



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 08:33 am BST

PDB ID : 6DJ9
Title : Structure of the USP15 DUSP domain in complex with a high-affinity Ubiquitin Variant (UbV)
Authors : Singer, A.U.; Teyra, J.; Boehmelt, G.; Lenter, M.; Sicheri, F.; Sidhu, S.S.
Deposited on : 2018-05-24
Resolution : 3.10 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

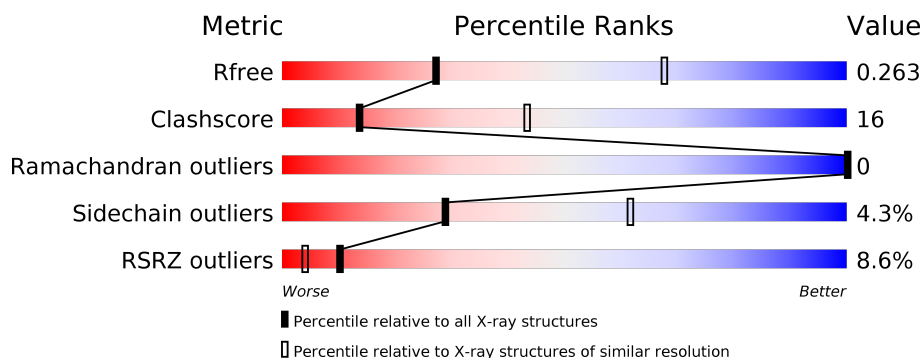
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	141	<div> <div>14%</div> <div> <div></div> <div>62%</div> <div>30%</div> <div>7%</div> </div> </div>
1	B	141	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>13%</div> </div> </div>
1	C	141	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>33%</div> <div>13%</div> </div> </div>
1	D	141	<div> <div>11%</div> <div> <div></div> <div>54%</div> <div>32%</div> <div>13%</div> </div> </div>
1	E	141	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>11%</div> </div> </div>
1	F	141	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	86	
2	H	86	
2	I	86	
2	J	86	
2	K	86	
2	L	86	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9759 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 Ubiquitin carboxyl-terminal hydrolase 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	1	0
			1055	680	176	195	4			
1	B	123	Total	C	N	O	S	0	0	0
			991	642	162	184	3			
1	C	123	Total	C	N	O	S	0	0	0
			1008	649	165	190	4			
1	D	122	Total	C	N	O	S	0	1	0
			1003	647	165	187	4			
1	E	126	Total	C	N	O	S	0	0	0
			1007	651	165	188	3			
1	F	131	Total	C	N	O	S	0	0	0
			1056	681	173	198	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9Y4E8
A	-2	ALA	-	expression tag	UNP Q9Y4E8
A	-1	ALA	-	expression tag	UNP Q9Y4E8
A	0	ALA	-	expression tag	UNP Q9Y4E8
A	135	SER	-	expression tag	UNP Q9Y4E8
A	136	SER	-	expression tag	UNP Q9Y4E8
A	137	GLY	-	expression tag	UNP Q9Y4E8
B	-3	GLY	-	expression tag	UNP Q9Y4E8
B	-2	ALA	-	expression tag	UNP Q9Y4E8
B	-1	ALA	-	expression tag	UNP Q9Y4E8
B	0	ALA	-	expression tag	UNP Q9Y4E8
B	135	SER	-	expression tag	UNP Q9Y4E8
B	136	SER	-	expression tag	UNP Q9Y4E8
B	137	GLY	-	expression tag	UNP Q9Y4E8
C	-3	GLY	-	expression tag	UNP Q9Y4E8
C	-2	ALA	-	expression tag	UNP Q9Y4E8
C	-1	ALA	-	expression tag	UNP Q9Y4E8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP Q9Y4E8
C	135	SER	-	expression tag	UNP Q9Y4E8
C	136	SER	-	expression tag	UNP Q9Y4E8
C	137	GLY	-	expression tag	UNP Q9Y4E8
D	-3	GLY	-	expression tag	UNP Q9Y4E8
D	-2	ALA	-	expression tag	UNP Q9Y4E8
D	-1	ALA	-	expression tag	UNP Q9Y4E8
D	0	ALA	-	expression tag	UNP Q9Y4E8
D	135	SER	-	expression tag	UNP Q9Y4E8
D	136	SER	-	expression tag	UNP Q9Y4E8
D	137	GLY	-	expression tag	UNP Q9Y4E8
E	-3	GLY	-	expression tag	UNP Q9Y4E8
E	-2	ALA	-	expression tag	UNP Q9Y4E8
E	-1	ALA	-	expression tag	UNP Q9Y4E8
E	0	ALA	-	expression tag	UNP Q9Y4E8
E	135	SER	-	expression tag	UNP Q9Y4E8
E	136	SER	-	expression tag	UNP Q9Y4E8
E	137	GLY	-	expression tag	UNP Q9Y4E8
F	-3	GLY	-	expression tag	UNP Q9Y4E8
F	-2	ALA	-	expression tag	UNP Q9Y4E8
F	-1	ALA	-	expression tag	UNP Q9Y4E8
F	0	ALA	-	expression tag	UNP Q9Y4E8
F	135	SER	-	expression tag	UNP Q9Y4E8
F	136	SER	-	expression tag	UNP Q9Y4E8
F	137	GLY	-	expression tag	UNP Q9Y4E8

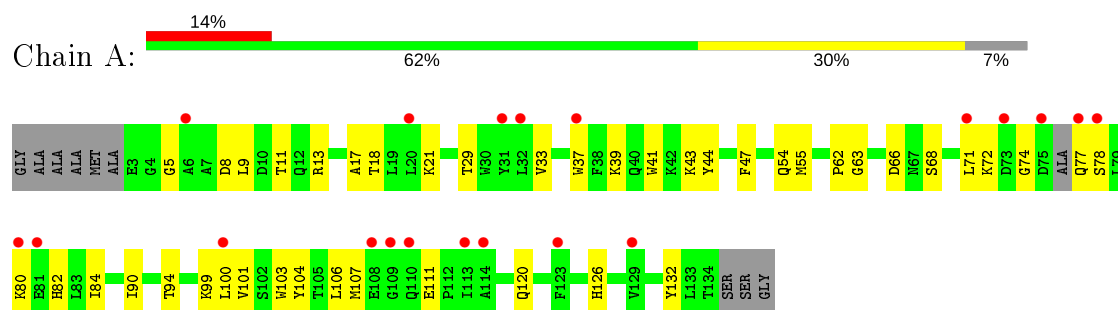
- Molecule 2 is a protein called Ubiquitin Variant UbV 15.D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	77	Total	C	N	O	S	0	0	0
			604	381	105	116	2			
2	H	78	Total	C	N	O	S	0	0	0
			611	386	107	116	2			
2	I	78	Total	C	N	O	S	0	0	0
			607	384	107	114	2			
2	J	77	Total	C	N	O	S	0	0	0
			611	387	107	115	2			
2	K	77	Total	C	N	O	S	0	0	0
			597	378	105	112	2			
2	L	78	Total	C	N	O	S	0	0	0
			609	386	105	116	2			

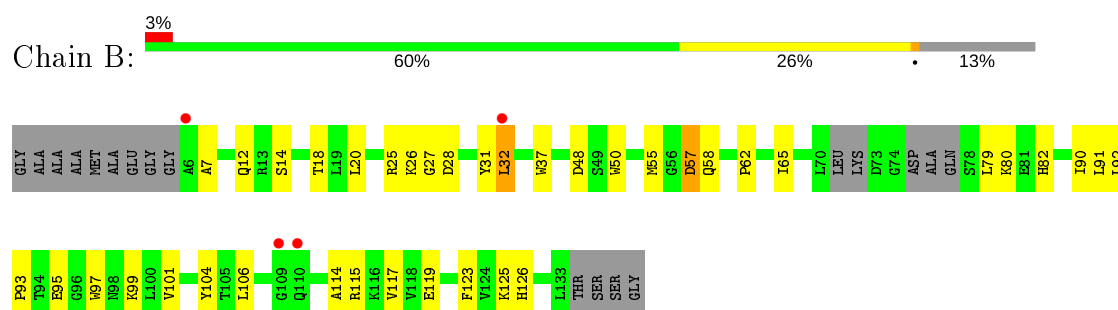
3 Residue-property plots [i](#)

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.

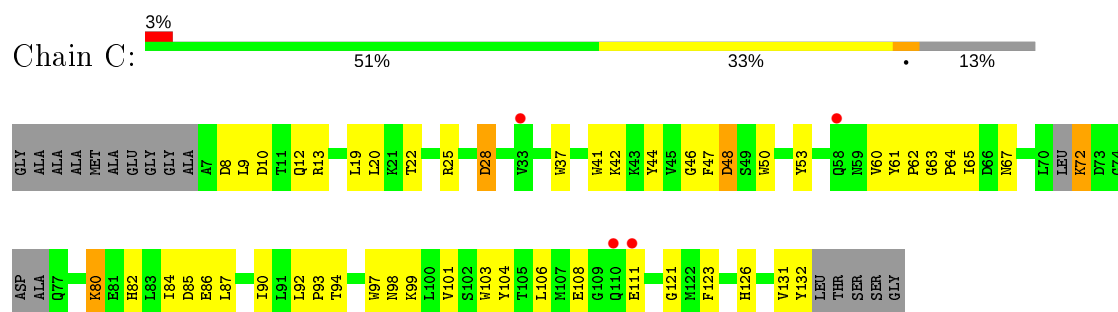
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15

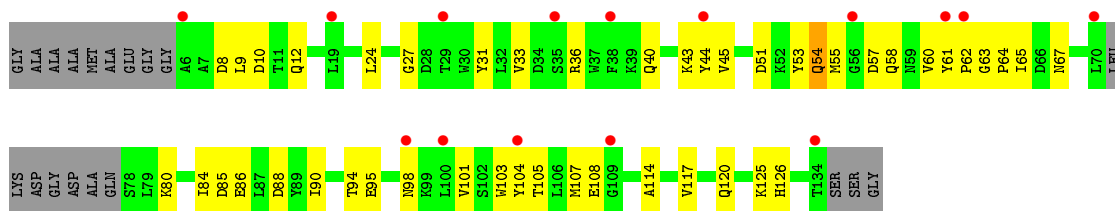


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15

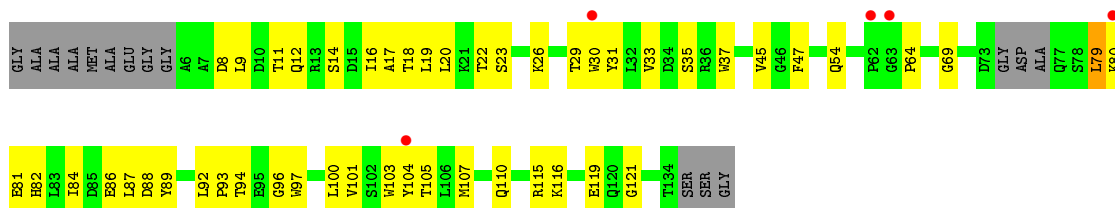


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15

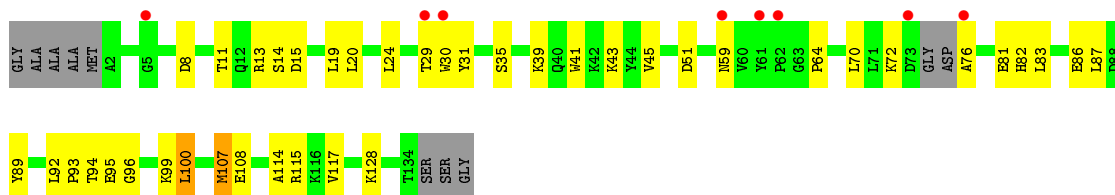




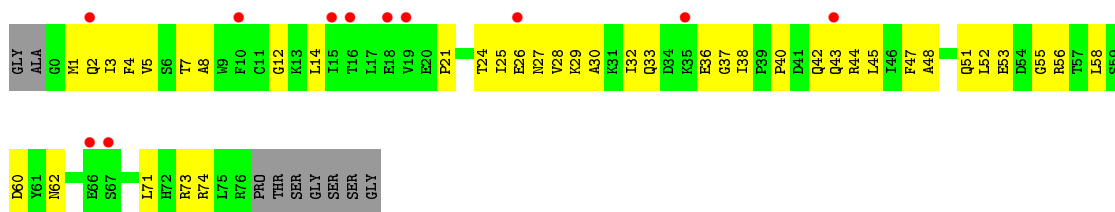
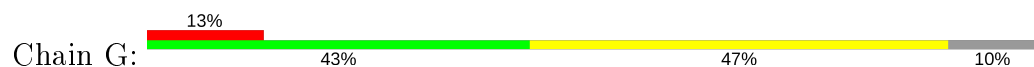
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15



• Molecule 2: Ubiquitin Variant UbV 15.D

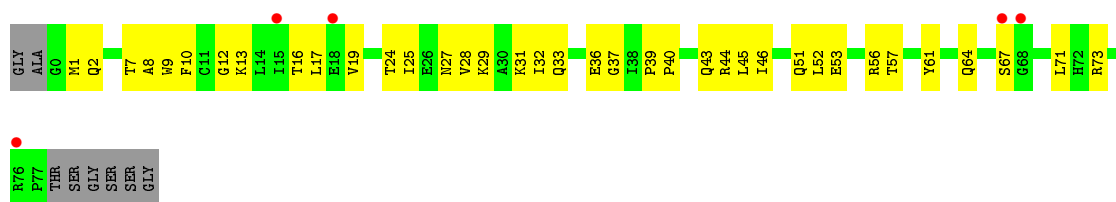


• Molecule 2: Ubiquitin Variant UbV 15.D

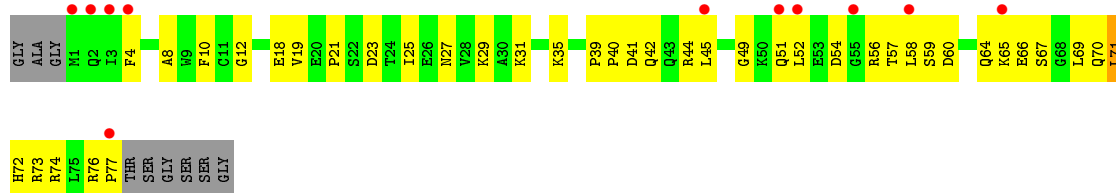
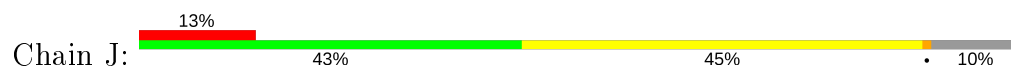


• Molecule 2: Ubiquitin Variant UbV 15.D

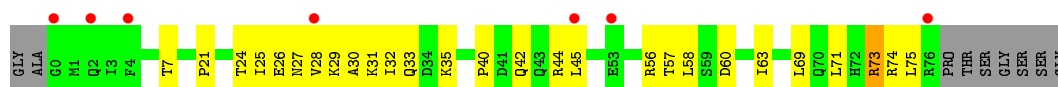




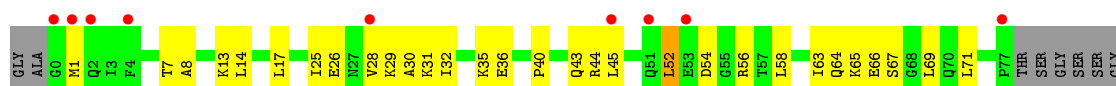
• Molecule 2: Ubiquitin Variant UbV 15.D



• Molecule 2: Ubiquitin Variant UbV 15.D



• Molecule 2: Ubiquitin Variant UbV 15.D



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	152.41Å 152.41Å 125.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.94 – 3.10 90.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.94-3.10) 99.9 (90.94-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	397.49 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.253 , 0.267 0.252 , 0.263	Depositor DCC
R_{free} test set	2199 reflections (7.30%)	wwPDB-VP
Wilson B-factor (Å ²)	99.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.438 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9759	wwPDB-VP
Average B, all atoms (Å ²)	112.0	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 54.16 % 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 3.8024e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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	0.25	0/1081	0.45	0/1465
1	B	0.26	0/1016	0.43	0/1378
1	C	0.25	0/1033	0.43	0/1397
1	D	0.25	0/1029	0.47	0/1396
1	E	0.25	0/1032	0.51	0/1403
1	F	0.25	0/1082	0.44	0/1466
2	G	0.25	0/613	0.50	0/826
2	H	0.26	0/621	0.48	0/838
2	I	0.26	0/617	0.46	0/833
2	J	0.25	0/621	0.47	0/837
2	K	0.24	0/606	0.51	0/817
2	L	0.24	0/619	0.47	0/835
All	All	0.25	0/9970	0.47	0/13491

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	D	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	63	GLY	Peptide
2	H	76	ARG	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	1055	0	1009	26	1
1	B	991	0	948	27	0
1	C	1008	0	965	33	0
1	D	1003	0	957	36	1
1	E	1007	0	954	33	0
1	F	1056	0	1019	26	0
2	G	604	0	602	32	0
2	H	611	0	611	23	0
2	I	607	0	607	30	0
2	J	611	0	619	30	0
2	K	597	0	596	19	0
2	L	609	0	611	31	0
All	All	9759	0	9498	306	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 306 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:D:54:GLN:HB2	1:D:60:VAL:HG21	1.60	0.82
1:D:10:ASP:H	2:H:49:GLY:HA2	1.47	0.80
1:A:55:MET:O	2:K:44:ARG:NH1	2.18	0.77
2:J:44:ARG:NH1	2:J:73:ARG:O	2.18	0.76
2:I:24:THR:HA	2:I:57:THR:HA	1.70	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:TYR:OH	1:D:80:LYS:O[3_675]	2.18	0.02

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	128/141 (91%)	113 (88%)	15 (12%)	0	100	100
1	B	117/141 (83%)	100 (86%)	17 (14%)	0	100	100
1	C	117/141 (83%)	97 (83%)	20 (17%)	0	100	100
1	D	119/141 (84%)	95 (80%)	24 (20%)	0	100	100
1	E	122/141 (86%)	100 (82%)	22 (18%)	0	100	100
1	F	127/141 (90%)	108 (85%)	19 (15%)	0	100	100
2	G	75/86 (87%)	68 (91%)	7 (9%)	0	100	100
2	H	76/86 (88%)	67 (88%)	9 (12%)	0	100	100
2	I	76/86 (88%)	69 (91%)	7 (9%)	0	100	100
2	J	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
2	K	75/86 (87%)	70 (93%)	5 (7%)	0	100	100
2	L	76/86 (88%)	63 (83%)	13 (17%)	0	100	100
All	All	1183/1362 (87%)	1021 (86%)	162 (14%)	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	109/119 (92%)	105 (96%)	4 (4%)	34	66
1	B	104/119 (87%)	99 (95%)	5 (5%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	108/119 (91%)	100 (93%)	8 (7%)	13	42
1	D	106/119 (89%)	98 (92%)	8 (8%)	13	42
1	E	104/119 (87%)	102 (98%)	2 (2%)	57	81
1	F	111/119 (93%)	106 (96%)	5 (4%)	27	60
2	G	65/73 (89%)	64 (98%)	1 (2%)	65	85
2	H	66/73 (90%)	63 (96%)	3 (4%)	27	60
2	I	65/73 (89%)	64 (98%)	1 (2%)	65	85
2	J	67/73 (92%)	63 (94%)	4 (6%)	19	49
2	K	63/73 (86%)	60 (95%)	3 (5%)	25	58
2	L	66/73 (90%)	65 (98%)	1 (2%)	65	85
All	All	1034/1152 (90%)	989 (96%)	45 (4%)	29	61

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	54	GLN
1	E	8	ASP
2	K	56	ARG
1	D	104	TYR
1	E	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no ligands in this entry.

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	131/141 (92%)	0.69	20 (15%)	2	1	82, 99, 121, 138	0
1	B	123/141 (87%)	0.18	4 (3%)	46	24	86, 103, 122, 152	0
1	C	123/141 (87%)	0.22	4 (3%)	46	24	87, 104, 142, 173	0
1	D	122/141 (86%)	0.62	15 (12%)	4	1	90, 108, 145, 159	0
1	E	126/141 (89%)	0.34	5 (3%)	38	19	101, 123, 170, 182	0
1	F	131/141 (92%)	0.37	8 (6%)	21	9	81, 109, 133, 150	0
2	G	77/86 (89%)	0.63	11 (14%)	2	1	89, 123, 167, 186	0
2	H	78/86 (90%)	0.58	6 (7%)	13	5	82, 121, 198, 208	0
2	I	78/86 (90%)	0.55	5 (6%)	19	8	80, 113, 146, 154	0
2	J	77/86 (89%)	0.57	11 (14%)	2	1	81, 111, 154, 168	0
2	K	77/86 (89%)	0.34	7 (9%)	9	3	83, 113, 135, 146	0
2	L	78/86 (90%)	0.49	9 (11%)	4	2	87, 110, 130, 138	0
All	All	1221/1362 (89%)	0.45	105 (8%)	10	4	80, 110, 146, 208	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	76	ARG	6.7
1	A	75	ASP	6.7
1	C	110	GLN	5.8
1	C	111	GLU	5.4
2	L	1	MET	5.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.