



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 12:07 am GMT

PDB ID : 4JSX
Title : structure of mTORDeltaN-mLST8-Torin2 complex
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2013-03-22
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

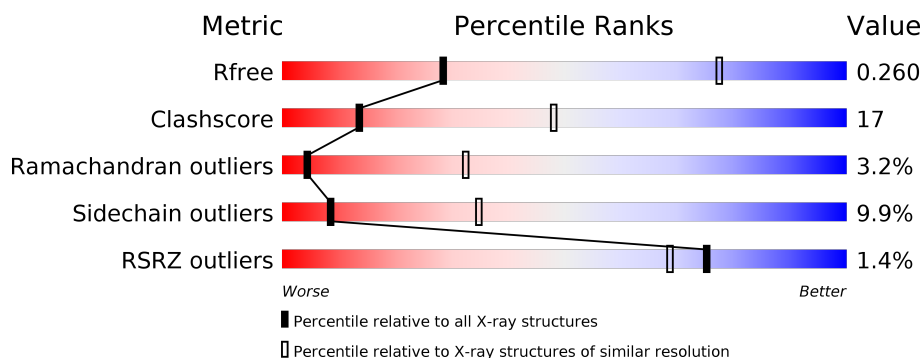
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	111664	1391 (3.60-3.40)
Clashscore	122126	1485 (3.60-3.40)
Ramachandran outliers	120053	1446 (3.60-3.40)
Sidechain outliers	120020	1447 (3.60-3.40)
RSRZ outliers	108989	1303 (3.60-3.40)

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. 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	1174	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>28%</div> <div>• • 10%</div> </div> </div>
1	B	1174	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>28%</div> <div>• • 10%</div> </div> </div>
2	C	326	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>38%</div> <div>7% • •</div> </div> </div>
2	D	326	<div> <div></div> <div> <div></div> <div>51%</div> <div>37%</div> <div>8% • •</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22160 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.

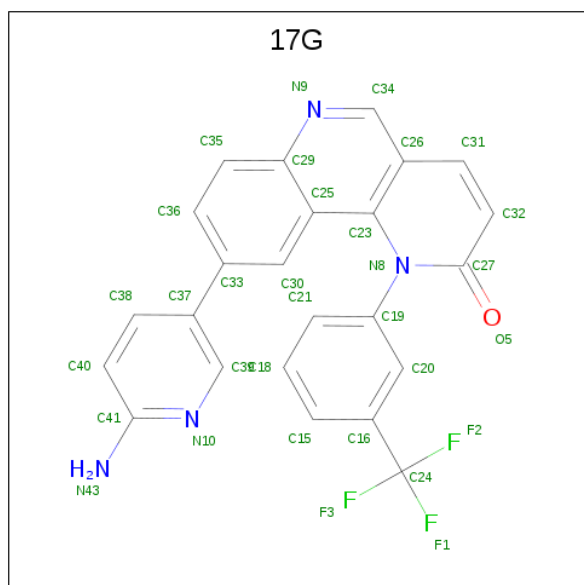
- Molecule 1 is a protein called Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0	0
			8607	5472	1520	1552	63			
1	A	1054	Total	C	N	O	S	0	0	0
			8577	5451	1517	1546	63			

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			
2	C	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			

- Molecule 3 is 9-(6-aminopyridin-3-yl)-1-[3-(trifluoromethyl)phenyl]benzo[h][1,6]naphthyridine-2(1H)-one (three-letter code: 17G) (formula: C₂₄H₁₅F₃N₄O).

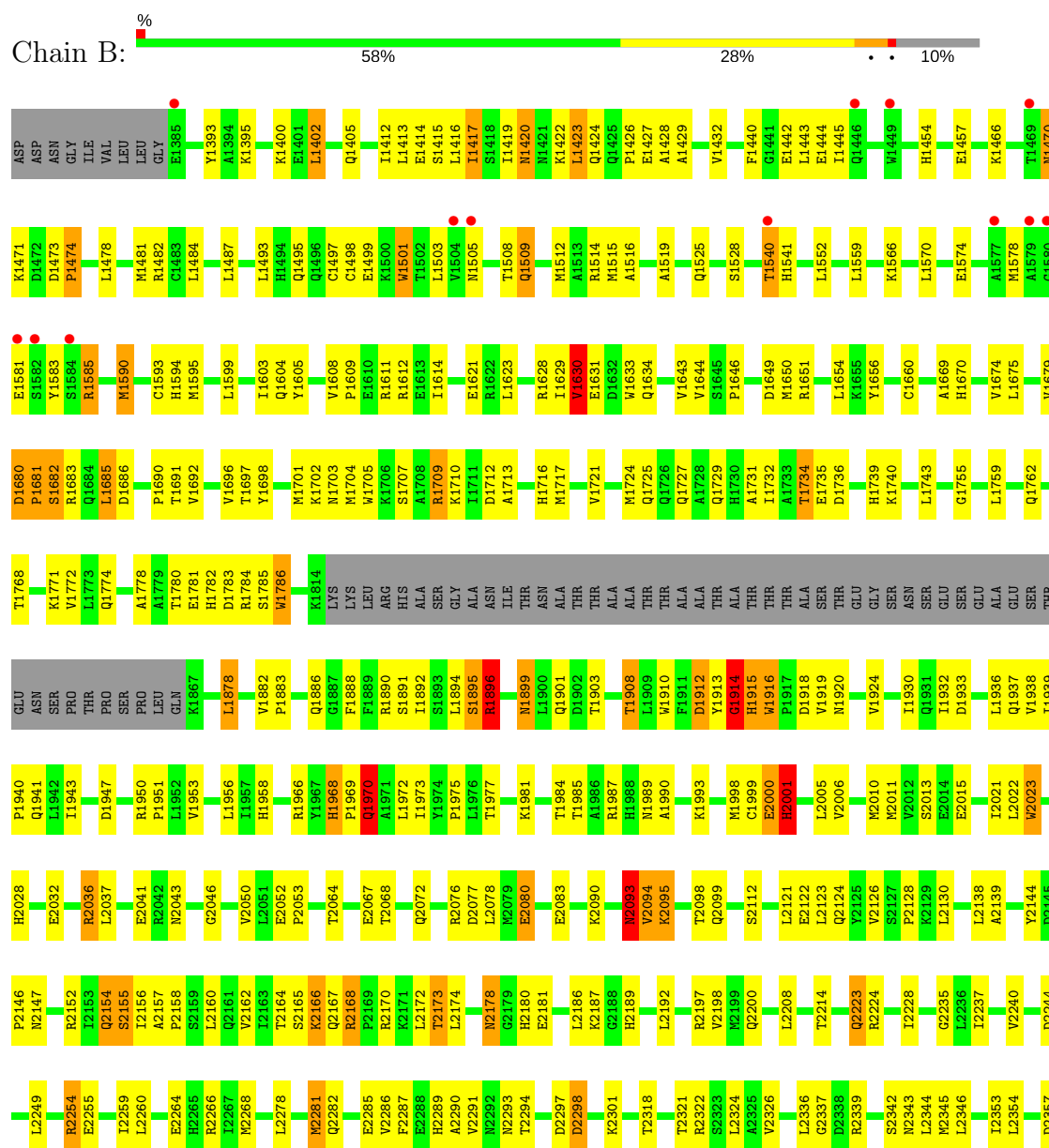


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			32	24	3	4	1		
3	A	1	Total	C	F	N	O	0	0
			32	24	3	4	1		

3 Residue-property plots

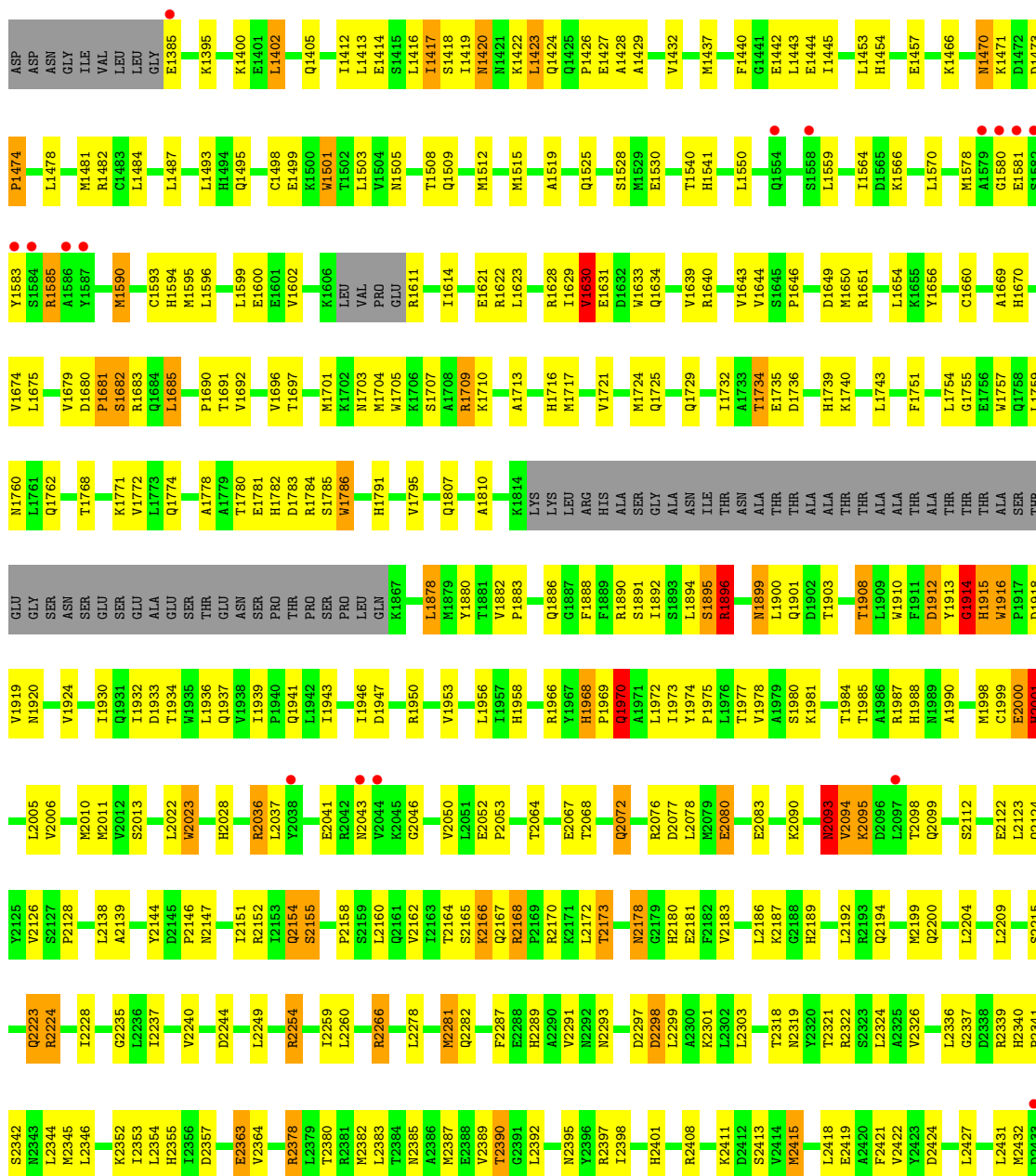
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

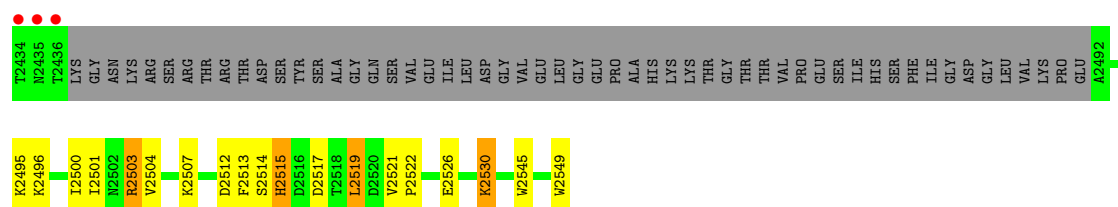
- Molecule 1: Serine/threonine-protein kinase mTOR



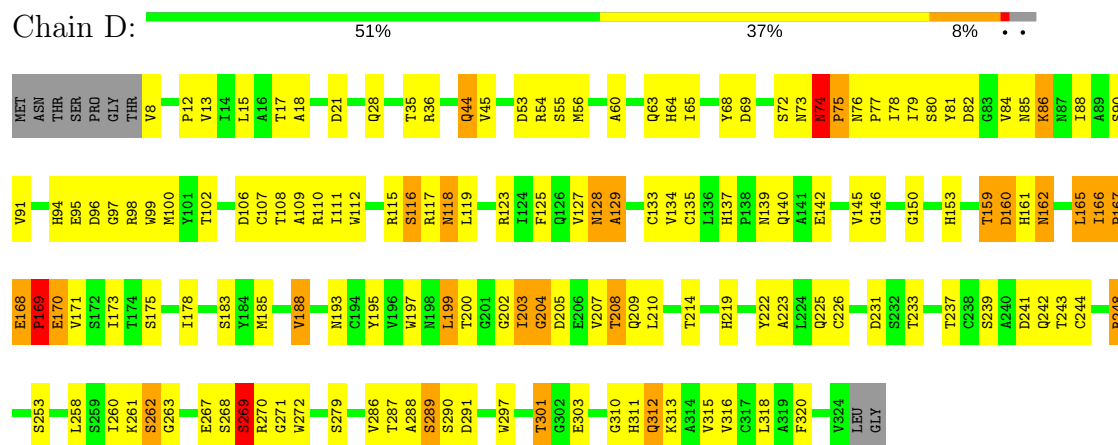


Chain A: 

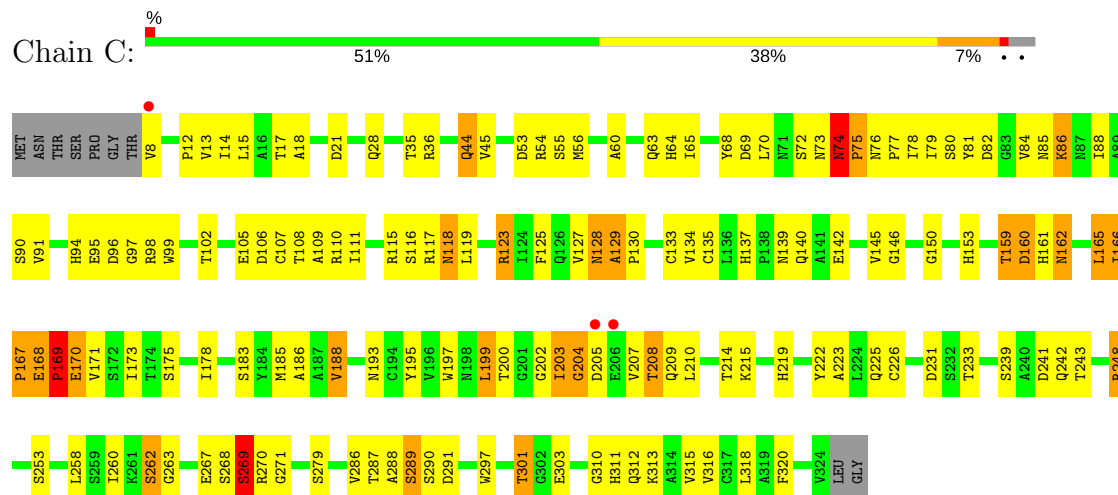




• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 2: Target of rapamycin complex subunit LST8



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.67 – 3.50 39.64 – 3.48	Depositor EDS
% Data completeness (in resolution range)	84.2 (39.67-3.50) 83.4 (39.64-3.48)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.257 0.226 , 0.260	Depositor DCC
R_{free} test set	1774 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22160	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5437e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 17G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/8772	0.61	1/11872 (0.0%)
1	B	0.35	0/8804	0.61	1/11918 (0.0%)
2	C	0.36	0/2514	0.66	0/3426
2	D	0.40	0/2514	0.68	0/3426
All	All	0.36	0/22604	0.62	2/30642 (0.0%)

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	2
1	B	0	2
2	C	0	1
2	D	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1915	HIS	N-CA-C	5.67	126.32	111.00
1	A	1915	HIS	N-CA-C	5.65	126.26	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1914	GLY	Peptide
1	A	2000	GLU	Peptide
1	B	1914	GLY	Peptide
1	B	2000	GLU	Peptide
2	D	169	PRO	Peptide

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	8577	0	8559	256	0
1	B	8607	0	8592	258	0
2	C	2456	0	2341	121	0
2	D	2456	0	2341	123	0
3	A	32	0	15	8	0
3	B	32	0	15	6	0
All	All	22160	0	21863	752	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 17.

The worst 5 of 752 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)
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.30	1.13
2:C:76:ASN:HB3	2:C:77:PRO:HD2	1.29	1.13
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.33	1.06
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.33	1.04
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.35	1.03

There are no symmetry-related clashes.

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	1046/1174 (89%)	922 (88%)	96 (9%)	28 (3%)	5	36
1	B	1052/1174 (90%)	925 (88%)	97 (9%)	30 (3%)	5	34
2	C	315/326 (97%)	275 (87%)	26 (8%)	14 (4%)	3	24
2	D	315/326 (97%)	272 (86%)	29 (9%)	14 (4%)	3	24
All	All	2728/3000 (91%)	2394 (88%)	248 (9%)	86 (3%)	4	32

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1630	VAL
1	B	1650	MET
1	B	1709	ARG
1	B	1896	ARG

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	927/1024 (90%)	838 (90%)	89 (10%)	9	36
1	B	930/1024 (91%)	839 (90%)	91 (10%)	9	35
2	C	269/276 (98%)	240 (89%)	29 (11%)	7	31
2	D	269/276 (98%)	240 (89%)	29 (11%)	7	31
All	All	2395/2600 (92%)	2157 (90%)	238 (10%)	8	35

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	169	PRO
1	A	1541	HIS
2	C	159	THR
2	D	188	VAL
1	A	1385	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	153	HIS
1	A	1687	HIS
2	C	137	HIS
2	D	242	GLN
1	A	1439	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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
3	17G	A	2601	-	35,36,36	1.34	5 (14%)	50,54,54	1.64	7 (14%)
3	17G	B	2601	-	35,36,36	1.26	5 (14%)	50,54,54	1.86	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	17G	A	2601	-	-	0/14/14/14	0/5/5/5
3	17G	B	2601	-	-	0/14/14/14	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	17G	C37-C33	-3.80	1.39	1.49
3	B	2601	17G	C37-C33	-3.54	1.40	1.49
3	A	2601	17G	C19-N8	-3.08	1.41	1.45
3	B	2601	17G	C19-N8	-2.36	1.42	1.45
3	A	2601	17G	C27-N8	2.11	1.41	1.37

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2601	17G	C26-C34-N9	-3.34	120.27	124.87
3	B	2601	17G	C31-C26-C34	-3.19	116.64	122.58
3	B	2601	17G	C21-C19-C20	-3.01	118.63	121.70
3	A	2601	17G	C26-C34-N9	-2.94	120.82	124.87
3	A	2601	17G	C31-C26-C34	-2.93	117.13	122.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	17G	8	0
3	B	2601	17G	6	0

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	1054/1174 (89%)	-0.20	19 (1%) 68 62	37, 70, 153, 188	0
1	B	1058/1174 (90%)	-0.30	17 (1%) 72 66	32, 61, 135, 180	0
2	C	317/326 (97%)	-0.23	3 (0%) 84 78	38, 70, 118, 156	0
2	D	317/326 (97%)	-0.38	0 100 100	29, 49, 97, 141	0
All	All	2746/3000 (91%)	-0.26	39 (1%) 75 69	29, 63, 144, 188	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1580	GLY	6.7
1	B	1446	GLN	5.3
1	B	1581	GLU	4.4
1	A	2436	THR	4.3
1	B	1582	SER	4.3

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, 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(\AA^2)	Q<0.9
3	17G	B	2601	32/32	0.96	0.21	36,37,38,38	0
3	17G	A	2601	32/32	0.96	0.20	38,40,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.