



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:46 PM UTC

PDB ID : 6RSU / pdb_00006rsu
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 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

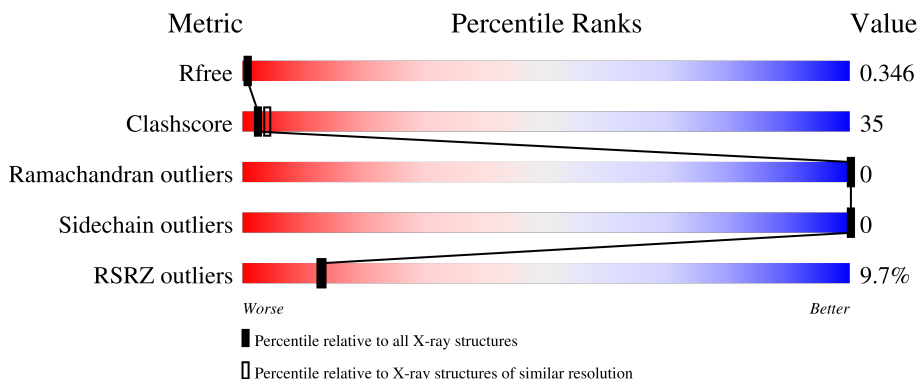
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	663	9% 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.

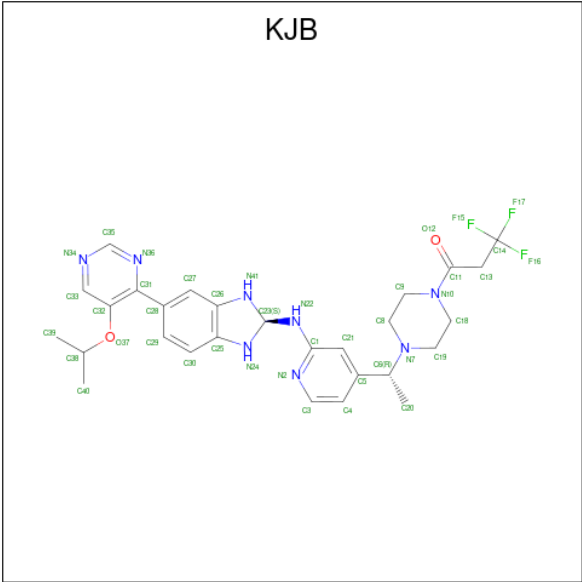
- Molecule 1 is a protein called Serine/threonine-protein kinase TBK1.

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-yloxy)pyrimidin-4-yl]-2,3-dihydro-1 {H}-benzimidazol-2-yl]amino]pyridin-4-yl]ethyl]piperazin-1-yl]propan-1-one (CCD ID: KJB) (formula: C₂₈H₃₃F₃N₈O₂) (labeled as "Ligand of Interest" by depositor).

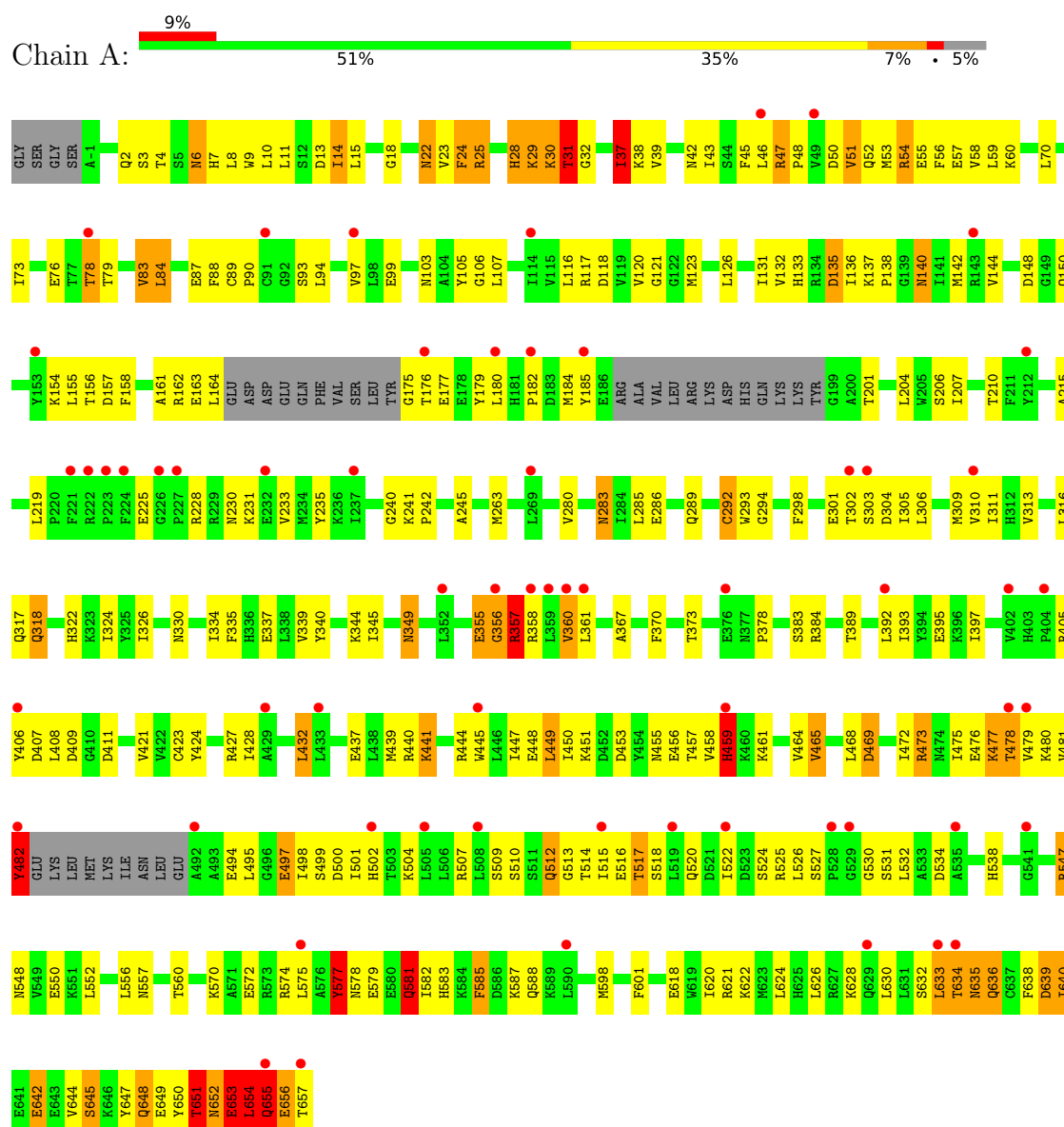


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	41	28	3	8	2	0	0

3 Residue-property plots

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: Serine/threonine-protein kinase TBK1



4 Data and refinement statistics

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 48.90 – 2.75	Depositor EDS
% Data completeness (in resolution range)	73.7 (48.90-2.75) 73.9 (48.90-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.289 , 0.351 0.288 , 0.346	Depositor DCC
R_{free} test set	8360 reflections (26.16%)	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 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	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.*

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: 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	1.65	62/5166 (1.2%)	1.54	109/6976 (1.6%)

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 (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	ARG	CZ-NH2	38.59	1.83	1.33
1	A	653	GLU	CD-OE1	26.89	1.76	1.25
1	A	581	GLN	CB-CG	25.90	2.30	1.52
1	A	654	LEU	CG-CD2	22.89	2.28	1.52
1	A	655	GLN	CD-OE1	22.46	1.66	1.23
1	A	581	GLN	CG-CD	22.18	2.07	1.52
1	A	653	GLU	CB-CG	22.10	2.18	1.52
1	A	653	GLU	CD-OE2	17.84	1.59	1.25
1	A	581	GLN	CD-NE2	17.17	1.69	1.33
1	A	581	GLN	CD-OE1	17.04	1.55	1.23
1	A	654	LEU	CG-CD1	-15.65	1.00	1.52
1	A	585	PHE	CE1-CZ	-14.73	0.94	1.38
1	A	585	PHE	CE2-CZ	-14.24	0.95	1.38
1	A	47	ARG	C-O	13.39	1.30	1.23
1	A	585	PHE	CG-CD1	-12.83	1.11	1.38
1	A	654	LEU	CA-C	12.75	1.69	1.52
1	A	31	THR	C-O	12.62	1.39	1.24
1	A	29	LYS	N-CA	12.28	1.62	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	HIS	ND1-CE1	-12.27	1.20	1.32
1	A	29	LYS	CA-C	12.25	1.69	1.52
1	A	356	GLY	C-O	12.21	1.41	1.23
1	A	28	HIS	C-N	12.01	1.50	1.34
1	A	653	GLU	CG-CD	11.70	1.81	1.52
1	A	656	GLU	CA-CB	11.17	1.72	1.53
1	A	655	GLN	CG-CD	11.09	1.79	1.52
1	A	654	LEU	CA-CB	11.07	1.71	1.53
1	A	654	LEU	CB-CG	11.04	1.75	1.53
1	A	29	LYS	C-N	-9.96	1.20	1.33
1	A	31	THR	C-N	-9.78	1.20	1.33
1	A	654	LEU	C-N	9.20	1.46	1.33
1	A	357	ARG	CD-NE	-8.95	1.33	1.46
1	A	482	TYR	CD1-CE1	-8.44	1.13	1.38
1	A	585	PHE	CD1-CE1	8.34	1.63	1.38
1	A	30	LYS	CD-CE	8.07	1.76	1.52
1	A	29	LYS	C-O	7.88	1.34	1.24
1	A	29	LYS	CE-NZ	-7.76	1.26	1.49
1	A	31	THR	CA-CB	-7.73	1.40	1.53
1	A	24	PHE	CE2-CZ	-7.63	1.15	1.38
1	A	357	ARG	NE-CZ	-7.28	1.25	1.33
1	A	47	ARG	CA-C	-7.26	1.47	1.53
1	A	24	PHE	CG-CD2	-7.10	1.24	1.38
1	A	28	HIS	C-O	7.03	1.32	1.23
1	A	482	TYR	CD2-CE2	-7.02	1.17	1.38
1	A	30	LYS	N-CA	6.65	1.54	1.46
1	A	441	LYS	C-O	-6.63	1.16	1.24
1	A	31	THR	CB-CG2	-6.14	1.32	1.52
1	A	357	ARG	CZ-NH1	6.01	1.41	1.32
1	A	150	GLN	CD-NE2	-6.00	1.20	1.33
1	A	655	GLN	CA-C	-5.79	1.45	1.52
1	A	577	TYR	CE1-CZ	5.66	1.51	1.38
1	A	459	HIS	CB-CG	-5.62	1.42	1.50
1	A	477	LYS	CG-CD	-5.60	1.35	1.52
1	A	140	ASN	CG-OD1	-5.55	1.13	1.23
1	A	31	THR	N-CA	5.54	1.53	1.46
1	A	656	GLU	N-CA	5.53	1.53	1.46
1	A	54	ARG	CZ-NH2	5.42	1.40	1.33
1	A	633	LEU	C-N	5.41	1.41	1.33
1	A	469	ASP	C-O	-5.27	1.18	1.24
1	A	577	TYR	CD1-CE1	5.09	1.53	1.38
1	A	54	ARG	CZ-NH1	5.01	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	THR	CB-CG2	-5.00	1.36	1.52
1	A	355	GLU	C-O	5.00	1.30	1.23

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	LEU	CB-CA-C	15.82	136.70	109.65
1	A	655	GLN	CA-C-O	-13.86	104.88	120.54
1	A	357	ARG	NH1-CZ-NH2	13.73	137.15	119.30
1	A	581	GLN	CB-CG-CD	-11.45	93.13	112.60
1	A	477	LYS	CG-CD-CE	-11.16	85.63	111.30
1	A	655	GLN	O-C-N	-10.67	111.05	123.22
1	A	357	ARG	NE-CZ-NH2	-10.39	109.85	119.20
1	A	656	GLU	N-CA-CB	10.39	127.76	111.24
1	A	30	LYS	CA-C-O	-9.86	107.98	120.31
1	A	654	LEU	N-CA-CB	-9.80	95.56	109.97
1	A	653	GLU	CA-C-N	-9.37	107.57	120.87
1	A	653	GLU	C-N-CA	-9.37	107.57	120.87
1	A	585	PHE	CD1-CG-CD2	-9.28	104.69	118.60
1	A	357	ARG	NE-CZ-NH1	-9.20	112.30	121.50
1	A	47	ARG	O-C-N	-9.17	117.31	121.53
1	A	31	THR	CB-CA-C	-9.11	94.02	110.70
1	A	653	GLU	CA-C-O	8.84	134.16	120.37
1	A	30	LYS	CA-CB-CG	-8.55	97.00	114.10
1	A	517	THR	CB-CA-C	-8.51	93.02	110.38
1	A	469	ASP	CB-CA-C	8.42	124.28	110.81
1	A	633	LEU	CA-C-N	-8.39	109.03	120.44
1	A	633	LEU	C-N-CA	-8.39	109.03	120.44
1	A	655	GLN	N-CA-CB	-8.33	96.42	110.16
1	A	30	LYS	O-C-N	8.23	133.42	122.30
1	A	577	TYR	N-CA-C	8.19	119.83	111.07
1	A	655	GLN	CA-CB-CG	8.07	130.23	114.10
1	A	654	LEU	O-C-N	-7.99	113.14	122.89
1	A	449	LEU	CB-CG-CD2	-7.91	86.97	110.70
1	A	356	GLY	O-C-N	-7.75	113.48	122.31
1	A	30	LYS	CD-CE-NZ	7.71	136.59	111.90
1	A	31	THR	CA-C-O	-7.61	111.79	120.24
1	A	54	ARG	CA-CB-CG	7.37	128.84	114.10
1	A	28	HIS	CA-C-O	-7.19	113.20	121.47
1	A	30	LYS	N-CA-C	7.08	122.23	112.04
1	A	655	GLN	CB-CG-CD	-6.98	100.73	112.60
1	A	653	GLU	O-C-N	-6.90	111.78	121.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ASN	N-CA-CB	6.84	120.61	110.49
1	A	292	CYS	N-CA-C	6.83	121.17	110.17
1	A	581	GLN	N-CA-CB	-6.78	99.86	110.30
1	A	581	GLN	CB-CA-C	-6.77	96.58	110.38
1	A	655	GLN	OE1-CD-NE2	6.76	129.37	122.60
1	A	31	THR	CA-CB-OG1	-6.73	99.51	109.60
1	A	449	LEU	CB-CG-CD1	6.66	130.68	110.70
1	A	477	LYS	CA-CB-CG	-6.66	100.78	114.10
1	A	585	PHE	CB-CG-CD2	6.57	131.86	120.70
1	A	14	ILE	CA-CB-CG2	6.51	121.56	110.50
1	A	655	GLN	CG-CD-NE2	-6.49	106.67	116.40
1	A	357	ARG	N-CA-CB	6.47	122.15	111.08
1	A	10	LEU	CB-CG-CD2	6.47	130.10	110.70
1	A	54	ARG	CB-CG-CD	-6.34	96.72	111.30
1	A	150	GLN	CA-CB-CG	-6.29	101.53	114.10
1	A	648	GLN	CA-C-N	6.28	133.54	121.54
1	A	648	GLN	C-N-CA	6.28	133.54	121.54
1	A	133	HIS	N-CA-C	6.27	120.80	111.96
1	A	29	LYS	CA-CB-CG	-6.25	101.60	114.10
1	A	360	VAL	CA-CB-CG2	6.22	120.98	110.40
1	A	458	VAL	N-CA-C	-6.16	104.33	110.62
1	A	547	ARG	CG-CD-NE	-6.07	98.65	112.00
1	A	656	GLU	CB-CA-C	-6.06	100.23	109.99
1	A	639	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	651	THR	CB-CA-C	6.01	122.20	110.67
1	A	473	ARG	CA-CB-CG	-5.98	102.13	114.10
1	A	459	HIS	CA-C-N	5.98	130.71	120.72
1	A	459	HIS	C-N-CA	5.98	130.71	120.72
1	A	263	MET	CA-CB-CG	-5.94	102.23	114.10
1	A	634	THR	CB-CA-C	-5.92	101.54	110.90
1	A	53	MET	CA-CB-CG	-5.92	102.26	114.10
1	A	459	HIS	CB-CA-C	-5.89	98.69	110.42
1	A	318	GLN	CB-CA-C	-5.87	99.44	109.65
1	A	31	THR	O-C-N	-5.87	114.61	122.23
1	A	459	HIS	CG-CD2-NE2	-5.84	101.36	107.20
1	A	653	GLU	CG-CD-OE2	-5.75	105.18	118.40
1	A	478	THR	CA-C-N	-5.71	110.93	120.30
1	A	478	THR	C-N-CA	-5.71	110.93	120.30
1	A	465	VAL	N-CA-C	5.64	115.72	110.42
1	A	648	GLN	CB-CA-C	-5.60	101.50	110.79
1	A	14	ILE	CG1-CB-CG2	-5.60	93.91	110.70
1	A	54	ARG	CB-CA-C	-5.58	100.30	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	THR	N-CA-C	5.56	117.42	111.36
1	A	469	ASP	CA-C-N	-5.55	111.87	120.31
1	A	469	ASP	C-N-CA	-5.55	111.87	120.31
1	A	155	LEU	CA-C-N	-5.51	111.02	121.54
1	A	155	LEU	C-N-CA	-5.51	111.02	121.54
1	A	651	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	219	LEU	CB-CG-CD2	5.49	127.16	110.70
1	A	497	GLU	CA-CB-CG	-5.43	103.23	114.10
1	A	654	LEU	CB-CG-CD2	5.39	126.88	110.70
1	A	31	THR	N-CA-CB	5.39	118.23	110.20
1	A	640	ILE	CA-CB-CG1	5.36	119.50	110.40
1	A	30	LYS	CA-C-N	5.30	129.64	120.58
1	A	30	LYS	C-N-CA	5.30	129.64	120.58
1	A	31	THR	CA-CB-CG2	5.29	119.50	110.50
1	A	39	VAL	CB-CA-C	-5.27	104.58	110.96
1	A	51	VAL	CA-C-N	-5.26	112.19	120.60
1	A	51	VAL	C-N-CA	-5.26	112.19	120.60
1	A	634	THR	CA-CB-CG2	5.26	119.44	110.50
1	A	652	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	355	GLU	O-C-N	5.20	129.38	122.41
1	A	78	THR	CB-CA-C	-5.18	100.27	110.11
1	A	22	ASN	CB-CA-C	-5.17	100.61	109.65
1	A	512	GLN	N-CA-C	-5.16	105.77	111.71
1	A	83	VAL	CG1-CB-CG2	5.12	122.07	110.80
1	A	432	LEU	CB-CG-CD2	5.12	126.05	110.70
1	A	132	VAL	CA-C-N	5.11	130.34	122.42
1	A	132	VAL	C-N-CA	5.11	130.34	122.42
1	A	37	ILE	CG1-CB-CG2	5.11	126.03	110.70
1	A	538	HIS	CB-CA-C	-5.08	102.03	110.81
1	A	494	GLU	CA-CB-CG	-5.04	104.03	114.10
1	A	156	THR	N-CA-C	5.00	121.45	110.80

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

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	5061	348	52
2	A	41	0	0	3	0
All	All	5103	5059	5061	351	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 35.

All (351) 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:CD	1:A:30:LYS:CE	1.76	1.63
1:A:654:LEU:CG	1:A:654:LEU:CB	1.75	1.57
1:A:655:GLN:CG	1:A:655:GLN:CD	1.79	1.53
1:A:653:GLU:CD	1:A:653:GLU:CG	1.81	1.51
1:A:581:GLN:CD	1:A:581:GLN:NE2	1.69	1.46
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	1.36
1:A:581:GLN:CD	1:A:581:GLN:CG	2.07	1.27
1:A:653:GLU:CD	1:A:653:GLU:OE1	1.76	1.27
1:A:29:LYS:O	1:A:30:LYS:HE2	1.35	1.25
1:A:653:GLU:CG	1:A:653:GLU:CB	2.18	1.21
1:A:654:LEU:CB	1:A:654:LEU:CD1	2.24	1.13
1:A:654:LEU:CG	1:A:654:LEU:CD2	2.28	1.12
1:A:29:LYS:C	1:A:30:LYS:HE2	1.75	1.10
1:A:581:GLN:CG	1:A:581:GLN:CB	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: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:137:LYS:H	1:A:140:ASN:CG	1.78	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: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:655:GLN:CD	1:A:655:GLN:CB	2.54	0.80
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:497:GLU:CD	1:A:500:ASP:CB	2.57	0.76
1:A:9:TRP:HE1	1:A:11:LEU:HD21	1.50	0.76
1:A:137:LYS:C	1:A:140:ASN:OD1	2.29	0.76
1:A:517:THR:OG1	1:A:518:SER:N	2.15	0.76
1:A:356:GLY:HA2	1:A:445:TRP:CE3	2.22	0.75
1:A:456:GLU:C	1:A:459:HIS:HB2	2.13	0.74
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:55:GLU:O	1:A:58:VAL:CG2	2.35	0.73
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:497:GLU:OE1	1:A:500:ASP:CG	2.34	0.71
1:A:73:ILE:CG1	1:A:84:LEU:CD1	2.68	0.70
1:A:547:ARG:NH2	1:A:550:GLU:CG	2.54	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:48:PRO:C	1:A:50:ASP:OD2	2.35	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:316:LEU:O	1:A:439:MET:HE1	1.94	0.68
1:A:8:LEU:C	1:A:8:LEU:HD12	2.19	0.67
1:A:78:THR:OG1	1:A:79:THR:HG23	1.95	0.67
1:A:497:GLU:OE1	1:A:500:ASP:CB	2.44	0.65
1:A:653:GLU:O	1:A:654:LEU:C	2.36	0.65
1:A:123:MET:SD	1:A:136:ILE:CD1	2.85	0.65
1:A:103:ASN:CG	1:A:107:LEU:HD23	2.21	0.65
1:A:655:GLN:CG	1:A:655:GLN:NE2	2.58	0.64
1:A:655:GLN:CD	1:A:655:GLN:HB3	2.23	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:456:GLU:C	1:A:459:HIS:CB	2.72	0.63
1:A:225:GLU:OE2	1:A:228:ARG:HD2	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:HD22	1:A:24:PHE:HZ	1.46	0.62
1:A:649:GLU:HG3	1:A:650:TYR:H	1.64	0.62
1:A:497:GLU:O	1:A:498:ILE:C	2.39	0.62
1:A:556:LEU:O	1:A:556:LEU:HD23	2.00	0.62
1:A:497:GLU:CD	1:A:500:ASP:HB2	2.24	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:465:VAL:HG22	1:A:512:GLN:CD	2.25	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: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
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:55:GLU:C	1:A:58:VAL:HG22	2.25	0.60
1:A:50:ASP:CG	1:A:51:VAL:H	2.10	0.59
1:A:29:LYS:C	1:A:30:LYS:CE	2.62	0.59
1:A:103:ASN:HB3	1:A:107:LEU:HD23	1.85	0.59
1:A:50:ASP:OD2	1:A:50:ASP:N	2.34	0.59
1:A:175:GLY:HA3	1:A:180:LEU:CD2	2.33	0.59
1:A:384:ARG:HH11	1:A:628:LYS:HE2	1.67	0.58
1:A:550:GLU:N	1:A:550:GLU:OE1	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:655:GLN:CG	1:A:655:GLN:O	2.49	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:468:LEU:C	1:A:468:LEU:HD23	2.30	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:656:GLU:CD	1:A:657:THR:H	2.13	0.57
1:A:313:VAL:O	1:A:322:HIS:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:HG12	1:A:84:LEU:HD11	1.87	0.56
1:A:48:PRO:C	1:A:50:ASP:H	2.13	0.56
1:A:649:GLU:CG	1:A:650:TYR:H	2.17	0.56
1:A:180:LEU:HD22	1:A:184:MET:HE2	1.88	0.56
1:A:360:VAL:HG13	1:A:360:VAL:O	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: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: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:473:ARG:HA	1:A:476:GLU:HB3	1.89	0.55
1:A:30:LYS:CD	1:A:30:LYS:HE2	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:73:ILE:CG1	1:A:84:LEU:HD11	2.37	0.54
1:A:654:LEU:CB	1:A:654:LEU:HD13	2.32	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: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: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:411:ASP:OD1	1:A:587:LYS:NZ	2.41	0.52
1:A:317:GLN:O	1:A:389:THR:HG22	2.09	0.52
1:A:57:GLU:O	1:A:60:LYS:HE3	2.10	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:PHE:CE1	1:A:642:GLU:OE2	2.59	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: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
1:A:9:TRP:CD1	1:A:11:LEU:CD2	2.93	0.51
1:A:103:ASN:OD1	1:A:107:LEU:CD2	2.58	0.51
1:A:135:ASP:CG	1:A:175:GLY:N	2.67	0.51
1:A:177:GLU:O	1:A:185:TYR:CE2	2.64	0.51
1:A:9:TRP:CD1	1:A:11:LEU:HD23	2.46	0.51
1:A:70:LEU:HD11	1:A:84:LEU:HD12	1.93	0.51
1:A:515:ILE:HD12	1:A:516:GLU:N	2.26	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:O	1:A:29:LYS:HG3	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:497:GLU:CD	1:A:500:ASP:HB3	2.37	0.50
1:A:201:THR:HG22	1:A:201:THR:O	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:48:PRO:C	1:A:50:ASP:N	2.69	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:42:ASN:OD1	1:A:45:PHE:HE1	1.95	0.49
1:A:136:ILE:HA	1:A:140:ASN:ND2	2.26	0.49
1:A:478:THR:HA	1:A:481:VAL:CG2	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LYS:HA	1:A:507:ARG:HB2	1.94	0.49
1:A:55:GLU:O	1:A:59:LEU:HG	2.13	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:50:ASP:CG	1:A:51:VAL:N	2.66	0.49
1:A:456:GLU:HA	1:A:459:HIS:HD2	1.66	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: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
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:531:SER:O	1:A:622:LYS:NZ	2.46	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:HG23	1:A:393:ILE:O	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:652:ASN:C	1:A:654:LEU:H	2.22	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:HH11	1:A:357:ARG:HD2	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:OD1	1:A:534:ASP:N	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:356:GLY:CA	1:A:445:TRP:CE3	2.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:497:GLU:CD	1:A:500:ASP:OD2	2.59	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:9:TRP:HE1	1:A:11:LEU:CD2	2.22	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:497:GLU:CD	1:A:500:ASP:CG	2.84	0.46
1:A:56:PHE:CD1	1:A:56:PHE:N	2.82	0.46
1:A:345:ILE:CG2	1:A:349:ASN:OD1	2.64	0.46
1:A:618:GLU:HA	1:A:621:ARG:NE	2.31	0.46
1:A:310:VAL:O	1:A:311:ILE:HD13	2.16	0.45
1:A:651:THR:C	1:A:654:LEU:CD1	2.89	0.45
1:A:656:GLU:CD	1:A:657:THR:N	2.74	0.45
1:A:526:LEU:N	1:A:526:LEU:HD23	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:572:GLU:C	1:A:574:ARG:H	2.24	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:137:LYS:O	1:A:140:ASN:CG	2.56	0.45
1:A:441:LYS:HZ2	1:A:444:ARG:HD2	1.82	0.45
1:A:138:PRO:HD3	1:A:210:THR:HG23	1.98	0.45
1:A:30:LYS:CD	1:A:30:LYS:HE3	2.19	0.45
1:A:406:TYR:O	1:A:407:ASP:C	2.60	0.45
1:A:448:GLU:HA	1:A:451:LYS:HG2	1.98	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: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:43:ILE:O	1:A:43:ILE:HG23	2.17	0.44
1:A:93:SER:HA	1:A:142:MET:HA	2.00	0.44
1:A:46:LEU:HB2	1:A:47:ARG:H	1.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:TYR:N	1:A:647:TYR:CD1	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:HH11	1:A:54:ARG:HD3	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
1:A:630:LEU:HD23	1:A:630:LEU:C	2.43	0.43
2:A:701:KJB:O37	2:A:701:KJB:C27	2.66	0.43
1:A:3:SER:OG	1:A:4:THR:N	2.52	0.43
1:A:29:LYS:O	1:A:30:LYS:CD	2.67	0.43
1:A:163:GLU:O	1:A:164:LEU:HG	2.19	0.43
1:A:309:MET:HE1	1:A:367:ALA:O	2.18	0.43
1:A:497:GLU:CG	1:A:500:ASP:OD2	2.66	0.42
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:638:PHE:CD1	1:A:638:PHE:C	2.96	0.42
1:A:94:LEU:HA	1:A:97:VAL:HG12	2.01	0.42
1:A:7:HIS:CD2	1:A:28:HIS:HA	2.54	0.42
1:A:649:GLU:O	1:A:653:GLU:N	2.53	0.42
1:A:88:PHE:O	1:A:90:PRO:HD3	2.19	0.42
1:A:241:LYS:HE2	1:A:285:LEU:O	2.20	0.42
1:A:316:LEU:O	1:A:439:MET:HE3	2.19	0.42
1:A:330:ASN:HB3	1:A:334:ILE:HD11	2.01	0.42
1:A:24:PHE:O	1:A:37:ILE:HG12	2.19	0.42
1:A:447:ILE:HG21	1:A:447:ILE:HD13	1.79	0.42
1:A:510:SER:O	1:A:513:GLY:N	2.53	0.42
1:A:620:ILE:O	1:A:621:ARG:C	2.61	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:583:HIS:C	1:A:583:HIS:CD2	2.98	0.41
1:A:137:LYS:CB	1:A:140:ASN:OD1	2.68	0.41
1:A:225:GLU:C	1:A:225:GLU:OE1	2.63	0.41
1:A:408:LEU:CD1	1:A:575:LEU:HD12	2.50	0.41
1:A:409:ASP:OD2	1:A:570:LYS:HE3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HG22	1:A:326:ILE:HG23	2.03	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:302:THR:O	1:A:303:SER:C	2.64	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:38:LYS:O	1:A:83:VAL:HA	2.20	0.41
1:A:406:TYR:N	1:A:406:TYR:CD1	2.87	0.41
1:A:500:ASP:O	1:A:504:LYS:HD3	2.20	0.41
1:A:14:ILE:HD13	1:A:14:ILE:HG21	1.88	0.41
1:A:179:TYR:O	1:A:206:SER:OG	2.28	0.41
1:A:283:ASN:HB3	1:A:293:TRP:CE2	2.56	0.40
1:A:177:GLU:O	1:A:185:TYR:HE2	2.03	0.40
1:A:468:LEU:O	1:A:469:ASP:C	2.63	0.40
1:A:60:LYS:HE3	1:A:60:LYS:HB3	1.80	0.40
1:A:579:GLU:N	1:A:579:GLU:CD	2.79	0.40
1:A:103:ASN:CG	1:A:107:LEU:CD2	2.93	0.40
1:A:204:LEU:HA	1:A:207:ILE:HD13	2.03	0.40
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:54:ARG:HH21	1:A:513:GLY:O[3_544]	0.87	0.73
1:A:459:HIS:CE1	1:A:459:HIS:HE1[4_555]	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:O	1:A:655:GLN:OE1[6_454]	1.61	0.59
1:A:581:GLN:HE22	1:A:653:GLU:HA[3_545]	1.01	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:29:LYS:NZ	1:A:655:GLN:O[6_454]	1.86	0.34
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: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
1:A:18:GLY:O	1:A:42:ASN:ND2[6_554]	2.03	0.17
1:A:28:HIS:C	1:A:655:GLN:NE2[6_454]	2.04	0.16
1:A:30:LYS:O	1:A:585:PHE:HZ[4_555]	1.44	0.16
1:A:148:ASP:O	1:A:547:ARG:HH12[4_555]	1.45	0.15
1:A:459:HIS:CE1	1:A:459:HIS:NE2[4_555]	2.06	0.14
1:A:581:GLN:CB	1:A:653:GLU:OE2[3_545]	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:29:LYS:C	1:A:655:GLN:CD[6_454]	2.12	0.08
1:A:148:ASP:O	1:A:547:ARG:NH1[4_555]	2.12	0.08
1:A:30:LYS:HZ3	1:A:655:GLN:N[6_454]	1.53	0.07
1:A:30:LYS:HZ2	1:A:654:LEU:CA[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: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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	620/663 (94%)	587 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	557/589 (95%)	557 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	7	HIS
1	A	22	ASN
1	A	124	ASN
1	A	297	GLN
1	A	368	GLN
1	A	459	HIS
1	A	502	HIS
1	A	583	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3.11	11 (26%)	56,65,65	4.73	32 (57%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	KJB	C25-N24	-12.39	1.19	1.39
2	A	701	KJB	C28-C31	-9.43	1.38	1.49
2	A	701	KJB	C26-N41	-6.34	1.29	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	KJB	C13-C11	5.30	1.57	1.51
2	A	701	KJB	C21-C1	4.55	1.51	1.39
2	A	701	KJB	C26-C25	3.90	1.49	1.40
2	A	701	KJB	C1-N2	-3.00	1.28	1.34
2	A	701	KJB	C9-N10	-2.94	1.41	1.47
2	A	701	KJB	C18-N10	2.67	1.51	1.47
2	A	701	KJB	O37-C38	-2.43	1.39	1.45
2	A	701	KJB	C11-N10	-2.19	1.31	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	KJB	C30-C25-N24	17.72	151.99	127.98
2	A	701	KJB	C14-C13-C11	-12.04	104.36	113.60
2	A	701	KJB	C26-N41-C23	-10.61	92.27	108.85
2	A	701	KJB	C3-N2-C1	9.11	130.22	117.21
2	A	701	KJB	C30-C25-C26	-8.62	108.76	121.11
2	A	701	KJB	C4-C3-N2	-8.32	113.77	123.97
2	A	701	KJB	C26-C25-N24	-7.10	98.79	108.68
2	A	701	KJB	C25-N24-C23	6.97	119.75	108.85
2	A	701	KJB	C32-C31-N36	-5.45	117.51	121.69
2	A	701	KJB	O37-C38-C40	-5.24	87.96	107.89
2	A	701	KJB	C4-C5-C21	5.22	124.79	118.74
2	A	701	KJB	C19-C18-N10	-4.89	100.69	110.42
2	A	701	KJB	C27-C26-N41	-4.60	119.69	127.88
2	A	701	KJB	C21-C1-N2	-4.59	116.91	122.92
2	A	701	KJB	C5-C6-N7	4.58	122.29	110.54
2	A	701	KJB	C25-C26-N41	4.45	114.88	108.68
2	A	701	KJB	C29-C30-C25	4.26	127.79	119.57
2	A	701	KJB	C8-C9-N10	-4.01	102.43	110.42
2	A	701	KJB	C32-O37-C38	-3.84	112.46	119.53
2	A	701	KJB	C20-C6-C5	-3.42	104.86	113.36
2	A	701	KJB	N34-C35-N36	-3.17	121.95	127.33
2	A	701	KJB	C27-C26-C25	2.99	125.07	121.77
2	A	701	KJB	C33-N34-C35	2.90	119.22	115.80
2	A	701	KJB	N22-C1-N2	-2.58	112.67	116.85
2	A	701	KJB	C18-N10-C9	2.57	117.93	112.68
2	A	701	KJB	C35-N36-C31	2.45	121.66	117.87
2	A	701	KJB	C20-C6-N7	-2.38	107.23	112.46
2	A	701	KJB	C18-N10-C11	-2.31	115.22	122.83
2	A	701	KJB	C18-C19-N7	-2.29	106.57	110.61
2	A	701	KJB	O37-C32-C33	-2.12	120.50	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	KJB	C29-C28-C31	-2.09	117.22	120.62
2	A	701	KJB	C32-C33-N34	-2.07	120.22	122.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

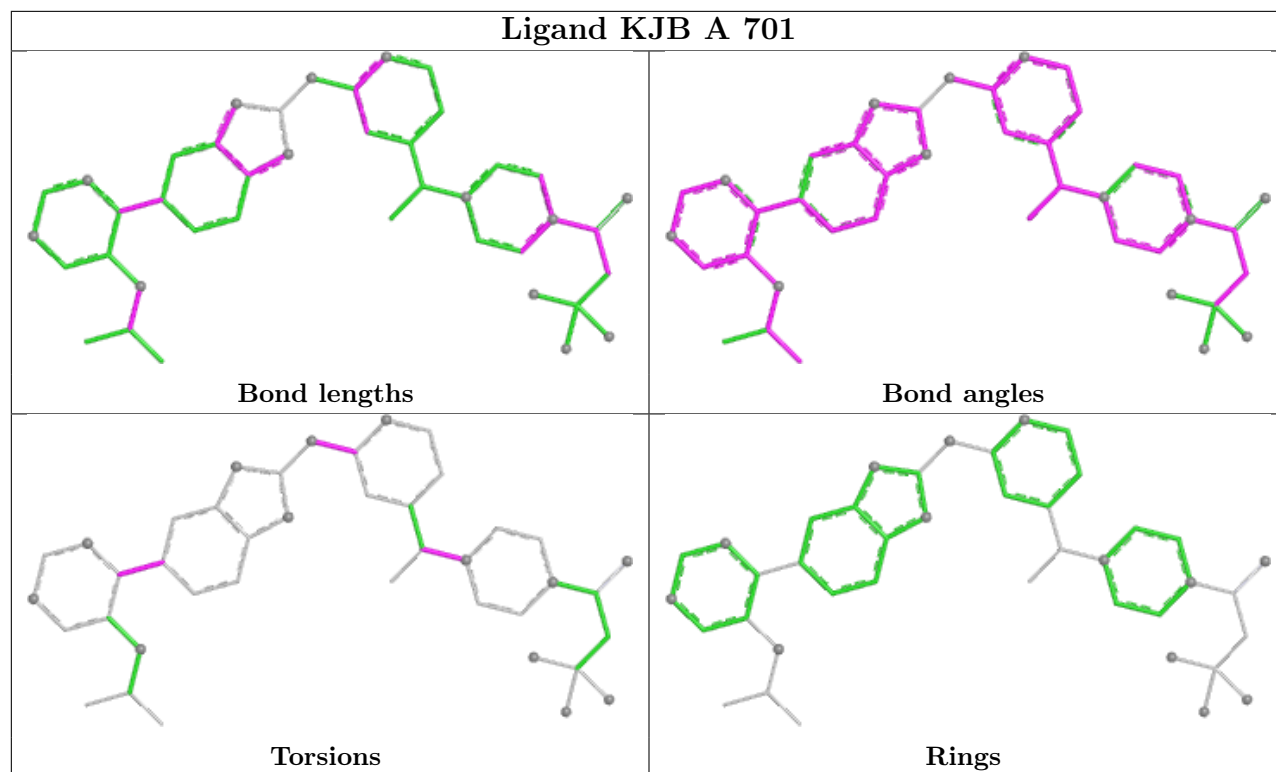
Mol	Chain	Res	Type	Atoms
2	A	701	KJB	C29-C28-C31-N36
2	A	701	KJB	C27-C28-C31-N36
2	A	701	KJB	C5-C6-N7-C19
2	A	701	KJB	C21-C1-N22-C23

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 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](#)

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, 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	628/663 (94%)	0.77	61 (9%) 13 13	54, 94, 126, 147	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	CYS	6.0
1	A	482	TYR	5.6
1	A	459	HIS	4.7
1	A	634	THR	4.5
1	A	222	ARG	3.9
1	A	176	THR	3.8
1	A	185	TYR	3.8
1	A	153	TYR	3.7
1	A	310	VAL	3.5
1	A	519	LEU	3.4
1	A	226	GLY	3.4
1	A	227	PRO	3.4
1	A	361	LEU	3.4
1	A	182	PRO	3.1
1	A	505	LEU	3.1
1	A	629	GLN	3.0
1	A	114	ILE	3.0
1	A	515	ILE	3.0
1	A	492	ALA	2.9
1	A	212	TYR	2.8
1	A	180	LEU	2.8
1	A	575	LEU	2.8
1	A	478	THR	2.7
1	A	392	LEU	2.6
1	A	143	ARG	2.6
1	A	508	LEU	2.6
1	A	406	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	356	GLY	2.5
1	A	657	THR	2.5
1	A	360	VAL	2.5
1	A	358	ARG	2.4
1	A	97	VAL	2.4
1	A	224	PHE	2.4
1	A	429	ALA	2.4
1	A	479	VAL	2.3
1	A	221	PHE	2.3
1	A	433	LEU	2.3
1	A	223	PRO	2.3
1	A	529	GLY	2.3
1	A	404	PRO	2.3
1	A	46	LEU	2.3
1	A	359	LEU	2.3
1	A	633	LEU	2.2
1	A	522	ILE	2.2
1	A	376	GLU	2.2
1	A	502	HIS	2.2
1	A	78	THR	2.2
1	A	302	THR	2.2
1	A	402	VAL	2.2
1	A	541	GLY	2.1
1	A	49	VAL	2.1
1	A	655	GLN	2.1
1	A	303	SER	2.1
1	A	528	PRO	2.1
1	A	352	LEU	2.1
1	A	232	GLU	2.0
1	A	445	TRP	2.0
1	A	590	LEU	2.0
1	A	535	ALA	2.0
1	A	269	LEU	2.0
1	A	237	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

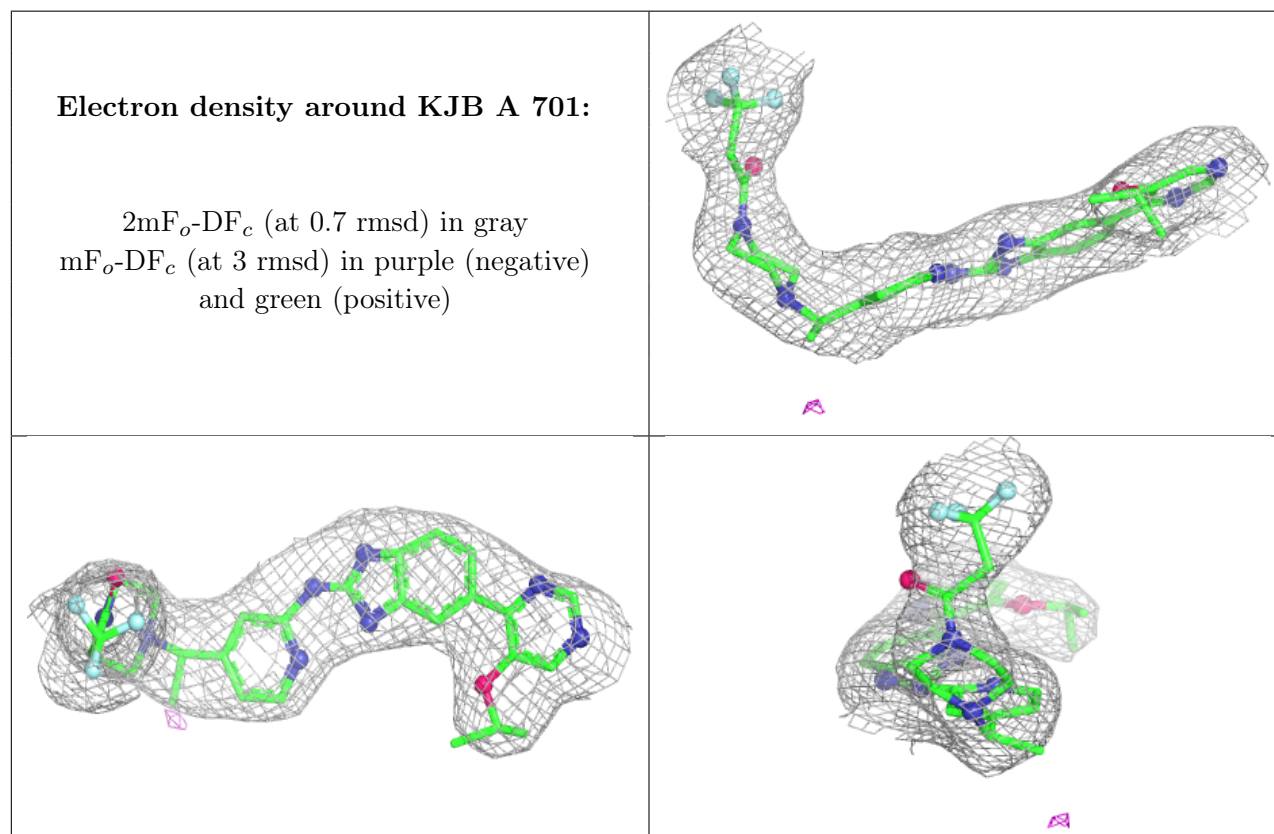
There are no oligosaccharides in this entry.

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	KJB	A	701	41/41	0.93	0.10	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.