



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:47 AM UTC

PDB ID : 5CYM / pdb_00005cym
Title : HIV-1 reverse transcriptase complexed with 4-iodopyrazole
Authors : Bauman, J.D.; Arnold, E.
Deposited on : 2015-07-30
Resolution : 2.10 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

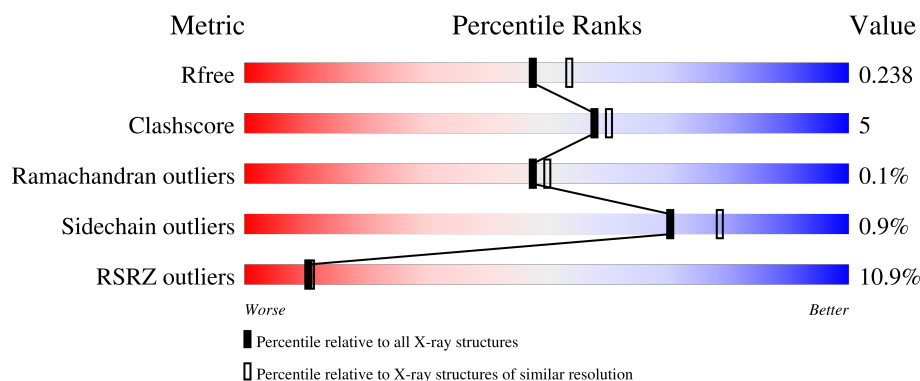
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	557	10% 90% 8% .
2	B	428	12% 86% 9% 5%

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
6	IOD	A	613	-	-	X	-
6	IOD	A	614	-	-	X	-
6	IOD	A	615	-	-	X	-
6	IOD	A	616	-	-	X	-
7	PYZ	B	509	-	-	X	-
8	DMS	B	514	-	-	-	X
8	DMS	B	515	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16183 atoms, of which 7992 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 HIV-1 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	546	Total	C	H	N	O	S	0	1	0
			8935	2878	4493	737	819	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

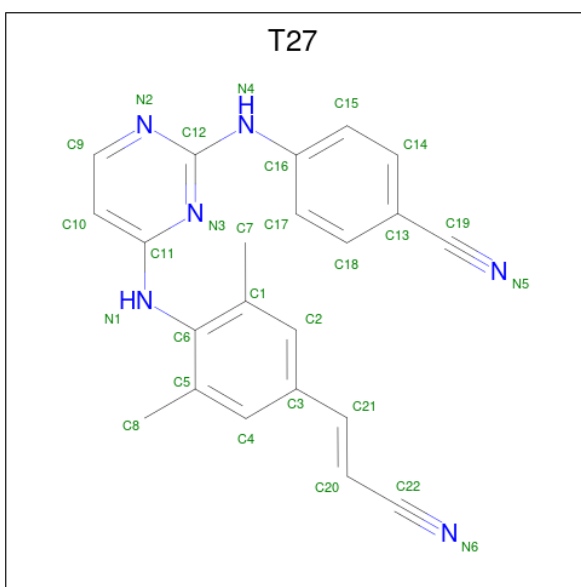
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	408	Total	C	H	N	O	S	0	2	0
			6788	2201	3409	559	612	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-{{4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (CCD ID: T27) (formula: C₂₂H₁₈N₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			46	22	18	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

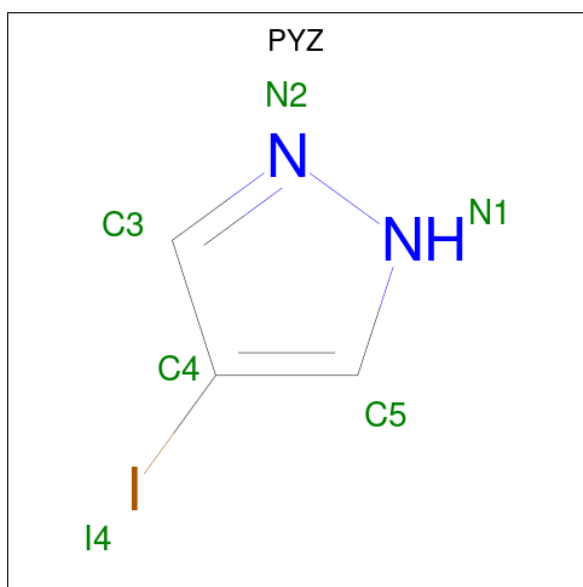


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	I	0	0
			10	10		
6	B	4	Total	I	0	0
			4	4		

- Molecule 7 is 4-IODOPYRAZOLE (CCD ID: PYZ) (formula: C₃H₃IN₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	A	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		
7	B	1	Total	C	H	I	N	0	0
			9	3	3	1	2		

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
8	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

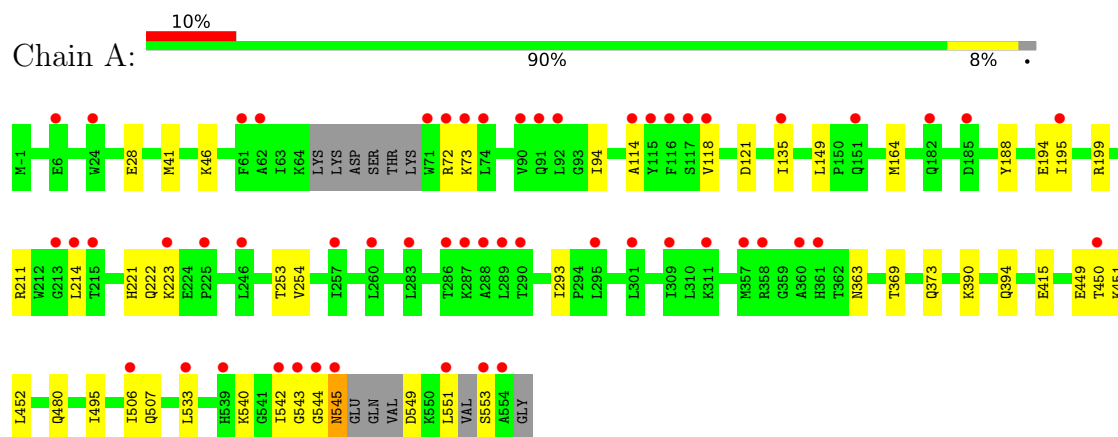
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	150	Total	O	0	0
			150	150		
9	B	86	Total	O	0	0
			86	86		

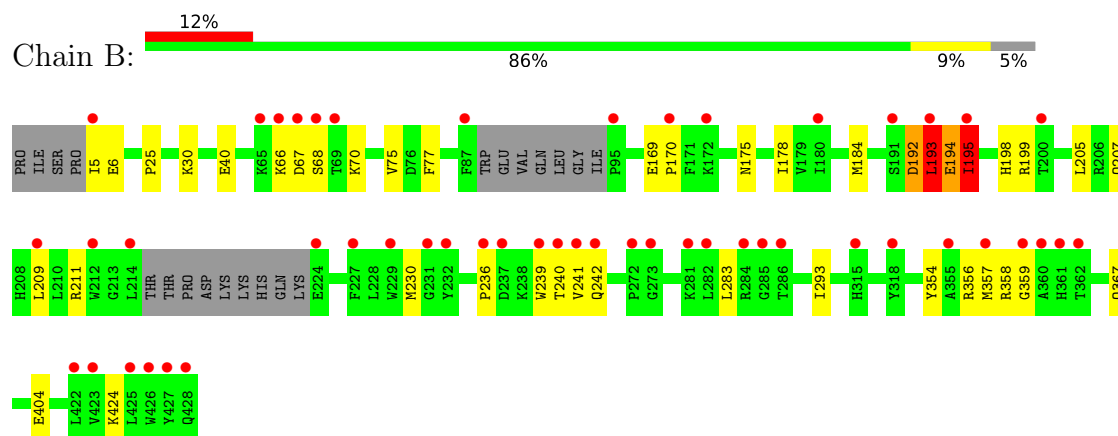
3 Residue-property plots [i](#)

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: HIV-1 reverse transcriptase, p66 subunit



- Molecule 2: HIV-1 reverse transcriptase, p51 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.84Å 73.48Å 109.58Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	43.17 – 2.10 43.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.17-2.10) 98.4 (43.17-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX dev_1988	Depositor
R, R_{free}	0.195 , 0.229 0.203 , 0.238	Depositor DCC
R_{free} test set	3742 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.8	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	0.95	EDS
Total number of atoms	16183	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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, IOD, SO4, PYZ, EDO, T27

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	0.43	0/4560	0.68	0/6196
2	B	0.44	0/3484	0.73	4/4730 (0.1%)
All	All	0.44	0/8044	0.70	4/10926 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	192	ASP	N-CA-C	-10.63	94.51	110.14
2	B	195	ILE	N-CA-C	6.43	117.95	110.62
2	B	194	GLU	N-CA-C	6.32	119.54	109.24
2	B	192	ASP	CA-C-O	-5.65	114.55	121.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	193	LEU	Peptide

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	4442	4493	4490	36	0
2	B	3379	3409	3394	35	0
3	A	28	18	18	2	0
4	A	15	0	0	0	0
4	B	5	0	0	1	0
5	A	8	12	12	0	0
5	B	8	12	12	0	0
6	A	10	0	0	10	0
6	B	4	0	0	0	0
7	A	12	6	6	0	0
7	B	24	12	12	2	0
8	A	4	6	6	0	0
8	B	16	24	24	1	0
9	A	150	0	0	4	0
9	B	86	0	0	3	0
All	All	8191	7992	7974	72	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 5.

All (72) 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)
2:B:192:ASP:O	2:B:193:LEU:HB2	1.76	0.84
1:A:543:GLY:N	2:B:283:LEU:O	2.09	0.84
6:A:614:IOD:I	6:A:615:IOD:I	3.36	0.84
1:A:394:GLN:NE2	9:A:702:HOH:O	2.16	0.79
2:B:40:GLU:OE1	9:B:601:HOH:O	2.02	0.77
1:A:390:LYS:NZ	1:A:415:GLU:OE1	2.22	0.73
2:B:293:ILE:O	9:B:602:HOH:O	2.10	0.70
1:A:195:ILE:O	1:A:199:ARG:HG3	1.94	0.67
1:A:449:GLU:OE1	1:A:449:GLU:N	2.28	0.66
2:B:193:LEU:HD23	2:B:194:GLU:C	2.20	0.66
1:A:543:GLY:CA	2:B:283:LEU:O	2.44	0.65
2:B:193:LEU:HD22	2:B:198:HIS:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:OD1	9:A:701:HOH:O	2.16	0.61
1:A:164:MET:HE2	6:A:607:IOD:I	2.71	0.61
6:A:613:IOD:I	6:A:616:IOD:I	3.59	0.60
1:A:222:GLN:O	1:A:222:GLN:NE2	2.34	0.60
1:A:506:ILE:HD11	1:A:533:LEU:HD23	1.83	0.60
1:A:543:GLY:HA3	2:B:283:LEU:O	2.01	0.59
2:B:25:PRO:HA	8:B:515:DMS:H12	1.85	0.59
1:A:506:ILE:CD1	1:A:533:LEU:HD23	2.34	0.57
2:B:240:THR:OG1	2:B:241:VAL:N	2.33	0.56
2:B:357:MET:HB3	2:B:367:GLN:HG2	1.88	0.55
1:A:549:ASP:O	6:A:616:IOD:I	2.95	0.55
1:A:544:GLY:O	6:A:615:IOD:I	2.95	0.55
1:A:480[B]:GLN:NE2	9:A:707:HOH:O	2.39	0.54
2:B:30:LYS:NZ	9:B:603:HOH:O	2.39	0.54
2:B:193:LEU:CD2	2:B:194:GLU:O	2.56	0.54
2:B:354:TYR:HB3	2:B:357:MET:HE3	1.89	0.53
1:A:506:ILE:HG13	1:A:507:GLN:N	2.24	0.53
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.45	0.52
2:B:193:LEU:CD2	2:B:198:HIS:HB2	2.40	0.51
1:A:553:SER:N	6:A:616:IOD:I	3.14	0.51
2:B:193:LEU:HD21	2:B:194:GLU:O	2.11	0.50
1:A:450:THR:O	1:A:451:LYS:HG2	2.12	0.50
1:A:551:LEU:HD12	6:A:614:IOD:I	2.82	0.49
3:A:601:T27:N3	3:A:601:T27:H17	2.29	0.48
2:B:5:ILE:HD12	2:B:6:GLU:N	2.29	0.48
1:A:41:MET:HE3	1:A:46:LYS:HE2	1.96	0.47
1:A:495:ILE:O	1:A:533:LEU:HD12	2.15	0.47
1:A:451:LYS:HG3	9:A:710:HOH:O	2.13	0.47
2:B:205:LEU:O	2:B:209:LEU:CD1	2.62	0.47
2:B:68:SER:HB2	2:B:230:MET:CE	2.45	0.46
2:B:207:GLN:O	2:B:211:ARG:HG3	2.15	0.46
2:B:77:PHE:H	7:B:509:PYZ:HN1	1.62	0.46
2:B:66:LYS:NZ	2:B:67:ASP:OD1	2.49	0.46
1:A:253:THR:O	1:A:254:VAL:C	2.59	0.45
1:A:369:THR:O	1:A:373:GLN:HG2	2.17	0.45
2:B:205:LEU:O	2:B:209:LEU:HD13	2.17	0.45
1:A:545:ASN:HA	6:A:615:IOD:I	2.87	0.45
2:B:358:ARG:HD2	2:B:359:GLY:N	2.32	0.44
1:A:450:THR:HG23	1:A:452:LEU:H	1.82	0.44
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.99	0.44
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:ARG:C	2:B:358:ARG:CD	2.91	0.43
1:A:28:GLU:HG3	1:A:135:ILE:HD12	2.00	0.43
1:A:254:VAL:HG23	1:A:293:ILE:HD11	2.00	0.43
2:B:175:ASN:HB3	2:B:178:ILE:HG12	2.00	0.43
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.48	0.42
2:B:357:MET:HE2	2:B:357:MET:H	1.83	0.42
1:A:221:HIS:HD2	1:A:223:LYS:H	1.68	0.42
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.50	0.42
6:A:613:IOD:I	6:A:614:IOD:I	3.77	0.42
2:B:424:LYS:NZ	4:B:501:SO4:O3	2.52	0.42
1:A:188:TYR:CD1	3:A:601:T27:H20	2.55	0.42
2:B:5:ILE:HD12	2:B:5:ILE:C	2.45	0.41
1:A:363:ASN:OD1	1:A:363:ASN:C	2.63	0.41
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.55	0.41
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.03	0.41
1:A:549:ASP:HA	6:A:616:IOD:I	2.90	0.41
1:A:72:ARG:HG3	1:A:73:LYS:N	2.36	0.41
2:B:184:MET:HE2	7:B:509:PYZ:I4	2.90	0.40
1:A:114:ALA:HA	1:A:214:LEU:HD22	2.03	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	539/557 (97%)	527 (98%)	12 (2%)	0	100	100
2	B	404/428 (94%)	392 (97%)	11 (3%)	1 (0%)	43	44
All	All	943/985 (96%)	919 (98%)	23 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	LEU

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	486/495 (98%)	482 (99%)	4 (1%)	73	81
2	B	372/390 (95%)	368 (99%)	4 (1%)	65	74
All	All	858/885 (97%)	850 (99%)	8 (1%)	70	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	194	GLU
1	A	211	ARG
1	A	545	ASN
2	B	70	LYS
2	B	195	ILE
2	B	242	GLN
2	B	356	ARG

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	147	ASN
1	A	315	HIS
1	A	524	GLN
1	A	545	ASN
2	B	255	ASN

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 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 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	EDO	A	606	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	B	502	-	3,3,3	0.41	0	2,2,2	0.33	0
7	PYZ	A	618	-	6,6,6	2.78	3 (50%)	7,7,7	1.14	1 (14%)
8	DMS	B	512	-	3,3,3	0.71	0	3,3,3	0.59	0
4	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.11	0
7	PYZ	A	617	-	6,6,6	3.01	4 (66%)	7,7,7	1.31	1 (14%)
4	SO4	A	602	-	4,4,4	0.25	0	6,6,6	0.21	0
5	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.31	0
3	T27	A	601	-	30,30,30	1.15	3 (10%)	37,40,40	1.74	5 (13%)
8	DMS	A	619	-	3,3,3	0.64	0	3,3,3	0.74	0
8	DMS	B	513	-	3,3,3	0.65	0	3,3,3	0.52	0
7	PYZ	B	511	-	6,6,6	2.66	3 (50%)	7,7,7	1.10	1 (14%)
7	PYZ	B	510	-	6,6,6	2.71	2 (33%)	7,7,7	1.13	1 (14%)
4	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.12	0
7	PYZ	B	508	-	6,6,6	2.71	3 (50%)	7,7,7	1.15	1 (14%)
7	PYZ	B	509	-	6,6,6	2.53	3 (50%)	7,7,7	0.94	1 (14%)
8	DMS	B	515	-	3,3,3	0.65	0	3,3,3	0.55	0
8	DMS	B	514	-	3,3,3	0.68	0	3,3,3	0.55	0
4	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.11	0
5	EDO	B	503	-	3,3,3	0.40	0	2,2,2	0.30	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
7	PYZ	B	511	-	-	-	0/1/1/1
5	EDO	A	606	-	-	0/1/1/1	-
7	PYZ	B	510	-	-	-	0/1/1/1
7	PYZ	B	508	-	-	-	0/1/1/1
7	PYZ	A	617	-	-	-	0/1/1/1
5	EDO	B	502	-	-	0/1/1/1	-
5	EDO	A	605	-	-	0/1/1/1	-
7	PYZ	A	618	-	-	-	0/1/1/1
7	PYZ	B	509	-	-	-	0/1/1/1
5	EDO	B	503	-	-	0/1/1/1	-
3	T27	A	601	-	-	0/13/14/14	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	618	PYZ	C5-N1	5.58	1.42	1.34
7	B	510	PYZ	C5-N1	5.52	1.42	1.34
7	A	617	PYZ	C5-N1	5.48	1.42	1.34
7	B	508	PYZ	C5-N1	5.45	1.42	1.34
7	B	511	PYZ	C5-N1	5.34	1.42	1.34
7	B	509	PYZ	C5-N1	4.81	1.41	1.34
7	A	617	PYZ	C4-I4	-3.45	2.01	2.08
3	A	601	T27	C12-N4	3.41	1.43	1.36
7	A	618	PYZ	C3-N2	2.75	1.38	1.33
3	A	601	T27	C11-N1	2.70	1.43	1.38
7	B	508	PYZ	C3-N2	2.68	1.38	1.33
7	B	510	PYZ	C3-N2	2.68	1.38	1.33
7	B	509	PYZ	C3-C4	2.62	1.44	1.39
7	B	511	PYZ	C3-N2	2.41	1.37	1.33
7	B	508	PYZ	C3-C4	2.35	1.44	1.39
7	A	617	PYZ	C3-N2	2.32	1.37	1.33
3	A	601	T27	C13-C19	2.24	1.49	1.44
7	A	618	PYZ	C3-C4	2.20	1.43	1.39
7	A	617	PYZ	C3-C4	2.15	1.43	1.39
7	B	509	PYZ	C4-I4	-2.06	2.04	2.08
7	B	511	PYZ	C4-I4	-2.04	2.04	2.08

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	T27	C9-N2-C12	6.01	120.44	115.42
3	A	601	T27	N2-C12-N3	-4.45	122.12	126.42
3	A	601	T27	C10-C9-N2	-4.27	118.74	123.97
3	A	601	T27	C10-C11-N3	-2.84	118.40	123.15
7	A	617	PYZ	C4-C3-N2	-2.80	109.64	111.81
7	B	510	PYZ	C4-C3-N2	-2.57	109.82	111.81
7	A	618	PYZ	C4-C3-N2	-2.50	109.87	111.81
7	B	511	PYZ	C4-C3-N2	-2.46	109.91	111.81
7	B	508	PYZ	C4-C3-N2	-2.44	109.92	111.81
3	A	601	T27	C6-N1-C11	-2.08	120.36	124.11
7	B	509	PYZ	C4-C3-N2	-2.02	110.24	111.81

There are no chirality outliers.

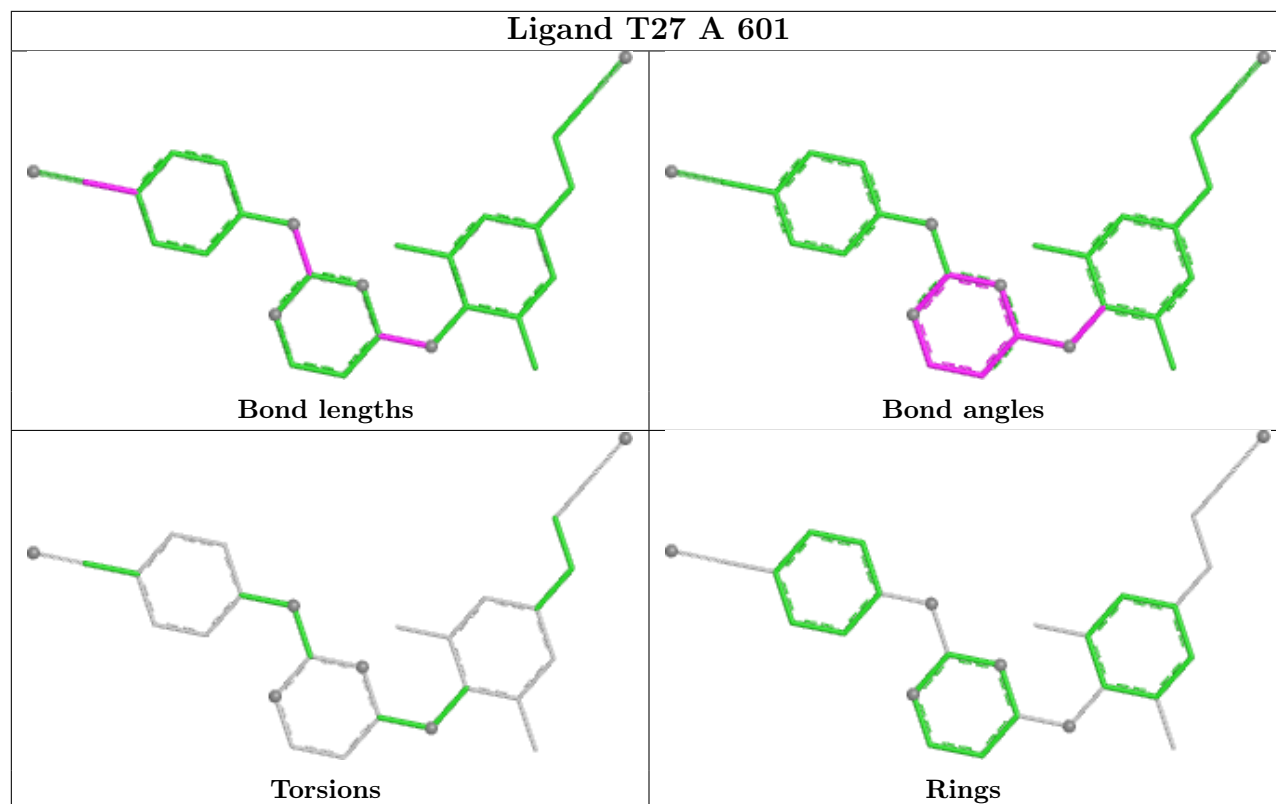
There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	SO4	1	0
3	A	601	T27	2	0
7	B	509	PYZ	2	0
8	B	515	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	546/557 (98%)	0.59	54 (9%)	13 13	30, 63, 120, 195	1 (0%)
2	B	408/428 (95%)	0.72	50 (12%)	8 8	24, 67, 124, 171	1 (0%)
All	All	954/985 (96%)	0.65	104 (10%)	10 11	24, 64, 124, 195	2 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	PHE	8.5
2	B	241	VAL	6.9
1	A	554	ALA	6.2
1	A	544	GLY	5.8
2	B	87	PHE	5.7
2	B	232	TYR	5.7
1	A	114	ALA	5.3
2	B	214	LEU	5.3
1	A	115	TYR	5.0
1	A	24	TRP	5.0
2	B	423	VAL	4.9
1	A	288	ALA	4.6
2	B	425	LEU	4.6
2	B	95	PRO	4.6
1	A	551	LEU	4.5
1	A	542	ILE	4.4
1	A	90	VAL	4.1
1	A	117	SER	4.1
2	B	359	GLY	4.0
2	B	422	LEU	4.0
2	B	242	GLN	4.0
1	A	545	ASN	3.9
1	A	543	GLY	3.9
2	B	355	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	193	LEU	3.7
2	B	240	THR	3.6
2	B	236	PRO	3.6
2	B	212	TRP	3.6
2	B	5	ILE	3.5
2	B	224	GLU	3.5
1	A	71	TRP	3.5
2	B	361	HIS	3.5
2	B	239	TRP	3.4
1	A	260	LEU	3.3
2	B	357	MET	3.3
1	A	553	SER	3.2
2	B	318	TYR	3.2
1	A	213	GLY	3.2
1	A	506	ILE	3.2
1	A	286	THR	3.1
2	B	426	TRP	3.1
2	B	65	LYS	3.0
1	A	151	GLN	3.0
2	B	195	ILE	3.0
1	A	92	LEU	3.0
1	A	6	GLU	3.0
1	A	257	ILE	3.0
1	A	283	LEU	2.9
2	B	272	PRO	2.8
2	B	66	LYS	2.8
1	A	533	LEU	2.8
2	B	180	ILE	2.8
1	A	223	LYS	2.7
1	A	301	LEU	2.7
1	A	311	LYS	2.7
1	A	357	MET	2.6
1	A	539	HIS	2.6
1	A	450	THR	2.6
1	A	182	GLN	2.6
1	A	360	ALA	2.6
2	B	360	ALA	2.6
2	B	237	ASP	2.6
1	A	195	ILE	2.5
2	B	209	LEU	2.5
1	A	290	THR	2.5
1	A	289	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	361	HIS	2.5
2	B	285	GLY	2.5
1	A	135	ILE	2.5
1	A	309	ILE	2.5
1	A	91	GLN	2.4
2	B	67	ASP	2.4
2	B	229	TRP	2.4
2	B	286	THR	2.4
2	B	315	HIS	2.4
2	B	273	GLY	2.4
2	B	227	PHE	2.4
1	A	295	LEU	2.4
2	B	231	GLY	2.4
2	B	362	THR	2.4
1	A	185	ASP	2.3
1	A	73	LYS	2.3
1	A	74	LEU	2.3
2	B	282	LEU	2.3
1	A	118	VAL	2.3
2	B	69	THR	2.3
1	A	62	ALA	2.3
2	B	427	TYR	2.3
2	B	170	PRO	2.2
2	B	200	THR	2.2
1	A	72	ARG	2.2
2	B	281	LYS	2.2
1	A	61	PHE	2.2
2	B	68	SER	2.2
2	B	428	GLN	2.2
1	A	358	ARG	2.2
1	A	214	LEU	2.1
1	A	246	LEU	2.1
1	A	287	LYS	2.1
2	B	191	SER	2.1
1	A	225	PRO	2.1
2	B	172	LYS	2.1
1	A	215	THR	2.0
2	B	284	ARG	2.0

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

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
7	PYZ	A	618	6/6	0.52	0.22	112,119,144,258	0
8	DMS	B	514	4/4	0.56	0.47	119,148,148,148	0
6	IOD	A	611	1/1	0.66	0.26	389,389,389,389	0
6	IOD	B	507	1/1	0.66	0.20	198,198,198,198	0
4	SO4	A	604	5/5	0.69	0.13	133,134,136,139	0
8	DMS	B	515	4/4	0.72	0.41	118,142,143,143	0
4	SO4	A	603	5/5	0.74	0.11	119,121,124,135	0
7	PYZ	B	509	6/6	0.75	0.25	89,102,129,326	0
7	PYZ	B	510	6/6	0.79	0.28	136,146,173,176	0
7	PYZ	B	511	6/6	0.79	0.19	93,101,121,172	0
6	IOD	A	612	1/1	0.81	0.16	229,229,229,229	0
8	DMS	B	512	4/4	0.81	0.24	88,106,107,107	0
6	IOD	A	614	1/1	0.82	0.34	198,198,198,198	0
8	DMS	A	619	4/4	0.84	0.25	93,112,120,120	0
5	EDO	B	502	4/4	0.84	0.26	67,80,97,113	0
6	IOD	B	506	1/1	0.85	0.14	216,216,216,216	0
6	IOD	A	610	1/1	0.85	0.20	182,182,182,182	0
6	IOD	A	616	1/1	0.86	0.18	87,87,87,87	1
6	IOD	B	505	1/1	0.86	0.30	160,160,160,160	0
5	EDO	A	606	4/4	0.87	0.18	67,87,109,109	0
4	SO4	A	602	5/5	0.88	0.08	89,95,101,103	0
4	SO4	B	501	5/5	0.88	0.16	122,123,126,130	0
6	IOD	B	504	1/1	0.89	0.19	112,112,112,112	0
6	IOD	A	609	1/1	0.90	0.16	153,153,153,153	0
7	PYZ	A	617	6/6	0.90	0.14	47,58,74,106	0
8	DMS	B	513	4/4	0.91	0.29	132,167,168,168	0
6	IOD	A	608	1/1	0.92	0.30	162,162,162,162	0
6	IOD	A	615	1/1	0.93	0.12	73,73,73,73	1
5	EDO	B	503	4/4	0.93	0.16	54,66,88,97	0
7	PYZ	B	508	6/6	0.95	0.16	97,98,117,118	0
5	EDO	A	605	4/4	0.95	0.10	57,72,80,96	0
3	T27	A	601	28/28	0.95	0.10	34,45,63,68	0

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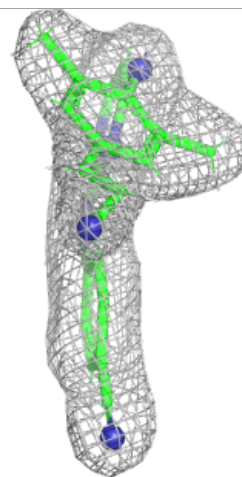
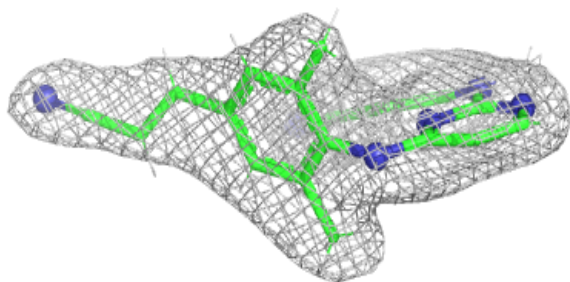
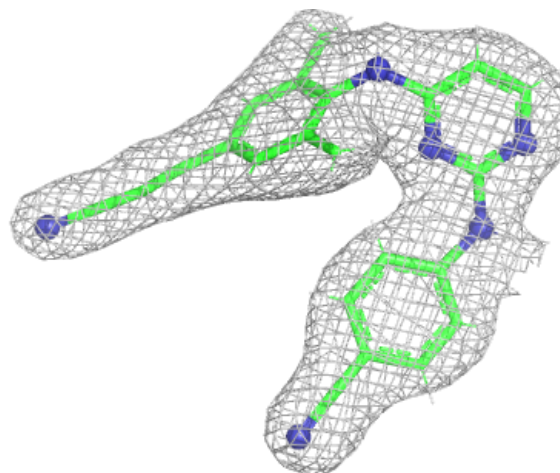
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IOD	A	607	1/1	0.96	0.28	132,132,132,132	0
6	IOD	A	613	1/1	0.96	0.17	100,100,100,100	0

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 601:

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 ⓘ

There are no such residues in this entry.