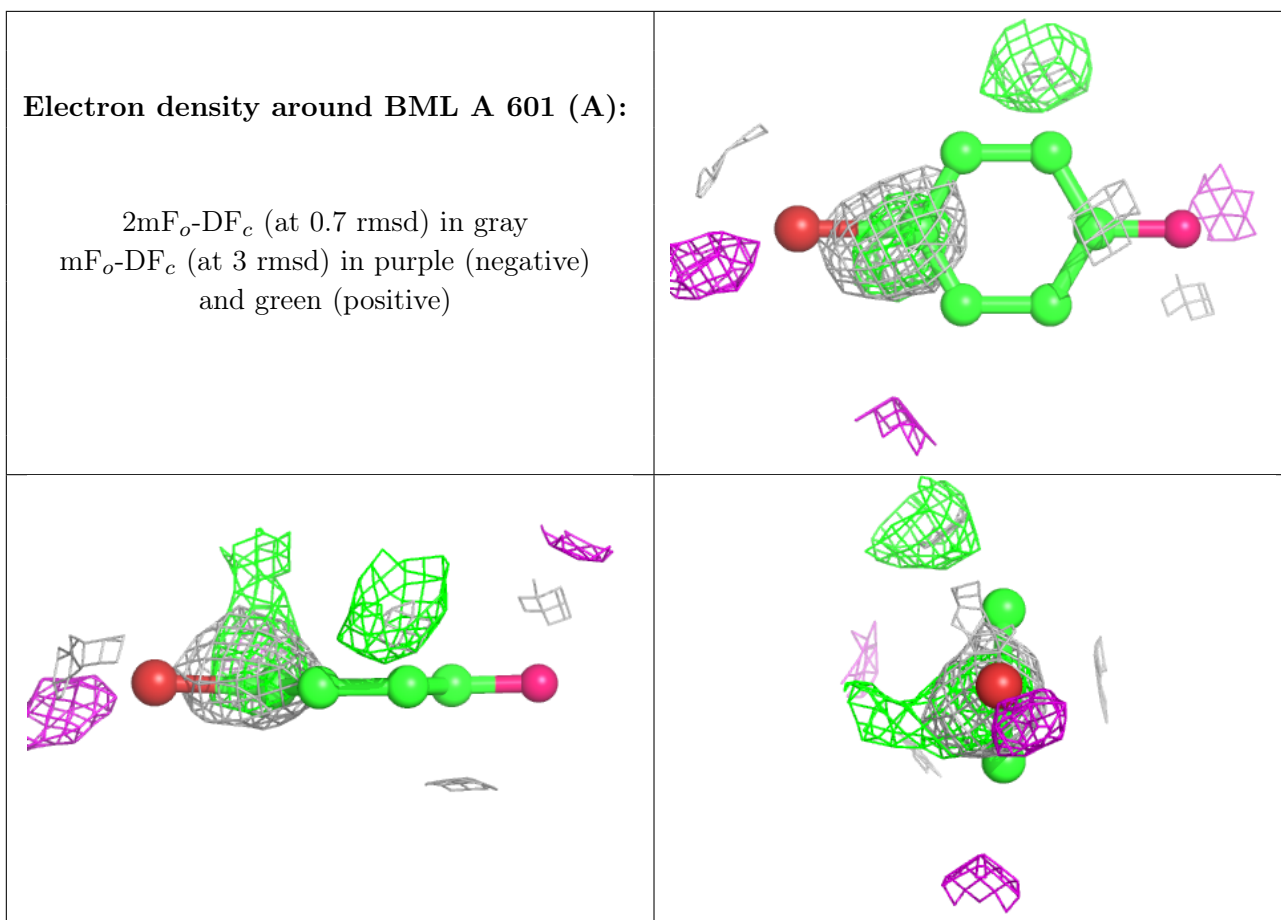
There are no monosaccharides in this entry.

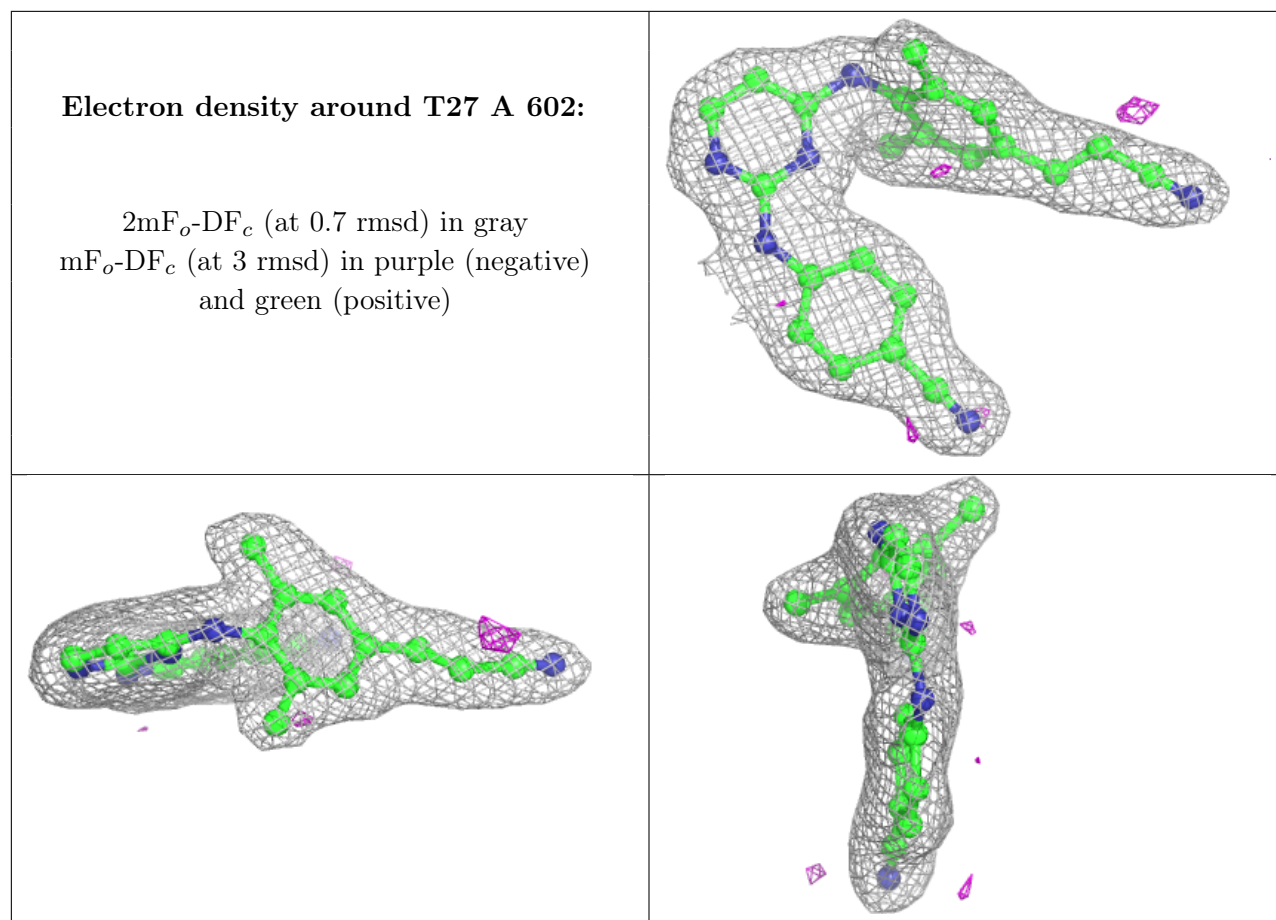
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	BML	A	601[A]	8/8	0.45	0.79	48,53,56,91	8
6	MG	A	607	1/1	0.80	0.17	63,63,63,63	0
5	DMS	A	606	4/4	0.85	0.15	47,60,62,77	0
5	DMS	B	503	4/4	0.86	0.20	66,75,79,82	0
5	DMS	B	505	4/4	0.88	0.18	51,55,58,70	0
7	SO4	A	608	5/5	0.89	0.22	85,86,89,97	0
5	DMS	A	604	4/4	0.91	0.32	53,58,66,77	0
5	DMS	B	502	4/4	0.93	0.20	43,44,57,59	0
8	EDO	B	506	4/4	0.93	0.22	44,44,50,51	0
5	DMS	A	603	4/4	0.95	0.11	60,63,68,69	0
5	DMS	B	501	4/4	0.95	0.13	42,46,49,52	0
5	DMS	A	605	4/4	0.96	0.14	37,42,44,45	0
5	DMS	B	504	4/4	0.96	0.19	39,42,55,57	0
7	SO4	A	609	5/5	0.96	0.29	60,77,82,84	0
7	SO4	A	610	5/5	0.96	0.25	42,54,61,63	0
4	T27	A	602	28/28	0.96	0.13	29,34,40,42	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.