



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:53 PM UTC

PDB ID : 3H1V / pdb_00003h1v
Title : Human glucokinase in complex with a synthetic activator
Authors : Kamata, K.; Takahashi, K.
Deposited on : 2009-04-14
Resolution : 2.11 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

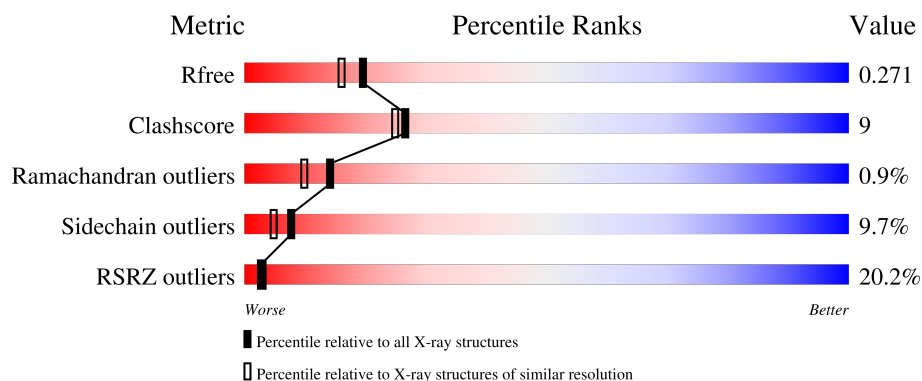
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	451	20% 69% 25% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3659 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.

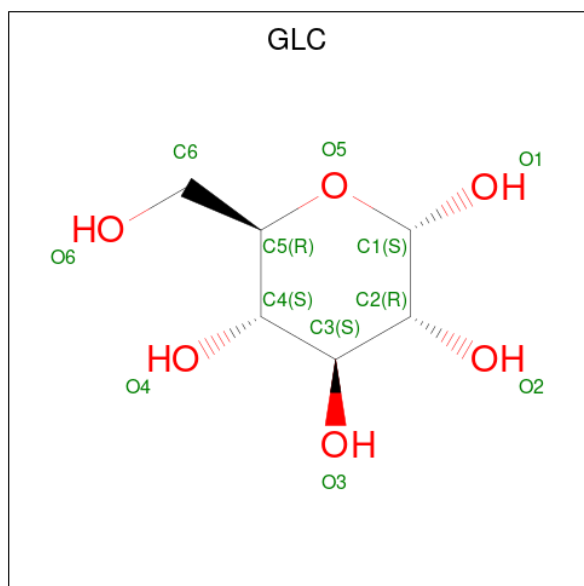
- Molecule 1 is a protein called Glucokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	446	3492	2170	607	683	32	0	0	0

There is a discrepancy between the modelled and reference sequences:

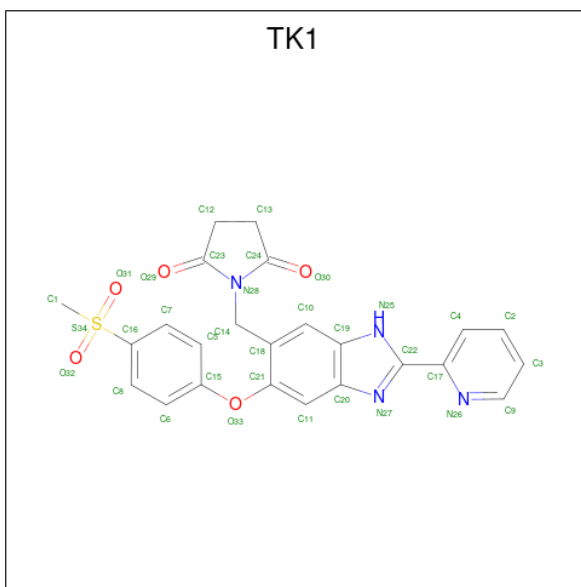
Chain	Residue	Modelled	Actual	Comment	Reference
X	15	MET	-	initiating methionine	UNP P35557

- 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 1-({5-[4-(methylsulfonyl)phenoxy]-2-pyridin-2-yl-1H-benzimidazol-6-yl}methyl)pyrrolidine-2,5-dione (CCD ID: TK1) (formula: C₂₄H₂₀N₄O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	C	N	O	S	0	0
			34	24	4	5	1		

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

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

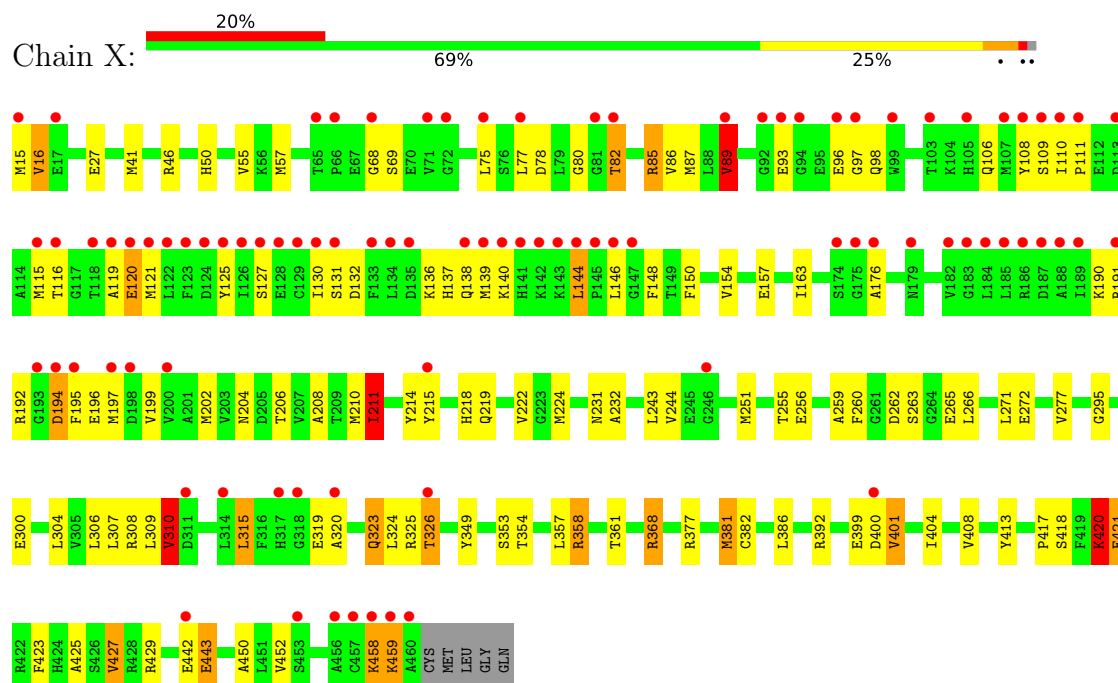
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	120	Total	O	0	0
			120	120		

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: Glucokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.79Å 79.79Å 326.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.46 – 2.11 47.46 – 2.11	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.46-2.11) 86.8 (47.46-2.11)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.284 (Not available) , 0.271	Depositor DCC
R_{free} test set	1733 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3659	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: GLC, NA, TK1

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	1.39	17/3545 (0.5%)	1.30	20/4764 (0.4%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	425	ALA	N-CA	7.12	1.54	1.46
1	X	55	VAL	CA-CB	6.77	1.60	1.53
1	X	206	THR	C-O	-6.43	1.16	1.24
1	X	89	VAL	CA-CB	6.24	1.62	1.54
1	X	232	ALA	CA-CB	5.85	1.64	1.53
1	X	208	ALA	C-O	5.64	1.30	1.24
1	X	57	MET	CA-C	5.45	1.59	1.53
1	X	255	THR	CA-C	-5.44	1.45	1.52
1	X	310	VAL	CA-CB	5.43	1.61	1.54
1	X	408	VAL	C-O	-5.41	1.18	1.24
1	X	211	ILE	CA-CB	5.30	1.60	1.54
1	X	210	MET	C-O	5.30	1.30	1.24
1	X	429	ARG	C-O	-5.20	1.18	1.24
1	X	150	PHE	N-CA	-5.20	1.40	1.46
1	X	382	CYS	C-O	5.19	1.30	1.24
1	X	16	VAL	C-O	-5.06	1.18	1.24
1	X	295	GLY	C-O	-5.04	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	157	GLU	N-CA-C	-9.69	101.96	113.88
1	X	417	PRO	CA-C-N	-8.05	109.59	122.23
1	X	417	PRO	C-N-CA	-8.05	109.59	122.23
1	X	206	THR	N-CA-C	-6.94	103.64	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	458	LYS	N-CA-C	-6.88	105.51	114.04
1	X	427	VAL	CB-CA-C	-6.67	103.14	112.14
1	X	139	MET	N-CA-C	6.14	121.82	112.54
1	X	420	LYS	CB-CA-C	-6.12	101.28	110.88
1	X	224	MET	CA-C-N	-5.82	115.97	123.19
1	X	224	MET	C-N-CA	-5.82	115.97	123.19
1	X	86	VAL	N-CA-C	-5.75	99.89	108.46
1	X	204	ASN	CB-CA-C	5.52	119.62	109.46
1	X	443	GLU	CA-C-N	5.22	125.63	119.94
1	X	443	GLU	C-N-CA	5.22	125.63	119.94
1	X	421	GLU	CB-CG-CD	5.21	121.47	112.60
1	X	69	SER	N-CA-C	5.21	117.56	108.76
1	X	368	ARG	CA-CB-CG	5.13	124.36	114.10
1	X	300	GLU	N-CA-C	5.05	116.78	111.28
1	X	222	VAL	CA-C-N	5.03	125.07	121.65
1	X	222	VAL	C-N-CA	5.03	125.07	121.65

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	3492	0	3429	65	1
2	X	12	0	12	0	0
3	X	34	0	20	3	0
4	X	1	0	0	0	0
5	X	120	0	0	2	0
All	All	3659	0	3461	65	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 9.

All (65) 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:349:TYR:OH	1:X:358:ARG:NH2	1.95	1.00
1:X:85:ARG:HG2	1:X:85:ARG:HH11	1.32	0.93
1:X:132:ASP:O	1:X:136:LYS:HB2	1.78	0.83
1:X:96:GLU:HB2	1:X:215:TYR:CE1	2.17	0.79
1:X:98:GLN:NE2	3:X:501:TK1:H1A	1.98	0.77
1:X:323:GLN:HE21	1:X:323:GLN:H	1.33	0.76
1:X:132:ASP:OD2	1:X:136:LYS:HD2	1.87	0.73
1:X:459:LYS:HE2	1:X:459:LYS:H	1.54	0.71
1:X:97:GLY:HA3	3:X:501:TK1:H1	1.78	0.64
1:X:146:LEU:HD22	1:X:199:VAL:HG22	1.80	0.63
1:X:131:SER:HG	1:X:195:PHE:HE2	1.51	0.58
1:X:119:ALA:HB2	1:X:176:ALA:HB2	1.86	0.58
1:X:82:THR:O	1:X:110:ILE:HD12	2.04	0.57
1:X:85:ARG:HH11	1:X:85:ARG:CG	2.13	0.57
1:X:154:VAL:HG11	1:X:202:MET:HE3	1.87	0.56
1:X:310:VAL:HG21	1:X:320:ALA:HB2	1.88	0.55
1:X:41:MET:HE2	1:X:392:ARG:HD3	1.87	0.55
1:X:50:HIS:CD2	1:X:243:LEU:HD11	2.41	0.55
1:X:400:ASP:CG	1:X:401:VAL:H	2.15	0.55
1:X:111:PRO:HD3	1:X:125:TYR:CZ	2.42	0.55
1:X:259:ALA:HB1	1:X:262:ASP:OD2	2.08	0.54
1:X:190:LYS:C	1:X:192:ARG:H	2.17	0.53
1:X:110:ILE:HB	1:X:115:MET:CE	2.39	0.53
1:X:306:LEU:O	1:X:310:VAL:HG13	2.10	0.52
1:X:120:GLU:H	1:X:120:GLU:CD	2.16	0.52
1:X:190:LYS:O	1:X:192:ARG:N	2.42	0.51
1:X:310:VAL:HG12	1:X:315:LEU:HB3	1.91	0.51
1:X:377:ARG:O	1:X:381:MET:HB2	2.11	0.50
1:X:214:TYR:O	1:X:218:HIS:HD2	1.94	0.50
1:X:263:SER:HB2	1:X:265:GLU:OE2	2.12	0.49
1:X:110:ILE:HB	1:X:115:MET:HE2	1.93	0.49
1:X:211:ILE:HD13	1:X:452:VAL:CG2	2.43	0.48
1:X:196:GLU:O	1:X:197:MET:HE2	2.14	0.48
1:X:320:ALA:HB1	1:X:324:LEU:HD23	1.96	0.48
1:X:106:GLN:HG2	1:X:108:TYR:CZ	2.49	0.47
1:X:121:MET:HB3	5:X:653:HOH:O	2.15	0.47
1:X:144:LEU:HD12	1:X:197:MET:HE1	1.97	0.46
1:X:89:VAL:CG1	1:X:450:ALA:HB2	2.46	0.46
1:X:98:GLN:NE2	3:X:501:TK1:C1	2.73	0.46
1:X:413:TYR:CZ	1:X:420:LYS:HG2	2.50	0.46
1:X:75:LEU:HD23	1:X:146:LEU:HD12	1.98	0.45
1:X:77:LEU:HB2	1:X:148:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:219:GLN:NE2	5:X:725:HOH:O	2.45	0.45
1:X:78:ASP:HB3	1:X:85:ARG:HB2	1.98	0.44
1:X:354:THR:O	1:X:354:THR:HG22	2.17	0.44
1:X:423:PHE:O	1:X:427:VAL:HG23	2.18	0.44
1:X:163:ILE:O	1:X:163:ILE:HG13	2.16	0.44
1:X:244:VAL:HG11	1:X:251:MET:HE1	2.00	0.44
1:X:85:ARG:HG2	1:X:85:ARG:NH1	2.11	0.43
1:X:260:PHE:CE2	1:X:266:LEU:HD21	2.53	0.43
1:X:323:GLN:HA	1:X:326:THR:HG23	2.01	0.43
1:X:137:HIS:O	1:X:138:GLN:HB2	2.19	0.42
1:X:93:GLU:OE2	1:X:98:GLN:OE1	2.37	0.42
1:X:140:LYS:HG2	1:X:140:LYS:O	2.19	0.42
1:X:127:SER:HA	1:X:130:ILE:HD12	2.01	0.42
1:X:442:GLU:O	1:X:443:GLU:C	2.62	0.42
1:X:96:GLU:HB2	1:X:215:TYR:CD1	2.54	0.41
1:X:82:THR:HA	1:X:115:MET:HE1	2.02	0.41
1:X:358:ARG:HE	1:X:358:ARG:HB3	1.47	0.41
1:X:231:ASN:OD1	1:X:256:GLU:HA	2.21	0.41
1:X:353:SER:HA	1:X:357:LEU:O	2.19	0.41
1:X:85:ARG:CG	1:X:85:ARG:NH1	2.78	0.41
1:X:131:SER:OG	1:X:195:PHE:HE2	2.03	0.41
1:X:272:GLU:OE1	1:X:308:ARG:NH1	2.54	0.41
1:X:421:GLU:H	1:X:421:GLU:CD	2.28	0.41

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]	1.29	0.91

5.3 Torsion angles

5.3.1 Protein backbone

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	444/451 (98%)	418 (94%)	22 (5%)	4 (1%)	14 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	191	ARG
1	X	194	ASP
1	X	68	GLY
1	X	80	GLY

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	382/386 (99%)	345 (90%)	37 (10%)	8 5

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	15	MET
1	X	16	VAL
1	X	27	GLU
1	X	46	ARG
1	X	82	THR
1	X	85	ARG
1	X	87	MET
1	X	89	VAL
1	X	109	SER
1	X	116	THR
1	X	120	GLU
1	X	144	LEU
1	X	194	ASP
1	X	211	ILE
1	X	271	LEU
1	X	277	VAL
1	X	304	LEU

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Mol	Chain	Res	Type
1	X	307	LEU
1	X	309	LEU
1	X	310	VAL
1	X	315	LEU
1	X	319	GLU
1	X	323	GLN
1	X	325	ARG
1	X	326	THR
1	X	358	ARG
1	X	361	THR
1	X	368	ARG
1	X	381	MET
1	X	386	LEU
1	X	399	GLU
1	X	401	VAL
1	X	404	ILE
1	X	418	SER
1	X	420	LYS
1	X	458	LYS
1	X	459	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	X	83	ASN
1	X	98	GLN
1	X	218	HIS
1	X	219	GLN
1	X	286	GLN
1	X	323	GLN
1	X	337	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	TK1	X	501	-	38,38,38	0.85	1 (2%)	56,56,56	2.00	16 (28%)
2	GLC	X	500	-	12,12,12	1.11	2 (16%)	17,17,17	1.27	4 (23%)

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	TK1	X	501	-	-	4/18/31/31	0/5/5/5
2	GLC	X	500	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	501	TK1	C7-C5	-2.07	1.35	1.38
2	X	500	GLC	O1-C1	2.05	1.46	1.39
2	X	500	GLC	O3-C3	2.01	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	501	TK1	O31-S34-C16	-6.30	103.33	108.23
3	X	501	TK1	C13-C24-N28	3.97	111.47	108.03
3	X	501	TK1	C6-C8-C16	-3.40	116.14	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	501	TK1	C19-C10-C18	-3.34	116.77	121.81
3	X	501	TK1	C12-C13-C24	-3.31	101.85	105.24
3	X	501	TK1	C7-C16-S34	-3.28	116.67	119.58
3	X	501	TK1	C8-C16-C7	3.19	124.62	120.47
3	X	501	TK1	O31-S34-C1	3.14	113.08	108.47
3	X	501	TK1	C24-N28-C23	-3.08	111.59	112.94
3	X	501	TK1	C11-C21-C18	3.00	123.59	120.49
3	X	501	TK1	C1-S34-C16	-2.88	101.38	104.55
3	X	501	TK1	O32-S34-O31	2.29	121.88	117.99
2	X	500	GLC	O3-C3-C4	-2.28	104.99	110.38
3	X	501	TK1	O30-C24-N28	-2.28	121.49	123.94
2	X	500	GLC	O3-C3-C2	2.25	115.68	110.38
3	X	501	TK1	C14-N28-C24	-2.21	120.52	123.23
3	X	501	TK1	O33-C21-C11	-2.13	115.47	121.63
2	X	500	GLC	O4-C4-C3	-2.08	105.47	110.38
2	X	500	GLC	O5-C5-C6	2.04	111.49	106.44
3	X	501	TK1	C14-C18-C10	-2.03	116.78	120.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	501	TK1	C7-C16-S34-O32
3	X	501	TK1	C8-C16-S34-O32
3	X	501	TK1	C8-C16-S34-C1
3	X	501	TK1	C7-C16-S34-C1

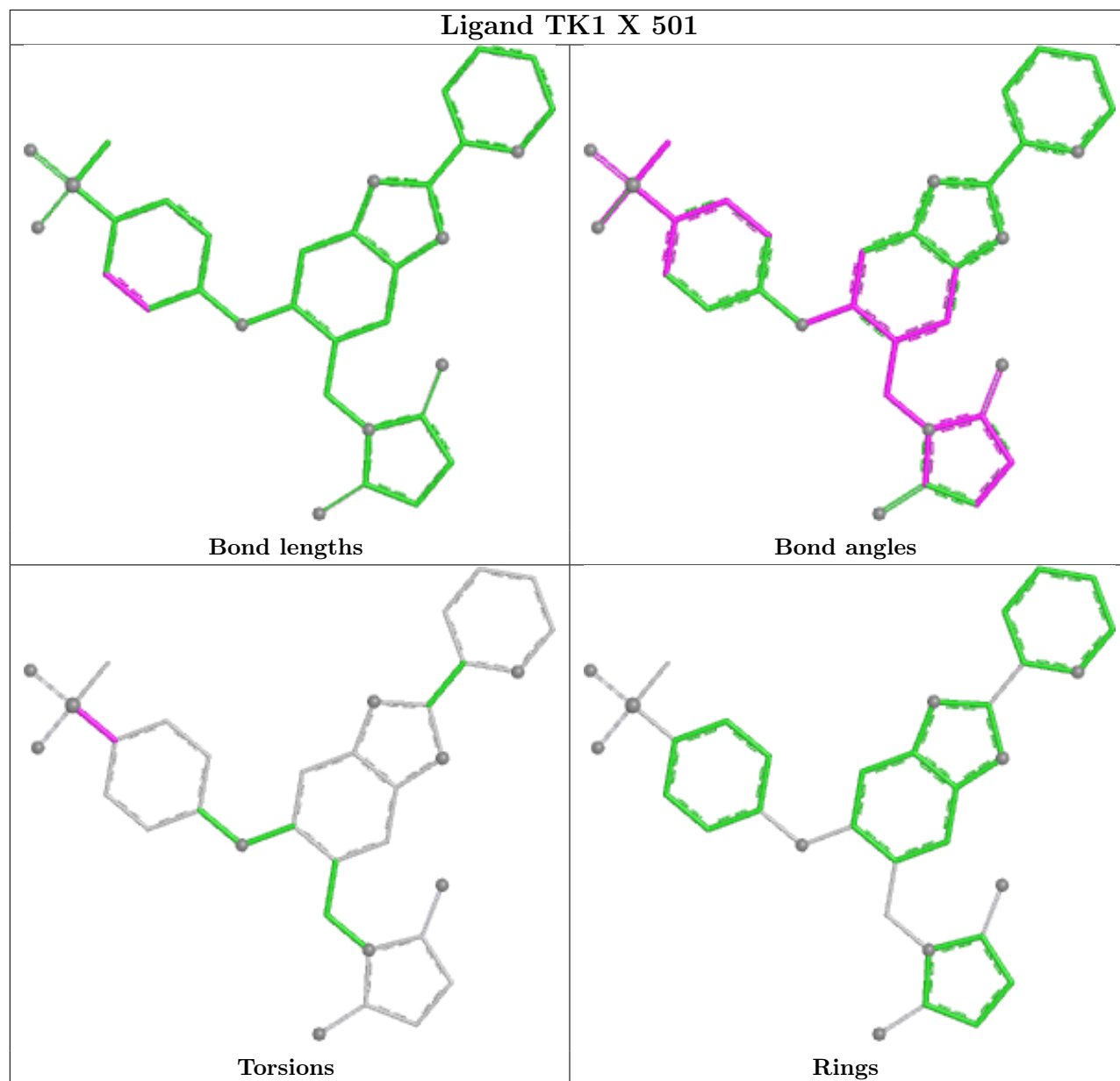
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	501	TK1	3	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	446/451 (98%)	0.89	90 (20%) 3 3	16, 35, 77, 88	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	460	ALA	5.9
1	X	65	THR	4.5
1	X	92	GLY	4.3
1	X	141	HIS	4.2
1	X	144	LEU	4.2
1	X	131	SER	4.2
1	X	189	ILE	4.1
1	X	66	PRO	4.1
1	X	195	PHE	4.1
1	X	193	GLY	4.0
1	X	72	GLY	4.0
1	X	126	ILE	3.9
1	X	174	SER	3.8
1	X	122	LEU	3.7
1	X	459	LYS	3.7
1	X	175	GLY	3.7
1	X	197	MET	3.7
1	X	119	ALA	3.7
1	X	183	GLY	3.6
1	X	15	MET	3.5
1	X	110	ILE	3.5
1	X	75	LEU	3.5
1	X	111	PRO	3.4
1	X	81	GLY	3.4
1	X	82	THR	3.4
1	X	191	ARG	3.3
1	X	400	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	X	121	MET	3.2
1	X	182	VAL	3.2
1	X	123	PHE	3.2
1	X	129	CYS	3.2
1	X	127	SER	3.1
1	X	113	ASP	3.1
1	X	317	HIS	3.1
1	X	194	ASP	3.0
1	X	186	ARG	3.0
1	X	116	THR	3.0
1	X	94	GLY	3.0
1	X	108	TYR	2.9
1	X	188	ALA	2.9
1	X	71	VAL	2.9
1	X	198	ASP	2.8
1	X	453	SER	2.8
1	X	146	LEU	2.8
1	X	457	CYS	2.8
1	X	17	GLU	2.7
1	X	184	LEU	2.7
1	X	320	ALA	2.7
1	X	77	LEU	2.7
1	X	456	ALA	2.6
1	X	133	PHE	2.6
1	X	187	ASP	2.6
1	X	89	VAL	2.6
1	X	93	GLU	2.6
1	X	103	THR	2.6
1	X	326	THR	2.6
1	X	96	GLU	2.5
1	X	145	PRO	2.5
1	X	134	LEU	2.5
1	X	109	SER	2.5
1	X	107	MET	2.5
1	X	318	GLY	2.5
1	X	124	ASP	2.4
1	X	115	MET	2.4
1	X	125	TYR	2.4
1	X	215	TYR	2.4
1	X	176	ALA	2.4
1	X	185	LEU	2.4
1	X	147	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	X	179	ASN	2.4
1	X	142	LYS	2.3
1	X	458	LYS	2.3
1	X	118	THR	2.3
1	X	68	GLY	2.3
1	X	140	LYS	2.3
1	X	130	ILE	2.3
1	X	138	GLN	2.3
1	X	135	ASP	2.2
1	X	139	MET	2.2
1	X	200	VAL	2.2
1	X	311	ASP	2.2
1	X	128	GLU	2.2
1	X	442	GLU	2.2
1	X	120	GLU	2.1
1	X	99	TRP	2.1
1	X	246	GLY	2.1
1	X	143	LYS	2.1
1	X	97	GLY	2.1
1	X	314	LEU	2.0
1	X	105	HIS	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.

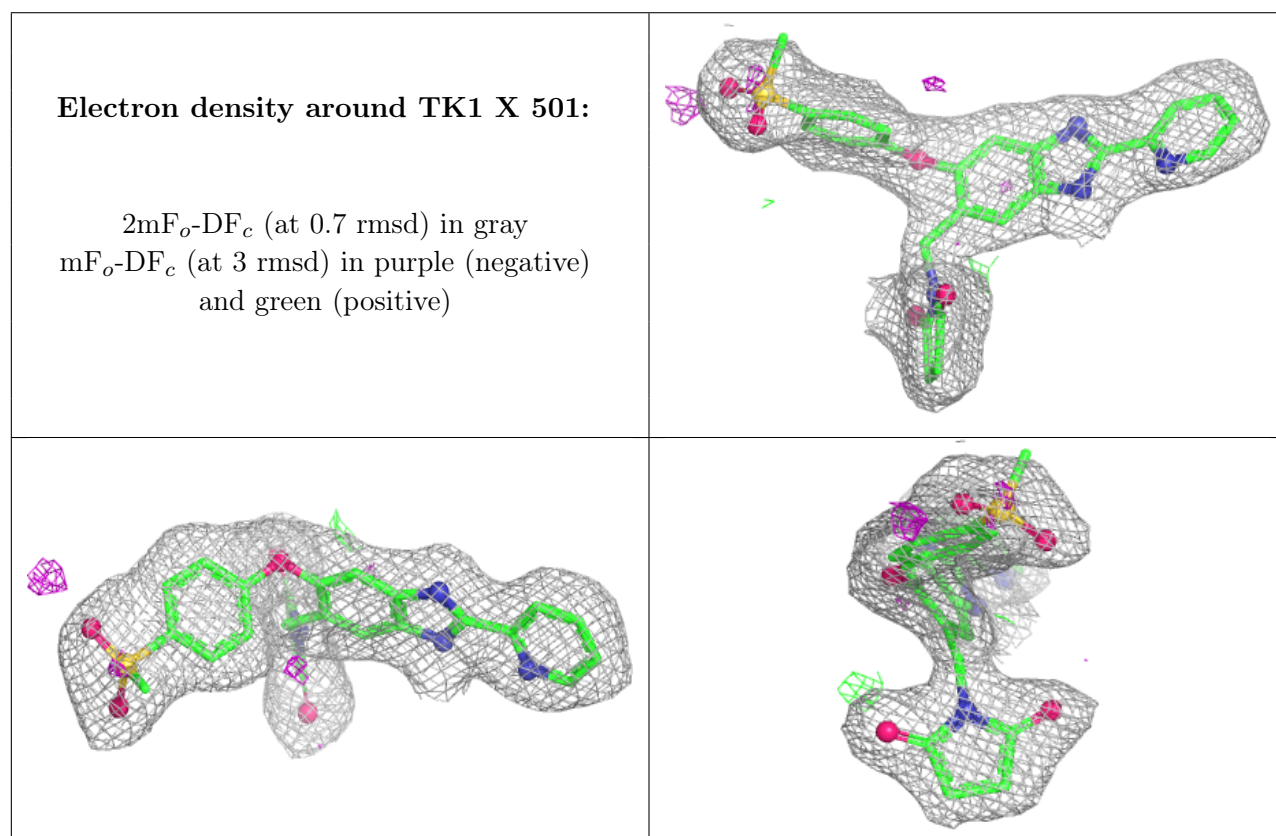
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	X	600	1/1	0.94	0.08	38,38,38,38	0
3	TK1	X	501	34/34	0.95	0.08	22,29,39,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	X	500	12/12	0.96	0.07	14,21,26,27	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.