



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:56 PM UTC

PDB ID : 8DXK / pdb_00008dxk
Title : HIV-1 reverse transcriptase/rilpivirine with bound fragment 4-bromopyrazole at multiple sites
Authors : Chopra, A.; Ruiz, F.X.; Bauman, J.D.; Arnold, E.
Deposited on : 2022-08-02
Resolution : 2.00 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

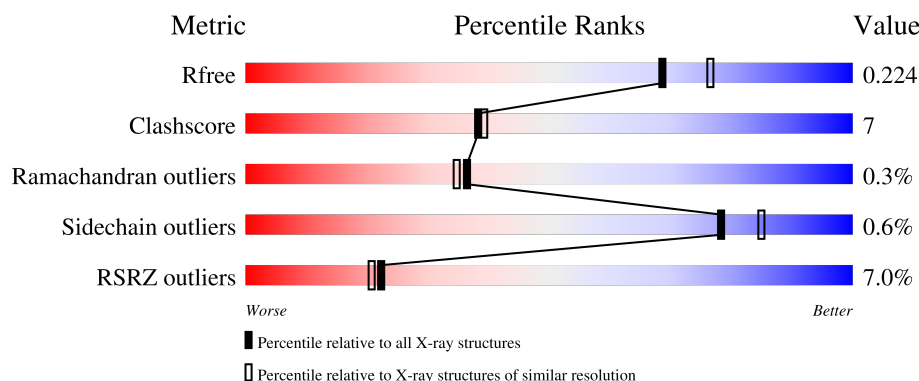
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	
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
8	BYZ	A	609[A]	-	-	X	X
8	BYZ	A	611	-	-	X	-
8	BYZ	A	612	-	-	X	-
8	BYZ	B	508[A]	-	-	X	-
8	BYZ	B	509	-	-	X	-
8	BYZ	B	510	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8818 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	7	0
			4566	2953	760	845	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

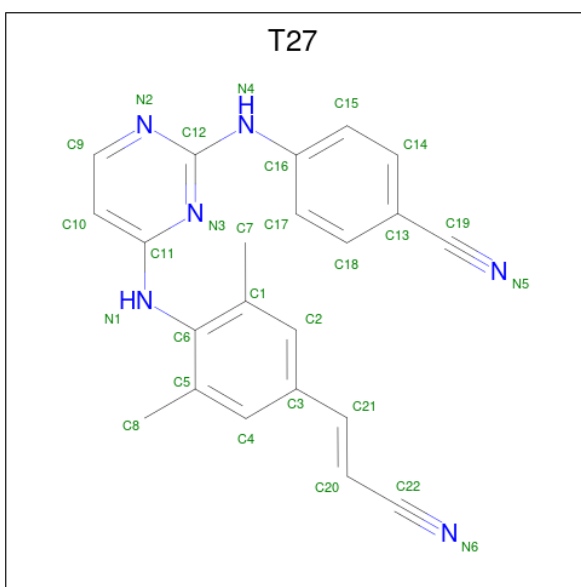
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	5	0
			3460	2261	568	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-{{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	N	0	0
			28	22	6		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



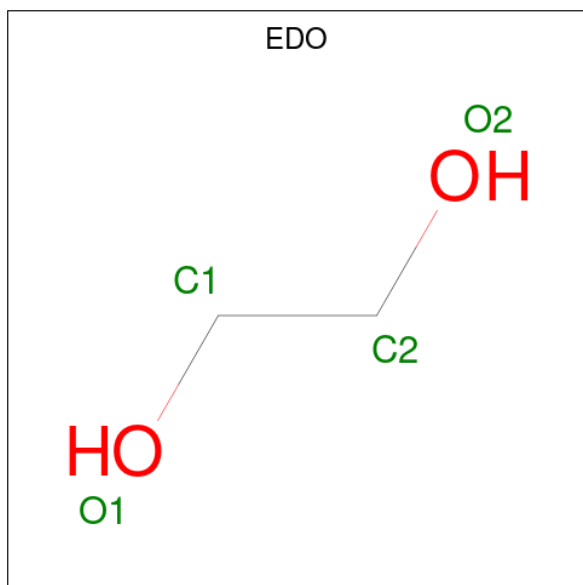
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

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

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



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

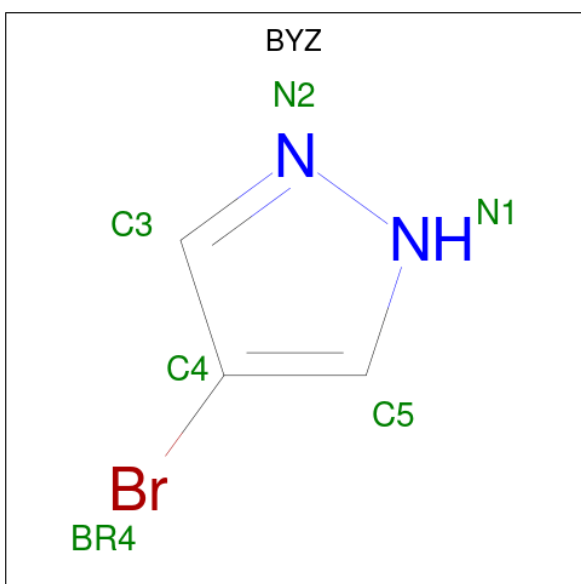
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- 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		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is 4-bromo-1H-pyrazole (CCD ID: BYZ) (formula: $C_3H_3BrN_2$) (labeled as "Ligand of Interest" by depositor).



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

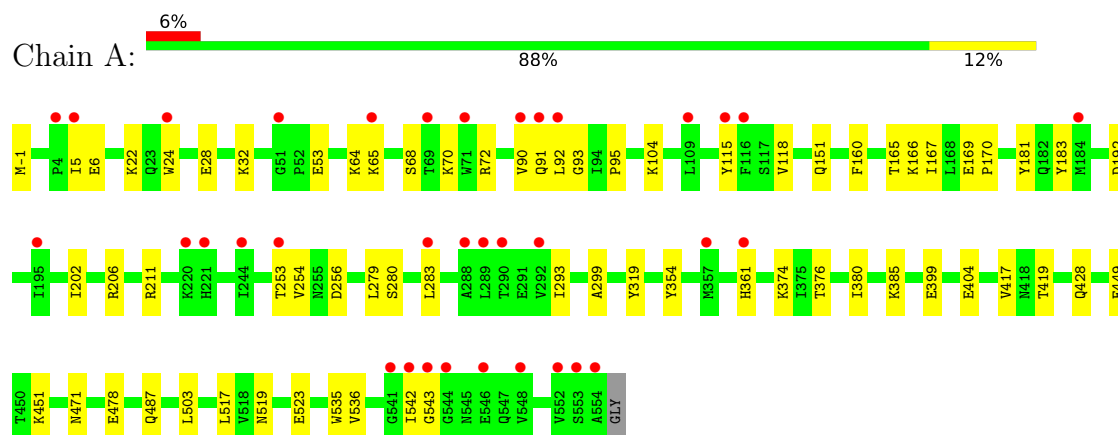
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	395	Total 395	O 395	0	1
9	B	264	Total 264	O 264	0	2

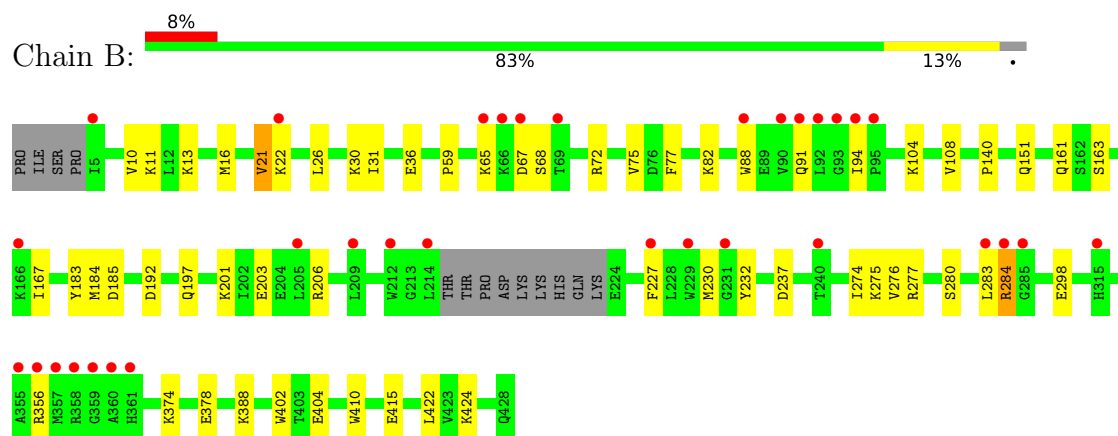
3 Residue-property plots

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	162.47Å 72.98Å 109.32Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	38.00 – 2.00 38.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.00-2.00) 99.9 (38.00-2.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.00Å)	Xtriage
Refinement program	PHENIX dev_3051	Depositor
R, R_{free}	0.181 , 0.215 (Not available) , 0.224	Depositor DCC
R_{free} test set	2000 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	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	8818	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BYZ, T27, SO4, DMS, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/4695	0.53	0/6381
2	B	0.37	0/3575	0.53	0/4860
All	All	0.37	0/8270	0.53	0/11241

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	4566	0	4619	59	0
2	B	3460	0	3484	55	0
3	A	28	0	18	1	0
4	A	4	0	6	2	0
4	B	20	0	30	3	0
5	A	8	0	12	0	0
5	B	4	0	6	0	0
6	A	1	0	0	0	0
7	A	15	0	0	0	0
7	B	5	0	0	1	0
8	A	30	0	15	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	18	0	9	8	0
9	A	395	0	0	5	0
9	B	264	0	0	6	0
All	All	8818	0	8199	113	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 7.

All (113) 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:428:GLN:H	4:A:602:DMS:H23	1.20	1.04
1:A:404:GLU:O	8:A:611:BYZ:H1	1.67	0.93
1:A:169[B]:GLU:HG2	1:A:170:PRO:HD3	1.61	0.80
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.68	0.76
1:A:65:LYS:HD2	1:A:72:ARG:HH12	1.51	0.75
1:A:428:GLN:N	4:A:602:DMS:H23	2.01	0.73
2:B:388:LYS:HE3	2:B:415:GLU:HG2	1.71	0.72
2:B:68:SER:HB2	2:B:230:MET:HE1	1.75	0.69
2:B:104:LYS:HA	2:B:237:ASP:HB2	1.75	0.69
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.74	0.68
2:B:77:PHE:H	8:B:510:BYZ:H2	1.41	0.68
2:B:410:TRP:HA	8:B:510:BYZ:H3	1.77	0.67
2:B:13:LYS:HB2	2:B:16:MET:HE2	1.79	0.65
1:A:211[A]:ARG:NH1	9:A:707:HOH:O	2.31	0.64
1:A:91:GLN:C	1:A:93:GLY:H	2.06	0.63
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.78	0.63
2:B:94:ILE:HG21	2:B:161:GLN:HE22	1.63	0.62
3:A:601:T27:N3	3:A:601:T27:H17	2.14	0.62
2:B:276:VAL:H	2:B:277:ARG:HH11	1.47	0.62
8:A:611:BYZ:H3	2:B:424:LYS:HD3	1.82	0.62
2:B:356:ARG:HD3	2:B:374:LYS:HZ1	1.64	0.61
2:B:94:ILE:CG2	2:B:161:GLN:HE22	2.13	0.61
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.83	0.60
4:B:502:DMS:H23	9:B:750:HOH:O	2.00	0.59
2:B:11:LYS:HE3	2:B:11:LYS:HA	1.85	0.58
2:B:402:TRP:HE1	4:B:501:DMS:H21	1.67	0.58
1:A:165:THR:HG23	8:A:610:BYZ:H3	1.85	0.58
1:A:449:GLU:OE2	1:A:449:GLU:N	2.30	0.57
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.06	0.56
1:A:253:THR:HG23	1:A:256:ASP:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.06	0.55
2:B:356:ARG:H	2:B:356:ARG:HD2	1.71	0.55
2:B:388:LYS:HE3	2:B:415:GLU:CG	2.35	0.55
2:B:104:LYS:HG2	2:B:192:ASP:HA	1.89	0.55
2:B:30:LYS:NZ	9:B:612:HOH:O	2.40	0.54
2:B:424:LYS:HE3	9:B:700:HOH:O	2.08	0.53
1:A:95:PRO:HD3	8:A:612:BYZ:H3	1.90	0.53
2:B:163:SER:O	2:B:167:ILE:HD12	2.08	0.53
2:B:26:LEU:O	8:B:508[A]:BYZ:N1	2.42	0.53
1:A:503:LEU:CD2	2:B:422:LEU:HD21	2.39	0.52
1:A:6:GLU:OE1	1:A:166:LYS:HE2	2.09	0.52
2:B:65:LYS:NZ	2:B:72:ARG:HB2	2.25	0.52
1:A:53:GLU:H	1:A:53:GLU:CD	2.18	0.52
2:B:410:TRP:HA	8:B:510:BYZ:C3	2.40	0.52
2:B:10:VAL:O	2:B:11:LYS:HD2	2.10	0.51
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.92	0.51
1:A:24:TRP:H	1:A:24:TRP:CD1	2.29	0.51
1:A:211[B]:ARG:NH2	9:A:703:HOH:O	2.25	0.51
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.39	0.51
1:A:65:LYS:HD3	1:A:68:SER:HB3	1.92	0.50
2:B:277:ARG:H	2:B:277:ARG:CD	2.25	0.50
2:B:356:ARG:HD3	2:B:374:LYS:NZ	2.27	0.50
1:A:519:ASN:O	1:A:523:GLU:HG2	2.11	0.50
2:B:65:LYS:HZ1	2:B:72:ARG:HB2	1.77	0.50
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.94	0.49
1:A:68:SER:OG	1:A:70:LYS:HE3	2.12	0.49
1:A:118:VAL:HG22	8:A:609[A]:BYZ:BR4	2.68	0.49
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.95	0.48
1:A:28:GLU:HG2	1:A:32:LYS:HE3	1.95	0.48
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.48	0.48
2:B:298:GLU:H	2:B:298:GLU:CD	2.20	0.48
2:B:75:VAL:O	8:B:510:BYZ:N1	2.47	0.47
2:B:65:LYS:HE3	2:B:227:PHE:CG	2.49	0.47
1:A:151:GLN:OE1	9:A:701:HOH:O	2.20	0.47
1:A:543:GLY:HA3	2:B:284:ARG:N	2.30	0.47
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.43	0.47
2:B:104:LYS:HB2	2:B:104:LYS:HE2	1.70	0.47
1:A:354:TYR:CD1	1:A:374:LYS:HD3	2.50	0.46
1:A:167:ILE:HD11	8:A:609[A]:BYZ:H3	1.97	0.46
2:B:88:TRP:HA	2:B:91:GLN:O	2.16	0.46
1:A:91:GLN:HG2	1:A:91:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169[B]:GLU:HG2	1:A:170:PRO:CD	2.38	0.45
1:A:280:SER:HA	1:A:283:LEU:CD1	2.46	0.45
1:A:354:TYR:HD1	1:A:374:LYS:HD3	1.82	0.45
2:B:11:LYS:HA	2:B:11:LYS:CE	2.47	0.45
2:B:277:ARG:N	2:B:277:ARG:HD2	2.32	0.45
1:A:65:LYS:HD3	1:A:68:SER:CB	2.48	0.44
1:A:95:PRO:HD3	8:A:612:BYZ:C3	2.47	0.44
7:B:507:SO4:O3	8:B:509:BYZ:H1	2.18	0.44
2:B:203:GLU:OE2	2:B:206:ARG:HD2	2.18	0.44
1:A:91:GLN:C	1:A:93:GLY:N	2.72	0.43
1:A:404:GLU:C	8:A:611:BYZ:H1	2.41	0.43
1:A:451:LYS:HE3	1:A:471:ASN:HA	2.00	0.43
2:B:36:GLU:HG3	9:B:741:HOH:O	2.18	0.43
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.19	0.43
2:B:82:LYS:NZ	9:B:626:HOH:O	2.51	0.43
2:B:184:MET:HE3	9:B:606:HOH:O	2.19	0.43
1:A:478:GLU:HG2	9:A:749:HOH:O	2.18	0.43
1:A:64:LYS:HE3	1:A:68:SER:O	2.18	0.43
2:B:402:TRP:HE1	4:B:501:DMS:C2	2.31	0.43
2:B:197:GLN:O	2:B:201:LYS:HG2	2.20	0.42
2:B:31:ILE:HD11	8:B:508[A]:BYZ:N2	2.33	0.42
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.42
2:B:65:LYS:HE2	2:B:65:LYS:HB2	1.79	0.42
2:B:274:ILE:C	2:B:275:LYS:HD2	2.45	0.42
2:B:280:SER:O	2:B:283:LEU:O	2.38	0.42
2:B:378:GLU:HG3	8:B:509:BYZ:H3	2.01	0.42
1:A:22:LYS:HE3	1:A:22:LYS:HB3	1.87	0.42
1:A:253:THR:HG22	1:A:256:ASP:CG	2.45	0.42
2:B:108:VAL:HB	2:B:232:TYR:HB3	2.02	0.42
1:A:376:THR:O	1:A:380:ILE:HG12	2.19	0.42
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.55	0.42
1:A:503:LEU:HD23	2:B:422:LEU:HD21	2.02	0.41
1:A:181:TYR:HE1	8:A:612:BYZ:C3	2.33	0.41
1:A:90:VAL:HG11	2:B:140:PRO:HB3	2.02	0.41
1:A:-1:MET:HE2	1:A:-1:MET:HB2	1.82	0.41
1:A:115:TYR:HA	1:A:160:PHE:CE1	2.56	0.41
1:A:202:ILE:O	1:A:206:ARG:HG3	2.21	0.41
2:B:388:LYS:HD3	2:B:388:LYS:C	2.46	0.40
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.03	0.40
1:A:65:LYS:HB2	1:A:72:ARG:NH1	2.36	0.40
1:A:487:GLN:OE1	9:A:702:HOH:O	2.22	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	561/557 (101%)	550 (98%)	10 (2%)	1 (0%)	43	42
2	B	416/428 (97%)	394 (95%)	20 (5%)	2 (0%)	24	21
All	All	977/985 (99%)	944 (97%)	30 (3%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
2	B	284	ARG
2	B	67	ASP

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	502/495 (101%)	498 (99%)	4 (1%)	73	80
2	B	380/390 (97%)	378 (100%)	2 (0%)	81	87
All	All	882/885 (100%)	876 (99%)	6 (1%)	78	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5[A]	ILE
1	A	5[B]	ILE
1	A	361	HIS
1	A	399	GLU
2	B	21	VAL
2	B	22	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	222	GLN
1	A	235	HIS
1	A	315	HIS
1	A	520	GLN
2	B	161	GLN
2	B	269	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 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	603	-	3,3,3	0.42	0	2,2,2	0.55	0
5	EDO	A	604	-	3,3,3	0.32	0	2,2,2	0.75	0
8	BYZ	A	609[A]	-	6,6,6	0.91	0	6,7,7	3.33	4 (66%)
7	SO4	A	606	-	4,4,4	0.25	0	6,6,6	0.09	0
4	DMS	B	504	-	3,3,3	0.71	0	3,3,3	0.74	0
8	BYZ	B	508[A]	-	6,6,6	0.89	0	6,7,7	3.33	4 (66%)
4	DMS	B	502	-	3,3,3	0.56	0	3,3,3	0.64	0
8	BYZ	B	509	-	6,6,6	0.91	0	6,7,7	3.35	4 (66%)
5	EDO	B	506	-	3,3,3	0.39	0	2,2,2	0.28	0
3	T27	A	601	-	30,30,30	2.90	5 (16%)	37,40,40	5.25	11 (29%)
4	DMS	B	501	-	3,3,3	2.56	1 (33%)	3,3,3	0.34	0
8	BYZ	B	510	-	6,6,6	0.89	0	6,7,7	3.34	4 (66%)
7	SO4	A	607	-	4,4,4	0.24	0	6,6,6	0.18	0
8	BYZ	A	610	-	6,6,6	0.90	0	6,7,7	3.38	4 (66%)
8	BYZ	A	611	-	6,6,6	0.99	0	6,7,7	3.37	4 (66%)
8	BYZ	A	612	-	6,6,6	0.92	0	6,7,7	3.35	4 (66%)
7	SO4	B	507	-	4,4,4	0.27	0	6,6,6	0.07	0
7	SO4	A	608	-	4,4,4	0.26	0	6,6,6	0.15	0
4	DMS	B	505	-	3,3,3	0.71	0	3,3,3	0.63	0
8	BYZ	A	613	-	6,6,6	0.87	0	6,7,7	3.38	4 (66%)
4	DMS	A	602	-	3,3,3	0.56	0	3,3,3	0.88	0
4	DMS	B	503	-	3,3,3	0.65	0	3,3,3	0.64	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
5	EDO	A	603	-	-	0/1/1/1	-
8	BYZ	A	612	-	-	-	0/1/1/1
8	BYZ	B	509	-	-	-	0/1/1/1
5	EDO	A	604	-	-	0/1/1/1	-
8	BYZ	B	510	-	-	-	0/1/1/1
8	BYZ	A	609[A]	-	-	-	0/1/1/1
5	EDO	B	506	-	-	0/1/1/1	-
8	BYZ	A	611	-	-	-	0/1/1/1
8	BYZ	A	610	-	-	-	0/1/1/1
3	T27	A	601	-	-	0/13/14/14	0/3/3/3
8	BYZ	B	508[A]	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BYZ	A	613	-	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	T27	C19-N5	12.46	1.42	1.14
3	A	601	T27	C12-N4	4.71	1.46	1.36
3	A	601	T27	C22-N6	4.53	1.25	1.14
4	B	501	DMS	O-S	4.37	1.79	1.50
3	A	601	T27	C13-C19	4.17	1.53	1.44
3	A	601	T27	C11-N1	3.55	1.44	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	T27	C13-C19-N5	-25.17	115.74	177.87
3	A	601	T27	C20-C22-N6	-15.14	123.13	176.36
3	A	601	T27	C9-N2-C12	7.14	121.39	115.42
8	A	613	BYZ	C4-C3-N2	-6.37	105.83	110.60
8	A	610	BYZ	C4-C3-N2	-6.36	105.83	110.60
8	A	612	BYZ	C4-C3-N2	-6.35	105.85	110.60
8	B	509	BYZ	C4-C3-N2	-6.32	105.86	110.60
8	A	609[A]	BYZ	C4-C3-N2	-6.28	105.90	110.60
8	B	510	BYZ	C4-C3-N2	-6.28	105.90	110.60
8	B	508[A]	BYZ	C4-C3-N2	-6.26	105.91	110.60
8	A	611	BYZ	C4-C3-N2	-6.24	105.93	110.60
3	A	601	T27	N2-C12-N3	-5.21	121.38	126.42
3	A	601	T27	C10-C9-N2	-4.48	118.48	123.97
8	A	611	BYZ	C3-N2-N1	3.48	112.55	105.75
8	A	610	BYZ	C3-N2-N1	3.47	112.53	105.75
8	A	613	BYZ	C3-N2-N1	3.45	112.50	105.75
8	B	509	BYZ	C3-N2-N1	3.42	112.44	105.75
8	A	609[A]	BYZ	C3-N2-N1	3.42	112.44	105.75
8	B	510	BYZ	C3-N2-N1	3.42	112.43	105.75
8	A	612	BYZ	C3-N2-N1	3.42	112.42	105.75
8	B	508[A]	BYZ	C3-N2-N1	3.41	112.41	105.75
8	A	611	BYZ	C5-N1-N2	-3.11	104.85	111.25
8	A	610	BYZ	C5-N1-N2	-3.08	104.91	111.25
8	A	613	BYZ	C5-N1-N2	-3.04	104.98	111.25
8	A	609[A]	BYZ	C5-N1-N2	-3.04	104.98	111.25
8	B	510	BYZ	C5-N1-N2	-3.04	104.98	111.25
8	B	508[A]	BYZ	C5-N1-N2	-3.04	104.99	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	612	BYZ	C5-N1-N2	-3.03	105.01	111.25
8	B	509	BYZ	C5-N1-N2	-3.03	105.01	111.25
3	A	601	T27	C14-C13-C19	2.89	124.68	119.97
3	A	601	T27	C6-N1-C11	-2.76	119.15	124.11
3	A	601	T27	C18-C13-C19	-2.70	115.57	119.97
3	A	601	T27	C7-C1-C6	-2.63	118.22	121.42
8	A	611	BYZ	BR4-C4-C5	2.39	128.44	125.70
3	A	601	T27	C10-C11-N3	-2.30	119.29	123.15
8	A	613	BYZ	BR4-C4-C5	2.28	128.32	125.70
8	B	510	BYZ	BR4-C4-C5	2.26	128.30	125.70
8	B	508[A]	BYZ	BR4-C4-C5	2.26	128.30	125.70
8	A	610	BYZ	BR4-C4-C5	2.23	128.26	125.70
8	A	609[A]	BYZ	BR4-C4-C5	2.23	128.26	125.70
8	B	509	BYZ	BR4-C4-C5	2.21	128.24	125.70
8	A	612	BYZ	BR4-C4-C5	2.19	128.22	125.70
3	A	601	T27	C4-C3-C21	-2.02	114.57	120.61

There are no chirality outliers.

There are no torsion outliers.

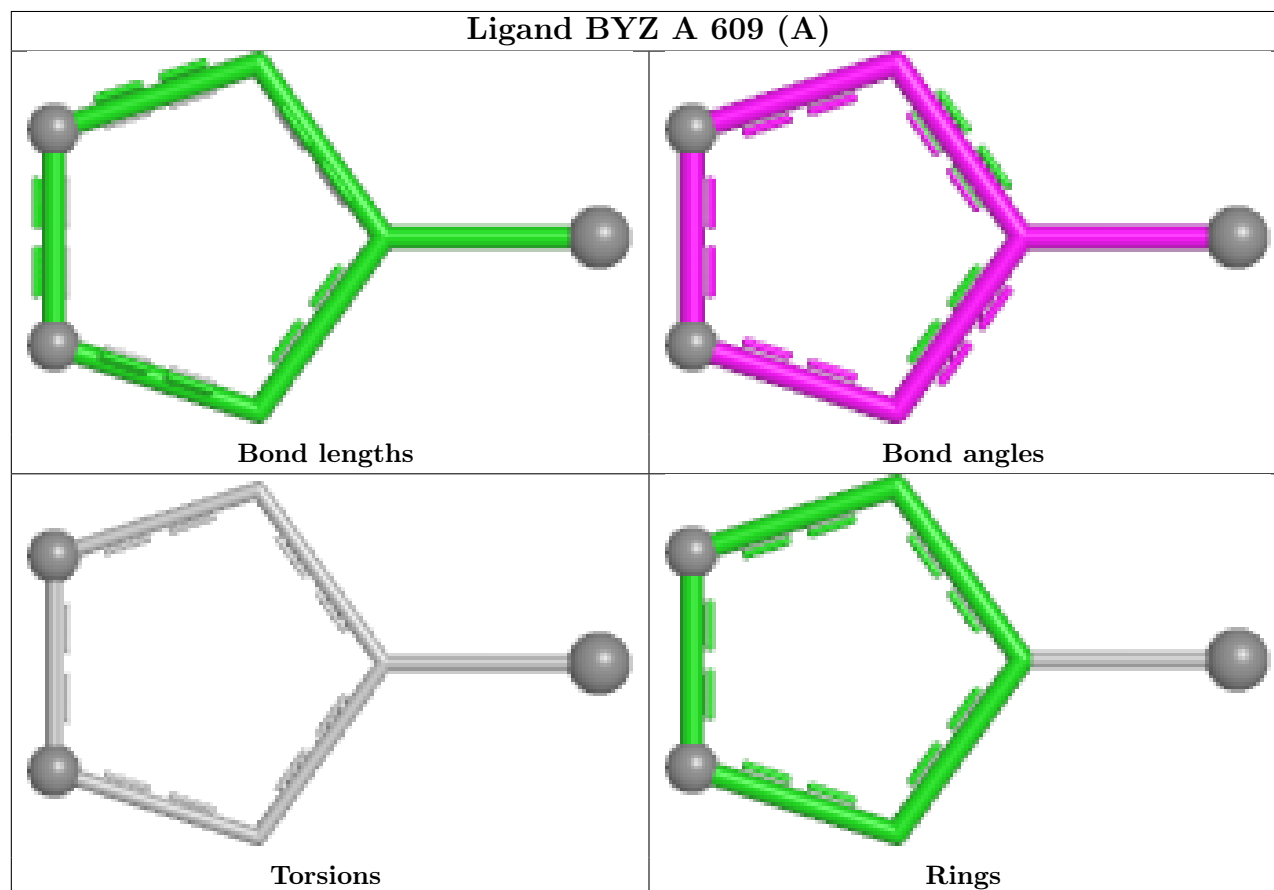
There are no ring outliers.

12 monomers are involved in 23 short contacts:

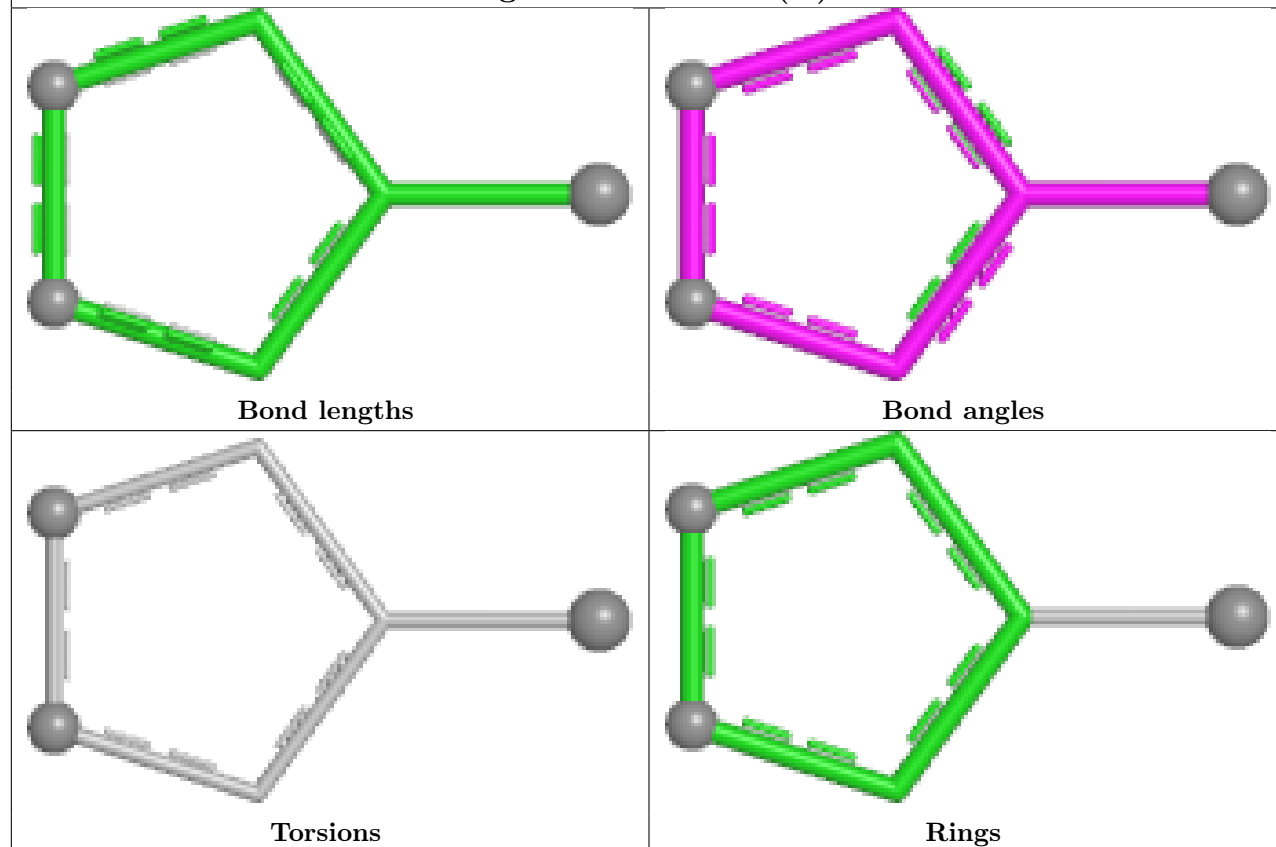
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	609[A]	BYZ	2	0
8	B	508[A]	BYZ	2	0
4	B	502	DMS	1	0
8	B	509	BYZ	2	0
3	A	601	T27	1	0
4	B	501	DMS	2	0
8	B	510	BYZ	4	0
8	A	610	BYZ	1	0
8	A	611	BYZ	3	0
8	A	612	BYZ	3	0
7	B	507	SO4	1	0
4	A	602	DMS	2	0

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.

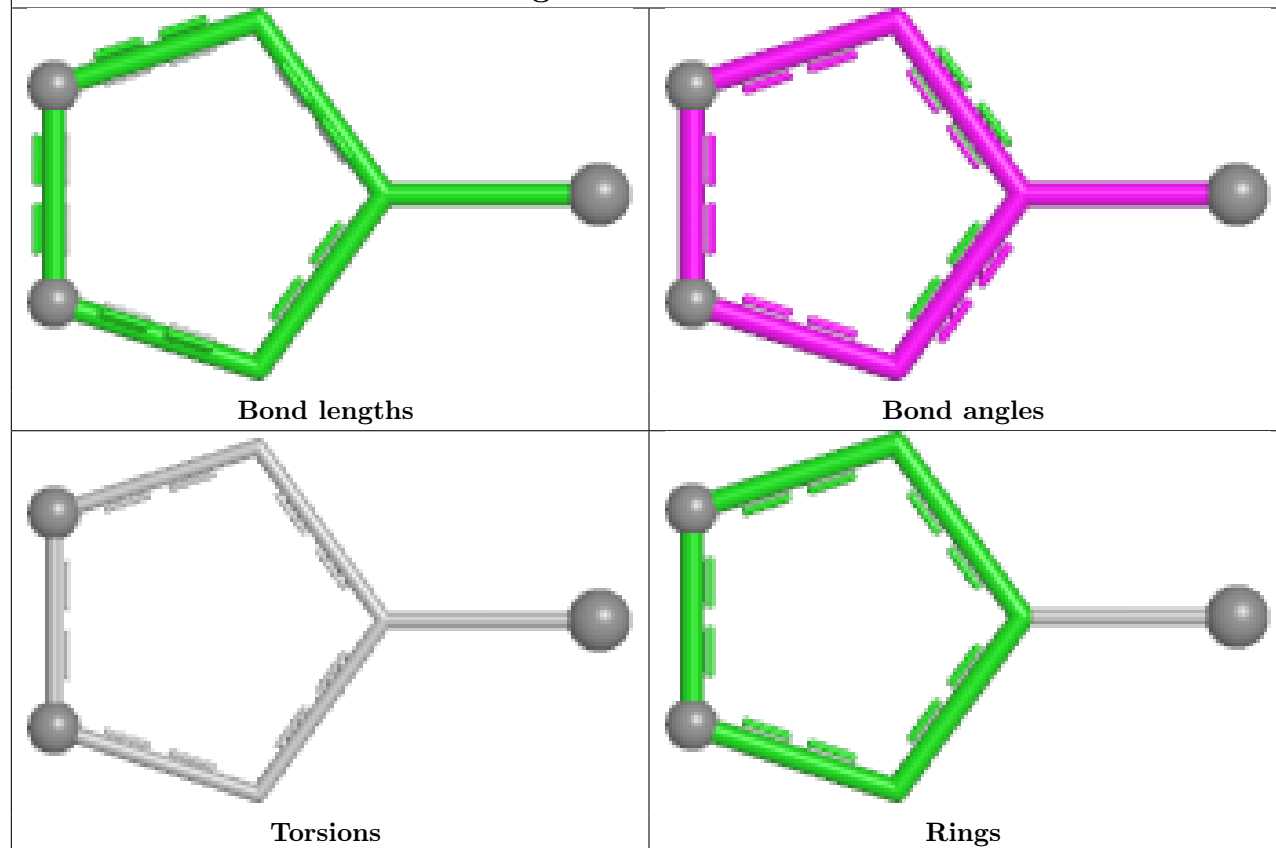
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

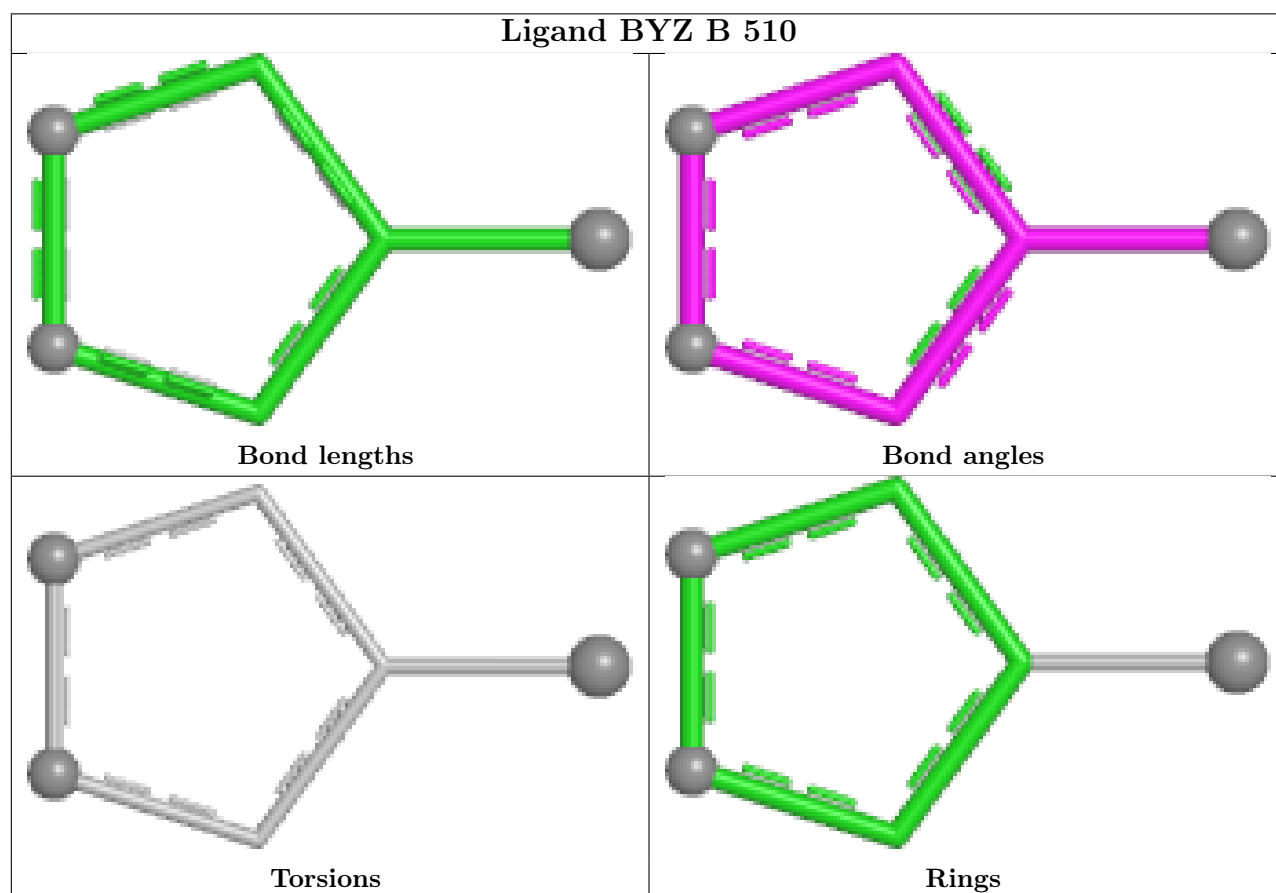
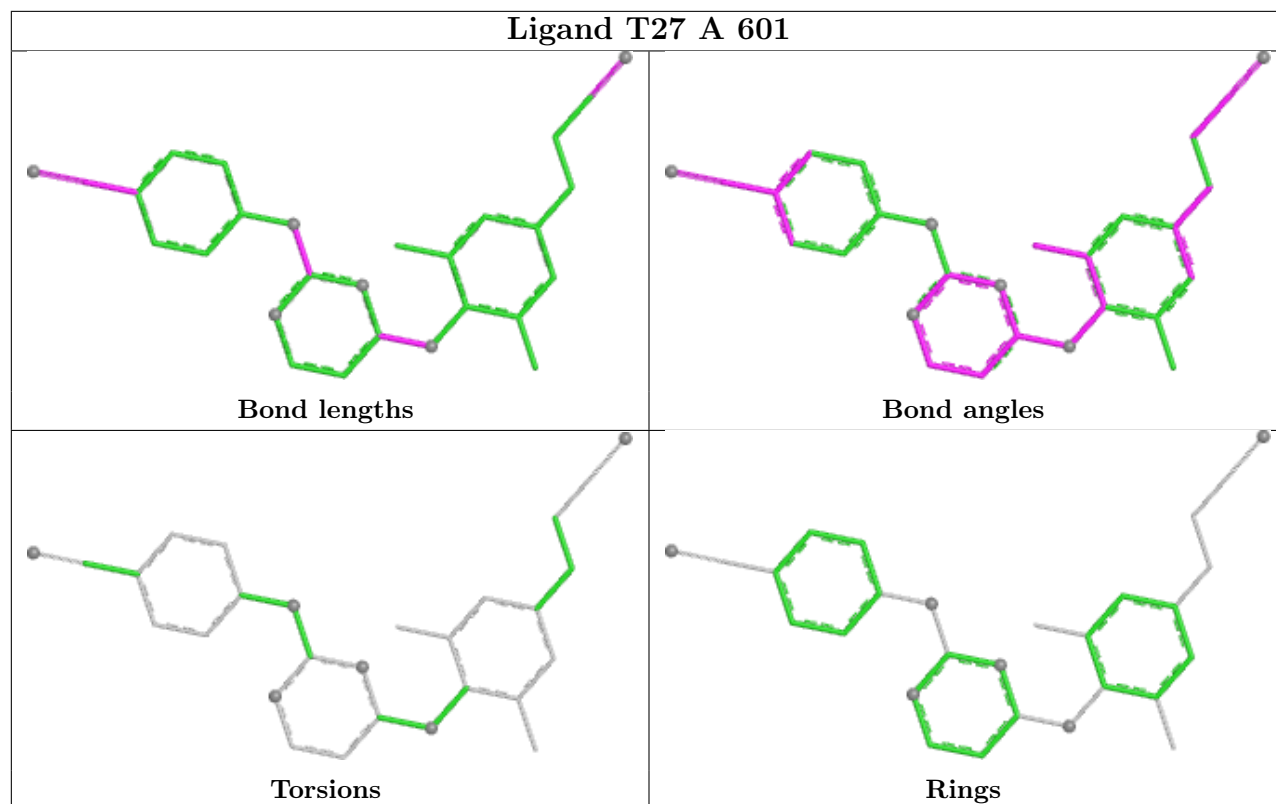


Ligand BYZ B 508 (A)

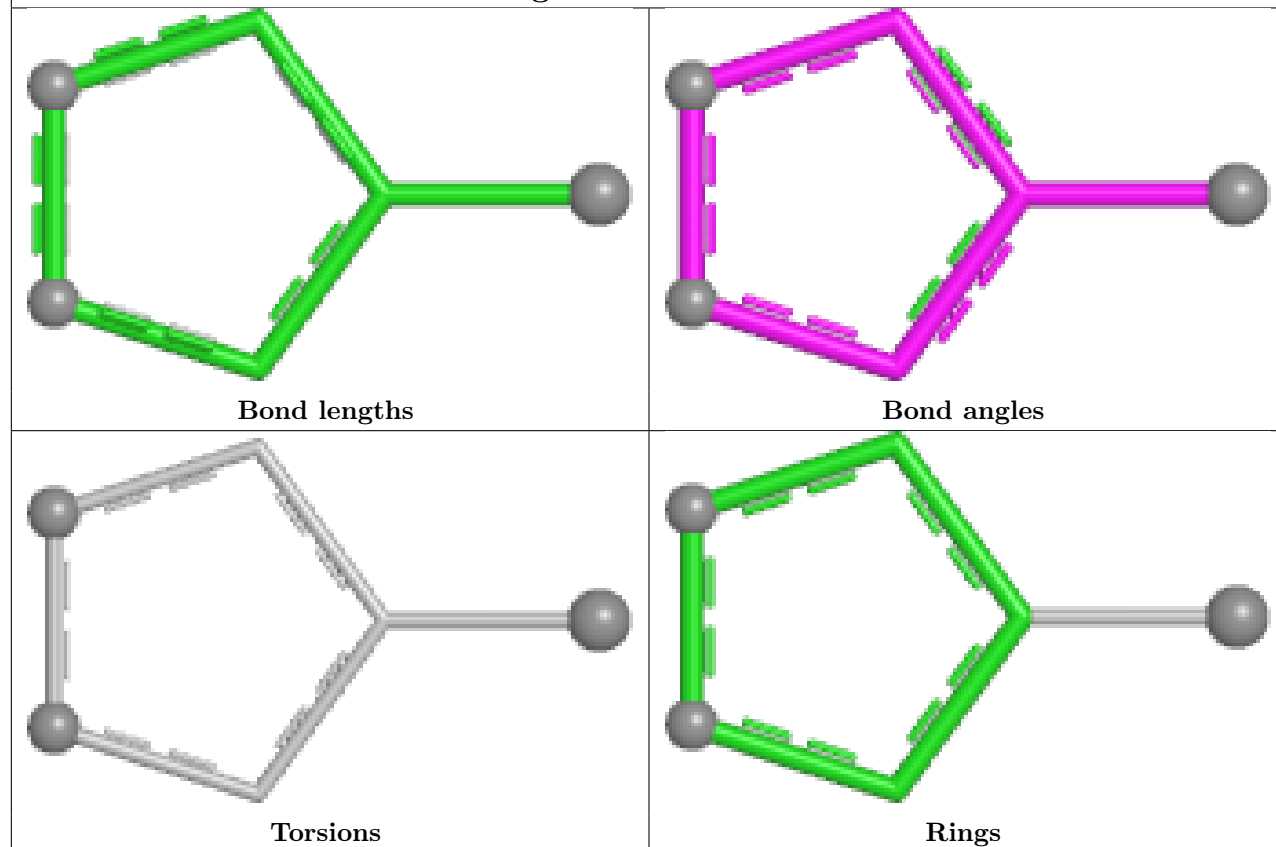


Ligand BYZ B 509

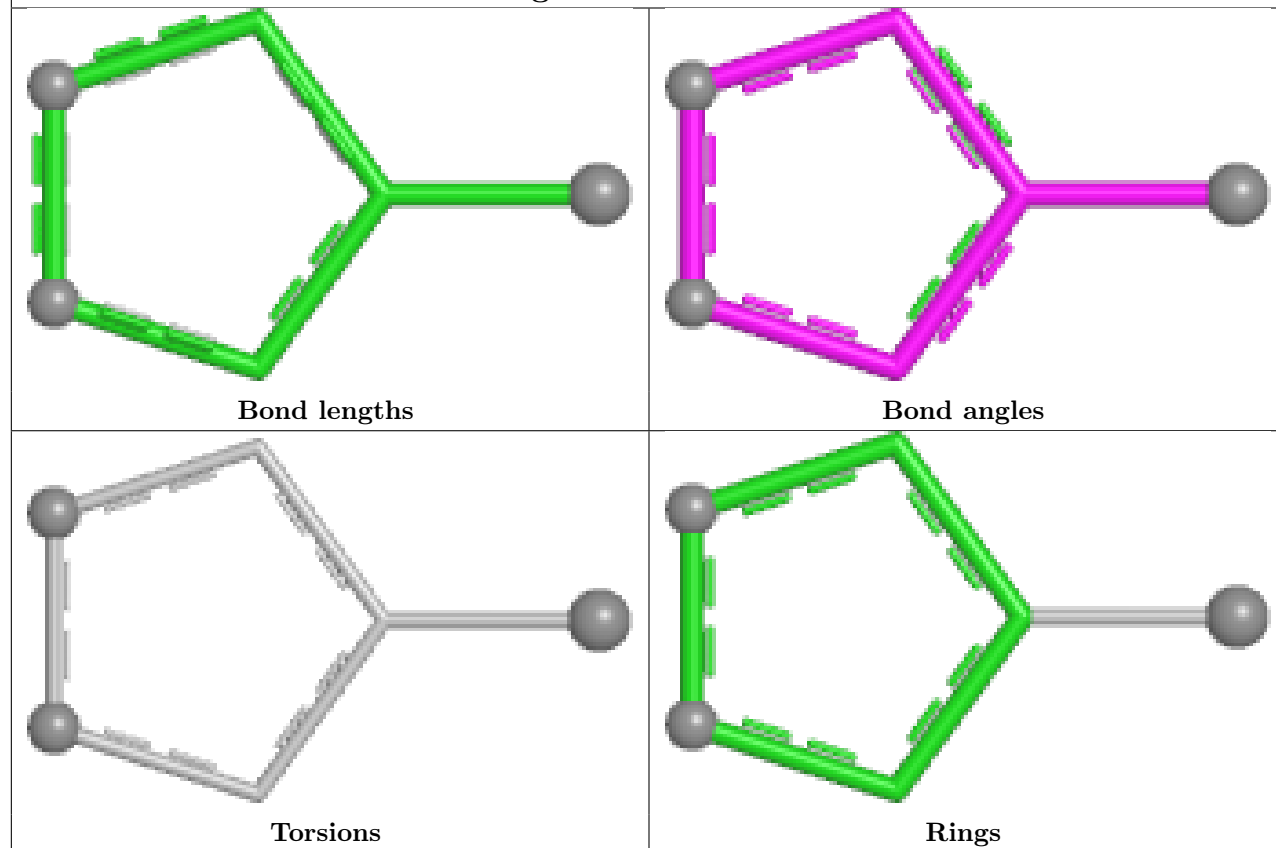




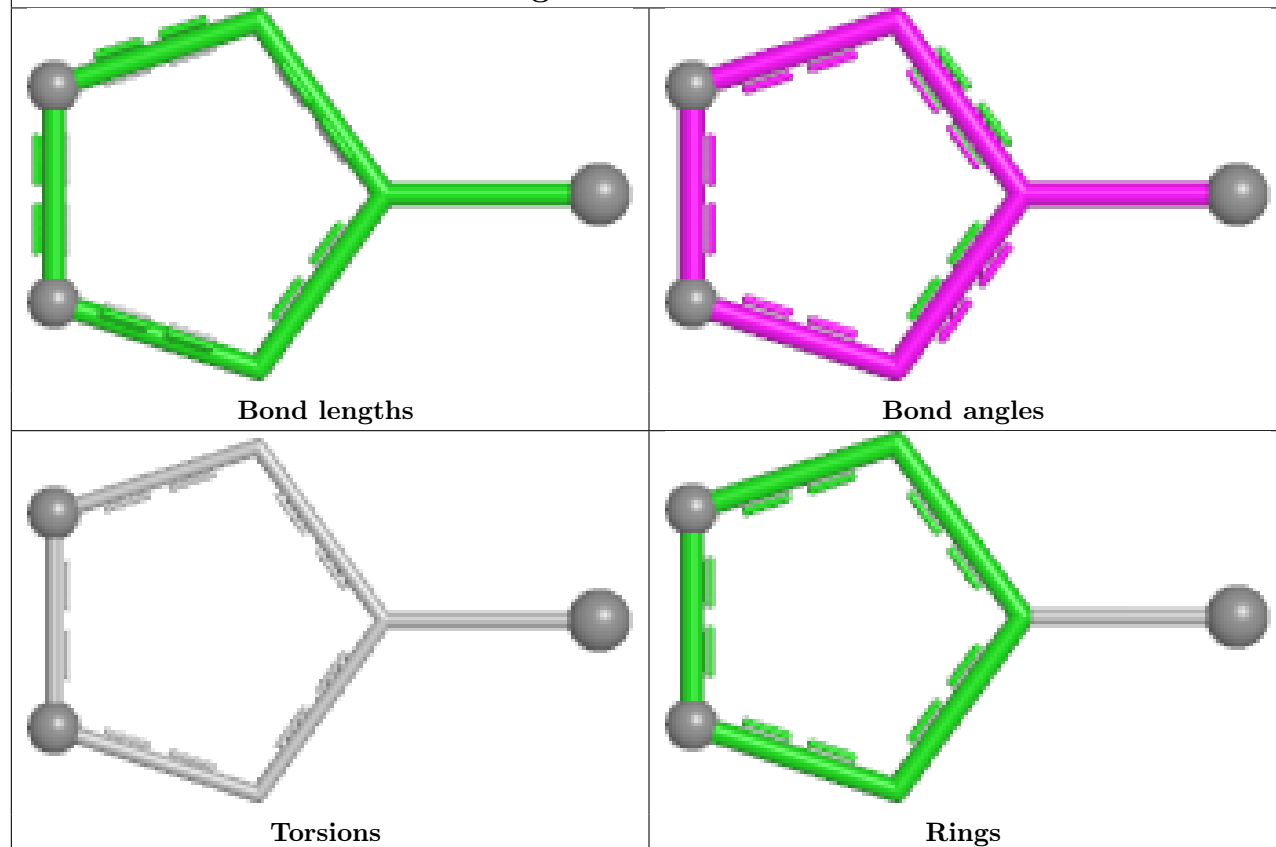
Ligand BYZ A 610



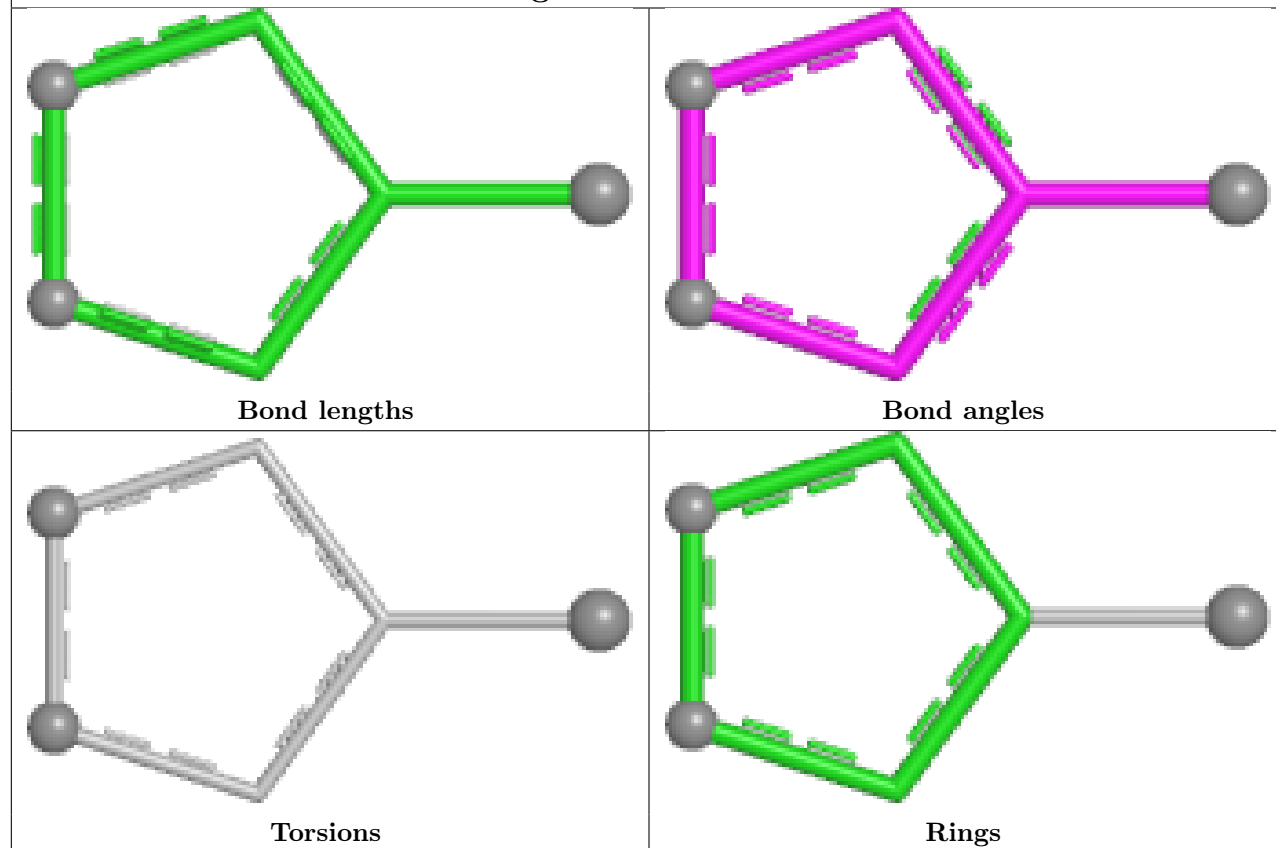
Ligand BYZ A 611



Ligand BYZ A 612



Ligand BYZ A 613



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%)	0.21	35 (6%) 26 24	13, 39, 92, 178	6 (1%)
2	B	415/428 (96%)	0.30	33 (7%) 18 17	14, 40, 90, 184	5 (1%)
All	All	971/985 (98%)	0.25	68 (7%) 22 21	13, 40, 92, 184	11 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	7.8
1	A	5[A]	ILE	6.7
2	B	92	LEU	6.1
2	B	94	ILE	5.4
1	A	544	GLY	5.1
2	B	284	ARG	4.8
1	A	543	GLY	4.7
1	A	24	TRP	4.4
2	B	95	PRO	4.3
1	A	554	ALA	4.2
2	B	5	ILE	4.1
2	B	90	VAL	4.1
2	B	357	MET	4.0
1	A	90	VAL	3.8
2	B	69	THR	3.6
2	B	93	GLY	3.6
2	B	209	LEU	3.6
2	B	359	GLY	3.6
1	A	220	LYS	3.5
2	B	214	LEU	3.4
1	A	116	PHE	3.3
2	B	360	ALA	3.2
1	A	546	GLU	3.1
1	A	553	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	3.0
1	A	289	LEU	3.0
1	A	292	VAL	3.0
2	B	240	THR	3.0
2	B	65	LYS	3.0
2	B	356	ARG	3.0
2	B	88	TRP	3.0
2	B	361	HIS	2.9
1	A	115	TYR	2.9
2	B	283	LEU	2.8
2	B	315[A]	HIS	2.8
1	A	548	VAL	2.7
1	A	109	LEU	2.6
1	A	184	MET	2.6
1	A	552	VAL	2.6
1	A	91	GLN	2.6
1	A	65	LYS	2.5
1	A	541	GLY	2.5
2	B	212	TRP	2.5
2	B	22	LYS	2.4
1	A	542	ILE	2.4
2	B	91	GLN	2.4
1	A	357	MET	2.4
1	A	195	ILE	2.4
1	A	253	THR	2.3
1	A	283	LEU	2.3
1	A	290	THR	2.3
1	A	288	ALA	2.3
2	B	285	GLY	2.3
2	B	66	LYS	2.3
2	B	229	TRP	2.3
2	B	231	GLY	2.2
1	A	361	HIS	2.2
1	A	244	ILE	2.2
2	B	205	LEU	2.2
2	B	355	ALA	2.2
1	A	71	TRP	2.2
1	A	221	HIS	2.1
2	B	166	LYS	2.1
1	A	69	THR	2.1
1	A	4	PRO	2.1
2	B	358	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	51	GLY	2.0
2	B	227	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

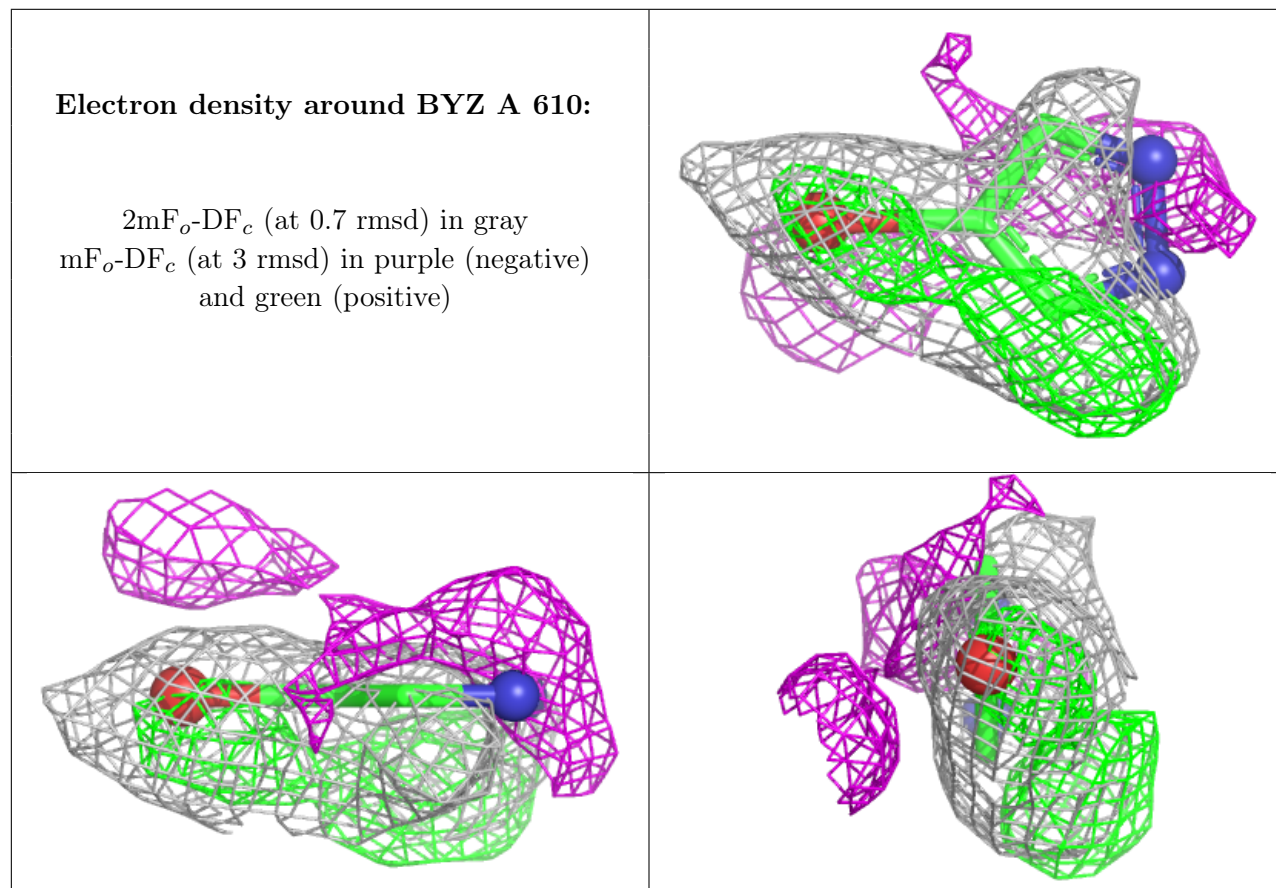
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	A	607	5/5	0.59	0.17	105,108,121,121	0
5	EDO	A	603	4/4	0.68	0.22	55,65,65,67	0
8	BYZ	A	610	6/6	0.69	0.33	86,93,106,208	0
8	BYZ	A	612	6/6	0.71	0.24	99,115,121,208	0
8	BYZ	A	613	6/6	0.72	0.18	111,115,121,227	0
8	BYZ	B	510	6/6	0.72	0.23	66,75,85,197	0
7	SO4	A	606	5/5	0.76	0.12	103,112,114,114	0
8	BYZ	A	609[A]	6/6	0.78	0.55	160,167,176,278	6
8	BYZ	A	611	6/6	0.79	0.23	75,82,89,171	0
4	DMS	B	504	4/4	0.82	0.22	58,72,80,82	0
8	BYZ	B	509	6/6	0.83	0.24	106,127,137,219	0
7	SO4	A	608	5/5	0.85	0.10	69,71,89,92	0
8	BYZ	B	508[A]	6/6	0.88	0.30	43,45,47,114	6
5	EDO	B	506	4/4	0.89	0.12	42,46,55,56	0
4	DMS	B	503	4/4	0.89	0.19	43,47,56,62	0
7	SO4	B	507	5/5	0.90	0.09	70,77,88,96	0
4	DMS	B	501	4/4	0.91	0.17	27,38,52,65	0
5	EDO	A	604	4/4	0.92	0.12	27,30,42,50	0
4	DMS	B	505	4/4	0.92	0.14	36,47,54,57	0
6	MG	A	605	1/1	0.92	0.07	72,72,72,72	0
4	DMS	B	502	4/4	0.93	0.14	36,44,57,58	0

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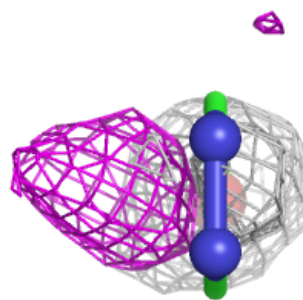
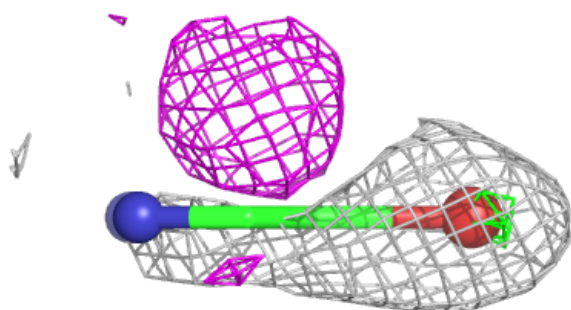
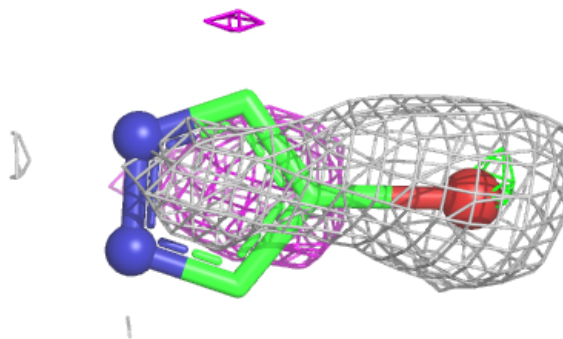
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	602	4/4	0.96	0.12	33,34,40,48	0
3	T27	A	601	28/28	0.96	0.07	25,28,35,43	0

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.

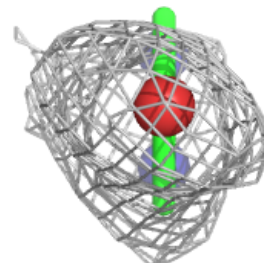
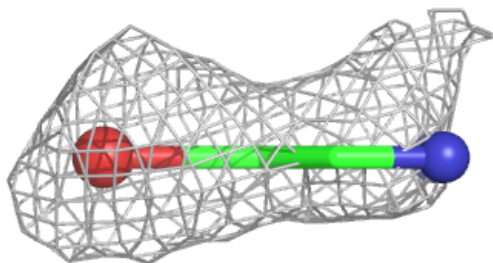
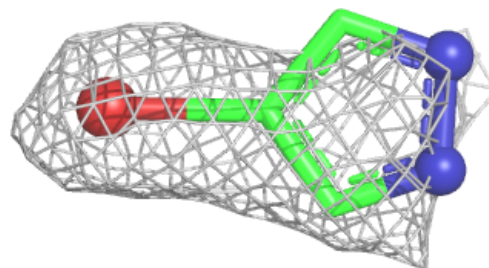


Electron density around BYZ A 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

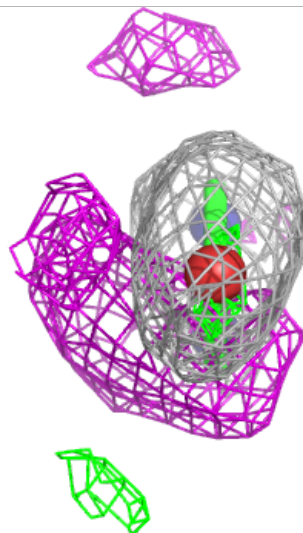
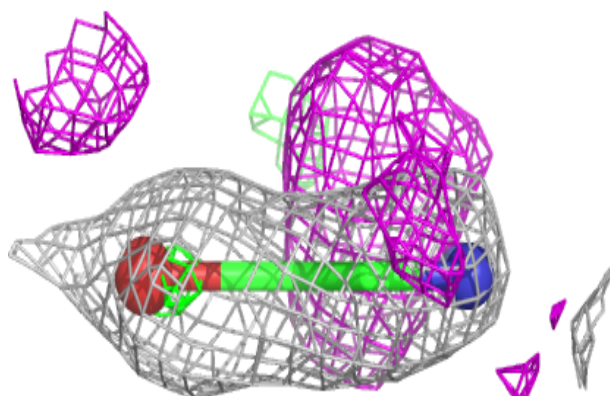
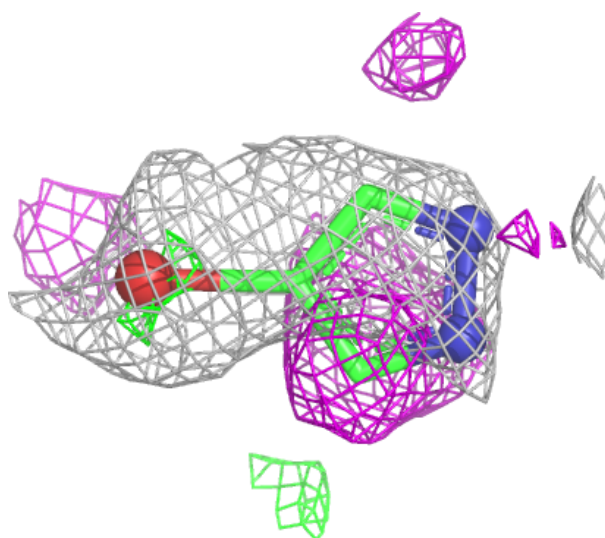
**Electron density around BYZ A 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



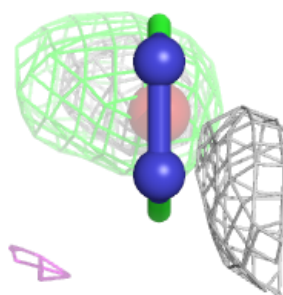
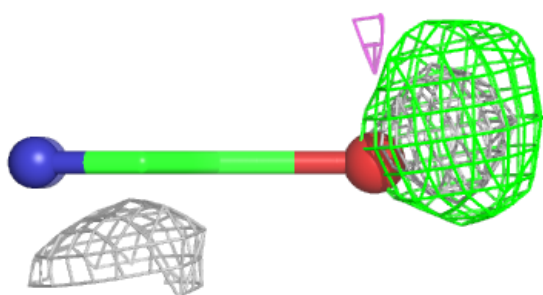
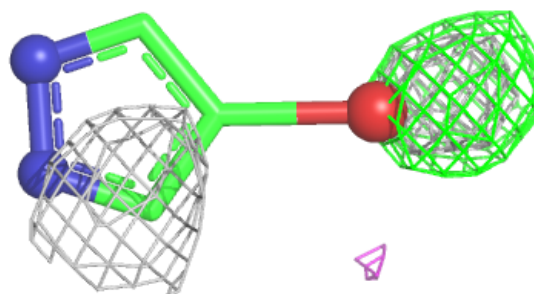
Electron density around BYZ B 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

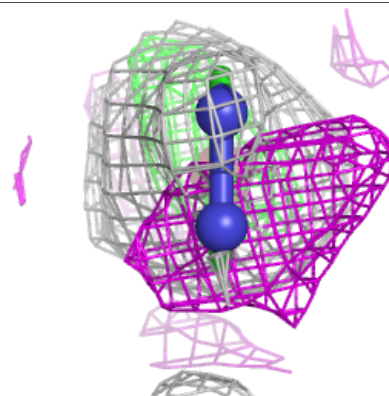
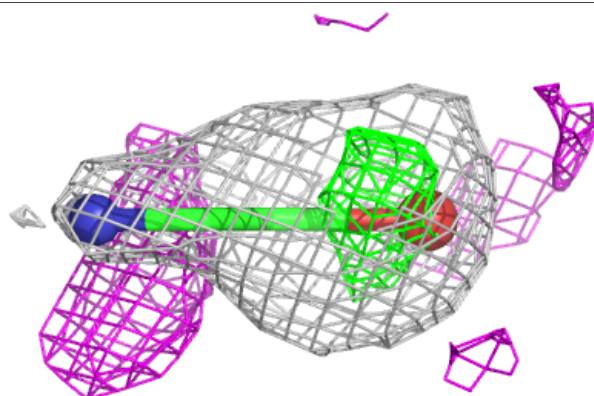
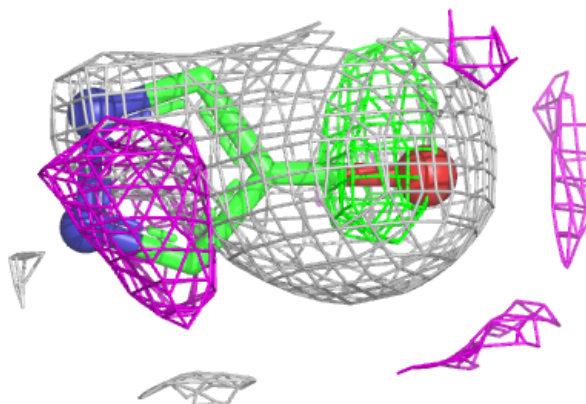


Electron density around BYZ A 609 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

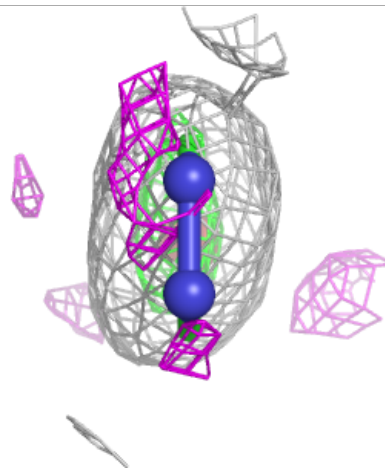
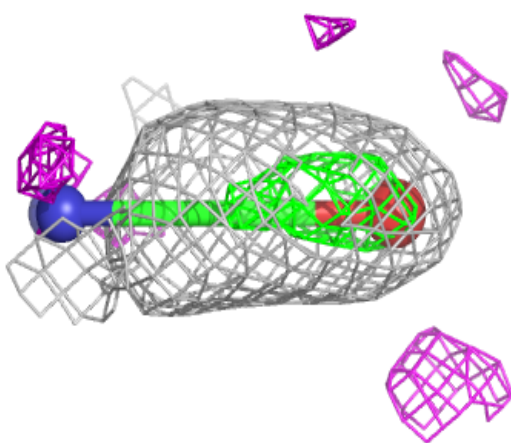
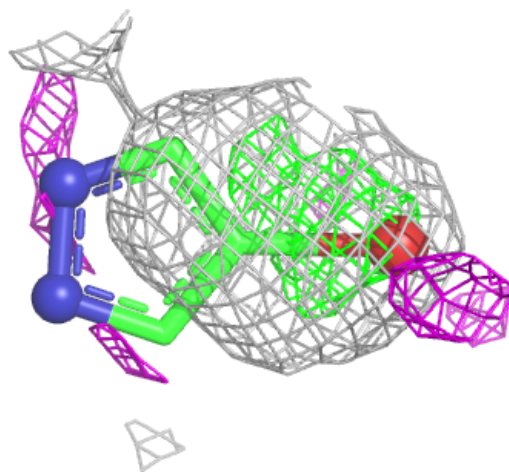
**Electron density around BYZ A 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



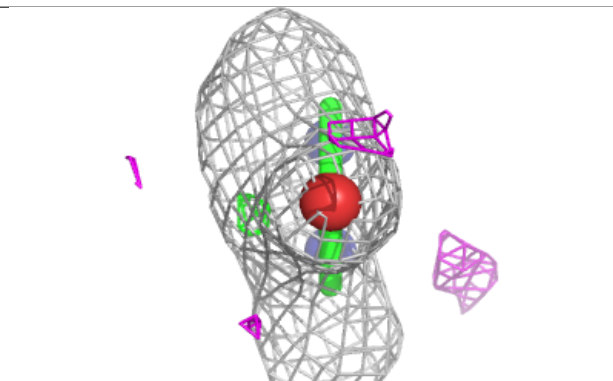
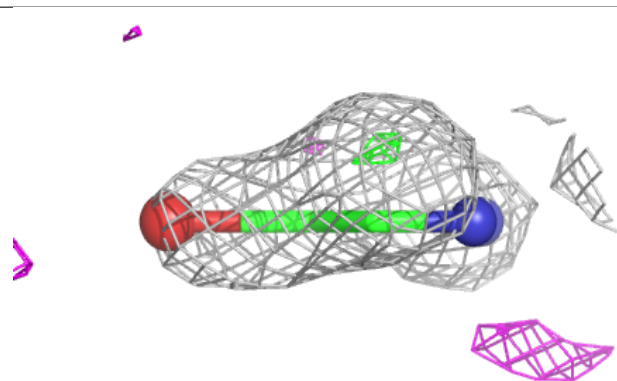
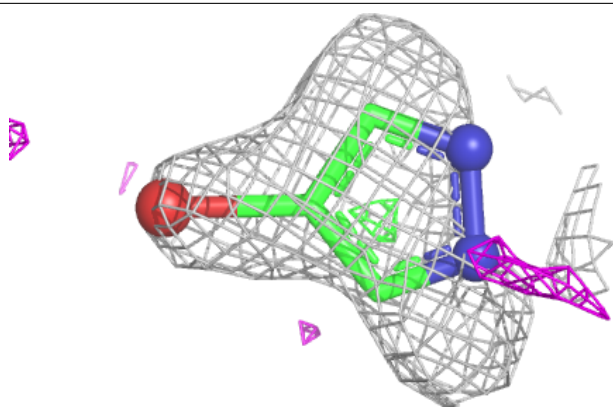
Electron density around BYZ B 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



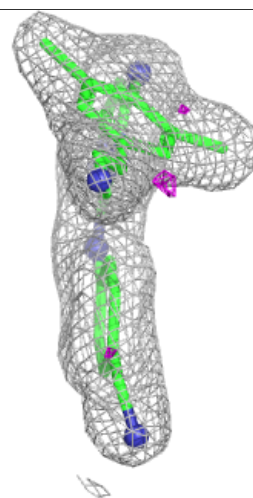
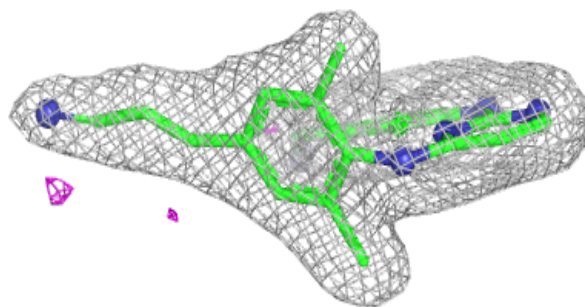
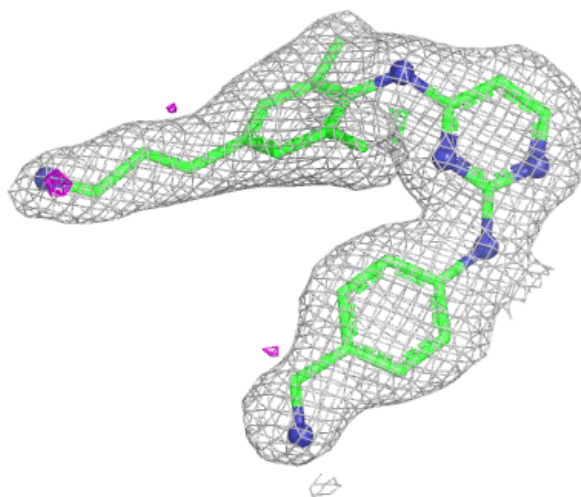
Electron density around BYZ B 508 (A):

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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.