



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:41 AM EDT

PDB ID : 1V4S / pdb_00001v4s
Title : Crystal structure of human glucokinase
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Deposited on : 2003-11-19
Resolution : 2.30 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

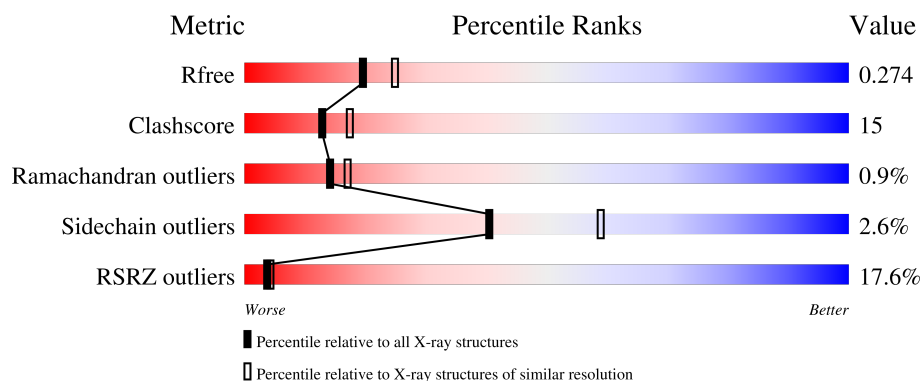
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	455	17% 68% 27% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3690 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.

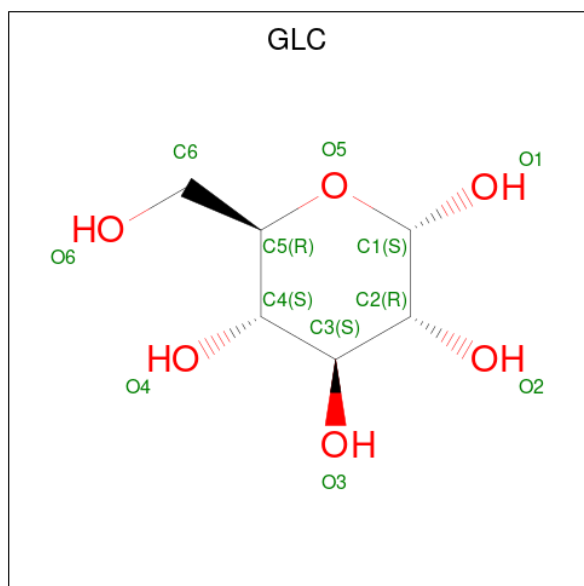
- Molecule 1 is a protein called glucokinase isoform 2.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP P35557

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

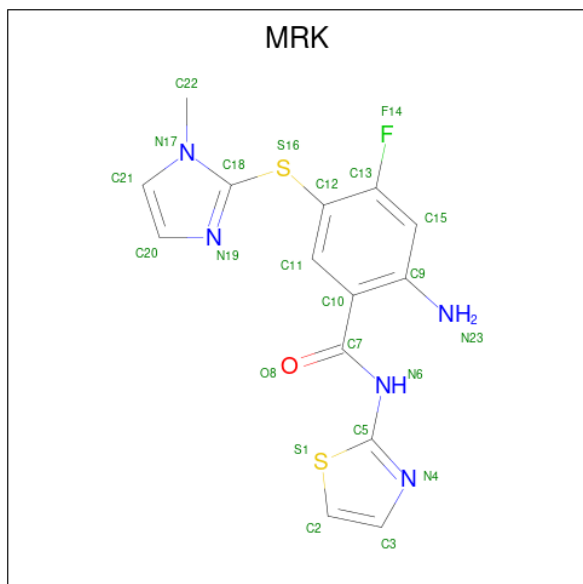


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is 2-AMINO-4-FLUORO-5-[(1-METHYL-1H-IMIDAZOL-2-YL)SULFANYL]-N-(1,3-THIAZOL-2-YL)BENZAMIDE (CCD ID: MRK) (formula: $C_{14}H_{12}FN_5OS_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			23	14	1	5	1	2		

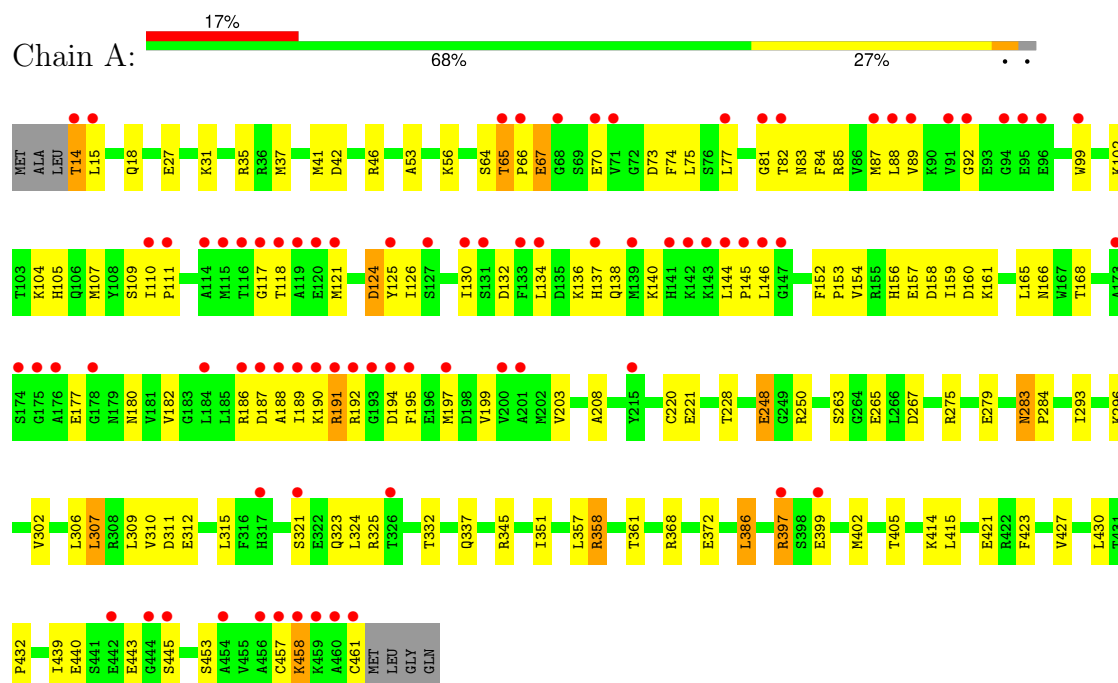
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	149	Total O 149 149	0	0

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 isoform 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.86Å 79.86Å 322.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.42 – 2.30 42.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (42.42-2.30) 98.6 (42.42-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.29Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.232 , 0.273 0.236 , 0.274	Depositor DCC
R_{free} test set	1919 reflections (6.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	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	0.93	EDS
Total number of atoms	3690	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GLC, MRK

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	0.40	0/3558	0.94	13/4783 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	GLU	N-CA-C	-10.35	100.78	113.41
1	A	293	ILE	N-CA-C	8.00	117.94	111.62
1	A	358	ARG	CA-C-N	7.25	127.18	119.85
1	A	358	ARG	C-N-CA	7.25	127.18	119.85
1	A	191	ARG	N-CA-C	-7.24	104.88	113.21
1	A	56	LYS	N-CA-C	7.00	120.70	111.75
1	A	283	ASN	CA-C-N	5.93	127.25	119.84
1	A	283	ASN	C-N-CA	5.93	127.25	119.84
1	A	415	LEU	N-CA-C	5.64	120.44	113.50
1	A	312	GLU	N-CA-C	-5.47	106.37	113.16
1	A	124	ASP	N-CA-C	-5.42	105.02	111.03
1	A	267	ASP	N-CA-C	5.05	117.45	111.33
1	A	458	LYS	N-CA-C	-5.03	107.29	112.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3505	0	3443	106	1
2	A	12	0	12	0	0
3	A	1	0	0	0	0
4	A	23	0	12	0	0
5	A	149	0	0	8	0
All	All	3690	0	3467	106	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 15.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:O	1:A:190:LYS:HD3	1.82	0.80
1:A:263:SER:HB2	1:A:265:GLU:OE2	1.81	0.80
1:A:14:THR:CG2	1:A:18:GLN:HE21	1.96	0.79
1:A:337:GLN:HE21	1:A:351:ILE:HD11	1.45	0.79
1:A:307:LEU:O	1:A:310:VAL:HG22	1.83	0.79
1:A:77:LEU:HG	1:A:146:LEU:HD11	1.65	0.78
1:A:118:THR:H	1:A:121:MET:HE3	1.50	0.76
1:A:118:THR:N	1:A:121:MET:HE3	2.04	0.73
1:A:192:ARG:C	1:A:194:ASP:H	1.95	0.72
1:A:14:THR:HG22	1:A:18:GLN:HE21	1.55	0.70
1:A:85:ARG:NH2	1:A:87:MET:HE1	2.06	0.70
1:A:104:LYS:HD3	1:A:137:HIS:HD2	1.57	0.69
1:A:15:LEU:H	1:A:15:LEU:HD12	1.57	0.69
1:A:161:LYS:HG3	1:A:180:ASN:ND2	2.08	0.69
1:A:104:LYS:HD3	1:A:137:HIS:CD2	2.35	0.62
1:A:74:PHE:O	1:A:88:LEU:HD12	2.00	0.61
1:A:92:GLY:HA3	1:A:99:TRP:CZ2	2.37	0.59
1:A:75:LEU:HD23	1:A:146:LEU:HD13	1.84	0.59
1:A:457:CYS:O	1:A:461:CYS:HB3	2.02	0.59
1:A:111:PRO:HG2	1:A:125:TYR:CE2	2.37	0.59
1:A:102:LYS:CE	1:A:443:GLU:HG3	2.33	0.58
1:A:126:ILE:O	1:A:130:ILE:HG13	2.02	0.58
1:A:187:ASP:O	1:A:191:ARG:HG3	2.04	0.58
1:A:453:SER:O	1:A:457:CYS:HB2	2.05	0.57
1:A:160:ASP:O	1:A:182:VAL:HG21	2.05	0.57
1:A:345:ARG:CZ	1:A:361:THR:HG23	2.35	0.57
1:A:248:GLU:HA	1:A:248:GLU:OE1	2.04	0.56
1:A:109:SER:O	1:A:111:PRO:HD3	2.07	0.55
1:A:92:GLY:HA3	1:A:99:TRP:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:HB1	1:A:445:SER:HA	1.88	0.55
1:A:31:LYS:O	1:A:35:ARG:HG3	2.07	0.55
1:A:130:ILE:O	1:A:134:LEU:HG	2.07	0.54
1:A:368:ARG:NH1	1:A:372:GLU:OE2	2.40	0.54
1:A:74:PHE:CD2	1:A:145:PRO:HB2	2.43	0.53
1:A:283:ASN:N	1:A:284:PRO:HD3	2.23	0.53
1:A:53:ALA:HB1	5:A:685:HOH:O	2.08	0.53
1:A:397:ARG:HG3	1:A:399:GLU:OE2	2.08	0.53
1:A:166:ASN:HA	1:A:177:GLU:HG2	1.91	0.53
1:A:386:LEU:HD12	1:A:423:PHE:HZ	1.74	0.53
1:A:423:PHE:O	1:A:427:VAL:HG23	2.10	0.52
1:A:82:THR:HA	1:A:110:ILE:HD12	1.90	0.52
1:A:102:LYS:HE3	1:A:443:GLU:HG3	1.90	0.52
1:A:84:PHE:CZ	1:A:126:ILE:HG23	2.45	0.52
1:A:192:ARG:C	1:A:194:ASP:N	2.63	0.52
1:A:102:LYS:HD3	1:A:105:HIS:HB3	1.92	0.52
1:A:439:ILE:HD11	5:A:642:HOH:O	2.10	0.52
1:A:190:LYS:C	1:A:192:ARG:H	2.16	0.52
1:A:386:LEU:HD12	1:A:423:PHE:CZ	2.45	0.51
1:A:121:MET:O	1:A:124:ASP:HB2	2.09	0.51
1:A:158:ASP:OD2	1:A:159:ILE:N	2.39	0.51
1:A:152:PHE:HB3	1:A:153:PRO:HD2	1.93	0.51
1:A:189:ILE:HG23	1:A:195:PHE:CE1	2.46	0.51
1:A:221:GLU:OE1	1:A:250:ARG:NH2	2.44	0.51
1:A:81:GLY:HA3	5:A:722:HOH:O	2.10	0.51
1:A:154:VAL:HG12	1:A:156:HIS:HD2	1.77	0.50
1:A:134:LEU:HB3	1:A:140:LYS:HA	1.92	0.50
1:A:306:LEU:O	1:A:310:VAL:HG13	2.12	0.50
1:A:203:VAL:HG12	5:A:728:HOH:O	2.11	0.50
1:A:85:ARG:HD3	1:A:107:MET:HE3	1.93	0.49
1:A:132:ASP:OD2	1:A:136:LYS:HE2	2.12	0.49
1:A:345:ARG:NH1	5:A:718:HOH:O	2.40	0.49
1:A:102:LYS:HE2	1:A:443:GLU:HG3	1.95	0.48
1:A:430:LEU:C	1:A:432:PRO:HD3	2.38	0.48
1:A:154:VAL:HG12	1:A:156:HIS:CD2	2.49	0.48
1:A:73:ASP:O	1:A:144:LEU:HD23	2.13	0.47
1:A:137:HIS:O	1:A:138:GLN:C	2.57	0.47
1:A:321:SER:O	1:A:325:ARG:HG3	2.13	0.47
1:A:85:ARG:HH22	1:A:87:MET:HE1	1.79	0.47
1:A:85:ARG:CD	1:A:107:MET:HE3	2.45	0.46
1:A:345:ARG:NE	1:A:361:THR:HG23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ARG:O	1:A:372:GLU:HG3	2.14	0.46
1:A:421:GLU:H	1:A:421:GLU:CD	2.23	0.46
1:A:37:MET:O	1:A:41:MET:HG3	2.16	0.46
1:A:144:LEU:O	1:A:197:MET:HE3	2.16	0.45
1:A:397:ARG:NE	5:A:697:HOH:O	2.48	0.45
1:A:75:LEU:HD22	1:A:197:MET:HE2	1.98	0.45
1:A:161:LYS:HG3	1:A:180:ASN:HD21	1.80	0.45
1:A:307:LEU:HD12	1:A:307:LEU:HA	1.73	0.44
1:A:14:THR:O	1:A:18:GLN:HG3	2.17	0.44
1:A:307:LEU:HD11	1:A:324:LEU:HG	1.98	0.44
1:A:186:ARG:HG2	1:A:190:LYS:HZ3	1.81	0.44
1:A:397:ARG:HG2	1:A:402:MET:HG3	1.99	0.44
1:A:168:THR:HG22	5:A:624:HOH:O	2.18	0.44
1:A:275:ARG:O	1:A:279:GLU:HG3	2.18	0.43
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.80	0.43
1:A:188:ALA:HA	1:A:191:ARG:CD	2.49	0.43
1:A:65:THR:O	1:A:65:THR:HG23	2.18	0.43
1:A:70:GLU:OE1	1:A:458:LYS:HG3	2.18	0.43
1:A:220:CYS:HA	1:A:405:THR:HB	2.00	0.43
1:A:228:THR:HG23	1:A:296:LYS:HB2	2.01	0.43
1:A:208:ALA:CB	1:A:445:SER:HA	2.48	0.42
1:A:42:ASP:O	1:A:46:ARG:HG2	2.19	0.41
1:A:323:GLN:HG3	5:A:720:HOH:O	2.19	0.41
1:A:81:GLY:C	1:A:83:ASN:H	2.27	0.41
1:A:421:GLU:CD	1:A:421:GLU:N	2.78	0.41
1:A:75:LEU:CD2	1:A:197:MET:HE2	2.50	0.41
1:A:302:VAL:O	1:A:306:LEU:HG	2.21	0.41
1:A:220:CYS:HA	1:A:405:THR:O	2.21	0.41
1:A:414:LYS:HE2	1:A:440:GLU:HB3	2.02	0.41
1:A:75:LEU:O	1:A:146:LEU:HD12	2.21	0.41
1:A:64:SER:O	1:A:65:THR:C	2.63	0.41
1:A:358:ARG:HD3	1:A:358:ARG:HA	1.91	0.40
1:A:321:SER:HB2	1:A:357:LEU:CD2	2.51	0.40
1:A:66:PRO:O	1:A:67:GLU:C	2.63	0.40
1:A:310:VAL:HG23	1:A:311:ASP:N	2.37	0.40
1:A:307:LEU:CD1	1:A:324:LEU:HG	2.51	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:A:421:GLU:OE2	1:A:421:GLU:OE2[11_655]	1.62	0.58

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	446/455 (98%)	416 (93%)	26 (6%)	4 (1%)	14 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	199	VAL
1	A	65	THR
1	A	117	GLY

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	384/389 (99%)	374 (97%)	10 (3%)	40 59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	27	GLU

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Mol	Chain	Res	Type
1	A	89	VAL
1	A	248	GLU
1	A	307	LEU
1	A	309	LEU
1	A	315	LEU
1	A	332	THR
1	A	386	LEU
1	A	397	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	26	GLN
1	A	204	ASN
1	A	313	ASN
1	A	323	GLN
1	A	337	GLN
1	A	347	GLN
1	A	416	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
4	MRK	A	501	-	25,25,25	1.98	9 (36%)	33,35,35	3.02	11 (33%)
2	GLC	A	500	-	12,12,12	1.16	2 (16%)	17,17,17	0.98	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
4	MRK	A	501	-	-	2/12/12/12	0/3/3/3
2	GLC	A	500	-	-	0/2/22/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	MRK	C7-N6	3.86	1.44	1.37
4	A	501	MRK	C18-N19	3.62	1.38	1.31
4	A	501	MRK	C18-N17	3.54	1.39	1.36
4	A	501	MRK	C11-C10	3.07	1.44	1.39
4	A	501	MRK	C12-C13	2.75	1.42	1.38
4	A	501	MRK	C10-C9	2.71	1.45	1.41
2	A	500	GLC	C1-C2	2.66	1.58	1.52
4	A	501	MRK	C15-C13	2.65	1.42	1.37
4	A	501	MRK	C10-C7	2.33	1.54	1.50
4	A	501	MRK	C21-C20	2.19	1.40	1.35
2	A	500	GLC	C4-C5	2.17	1.57	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	MRK	C9-C10-C7	10.92	128.15	120.14
4	A	501	MRK	S16-C18-N19	-6.42	121.77	124.96
4	A	501	MRK	N17-C18-N19	5.51	119.76	111.58
4	A	501	MRK	C21-N17-C18	-4.93	99.19	106.81
4	A	501	MRK	C20-C21-N17	4.61	110.65	106.46
4	A	501	MRK	C22-N17-C21	3.16	130.37	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	MRK	C20-N19-C18	-2.87	99.07	106.98
4	A	501	MRK	C5-N6-C7	2.78	128.28	123.67
4	A	501	MRK	C15-C13-C12	-2.59	119.34	122.98
4	A	501	MRK	F14-C13-C12	2.32	121.89	118.40
4	A	501	MRK	C22-N17-C18	2.07	130.44	127.02

There are no chirality outliers.

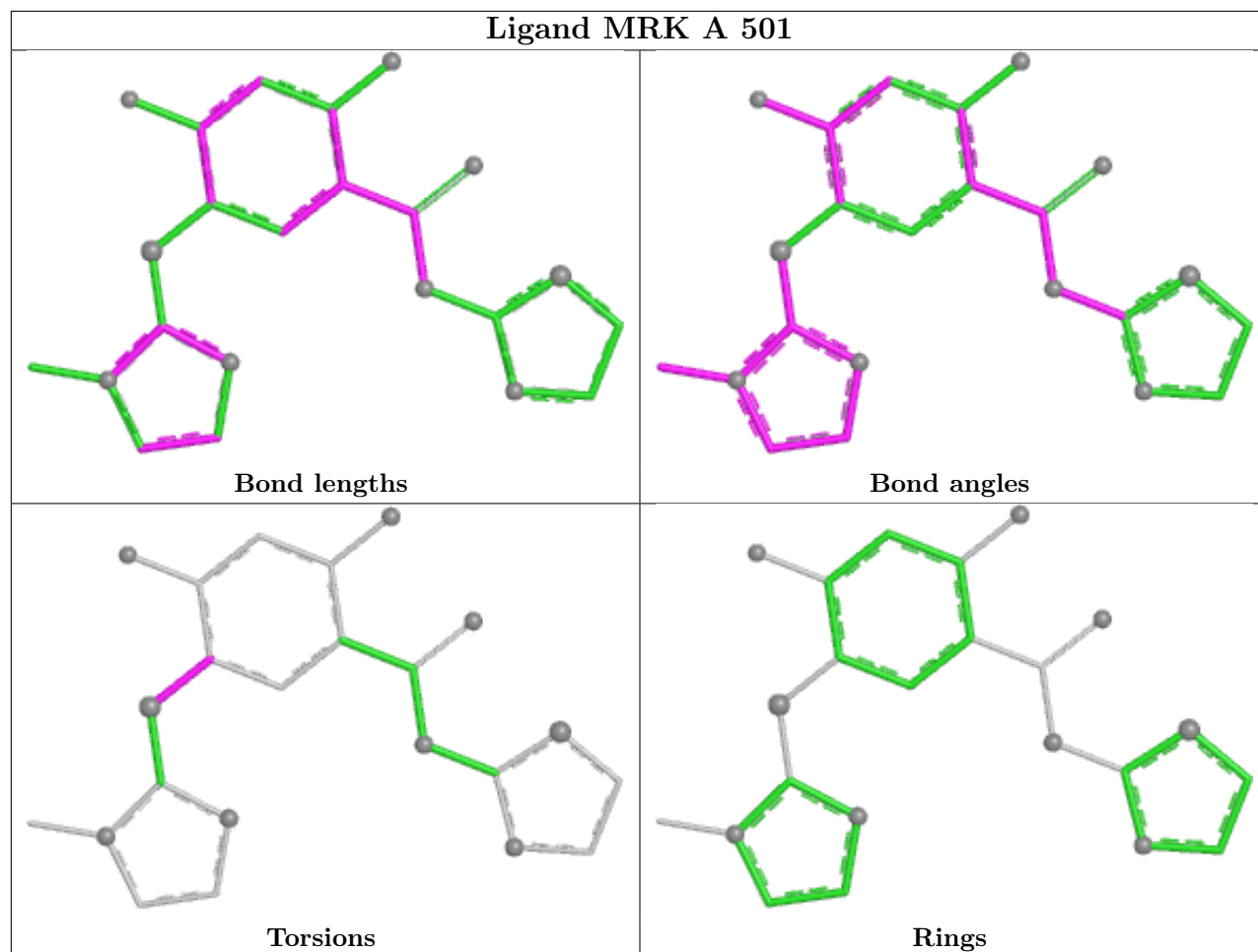
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	MRK	C11-C12-S16-C18
4	A	501	MRK	C13-C12-S16-C18

There are no ring outliers.

No monomer is involved in short contacts.

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	A	448/455 (98%)	0.86	79 (17%) 4 4	20, 42, 90, 104	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	LEU	7.1
1	A	147	GLY	4.8
1	A	461	CYS	4.5
1	A	197	MET	4.5
1	A	189	ILE	4.4
1	A	66	PRO	4.3
1	A	460	ALA	4.1
1	A	116	THR	4.1
1	A	459	LYS	3.8
1	A	65	THR	3.7
1	A	119	ALA	3.7
1	A	195	PHE	3.7
1	A	190	LYS	3.7
1	A	139	MET	3.6
1	A	141	HIS	3.6
1	A	89	VAL	3.5
1	A	145	PRO	3.5
1	A	15	LEU	3.5
1	A	457	CYS	3.5
1	A	96	GLU	3.5
1	A	146	LEU	3.4
1	A	114	ALA	3.4
1	A	187	ASP	3.4
1	A	137	HIS	3.1
1	A	133	PHE	3.1
1	A	127	SER	3.1
1	A	71	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	118	THR	3.0
1	A	92	GLY	3.0
1	A	88	LEU	3.0
1	A	456	ALA	2.9
1	A	94	GLY	2.9
1	A	143	LYS	2.9
1	A	200	VAL	2.9
1	A	110	ILE	2.9
1	A	81	GLY	2.8
1	A	115	MET	2.8
1	A	142	LYS	2.8
1	A	397	ARG	2.8
1	A	175	GLY	2.8
1	A	193	GLY	2.7
1	A	70	GLU	2.7
1	A	95	GLU	2.7
1	A	191	ARG	2.7
1	A	134	LEU	2.7
1	A	188	ALA	2.6
1	A	91	VAL	2.6
1	A	317	HIS	2.6
1	A	442	GLU	2.5
1	A	444	GLY	2.5
1	A	130	ILE	2.5
1	A	192	ARG	2.5
1	A	173	ALA	2.4
1	A	445	SER	2.4
1	A	215	TYR	2.4
1	A	194	ASP	2.4
1	A	201	ALA	2.4
1	A	120	GLU	2.4
1	A	99	TRP	2.4
1	A	125	TYR	2.3
1	A	68	GLY	2.3
1	A	458	LYS	2.3
1	A	174	SER	2.3
1	A	176	ALA	2.3
1	A	14	THR	2.3
1	A	82	THR	2.3
1	A	321	SER	2.2
1	A	77	LEU	2.2
1	A	454	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	87	MET	2.2
1	A	117	GLY	2.2
1	A	184	LEU	2.1
1	A	178	GLY	2.1
1	A	399	GLU	2.1
1	A	111	PRO	2.1
1	A	326	THR	2.0
1	A	186	ARG	2.0
1	A	121	MET	2.0
1	A	131	SER	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](#)

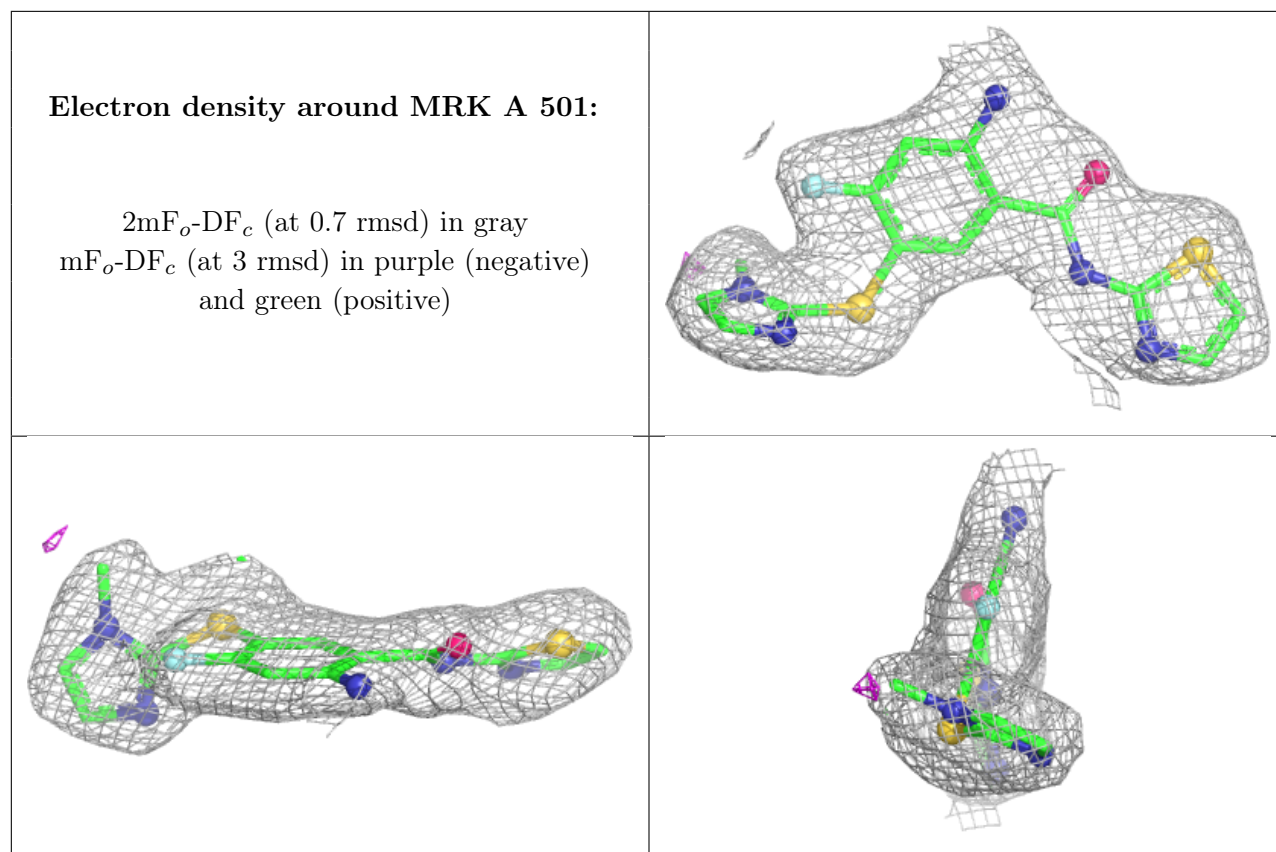
There are no oligosaccharides in this entry.

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	MRK	A	501	23/23	0.93	0.09	33,46,50,50	0
2	GLC	A	500	12/12	0.94	0.08	27,30,33,37	0
3	NA	A	600	1/1	0.96	0.06	48,48,48,48	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.