



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:02 PM UTC

PDB ID : 8S99 / pdb_00008s99
Title : Crystal structure of the TYK2 pseudokinase domain in complex with compound 11
Authors : Toms, A.V.; Leit, S.; Greenwood, J.R.; Carriero, S.; Mondal, S.; Abel, R.; Ashwell, M.; Blanchette, H.; Boyles, N.; Cartwright, M.; Collis, A.; Feng, S.; Ghanakota, P.; Harriman, G.C.; Hosagrahara, V.; Kaila, N.; Kapeller, R.; Rafi, S.; Romero, D.L.; Tarantino, P.; Timaniya, J.; Wester, R.T.; Westlin, W.; Srivastava, B.; Miao, W.; Tummino, P.; McElwee, J.J.; Edmondson, S.D.; Massee, C.E.
Deposited on : 2023-03-27
Resolution : 1.71 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)

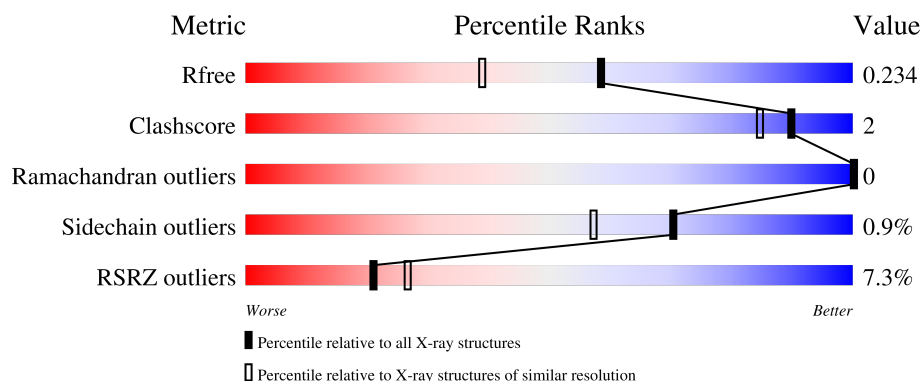
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	295	8% 83% 6% 12%
1	B	295	6% 85% • 12%

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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

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Mol	Chain	Length	Quality of chain
1	C	295	5% 83% 5% 12%

2 Entry composition [i](#)

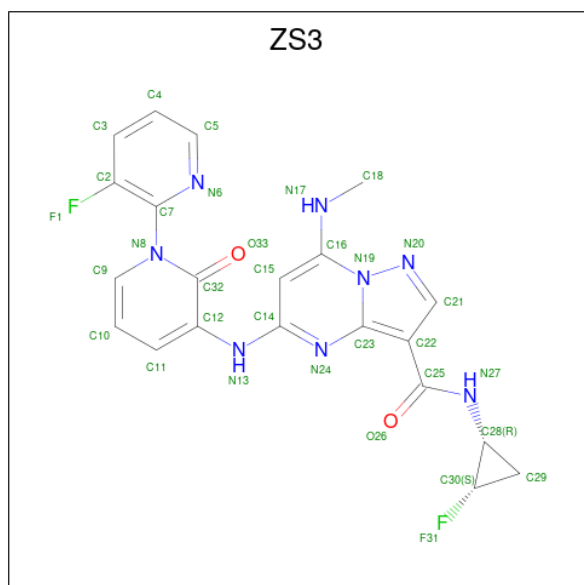
There are 5 unique types of molecules in this entry. The entry contains 7307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Non-receptor tyrosine-protein kinase TYK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	28	12	0
			2175	1365	400	399	11			
1	B	261	Total	C	N	O	S	20	13	0
			2183	1373	401	398	11			
1	C	260	Total	C	N	O	S	33	7	0
			2122	1335	390	386	11			

- Molecule 2 is (8S)-N-[(1R,2S)-2-fluorocyclopropyl]-5-[[[(1M,2'M)-3'-fluoro-2-oxo-2H-[1,2'-bipyridin]-3-yl]amino}-7-(methylamino)pyrazolo[1,5-a]pyrimidine-3-carboxamide (CCD ID: ZS3) (formula: C₂₁H₁₈F₂N₈O₂) (labeled as "Ligand of Interest" by depositor).



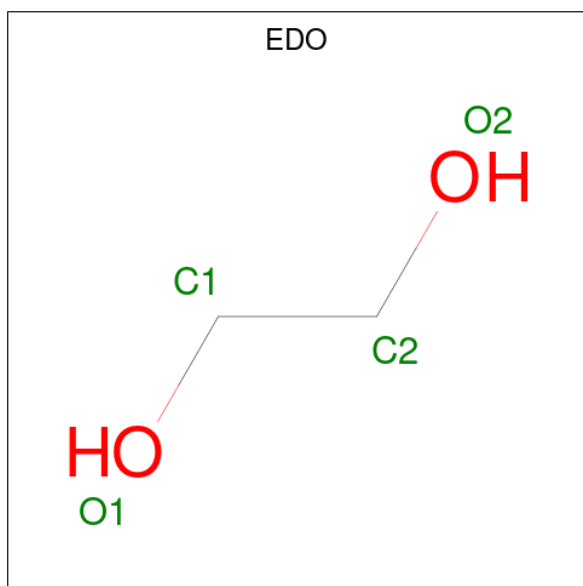
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	1
			40	25	3	9	3		
2	B	1	Total	C	F	N	O	0	1
			40	25	3	9	3		

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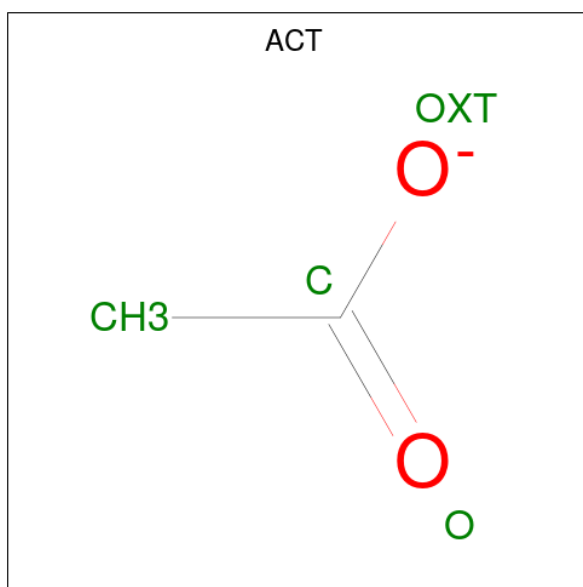
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	1
			40	25	3	9	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

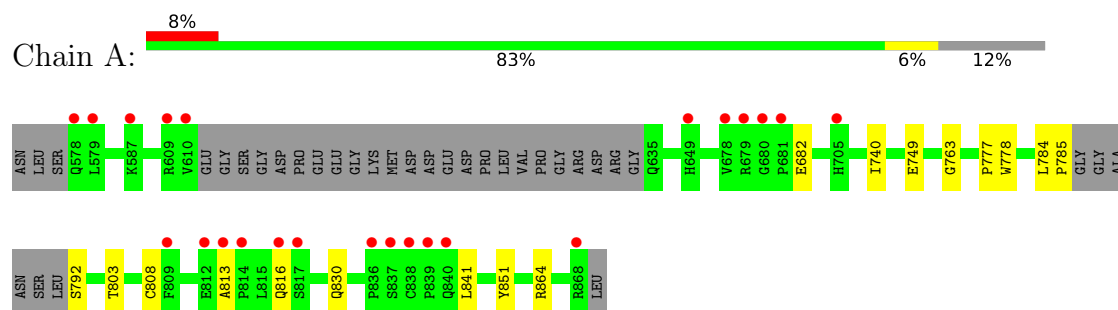
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	219	Total	O	0	0
			219	219		
5	B	225	Total	O	0	0
			225	225		
5	C	227	Total	O	0	0
			227	227		

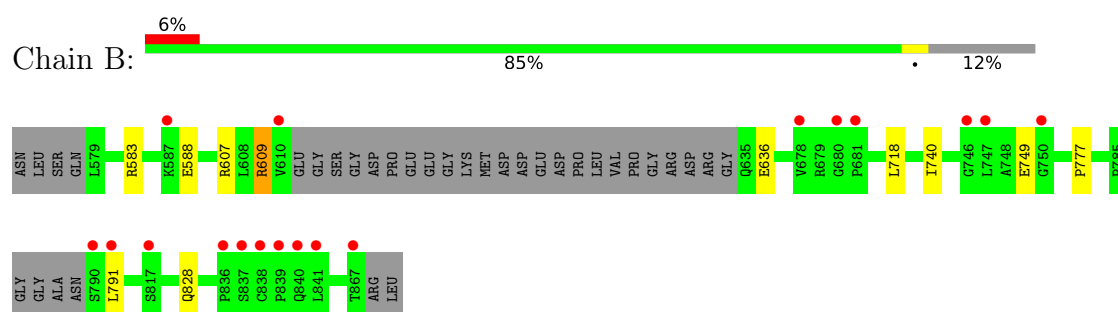
3 Residue-property plots [i](#)

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.

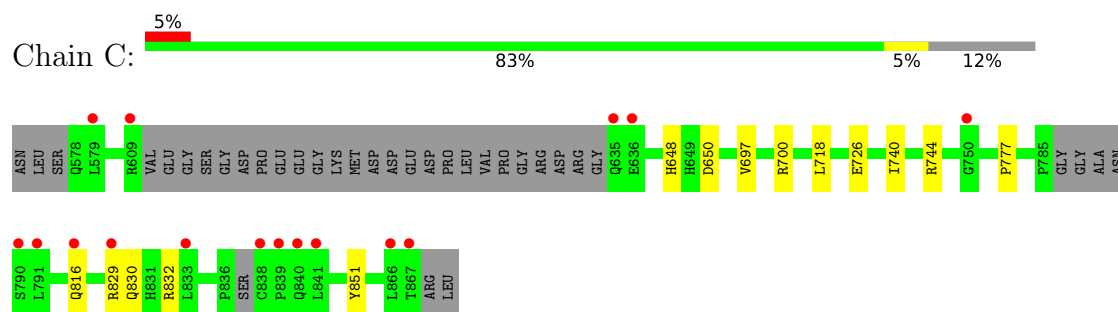
- Molecule 1: Non-receptor tyrosine-protein kinase TYK2



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.21Å 112.72Å 157.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.62 – 1.71 47.62 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.62-1.71) 99.2 (47.62-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.225 0.199 , 0.234	Depositor DCC
R_{free} test set	3022 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7307	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.21% 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: EDO, ACT, ZS3

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	0.99	2/2223 (0.1%)	1.19	0/3012
1	B	0.98	2/2231 (0.1%)	1.24	3/3023 (0.1%)
1	C	0.96	0/2168	1.20	0/2937
All	All	0.98	4/6622 (0.1%)	1.21	3/8972 (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
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	583	ARG	NE-CZ	8.45	1.42	1.33
1	A	816	GLN	CB-CG	5.82	1.70	1.52
1	B	791	LEU	CG-CD2	5.73	1.71	1.52
1	A	864	ARG	CD-NE	-5.70	1.38	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	749	GLU	CB-CG-CD	8.45	126.97	112.60
1	B	609	ARG	NE-CZ-NH2	8.45	126.80	119.20
1	B	609	ARG	NE-CZ-NH1	-8.38	113.12	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	609	ARG	Sidechain

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	2175	0	2147	6	0
1	B	2183	0	2164	4	0
1	C	2122	0	2108	11	0
2	A	40	0	0	1	0
2	B	40	0	0	0	0
2	C	40	0	0	1	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
5	A	219	0	0	1	0
5	B	225	0	0	0	0
5	C	227	0	0	2	0
All	All	7307	0	6464	23	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 (23) 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:B:828[B]:GLN:OE1	1:B:828[B]:GLN:HA	1.90	0.72
1:A:784:LEU:HB3	1:A:785:PRO:HD3	1.77	0.65
1:B:607:ARG:HB3	1:B:636:GLU:HG3	1.80	0.62
1:C:744[B]:ARG:NH2	5:C:1002:HOH:O	2.33	0.62
1:A:808:CYS:SG	1:A:841:LEU:HD21	2.48	0.54
1:C:816:GLN:HA	1:C:816:GLN:HE21	1.80	0.47
1:B:588[B]:GLU:HA	1:B:588[B]:GLU:OE2	2.16	0.46
1:B:718:LEU:HD22	1:B:740[A]:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:HIS:HD2	1:C:650:ASP:H	1.64	0.45
1:C:726:GLU:OE1	5:C:1001:HOH:O	2.21	0.45
1:C:697[B]:VAL:HG12	1:C:700:ARG:HH21	1.81	0.45
1:C:648:HIS:CD2	1:C:650:ASP:H	2.35	0.44
1:A:830:GLN:HA	1:A:851:TYR:CZ	2.54	0.43
1:A:740:ILE:HD11	1:A:803:THR:HG21	2.01	0.42
1:C:832:ARG:HD2	1:C:832:ARG:HA	1.88	0.42
1:C:829[B]:ARG:HD3	1:C:829[B]:ARG:HA	1.85	0.42
1:C:816:GLN:HA	1:C:816:GLN:NE2	2.34	0.42
1:A:778:TRP:CZ2	1:A:813:ALA:CB	3.02	0.42
1:A:763:GLY:HA3	5:A:1005:HOH:O	2.21	0.41
1:C:830:GLN:HA	1:C:851:TYR:CZ	2.56	0.40
1:C:718:LEU:HD22	1:C:740:ILE:HD11	2.04	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	267/295 (90%)	261 (98%)	6 (2%)	0	100	100
1	B	268/295 (91%)	262 (98%)	6 (2%)	0	100	100
1	C	259/295 (88%)	254 (98%)	5 (2%)	0	100	100
All	All	794/885 (90%)	777 (98%)	17 (2%)	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	240/254 (94%)	236 (98%)	4 (2%)	53	31
1	B	241/254 (95%)	240 (100%)	1 (0%)	84	76
1	C	234/254 (92%)	233 (100%)	1 (0%)	84	76
All	All	715/762 (94%)	709 (99%)	6 (1%)	70	61

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

Mol	Chain	Res	Type
1	A	682	GLU
1	A	749	GLU
1	A	777	PRO
1	A	792	SER
1	B	777	PRO
1	C	777	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	734	ASN
1	A	830	GLN
1	B	597	GLN
1	B	602	ASN
1	B	727	ASN
1	B	739	ASN
1	B	831	HIS
1	C	648	HIS
1	C	674	HIS
1	C	727	ASN
1	C	739	ASN
1	C	816	GLN

5.3.3 RNA ⓘ

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](#)

15 ligands are modelled in this entry.

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	$\# Z > 2$
2	ZS3	B	901[B]	-	36,37,37	2.17	12 (33%)	39,54,54	2.43	14 (35%)
3	EDO	A	902	-	3,3,3	0.18	0	2,2,2	0.15	0
3	EDO	B	902	-	3,3,3	0.13	0	2,2,2	0.19	0
2	ZS3	A	901[B]	-	36,37,37	2.37	16 (44%)	39,54,54	2.30	15 (38%)
2	ZS3	C	901[B]	-	36,37,37	2.30	13 (36%)	39,54,54	2.50	17 (43%)
2	ZS3	B	901[A]	-	36,37,37	2.10	10 (27%)	39,54,54	2.42	14 (35%)
2	ZS3	C	901[A]	-	36,37,37	2.11	11 (30%)	39,54,54	2.50	16 (41%)
3	EDO	C	904	-	3,3,3	0.05	0	2,2,2	0.04	0
3	EDO	B	903	-	3,3,3	0.10	0	2,2,2	0.21	0
3	EDO	C	902	-	3,3,3	0.14	0	2,2,2	0.14	0
2	ZS3	A	901[A]	-	36,37,37	2.27	15 (41%)	39,54,54	2.29	15 (38%)
4	ACT	A	903	-	3,3,3	1.03	0	3,3,3	0.78	0
4	ACT	B	904	-	3,3,3	1.00	0	3,3,3	0.79	0
4	ACT	C	903	-	3,3,3	0.99	0	3,3,3	0.81	0
3	EDO	A	904	-	3,3,3	0.12	0	2,2,2	0.28	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
2	ZS3	B	901[B]	-	-	2/15/23/23	0/5/5/5
3	EDO	A	902	-	-	0/1/1/1	-
3	EDO	B	902	-	-	0/1/1/1	-
2	ZS3	A	901[B]	-	-	2/15/23/23	0/5/5/5
2	ZS3	C	901[B]	-	-	2/15/23/23	0/5/5/5
2	ZS3	B	901[A]	-	-	1/15/23/23	0/5/5/5
2	ZS3	C	901[A]	-	-	1/15/23/23	0/5/5/5
3	EDO	C	904	-	-	0/1/1/1	-
3	EDO	B	903	-	-	1/1/1/1	-
3	EDO	C	902	-	-	0/1/1/1	-
2	ZS3	A	901[A]	-	-	1/15/23/23	0/5/5/5
3	EDO	A	904	-	-	0/1/1/1	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901[A]	ZS3	C21-C22	-5.42	1.34	1.41
2	C	901[B]	ZS3	C21-C22	-5.42	1.34	1.41
2	B	901[A]	ZS3	C21-C22	-5.20	1.34	1.41
2	B	901[B]	ZS3	C21-C22	-5.20	1.34	1.41
2	C	901[A]	ZS3	C22-C25	-4.90	1.35	1.49
2	C	901[B]	ZS3	F31-C30	-4.81	1.29	1.40
2	A	901[B]	ZS3	C22-C25	-4.78	1.35	1.49
2	A	901[A]	ZS3	C16-N19	-4.71	1.33	1.37
2	A	901[B]	ZS3	C16-N19	-4.71	1.33	1.37
2	A	901[A]	ZS3	C22-C25	-4.67	1.36	1.49
2	B	901[A]	ZS3	C22-C25	-4.64	1.36	1.49
2	C	901[B]	ZS3	C22-C25	-4.62	1.36	1.49
2	B	901[B]	ZS3	C22-C25	-4.54	1.36	1.49
2	A	901[A]	ZS3	C21-C22	-4.36	1.35	1.41
2	A	901[B]	ZS3	C21-C22	-4.36	1.35	1.41
2	A	901[A]	ZS3	C5-N6	3.93	1.42	1.34
2	A	901[B]	ZS3	C5-N6	3.93	1.42	1.34
2	C	901[A]	ZS3	C22-C23	-3.91	1.35	1.45
2	C	901[B]	ZS3	C22-C23	-3.91	1.35	1.45
2	A	901[A]	ZS3	C22-C23	-3.78	1.35	1.45
2	A	901[B]	ZS3	C22-C23	-3.78	1.35	1.45
2	B	901[A]	ZS3	C22-C23	-3.62	1.35	1.45
2	B	901[B]	ZS3	C22-C23	-3.62	1.35	1.45
2	C	901[A]	ZS3	C5-N6	3.61	1.42	1.34
2	C	901[B]	ZS3	C5-N6	3.61	1.42	1.34
2	A	901[B]	ZS3	F31-C30	-3.58	1.32	1.40
2	B	901[A]	ZS3	C5-N6	3.57	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901[B]	ZS3	C5-N6	3.57	1.42	1.34
2	C	901[A]	ZS3	C16-N19	-3.55	1.34	1.37
2	C	901[B]	ZS3	C16-N19	-3.55	1.34	1.37
2	B	901[A]	ZS3	C7-N8	-3.50	1.35	1.42
2	B	901[B]	ZS3	C7-N8	-3.50	1.35	1.42
2	A	901[A]	ZS3	C7-N8	-3.28	1.36	1.42
2	A	901[B]	ZS3	C7-N8	-3.28	1.36	1.42
2	C	901[A]	ZS3	C7-N8	-3.23	1.36	1.42
2	C	901[B]	ZS3	C7-N8	-3.23	1.36	1.42
2	B	901[A]	ZS3	C16-N19	-3.17	1.34	1.37
2	B	901[B]	ZS3	C16-N19	-3.17	1.34	1.37
2	A	901[A]	ZS3	F1-C2	-3.12	1.27	1.35
2	A	901[B]	ZS3	F1-C2	-3.12	1.27	1.35
2	A	901[A]	ZS3	C7-C2	-3.04	1.38	1.42
2	A	901[B]	ZS3	C7-C2	-3.04	1.38	1.42
2	C	901[B]	ZS3	C29-C28	2.89	1.53	1.49
2	B	901[A]	ZS3	C12-C32	-2.84	1.41	1.48
2	B	901[B]	ZS3	C12-C32	-2.84	1.41	1.48
2	A	901[B]	ZS3	C29-C28	2.79	1.53	1.49
2	C	901[A]	ZS3	C12-C32	-2.73	1.41	1.48
2	C	901[B]	ZS3	C12-C32	-2.73	1.41	1.48
2	B	901[A]	ZS3	C21-N20	2.71	1.36	1.32
2	B	901[B]	ZS3	C21-N20	2.71	1.36	1.32
2	B	901[B]	ZS3	C29-C28	2.71	1.52	1.49
2	A	901[A]	ZS3	C12-C32	-2.64	1.41	1.48
2	A	901[B]	ZS3	C12-C32	-2.64	1.41	1.48
2	C	901[A]	ZS3	C32-N8	-2.50	1.36	1.41
2	C	901[B]	ZS3	C32-N8	-2.50	1.36	1.41
2	A	901[A]	ZS3	C23-N19	-2.47	1.34	1.38
2	A	901[B]	ZS3	C23-N19	-2.47	1.34	1.38
2	B	901[A]	ZS3	C32-N8	-2.44	1.36	1.41
2	B	901[B]	ZS3	C32-N8	-2.44	1.36	1.41
2	A	901[A]	ZS3	C32-N8	-2.36	1.36	1.41
2	A	901[B]	ZS3	C32-N8	-2.36	1.36	1.41
2	C	901[A]	ZS3	C23-N19	-2.34	1.35	1.38
2	C	901[B]	ZS3	C23-N19	-2.34	1.35	1.38
2	C	901[A]	ZS3	C7-C2	-2.32	1.39	1.42
2	C	901[B]	ZS3	C7-C2	-2.32	1.39	1.42
2	A	901[A]	ZS3	C29-C28	2.29	1.52	1.49
2	A	901[A]	ZS3	C18-N17	2.26	1.49	1.45
2	A	901[B]	ZS3	C18-N17	2.26	1.49	1.45
2	B	901[A]	ZS3	C7-C2	-2.24	1.39	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901[B]	ZS3	C7-C2	-2.24	1.39	1.42
2	A	901[A]	ZS3	C14-N13	-2.22	1.36	1.39
2	A	901[B]	ZS3	C14-N13	-2.22	1.36	1.39
2	C	901[A]	ZS3	C14-N13	-2.15	1.36	1.39
2	C	901[B]	ZS3	C14-N13	-2.15	1.36	1.39
2	B	901[B]	ZS3	F31-C30	-2.11	1.35	1.40
2	A	901[A]	ZS3	C12-N13	-2.08	1.35	1.41
2	A	901[B]	ZS3	C12-N13	-2.08	1.35	1.41

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901[A]	ZS3	N13-C14-N24	6.30	124.10	113.87
2	C	901[B]	ZS3	N13-C14-N24	6.30	124.10	113.87
2	B	901[A]	ZS3	N13-C14-N24	6.15	123.85	113.87
2	B	901[B]	ZS3	N13-C14-N24	6.15	123.85	113.87
2	A	901[A]	ZS3	N13-C14-N24	6.10	123.77	113.87
2	A	901[B]	ZS3	N13-C14-N24	6.10	123.77	113.87
2	B	901[A]	ZS3	C22-C23-N19	6.04	108.74	105.58
2	B	901[B]	ZS3	C22-C23-N19	6.04	108.74	105.58
2	C	901[A]	ZS3	C21-N20-N19	5.61	107.37	103.43
2	C	901[B]	ZS3	C21-N20-N19	5.61	107.37	103.43
2	A	901[A]	ZS3	C21-C22-C23	5.11	108.39	104.57
2	A	901[B]	ZS3	C21-C22-C23	5.11	108.39	104.57
2	B	901[A]	ZS3	C21-N20-N19	4.97	106.92	103.43
2	B	901[B]	ZS3	C21-N20-N19	4.97	106.92	103.43
2	C	901[A]	ZS3	C21-C22-C23	4.85	108.19	104.57
2	C	901[B]	ZS3	C21-C22-C23	4.85	108.19	104.57
2	B	901[A]	ZS3	C23-N19-N20	-4.46	107.54	112.24
2	B	901[B]	ZS3	C23-N19-N20	-4.46	107.54	112.24
2	A	901[A]	ZS3	C21-N20-N19	4.27	106.43	103.43
2	A	901[B]	ZS3	C21-N20-N19	4.27	106.43	103.43
2	C	901[A]	ZS3	C22-C23-N19	4.23	107.80	105.58
2	C	901[B]	ZS3	C22-C23-N19	4.23	107.80	105.58
2	A	901[A]	ZS3	N6-C7-N8	3.99	119.21	114.66
2	A	901[B]	ZS3	N6-C7-N8	3.99	119.21	114.66
2	C	901[A]	ZS3	C23-N19-N20	-3.98	108.04	112.24
2	C	901[B]	ZS3	C23-N19-N20	-3.98	108.04	112.24
2	B	901[A]	ZS3	C21-C22-C23	3.98	107.54	104.57
2	B	901[B]	ZS3	C21-C22-C23	3.98	107.54	104.57
2	A	901[A]	ZS3	C22-C23-N19	3.90	107.63	105.58
2	A	901[B]	ZS3	C22-C23-N19	3.90	107.63	105.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901[A]	ZS3	C32-C12-N13	3.85	115.58	112.00
2	C	901[B]	ZS3	C32-C12-N13	3.85	115.58	112.00
2	C	901[A]	ZS3	C22-C23-N24	3.48	133.01	123.54
2	C	901[B]	ZS3	C22-C23-N24	3.48	133.01	123.54
2	A	901[A]	ZS3	C22-C23-N24	3.40	132.80	123.54
2	A	901[B]	ZS3	C22-C23-N24	3.40	132.80	123.54
2	B	901[A]	ZS3	C22-C23-N24	3.28	132.46	123.54
2	B	901[B]	ZS3	C22-C23-N24	3.28	132.46	123.54
2	A	901[A]	ZS3	C23-N19-N20	-3.28	108.78	112.24
2	A	901[B]	ZS3	C23-N19-N20	-3.28	108.78	112.24
2	C	901[A]	ZS3	C22-C21-N20	-3.12	108.57	112.45
2	C	901[B]	ZS3	C22-C21-N20	-3.12	108.57	112.45
2	B	901[A]	ZS3	N19-C23-N24	-3.02	118.80	122.15
2	B	901[B]	ZS3	N19-C23-N24	-3.02	118.80	122.15
2	B	901[A]	ZS3	C14-N24-C23	3.02	121.46	117.18
2	B	901[B]	ZS3	C14-N24-C23	3.02	121.46	117.18
2	C	901[A]	ZS3	C14-N24-C23	3.01	121.45	117.18
2	C	901[B]	ZS3	C14-N24-C23	3.01	121.45	117.18
2	A	901[A]	ZS3	C22-C21-N20	-2.97	108.76	112.45
2	A	901[B]	ZS3	C22-C21-N20	-2.97	108.76	112.45
2	C	901[A]	ZS3	N6-C7-N8	2.78	117.83	114.66
2	C	901[B]	ZS3	N6-C7-N8	2.78	117.83	114.66
2	C	901[A]	ZS3	N19-C23-N24	-2.68	119.18	122.15
2	C	901[B]	ZS3	N19-C23-N24	-2.68	119.18	122.15
2	C	901[A]	ZS3	C5-N6-C7	2.64	121.03	115.05
2	C	901[B]	ZS3	C5-N6-C7	2.64	121.03	115.05
2	A	901[A]	ZS3	C5-N6-C7	2.59	120.91	115.05
2	A	901[B]	ZS3	C5-N6-C7	2.59	120.91	115.05
2	B	901[A]	ZS3	C22-C21-N20	-2.57	109.25	112.45
2	B	901[B]	ZS3	C22-C21-N20	-2.57	109.25	112.45
2	C	901[A]	ZS3	C4-C5-N6	-2.55	119.38	123.42
2	C	901[B]	ZS3	C4-C5-N6	-2.55	119.38	123.42
2	A	901[A]	ZS3	C14-N24-C23	2.53	120.77	117.18
2	A	901[B]	ZS3	C14-N24-C23	2.53	120.77	117.18
2	C	901[A]	ZS3	C15-C14-N24	-2.52	118.67	122.75
2	C	901[B]	ZS3	C15-C14-N24	-2.52	118.67	122.75
2	B	901[A]	ZS3	C4-C5-N6	-2.52	119.43	123.42
2	B	901[B]	ZS3	C4-C5-N6	-2.52	119.43	123.42
2	A	901[A]	ZS3	C15-C14-N24	-2.51	118.69	122.75
2	A	901[B]	ZS3	C15-C14-N24	-2.51	118.69	122.75
2	B	901[A]	ZS3	N6-C7-N8	2.50	117.51	114.66
2	B	901[B]	ZS3	N6-C7-N8	2.50	117.51	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901[A]	ZS3	C5-N6-C7	2.43	120.56	115.05
2	B	901[B]	ZS3	C5-N6-C7	2.43	120.56	115.05
2	B	901[A]	ZS3	C15-C14-N24	-2.40	118.86	122.75
2	B	901[B]	ZS3	C15-C14-N24	-2.40	118.86	122.75
2	A	901[A]	ZS3	C32-C12-N13	2.38	114.21	112.00
2	A	901[B]	ZS3	C32-C12-N13	2.38	114.21	112.00
2	B	901[A]	ZS3	C32-C12-N13	2.36	114.19	112.00
2	B	901[B]	ZS3	C32-C12-N13	2.36	114.19	112.00
2	A	901[A]	ZS3	N19-C23-N24	-2.33	119.57	122.15
2	A	901[B]	ZS3	N19-C23-N24	-2.33	119.57	122.15
2	A	901[A]	ZS3	F1-C2-C7	-2.27	117.71	119.87
2	A	901[B]	ZS3	F1-C2-C7	-2.27	117.71	119.87
2	C	901[A]	ZS3	C3-C2-C7	-2.20	120.25	121.69
2	C	901[B]	ZS3	C3-C2-C7	-2.20	120.25	121.69
2	C	901[B]	ZS3	C21-C22-C25	-2.07	123.42	129.45
2	A	901[A]	ZS3	C4-C5-N6	-2.03	120.20	123.42
2	A	901[B]	ZS3	C4-C5-N6	-2.03	120.20	123.42
2	C	901[A]	ZS3	C11-C12-C32	-2.01	118.99	120.46
2	C	901[B]	ZS3	C11-C12-C32	-2.01	118.99	120.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

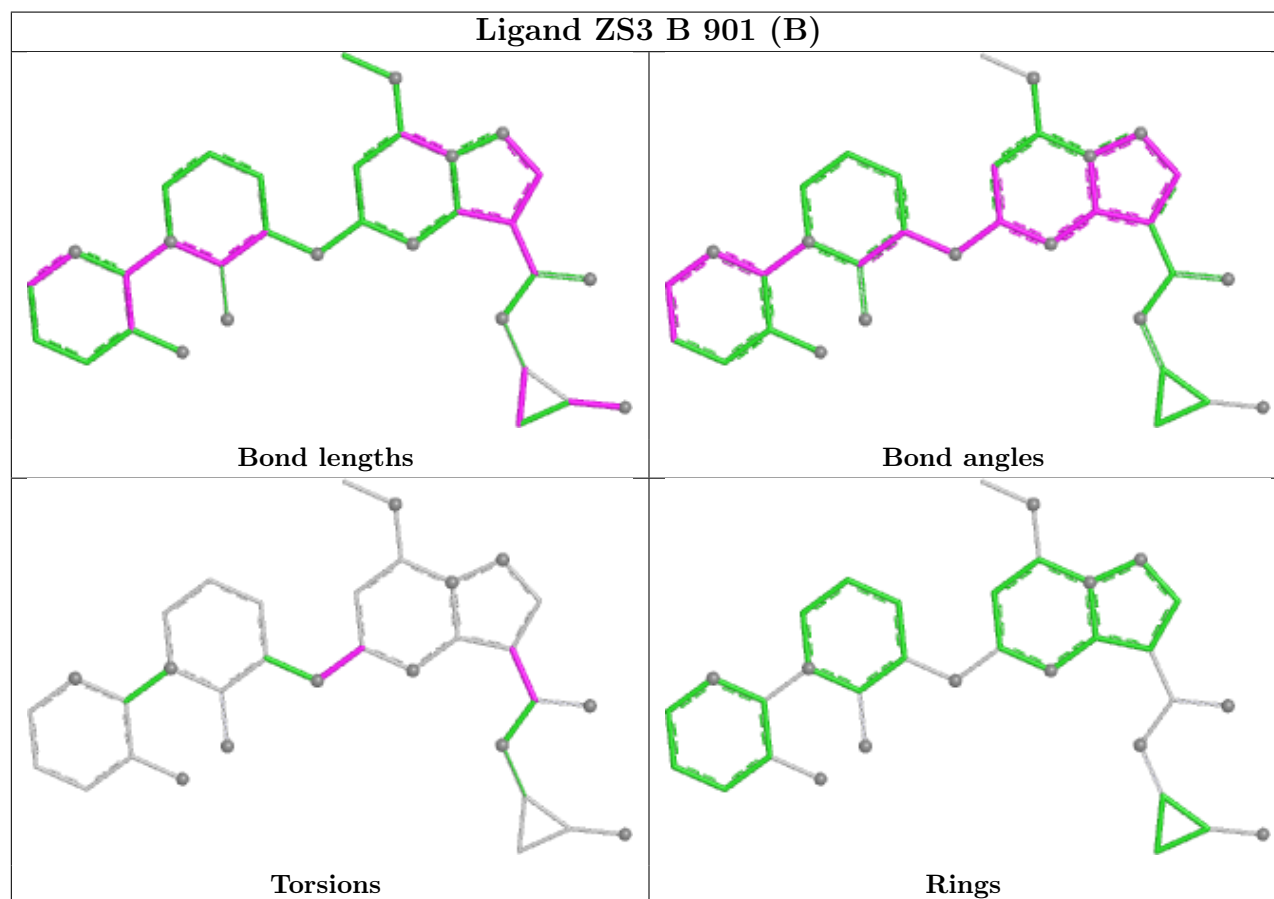
Mol	Chain	Res	Type	Atoms
2	A	901[B]	ZS3	C21-C22-C25-N27
2	B	901[B]	ZS3	C21-C22-C25-N27
2	C	901[B]	ZS3	C21-C22-C25-N27
3	B	903	EDO	O1-C1-C2-O2
2	A	901[A]	ZS3	N24-C14-N13-C12
2	A	901[B]	ZS3	N24-C14-N13-C12
2	B	901[A]	ZS3	N24-C14-N13-C12
2	B	901[B]	ZS3	N24-C14-N13-C12
2	C	901[A]	ZS3	N24-C14-N13-C12
2	C	901[B]	ZS3	N24-C14-N13-C12

There are no ring outliers.

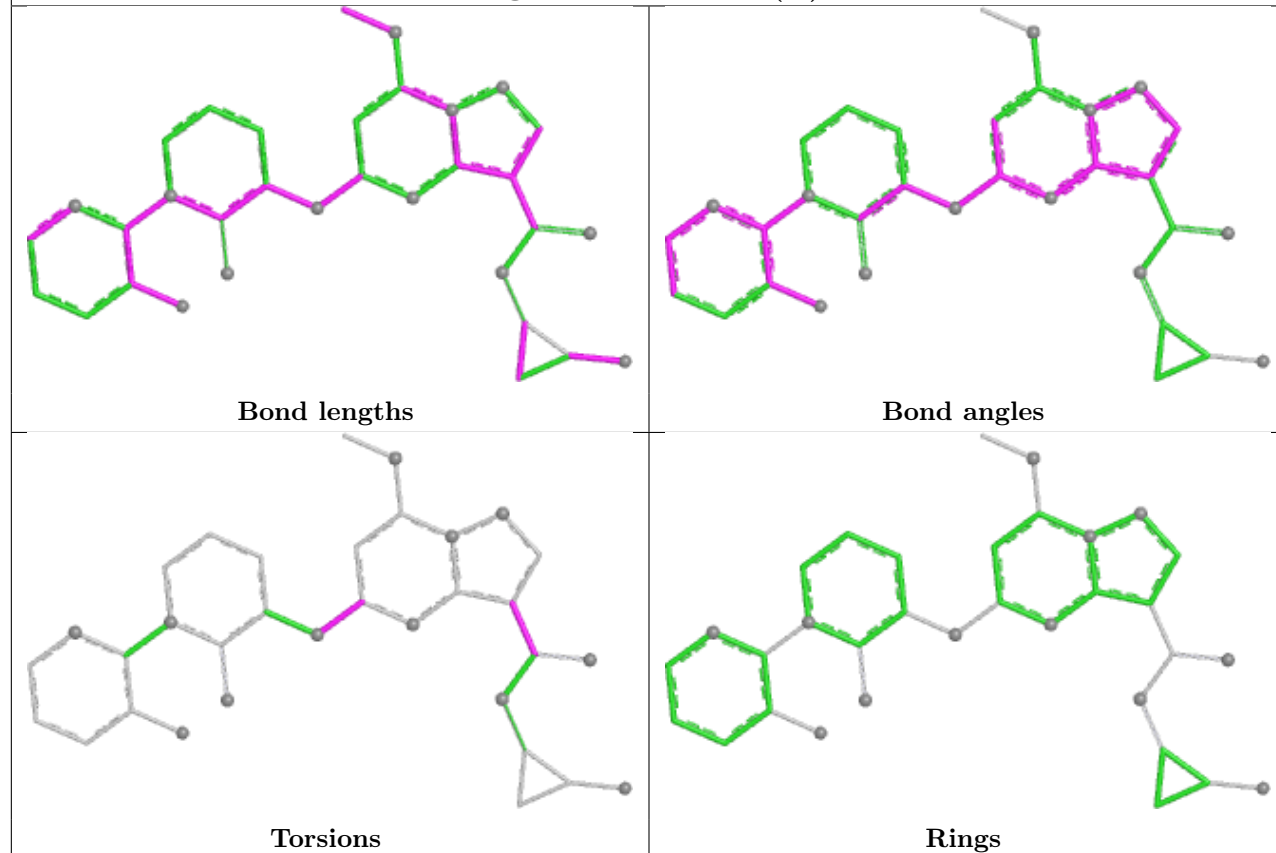
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901[A]	ZS3	1	0
2	A	901[A]	ZS3	1	0

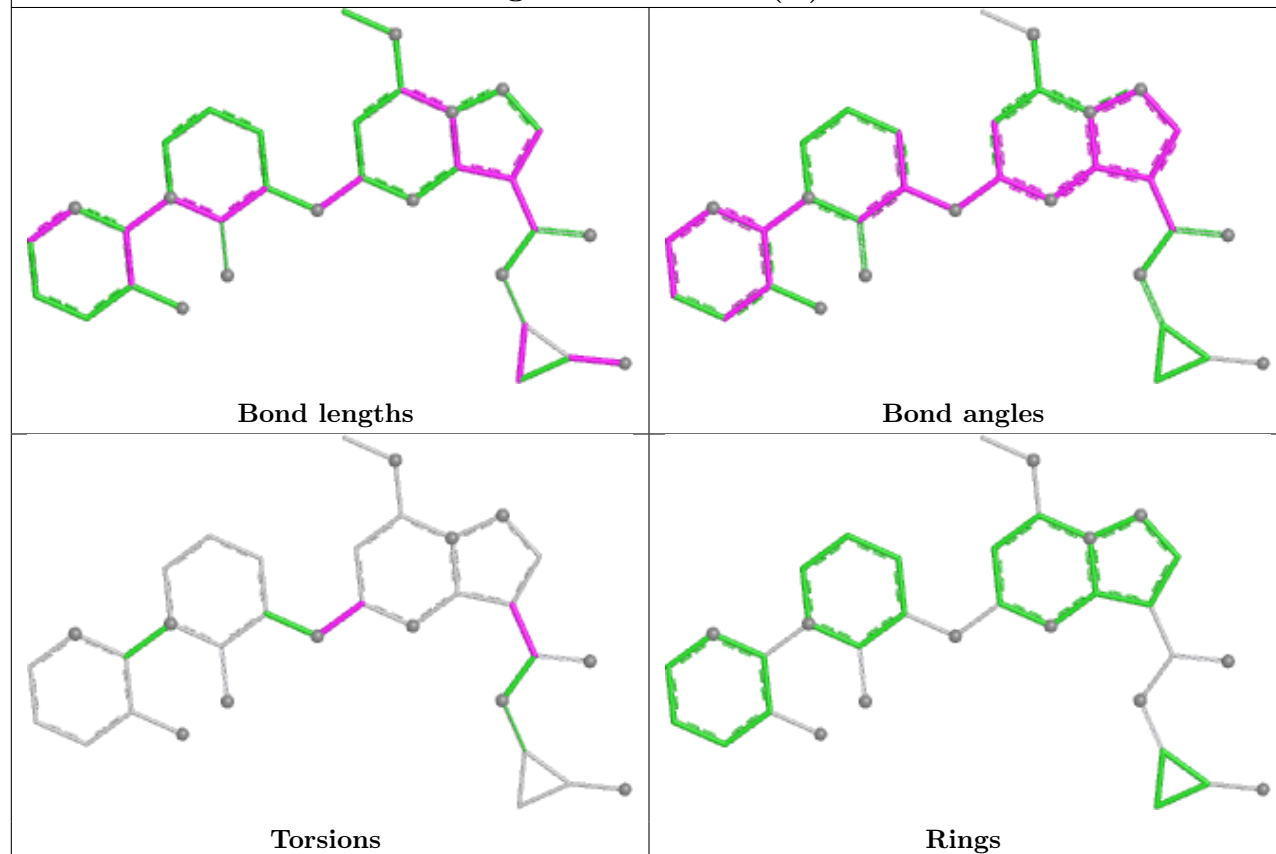
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



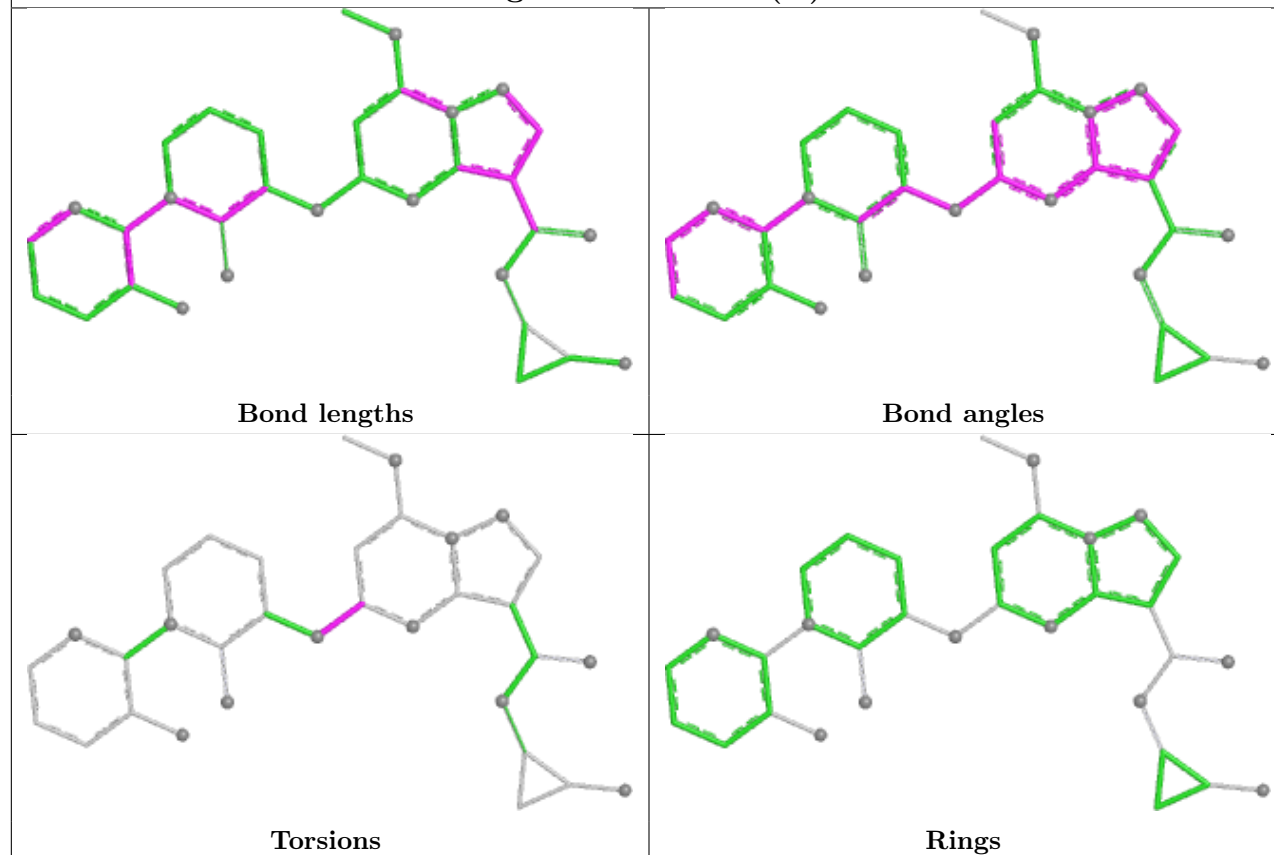
Ligand ZS3 A 901 (B)



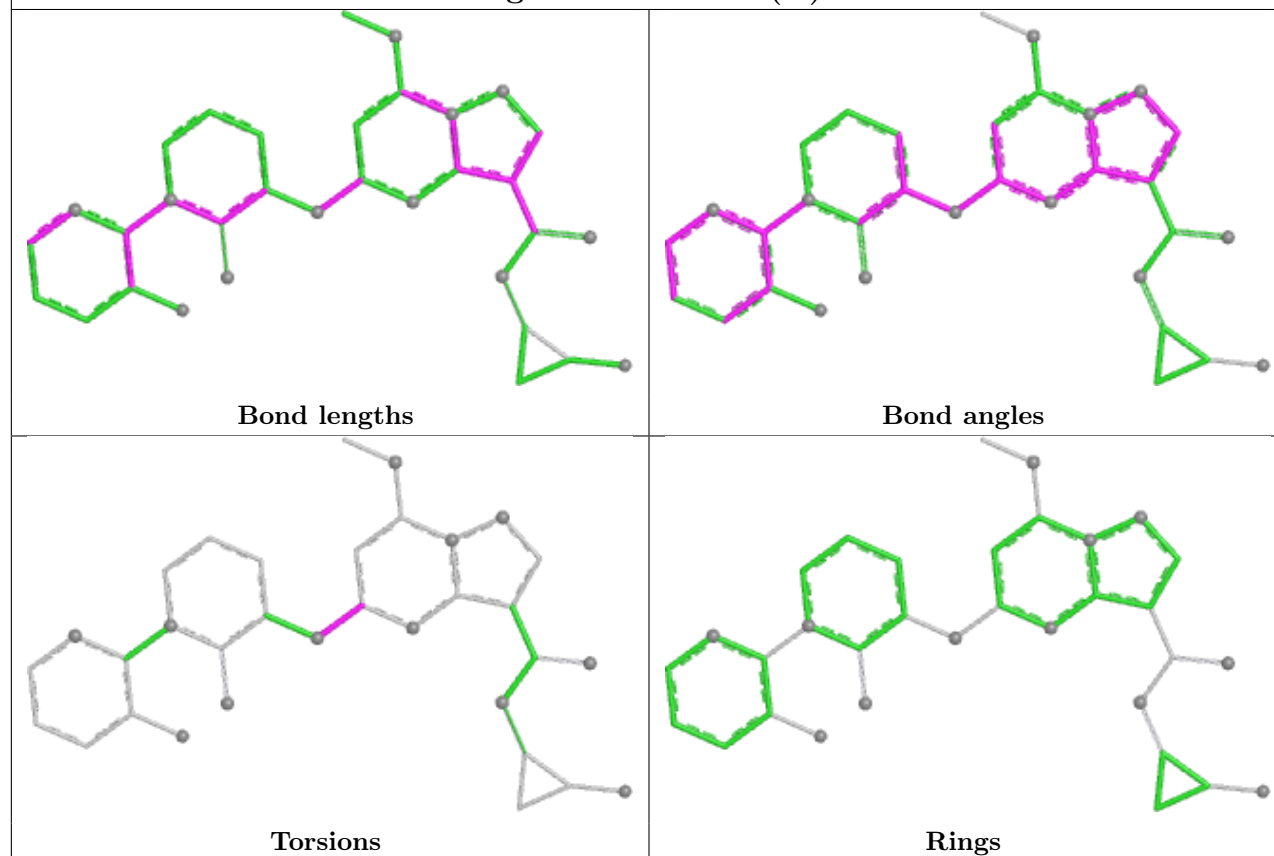
Ligand ZS3 C 901 (B)

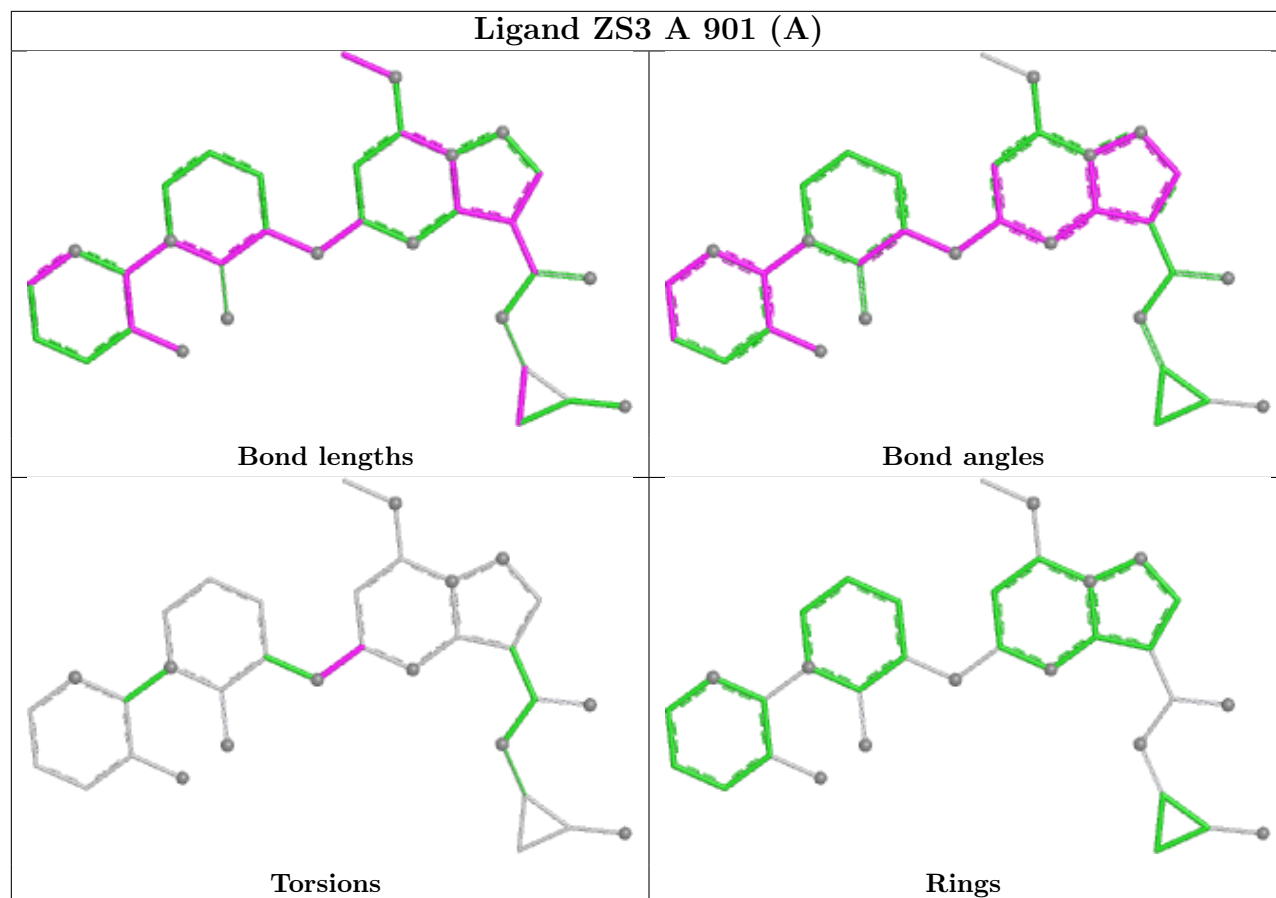


Ligand ZS3 B 901 (A)



Ligand ZS3 C 901 (A)





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	261/295 (88%)	0.35	23 (8%) 15 21	7, 20, 40, 60	20 (7%)
1	B	261/295 (88%)	0.34	18 (6%) 23 28	6, 20, 35, 53	20 (7%)
1	C	260/295 (88%)	0.20	16 (6%) 26 32	6, 19, 36, 61	17 (6%)
All	All	782/885 (88%)	0.29	57 (7%) 21 27	6, 20, 38, 61	57 (7%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	SER	5.9
1	B	791	LEU	5.5
1	B	839	PRO	5.0
1	A	837	SER	4.8
1	C	838	CYS	4.8
1	A	681	PRO	4.3
1	A	610	VAL	4.3
1	C	791	LEU	4.1
1	C	840	GLN	4.1
1	A	836	PRO	4.0
1	B	838	CYS	3.9
1	A	839	PRO	3.5
1	C	839	PRO	3.5
1	C	841	LEU	3.5
1	B	836	PRO	3.5
1	A	838	CYS	3.3
1	C	635	GLN	3.3
1	A	679	ARG	3.0
1	B	681	PRO	3.0
1	C	609	ARG	2.9
1	A	868	ARG	2.8
1	A	816	GLN	2.8
1	B	837	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	680	GLY	2.8
1	C	790	SER	2.8
1	B	840	GLN	2.8
1	A	812	GLU	2.7
1	A	680	GLY	2.7
1	B	610	VAL	2.7
1	C	816	GLN	2.7
1	B	747	LEU	2.7
1	A	649	HIS	2.6
1	A	579	LEU	2.5
1	A	678	VAL	2.5
1	B	750	GLY	2.5
1	C	750	GLY	2.5
1	A	809	PHE	2.5
1	B	841	LEU	2.5
1	A	814	PRO	2.4
1	B	817	SER	2.3
1	C	867	THR	2.3
1	A	813	ALA	2.3
1	A	705	HIS	2.3
1	A	840	GLN	2.3
1	A	609	ARG	2.3
1	B	790	SER	2.3
1	B	678	VAL	2.2
1	B	746	GLY	2.2
1	C	829[A]	ARG	2.2
1	B	587[A]	LYS	2.2
1	C	636	GLU	2.1
1	A	578	GLN	2.1
1	C	579	LEU	2.1
1	C	866	LEU	2.1
1	B	867	THR	2.1
1	C	833	LEU	2.0
1	A	587[A]	LYS	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](#)

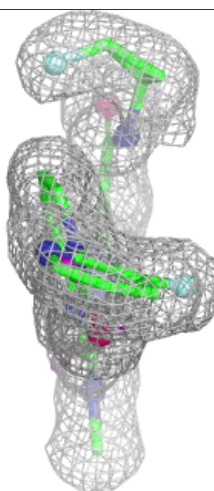
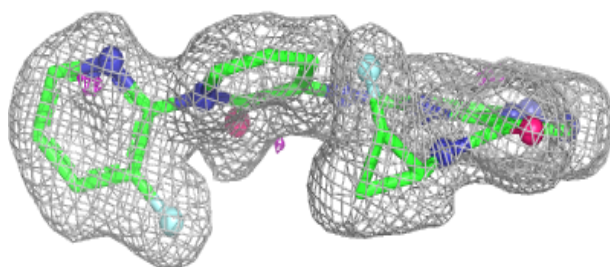
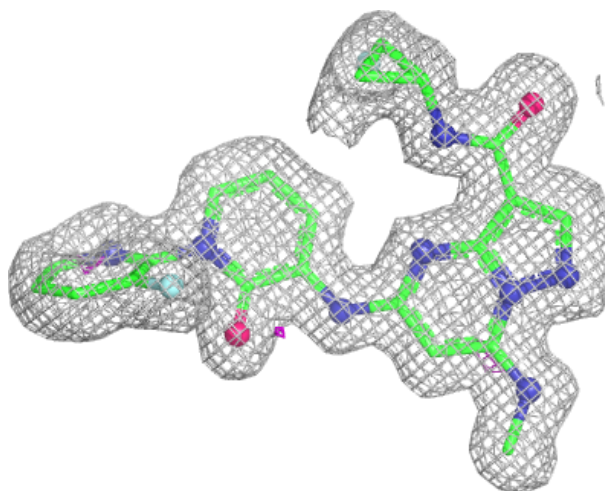
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	C	903	4/4	0.63	0.23	40,42,42,42	0
4	ACT	B	904	4/4	0.67	0.22	37,38,38,41	0
4	ACT	A	903	4/4	0.79	0.18	34,34,34,36	0
3	EDO	B	903	4/4	0.87	0.12	26,29,31,33	0
3	EDO	A	904	4/4	0.88	0.14	36,37,38,38	0
3	EDO	C	904	4/4	0.89	0.11	35,35,37,38	0
3	EDO	C	902	4/4	0.92	0.13	17,21,22,22	0
3	EDO	A	902	4/4	0.93	0.10	20,23,23,24	0
2	ZS3	B	901[B]	33/33	0.95	0.07	12,13,21,22	7
2	ZS3	A	901[A]	33/33	0.95	0.07	12,13,22,23	7
2	ZS3	A	901[B]	33/33	0.95	0.07	12,14,22,23	7
3	EDO	B	902	4/4	0.95	0.09	20,23,23,23	0
2	ZS3	B	901[A]	33/33	0.95	0.07	12,15,21,22	7
2	ZS3	C	901[B]	33/33	0.97	0.05	12,12,20,20	7
2	ZS3	C	901[A]	33/33	0.97	0.05	12,14,20,20	7

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.

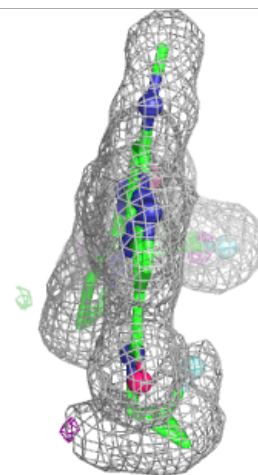
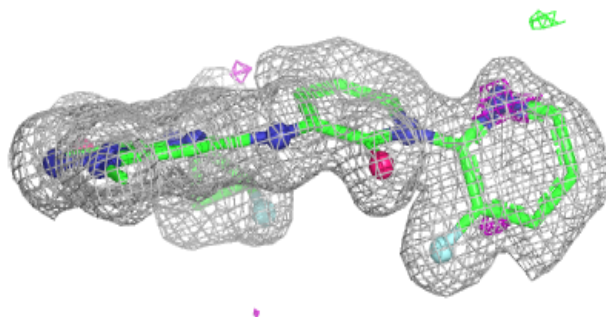
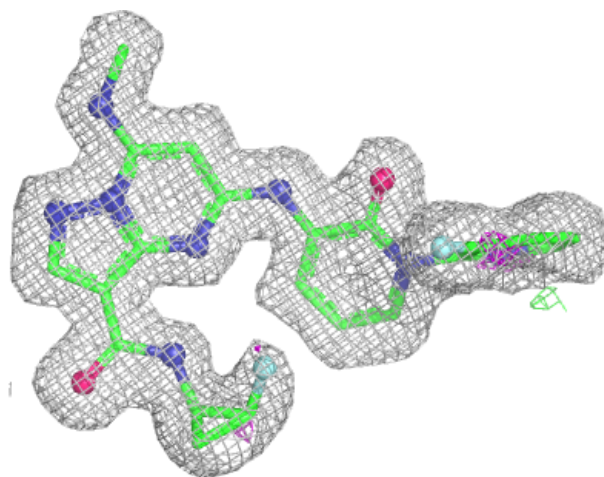
Electron density around ZS3 B 901 (B):

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



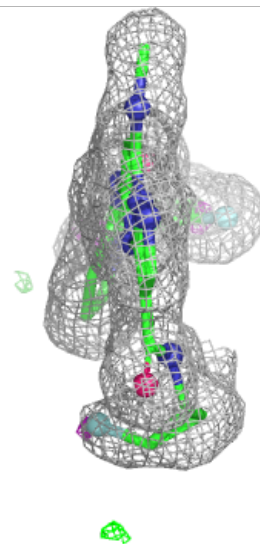
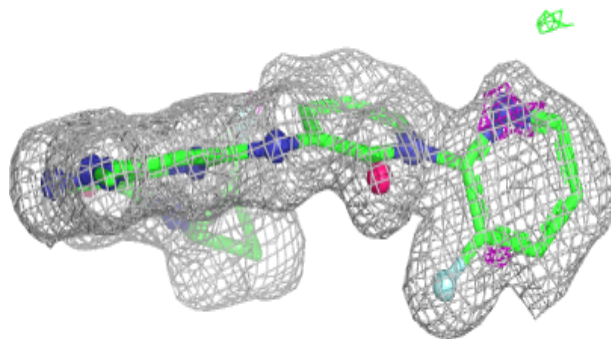
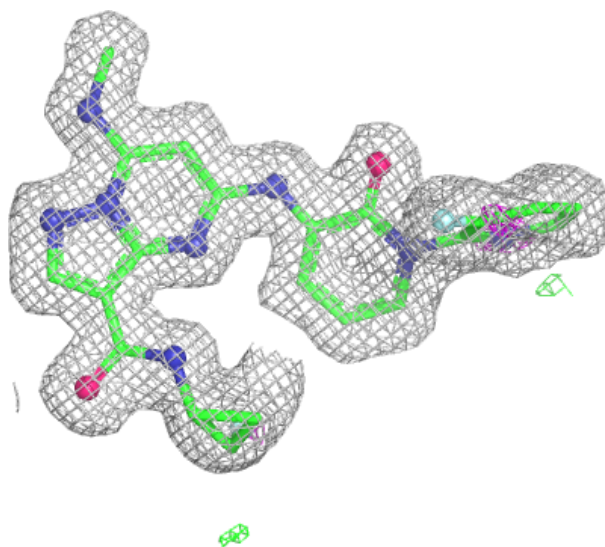
Electron density around ZS3 A 901 (A):

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



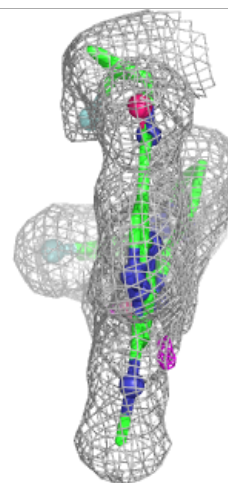
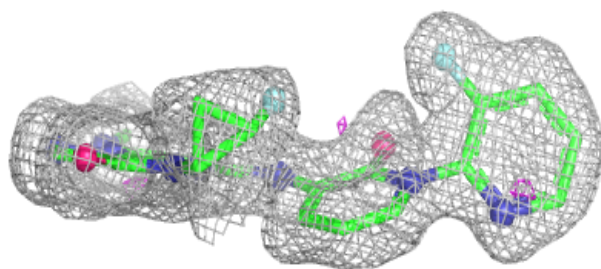
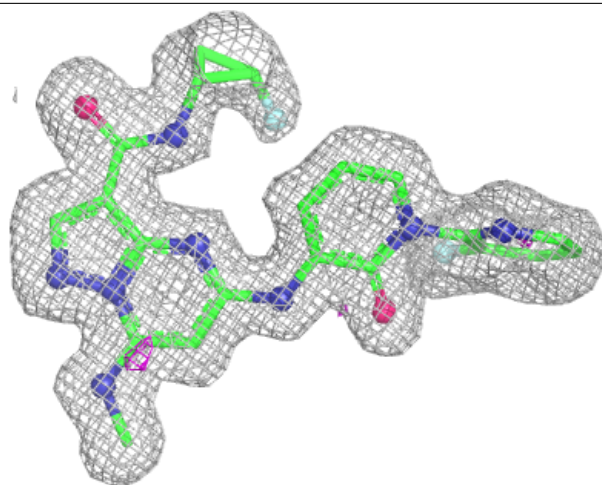
Electron density around ZS3 A 901 (B):

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



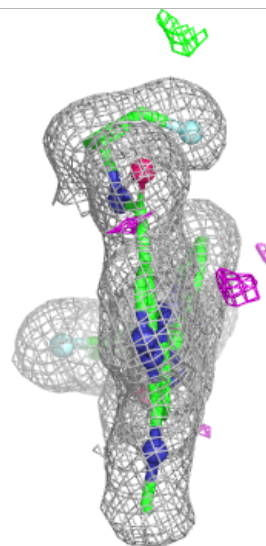
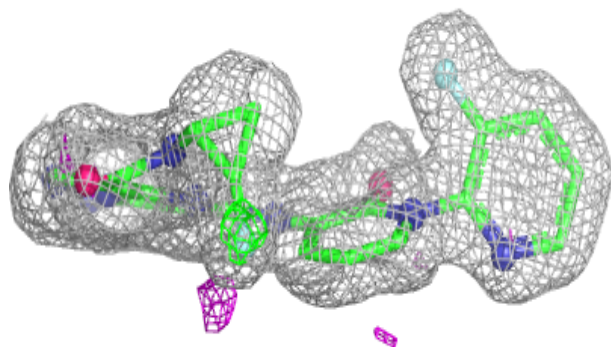
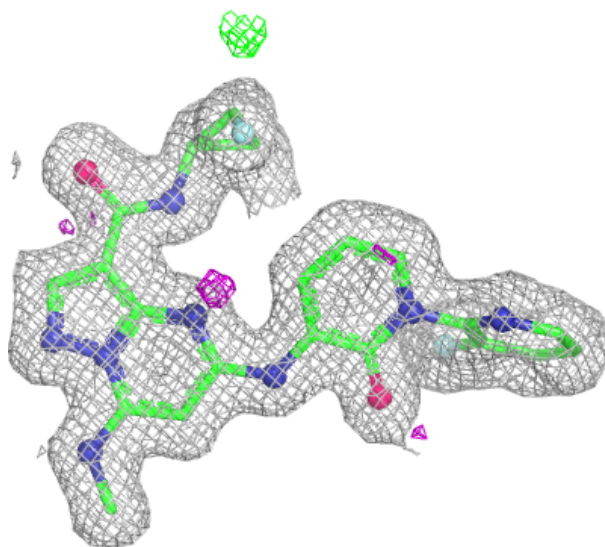
Electron density around ZS3 B 901 (A):

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



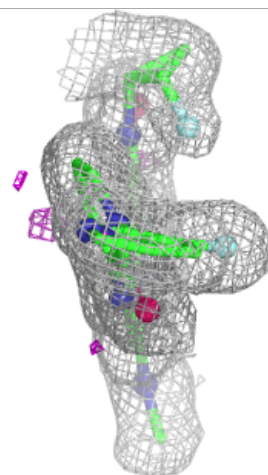
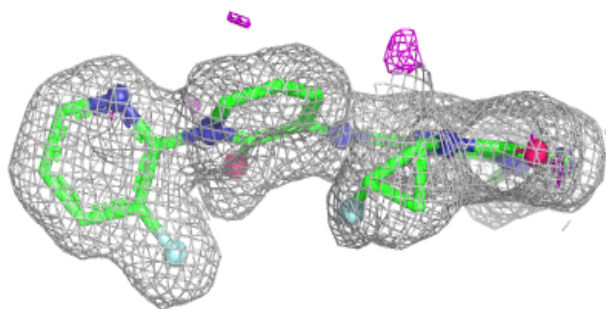
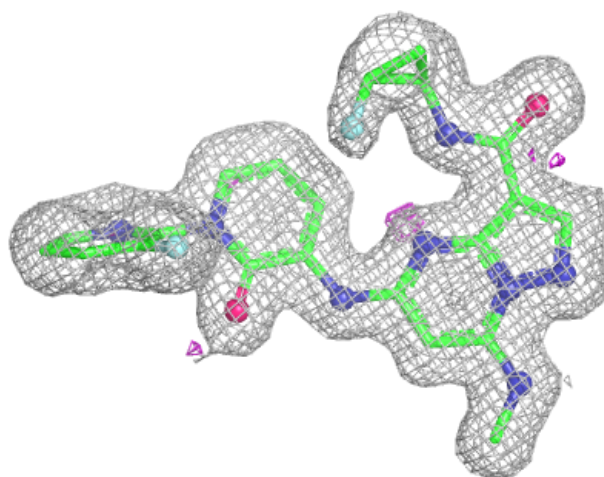
Electron density around ZS3 C 901 (B):

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



Electron density around ZS3 C 901 (A):

$2mF_o-DF_c$ (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.