



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:07 AM UTC

PDB ID : 3V5L / pdb_00003v5l
Title : Crystal Structure of Interleukin-2 Inducible T-cell Kinase Itk Catalytic Domain with Thienopyrazolylindole Inhibitor 542
Authors : McLean, L.R.; Zhang, Y.
Deposited on : 2011-12-16
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

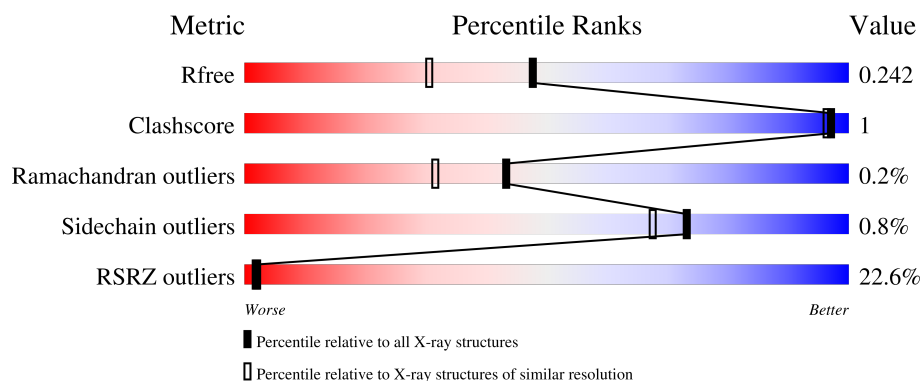
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	266	28% 88% • 10%
1	B	266	20% 89% • 9%
1	C	266	13% 87% 5% 8%
1	D	266	22% 86% 6% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8085 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.

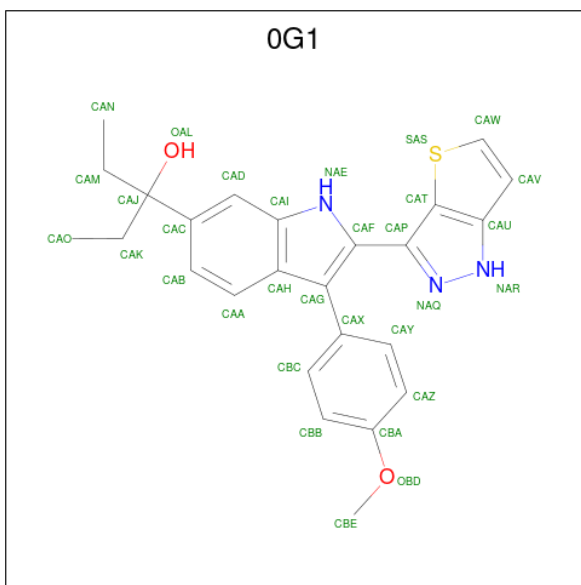
- Molecule 1 is a protein called Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1853	1193	306	338	16			
1	B	241	Total	C	N	O	S	0	0	0
			1860	1200	304	340	16			
1	C	244	Total	C	N	O	S	0	0	0
			1904	1223	316	348	17			
1	D	246	Total	C	N	O	S	0	0	0
			1915	1228	317	354	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	expression tag	UNP Q08881
A	356	SER	-	expression tag	UNP Q08881
B	355	GLY	-	expression tag	UNP Q08881
B	356	SER	-	expression tag	UNP Q08881
C	355	GLY	-	expression tag	UNP Q08881
C	356	SER	-	expression tag	UNP Q08881
D	355	GLY	-	expression tag	UNP Q08881
D	356	SER	-	expression tag	UNP Q08881

- Molecule 2 is 3-[3-(4-methoxyphenyl)-2-(1H-thieno[3,2-c]pyrazol-3-yl)-1H-indol-6-yl]pentan-3-ol (CCD ID: 0G1) (formula: C₂₅H₂₅N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	25	3	2	1		
2	B	1	Total	C	N	O	S	0	0
			31	25	3	2	1		
2	C	1	Total	C	N	O	S	0	0
			31	25	3	2	1		
2	D	1	Total	C	N	O	S	0	0
			31	25	3	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

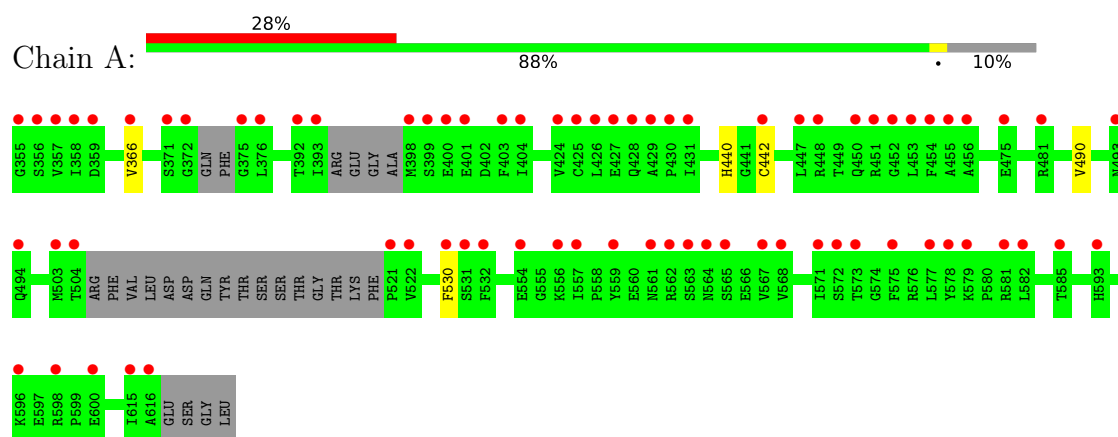
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	86	Total	O		0	0
			86	86			
4	B	119	Total	O		0	0
			119	119			
4	C	122	Total	O		0	0
			122	122			
4	D	97	Total	O		0	0
			97	97			

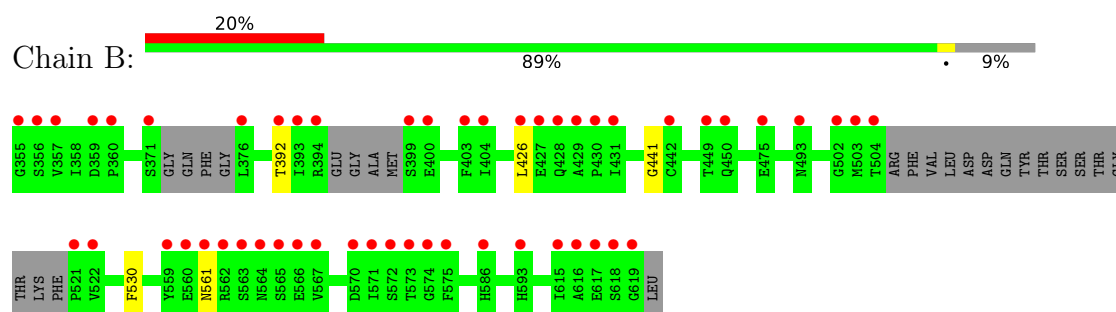
3 Residue-property plots [i](#)

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.

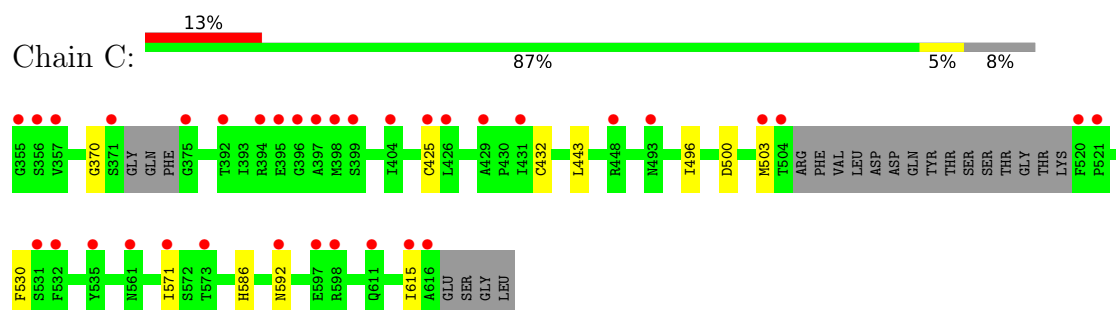
- Molecule 1: Tyrosine-protein kinase ITK/TSK



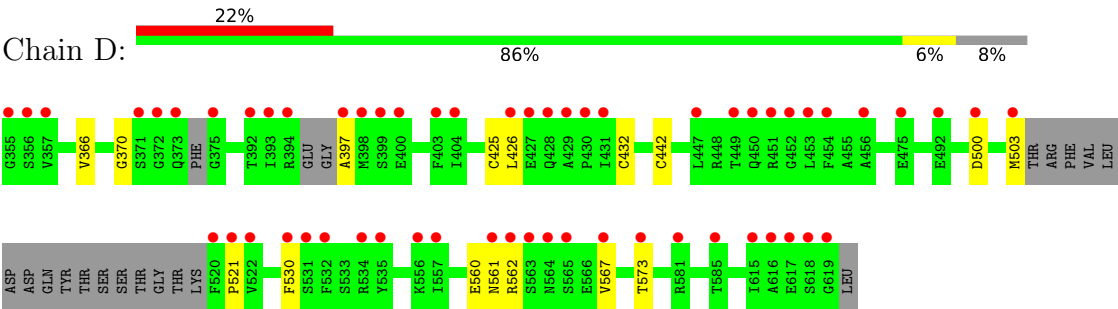
- Molecule 1: Tyrosine-protein kinase ITK/TSK



- Molecule 1: Tyrosine-protein kinase ITK/TSK



- Molecule 1: Tyrosine-protein kinase ITK/TSK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.97Å 68.91Å 140.03Å 90.00° 100.52° 90.00°	Depositor
Resolution (Å)	47.58 – 1.86 47.58 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.58-1.86) 98.7 (47.58-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.87Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.1, BUSTER 2.9.1	Depositor
R, R_{free}	0.232 , 0.252 (Not available) , 0.242	Depositor DCC
R_{free} test set	5316 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8085	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3986e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, OG1

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	0.70	0/1894	1.24	1/2561 (0.0%)
1	B	0.70	0/1901	1.23	3/2572 (0.1%)
1	C	0.68	0/1946	1.20	1/2631 (0.0%)
1	D	0.70	0/1956	1.24	3/2643 (0.1%)
All	All	0.70	0/7697	1.23	8/10407 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	PHE	CA-CB-CG	6.13	119.93	113.80
1	D	530	PHE	CA-CB-CG	6.09	119.89	113.80
1	C	530	PHE	CA-CB-CG	6.03	119.83	113.80
1	D	397	ALA	CA-C-N	6.02	132.53	121.70
1	D	397	ALA	C-N-CA	6.02	132.53	121.70
1	A	530	PHE	CA-CB-CG	5.71	119.51	113.80
1	B	441	GLY	CA-C-N	5.33	128.33	120.82
1	B	441	GLY	C-N-CA	5.33	128.33	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1853	0	1776	3	0
1	B	1860	0	1794	1	0
1	C	1904	0	1849	5	0
1	D	1915	0	1842	7	0
2	A	31	0	25	1	0
2	B	31	0	25	0	0
2	C	31	0	25	1	0
2	D	31	0	25	2	0
3	B	5	0	0	0	0
4	A	86	0	0	0	0
4	B	119	0	0	0	0
4	C	122	0	0	0	0
4	D	97	0	0	0	0
All	All	8085	0	7361	14	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 1.

All (14) 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:C:370:GLY:HA3	2:C:701:OG1:H6	1.93	0.50
1:D:500:ASP:HB3	1:D:503:MET:HE3	1.97	0.46
1:C:500:ASP:HB3	1:C:503:MET:HE3	1.98	0.45
1:C:425:CYS:HB3	1:C:432:CYS:SG	2.57	0.45
1:D:442:CYS:HB3	2:D:701:OG1:H4	1.99	0.44
1:D:370:GLY:HA3	2:D:701:OG1:H6	1.99	0.43
1:A:442:CYS:HB3	2:A:701:OG1:H4	2.01	0.43
1:B:561:ASN:HD22	1:D:573:THR:HG22	1.84	0.42
1:D:560:GLU:HA	1:D:561:ASN:HA	1.75	0.42
1:D:425:CYS:HB3	1:D:432:CYS:SG	2.60	0.41
1:A:440:HIS:HB2	1:A:490:VAL:HB	2.02	0.41
1:C:586:HIS:HB3	1:C:615:ILE:HD12	2.02	0.41
1:A:366:VAL:HG11	1:D:366:VAL:HG11	2.03	0.40
1:C:443:LEU:HD13	1:C:496:ILE:HD12	2.03	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	232/266 (87%)	227 (98%)	5 (2%)	0	100	100
1	B	233/266 (88%)	229 (98%)	4 (2%)	0	100	100
1	C	238/266 (90%)	235 (99%)	3 (1%)	0	100	100
1	D	238/266 (90%)	230 (97%)	6 (2%)	2 (1%)	16	6
All	All	941/1064 (88%)	921 (98%)	18 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	521	PRO
1	D	562	ARG

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	192/233 (82%)	192 (100%)	0	100	100
1	B	196/233 (84%)	194 (99%)	2 (1%)	68	60
1	C	202/233 (87%)	200 (99%)	2 (1%)	68	60
1	D	201/233 (86%)	199 (99%)	2 (1%)	68	60
All	All	791/932 (85%)	785 (99%)	6 (1%)	73	67

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

Mol	Chain	Res	Type
1	B	392	THR
1	B	426	LEU
1	C	571	ILE
1	C	592	ASN
1	D	426	LEU
1	D	567	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	GLN
1	A	384	ASN
1	A	440	HIS
1	A	592	ASN
1	B	378	HIS
1	B	384	ASN
1	B	440	HIS
1	B	561	ASN
1	B	589	GLN
1	B	592	ASN
1	C	384	ASN
1	D	593	HIS
1	D	611	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](#)

5 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	0G1	D	701	-	33,35,35	2.07	6 (18%)	45,52,52	2.14	10 (22%)
3	SO4	B	702	-	4,4,4	0.24	0	6,6,6	0.08	0
2	0G1	C	701	-	33,35,35	2.05	6 (18%)	45,52,52	2.14	11 (24%)
2	0G1	B	701	-	33,35,35	2.08	7 (21%)	45,52,52	2.12	10 (22%)
2	0G1	A	701	-	33,35,35	2.09	8 (24%)	45,52,52	2.16	11 (24%)

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	0G1	B	701	-	-	2/22/22/22	0/5/5/5
2	0G1	C	701	-	-	2/22/22/22	0/5/5/5
2	0G1	D	701	-	-	2/22/22/22	0/5/5/5
2	0G1	A	701	-	-	2/22/22/22	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	0G1	NAR-NAQ	-6.08	1.23	1.36
2	D	701	0G1	NAR-NAQ	-6.04	1.24	1.36
2	A	701	0G1	NAR-NAQ	-6.04	1.24	1.36
2	C	701	0G1	NAR-NAQ	-6.04	1.24	1.36
2	A	701	0G1	CAX-CAG	-5.83	1.39	1.49
2	D	701	0G1	CAX-CAG	-5.80	1.39	1.49
2	C	701	0G1	CAX-CAG	-5.77	1.39	1.49
2	B	701	0G1	CAX-CAG	-5.76	1.39	1.49
2	A	701	0G1	CAV-CAU	-3.87	1.35	1.43
2	D	701	0G1	CAV-CAU	-3.85	1.35	1.43
2	C	701	0G1	CAV-CAU	-3.83	1.35	1.43
2	B	701	0G1	CAV-CAU	-3.81	1.35	1.43
2	B	701	0G1	CAH-CAG	-3.67	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	0G1	CAH-CAG	-3.66	1.39	1.47
2	D	701	0G1	CAH-CAG	-3.63	1.39	1.47
2	C	701	0G1	CAH-CAG	-3.59	1.39	1.47
2	A	701	0G1	CAF-NAE	-2.99	1.34	1.38
2	A	701	0G1	CAI-NAE	-2.94	1.33	1.38
2	B	701	0G1	CAF-NAE	-2.93	1.34	1.38
2	C	701	0G1	CAF-NAE	-2.85	1.34	1.38
2	D	701	0G1	CAI-NAE	-2.83	1.33	1.38
2	B	701	0G1	CAI-NAE	-2.82	1.33	1.38
2	C	701	0G1	CAI-NAE	-2.69	1.33	1.38
2	D	701	0G1	CAF-NAE	-2.69	1.34	1.38
2	B	701	0G1	CAT-SAS	-2.28	1.69	1.72
2	A	701	0G1	CAJ-CAC	2.09	1.55	1.53
2	A	701	0G1	CAT-SAS	-2.03	1.69	1.72

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	0G1	CAU-CAT-SAS	-6.51	105.36	110.78
2	D	701	0G1	CAU-CAT-SAS	-6.41	105.44	110.78
2	A	701	0G1	CAU-CAT-SAS	-6.30	105.54	110.78
2	B	701	0G1	CAU-CAT-SAS	-6.18	105.63	110.78
2	A	701	0G1	CAW-SAS-CAT	5.53	97.04	91.38
2	A	701	0G1	CAW-CAV-CAU	5.48	116.86	111.14
2	B	701	0G1	CAW-SAS-CAT	5.48	96.98	91.38
2	D	701	0G1	CAW-SAS-CAT	5.46	96.96	91.38
2	C	701	0G1	CAW-CAV-CAU	5.41	116.79	111.14
2	D	701	0G1	CAW-CAV-CAU	5.35	116.73	111.14
2	C	701	0G1	CAW-SAS-CAT	5.34	96.84	91.38
2	B	701	0G1	CAW-CAV-CAU	5.16	116.52	111.14
2	C	701	0G1	CAG-CAF-NAE	-4.47	106.50	109.80
2	D	701	0G1	CAG-CAF-NAE	-4.36	106.58	109.80
2	A	701	0G1	CAG-CAF-NAE	-4.34	106.60	109.80
2	B	701	0G1	CAG-CAF-NAE	-4.10	106.77	109.80
2	D	701	0G1	CAP-NAQ-NAR	3.99	111.69	104.90
2	A	701	0G1	CAP-NAQ-NAR	3.96	111.64	104.90
2	C	701	0G1	CAP-NAQ-NAR	3.96	111.63	104.90
2	B	701	0G1	CAP-NAQ-NAR	3.81	111.39	104.90
2	B	701	0G1	CBE-OB-D-CBA	-3.76	109.44	117.50
2	A	701	0G1	CAV-CAW-SAS	-3.54	106.52	112.86
2	C	701	0G1	CBE-OB-D-CBA	-3.51	109.98	117.50
2	D	701	0G1	CAV-CAW-SAS	-3.47	106.64	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	0G1	CAV-CAW-SAS	-3.47	106.65	112.86
2	A	701	0G1	CBE-OBDB-CBA	-3.43	110.13	117.50
2	C	701	0G1	CAV-CAW-SAS	-3.39	106.79	112.86
2	C	701	0G1	CAT-CAP-NAQ	-3.13	105.74	111.52
2	D	701	0G1	CAT-CAP-NAQ	-3.12	105.76	111.52
2	A	701	0G1	CAT-CAP-NAQ	-3.10	105.80	111.52
2	D	701	0G1	CBE-OBDB-CBA	-3.10	110.86	117.50
2	B	701	0G1	CAT-CAP-NAQ	-3.09	105.81	111.52
2	D	701	0G1	CAD-CAI-CAH	-3.08	120.06	122.52
2	B	701	0G1	CAH-CAG-CAF	3.08	107.68	106.06
2	A	701	0G1	CAH-CAG-CAF	3.07	107.68	106.06
2	B	701	0G1	CAD-CAI-CAH	-3.07	120.07	122.52
2	A	701	0G1	CAD-CAI-CAH	-3.04	120.09	122.52
2	C	701	0G1	CAD-CAI-CAH	-2.99	120.14	122.52
2	D	701	0G1	CAH-CAG-CAF	2.89	107.59	106.06
2	C	701	0G1	CAH-CAG-CAF	2.76	107.52	106.06
2	C	701	0G1	CAI-NAE-CAF	2.25	111.47	109.00
2	A	701	0G1	CAI-NAE-CAF	2.07	111.27	109.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	0G1	CAZ-CBA-OBDB-CBE
2	B	701	0G1	CBB-CBA-OBDB-CBE
2	B	701	0G1	CAZ-CBA-OBDB-CBE
2	A	701	0G1	CBB-CBA-OBDB-CBE
2	C	701	0G1	CBB-CBA-OBDB-CBE
2	C	701	0G1	CAZ-CBA-OBDB-CBE
2	D	701	0G1	CBB-CBA-OBDB-CBE
2	D	701	0G1	CAZ-CBA-OBDB-CBE

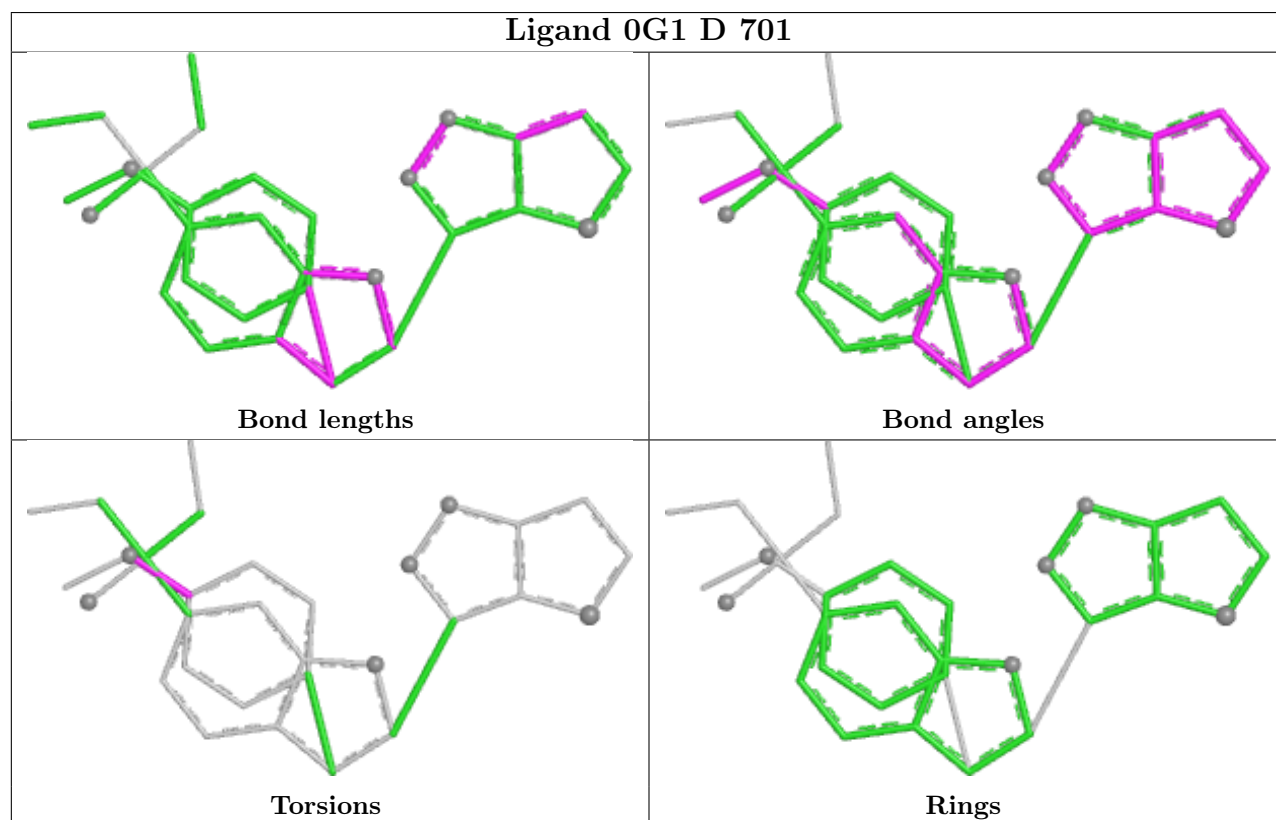
There are no ring outliers.

3 monomers are involved in 4 short contacts:

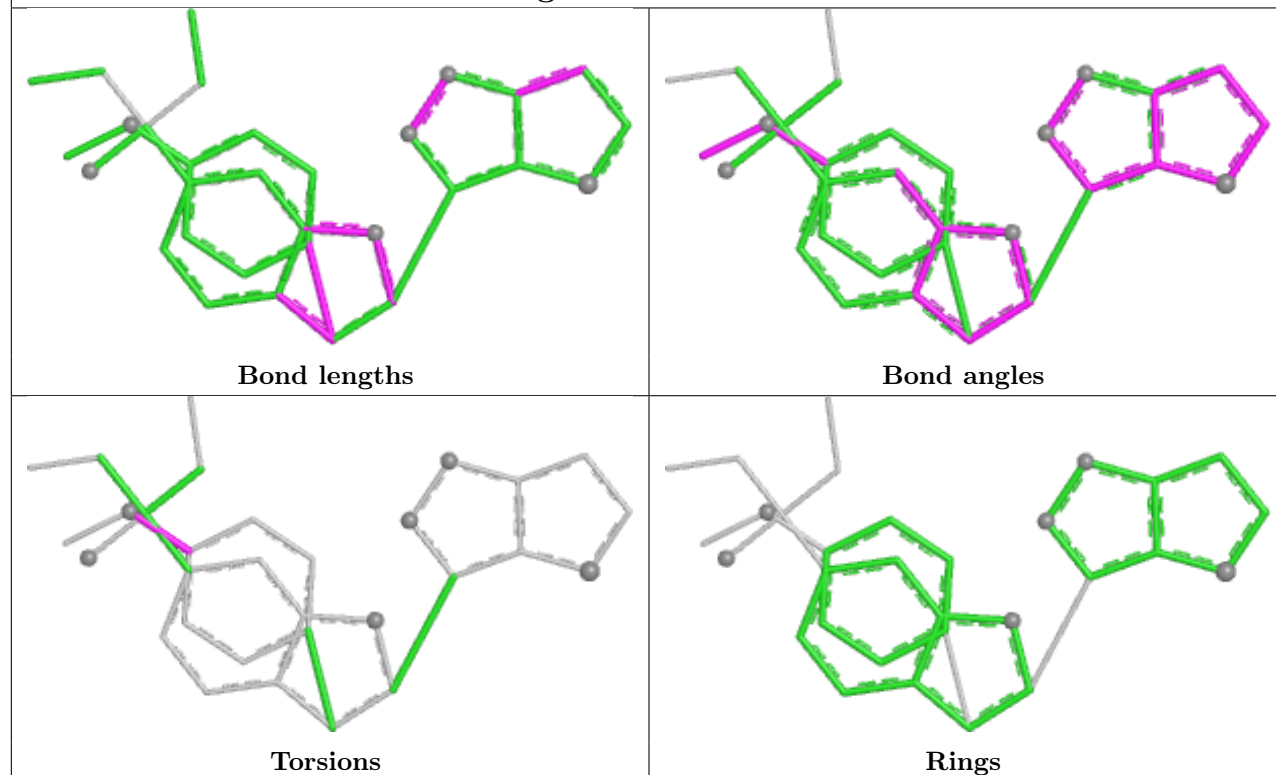
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	0G1	2	0
2	C	701	0G1	1	0
2	A	701	0G1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

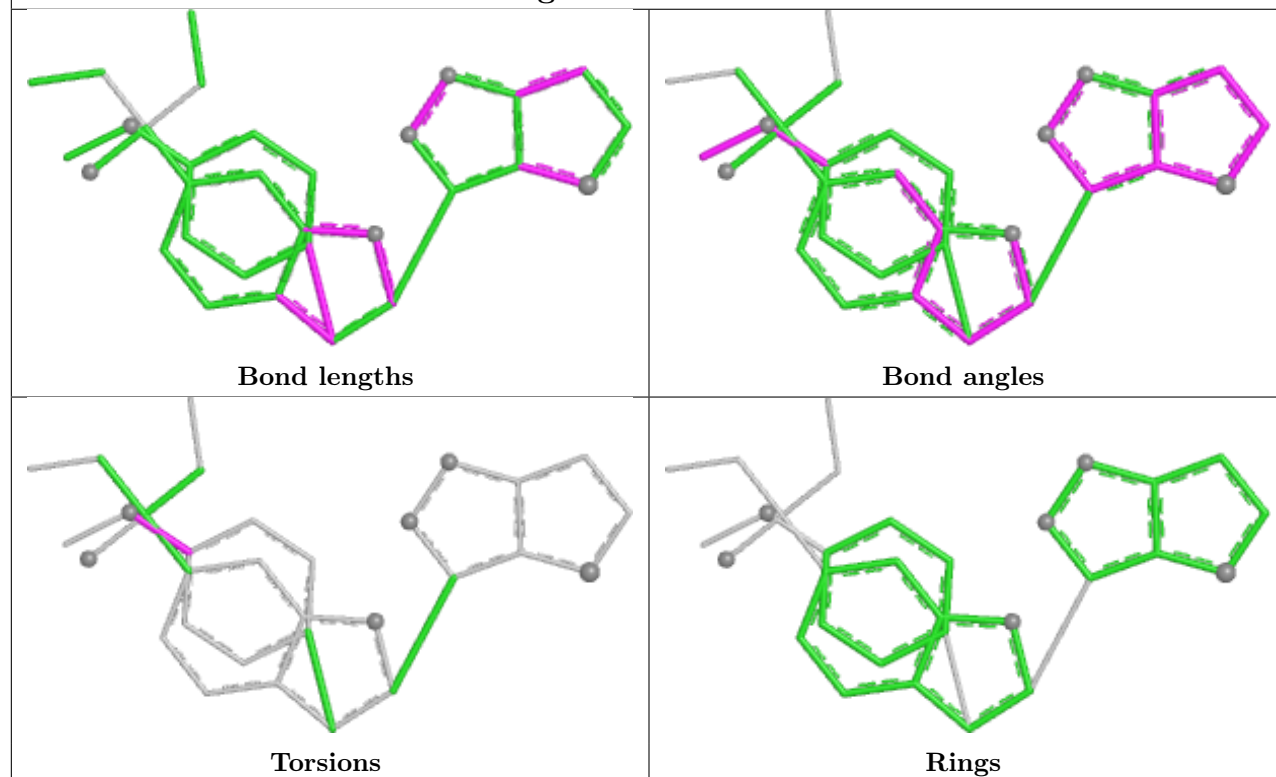
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

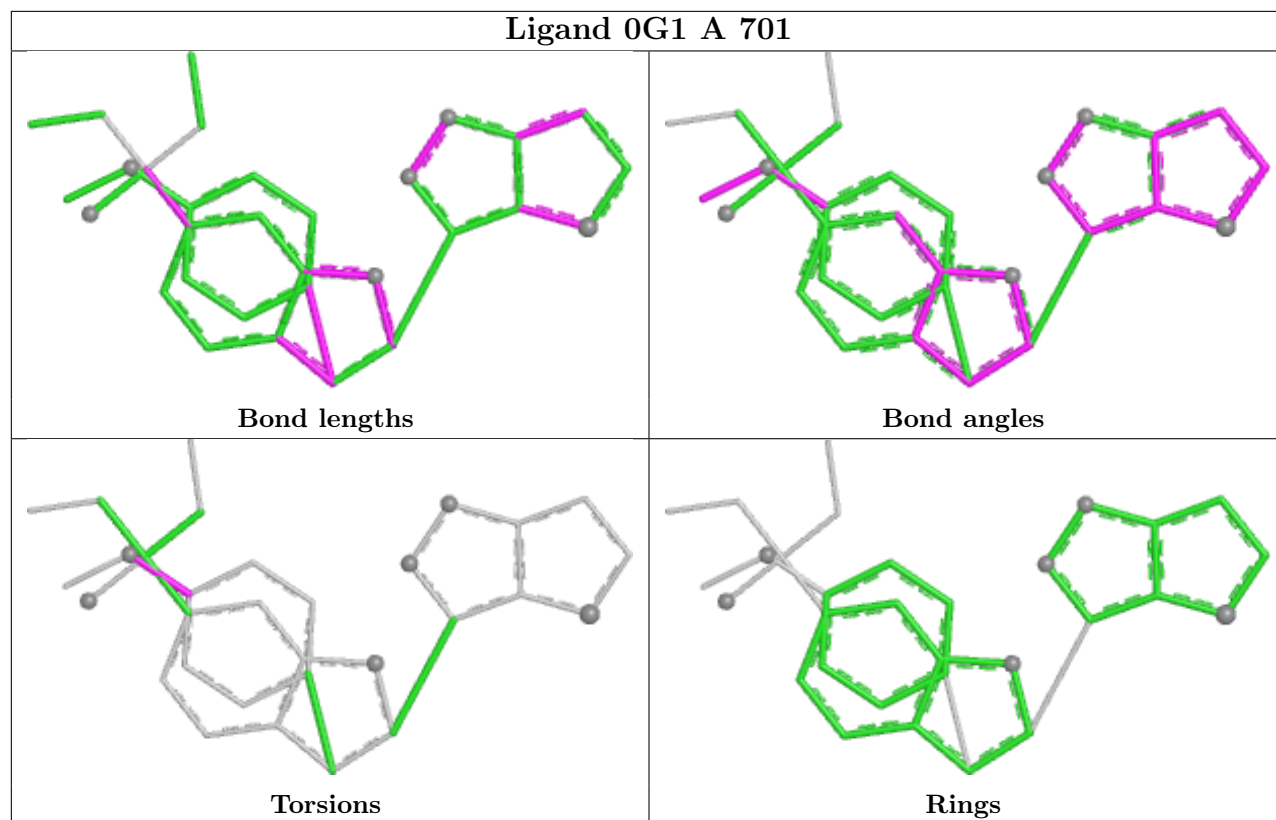


Ligand 0G1 C 701



Ligand 0G1 B 701





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	240/266 (90%)	1.42	74 (30%) 1 1	16, 30, 50, 69	0
1	B	241/266 (90%)	1.05	52 (21%) 2 2	13, 25, 46, 65	0
1	C	244/266 (91%)	0.85	35 (14%) 6 6	12, 23, 41, 64	0
1	D	246/266 (92%)	1.35	58 (23%) 2 1	14, 28, 47, 71	0
All	All	971/1064 (91%)	1.17	219 (22%) 2 2	12, 27, 47, 71	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	THR	9.3
1	D	520	PHE	8.9
1	B	504	THR	8.7
1	B	619	GLY	7.9
1	A	616	ALA	7.6
1	C	504	THR	7.5
1	C	616	ALA	7.3
1	A	393	ILE	7.2
1	D	394	ARG	7.2
1	A	372	GLY	6.5
1	D	397	ALA	6.4
1	D	373	GLN	6.3
1	D	561	ASN	6.1
1	D	521	PRO	6.0
1	A	429	ALA	6.0
1	C	520	PHE	5.8
1	A	521	PRO	5.7
1	D	355	GLY	5.6
1	D	503	MET	5.6
1	C	396	GLY	5.4
1	D	619	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	618	SER	5.4
1	B	429	ALA	5.3
1	B	575	PHE	5.1
1	A	355	GLY	5.0
1	C	371	SER	5.0
1	C	397	ALA	4.8
1	B	371	SER	4.7
1	C	355	GLY	4.7
1	D	356	SER	4.7
1	B	573	THR	4.6
1	A	561	ASN	4.5
1	B	394	ARG	4.5
1	B	521	PRO	4.5
1	B	355	GLY	4.4
1	A	426	LEU	4.4
1	A	427	GLU	4.4
1	B	567	VAL	4.3
1	D	617	GLU	4.3
1	D	372	GLY	4.3
1	A	356	SER	4.2
1	C	521	PRO	4.2
1	A	428	GLN	4.1
1	C	394	ARG	4.1
1	B	427	GLU	4.1
1	B	617	GLU	4.1
1	A	573	THR	4.0
1	B	565	SER	3.8
1	D	429	ALA	3.8
1	A	451	ARG	3.8
1	D	565	SER	3.7
1	D	556	LYS	3.7
1	B	399	SER	3.7
1	D	453	LEU	3.7
1	D	563	SER	3.7
1	D	562	ARG	3.7
1	B	426	LEU	3.6
1	D	426	LEU	3.6
1	A	581	ARG	3.6
1	A	564	ASN	3.5
1	A	565	SER	3.5
1	A	522	VAL	3.5
1	D	357	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	430	PRO	3.5
1	A	357	VAL	3.4
1	A	398	MET	3.4
1	A	567	VAL	3.4
1	C	395	GLU	3.4
1	B	404	ILE	3.4
1	B	571	ILE	3.4
1	A	456	ALA	3.4
1	B	561	ASN	3.4
1	B	393	ILE	3.3
1	A	450	GLN	3.3
1	A	455	ALA	3.3
1	A	403	PHE	3.3
1	A	494	GLN	3.3
1	D	451	ARG	3.3
1	C	356	SER	3.3
1	A	493	ASN	3.2
1	A	431	ILE	3.2
1	B	431	ILE	3.2
1	C	573	THR	3.2
1	D	454	PHE	3.2
1	C	615	ILE	3.1
1	D	564	ASN	3.1
1	B	503	MET	3.1
1	D	616	ALA	3.1
1	D	428	GLN	3.1
1	A	571	ILE	3.1
1	B	357	VAL	3.1
1	D	398	MET	3.1
1	C	448	ARG	3.1
1	D	534	ARG	3.1
1	A	371	SER	3.0
1	D	618	SER	3.0
1	B	493	ASN	3.0
1	C	561	ASN	3.0
1	B	562	ARG	3.0
1	A	503	MET	3.0
1	B	616	ALA	3.0
1	D	393	ILE	3.0
1	C	357	VAL	2.9
1	B	615	ILE	2.9
1	C	503	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	375	GLY	2.9
1	B	403	PHE	2.9
1	A	400	GLU	2.9
1	D	427	GLU	2.9
1	B	392	THR	2.8
1	D	532	PHE	2.8
1	D	522	VAL	2.8
1	C	532	PHE	2.8
1	D	371	SER	2.8
1	A	557	ILE	2.8
1	B	400	GLU	2.8
1	C	592	ASN	2.8
1	D	456	ALA	2.7
1	A	375	GLY	2.7
1	A	453	LEU	2.7
1	D	430	PRO	2.7
1	A	399	SER	2.7
1	B	563	SER	2.7
1	A	452	GLY	2.6
1	C	429	ALA	2.6
1	A	562	ARG	2.6
1	C	392	THR	2.6
1	C	426	LEU	2.6
1	A	404	ILE	2.6
1	A	572	SER	2.6
1	B	564	ASN	2.6
1	D	567	VAL	2.6
1	B	586	HIS	2.5
1	C	598	ARG	2.5
1	D	399	SER	2.5
1	B	449	THR	2.5
1	D	585	THR	2.5
1	A	447	LEU	2.5
1	A	582	LEU	2.5
1	D	452	GLY	2.5
1	A	593	HIS	2.5
1	C	399	SER	2.5
1	A	392	THR	2.5
1	D	392	THR	2.5
1	D	449	THR	2.5
1	B	430	PRO	2.5
1	C	597	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	600	GLU	2.4
1	B	442	CYS	2.4
1	D	531	SER	2.4
1	B	428	GLN	2.4
1	C	375	GLY	2.4
1	C	531	SER	2.4
1	D	447	LEU	2.4
1	B	559	TYR	2.4
1	D	535	TYR	2.4
1	A	532	PHE	2.4
1	D	615	ILE	2.4
1	D	403	PHE	2.3
1	B	475	GLU	2.3
1	B	502	GLY	2.3
1	B	356	SER	2.3
1	D	492	GLU	2.3
1	A	578	TYR	2.3
1	B	593	HIS	2.3
1	C	493	ASN	2.3
1	D	581	ARG	2.3
1	D	400	GLU	2.3
1	C	611	GLN	2.3
1	A	585	THR	2.3
1	A	454	PHE	2.3
1	A	556	LYS	2.3
1	D	530	PHE	2.2
1	A	596	LYS	2.2
1	A	598	ARG	2.2
1	B	360	PRO	2.2
1	D	557	ILE	2.2
1	A	475	GLU	2.2
1	B	376	LEU	2.2
1	B	572	SER	2.2
1	A	559	TYR	2.2
1	C	431	ILE	2.2
1	C	571	ILE	2.2
1	D	404	ILE	2.2
1	A	366	VAL	2.2
1	B	574	GLY	2.2
1	A	554	GLU	2.1
1	D	475	GLU	2.1
1	A	615	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	404	ILE	2.1
1	B	450	GLN	2.1
1	A	359	ASP	2.1
1	D	573	THR	2.1
1	A	442	CYS	2.1
1	A	376	LEU	2.1
1	A	575	PHE	2.1
1	D	450	GLN	2.1
1	A	579	LYS	2.1
1	B	560	GLU	2.1
1	B	566	GLU	2.1
1	C	398	MET	2.1
1	C	425	CYS	2.1
1	A	358	ILE	2.1
1	A	577	LEU	2.1
1	B	359	ASP	2.1
1	B	570	ASP	2.1
1	A	530	PHE	2.0
1	A	531	SER	2.0
1	D	431	ILE	2.0
1	C	535	TYR	2.0
1	A	568	VAL	2.0
1	B	522	VAL	2.0
1	A	425	CYS	2.0
1	A	448	ARG	2.0
1	A	481	ARG	2.0
1	D	500	ASP	2.0
1	A	401	GLU	2.0
1	A	563	SER	2.0
1	A	424	VAL	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 ⓘ

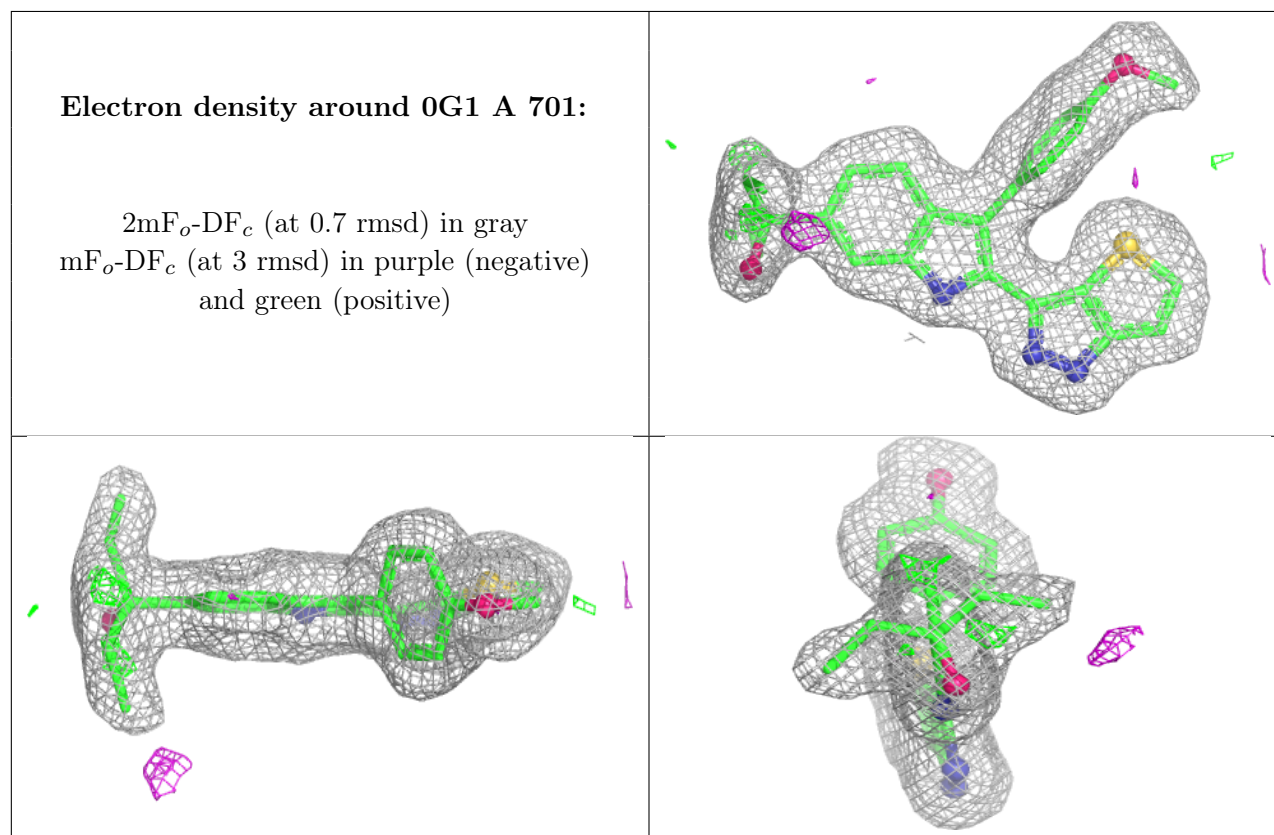
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

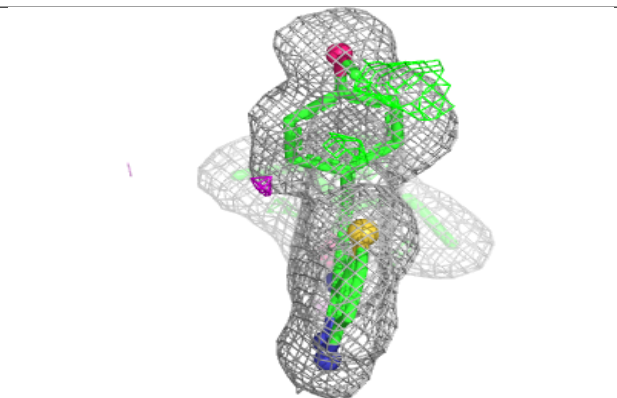
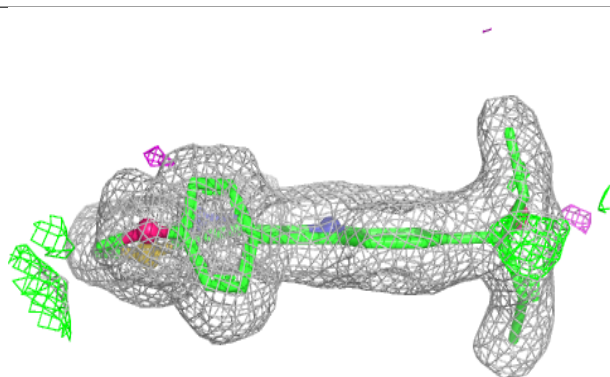
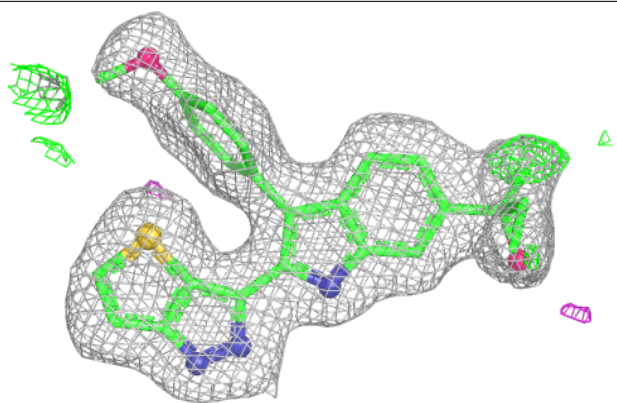
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	0G1	A	701	31/31	0.94	0.10	16,24,37,43	0
2	0G1	B	701	31/31	0.96	0.09	13,18,40,58	0
2	0G1	D	701	31/31	0.96	0.09	14,21,35,66	0
2	0G1	C	701	31/31	0.97	0.09	11,17,36,99	0
3	SO4	B	702	5/5	0.98	0.06	24,29,29,30	0

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.

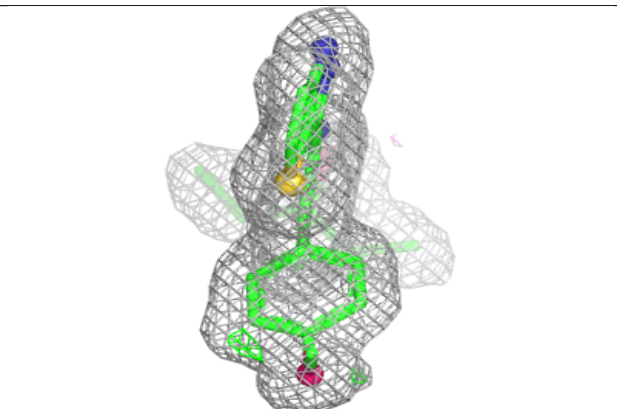
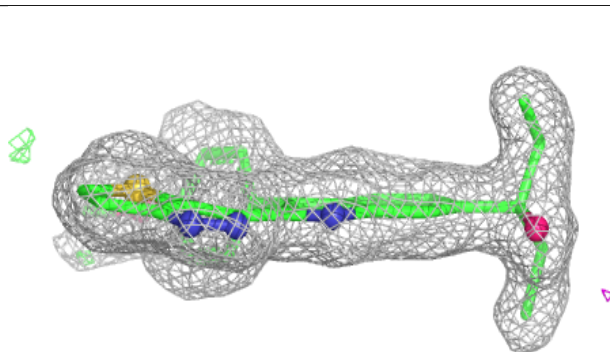
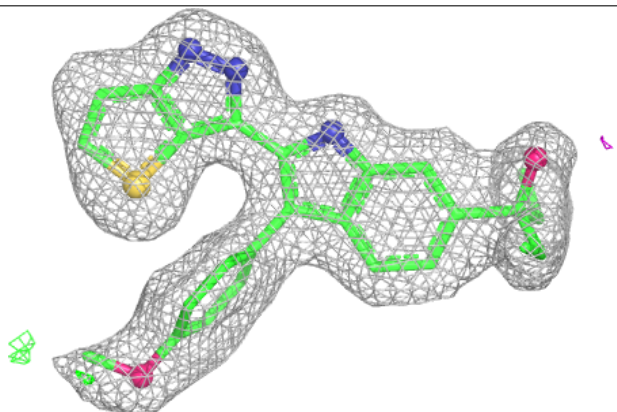


Electron density around 0G1 B 701:

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

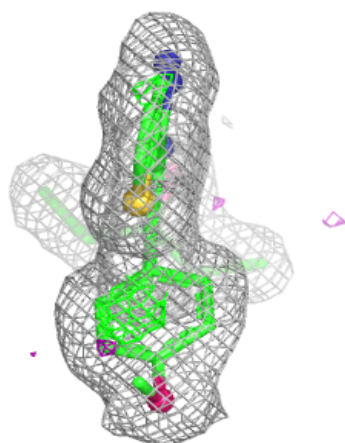
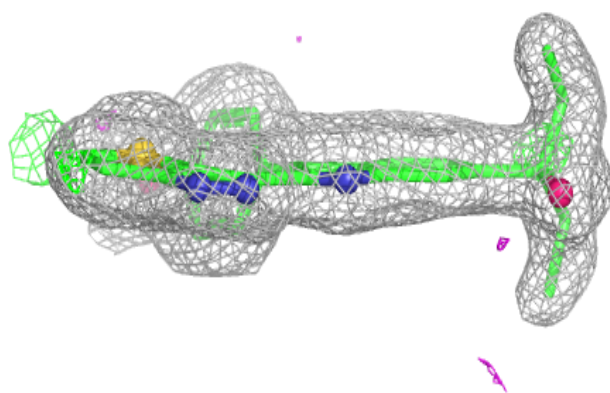
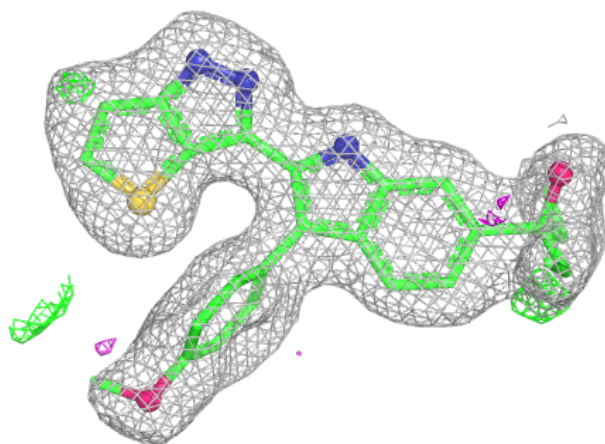
**Electron density around 0G1 D 701:**

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



Electron density around 0G1 C 701:

$2mF_o-DF_c$ (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.