Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 07:52 PM EDT

PDB ID	:	5CYQ
Title	:	HIV-1 reverse transcriptase complexed with 4-bromopyrazole
Authors	:	Bauman, J.D.; Arnold, E.
Deposited on	:	2015-07-30
Resolution	:	2.15 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 (i) 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 (i)) were used in the production of this report:

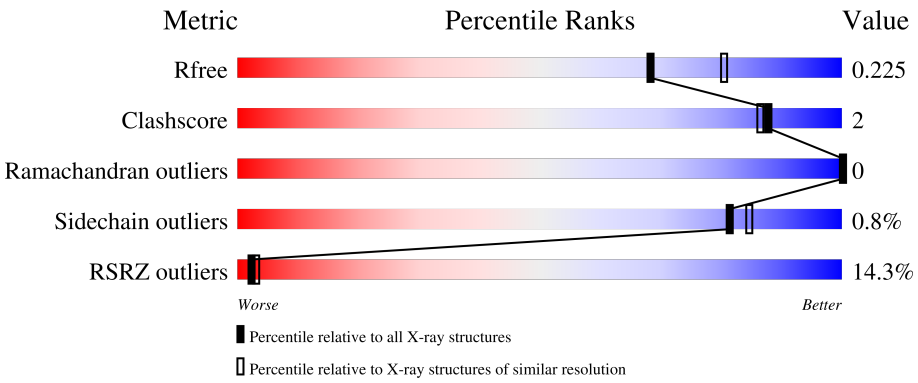
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	12% 94% 5% •
2	B	428	16% 93% • •

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
4	BYZ	A	602	-	-	X	X
4	BYZ	A	604	-	-	-	X
4	BYZ	A	606	-	-	-	X
4	BYZ	A	609	-	-	-	X
4	BYZ	B	501	-	-	-	X
4	BYZ	B	505	-	-	-	X
4	BYZ	B	506	-	-	-	X
4	BYZ	B	507	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16519 atoms, of which 8099 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
			Total	C	H	N	O	S			
1	A	548	8986	2891	4521	743	823	8	0	1	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

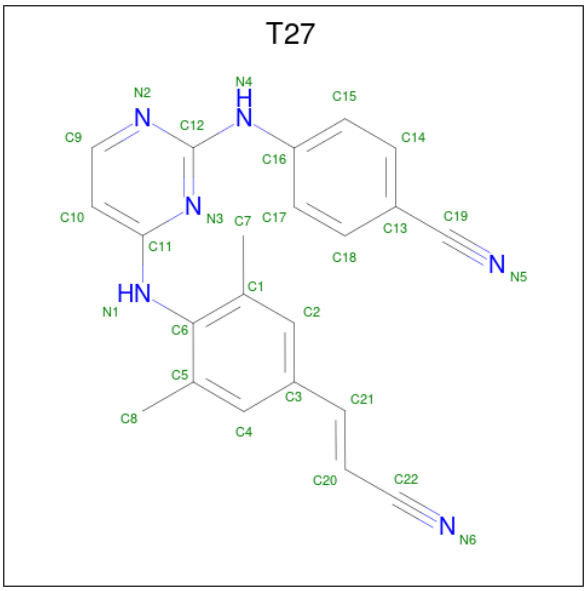
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	415	6918	2245	3476	568	622	7	0	3	0

There is a discrepancy between the modelled and reference sequences:

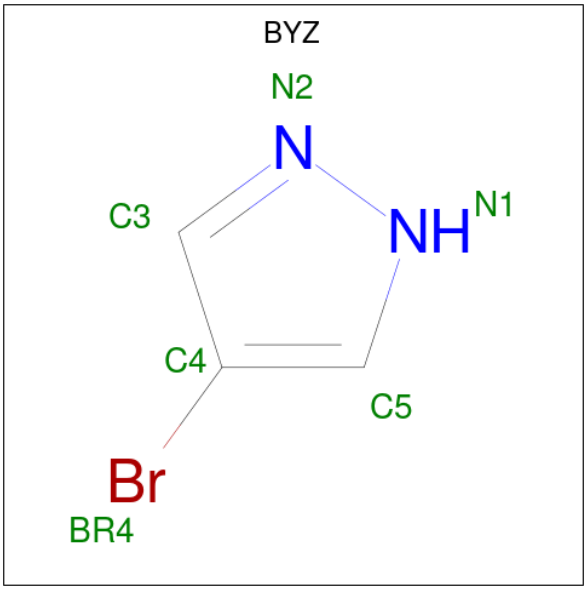
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (three-letter code: T27) (formula: $C_{22}H_{18}N_6$).



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

- Molecule 4 is 4-bromo-1H-pyrazole (three-letter code: BYZ) (formula: $C_3H_3BrN_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	H	N		
4	A	1	9	1	3	3	2	0	0
			Total	Br	C	H	N		
4	A	1	9	1	3	3	2	0	0
			Total	Br	C	H	N		
4	A	1	9	1	3	3	2	0	0

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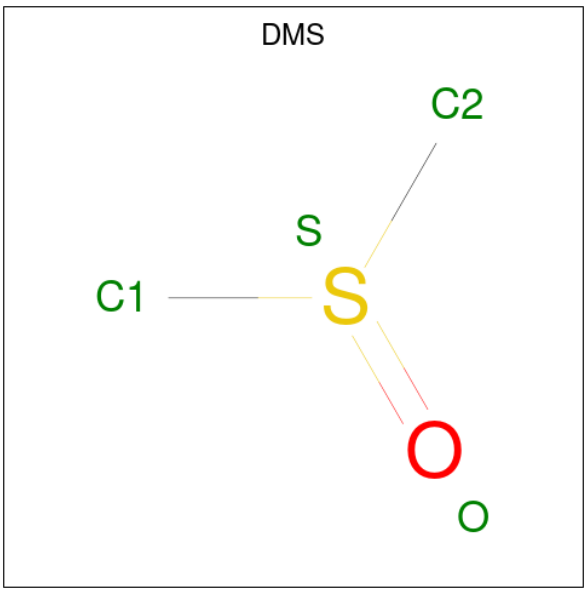
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Br C N 6 1 3 2	0	0
4	A	1	Total Br C N 6 1 3 2	0	0
4	A	1	Total Br C N 6 1 3 2	0	0
4	A	1	Total Br C H N 9 1 3 3 2	0	0
4	A	1	Total Br C H N 9 1 3 3 2	0	0
4	B	1	Total Br C H N 9 1 3 3 2	0	0
4	B	1	Total Br C H N 9 1 3 3 2	0	0
4	B	1	Total Br C H N 9 1 3 3 2	0	0
4	B	1	Total Br C H N 9 1 3 3 2	0	0
4	B	1	Total Br C H N 9 1 3 3 2	0	0
4	B	1	Total Br C N 6 1 3 2	0	0
4	B	1	Total Br C N 6 1 3 2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O S 10 2 6 1 1	0	0
5	A	1	Total C H O S 10 2 6 1 1	0	0
5	A	1	Total C H O S 10 2 6 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C H O S 10 2 6 1 1	0	0
5	B	1	Total C H O S 10 2 6 1 1	0	0
5	B	1	Total C H O S 10 2 6 1 1	0	0
5	B	1	Total C H O S 10 2 6 1 1	0	0
5	B	1	Total C H O S 10 2 6 1 1	0	0
5	B	1	Total C H O S 10 2 6 1 1	0	0

- Molecule 6 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Br 3 3	0	0

- Molecule 7 is water.

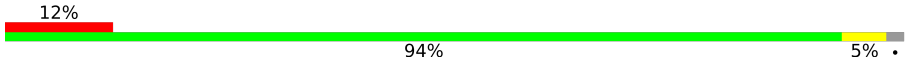
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	233	Total O 233 233	0	0
7	B	119	Total O 119 119	0	0

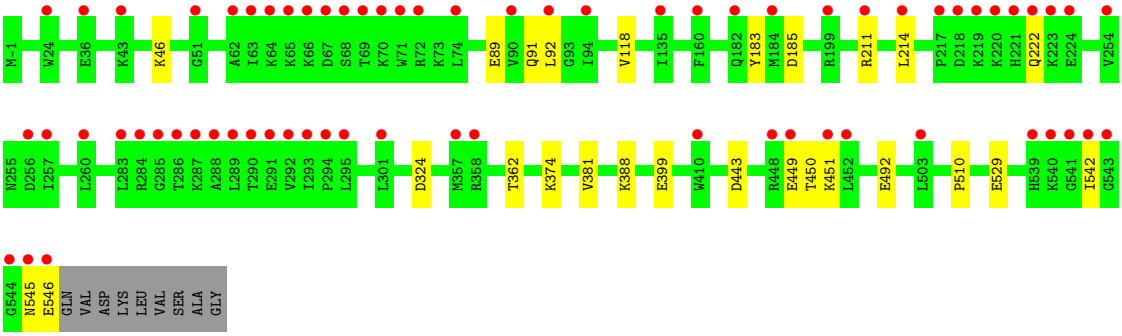
3 Residue-property plots (i)

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: HIV-1 reverse transcriptase, p66 subunit

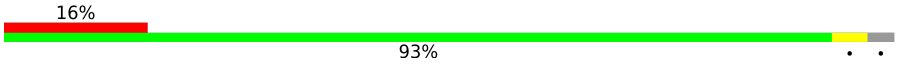
Chain A:

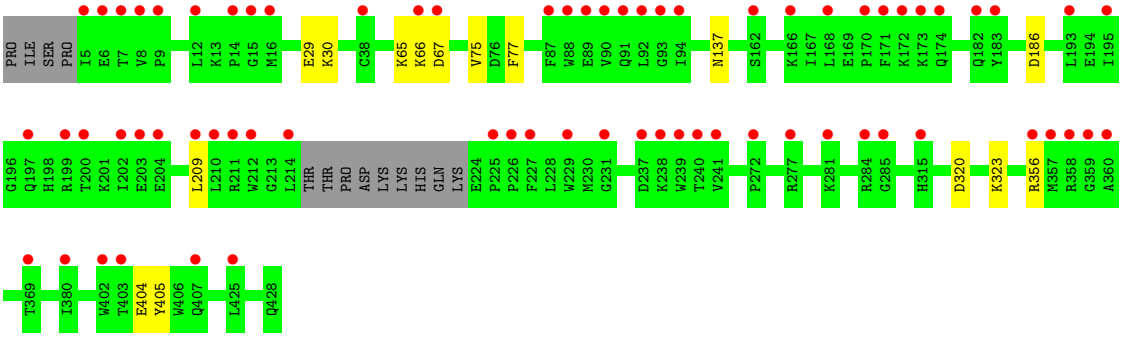




• Molecule 2: HIV-1 reverse transcriptase, p51 subunit

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.89Å 73.17Å 108.89Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	39.75 – 2.15 39.75 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.7 (39.75-2.15) 91.0 (39.75-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.14Å)	Xtriage
Refinement program	PHENIX dev_1988	Depositor
R, R_{free}	0.203 , 0.224 0.204 , 0.225	Depositor DCC
R_{free} test set	1975 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16519	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BR, T27, DMS, BYZ

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	0.23	0/4586	0.39	0/6233
2	B	0.22	0/3553	0.38	0/4828
All	All	0.23	0/8139	0.39	0/11061

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4465	4521	4521	20	0
2	B	3442	3476	3462	11	0
3	A	28	18	18	1	0
4	A	48	15	24	2	0
4	B	42	15	21	4	0
5	A	16	18	24	1	0
5	B	24	36	36	1	0
6	A	3	0	0	1	0
7	A	233	0	0	10	0
7	B	119	0	0	6	0
All	All	8420	8099	8106	33	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 2.

All (33) 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:183:TYR:OH	7:A:701:HOH:O	1.83	0.97
2:B:29:GLU:OE2	7:B:601:HOH:O	1.89	0.89
5:B:512:DMS:S	7:B:673:HOH:O	2.36	0.84
2:B:405:TYR:OH	7:B:602:HOH:O	1.96	0.83
1:A:492:GLU:OE2	7:A:703:HOH:O	2.03	0.75
2:B:137:ASN:ND2	7:B:604:HOH:O	2.22	0.70
1:A:449:GLU:OE1	1:A:449:GLU:N	2.25	0.69
1:A:443:ASP:OD1	7:A:705:HOH:O	2.15	0.65
1:A:529:GLU:OE1	7:A:703:HOH:O	2.14	0.65
1:A:362:THR:OG1	7:A:704:HOH:O	2.14	0.64
2:B:186:ASP:OD2	4:B:506:BYZ:H1	2.01	0.60
1:A:399:GLU:OE1	7:A:706:HOH:O	2.15	0.59
1:A:46:LYS:HD3	6:A:616:BR:BR	2.58	0.58
2:B:186:ASP:OD1	7:B:603:HOH:O	2.17	0.57
2:B:75:VAL:O	4:B:507:BYZ:N1	2.41	0.53
1:A:542:ILE:O	1:A:546:GLU:N	2.40	0.53
1:A:451:LYS:HG3	7:A:717:HOH:O	2.09	0.53
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.35	0.52
1:A:222:GLN:O	1:A:222:GLN:NE2	2.42	0.52
3:A:601:T27:N3	3:A:601:T27:H17	2.27	0.50
1:A:381:VAL:HG13	4:B:502:BYZ:BR4	2.71	0.46
1:A:211[A]:ARG:NH1	7:A:728:HOH:O	2.49	0.45
1:A:118:VAL:HG22	4:A:602:BYZ:BR4	2.72	0.44
2:B:66:LYS:O	2:B:67:ASP:HB2	2.17	0.44
1:A:450:THR:O	1:A:451:LYS:HG2	2.18	0.43
2:B:65:LYS:HB2	7:B:606:HOH:O	2.17	0.43
1:A:214:LEU:CD2	4:A:602:BYZ:N2	2.82	0.43
2:B:320:ASP:OD2	2:B:323:LYS:NZ	2.50	0.43
1:A:324:ASP:OD2	1:A:388:LYS:NZ	2.51	0.43
1:A:510:PRO:C	5:A:613:DMS:H21	2.40	0.43
1:A:374:LYS:NZ	7:A:720:HOH:O	2.45	0.41
2:B:77:PHE:N	4:B:507:BYZ:N2	2.61	0.41
1:A:211[B]:ARG:NE	7:A:719:HOH:O	2.44	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	547/557 (98%)	530 (97%)	17 (3%)	0	100	100
2	B	414/428 (97%)	398 (96%)	16 (4%)	0	100	100
All	All	961/985 (98%)	928 (97%)	33 (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	489/495 (99%)	484 (99%)	5 (1%)	76	79
2	B	379/390 (97%)	377 (100%)	2 (0%)	88	91
All	All	868/885 (98%)	861 (99%)	7 (1%)	81	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	91	GLN
1	A	92	LEU
1	A	185	ASP
1	A	545	ASN
2	B	209	LEU
2	B	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
4	BYZ	B	501	-	6,6,6	2.19	1 (16%)	3,7,7	2.86	2 (66%)
4	BYZ	B	502	-	6,6,6	2.13	1 (16%)	3,7,7	3.01	2 (66%)
5	DMS	A	613	-	3,3,3	0.64	0	3,3,3	0.52	0
5	DMS	B	513	-	3,3,3	0.64	0	3,3,3	0.39	0
5	DMS	B	508	-	3,3,3	0.66	0	3,3,3	0.51	0
5	DMS	A	612	-	3,3,3	0.66	0	3,3,3	0.68	0
4	BYZ	B	507	-	6,6,6	2.20	2 (33%)	3,7,7	3.14	3 (100%)
5	DMS	B	511	-	3,3,3	0.65	0	3,3,3	0.50	0
4	BYZ	A	607	-	6,6,6	2.18	2 (33%)	3,7,7	3.18	3 (100%)
3	T27	A	601	-	30,30,30	1.18	3 (10%)	39,40,40	1.84	7 (17%)
5	DMS	B	510	-	3,3,3	0.65	0	3,3,3	0.46	0
4	BYZ	A	602	-	6,6,6	2.03	1 (16%)	3,7,7	3.18	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BYZ	B	504	-	6,6,6	2.14	1 (16%)	3,7,7	2.97	3 (100%)
4	BYZ	A	609	-	6,6,6	2.10	1 (16%)	3,7,7	3.04	3 (100%)
4	BYZ	A	606	-	6,6,6	2.20	2 (33%)	3,7,7	3.15	3 (100%)
4	BYZ	A	604	-	6,6,6	2.18	1 (16%)	3,7,7	2.90	3 (100%)
4	BYZ	B	503	-	6,6,6	2.16	1 (16%)	3,7,7	2.89	2 (66%)
4	BYZ	B	505	-	6,6,6	2.20	1 (16%)	3,7,7	2.90	2 (66%)
5	DMS	B	509	-	3,3,3	0.66	0	3,3,3	0.49	0
5	DMS	B	512	-	3,3,3	0.66	0	3,3,3	0.47	0
4	BYZ	B	506	-	6,6,6	2.15	2 (33%)	3,7,7	3.17	3 (100%)
5	DMS	A	610	-	3,3,3	0.64	0	3,3,3	0.57	0
5	DMS	A	611	-	3,3,3	0.66	0	3,3,3	0.53	0
4	BYZ	A	608	-	6,6,6	2.21	1 (16%)	3,7,7	2.91	3 (100%)
4	BYZ	A	605	-	6,6,6	2.20	2 (33%)	3,7,7	3.14	3 (100%)
4	BYZ	A	603	-	6,6,6	2.13	1 (16%)	3,7,7	2.99	3 (100%)

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
4	BYZ	A	606	-	-	-	0/1/1/1
4	BYZ	B	507	-	-	-	0/1/1/1
4	BYZ	A	604	-	-	-	0/1/1/1
4	BYZ	B	506	-	-	-	0/1/1/1
4	BYZ	B	503	-	-	-	0/1/1/1
4	BYZ	A	608	-	-	-	0/1/1/1
4	BYZ	A	607	-	-	-	0/1/1/1
4	BYZ	B	505	-	-	-	0/1/1/1
3	T27	A	601	-	-	0/13/14/14	0/3/3/3
4	BYZ	B	501	-	-	-	0/1/1/1
4	BYZ	B	502	-	-	-	0/1/1/1
4	BYZ	A	605	-	-	-	0/1/1/1
4	BYZ	A	602	-	-	-	0/1/1/1
4	BYZ	A	603	-	-	-	0/1/1/1
4	BYZ	B	504	-	-	-	0/1/1/1
4	BYZ	A	609	-	-	-	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	BYZ	BR4-C4	4.86	2.00	1.90
4	A	608	BYZ	BR4-C4	4.85	2.00	1.90
4	B	501	BYZ	BR4-C4	4.83	2.00	1.90
4	B	507	BYZ	BR4-C4	4.82	2.00	1.90
4	A	604	BYZ	BR4-C4	4.79	2.00	1.90
4	A	606	BYZ	BR4-C4	4.79	2.00	1.90
4	A	605	BYZ	BR4-C4	4.79	2.00	1.90
4	B	503	BYZ	BR4-C4	4.74	1.99	1.90
4	A	607	BYZ	BR4-C4	4.74	1.99	1.90
4	B	504	BYZ	BR4-C4	4.70	1.99	1.90
4	B	506	BYZ	BR4-C4	4.69	1.99	1.90
4	B	502	BYZ	BR4-C4	4.69	1.99	1.90
4	A	603	BYZ	BR4-C4	4.66	1.99	1.90
4	A	609	BYZ	BR4-C4	4.57	1.99	1.90
4	A	602	BYZ	BR4-C4	4.57	1.99	1.90
3	A	601	T27	C12-N4	4.02	1.44	1.36
3	A	601	T27	C11-N1	3.08	1.44	1.38
3	A	601	T27	C13-C19	2.35	1.49	1.44
4	A	606	BYZ	N2-N1	2.13	1.41	1.37
4	A	607	BYZ	N2-N1	2.10	1.41	1.37
4	A	605	BYZ	N2-N1	2.08	1.41	1.37
4	B	507	BYZ	N2-N1	2.05	1.41	1.37
4	B	506	BYZ	N2-N1	2.02	1.41	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	T27	N2-C12-N3	-5.80	121.05	126.55
3	A	601	T27	C9-N2-C12	5.79	120.59	115.45
4	A	607	BYZ	C5-C4-C3	4.52	114.55	106.51
4	B	506	BYZ	C5-C4-C3	4.50	114.53	106.51
4	A	606	BYZ	C5-C4-C3	4.47	114.48	106.51
4	A	605	BYZ	C5-C4-C3	4.46	114.46	106.51
4	B	507	BYZ	C5-C4-C3	4.46	114.45	106.51
4	A	609	BYZ	C5-C4-C3	4.31	114.18	106.51
4	A	603	BYZ	C5-C4-C3	4.25	114.07	106.51
4	A	602	BYZ	C5-C4-C3	4.22	114.03	106.51
4	B	504	BYZ	C5-C4-C3	4.22	114.02	106.51
4	B	502	BYZ	C5-C4-C3	4.21	114.00	106.51
4	A	608	BYZ	C5-C4-C3	4.13	113.86	106.51
4	B	505	BYZ	C5-C4-C3	4.12	113.84	106.51
4	A	604	BYZ	C5-C4-C3	4.11	113.84	106.51
4	B	503	BYZ	C5-C4-C3	4.08	113.78	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	BYZ	C5-C4-C3	4.06	113.73	106.51
3	A	601	T27	C10-C9-N2	-3.63	119.45	123.96
3	A	601	T27	C9-C10-C11	3.57	119.09	116.76
4	A	602	BYZ	BR4-C4-C3	-3.45	120.51	126.78
3	A	601	T27	C10-C11-N3	-2.83	118.38	123.16
4	B	502	BYZ	BR4-C4-C5	-2.74	121.79	126.78
3	A	601	T27	C12-N3-C11	2.58	121.43	116.28
4	B	503	BYZ	BR4-C4-C5	-2.33	122.54	126.78
4	A	607	BYZ	BR4-C4-C3	-2.25	122.70	126.78
4	B	507	BYZ	BR4-C4-C3	-2.23	122.73	126.78
4	B	506	BYZ	BR4-C4-C3	-2.23	122.73	126.78
4	B	506	BYZ	BR4-C4-C5	-2.22	122.74	126.78
4	A	605	BYZ	BR4-C4-C5	-2.22	122.75	126.78
4	A	607	BYZ	BR4-C4-C5	-2.22	122.75	126.78
4	A	606	BYZ	BR4-C4-C5	-2.21	122.76	126.78
4	A	606	BYZ	BR4-C4-C3	-2.21	122.77	126.78
4	A	605	BYZ	BR4-C4-C3	-2.19	122.79	126.78
4	B	505	BYZ	BR4-C4-C5	-2.19	122.80	126.78
4	B	507	BYZ	BR4-C4-C5	-2.18	122.82	126.78
4	A	603	BYZ	BR4-C4-C3	-2.17	122.83	126.78
4	A	609	BYZ	BR4-C4-C5	-2.15	122.86	126.78
4	B	501	BYZ	BR4-C4-C3	-2.13	122.92	126.78
3	A	601	T27	C6-N1-C11	-2.12	120.35	124.18
4	B	504	BYZ	BR4-C4-C5	-2.11	122.94	126.78
4	A	609	BYZ	BR4-C4-C3	-2.10	122.95	126.78
4	B	504	BYZ	BR4-C4-C3	-2.06	123.04	126.78
4	A	604	BYZ	BR4-C4-C3	-2.05	123.06	126.78
4	A	608	BYZ	BR4-C4-C3	-2.04	123.07	126.78
4	A	608	BYZ	BR4-C4-C5	-2.04	123.08	126.78
4	A	603	BYZ	BR4-C4-C5	-2.03	123.10	126.78
4	A	604	BYZ	BR4-C4-C5	-2.02	123.10	126.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	BYZ	1	0
5	A	613	DMS	1	0
4	B	507	BYZ	2	0

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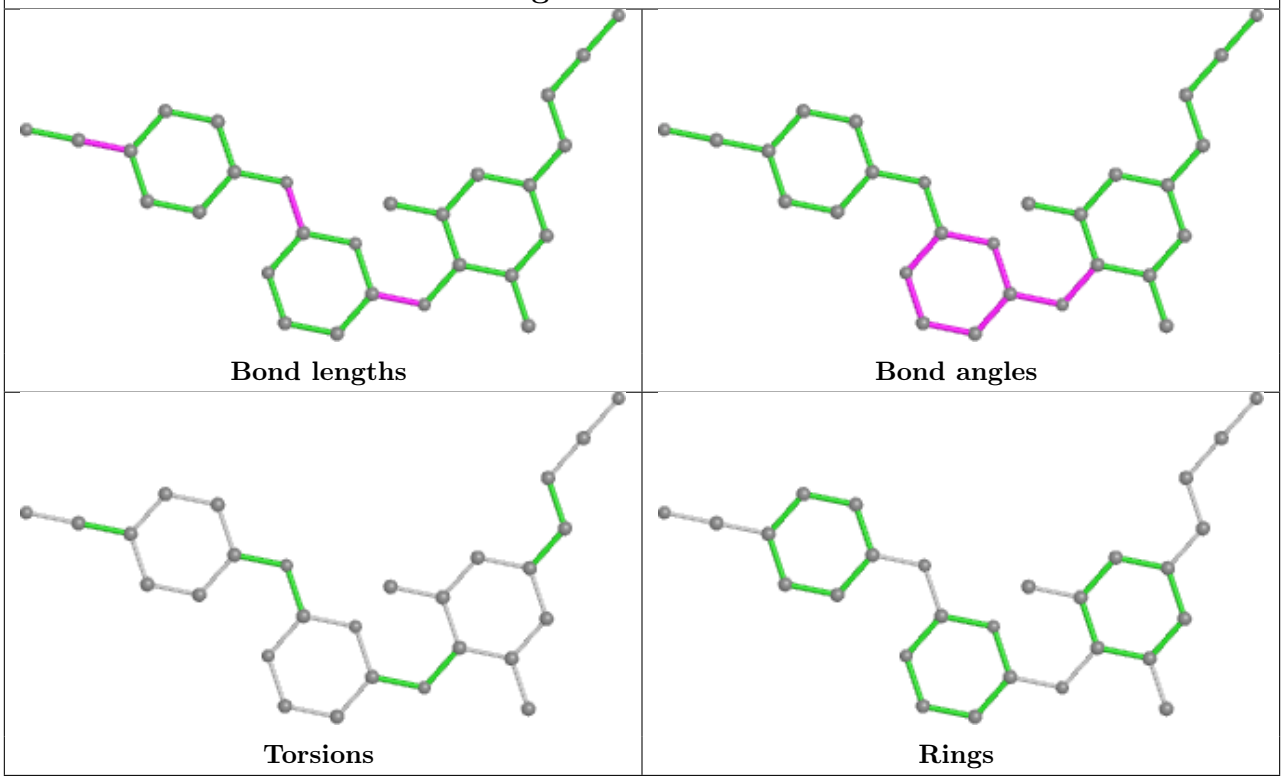
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	T27	1	0
4	A	602	BYZ	2	0
5	B	512	DMS	1	0
4	B	506	BYZ	1	0

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 then 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.

Ligand T27 A 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	548/557 (98%)	0.73	68 (12%)	4	5	23, 46, 104, 138	0
2	B	415/428 (96%)	1.04	70 (16%)	1	1	27, 53, 112, 142	0
All	All	963/985 (97%)	0.87	138 (14%)	2	3	23, 50, 109, 142	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	90	VAL	15.8
1	A	67	ASP	9.8
2	B	88	TRP	9.5
1	A	69	THR	8.6
2	B	92	LEU	8.5
2	B	89	GLU	8.3
1	A	285	GLY	8.0
1	A	543	GLY	7.3
1	A	219	LYS	7.3
1	A	24	TRP	7.2
1	A	546	GLU	7.1
1	A	289	LEU	7.0
1	A	68	SER	6.8
2	B	240	THR	6.4
2	B	91	GLN	6.4
2	B	226	PRO	6.2
2	B	357	MET	6.1
2	B	5	ILE	6.1
2	B	66	LYS	6.0
1	A	287	LYS	6.0
2	B	94	ILE	5.9
1	A	90	VAL	5.9
2	B	356	ARG	5.7
2	B	212	TRP	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	286	THR	5.7
1	A	288	ALA	5.5
2	B	359	GLY	5.5
1	A	290	THR	5.4
2	B	214	LEU	5.4
1	A	542	ILE	5.3
1	A	64	LYS	5.2
1	A	218	ASP	5.2
1	A	358	ARG	5.1
1	A	541	GLY	5.1
1	A	70	LYS	5.0
1	A	220	LYS	5.0
1	A	292	VAL	4.8
1	A	291	GLU	4.8
2	B	93	GLY	4.8
1	A	63	ILE	4.8
1	A	66	LYS	4.7
2	B	358	ARG	4.6
1	A	72	ARG	4.6
1	A	92	LEU	4.5
1	A	65	LYS	4.4
2	B	197	GLN	4.4
1	A	221	HIS	4.3
1	A	544	GLY	4.3
2	B	360	ALA	4.3
2	B	200	THR	4.3
2	B	14	PRO	4.3
2	B	425	LEU	4.1
1	A	217	PRO	4.0
2	B	7	THR	4.0
2	B	209	LEU	4.0
1	A	545	ASN	4.0
2	B	173	LYS	3.9
2	B	229	TRP	3.9
1	A	71	TRP	3.8
1	A	224	GLU	3.8
2	B	211	ARG	3.7
2	B	174	GLN	3.6
1	A	301	LEU	3.6
1	A	223	LYS	3.5
2	B	227	PHE	3.5
1	A	283	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	168	LEU	3.4
2	B	195	ILE	3.4
1	A	449	GLU	3.4
2	B	67	ASP	3.4
2	B	225	PRO	3.3
2	B	237	ASP	3.3
2	B	6	GLU	3.2
1	A	257	ILE	3.2
2	B	170	PRO	3.1
1	A	222	GLN	3.1
2	B	12	LEU	3.1
2	B	202	ILE	3.1
2	B	87	PHE	3.1
2	B	277	ARG	3.0
2	B	204	GLU	2.9
2	B	166	LYS	2.9
2	B	193	LEU	2.8
1	A	410	TRP	2.8
1	A	284	ARG	2.8
2	B	171	PHE	2.7
2	B	284	ARG	2.7
1	A	452	LEU	2.7
2	B	15	GLY	2.7
2	B	203	GLU	2.6
2	B	38	CYS	2.6
1	A	448	ARG	2.6
1	A	539	HIS	2.6
1	A	254	VAL	2.6
1	A	256	ASP	2.6
2	B	199	ARG	2.6
2	B	369	THR	2.6
2	B	210	LEU	2.6
1	A	51	GLY	2.5
1	A	451	LYS	2.5
2	B	238	LYS	2.5
2	B	172	LYS	2.5
1	A	295	LEU	2.5
1	A	214	LEU	2.5
1	A	540	LYS	2.5
2	B	182	GLN	2.4
2	B	239	TRP	2.4
1	A	293	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	183	TYR	2.4
1	A	43	LYS	2.4
1	A	211[A]	ARG	2.4
2	B	403	THR	2.4
2	B	315	HIS	2.3
2	B	380[A]	ILE	2.3
1	A	94	ILE	2.3
1	A	74	LEU	2.3
1	A	260	LEU	2.3
1	A	36	GLU	2.3
2	B	8	VAL	2.3
1	A	182	GLN	2.3
1	A	357	MET	2.2
2	B	402	TRP	2.2
1	A	503	LEU	2.2
2	B	241	VAL	2.2
1	A	135	ILE	2.2
2	B	407	GLN	2.2
2	B	272	PRO	2.2
1	A	184	MET	2.2
1	A	160	PHE	2.2
2	B	16	MET	2.2
1	A	199	ARG	2.1
2	B	231	GLY	2.1
1	A	294	PRO	2.1
2	B	281	LYS	2.1
2	B	9	PRO	2.0
2	B	285	GLY	2.0
2	B	162	SER	2.0
1	A	62	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 monosaccharides in this entry.

6.4 Ligands (i)

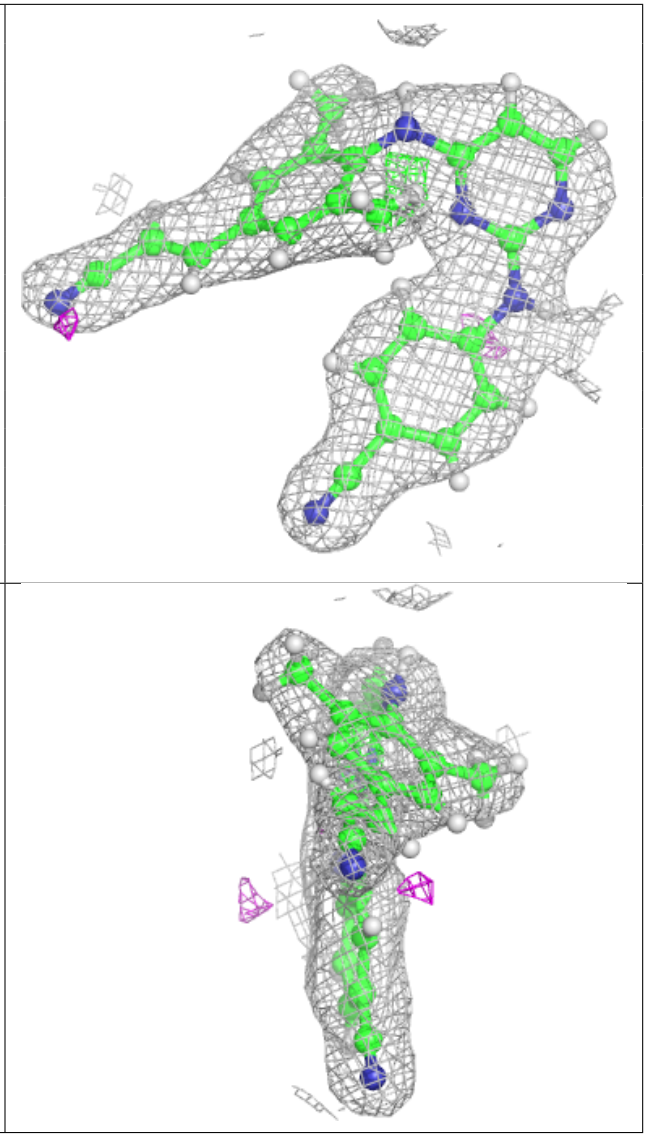
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BYZ	B	506	6/6	0.25	0.88	270,271,271,271	0
4	BYZ	B	501	6/6	0.47	0.77	230,350,421,475	0
4	BYZ	A	606	6/6	0.48	0.76	242,242,243,243	0
6	BR	A	614	1/1	0.51	0.37	175,175,175,175	0
4	BYZ	B	505	6/6	0.57	0.46	107,110,132,132	9
4	BYZ	A	604	6/6	0.59	0.57	164,166,199,200	0
4	BYZ	A	609	6/6	0.64	0.42	131,131,157,157	0
4	BYZ	B	502	6/6	0.70	0.30	103,103,124,124	0
6	BR	A	616	1/1	0.72	0.28	171,171,171,171	0
4	BYZ	A	602	6/6	0.76	0.49	147,148,177,177	9
4	BYZ	A	607	6/6	0.80	0.41	205,206,206,206	0
4	BYZ	A	605	6/6	0.80	0.26	144,148,149,149	0
4	BYZ	A	603	6/6	0.81	0.21	72,73,87,88	0
4	BYZ	B	504	6/6	0.82	0.47	93,93,112,112	9
4	BYZ	B	507	6/6	0.83	0.39	68,69,70,75	6
5	DMS	B	513	4/4	0.84	0.34	103,124,126,126	0
4	BYZ	B	503	6/6	0.86	0.34	96,98,118,119	9
5	DMS	B	510	4/4	0.86	0.30	79,96,97,97	0
5	DMS	B	511	4/4	0.86	0.27	80,97,98,98	0
5	DMS	A	610	4/4	0.90	0.20	84,101,102,102	0
5	DMS	B	512	4/4	0.92	0.33	59,76,77,77	0
5	DMS	B	509	4/4	0.92	0.24	59,71,76,76	0
6	BR	A	615	1/1	0.93	0.15	169,169,169,169	0
5	DMS	A	611	4/4	0.93	0.20	67,81,85,85	0
3	T27	A	601	28/28	0.95	0.15	27,33,41,42	0
4	BYZ	A	608	6/6	0.95	0.15	93,93,112,112	0
5	DMS	A	613	4/4	0.95	0.19	55,60,62,63	0
5	DMS	B	508	4/4	0.95	0.19	66,80,80,80	0
5	DMS	A	612	4/4	0.96	0.19	52,65,66,66	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 (i)

There are no such residues in this entry.