



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:51 AM UTC

PDB ID : 8DXM / pdb_00008dxm
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	:	4-5-2 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

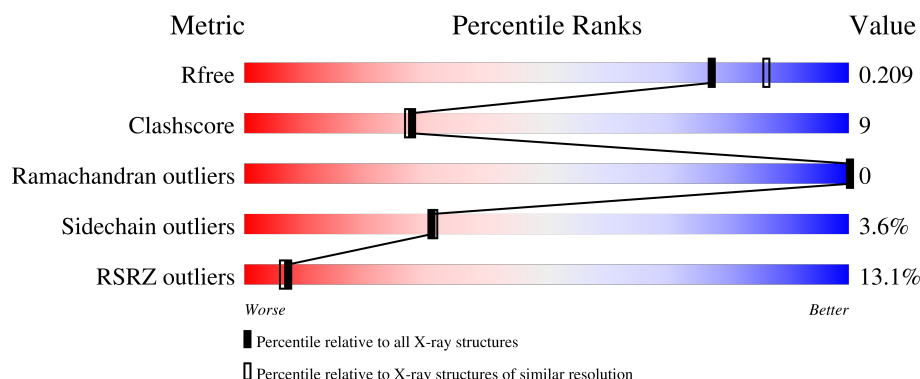
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	11% 83% 16% .
2	B	428	15% 82% 14% ..

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

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
1	A	556	Total	C	N	O	S	0	0	0
			4516	2923	750	835	8			

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

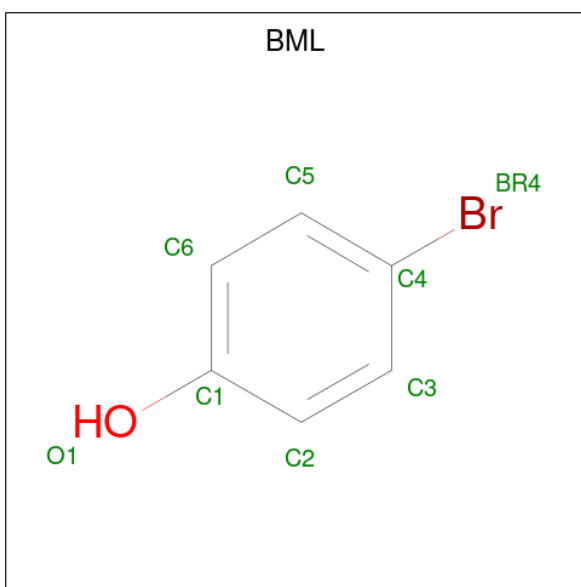
- Molecule 2 is a protein called p51 RT.

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

There is a discrepancy between the modelled and reference sequences:

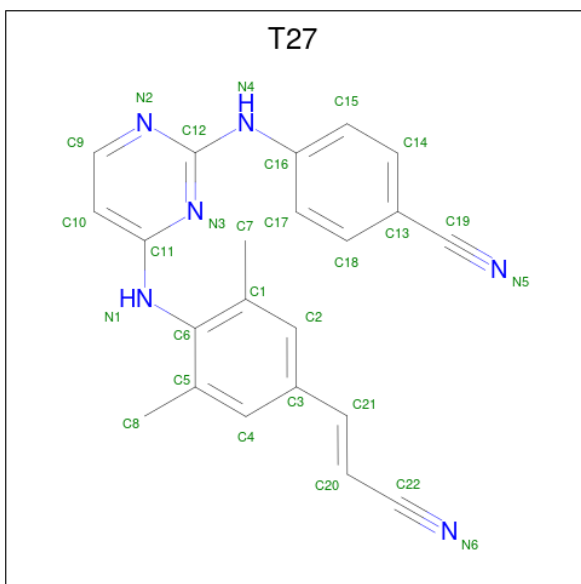
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

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



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

- Molecule 4 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (CCD ID: T27) (formula: $C_{22}H_{18}N_6$).



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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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 (CCD ID: MG) (formula: Mg).

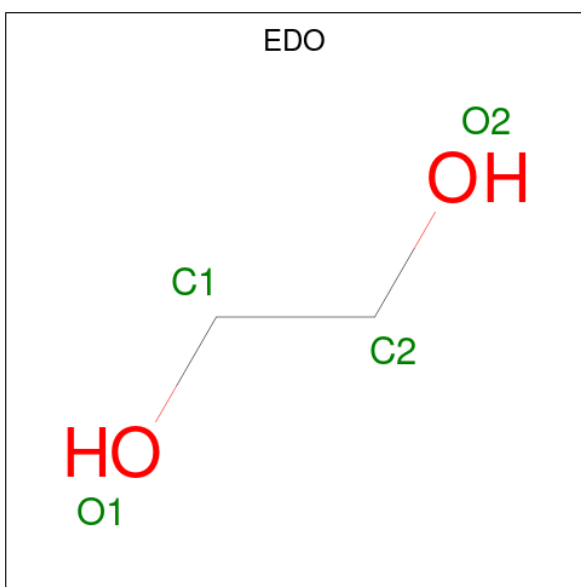
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

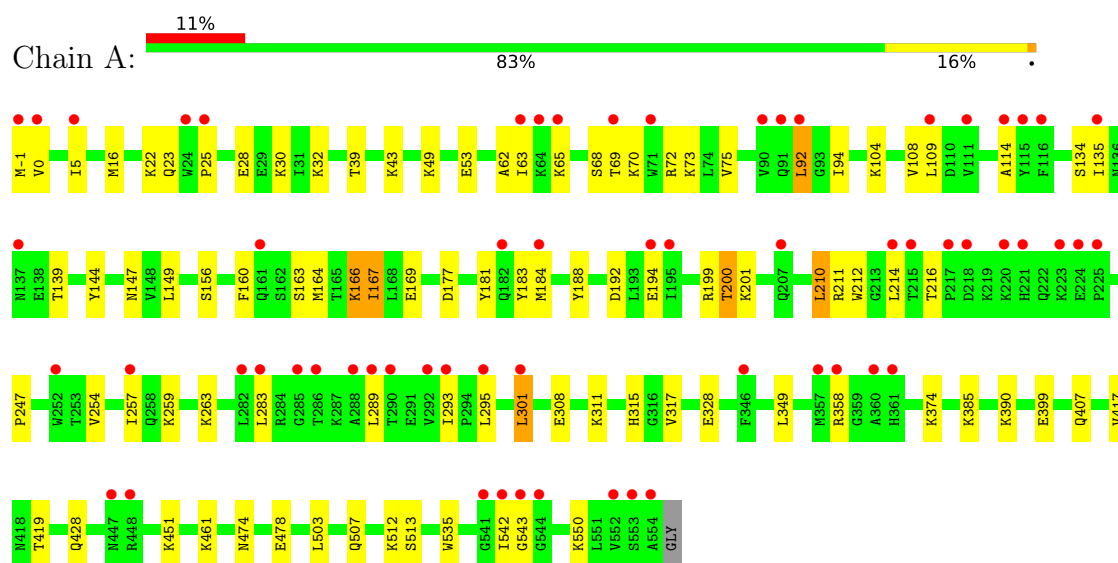
- Molecule 9 is water.

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

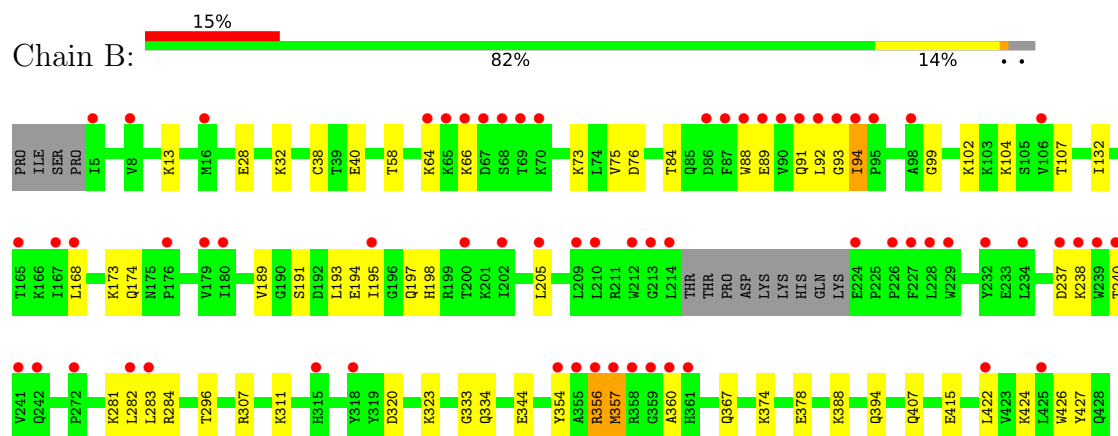
3 Residue-property plots [i](#)

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)	Xtriage
Refinement program	PHENIX dev_3051	Depositor
R, R_{free}	0.197 , 0.208 0.197 , 0.209	Depositor DCC
R_{free} test set	2000 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8552	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage'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, T27, EDO, 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	0.54	0/4634	0.84	9/6299 (0.1%)
2	B	0.40	0/3570	0.70	5/4852 (0.1%)
All	All	0.48	0/8204	0.78	14/11151 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	356	ARG	CA-C-N	-8.19	109.71	121.42
2	B	356	ARG	C-N-CA	-8.19	109.71	121.42
1	A	72	ARG	CA-C-N	6.57	130.82	121.42
1	A	72	ARG	C-N-CA	6.57	130.82	121.42
1	A	513	SER	CA-C-N	6.54	129.70	120.28
1	A	513	SER	C-N-CA	6.54	129.70	120.28
1	A	147	ASN	N-CA-C	-6.39	105.79	113.97
2	B	357	MET	O-C-N	6.04	130.13	123.01
1	A	200	THR	CB-CA-C	-5.78	101.81	110.88
2	B	427	TYR	CA-C-N	-5.65	111.52	121.70
2	B	427	TYR	C-N-CA	-5.65	111.52	121.70
1	A	69	THR	N-CA-C	-5.34	106.61	113.02
1	A	184	MET	CB-CA-C	-5.21	110.59	116.63
1	A	65	LYS	N-CA-C	-5.11	102.35	109.96

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	96	0
2	B	3459	0	3488	50	0
3	A	8	0	4	27	0
4	A	28	0	18	1	0
5	A	16	0	24	5	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	8	0
9	B	198	0	0	5	0
All	All	8552	0	8142	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (146) 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:428:GLN:H	5:A:605:DMS:H23	1.41	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:A:701:HOH:O	2:B:283:LEU:C	2.33	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
2:B:354:TYR:CB	2:B:357:MET:HE1	2.21	0.70
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
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:104:LYS:HD2	2:B:237:ASP:CG	2.21	0.65
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
2:B:107:THR:HG1	2:B:198:HIS:HE2	1.47	0.63
1:A:503:LEU:HD11	1:A:535:TRP:HB2	1.80	0.63
1:A:104:LYS:HB3	1:A:104:LYS:HZ1	1.62	0.63
2:B:281:LYS:O	2:B:281:LYS:HG3	2.00	0.62
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
1:A:428:GLN:N	5:A:605:DMS:H23	2.13	0.61
1:A:53:GLU:H	1:A:53:GLU:CD	2.10	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
2:B:354:TYR:HB3	2:B:357:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H11	9:B:757:HOH:O	2.07	0.55
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:22:LYS:C	1:A:22:LYS:HD2	2.34	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
2:B:73:LYS:HZ1	2:B:75:VAL:CG2	2.23	0.51
1:A:315:HIS:HB2	5:A:604:DMS:H23	1.92	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: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: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
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
2:B:354:TYR:HB2	2:B:357:MET:HE1	1.95	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:-1:MET:HE2	1:A:0:VAL:O	2.14	0.47
1:A:104:LYS:HD3	1:A:192:ASP:O	2.15	0.47
1:A:108:VAL:C	1:A:109:LEU:HD12	2.39	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:512:LYS:HE2	5:A:603:DMS:H13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:91:GLN:C	2:B:93:GLY:N	2.76	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
2:B:92:LEU:HD23	2:B:92:LEU:C	2.44	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
2:B:195:ILE:HA	2:B:198:HIS:HB3	2.01	0.42
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
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:474:ASN:HD22	5:A:606:DMS:H12	1.84	0.42
1:A:32:LYS:HB2	1:A:32:LYS:HE3	1.79	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.20	0.42
2:B:73:LYS:NZ	2:B:75:VAL:CG2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HG3	1:A:259:LYS:HZ2	1.85	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
2:B:333:GLY:O	2:B:334:GLN:HB2	2.20	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%)	473 (96%)	22 (4%)	25	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	380/390 (97%)	371 (98%)	9 (2%)	43	47
All	All	875/885 (99%)	844 (96%)	31 (4%)	31	32

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
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	289	LEU
1	A	295	LEU
1	A	301	LEU
1	A	358	ARG
1	A	374	LYS
1	A	399	GLU
1	A	451	LYS
1	A	461	LYS
2	B	64	LYS
2	B	66	LYS
2	B	88	TRP
2	B	89	GLU
2	B	94	ILE
2	B	173	LYS
2	B	238	LYS
2	B	240	THR
2	B	407	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	161	GLN
1	A	207	GLN
1	A	520	GLN
2	B	151	GLN
2	B	161	GLN
2	B	182	GLN
2	B	258	GLN
2	B	278	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 oligosaccharides 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	503	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
5	DMS	B	505	-	3,3,3	2.62	1 (33%)	3,3,3	0.36	0
7	SO4	A	609	-	4,4,4	0.40	0	6,6,6	0.09	0
5	DMS	B	501	-	3,3,3	2.71	1 (33%)	3,3,3	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	608	-	4,4,4	0.41	0	6,6,6	0.09	0
5	DMS	A	603	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
5	DMS	A	606	-	3,3,3	2.76	1 (33%)	3,3,3	0.61	0
5	DMS	B	504	-	3,3,3	2.60	1 (33%)	3,3,3	0.47	0
5	DMS	A	604	-	3,3,3	2.60	1 (33%)	3,3,3	0.68	0
5	DMS	A	605	-	3,3,3	2.83	1 (33%)	3,3,3	0.81	0
7	SO4	A	610	-	4,4,4	0.39	0	6,6,6	0.09	0
3	BML	A	601[A]	-	8,8,8	0.38	0	10,10,10	0.16	0
8	EDO	B	506	-	3,3,3	0.21	0	2,2,2	0.16	0
4	T27	A	602	-	30,30,30	1.12	3 (10%)	37,40,40	1.64	4 (10%)
5	DMS	B	502	-	3,3,3	2.62	1 (33%)	3,3,3	0.41	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
4	T27	A	602	-	-	2/13/14/14	0/3/3/3
8	EDO	B	506	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	DMS	O-S	4.78	1.81	1.50
5	A	606	DMS	O-S	4.62	1.80	1.50
5	B	503	DMS	O-S	4.58	1.80	1.50
5	A	603	DMS	O-S	4.57	1.80	1.50
5	B	501	DMS	O-S	4.56	1.80	1.50
5	B	502	DMS	O-S	4.46	1.79	1.50
5	B	505	DMS	O-S	4.39	1.79	1.50
5	A	604	DMS	O-S	4.39	1.79	1.50
5	B	504	DMS	O-S	4.37	1.79	1.50
4	A	602	T27	C12-N4	3.74	1.44	1.36
4	A	602	T27	C11-N1	2.90	1.43	1.38
4	A	602	T27	C13-C19	2.24	1.49	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	T27	C9-N2-C12	5.78	120.25	115.42
4	A	602	T27	N2-C12-N3	-4.66	121.91	126.42
4	A	602	T27	C10-C9-N2	-4.00	119.07	123.97
4	A	602	T27	C10-C11-N3	-2.71	118.61	123.15

There are no chirality outliers.

All (3) torsion outliers are listed below:

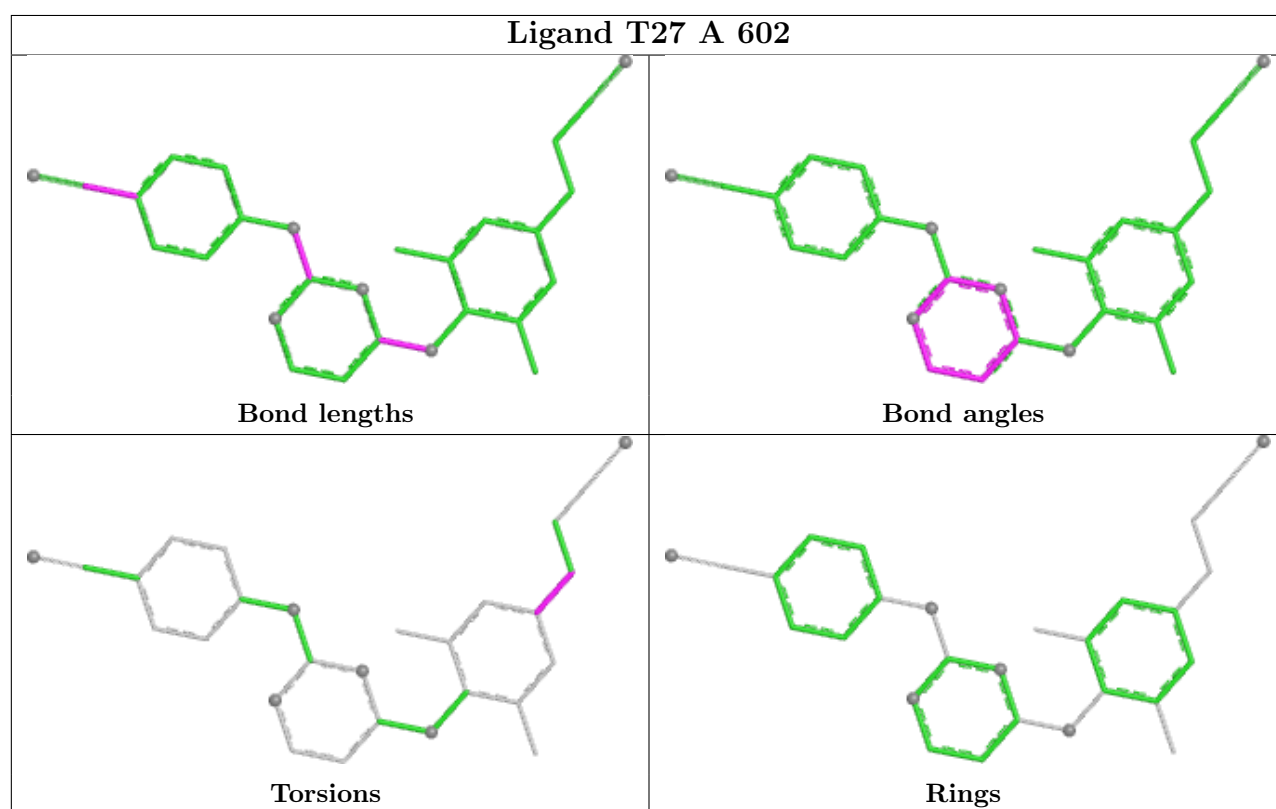
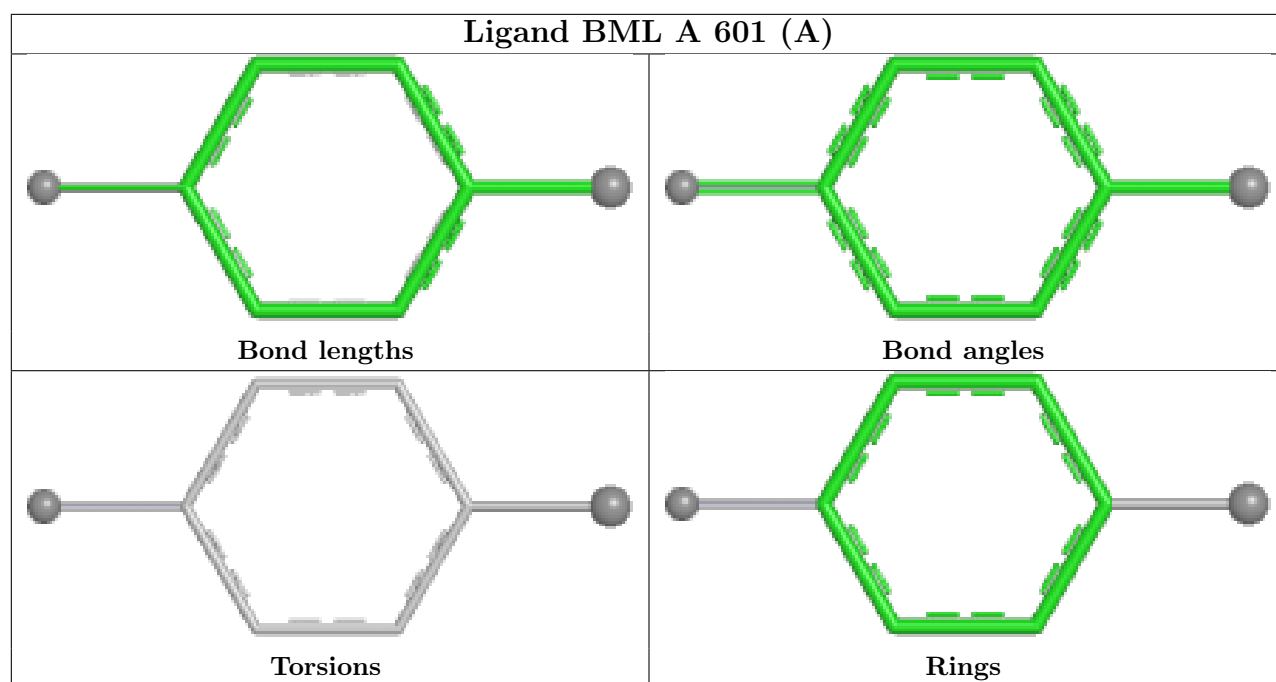
Mol	Chain	Res	Type	Atoms
4	A	602	T27	C20-C21-C3-C4
4	A	602	T27	C20-C21-C3-C2
8	B	506	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	DMS	1	0
5	B	501	DMS	1	0
5	A	603	DMS	1	0
5	A	606	DMS	1	0
5	A	604	DMS	1	0
5	A	605	DMS	2	0
3	A	601[A]	BML	27	0
4	A	602	T27	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 ⓘ

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	556/557 (99%)	0.66	62 (11%) 10 9	25, 45, 95, 177	0
2	B	415/428 (96%)	0.83	65 (15%) 5 4	18, 46, 108, 226	4 (0%)
All	All	971/985 (98%)	0.73	127 (13%) 7 6	18, 46, 104, 226	4 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	TRP	9.0
2	B	94	ILE	7.5
1	A	115	TYR	6.1
2	B	241	VAL	5.9
2	B	92	LEU	5.7
2	B	5	ILE	5.5
2	B	95	PRO	5.1
1	A	288	ALA	4.9
1	A	554	ALA	4.8
2	B	90	VAL	4.6
2	B	214	LEU	4.3
1	A	116	PHE	4.2
2	B	229	TRP	4.1
2	B	355	ALA	4.1
1	A	5	ILE	4.0
2	B	359	GLY	3.9
1	A	289	LEU	3.9
2	B	209	LEU	3.8
2	B	88	TRP	3.8
1	A	295	LEU	3.8
1	A	65	LYS	3.8
1	A	90	VAL	3.8
1	A	92	LEU	3.7
2	B	357	MET	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	93	GLY	3.7
2	B	356	ARG	3.6
1	A	292	VAL	3.6
2	B	66	LYS	3.6
1	A	543	GLY	3.6
1	A	544	GLY	3.5
1	A	282	LEU	3.5
2	B	283	LEU	3.5
1	A	286	THR	3.4
2	B	69	THR	3.4
2	B	240	THR	3.4
2	B	425	LEU	3.4
1	A	290	THR	3.4
1	A	109	LEU	3.4
1	A	357	MET	3.4
1	A	541	GLY	3.3
1	A	220	LYS	3.3
2	B	361	HIS	3.3
1	A	293	ILE	3.3
2	B	202	ILE	3.3
2	B	239	TRP	3.3
2	B	360	ALA	3.3
1	A	218	ASP	3.2
1	A	552	VAL	3.1
2	B	70	LYS	3.1
2	B	212	TRP	3.1
2	B	354	TYR	3.1
2	B	200	THR	3.1
1	A	25	PRO	3.1
1	A	257	ILE	3.1
2	B	87	PHE	3.0
2	B	242	GLN	3.0
1	A	553	SER	2.9
1	A	91	GLN	2.9
1	A	195	ILE	2.9
1	A	137	ASN	2.8
2	B	315	HIS	2.8
1	A	71	TRP	2.8
2	B	180	ILE	2.8
2	B	205	LEU	2.8
2	B	179	VAL	2.8
2	B	16	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	228	LEU	2.7
2	B	227	PHE	2.7
1	A	69	THR	2.7
1	A	225	PRO	2.7
1	A	135	ILE	2.7
2	B	89	GLU	2.7
1	A	301	LEU	2.7
2	B	68	SER	2.6
2	B	226	PRO	2.6
1	A	-1	MET	2.6
2	B	67	ASP	2.6
2	B	358	ARG	2.6
1	A	361	HIS	2.5
2	B	64	LYS	2.5
2	B	318	TYR	2.5
2	B	422	LEU	2.5
2	B	8	VAL	2.5
2	B	237	ASP	2.5
1	A	214	LEU	2.5
1	A	358	ARG	2.4
2	B	168	LEU	2.4
2	B	167	ILE	2.4
1	A	346	PHE	2.4
2	B	238	LYS	2.4
1	A	182	GLN	2.4
1	A	111	VAL	2.4
2	B	234	LEU	2.3
1	A	223	LYS	2.3
1	A	0	VAL	2.3
1	A	217	PRO	2.3
2	B	224	GLU	2.3
2	B	91	GLN	2.3
2	B	282	LEU	2.3
2	B	65	LYS	2.3
1	A	448	ARG	2.2
1	A	63	ILE	2.2
2	B	86	ASP	2.2
2	B	106	VAL	2.2
1	A	221	HIS	2.2
1	A	184	MET	2.2
1	A	161	GLN	2.2
1	A	542	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	64	LYS	2.2
1	A	194	GLU	2.2
1	A	114	ALA	2.2
2	B	98	ALA	2.2
1	A	207	GLN	2.1
2	B	165	THR	2.1
2	B	213	GLY	2.1
1	A	360	ALA	2.1
1	A	252	TRP	2.1
2	B	210	LEU	2.1
2	B	232	TYR	2.1
1	A	224	GLU	2.1
2	B	195	ILE	2.0
1	A	215	THR	2.0
1	A	283	LEU	2.0
1	A	285	GLY	2.0
1	A	447	ASN	2.0
2	B	176	PRO	2.0
2	B	272	PRO	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.

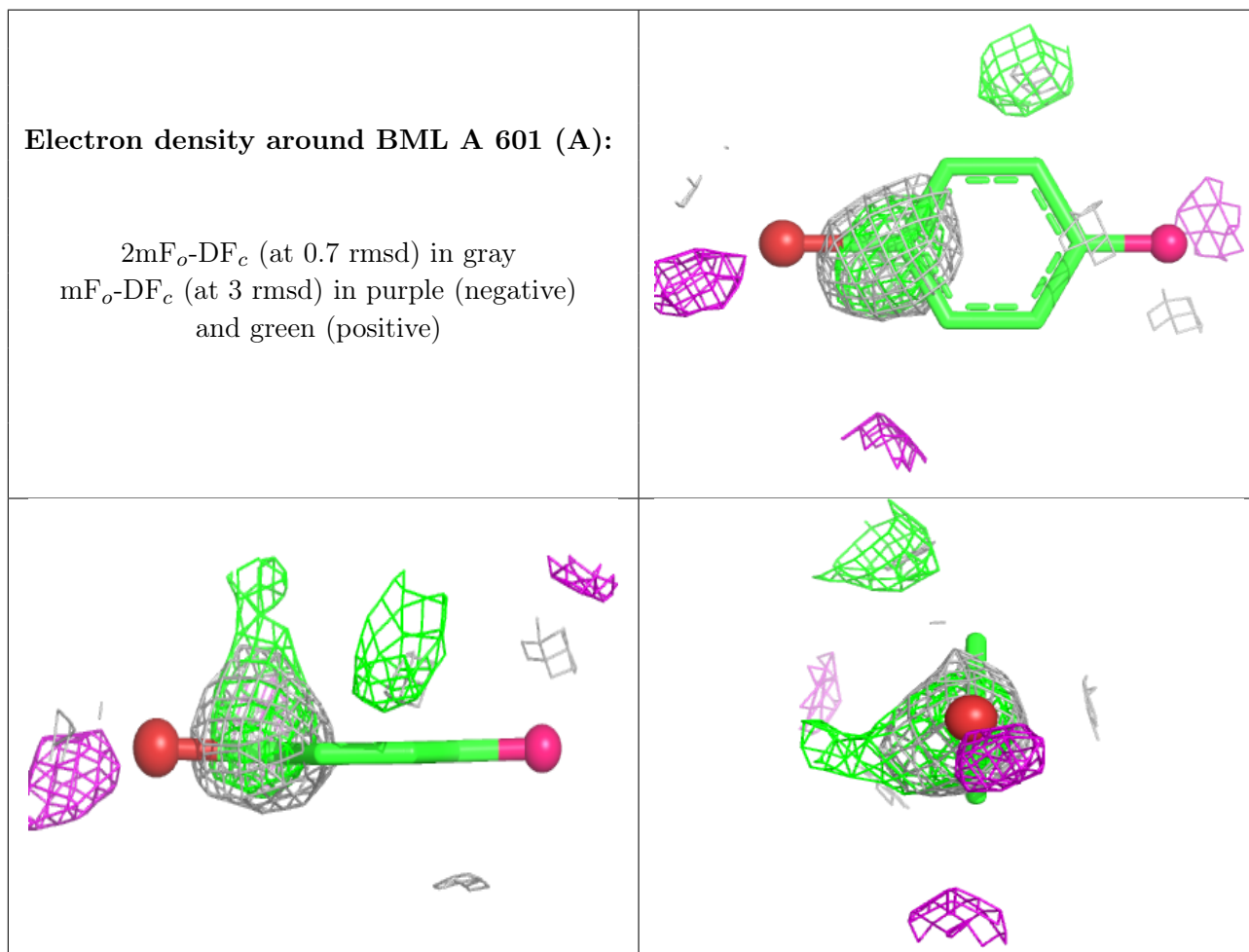
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	A	608	5/5	0.65	0.12	85,86,89,97	0
3	BML	A	601[A]	8/8	0.77	0.61	48,53,56,91	8
5	DMS	A	606	4/4	0.78	0.18	47,60,62,77	0
7	SO4	A	609	5/5	0.78	0.13	60,77,82,84	0

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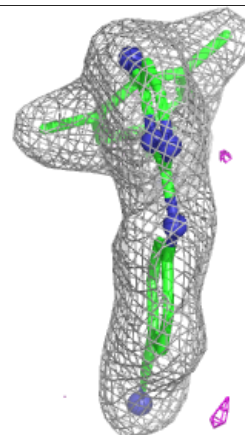
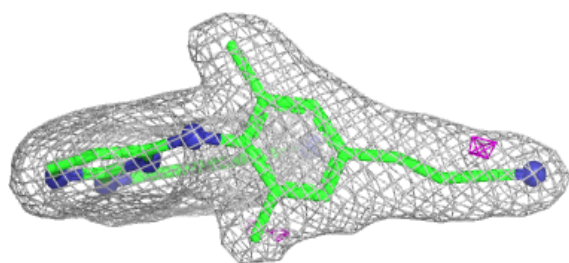
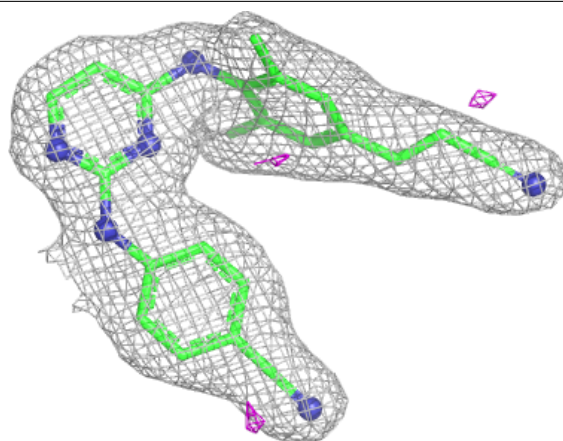
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	604	4/4	0.79	0.18	53,58,66,77	0
5	DMS	B	503	4/4	0.80	0.19	66,75,79,82	0
5	DMS	B	505	4/4	0.80	0.21	51,55,58,70	0
5	DMS	A	603	4/4	0.84	0.20	60,63,68,69	0
7	SO4	A	610	5/5	0.87	0.13	42,54,61,63	0
8	EDO	B	506	4/4	0.90	0.14	44,44,50,51	0
5	DMS	B	501	4/4	0.91	0.17	42,46,49,52	0
5	DMS	B	502	4/4	0.91	0.16	43,44,57,59	0
6	MG	A	607	1/1	0.92	0.12	63,63,63,63	0
4	T27	A	602	28/28	0.95	0.09	29,34,40,42	0
5	DMS	B	504	4/4	0.95	0.12	39,42,55,57	0
5	DMS	A	605	4/4	0.96	0.10	37,42,44,45	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 T27 A 602:

$2mF_o-DF_c$ (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.