



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:34 PM UTC

PDB ID : 3A0I / pdb_00003a0i
Title : Human glucokinase in complex with a synthetic activator
Authors : Kamata, K.; Mitsuya, M.
Deposited on : 2009-03-19
Resolution : 2.20 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

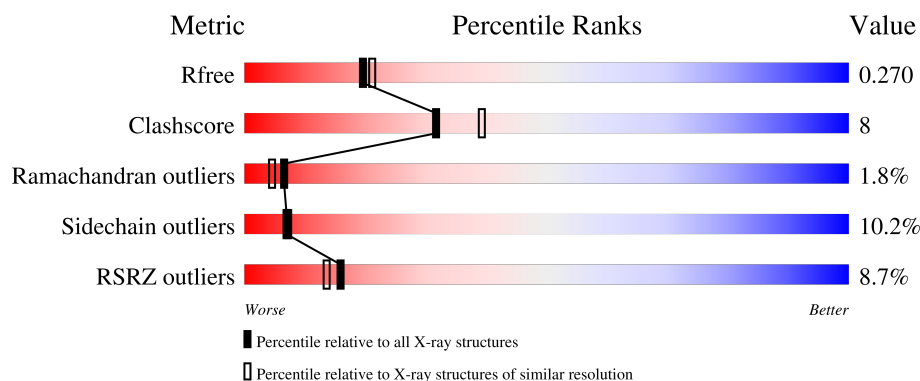
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	X	455	9% 69% 25% ...

2 Entry composition [i](#)

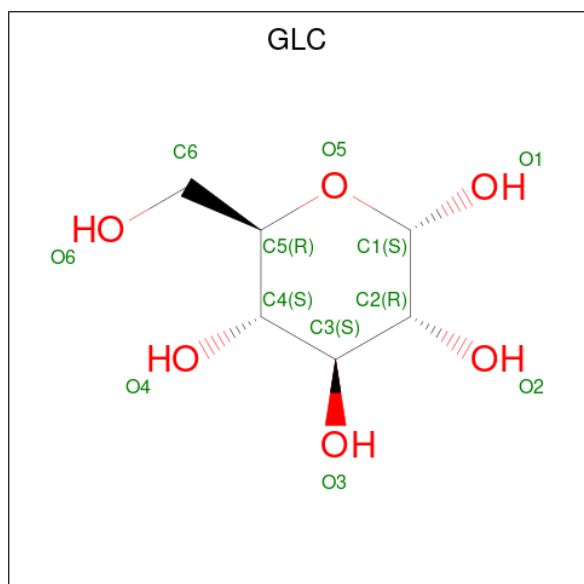
There are 5 unique types of molecules in this entry. The entry contains 3685 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucokinase.

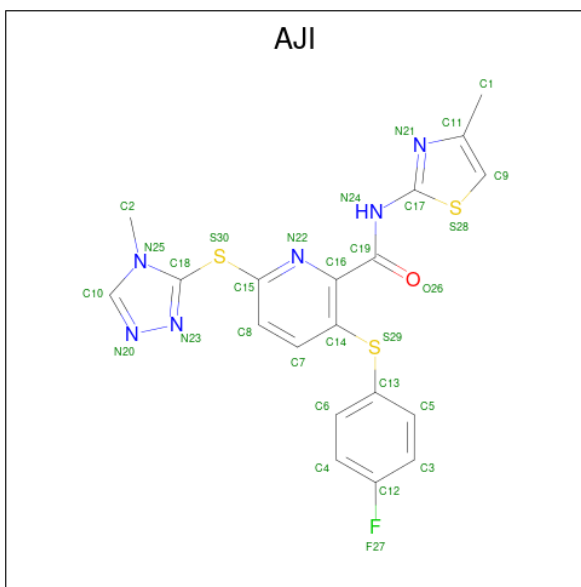
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	448	3505	2178	609	686	32	0	0	0

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	X	1	12	6	6	0	0

- Molecule 3 is 3-[(4-fluorophenyl)sulfanyl]-N-(4-methyl-1,3-thiazol-2-yl)-6-[(4-methyl-4H-1,2,4-triazol-3-yl)sulfanyl]pyridine-2-carboxamide (CCD ID: AJI) (formula: C₁₉H₁₅FN₆OS₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	C	F	N	O	S	
			30	19	1	6	1	3	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total	Na		
			1	1	0	0

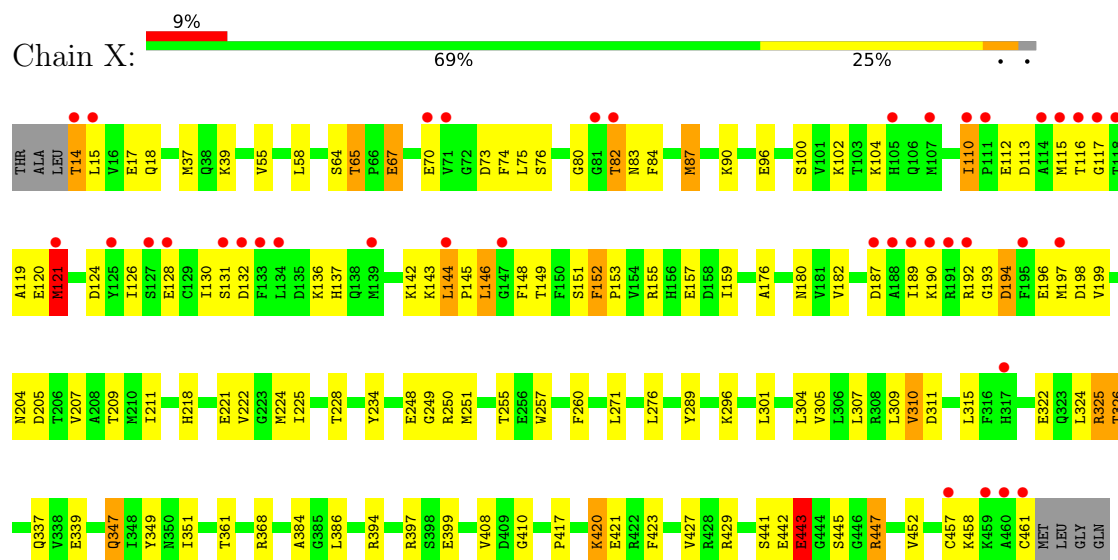
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	137	Total	O		
			137	137	0	0

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: Glucokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.73Å 79.73Å 321.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.37 – 2.20 42.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (42.37-2.20) 94.7 (42.37-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.277 0.220 , 0.270	Depositor DCC
R_{free} test set	1529 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	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	0.94	EDS
Total number of atoms	3685	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: AJI, NA, GLC

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	X	1.42	15/3558 (0.4%)	1.33	18/4783 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	225	ILE	CA-CB	7.54	1.63	1.54
1	X	211	ILE	CA-CB	6.57	1.62	1.54
1	X	87	MET	CG-SD	5.69	1.95	1.80
1	X	55	VAL	CA-CB	5.62	1.60	1.53
1	X	148	PHE	CA-C	5.55	1.59	1.52
1	X	443	GLU	CA-C	-5.55	1.45	1.53
1	X	222	VAL	CA-CB	5.49	1.62	1.54
1	X	408	VAL	CA-CB	5.42	1.64	1.55
1	X	37	MET	C-O	-5.37	1.17	1.24
1	X	452	VAL	CA-CB	5.36	1.61	1.54
1	X	234	TYR	CA-CB	5.29	1.62	1.53
1	X	207	VAL	N-CA	5.20	1.52	1.46
1	X	255	THR	CA-CB	5.11	1.61	1.53
1	X	384	ALA	CA-CB	5.06	1.61	1.53
1	X	410	GLY	C-O	-5.02	1.18	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	442	GLU	CA-C-N	-12.61	106.13	123.03
1	X	442	GLU	C-N-CA	-12.61	106.13	123.03
1	X	157	GLU	N-CA-C	-9.58	102.10	113.88
1	X	339	GLU	N-CA-C	7.13	121.57	113.01
1	X	276	LEU	N-CA-C	6.13	117.63	111.07
1	X	58	LEU	CA-C-N	-5.59	114.19	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	58	LEU	C-N-CA	-5.59	114.19	119.90
1	X	427	VAL	CB-CA-C	-5.45	104.78	112.14
1	X	443	GLU	N-CA-C	-5.40	99.58	108.49
1	X	204	ASN	CB-CA-C	5.38	119.36	109.46
1	X	152	PHE	CA-C-N	-5.35	113.65	120.23
1	X	152	PHE	C-N-CA	-5.35	113.65	120.23
1	X	442	GLU	O-C-N	-5.25	116.28	122.32
1	X	251	MET	CG-SD-CE	-5.24	89.37	100.90
1	X	417	PRO	CA-C-N	-5.20	113.88	121.99
1	X	417	PRO	C-N-CA	-5.20	113.88	121.99
1	X	310	VAL	N-CA-CB	5.07	117.44	110.54
1	X	83	ASN	N-CA-C	5.03	117.16	109.07

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	X	3505	0	3443	55	1
2	X	12	0	12	0	0
3	X	30	0	15	2	0
4	X	1	0	0	0	0
5	X	137	0	0	3	0
All	All	3685	0	3470	57	1

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 8.

All (57) 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:X:119:ALA:HB2	1:X:176:ALA:HB2	1.56	0.86
1:X:14:THR:CG2	1:X:18:GLN:HE21	1.93	0.82
1:X:397:ARG:HG3	1:X:399:GLU:OE1	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:322:GLU:O	1:X:326:THR:HG23	1.83	0.78
1:X:82:THR:O	1:X:110:ILE:HD12	1.92	0.67
1:X:128:GLU:O	1:X:131:SER:OG	2.11	0.67
1:X:75:LEU:HD23	1:X:146:LEU:HD12	1.75	0.67
1:X:14:THR:HG23	1:X:18:GLN:HE21	1.61	0.65
1:X:84:PHE:CZ	1:X:126:ILE:HG23	2.32	0.65
1:X:209:THR:HG23	1:X:441:SER:HB3	1.81	0.61
1:X:325:ARG:NH1	5:X:777:HOH:O	2.35	0.60
3:X:501:AJI:O26	3:X:501:AJI:S29	2.61	0.58
1:X:420:LYS:HG2	1:X:421:GLU:N	2.19	0.56
1:X:14:THR:HG22	1:X:18:GLN:HE21	1.68	0.55
1:X:301:LEU:O	1:X:305:VAL:HG23	2.07	0.54
1:X:75:LEU:HD23	1:X:146:LEU:CD1	2.37	0.54
1:X:143:LYS:HG3	1:X:196:GLU:O	2.08	0.53
1:X:421:GLU:H	1:X:421:GLU:CD	2.17	0.52
1:X:307:LEU:HD11	1:X:324:LEU:HG	1.92	0.52
1:X:347:GLN:HA	1:X:347:GLN:OE1	2.10	0.51
1:X:144:LEU:O	1:X:197:MET:HE3	2.11	0.51
1:X:443:GLU:O	1:X:447:ARG:HB2	2.11	0.50
1:X:14:THR:HG22	1:X:18:GLN:NE2	2.27	0.49
1:X:149:THR:HG21	1:X:445:SER:OG	2.13	0.49
1:X:192:ARG:O	1:X:194:ASP:N	2.40	0.48
1:X:14:THR:HA	1:X:17:GLU:HB2	1.94	0.48
1:X:152:PHE:HB3	1:X:153:PRO:HD2	1.97	0.47
1:X:337:GLN:HE21	1:X:347:GLN:NE2	2.13	0.47
1:X:80:GLY:HA2	1:X:152:PHE:CE1	2.50	0.47
1:X:132:ASP:OD1	1:X:136:LYS:HE2	2.16	0.46
1:X:205:ASP:OD2	1:X:205:ASP:N	2.47	0.46
1:X:104:LYS:HD3	1:X:137:HIS:CD2	2.51	0.46
1:X:100:SER:HB2	1:X:447:ARG:HG2	1.98	0.46
1:X:115:MET:C	1:X:117:GLY:H	2.24	0.45
1:X:126:ILE:O	1:X:130:ILE:HG13	2.15	0.45
1:X:82:THR:O	1:X:110:ILE:CD1	2.62	0.45
1:X:221:GLU:OE1	1:X:250:ARG:NH2	2.50	0.44
1:X:80:GLY:HA3	1:X:151:SER:HB2	1.98	0.44
1:X:218:HIS:HE1	5:X:829:HOH:O	1.99	0.44
1:X:349:TYR:CD2	1:X:349:TYR:C	2.95	0.44
1:X:73:ASP:OD1	1:X:90:LYS:NZ	2.50	0.44
1:X:76:SER:HB2	1:X:87:MET:HG2	1.99	0.44
1:X:74:PHE:CE2	1:X:145:PRO:HG2	2.53	0.43
1:X:249:GLY:C	1:X:250:ARG:HG3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:501:AJI:O26	3:X:501:AJI:S28	2.76	0.43
1:X:257:TRP:C	1:X:257:TRP:CD1	2.97	0.42
1:X:260:PHE:O	1:X:289:TYR:HB2	2.19	0.42
1:X:189:ILE:HG22	1:X:190:LYS:HD2	2.02	0.41
1:X:182:VAL:HG13	1:X:199:VAL:HG11	2.02	0.41
1:X:119:ALA:CB	1:X:176:ALA:HB2	2.39	0.41
1:X:228:THR:HG23	1:X:296:LYS:HB2	2.03	0.41
1:X:180:ASN:OD1	1:X:180:ASN:C	2.64	0.41
1:X:155:ARG:NE	5:X:767:HOH:O	2.38	0.40
1:X:144:LEU:HD12	1:X:197:MET:HE1	2.04	0.40
1:X:64:SER:O	1:X:65:THR:C	2.63	0.40
1:X:121:MET:O	1:X:124:ASP:HB2	2.22	0.40
1:X:224:MET:HE1	1:X:423:PHE:CZ	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:421:GLU:OE2	1:X:421:GLU:OE2[11_655]	1.44	0.76

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	X	446/455 (98%)	406 (91%)	32 (7%)	8 (2%)	6 4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	67	GLU
1	X	194	ASP
1	X	112	GLU

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Mol	Chain	Res	Type
1	X	142	LYS
1	X	187	ASP
1	X	193	GLY
1	X	458	LYS
1	X	121	MET

5.3.2 Protein sidechains ⓘ

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	X	384/389 (99%)	345 (90%)	39 (10%)	7 7

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	14	THR
1	X	15	LEU
1	X	39	LYS
1	X	65	THR
1	X	67	GLU
1	X	70	GLU
1	X	82	THR
1	X	96	GLU
1	X	102	LYS
1	X	110	ILE
1	X	113	ASP
1	X	116	THR
1	X	120	GLU
1	X	121	MET
1	X	144	LEU
1	X	146	LEU
1	X	159	ILE
1	X	198	ASP
1	X	248	GLU
1	X	271	LEU
1	X	304	LEU

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Mol	Chain	Res	Type
1	X	309	LEU
1	X	310	VAL
1	X	311	ASP
1	X	315	LEU
1	X	325	ARG
1	X	326	THR
1	X	347	GLN
1	X	351	ILE
1	X	361	THR
1	X	368	ARG
1	X	386	LEU
1	X	394	ARG
1	X	420	LYS
1	X	429	ARG
1	X	443	GLU
1	X	447	ARG
1	X	457	CYS
1	X	461	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	18	GLN
1	X	218	HIS
1	X	337	GLN
1	X	416	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
3	AJI	X	501	-	33,33,33	1.49	6 (18%)	40,46,46	2.15	12 (30%)
2	GLC	X	500	-	12,12,12	1.01	1 (8%)	17,17,17	1.31	3 (17%)

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
3	AJI	X	501	-	-	2/16/16/16	0/4/4/4
2	GLC	X	500	-	-	0/2/22/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	501	AJI	C18-N25	4.21	1.40	1.36
3	X	501	AJI	C16-C19	-3.62	1.45	1.50
2	X	500	GLC	O3-C3	2.72	1.49	1.43
3	X	501	AJI	C17-S28	-2.68	1.70	1.74
3	X	501	AJI	C2-N25	-2.46	1.41	1.46
3	X	501	AJI	C13-S29	-2.23	1.73	1.77
3	X	501	AJI	C16-C14	-2.11	1.36	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	501	AJI	C7-C14-C16	-4.66	113.12	119.32
3	X	501	AJI	C11-C9-S28	-4.54	108.05	111.23
3	X	501	AJI	O26-C19-N24	4.52	128.88	122.27
3	X	501	AJI	C9-S28-C17	4.13	91.61	88.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	501	AJI	N24-C17-N21	3.67	127.52	121.18
3	X	501	AJI	C13-S29-C14	-3.53	98.34	102.97
3	X	501	AJI	C14-C16-N22	3.27	126.09	121.77
3	X	501	AJI	C8-C15-N22	-3.09	120.15	123.47
3	X	501	AJI	S28-C17-N21	-2.61	112.94	115.69
3	X	501	AJI	C19-C16-N22	-2.55	113.52	116.02
2	X	500	GLC	C1-C2-C3	2.51	115.47	110.36
2	X	500	GLC	O2-C2-C3	2.23	115.64	110.38
3	X	501	AJI	S28-C17-N24	-2.11	119.53	123.29
2	X	500	GLC	O5-C5-C4	2.03	113.36	109.70
3	X	501	AJI	C7-C14-S29	2.02	124.52	119.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

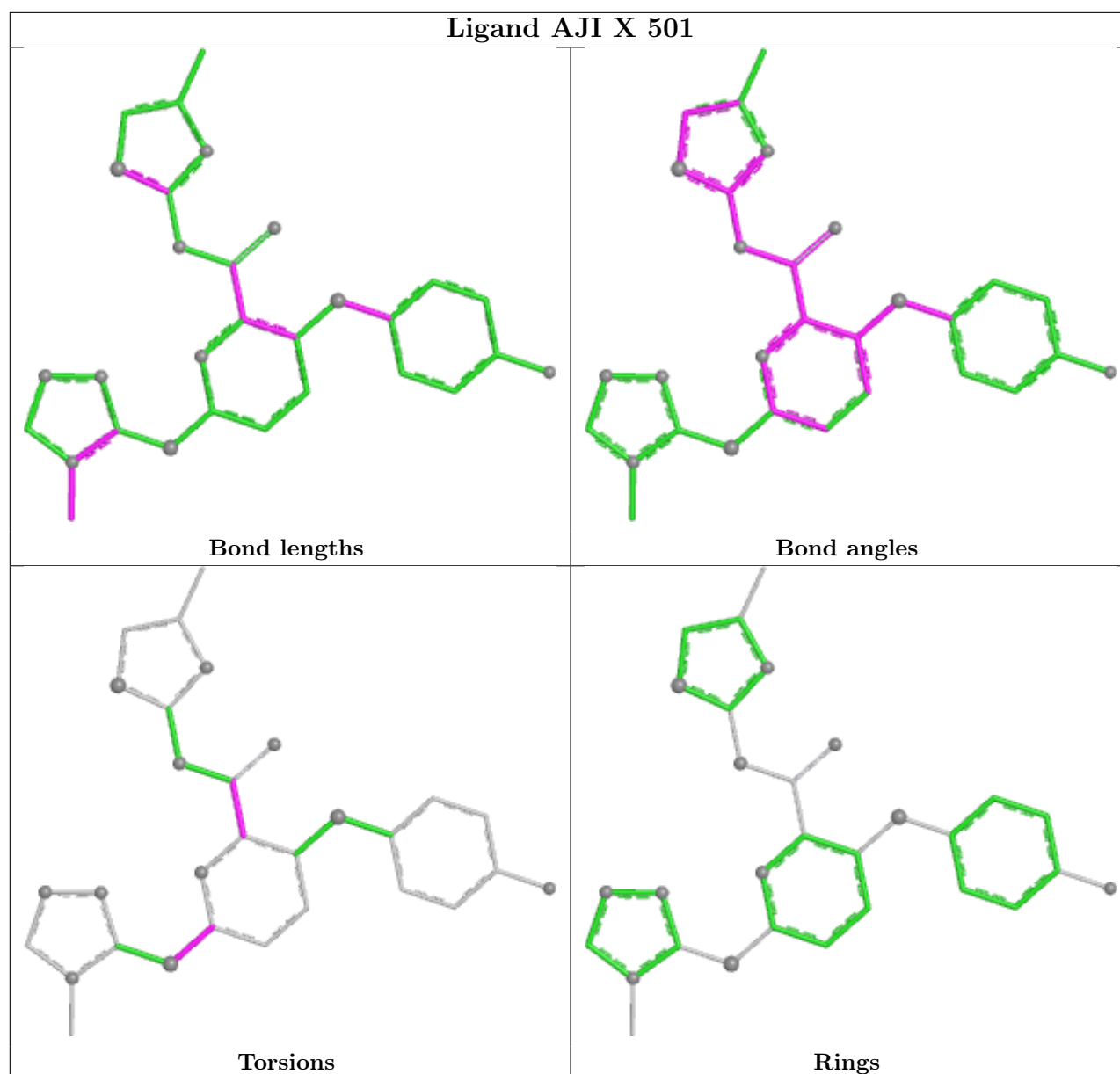
Mol	Chain	Res	Type	Atoms
3	X	501	AJI	N22-C15-S30-C18
3	X	501	AJI	C14-C16-C19-N24

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	501	AJI	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.



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	X	448/455 (98%)	0.40	39 (8%) 16 13	13, 32, 68, 83	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	189	ILE	4.2
1	X	139	MET	4.0
1	X	110	ILE	3.9
1	X	191	ARG	3.9
1	X	114	ALA	3.8
1	X	195	PHE	3.7
1	X	131	SER	3.7
1	X	188	ALA	3.4
1	X	127	SER	3.4
1	X	460	ALA	3.2
1	X	147	GLY	3.2
1	X	15	LEU	3.1
1	X	190	LYS	3.0
1	X	461	CYS	2.9
1	X	144	LEU	2.9
1	X	118	THR	2.8
1	X	121	MET	2.8
1	X	81	GLY	2.7
1	X	116	THR	2.7
1	X	117	GLY	2.7
1	X	111	PRO	2.7
1	X	197	MET	2.7
1	X	125	TYR	2.6
1	X	133	PHE	2.5
1	X	82	THR	2.5
1	X	187	ASP	2.3
1	X	457	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	107	MET	2.3
1	X	317	HIS	2.3
1	X	134	LEU	2.2
1	X	14	THR	2.2
1	X	128	GLU	2.2
1	X	71	VAL	2.2
1	X	115	MET	2.2
1	X	70	GLU	2.2
1	X	132	ASP	2.1
1	X	192	ARG	2.0
1	X	105	HIS	2.0
1	X	459	LYS	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](#)

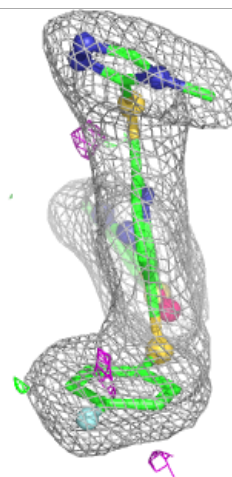
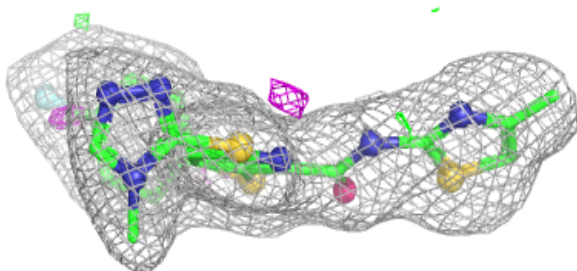
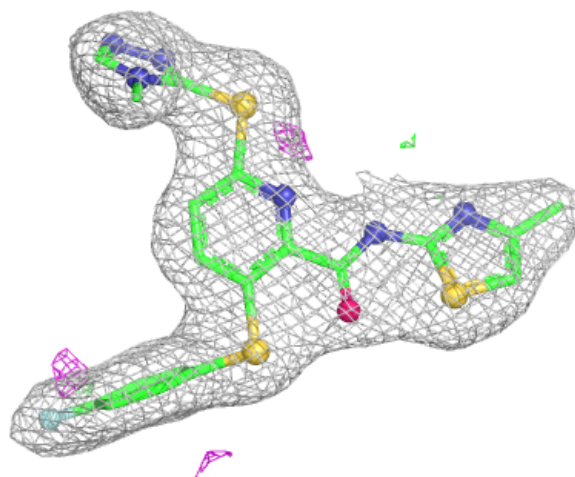
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	X	500	12/12	0.96	0.06	14,18,22,25	0
4	NA	X	600	1/1	0.96	0.04	37,37,37,37	0
3	AJI	X	501	30/30	0.97	0.06	20,24,28,29	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 AJI X 501:

$2mF_o-DF_c$ (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.