Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:33 am BST

PDB ID	:	6RSU
Title	:	TBK1 in complex with Inhibitor compound 35
Authors	:	Panne, D.; Hillig, R.C.; Rengachari, S.
Deposited on	:	2019-05-22
Resolution	:	2.75 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 following versions of software and data (see references ⓘ) were used in the production of this report:

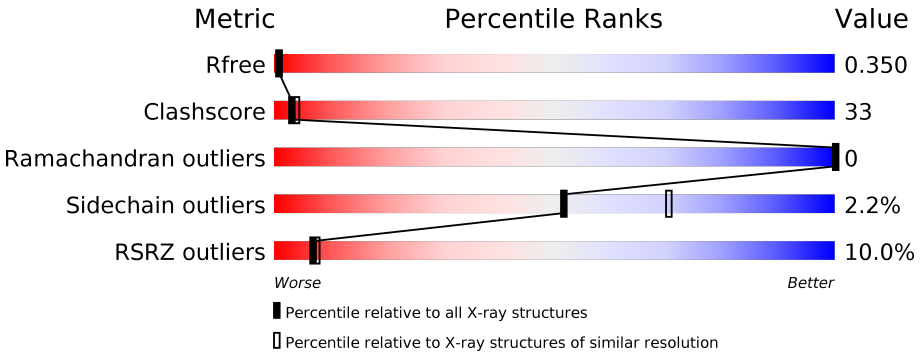
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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 <=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	663	10%, 51%, 35%, 7%, 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10162 atoms, of which 5059 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.

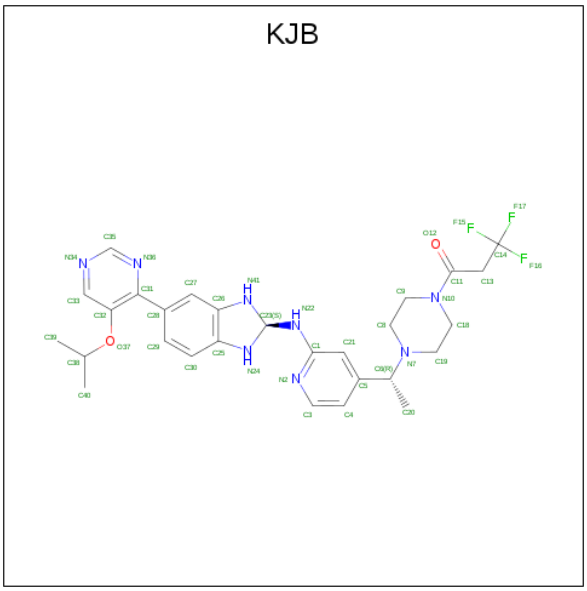
- Molecule 1 is a protein called Serine/threonine-protein kinase TBK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	628	Total	C	H	N	O	S	0	0	0
			10121	3225	5059	868	944	25			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9UHD2
A	-4	SER	-	expression tag	UNP Q9UHD2
A	-3	GLY	-	expression tag	UNP Q9UHD2
A	-2	SER	-	expression tag	UNP Q9UHD2
A	-1	ALA	-	expression tag	UNP Q9UHD2
A	0	MET	-	expression tag	UNP Q9UHD2
A	1	GLY	-	expression tag	UNP Q9UHD2

- Molecule 2 is 3,3,3-tris(fluoranyl)-1-[4-[(1 {R})-1-[2-[[(2 {S})-5-(5-propan-2-yloxypyrimidin-4-yl)-2,3-dihydro-1 {H}-benzimidazol-2-yl]amino]pyridin-4-yl]ethyl]piperazin-1-yl]propan-1-one (three-letter code: KJB) (formula: $C_{28}H_{33}F_3N_8O_2$) (labeled as "Ligand of Interest" by author).



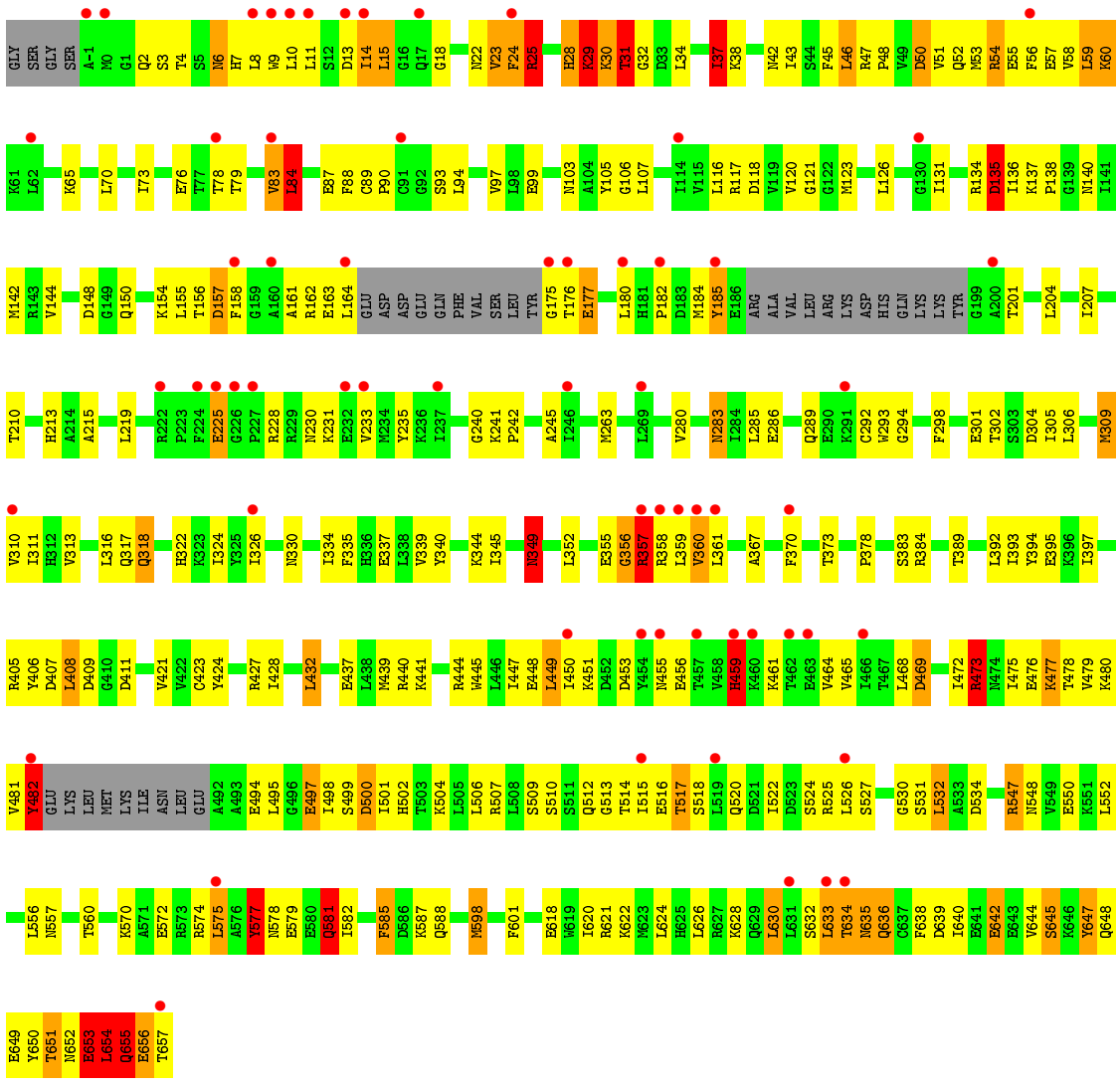
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	41	28	3	8	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Serine/threonine-protein kinase TBK1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.56Å 136.56Å 87.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.90 – 2.75 48.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	73.7 (48.90-2.75) 73.7 (48.95-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.289 , 0.351 0.289 , 0.350	Depositor DCC
R_{free} test set	892 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	99.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10162	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: KJB

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	1.77	54/5166 (1.0%)	1.44	103/6976 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	32

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	653	GLU	CD-OE1	46.18	1.76	1.25
1	A	357	ARG	CZ-NH2	38.90	1.83	1.33
1	A	653	GLU	CB-CG	35.06	2.18	1.52
1	A	653	GLU	CD-OE2	30.53	1.59	1.25
1	A	581	GLN	CB-CG	28.75	2.30	1.52
1	A	581	GLN	CG-CD	24.54	2.07	1.51
1	A	585	PHE	CE1-CZ	-22.57	0.94	1.37
1	A	585	PHE	CE2-CZ	-21.80	0.95	1.37
1	A	654	LEU	CG-CD2	20.61	2.28	1.51
1	A	653	GLU	CG-CD	19.56	1.81	1.51
1	A	655	GLN	CD-OE1	19.22	1.66	1.24
1	A	585	PHE	CG-CD1	-17.89	1.11	1.38
1	A	482	TYR	CD1-CE1	-17.34	1.13	1.39
1	A	581	GLN	CD-NE2	14.58	1.69	1.32
1	A	581	GLN	CD-OE1	14.54	1.55	1.24
1	A	482	TYR	CD2-CE2	-14.51	1.17	1.39
1	A	654	LEU	CG-CD1	-13.77	1.00	1.51
1	A	655	GLN	CG-CD	12.48	1.79	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	PHE	CD1-CE1	12.21	1.63	1.39
1	A	24	PHE	CE2-CZ	-11.36	1.15	1.37
1	A	356	GLY	C-O	11.02	1.41	1.23
1	A	577	TYR	CE1-CZ	10.22	1.51	1.38
1	A	30	LYS	CD-CE	10.16	1.76	1.51
1	A	24	PHE	CG-CD2	-9.88	1.24	1.38
1	A	577	TYR	CD1-CE1	9.71	1.53	1.39
1	A	29	LYS	CE-NZ	-9.19	1.26	1.49
1	A	31	THR	C-O	8.48	1.39	1.23
1	A	656	GLU	CA-CB	8.35	1.72	1.53
1	A	654	LEU	CB-CG	7.92	1.75	1.52
1	A	29	LYS	N-CA	7.84	1.62	1.46
1	A	497	GLU	CB-CG	7.82	1.67	1.52
1	A	654	LEU	CA-CB	7.79	1.71	1.53
1	A	357	ARG	CD-NE	-7.49	1.33	1.46
1	A	28	HIS	C-N	7.17	1.50	1.34
1	A	31	THR	C-N	-6.90	1.20	1.33
1	A	24	PHE	CE1-CZ	-6.47	1.25	1.37
1	A	654	LEU	CA-C	6.32	1.69	1.52
1	A	29	LYS	CA-C	6.28	1.69	1.52
1	A	357	ARG	CZ-NH1	6.24	1.41	1.33
1	A	357	ARG	NE-CZ	-6.16	1.25	1.33
1	A	29	LYS	C-N	-6.08	1.20	1.34
1	A	31	THR	CB-CG2	-6.08	1.32	1.52
1	A	360	VAL	CB-CG1	6.04	1.65	1.52
1	A	585	PHE	CB-CG	-6.01	1.41	1.51
1	A	30	LYS	CE-NZ	-5.84	1.34	1.49
1	A	656	GLU	CB-CG	5.83	1.63	1.52
1	A	459	HIS	ND1-CE1	-5.79	1.20	1.34
1	A	494	GLU	CB-CG	5.76	1.63	1.52
1	A	54	ARG	CZ-NH2	5.73	1.40	1.33
1	A	29	LYS	C-O	5.61	1.34	1.23
1	A	654	LEU	C-N	5.43	1.46	1.34
1	A	577	TYR	CD2-CE2	5.39	1.47	1.39
1	A	54	ARG	CZ-NH1	5.17	1.39	1.33
1	A	477	LYS	CD-CE	-5.16	1.38	1.51

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	ARG	NE-CZ-NH2	-20.90	109.85	120.30
1	A	357	ARG	NH1-CZ-NH2	16.13	137.15	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	ARG	NE-CZ-NH1	-15.99	112.30	120.30
1	A	585	PHE	CB-CG-CD2	15.80	131.86	120.80
1	A	449	LEU	CB-CG-CD2	-14.14	86.97	111.00
1	A	654	LEU	CB-CA-C	13.95	136.70	110.20
1	A	135	ASP	CB-CG-OD1	-12.12	107.39	118.30
1	A	449	LEU	CB-CG-CD1	11.57	130.68	111.00
1	A	10	LEU	CB-CG-CD2	11.24	130.10	111.00
1	A	30	LYS	CD-CE-NZ	10.82	136.59	111.70
1	A	585	PHE	CD1-CG-CD2	-10.47	104.69	118.30
1	A	655	GLN	CA-C-N	10.32	139.90	117.20
1	A	135	ASP	CB-CG-OD2	10.28	127.55	118.30
1	A	500	ASP	CB-CG-OD2	9.96	127.26	118.30
1	A	50	ASP	CB-CG-OD1	9.62	126.96	118.30
1	A	656	GLU	N-CA-CB	9.54	127.76	110.60
1	A	219	LEU	CB-CG-CD2	9.51	127.16	111.00
1	A	654	LEU	CB-CG-CD2	9.34	126.88	111.00
1	A	653	GLU	OE1-CD-OE2	-9.20	112.27	123.30
1	A	432	LEU	CB-CG-CD2	8.85	126.05	111.00
1	A	577	TYR	CB-CG-CD1	-8.84	115.70	121.00
1	A	24	PHE	CB-CG-CD2	8.82	126.97	120.80
1	A	477	LYS	CG-CD-CE	-8.76	85.63	111.90
1	A	185	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	A	14	ILE	CG1-CB-CG2	-7.95	93.91	111.40
1	A	655	GLN	N-CA-CB	-7.88	96.42	110.60
1	A	655	GLN	CA-CB-CG	7.65	130.23	113.40
1	A	185	TYR	CB-CG-CD1	7.56	125.54	121.00
1	A	408	LEU	CB-CG-CD2	7.54	123.81	111.00
1	A	30	LYS	CA-CB-CG	-7.45	97.00	113.40
1	A	654	LEU	N-CA-CB	-7.42	95.56	110.40
1	A	655	GLN	O-C-N	-7.28	111.05	122.70
1	A	655	GLN	CA-C-O	-7.25	104.88	120.10
1	A	497	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	A	581	GLN	CB-CG-CD	-7.10	93.13	111.60
1	A	585	PHE	CD1-CE1-CZ	7.06	128.57	120.10
1	A	46	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	A	54	ARG	CA-CB-CG	7.02	128.84	113.40
1	A	83	VAL	CG1-CB-CG2	6.98	122.07	110.90
1	A	469	ASP	CB-CA-C	6.94	124.28	110.40
1	A	581	GLN	CB-CA-C	-6.91	96.58	110.40
1	A	517	THR	CB-CA-C	-6.88	93.02	111.60
1	A	219	LEU	CB-CG-CD1	-6.87	99.32	111.00
1	A	653	GLU	O-C-N	-6.82	111.78	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	360	VAL	CA-CB-CG2	6.72	120.98	110.90
1	A	30	LYS	O-C-N	6.70	133.42	122.70
1	A	653	GLU	CA-C-O	6.70	134.16	120.10
1	A	352	LEU	CB-CG-CD2	6.70	122.38	111.00
1	A	37	ILE	CG1-CB-CG2	6.65	126.03	111.40
1	A	653	GLU	CG-CD-OE2	-6.56	105.18	118.30
1	A	134	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	A	263	MET	CA-CB-CG	-6.51	102.23	113.30
1	A	31	THR	CB-CA-C	-6.51	94.02	111.60
1	A	53	MET	CA-CB-CG	-6.49	102.26	113.30
1	A	357	ARG	N-CA-CB	6.42	122.15	110.60
1	A	219	LEU	CA-CB-CG	-6.39	100.60	115.30
1	A	547	ARG	CG-CD-NE	-6.26	98.65	111.80
1	A	53	MET	CG-SD-CE	-6.23	90.23	100.20
1	A	24	PHE	CZ-CE2-CD2	6.15	127.48	120.10
1	A	359	LEU	CB-CG-CD1	6.11	121.39	111.00
1	A	84	LEU	CB-CG-CD1	-6.11	100.62	111.00
1	A	630	LEU	CB-CG-CD2	-6.02	100.76	111.00
1	A	654	LEU	O-C-N	-5.97	113.14	122.70
1	A	581	GLN	N-CA-CB	-5.97	99.86	110.60
1	A	482	TYR	CG-CD2-CE2	-5.95	116.54	121.30
1	A	459	HIS	CB-CA-C	-5.86	98.69	110.40
1	A	30	LYS	CA-C-O	-5.77	107.98	120.10
1	A	356	GLY	O-C-N	-5.76	113.48	122.70
1	A	34	LEU	CA-CB-CG	-5.75	102.07	115.30
1	A	31	THR	CA-C-N	5.75	127.70	116.20
1	A	477	LYS	CA-CB-CG	-5.74	100.78	113.40
1	A	54	ARG	CB-CG-CD	-5.72	96.72	111.60
1	A	482	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	A	59	LEU	CB-CG-CD2	5.69	120.67	111.00
1	A	653	GLU	C-N-CA	-5.65	107.57	121.70
1	A	84	LEU	CB-CG-CD2	5.61	120.53	111.00
1	A	155	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	A	157	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	15	LEU	CB-CG-CD2	5.56	120.46	111.00
1	A	349	ASN	N-CA-CB	5.56	120.61	110.60
1	A	46	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	157	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	318	GLN	CB-CA-C	-5.48	99.44	110.40
1	A	577	TYR	CG-CD2-CE2	5.43	125.64	121.30
1	A	150	GLN	CA-CB-CG	-5.39	101.53	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	547	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	29	LYS	CA-CB-CG	-5.37	101.60	113.40
1	A	14	ILE	CA-CB-CG2	5.33	121.56	110.90
1	A	25	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	575	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	598	MET	CA-CB-CG	-5.27	104.34	113.30
1	A	394	TYR	CB-CG-CD1	5.15	124.09	121.00
1	A	473	ARG	CA-CB-CG	-5.12	102.13	113.40
1	A	656	GLU	CB-CA-C	-5.09	100.23	110.40
1	A	31	THR	CA-CB-CG2	5.07	119.50	112.40
1	A	633	LEU	C-N-CA	-5.07	109.03	121.70
1	A	31	THR	O-C-N	-5.06	114.61	123.20
1	A	54	ARG	CB-CA-C	-5.05	100.30	110.40
1	A	634	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	500	ASP	OD1-CG-OD2	-5.02	113.76	123.30
1	A	23	VAL	CG1-CB-CG2	5.02	118.93	110.90
1	A	506	LEU	CB-CA-C	5.01	119.72	110.20

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ASP	Sidechain
1	A	154	LYS	Mainchain
1	A	157	ASP	Mainchain
1	A	158	PHE	Mainchain
1	A	161	ALA	Mainchain
1	A	25	ARG	Mainchain
1	A	283	ASN	Mainchain
1	A	289	GLN	Mainchain
1	A	294	GLY	Mainchain
1	A	31	THR	Mainchain
1	A	357	ARG	Mainchain
1	A	37	ILE	Mainchain
1	A	459	HIS	Sidechain,Mainchain
1	A	464	VAL	Mainchain
1	A	482	TYR	Sidechain
1	A	577	TYR	Sidechain
1	A	581	GLN	Sidechain
1	A	6	ASN	Mainchain
1	A	635	ASN	Mainchain
1	A	636	GLN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	640	ILE	Mainchain
1	A	642	GLU	Mainchain
1	A	645	SER	Mainchain
1	A	651	THR	Mainchain
1	A	653	GLU	Sidechain,Mainchain
1	A	654	LEU	Mainchain
1	A	655	GLN	Mainchain
1	A	84	LEU	Mainchain
1	A	87	GLU	Sidechain
1	A	99	GLU	Sidechain

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	5062	5059	5059	337	52
2	A	41	0	0	3	0
All	All	5103	5059	5059	340	52

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 33.

All (340) 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:30:LYS:CE	1:A:30:LYS:CD	1.76	1.63
1:A:654:LEU:CB	1:A:654:LEU:CG	1.75	1.57
1:A:655:GLN:CD	1:A:655:GLN:CG	1.79	1.49
1:A:653:GLU:CG	1:A:653:GLU:CD	1.81	1.46
1:A:581:GLN:CD	1:A:581:GLN:NE2	1.69	1.42
1:A:357:ARG:NH2	1:A:357:ARG:CZ	1.83	1.37
1:A:655:GLN:CD	1:A:655:GLN:OE1	1.66	1.32
1:A:29:LYS:O	1:A:30:LYS:HE2	1.35	1.25
1:A:581:GLN:CG	1:A:581:GLN:CD	2.07	1.23
1:A:653:GLU:CD	1:A:653:GLU:OE1	1.76	1.22
1:A:653:GLU:CB	1:A:653:GLU:CG	2.18	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LEU:CB	1:A:654:LEU:CD1	2.24	1.13
1:A:654:LEU:CD2	1:A:654:LEU:CG	2.28	1.12
1:A:581:GLN:CB	1:A:581:GLN:CG	2.30	1.10
1:A:137:LYS:N	1:A:140:ASN:OD1	1.86	1.09
1:A:29:LYS:O	1:A:30:LYS:CE	2.01	1.08
1:A:135:ASP:OD1	1:A:175:GLY:HA2	1.52	1.08
1:A:29:LYS:C	1:A:30:LYS:HE2	1.75	1.06
1:A:135:ASP:OD1	1:A:175:GLY:CA	2.05	1.05
1:A:14:ILE:HG22	1:A:24:PHE:HE2	1.20	1.04
1:A:14:ILE:HG22	1:A:24:PHE:CE2	1.97	1.00
1:A:135:ASP:OD1	1:A:175:GLY:N	1.94	1.00
1:A:14:ILE:HA	1:A:24:PHE:HD2	1.30	0.97
1:A:46:LEU:HD21	1:A:164:LEU:CD1	1.96	0.96
1:A:456:GLU:O	1:A:459:HIS:HB3	1.66	0.95
1:A:46:LEU:HD21	1:A:164:LEU:HD12	1.50	0.94
1:A:137:LYS:O	1:A:140:ASN:OD1	1.87	0.93
1:A:55:GLU:O	1:A:58:VAL:HG22	1.70	0.92
1:A:651:THR:O	1:A:654:LEU:CD1	2.18	0.92
1:A:14:ILE:HA	1:A:24:PHE:CD2	2.05	0.91
1:A:31:THR:OG1	1:A:32:GLY:N	2.01	0.88
1:A:137:LYS:H	1:A:140:ASN:CG	1.78	0.87
1:A:456:GLU:HA	1:A:459:HIS:CD2	2.08	0.87
1:A:73:ILE:HG13	1:A:84:LEU:CD1	2.05	0.85
1:A:137:LYS:CA	1:A:140:ASN:OD1	2.24	0.84
1:A:28:HIS:HB3	1:A:31:THR:OG1	1.77	0.83
1:A:456:GLU:HA	1:A:459:HIS:HB2	1.60	0.83
1:A:73:ILE:HG13	1:A:84:LEU:HD12	1.60	0.82
1:A:547:ARG:NH2	1:A:550:GLU:HG2	1.97	0.80
1:A:478:THR:HA	1:A:481:VAL:HG22	1.65	0.78
1:A:577:TYR:CZ	1:A:581:GLN:HG3	2.18	0.78
1:A:517:THR:OG1	1:A:518:SER:N	2.15	0.77
1:A:651:THR:O	1:A:654:LEU:HD13	1.83	0.77
1:A:311:ILE:HG23	1:A:373:THR:HG21	1.65	0.77
1:A:456:GLU:O	1:A:459:HIS:CB	2.32	0.77
1:A:9:TRP:HE1	1:A:11:LEU:HD21	1.50	0.76
1:A:655:GLN:CB	1:A:655:GLN:CD	2.54	0.76
1:A:356:GLY:HA2	1:A:445:TRP:CE3	2.22	0.75
1:A:29:LYS:HG3	1:A:30:LYS:HE2	1.71	0.73
1:A:175:GLY:HA3	1:A:180:LEU:HD21	1.70	0.73
1:A:497:GLU:CD	1:A:500:ASP:CB	2.57	0.73
1:A:55:GLU:O	1:A:58:VAL:CG2	2.35	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:HB3	1:A:449:LEU:HD11	1.71	0.72
1:A:13:ASP:O	1:A:24:PHE:HB3	1.90	0.72
1:A:456:GLU:CA	1:A:459:HIS:HB2	2.19	0.72
1:A:137:LYS:C	1:A:140:ASN:OD1	2.29	0.71
1:A:547:ARG:NH2	1:A:550:GLU:CG	2.54	0.70
1:A:73:ILE:CG1	1:A:84:LEU:CD1	2.68	0.70
1:A:48:PRO:CA	1:A:50:ASP:OD2	2.39	0.70
1:A:456:GLU:HA	1:A:459:HIS:CB	2.21	0.70
1:A:577:TYR:CE1	1:A:581:GLN:CG	2.75	0.69
1:A:456:GLU:HA	1:A:459:HIS:CG	2.27	0.69
1:A:638:PHE:HE1	1:A:642:GLU:OE2	1.74	0.69
1:A:468:LEU:HD21	1:A:472:ILE:HD11	1.73	0.69
1:A:30:LYS:CE	1:A:30:LYS:CG	2.70	0.69
1:A:636:GLN:O	1:A:639:ASP:HB2	1.93	0.69
1:A:456:GLU:C	1:A:459:HIS:HB2	2.13	0.68
1:A:78:THR:OG1	1:A:79:THR:HG23	1.95	0.67
1:A:497:GLU:OE1	1:A:500:ASP:CG	2.34	0.66
1:A:497:GLU:OE1	1:A:500:ASP:CB	2.44	0.65
1:A:123:MET:SD	1:A:136:ILE:CD1	2.85	0.65
1:A:48:PRO:C	1:A:50:ASP:OD2	2.35	0.65
1:A:655:GLN:NE2	1:A:655:GLN:CG	2.58	0.64
1:A:316:LEU:O	1:A:439:MET:CE	2.46	0.64
1:A:577:TYR:CE1	1:A:581:GLN:HG3	2.33	0.64
1:A:22:ASN:HB3	1:A:24:PHE:CE1	2.34	0.63
1:A:225:GLU:OE2	1:A:228:ARG:HD2	1.99	0.63
1:A:22:ASN:HD22	1:A:24:PHE:HZ	1.46	0.62
1:A:8:LEU:C	1:A:8:LEU:HD12	2.19	0.62
1:A:649:GLU:HG3	1:A:650:TYR:H	1.64	0.62
1:A:556:LEU:O	1:A:556:LEU:HD23	2.00	0.62
1:A:201:THR:OG1	1:A:292:CYS:SG	2.53	0.62
1:A:301:GLU:O	1:A:304:ASP:HB3	2.00	0.62
1:A:497:GLU:HG2	1:A:500:ASP:OD2	1.99	0.62
1:A:620:ILE:O	1:A:624:LEU:HD12	1.99	0.62
1:A:525:ARG:HA	1:A:530:GLY:HA3	1.80	0.61
1:A:28:HIS:HB3	1:A:31:THR:HG1	1.61	0.61
1:A:6:ASN:O	1:A:29:LYS:N	2.32	0.61
1:A:653:GLU:O	1:A:654:LEU:C	2.36	0.61
1:A:392:LEU:HD23	1:A:432:LEU:CD2	2.29	0.61
1:A:46:LEU:HD21	1:A:164:LEU:HD11	1.80	0.61
1:A:498:ILE:O	1:A:501:ILE:HG13	2.01	0.61
1:A:633:LEU:HD12	1:A:633:LEU:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLU:OE1	1:A:500:ASP:OD2	2.19	0.60
1:A:649:GLU:HG3	1:A:650:TYR:N	2.16	0.60
1:A:642:GLU:OE1	1:A:642:GLU:HA	2.02	0.60
1:A:103:ASN:CG	1:A:107:LEU:HD23	2.21	0.60
1:A:655:GLN:CD	1:A:655:GLN:HB3	2.23	0.59
1:A:655:GLN:O	1:A:655:GLN:CG	2.49	0.59
1:A:103:ASN:HB3	1:A:107:LEU:HD23	1.85	0.59
1:A:175:GLY:HA3	1:A:180:LEU:CD2	2.33	0.59
1:A:50:ASP:N	1:A:50:ASP:OD2	2.34	0.59
1:A:384:ARG:HH11	1:A:628:LYS:HE2	1.67	0.58
1:A:550:GLU:OE1	1:A:550:GLU:N	2.32	0.58
1:A:54:ARG:O	1:A:58:VAL:HG13	2.03	0.58
1:A:497:GLU:O	1:A:500:ASP:N	2.36	0.58
1:A:547:ARG:HH21	1:A:550:GLU:HG2	1.68	0.58
1:A:655:GLN:O	1:A:655:GLN:HG2	2.03	0.58
1:A:497:GLU:CD	1:A:500:ASP:HB2	2.24	0.58
1:A:497:GLU:O	1:A:498:ILE:C	2.39	0.58
1:A:116:LEU:O	1:A:120:VAL:HG22	2.04	0.57
1:A:117:ARG:HB2	1:A:306:LEU:HD22	1.86	0.57
1:A:465:VAL:HG22	1:A:512:GLN:CD	2.25	0.57
1:A:497:GLU:OE1	1:A:500:ASP:HB3	2.04	0.57
1:A:137:LYS:H	1:A:140:ASN:ND2	2.02	0.57
1:A:384:ARG:NH1	1:A:628:LYS:HE2	2.20	0.57
1:A:313:VAL:O	1:A:322:HIS:N	2.38	0.56
1:A:316:LEU:O	1:A:439:MET:HE1	2.05	0.56
1:A:73:ILE:HG12	1:A:84:LEU:HD11	1.87	0.56
1:A:180:LEU:HD22	1:A:184:MET:HE2	1.88	0.56
1:A:649:GLU:CG	1:A:650:TYR:H	2.17	0.56
1:A:360:VAL:O	1:A:360:VAL:HG13	2.06	0.56
1:A:318:GLN:HA	1:A:389:THR:HA	1.88	0.56
1:A:579:GLU:HA	1:A:582:ILE:HG12	1.87	0.56
1:A:105:TYR:OH	1:A:421:VAL:HG22	2.05	0.56
1:A:456:GLU:C	1:A:459:HIS:CB	2.72	0.56
1:A:618:GLU:HA	1:A:621:ARG:HE	1.71	0.56
1:A:654:LEU:CB	1:A:654:LEU:HD12	2.32	0.56
1:A:473:ARG:O	1:A:477:LYS:N	2.39	0.55
1:A:55:GLU:C	1:A:58:VAL:HG22	2.25	0.55
1:A:11:LEU:N	1:A:11:LEU:HD23	2.20	0.55
1:A:14:ILE:CA	1:A:24:PHE:HD2	2.13	0.55
1:A:524:SER:O	1:A:527:SER:OG	2.24	0.55
1:A:50:ASP:CG	1:A:51:VAL:H	2.10	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HA	1:A:476:GLU:HB3	1.89	0.55
1:A:30:LYS:HE2	1:A:30:LYS:CD	2.19	0.55
1:A:577:TYR:CZ	1:A:581:GLN:CG	2.90	0.55
1:A:58:VAL:HG23	1:A:59:LEU:HD23	1.89	0.54
1:A:392:LEU:HD23	1:A:432:LEU:HD23	1.89	0.54
1:A:117:ARG:NH1	1:A:118:ASP:OD1	2.40	0.54
1:A:468:LEU:HD23	1:A:469:ASP:N	2.22	0.54
1:A:478:THR:CA	1:A:481:VAL:HG22	2.34	0.54
1:A:654:LEU:CB	1:A:654:LEU:HD13	2.32	0.54
1:A:73:ILE:CG1	1:A:84:LEU:HD11	2.37	0.54
1:A:656:GLU:OE2	1:A:657:THR:N	2.40	0.54
1:A:384:ARG:O	1:A:624:LEU:HD23	2.06	0.53
1:A:316:LEU:O	1:A:439:MET:HE3	2.07	0.53
1:A:45:PHE:CE2	1:A:46:LEU:HG	2.43	0.53
1:A:654:LEU:CB	1:A:654:LEU:HG	2.17	0.53
1:A:408:LEU:HD11	1:A:575:LEU:HD12	1.91	0.53
1:A:451:LYS:O	1:A:455:ASN:N	2.42	0.53
1:A:241:LYS:NZ	1:A:245:ALA:O	2.40	0.53
1:A:522:ILE:HG23	1:A:626:LEU:HD11	1.90	0.53
1:A:468:LEU:C	1:A:468:LEU:HD23	2.30	0.53
1:A:461:LYS:HE3	1:A:465:VAL:HG21	1.90	0.52
1:A:547:ARG:NH2	1:A:550:GLU:CB	2.73	0.52
1:A:577:TYR:CE1	1:A:581:GLN:HG2	2.44	0.52
1:A:48:PRO:CB	1:A:50:ASP:OD2	2.57	0.52
1:A:317:GLN:O	1:A:389:THR:HG22	2.09	0.52
1:A:240:GLY:O	1:A:242:PRO:HD3	2.10	0.52
1:A:356:GLY:N	1:A:445:TRP:CZ3	2.73	0.52
1:A:57:GLU:O	1:A:60:LYS:HE3	2.10	0.52
1:A:638:PHE:CE1	1:A:642:GLU:OE2	2.59	0.52
1:A:656:GLU:CD	1:A:657:THR:H	2.13	0.52
1:A:450:ILE:O	1:A:453:ASP:HB2	2.09	0.52
1:A:636:GLN:HA	1:A:639:ASP:HB2	1.91	0.52
1:A:48:PRO:C	1:A:50:ASP:H	2.13	0.52
1:A:103:ASN:CB	1:A:107:LEU:HD23	2.39	0.52
1:A:126:LEU:HD13	1:A:131:ILE:O	2.10	0.52
1:A:292:CYS:SG	1:A:293:TRP:N	2.82	0.51
1:A:392:LEU:HD23	1:A:432:LEU:HD21	1.92	0.51
1:A:633:LEU:HD12	1:A:633:LEU:N	2.25	0.51
1:A:48:PRO:HB2	1:A:50:ASP:OD2	2.11	0.51
1:A:231:LYS:O	1:A:231:LYS:HG2	2.11	0.51
1:A:340:TYR:O	1:A:344:LYS:HA	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TRP:CD1	1:A:11:LEU:CD2	2.93	0.51
1:A:29:LYS:C	1:A:30:LYS:CE	2.62	0.51
1:A:103:ASN:OD1	1:A:107:LEU:CD2	2.58	0.51
1:A:177:GLU:O	1:A:185:TYR:CE2	2.64	0.51
1:A:515:ILE:HD12	1:A:516:GLU:N	2.26	0.51
1:A:70:LEU:HD11	1:A:84:LEU:HD12	1.93	0.51
1:A:9:TRP:CD1	1:A:11:LEU:HD23	2.46	0.51
1:A:136:ILE:HA	1:A:140:ASN:HD21	1.76	0.51
1:A:367:ALA:HA	1:A:370:PHE:CD1	2.46	0.51
1:A:517:THR:O	1:A:520:GLN:NE2	2.44	0.50
1:A:479:VAL:HG23	1:A:480:LYS:HD2	1.92	0.50
1:A:649:GLU:CG	1:A:650:TYR:N	2.74	0.50
1:A:423:CYS:SG	1:A:556:LEU:HD11	2.51	0.50
1:A:280:VAL:HA	1:A:293:TRP:CZ3	2.47	0.50
1:A:29:LYS:HG3	1:A:29:LYS:O	2.10	0.50
1:A:123:MET:SD	1:A:136:ILE:HD11	2.52	0.50
1:A:468:LEU:O	1:A:472:ILE:HG13	2.11	0.50
1:A:201:THR:O	1:A:201:THR:HG22	2.10	0.50
1:A:9:TRP:NE1	1:A:11:LEU:HD21	2.21	0.50
1:A:29:LYS:HG3	1:A:30:LYS:CE	2.40	0.50
1:A:468:LEU:HD21	1:A:509:SER:HB2	1.92	0.50
1:A:441:LYS:NZ	1:A:444:ARG:HD2	2.27	0.49
1:A:645:SER:O	1:A:648:GLN:HB3	2.12	0.49
1:A:525:ARG:CB	1:A:530:GLY:O	2.61	0.49
1:A:654:LEU:CD1	1:A:654:LEU:HB2	2.36	0.49
1:A:136:ILE:HA	1:A:140:ASN:ND2	2.26	0.49
1:A:42:ASN:OD1	1:A:45:PHE:HE1	1.95	0.49
1:A:478:THR:HA	1:A:481:VAL:CG2	2.39	0.49
1:A:504:LYS:HA	1:A:507:ARG:HB2	1.94	0.49
1:A:313:VAL:CG2	1:A:324:ILE:CD1	2.91	0.49
1:A:313:VAL:HG21	1:A:324:ILE:CD1	2.43	0.49
1:A:55:GLU:O	1:A:59:LEU:HG	2.13	0.49
1:A:456:GLU:HA	1:A:459:HIS:HD2	1.66	0.49
1:A:50:ASP:CG	1:A:51:VAL:N	2.66	0.49
1:A:468:LEU:HD12	1:A:644:VAL:CG2	2.43	0.49
1:A:424:TYR:O	1:A:427:ARG:HG2	2.11	0.48
1:A:531:SER:O	1:A:622:LYS:NZ	2.46	0.48
1:A:356:GLY:HA2	1:A:445:TRP:CD2	2.49	0.48
1:A:525:ARG:HA	1:A:530:GLY:CA	2.42	0.48
1:A:23:VAL:HA	1:A:37:ILE:O	2.13	0.48
1:A:280:VAL:HA	1:A:293:TRP:CH2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG21	1:A:324:ILE:HD13	1.96	0.48
1:A:94:LEU:HD12	1:A:97:VAL:CG1	2.44	0.48
1:A:228:ARG:O	1:A:231:LYS:HE2	2.14	0.47
1:A:373:THR:OG1	1:A:378:PRO:HA	2.14	0.47
1:A:393:ILE:O	1:A:393:ILE:HG23	2.13	0.47
1:A:634:THR:OG1	1:A:635:ASN:N	2.47	0.47
1:A:630:LEU:O	1:A:634:THR:HG23	2.15	0.47
1:A:9:TRP:NE1	1:A:11:LEU:CD2	2.77	0.47
1:A:313:VAL:CG2	1:A:324:ILE:HD13	2.45	0.47
1:A:2:GLN:OE1	1:A:76:GLU:OE2	2.32	0.47
1:A:475:ILE:HG21	1:A:501:ILE:HD11	1.96	0.47
1:A:510:SER:O	1:A:514:THR:N	2.47	0.47
1:A:525:ARG:HA	1:A:530:GLY:O	2.15	0.47
1:A:9:TRP:CZ3	1:A:37:ILE:HG21	2.50	0.47
1:A:357:ARG:HD2	1:A:357:ARG:HH11	1.40	0.47
1:A:395:GLU:O	1:A:397:ILE:HG13	2.15	0.47
1:A:441:LYS:HD2	1:A:441:LYS:HA	1.75	0.47
1:A:548:ASN:O	1:A:552:LEU:HD12	2.14	0.47
1:A:120:VAL:HG23	1:A:121:GLY:N	2.30	0.47
1:A:642:GLU:OE1	1:A:642:GLU:CA	2.63	0.47
1:A:207:ILE:HD12	1:A:207:ILE:H	1.80	0.47
1:A:405:ARG:O	1:A:587:LYS:NZ	2.48	0.47
1:A:548:ASN:O	1:A:552:LEU:CD1	2.63	0.46
1:A:534:ASP:N	1:A:534:ASP:OD1	2.39	0.46
1:A:317:GLN:OE1	1:A:383:SER:O	2.34	0.46
1:A:578:ASN:O	1:A:581:GLN:HB2	2.15	0.46
1:A:135:ASP:CG	1:A:175:GLY:N	2.67	0.46
1:A:356:GLY:CA	1:A:445:TRP:CE3	2.95	0.46
1:A:461:LYS:HE3	1:A:465:VAL:CG2	2.46	0.46
1:A:504:LYS:HE3	1:A:507:ARG:HH21	1.80	0.46
1:A:479:VAL:HG23	1:A:480:LYS:CD	2.46	0.46
1:A:29:LYS:O	1:A:30:LYS:NZ	2.44	0.46
1:A:302:THR:O	1:A:305:ILE:N	2.49	0.46
1:A:468:LEU:CD2	1:A:472:ILE:HD11	2.44	0.46
1:A:547:ARG:HH22	1:A:550:GLU:HG2	1.77	0.46
1:A:201:THR:HG21	1:A:286:GLU:O	2.15	0.46
1:A:337:GLU:O	1:A:340:TYR:HB3	2.16	0.46
1:A:9:TRP:HE1	1:A:11:LEU:CD2	2.22	0.46
1:A:345:ILE:CG2	1:A:349:ASN:OD1	2.64	0.46
1:A:56:PHE:N	1:A:56:PHE:CD1	2.82	0.46
1:A:618:GLU:HA	1:A:621:ARG:NE	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:O	1:A:311:ILE:HD13	2.16	0.45
1:A:526:LEU:HD23	1:A:526:LEU:N	2.30	0.45
1:A:547:ARG:HH21	1:A:550:GLU:CG	2.27	0.45
1:A:89:CYS:HA	1:A:144:VAL:HG12	1.98	0.45
1:A:8:LEU:HD23	1:A:29:LYS:HD2	1.98	0.45
1:A:9:TRP:CE3	1:A:37:ILE:HG21	2.51	0.45
1:A:48:PRO:HA	1:A:50:ASP:OD2	2.15	0.45
1:A:632:SER:OG	1:A:636:GLN:OE1	2.35	0.45
1:A:52:GLN:HA	1:A:55:GLU:HB2	1.99	0.45
1:A:138:PRO:HD3	1:A:210:THR:HG23	1.98	0.45
1:A:30:LYS:HE3	1:A:30:LYS:CD	2.19	0.45
1:A:448:GLU:HA	1:A:451:LYS:HG2	1.98	0.45
1:A:48:PRO:C	1:A:50:ASP:N	2.69	0.45
1:A:499:SER:O	1:A:502:HIS:HB3	2.17	0.45
1:A:638:PHE:CD1	1:A:638:PHE:O	2.69	0.45
1:A:230:ASN:O	1:A:233:VAL:HG12	2.17	0.45
1:A:309:MET:HE1	1:A:367:ALA:O	2.17	0.45
1:A:335:PHE:O	1:A:339:VAL:HG23	2.17	0.44
1:A:15:LEU:HD21	1:A:25:ARG:HB2	1.99	0.44
1:A:93:SER:HA	1:A:142:MET:HA	2.00	0.44
1:A:43:ILE:O	1:A:43:ILE:HG23	2.17	0.44
1:A:46:LEU:HB2	1:A:47:ARG:H	1.58	0.44
1:A:647:TYR:CD1	1:A:647:TYR:N	2.86	0.44
1:A:478:THR:O	1:A:481:VAL:HG22	2.18	0.44
2:A:701:KJB:C21	2:A:701:KJB:C19	2.96	0.44
1:A:360:VAL:O	1:A:361:LEU:HD23	2.18	0.43
1:A:495:LEU:HA	1:A:498:ILE:HD12	2.00	0.43
1:A:54:ARG:HD3	1:A:54:ARG:HH11	1.60	0.43
1:A:650:TYR:O	1:A:653:GLU:HB3	2.18	0.43
1:A:531:SER:O	1:A:532:LEU:HD22	2.19	0.43
1:A:437:GLU:OE1	1:A:440:ARG:NH1	2.52	0.43
1:A:557:ASN:HA	1:A:560:THR:HG22	2.00	0.43
1:A:632:SER:HA	1:A:635:ASN:OD1	2.18	0.43
1:A:636:GLN:HA	1:A:639:ASP:OD2	2.19	0.43
1:A:58:VAL:HG23	1:A:59:LEU:N	2.33	0.43
2:A:701:KJB:O37	2:A:701:KJB:C27	2.66	0.43
1:A:163:GLU:O	1:A:164:LEU:HG	2.19	0.43
1:A:29:LYS:O	1:A:30:LYS:CD	2.67	0.43
1:A:3:SER:OG	1:A:4:THR:N	2.52	0.43
1:A:497:GLU:CG	1:A:500:ASP:OD2	2.66	0.42
1:A:652:ASN:C	1:A:654:LEU:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PRO:O	1:A:235:TYR:HE1	2.02	0.42
1:A:427:ARG:HG3	1:A:428:ILE:N	2.33	0.42
1:A:94:LEU:HA	1:A:97:VAL:HG12	2.01	0.42
1:A:649:GLU:O	1:A:653:GLU:N	2.53	0.42
1:A:7:HIS:CD2	1:A:28:HIS:HA	2.54	0.42
1:A:241:LYS:HE2	1:A:285:LEU:O	2.20	0.42
1:A:330:ASN:HB3	1:A:334:ILE:HD11	2.01	0.42
1:A:88:PHE:O	1:A:90:PRO:HD3	2.19	0.42
1:A:24:PHE:O	1:A:37:ILE:HG12	2.19	0.42
1:A:447:ILE:HD13	1:A:447:ILE:HG21	1.79	0.42
1:A:510:SER:O	1:A:513:GLY:N	2.53	0.42
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.83	0.42
1:A:106:GLY:HA3	1:A:215:ALA:O	2.20	0.42
1:A:137:LYS:CB	1:A:140:ASN:OD1	2.68	0.41
1:A:409:ASP:OD2	1:A:570:LYS:HE3	2.20	0.41
1:A:408:LEU:CD1	1:A:575:LEU:HD12	2.50	0.41
1:A:441:LYS:HZ2	1:A:444:ARG:HD2	1.85	0.41
1:A:324:ILE:HG22	1:A:326:ILE:HG23	2.03	0.41
1:A:497:GLU:CD	1:A:500:ASP:OD2	2.59	0.41
1:A:598:MET:HA	1:A:601:PHE:HB3	2.02	0.41
1:A:475:ILE:N	1:A:475:ILE:HD13	2.36	0.41
1:A:76:GLU:HB3	1:A:79:THR:OG1	2.20	0.41
1:A:162:ARG:HD2	1:A:162:ARG:HA	1.81	0.41
1:A:176:THR:O	1:A:180:LEU:HG	2.20	0.41
1:A:298:PHE:O	1:A:302:THR:HG22	2.21	0.41
2:A:701:KJB:C39	2:A:701:KJB:C33	2.90	0.41
1:A:406:TYR:CD1	1:A:406:TYR:N	2.87	0.41
1:A:644:VAL:CG1	1:A:644:VAL:O	2.67	0.41
1:A:656:GLU:CD	1:A:657:THR:N	2.74	0.41
1:A:38:LYS:O	1:A:83:VAL:HA	2.20	0.41
1:A:497:GLU:OE2	1:A:500:ASP:CB	2.69	0.41
1:A:500:ASP:O	1:A:504:LYS:HD3	2.20	0.41
1:A:14:ILE:HG21	1:A:14:ILE:HD13	1.88	0.41
1:A:283:ASN:HB3	1:A:293:TRP:CE2	2.56	0.40
1:A:411:ASP:OD1	1:A:587:LYS:NZ	2.41	0.40
1:A:572:GLU:C	1:A:574:ARG:H	2.24	0.40
1:A:177:GLU:O	1:A:185:TYR:HE2	2.03	0.40
1:A:60:LYS:HE3	1:A:60:LYS:HB3	1.80	0.40
1:A:156:THR:OG1	1:A:156:THR:O	2.33	0.40
1:A:204:LEU:HA	1:A:207:ILE:HD13	2.03	0.40
1:A:406:TYR:O	1:A:407:ASP:C	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:GLU:O	1:A:653:GLU:HB2	2.22	0.40

All (52) 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:356:GLY:O	1:A:357:ARG:NH2[4_555]	0.84	1.36
1:A:581:GLN:CD	1:A:653:GLU:OE2[3_545]	1.14	1.06
1:A:356:GLY:O	1:A:357:ARG:CZ[4_555]	1.29	0.91
1:A:482:TYR:OH	1:A:482:TYR:OH[4_555]	1.33	0.87
1:A:28:HIS:O	1:A:655:GLN:NE2[6_454]	1.37	0.83
1:A:459:HIS:CE1	1:A:459:HIS:CE1[4_555]	1.43	0.77
1:A:459:HIS:CE1	1:A:459:HIS:HE1[4_555]	0.87	0.73
1:A:54:ARG:HH21	1:A:513:GLY:O[3_544]	0.87	0.73
1:A:581:GLN:CG	1:A:653:GLU:OE2[3_545]	1.55	0.65
1:A:54:ARG:NH2	1:A:513:GLY:O[3_544]	1.58	0.62
1:A:581:GLN:OE1	1:A:653:GLU:O[3_545]	1.58	0.62
1:A:581:GLN:HE21	1:A:653:GLU:OE1[3_545]	0.99	0.61
1:A:581:GLN:NE2	1:A:653:GLU:OE1[3_545]	1.59	0.61
1:A:581:GLN:HE22	1:A:653:GLU:HA[3_545]	1.01	0.59
1:A:29:LYS:O	1:A:655:GLN:OE1[6_454]	1.61	0.59
1:A:459:HIS:HE1	1:A:459:HIS:HE1[4_555]	1.04	0.56
1:A:29:LYS:HZ2	1:A:655:GLN:O[6_454]	1.05	0.55
1:A:30:LYS:HZ3	1:A:655:GLN:H[6_454]	1.06	0.54
1:A:581:GLN:OE1	1:A:653:GLU:OE2[3_545]	1.68	0.52
1:A:29:LYS:O	1:A:655:GLN:CD[6_454]	1.72	0.48
1:A:356:GLY:O	1:A:357:ARG:HH22[4_555]	1.19	0.41
1:A:30:LYS:HZ2	1:A:654:LEU:HA[6_454]	1.21	0.39
1:A:577:TYR:OH	1:A:654:LEU:O[3_545]	1.81	0.39
1:A:28:HIS:O	1:A:655:GLN:HE21[6_454]	1.24	0.36
1:A:357:ARG:HH11	1:A:357:ARG:HH11[4_555]	1.25	0.35
1:A:357:ARG:NH1	1:A:357:ARG:NH1[4_555]	1.86	0.34
1:A:581:GLN:CD	1:A:653:GLU:CD[3_545]	1.86	0.34
1:A:29:LYS:NZ	1:A:655:GLN:O[6_454]	1.86	0.34
1:A:28:HIS:O	1:A:655:GLN:HE22[6_454]	1.28	0.32
1:A:581:GLN:NE2	1:A:653:GLU:HA[3_545]	1.28	0.32
1:A:357:ARG:HH11	1:A:357:ARG:HH12[4_555]	1.31	0.29
1:A:355:GLU:OE2	1:A:445:TRP:HE1[4_555]	1.33	0.27
1:A:357:ARG:NH1	1:A:357:ARG:HH11[4_555]	1.34	0.26
1:A:588:GLN:OE1	1:A:650:TYR:HH[3_545]	1.35	0.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:O	1:A:42:ASN:ND2[6_554]	2.03	0.17
1:A:30:LYS:O	1:A:585:PHE:HZ[4_555]	1.44	0.16
1:A:28:HIS:C	1:A:655:GLN:NE2[6_454]	2.04	0.16
1:A:148:ASP:O	1:A:547:ARG:HH12[4_555]	1.45	0.15
1:A:581:GLN:CB	1:A:653:GLU:OE2[3_545]	2.06	0.14
1:A:459:HIS:CE1	1:A:459:HIS:NE2[4_555]	2.06	0.14
1:A:356:GLY:C	1:A:357:ARG:HH22[4_555]	1.47	0.13
1:A:581:GLN:NE2	1:A:653:GLU:CD[3_545]	2.07	0.13
1:A:581:GLN:NE2	1:A:653:GLU:CA[3_545]	2.08	0.12
1:A:588:GLN:OE1	1:A:650:TYR:OH[3_545]	2.08	0.12
1:A:355:GLU:OE2	1:A:445:TRP:NE1[4_555]	2.10	0.10
1:A:148:ASP:O	1:A:547:ARG:NH1[4_555]	2.12	0.08
1:A:29:LYS:C	1:A:655:GLN:CD[6_454]	2.12	0.08
1:A:30:LYS:HZ3	1:A:655:GLN:N[6_454]	1.53	0.07
1:A:459:HIS:NE2	1:A:459:HIS:HE1[4_555]	1.53	0.07
1:A:30:LYS:HZ2	1:A:654:LEU:CA[6_454]	1.53	0.07
1:A:30:LYS:NZ	1:A:654:LEU:HA[6_454]	1.54	0.06
1:A:581:GLN:HE22	1:A:653:GLU:CA[3_545]	1.55	0.05

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	620/663 (94%)	587 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	557/589 (95%)	545 (98%)	12 (2%)	52 70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	60	LYS
1	A	65	LYS
1	A	135	ASP
1	A	177	GLU
1	A	213	HIS
1	A	225	GLU
1	A	309	MET
1	A	349	ASN
1	A	473	ARG
1	A	532	LEU
1	A	647	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	181	HIS
1	A	459	HIS
1	A	502	HIS
1	A	512	GLN
1	A	583	HIS
1	A	629	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	KJB	A	701	-	42,45,45	3.12	12 (28%)	53,65,65	4.58	32 (60%)

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	KJB	A	701	-	-	4/27/47/47	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	KJB	C25-N24	-12.57	1.19	1.39
2	A	701	KJB	C28-C31	-9.10	1.38	1.49
2	A	701	KJB	C26-N41	-6.41	1.29	1.39
2	A	701	KJB	C13-C11	5.16	1.57	1.51
2	A	701	KJB	C21-C1	4.55	1.51	1.39
2	A	701	KJB	C26-C25	3.61	1.49	1.40
2	A	701	KJB	C13-C14	3.07	1.53	1.49
2	A	701	KJB	C9-N10	-2.95	1.41	1.47
2	A	701	KJB	C1-N2	-2.86	1.28	1.34
2	A	701	KJB	C18-N10	2.69	1.51	1.47
2	A	701	KJB	O37-C38	-2.41	1.39	1.45
2	A	701	KJB	C11-N10	-2.10	1.31	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	KJB	C30-C25-N24	16.63	151.99	127.98
2	A	701	KJB	C26-N41-C23	-10.52	92.27	108.85
2	A	701	KJB	C3-N2-C1	9.16	130.22	117.22
2	A	701	KJB	C4-C3-N2	-8.20	113.77	123.96
2	A	701	KJB	C30-C25-C26	-7.86	108.76	121.03
2	A	701	KJB	C5-C21-C1	-7.20	112.02	119.02
2	A	701	KJB	C25-N24-C23	6.91	119.75	108.85
2	A	701	KJB	C26-C25-N24	-6.61	98.79	108.58
2	A	701	KJB	O37-C38-C40	-5.70	87.96	107.93
2	A	701	KJB	C32-C31-N36	-5.26	117.51	121.68
2	A	701	KJB	C4-C5-C21	5.23	124.79	118.76
2	A	701	KJB	N34-C35-N36	-5.23	121.95	127.70
2	A	701	KJB	C19-C18-N10	-4.55	100.70	110.44
2	A	701	KJB	C5-C6-N7	4.54	122.29	110.51
2	A	701	KJB	C27-C26-N41	-4.48	119.68	127.92
2	A	701	KJB	C25-C26-N41	4.25	114.88	108.58
2	A	701	KJB	C29-C30-C25	4.21	127.79	119.64
2	A	701	KJB	C21-C1-N2	-4.19	116.91	122.75
2	A	701	KJB	C8-C9-N10	-3.74	102.43	110.44
2	A	701	KJB	C32-O37-C38	-3.67	112.46	119.53
2	A	701	KJB	C27-C26-C25	3.60	125.07	121.54
2	A	701	KJB	C20-C6-C5	-3.33	104.86	113.24
2	A	701	KJB	F16-C14-C13	-3.32	107.51	112.36
2	A	701	KJB	C18-N10-C9	2.76	117.93	112.62
2	A	701	KJB	C33-N34-C35	2.68	119.22	115.80
2	A	701	KJB	N22-C1-N2	-2.54	112.66	116.84
2	A	701	KJB	C35-N36-C31	2.48	121.66	117.78
2	A	701	KJB	C20-C6-N7	-2.34	107.23	112.47
2	A	701	KJB	C18-N10-C11	-2.32	115.22	122.81
2	A	701	KJB	C29-C28-C31	-2.13	117.23	120.61
2	A	701	KJB	F17-C14-C13	2.11	115.46	112.36
2	A	701	KJB	C18-C19-N7	-2.10	106.57	110.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

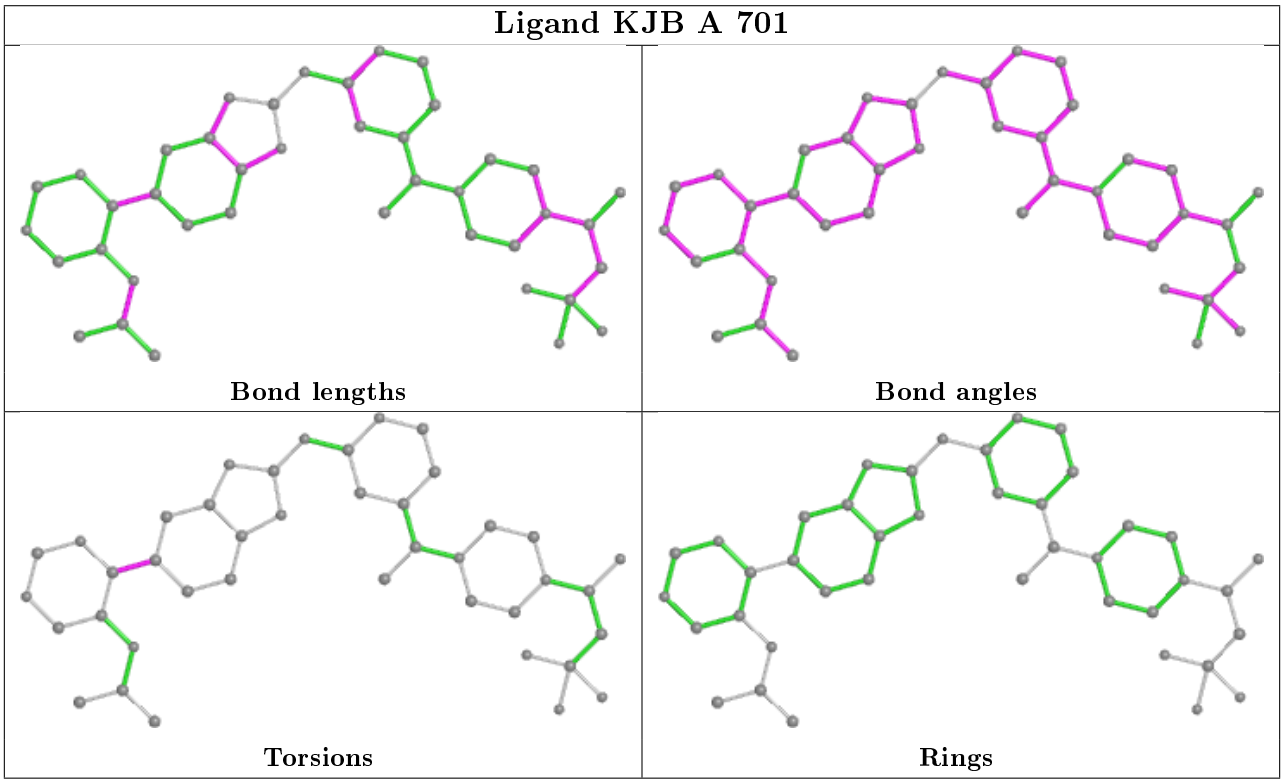
Mol	Chain	Res	Type	Atoms
2	A	701	KJB	C27-C28-C31-C32
2	A	701	KJB	C29-C28-C31-N36
2	A	701	KJB	C27-C28-C31-N36
2	A	701	KJB	C29-C28-C31-C32

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	KJB	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 then 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	29:LYS	C	30:LYS	N	1.20

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, 95^{th} 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	628/663 (94%)	0.65	63 (10%) 7 7	46, 85, 115, 133	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	HIS	11.7
1	A	482	TYR	11.5
1	A	460	LYS	8.1
1	A	226	GLY	8.1
1	A	78	THR	5.6
1	A	634	THR	5.6
1	A	-1	ALA	5.5
1	A	232	GLU	5.0
1	A	227	PRO	4.6
1	A	10	LEU	4.4
1	A	185	TYR	4.3
1	A	575	LEU	4.3
1	A	180	LEU	4.1
1	A	515	ILE	4.1
1	A	224	PHE	4.0
1	A	463	GLU	3.9
1	A	657	THR	3.8
1	A	182	PRO	3.7
1	A	360	VAL	3.6
1	A	519	LEU	3.5
1	A	361	LEU	3.4
1	A	176	THR	3.4
1	A	222	ARG	3.2
1	A	291	LYS	3.2
1	A	633	LEU	3.1
1	A	358	ARG	3.0
1	A	164	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	175	GLY	2.9
1	A	233	VAL	2.9
1	A	326	ILE	2.8
1	A	11	LEU	2.7
1	A	56	PHE	2.7
1	A	0	MET	2.7
1	A	359	LEU	2.7
1	A	462	THR	2.7
1	A	24	PHE	2.7
1	A	457	THR	2.6
1	A	225	GLU	2.5
1	A	200	ALA	2.4
1	A	14	ILE	2.4
1	A	455	ASN	2.4
1	A	237	ILE	2.4
1	A	450	ILE	2.4
1	A	246	ILE	2.3
1	A	466	ILE	2.3
1	A	62	LEU	2.3
1	A	526	LEU	2.3
1	A	631	LEU	2.2
1	A	130	GLY	2.2
1	A	370	PHE	2.2
1	A	269	LEU	2.2
1	A	8	LEU	2.2
1	A	9	TRP	2.2
1	A	158	PHE	2.2
1	A	83	VAL	2.1
1	A	17	GLN	2.1
1	A	310	VAL	2.1
1	A	91	CYS	2.1
1	A	13	ASP	2.1
1	A	357	ARG	2.1
1	A	454	TYR	2.0
1	A	114	ILE	2.0
1	A	160	ALA	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 carbohydrates in this entry.

6.4 Ligands (i)

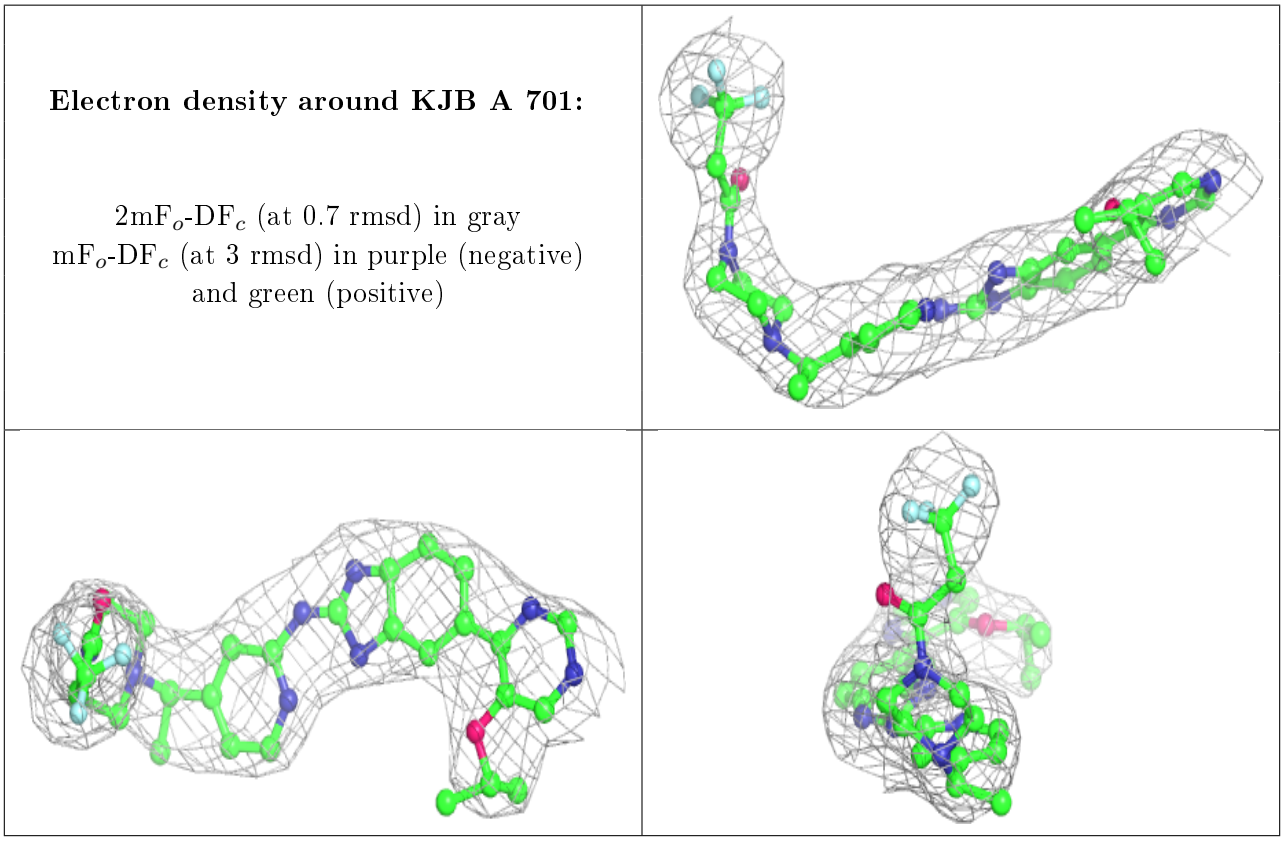
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KJB	A	701	41/41	0.94	0.24	47,64,85,105	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 KJB A 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.