



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:59 PM UTC

PDB ID : 6S2K / pdb_00006s2k
Title : Human Menin in complex with AJ21
Authors : Groves, M.R.; Gao, K.
Deposited on : 2019-06-21
Resolution : 3.10 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

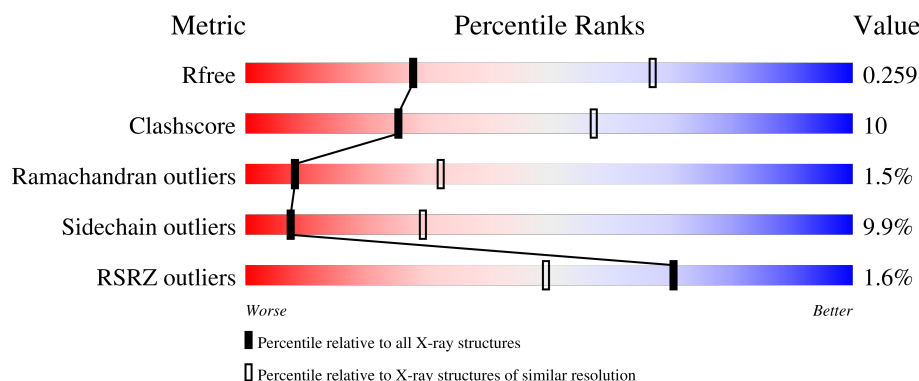
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	A	526	
1	B	526	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7284 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 Multiple endocrine neoplasia I, isoform CRA_b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3645	2343	616	672	14			
1	B	463	Total	C	N	O	S	0	0	0
			3610	2320	611	665	14			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A024R5E3
A	2	ALA	-	expression tag	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	TRP	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	SER	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	LEU	deletion	UNP A0A024R5E3
A	?	-	ASP	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	LEU	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLN	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	VAL	deletion	UNP A0A024R5E3
A	?	-	SER	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
B	1	GLY	-	expression tag	UNP A0A024R5E3
B	2	ALA	-	expression tag	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3

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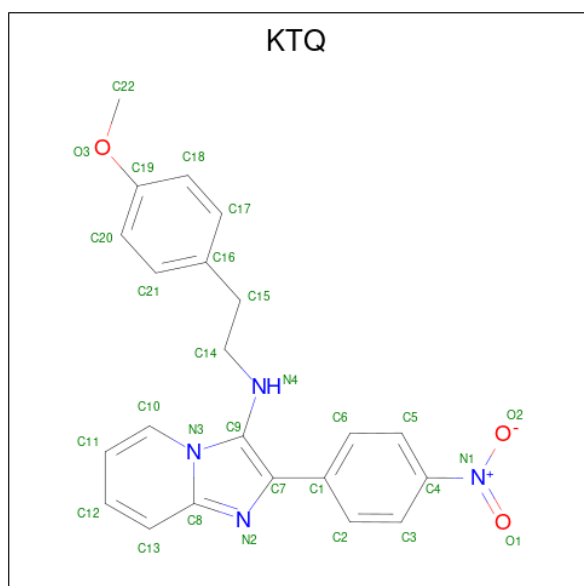
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	TRP	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	SER	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	LEU	deletion	UNP A0A024R5E3
B	?	-	ASP	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	LEU	deletion	UNP A0A024R5E3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	THR	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	GLN	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	VAL	deletion	UNP A0A024R5E3
B	?	-	SER	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3

- Molecule 2 is {N}-[2-(4-methoxyphenyl)ethyl]-2-(4-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (CCD ID: KTQ) (formula: C₂₂H₂₀N₄O₃).

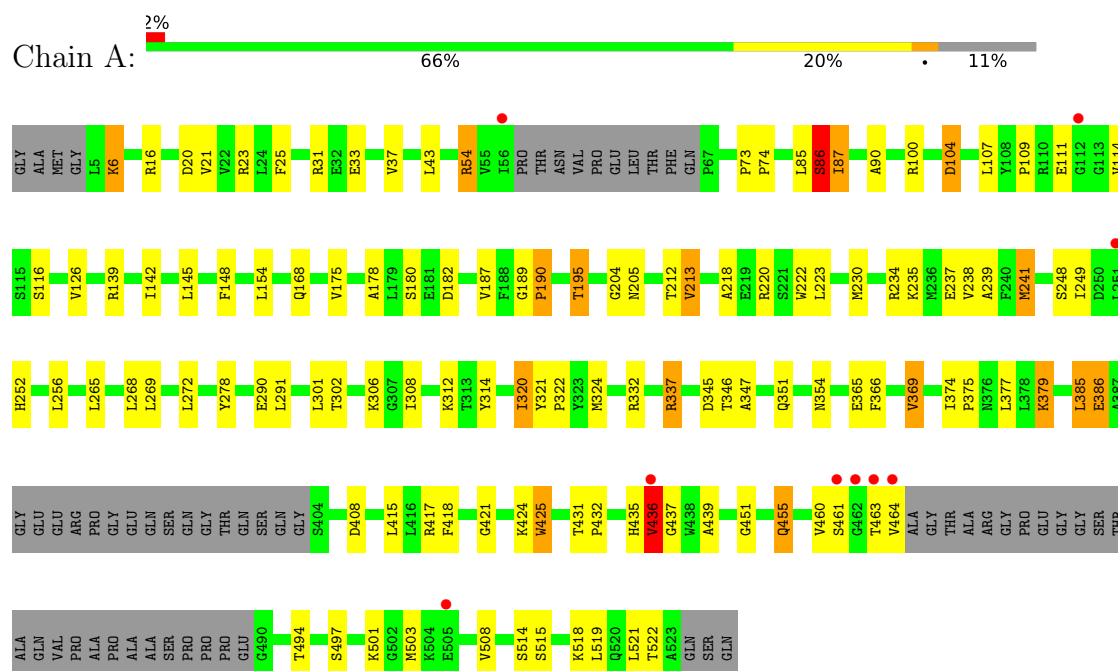


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			29	22	4	3		

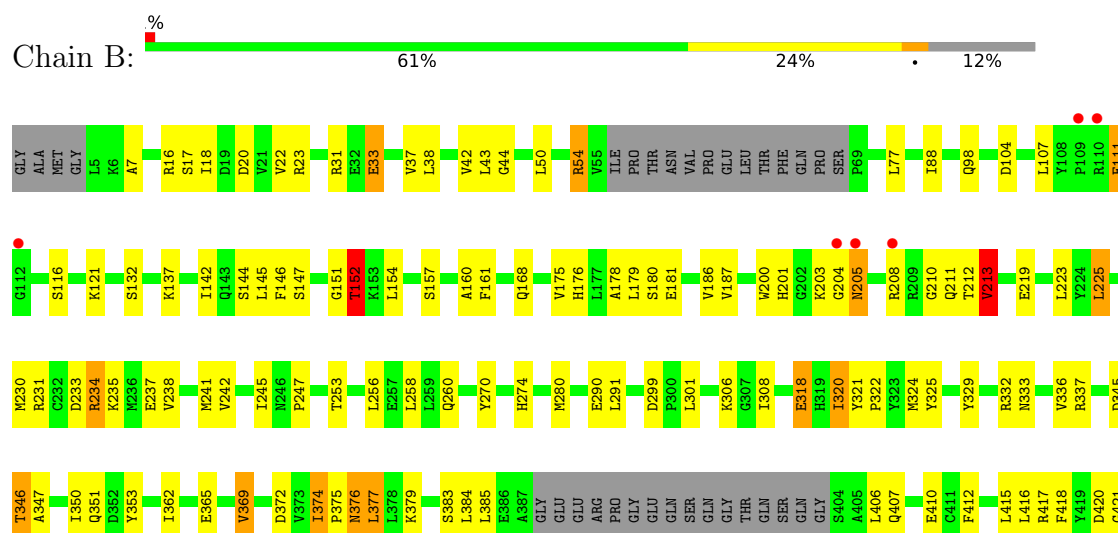
3 Residue-property plots [i](#)

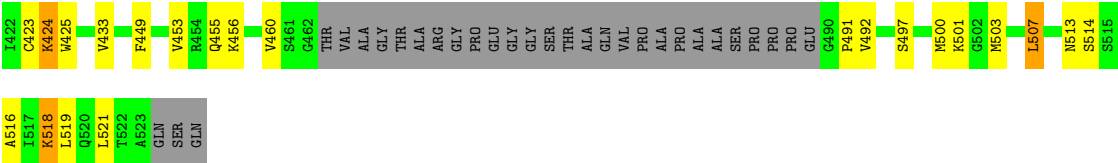
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Multiple endocrine neoplasia I, isoform CRA_b



- Molecule 1: Multiple endocrine neoplasia I, isoform CRA_b





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.40Å 101.31Å 126.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 3.10 47.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.04-3.10) 95.3 (47.04-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.300 (Not available) , 0.259	Depositor DCC
R_{free} test set	947 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7284	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.96% 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: KTQ

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	1.03	0/3729	1.54	16/5069 (0.3%)
1	B	1.03	0/3693	1.56	11/5018 (0.2%)
All	All	1.03	0/7422	1.55	27/10087 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	TRP	CA-C-N	6.17	129.36	120.79
1	B	425	TRP	C-N-CA	6.17	129.36	120.79
1	B	152	THR	CB-CA-C	6.03	120.30	111.73
1	A	522	THR	CA-C-O	-6.01	115.61	121.02
1	A	306	LYS	CA-C-N	5.92	126.39	119.94
1	A	306	LYS	C-N-CA	5.92	126.39	119.94
1	A	425	TRP	CA-C-N	5.69	129.36	120.82
1	A	425	TRP	C-N-CA	5.69	129.36	120.82
1	B	425	TRP	O-C-N	5.46	127.71	122.03
1	A	104	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	126	VAL	CA-C-N	5.24	127.25	120.70
1	A	126	VAL	C-N-CA	5.24	127.25	120.70
1	A	218	ALA	CA-C-N	5.24	128.03	120.38
1	A	218	ALA	C-N-CA	5.24	128.03	120.38
1	B	233	ASP	CA-C-O	-5.22	115.78	121.89
1	B	88	ILE	CA-C-N	5.21	127.26	120.28
1	B	88	ILE	C-N-CA	5.21	127.26	120.28
1	B	299	ASP	CB-CA-C	5.19	117.62	109.27
1	A	436	VAL	CA-C-N	5.16	125.71	119.98
1	A	436	VAL	C-N-CA	5.16	125.71	119.98
1	A	302	THR	CA-C-N	5.12	127.10	120.44
1	A	302	THR	C-N-CA	5.12	127.10	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	CA-C-N	5.11	125.65	119.98
1	A	100	ARG	C-N-CA	5.11	125.65	119.98
1	B	213	VAL	N-CA-C	-5.07	108.03	112.90
1	B	7	ALA	CA-C-N	5.05	127.30	120.38
1	B	7	ALA	C-N-CA	5.05	127.30	120.38

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	3645	0	3592	60	0
1	B	3610	0	3553	81	0
2	B	29	0	0	3	0
All	All	7284	0	7145	140	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 10.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:HG3	1:B:168:GLN:HE21	1.38	0.87
1:B:201:HIS:O	1:B:205:ASN:CB	2.30	0.80
1:A:234:ARG:HA	1:A:237:GLU:OE1	1.90	0.72
1:B:372:ASP:O	1:B:376:ASN:ND2	2.26	0.68
1:B:178:ALA:HB2	1:B:187:VAL:HG13	1.77	0.67
1:B:374:ILE:HB	1:B:375:PRO:HD3	1.76	0.67
1:A:290:GLU:OE1	1:A:332:ARG:NH1	2.28	0.66
1:B:369:VAL:HG12	2:B:601:KTQ:C22	2.27	0.65
1:A:43:LEU:HD12	1:A:241:MET:HG2	1.79	0.65
1:B:521:LEU:O	1:B:521:LEU:HG	1.97	0.64
1:A:521:LEU:HG	1:A:521:LEU:O	1.97	0.64
1:B:235:LYS:HG2	1:B:274:HIS:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLU:OE1	1:B:332:ARG:NH1	2.31	0.63
1:A:435:HIS:O	1:A:437:GLY:N	2.31	0.63
1:A:314:TYR:OH	1:B:235:LYS:NZ	2.32	0.62
1:B:208:ARG:NH2	1:B:213:VAL:HA	2.14	0.61
1:B:180:SER:OG	1:B:181:GLU:N	2.31	0.61
1:B:320:ILE:HG21	1:B:362:ILE:HD11	1.83	0.61
1:A:175:VAL:O	1:A:234:ARG:NH2	2.34	0.60
1:B:208:ARG:HH22	1:B:213:VAL:HA	1.66	0.60
1:B:514:SER:O	1:B:518:LYS:HG3	2.02	0.59
1:B:320:ILE:HG23	1:B:346:THR:CG2	2.33	0.58
1:B:142:ILE:O	1:B:154:LEU:HA	2.03	0.58
1:B:50:LEU:O	1:B:54:ARG:NH1	2.37	0.58
1:A:148:PHE:HB2	1:A:154:LEU:HD21	1.86	0.57
1:A:20:ASP:HA	1:A:23:ARG:HH11	1.70	0.57
1:B:320:ILE:HG23	1:B:346:THR:HG23	1.87	0.56
1:A:497:SER:O	1:A:501:LYS:HG3	2.05	0.56
1:A:230:MET:HE1	1:A:278:TYR:CD1	2.40	0.56
1:A:463:THR:HG22	1:A:501:LYS:HE3	1.87	0.56
1:B:20:ASP:OD1	1:B:23:ARG:NH1	2.39	0.55
1:B:456:LYS:O	1:B:491:PRO:HD2	2.07	0.55
1:A:182:ASP:HB2	1:A:222:TRP:CH2	2.41	0.55
1:A:234:ARG:O	1:A:237:GLU:HB2	2.08	0.54
1:A:54:ARG:HD2	1:A:249:ILE:HD13	1.90	0.54
1:B:180:SER:CB	1:B:223:LEU:O	2.56	0.54
1:B:324:MET:HE3	1:B:365:GLU:HG2	1.88	0.54
1:B:104:ASP:HB3	1:B:107:LEU:HD12	1.90	0.54
1:A:21:VAL:O	1:A:25:PHE:HD1	1.91	0.53
1:B:415:LEU:O	1:B:418:PHE:HB3	2.08	0.53
1:B:43:LEU:HD12	1:B:241:MET:HG2	1.90	0.53
1:A:114:VAL:HG13	1:A:189:GLY:HA2	1.92	0.52
1:A:415:LEU:O	1:A:418:PHE:HB3	2.10	0.52
1:B:208:ARG:O	1:B:211:GLN:HB2	2.10	0.51
1:A:238:VAL:O	1:A:241:MET:HB3	2.10	0.51
1:B:324:MET:HE2	1:B:346:THR:HG21	1.92	0.51
1:B:168:GLN:HG3	1:B:234:ARG:NH1	2.26	0.50
1:B:203:LYS:C	1:B:205:ASN:H	2.18	0.50
1:A:6:LYS:N	1:A:6:LYS:HD2	2.27	0.50
1:B:347:ALA:HA	1:B:350:ILE:HG22	1.93	0.50
1:A:37:VAL:HA	1:A:145:LEU:HD12	1.94	0.50
1:B:321:TYR:N	1:B:322:PRO:CD	2.74	0.49
1:A:351:GLN:HB2	1:A:424:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MET:HE1	1:A:278:TYR:CE1	2.48	0.49
1:A:239:ALA:HA	1:A:269:LEU:HD13	1.95	0.49
1:B:38:LEU:O	1:B:42:VAL:HG23	2.13	0.49
1:B:180:SER:OG	1:B:223:LEU:O	2.25	0.49
1:A:321:TYR:N	1:A:322:PRO:CD	2.76	0.49
1:B:374:ILE:HB	1:B:375:PRO:CD	2.41	0.49
1:A:375:PRO:O	1:A:379:LYS:HB2	2.13	0.49
1:B:321:TYR:CE1	2:B:601:KTQ:C11	2.96	0.48
1:B:497:SER:O	1:B:501:LYS:HG3	2.12	0.48
1:B:242:VAL:O	1:B:245:ILE:HG13	2.13	0.48
1:B:178:ALA:HA	1:B:230:MET:O	2.14	0.48
1:B:351:GLN:HB2	1:B:424:LYS:HB3	1.96	0.48
1:A:514:SER:O	1:A:518:LYS:HG3	2.13	0.48
1:A:33:GLU:HG3	1:A:168:GLN:HE21	1.78	0.47
1:B:176:HIS:HD2	1:B:237:GLU:OE2	1.97	0.47
1:B:376:ASN:HD22	1:B:376:ASN:N	2.12	0.47
1:A:345:ASP:OD1	1:A:417:ARG:NH2	2.47	0.47
1:A:195:THR:OG1	1:A:213:VAL:HB	2.15	0.47
1:B:180:SER:HB2	1:B:223:LEU:O	2.14	0.47
1:B:203:LYS:C	1:B:205:ASN:N	2.73	0.47
1:B:329:TYR:O	1:B:333:ASN:ND2	2.48	0.47
1:A:337:ARG:NE	1:A:408:ASP:OD2	2.48	0.47
1:A:104:ASP:OD2	1:A:107:LEU:CD1	2.63	0.46
1:A:180:SER:CB	1:A:223:LEU:O	2.63	0.46
1:A:451:GLY:O	1:A:455:GLN:NE2	2.48	0.46
1:B:347:ALA:HB1	1:B:421:GLY:HA3	1.98	0.46
1:B:423:CYS:HB3	1:B:497:SER:HB2	1.97	0.46
1:B:345:ASP:OD1	1:B:417:ARG:NH2	2.49	0.46
1:A:439:ALA:HB1	1:A:518:LYS:HG2	1.98	0.46
1:B:132:SER:OG	1:B:152:THR:HG23	2.16	0.45
1:B:321:TYR:O	1:B:325:TYR:HD2	1.99	0.45
1:B:178:ALA:O	1:B:179:LEU:HD23	2.16	0.45
1:B:247:PRO:HA	1:B:258:LEU:HD12	1.99	0.45
1:B:161:PHE:HZ	1:B:241:MET:HE2	1.82	0.45
1:A:37:VAL:HA	1:A:145:LEU:CD1	2.47	0.45
1:B:420:ASP:HA	1:B:500:MET:HG3	1.98	0.45
1:A:347:ALA:HB1	1:A:421:GLY:HA3	1.98	0.45
1:B:175:VAL:O	1:B:234:ARG:NH2	2.49	0.45
1:A:85:LEU:O	1:A:86:SER:C	2.60	0.45
1:A:515:SER:O	1:A:519:LEU:HD23	2.17	0.45
1:B:280:MET:SD	1:B:321:TYR:HD2	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HG22	1:A:366:PHE:CZ	2.53	0.44
1:A:424:LYS:O	1:A:425:TRP:C	2.60	0.44
1:B:238:VAL:HA	1:B:241:MET:HE3	2.00	0.44
1:B:208:ARG:NH2	1:B:212:THR:O	2.51	0.44
1:A:73:PRO:HA	1:A:74:PRO:HD3	1.93	0.43
1:A:104:ASP:OD2	1:A:107:LEU:HD13	2.18	0.43
1:A:265:LEU:O	1:A:269:LEU:HD12	2.18	0.43
1:A:142:ILE:O	1:A:154:LEU:HA	2.18	0.43
1:B:18:ILE:O	1:B:22:VAL:HG23	2.18	0.43
1:A:321:TYR:N	1:A:322:PRO:HD2	2.33	0.43
1:A:365:GLU:O	1:A:369:VAL:HG13	2.19	0.43
1:B:168:GLN:HG3	1:B:234:ARG:HH11	1.84	0.43
1:B:270:TYR:OH	1:B:306:LYS:HE3	2.18	0.43
1:B:407:GLN:HA	1:B:453:VAL:HG21	2.01	0.43
1:A:178:ALA:HB2	1:A:187:VAL:HG13	2.00	0.43
1:A:374:ILE:HB	1:A:375:PRO:HD3	2.00	0.42
1:B:121:LYS:HD3	1:B:210:GLY:HA2	2.00	0.42
1:A:461:SER:HB3	1:A:501:LYS:HD2	2.01	0.42
1:B:151:GLY:O	1:B:152:THR:HG22	2.20	0.42
1:A:324:MET:HE3	1:A:365:GLU:HG2	2.02	0.42
1:B:365:GLU:O	1:B:369:VAL:HG13	2.19	0.42
1:A:238:VAL:HA	1:A:241:MET:HE3	2.01	0.42
1:B:318:GLU:O	1:B:353:TYR:OH	2.32	0.42
1:A:220:ARG:HB2	1:A:354:ASN:HD22	1.84	0.42
1:A:321:TYR:O	1:A:322:PRO:C	2.62	0.42
1:B:142:ILE:HA	1:B:147:SER:OG	2.20	0.42
1:B:513:ASN:O	1:B:516:ALA:N	2.47	0.42
1:B:406:LEU:HA	1:B:449:PHE:CE2	2.55	0.41
1:B:142:ILE:HA	1:B:147:SER:CB	2.51	0.41
1:B:176:HIS:CD2	1:B:237:GLU:OE2	2.73	0.41
1:A:308:ILE:HG22	1:A:312:LYS:HD2	2.03	0.41
1:A:455:GLN:HE21	1:A:455:GLN:CA	2.34	0.41
1:B:336:VAL:HG22	1:B:377:LEU:HD22	2.02	0.41
1:A:320:ILE:HG23	1:A:346:THR:HG23	2.03	0.41
1:A:385:LEU:O	1:A:386:GLU:C	2.64	0.41
1:B:412:PHE:CE2	1:B:416:LEU:HD11	2.56	0.41
1:A:268:LEU:HD11	1:A:272:LEU:HD11	2.02	0.41
1:B:37:VAL:HA	1:B:145:LEU:HD12	2.01	0.41
1:B:137:LYS:HD2	1:B:200:TRP:CZ2	2.56	0.41
1:B:321:TYR:CZ	2:B:601:KTQ:C11	3.04	0.41
1:A:87:ILE:O	1:A:90:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:SER:O	1:B:160:ALA:HB3	2.21	0.40
1:B:161:PHE:CZ	1:B:241:MET:HE2	2.55	0.40
1:B:181:GLU:HG3	1:B:225:LEU:HD21	2.02	0.40
1:B:44:GLY:HA3	1:B:146:PHE:HB3	2.03	0.40
1:B:503:MET:O	1:B:507:LEU:HG	2.22	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	460/526 (88%)	403 (88%)	47 (10%)	10 (2%)	5	24
1	B	455/526 (86%)	412 (90%)	39 (9%)	4 (1%)	14	44
All	All	915/1052 (87%)	815 (89%)	86 (9%)	14 (2%)	8	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	VAL
1	B	111	GLU
1	A	139	ARG
1	A	204	GLY
1	B	225	LEU
1	A	241	MET
1	A	385	LEU
1	B	204	GLY
1	B	205	ASN
1	A	86	SER
1	A	190	PRO
1	A	205	ASN
1	A	386	GLU

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Mol	Chain	Res	Type
1	A	109	PRO

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	A	383/435 (88%)	351 (92%)	32 (8%)	10	35
1	B	378/435 (87%)	335 (89%)	43 (11%)	5	23
All	All	761/870 (88%)	686 (90%)	75 (10%)	7	29

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	16	ARG
1	A	31	ARG
1	A	54	ARG
1	A	86	SER
1	A	87	ILE
1	A	111	GLU
1	A	116	SER
1	A	190	PRO
1	A	195	THR
1	A	212	THR
1	A	213	VAL
1	A	235	LYS
1	A	248	SER
1	A	252	HIS
1	A	256	LEU
1	A	291	LEU
1	A	301	LEU
1	A	320	ILE
1	A	337	ARG
1	A	369	VAL
1	A	377	LEU

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Mol	Chain	Res	Type
1	A	379	LYS
1	A	431	THR
1	A	432	PRO
1	A	436	VAL
1	A	455	GLN
1	A	460	VAL
1	A	464	VAL
1	A	494	THR
1	A	503	MET
1	A	508	VAL
1	B	16	ARG
1	B	17	SER
1	B	31	ARG
1	B	33	GLU
1	B	54	ARG
1	B	77	LEU
1	B	98	GLN
1	B	111	GLU
1	B	116	SER
1	B	144	SER
1	B	152	THR
1	B	186	VAL
1	B	213	VAL
1	B	219	GLU
1	B	231	ARG
1	B	234	ARG
1	B	253	THR
1	B	256	LEU
1	B	260	GLN
1	B	291	LEU
1	B	301	LEU
1	B	308	ILE
1	B	318	GLU
1	B	320	ILE
1	B	337	ARG
1	B	346	THR
1	B	369	VAL
1	B	374	ILE
1	B	376	ASN
1	B	377	LEU
1	B	379	LYS
1	B	383	SER

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Mol	Chain	Res	Type
1	B	384	LEU
1	B	385	LEU
1	B	410	GLU
1	B	424	LYS
1	B	433	VAL
1	B	455	GLN
1	B	460	VAL
1	B	492	VAL
1	B	507	LEU
1	B	518	LYS
1	B	519	LEU

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

Mol	Chain	Res	Type
1	A	98	GLN
1	A	176	HIS
1	A	246	ASN
1	A	274	HIS
1	A	335	ASN
1	A	354	ASN
1	A	407	GLN
1	A	455	GLN
1	B	168	GLN
1	B	176	HIS
1	B	371	ASN
1	B	376	ASN

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

1 ligand is 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	KTQ	B	601	-	32,32,32	0.70	0	41,44,44	0.89	1 (2%)

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	KTQ	B	601	-	-	8/14/16/16	0/4/4/4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	KTQ	C13-C8-N3	2.59	120.86	118.41

There are no chirality outliers.

All (8) torsion outliers are listed below:

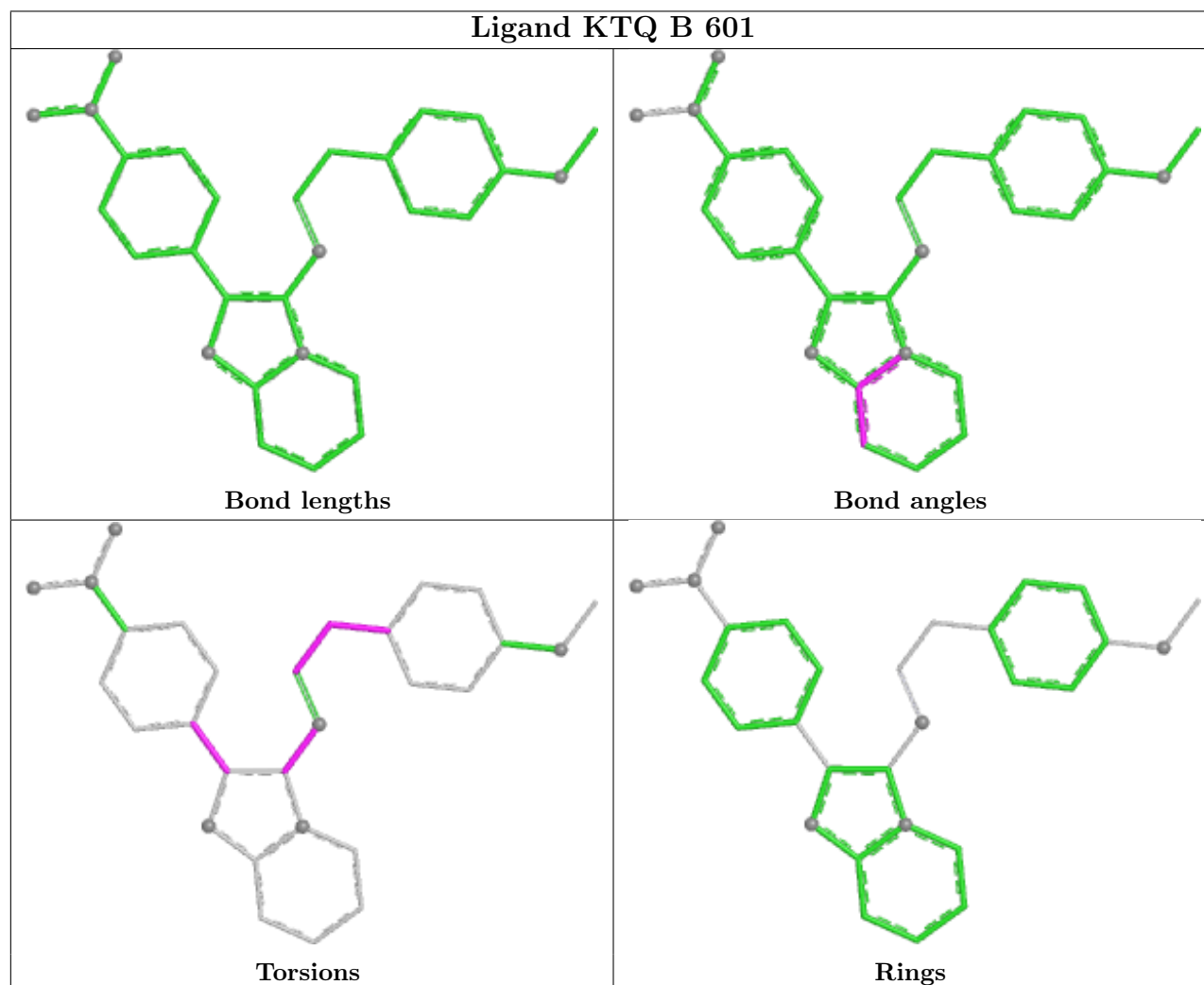
Mol	Chain	Res	Type	Atoms
2	B	601	KTQ	C2-C1-C7-C9
2	B	601	KTQ	C6-C1-C7-C9
2	B	601	KTQ	N4-C14-C15-C16
2	B	601	KTQ	C6-C1-C7-N2
2	B	601	KTQ	C2-C1-C7-N2
2	B	601	KTQ	C14-C15-C16-C21
2	B	601	KTQ	C14-C15-C16-C17
2	B	601	KTQ	C7-C9-N4-C14

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	KTQ	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	468/526 (88%)	-0.02	9 (1%) 66 45	16, 31, 57, 93	0
1	B	463/526 (88%)	0.00	6 (1%) 75 56	20, 31, 58, 79	0
All	All	931/1052 (88%)	-0.01	15 (1%) 70 49	16, 31, 58, 93	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ILE	3.7
1	A	464	VAL	2.8
1	B	112	GLY	2.8
1	B	110	ARG	2.7
1	A	505	GLU	2.6
1	A	461	SER	2.5
1	A	463	THR	2.5
1	B	204	GLY	2.5
1	A	462	GLY	2.4
1	B	109	PRO	2.4
1	A	112	GLY	2.3
1	A	436	VAL	2.3
1	B	208	ARG	2.3
1	A	251	LEU	2.3
1	B	205	ASN	2.1

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](#)

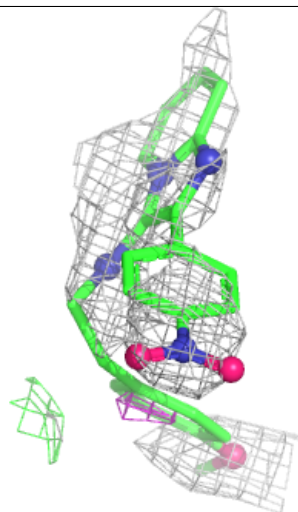
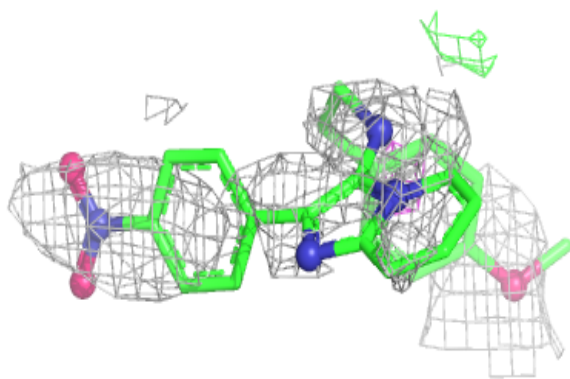
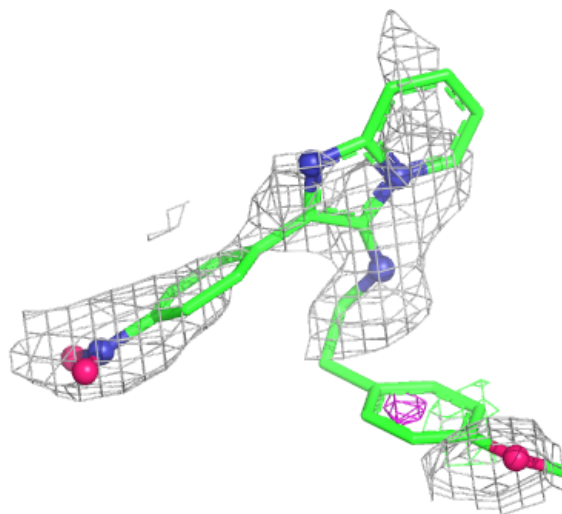
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	KTQ	B	601	29/29	0.78	0.26	77,100,120,123	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 KTQ B 601:

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.