wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 12:18 am BST

PDB ID	:	6UPU
Title	:	Crystal structure of the Orientia tsutsugamushi OtDUB in complex with three molecules of ubiquitin
Authors	:	Lim, C.S.; Ronau, J.A.; Xiong, Y.
Deposited on	:	2019-10-18
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

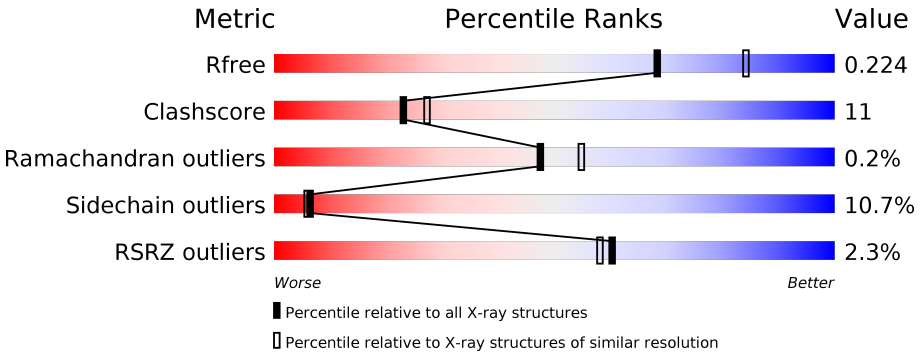
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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.



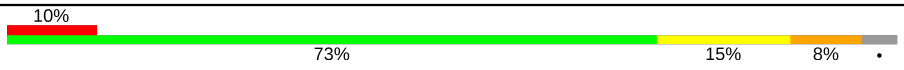
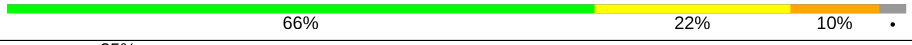
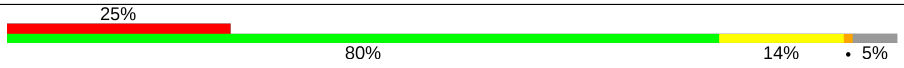
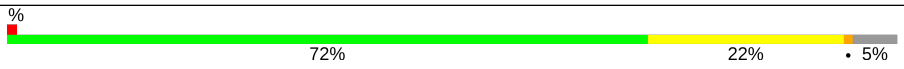
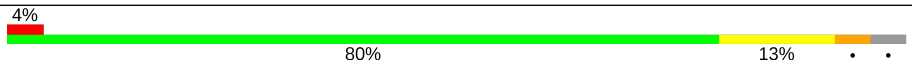
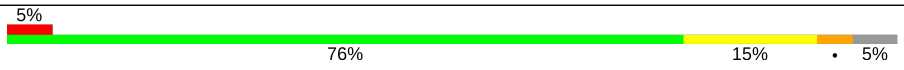
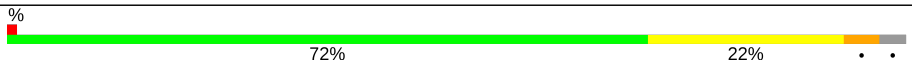
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	260	76% 18% 5%
1	E	260	74% 22%
1	I	260	75% 20%
1	M	260	% 76% 20%
2	B	79	63% 28% 6%
2	C	79	% 77% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	79	
2	F	79	
2	G	79	
2	H	79	
2	J	79	
2	K	79	
2	L	79	
2	N	79	
2	O	79	
2	P	79	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15824 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 ULP_PROTEASE domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2034	1269	354	401	10			
1	E	258	Total	C	N	O	S	0	0	0
			2029	1266	353	400	10			
1	I	258	Total	C	N	O	S	0	0	0
			2029	1266	353	400	10			
1	M	258	Total	C	N	O	S	0	0	0
			2029	1266	353	400	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B3CVM3
E	0	GLY	-	expression tag	UNP B3CVM3
I	0	GLY	-	expression tag	UNP B3CVM3
M	0	GLY	-	expression tag	UNP B3CVM3

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	S	0	0	0
			605	380	106	118	1			
2	C	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	D	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			
2	F	77	Total	C	N	O	S	0	0	0
			605	380	106	118	1			
2	G	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	H	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	77	Total	C	N	O	S	0	0	0
			605	380	106	118	1			
2	K	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	L	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			
2	N	78	Total	C	N	O	S	0	0	0
			609	382	107	119	1			
2	O	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	P	77	Total	C	N	O	S	0	0	0
			606	380	106	119	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP F5H388
B	-1	GLY	-	expression tag	UNP F5H388
B	0	GLY	-	expression tag	UNP F5H388
C	-2	GLY	-	expression tag	UNP F5H388
C	-1	GLY	-	expression tag	UNP F5H388
C	0	GLY	-	expression tag	UNP F5H388
D	-2	GLY	-	expression tag	UNP F5H388
D	-1	GLY	-	expression tag	UNP F5H388
D	0	GLY	-	expression tag	UNP F5H388
F	-2	GLY	-	expression tag	UNP F5H388
F	-1	GLY	-	expression tag	UNP F5H388
F	0	GLY	-	expression tag	UNP F5H388
G	-2	GLY	-	expression tag	UNP F5H388
G	-1	GLY	-	expression tag	UNP F5H388
G	0	GLY	-	expression tag	UNP F5H388
H	-2	GLY	-	expression tag	UNP F5H388
H	-1	GLY	-	expression tag	UNP F5H388
H	0	GLY	-	expression tag	UNP F5H388
J	-2	GLY	-	expression tag	UNP F5H388
J	-1	GLY	-	expression tag	UNP F5H388
J	0	GLY	-	expression tag	UNP F5H388
K	-2	GLY	-	expression tag	UNP F5H388
K	-1	GLY	-	expression tag	UNP F5H388
K	0	GLY	-	expression tag	UNP F5H388
L	-2	GLY	-	expression tag	UNP F5H388
L	-1	GLY	-	expression tag	UNP F5H388
L	0	GLY	-	expression tag	UNP F5H388

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	-2	GLY	-	expression tag	UNP F5H388
N	-1	GLY	-	expression tag	UNP F5H388
N	0	GLY	-	expression tag	UNP F5H388
O	-2	GLY	-	expression tag	UNP F5H388
O	-1	GLY	-	expression tag	UNP F5H388
O	0	GLY	-	expression tag	UNP F5H388
P	-2	GLY	-	expression tag	UNP F5H388
P	-1	GLY	-	expression tag	UNP F5H388
P	0	GLY	-	expression tag	UNP F5H388

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total O 73 73	0	0
3	B	20	Total O 20 20	0	0
3	C	14	Total O 14 14	0	0
3	D	5	Total O 5 5	0	0
3	E	68	Total O 68 68	0	0
3	F	31	Total O 31 31	0	0
3	G	8	Total O 8 8	0	0
3	H	14	Total O 14 14	0	0
3	I	61	Total O 61 61	0	0
3	J	26	Total O 26 26	0	0
3	K	11	Total O 11 11	0	0
3	L	7	Total O 7 7	0	0
3	M	89	Total O 89 89	0	0
3	N	23	Total O 23 23	0	0
3	O	10	Total O 10 10	0	0

Continued on next page...

Continued from previous page...

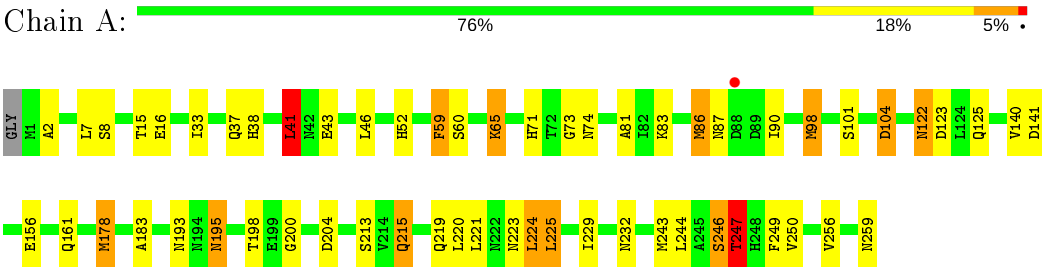
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	16	Total	O	0	0
			16	16		

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.

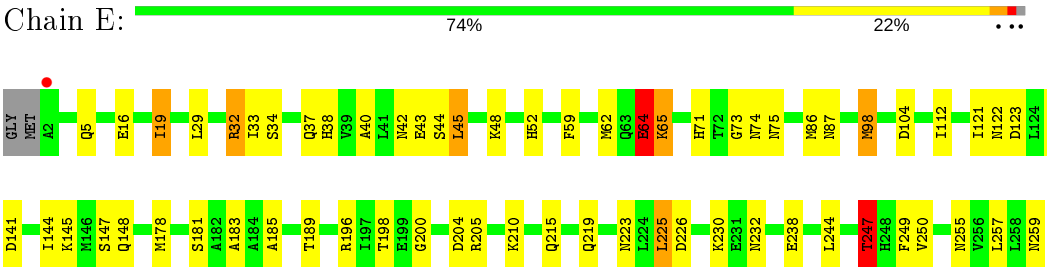
- Molecule 1: ULP_PROTEASE domain-containing protein

Chain A:



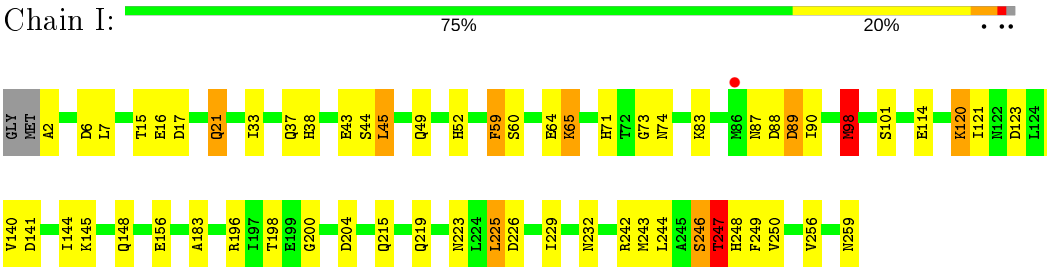
- Molecule 1: ULP_PROTEASE domain-containing protein

Chain E:



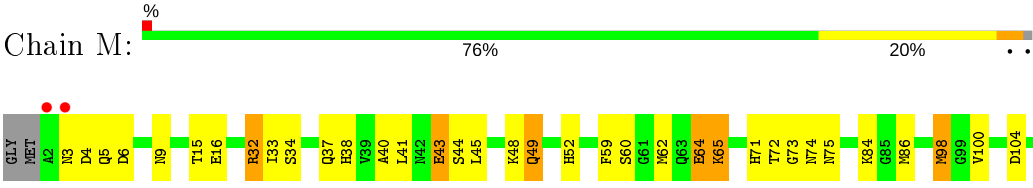
- Molecule 1: ULP_PROTEASE domain-containing protein

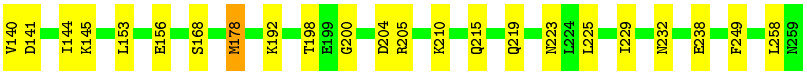
Chain I:



- Molecule 1: ULP_PROTEASE domain-containing protein

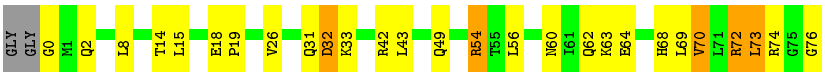
Chain M:





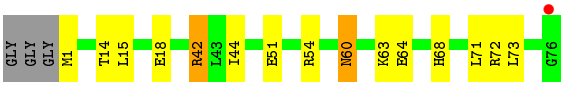
• Molecule 2: Ubiquitin

Chain B:



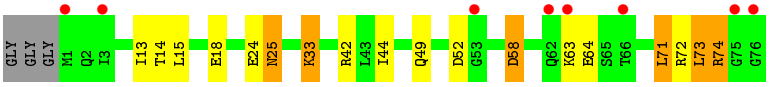
• Molecule 2: Ubiquitin

Chain C:



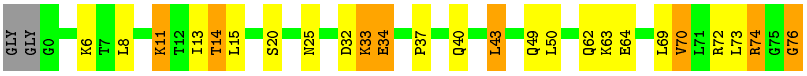
• Molecule 2: Ubiquitin

Chain D:



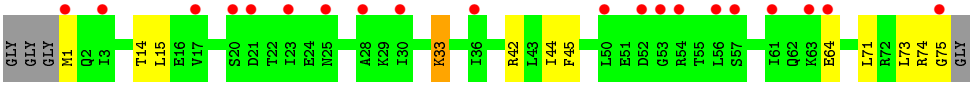
• Molecule 2: Ubiquitin

Chain F:



• Molecule 2: Ubiquitin

Chain G:

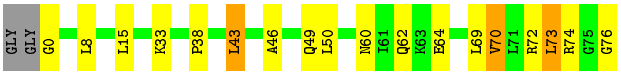


• Molecule 2: Ubiquitin

Chain H:

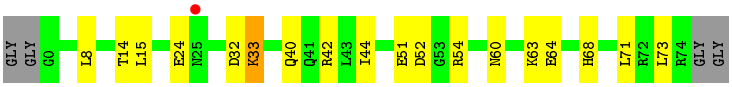
• Molecule 2: Ubiquitin

Chain J:



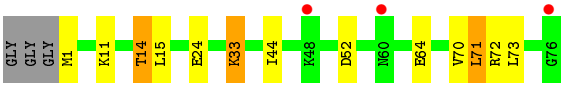
• Molecule 2: Ubiquitin

Chain K:



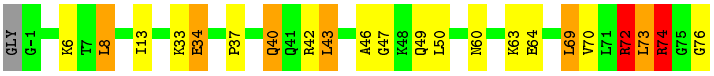
• Molecule 2: Ubiquitin

Chain L:



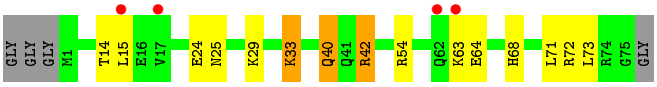
• Molecule 2: Ubiquitin

Chain N:



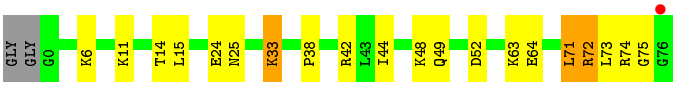
• Molecule 2: Ubiquitin

Chain O:



• Molecule 2: Ubiquitin

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.75Å 144.07Å 143.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.70 – 2.20 56.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (56.70-2.20) 98.5 (56.70-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.209 0.199 , 0.224	Depositor DCC
R_{free} test set	6079 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
Reported twinning fraction	0.742 for H, K, L 0.258 for -H, -L, -K	Depositor
Outliers	0 of 124051 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15824	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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

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	0.84	0/2058	1.01	4/2788 (0.1%)
1	E	0.90	2/2053 (0.1%)	1.03	6/2781 (0.2%)
1	I	0.82	0/2053	0.99	6/2781 (0.2%)
1	M	0.89	3/2053 (0.1%)	1.02	4/2781 (0.1%)
2	B	0.83	0/611	1.22	4/821 (0.5%)
2	C	0.75	0/607	1.00	2/816 (0.2%)
2	D	0.70	0/608	0.87	0/816
2	F	0.85	0/611	1.24	3/821 (0.4%)
2	G	0.67	0/603	0.83	0/811
2	H	0.81	1/607 (0.2%)	0.93	0/816
2	J	0.85	0/611	1.06	0/821
2	K	0.71	0/603	0.90	0/811
2	L	0.71	0/608	0.87	0/816
2	N	0.89	1/615 (0.2%)	1.11	4/826 (0.5%)
2	O	0.71	0/603	0.92	1/811 (0.1%)
2	P	0.77	0/612	0.93	1/821 (0.1%)
All	All	0.82	7/15516 (0.0%)	1.00	35/20938 (0.2%)

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	1
2	B	0	1
2	D	0	1
2	G	0	1
2	L	0	1
All	All	0	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	64	GLU	CD-OE1	6.72	1.33	1.25
1	M	43	GLU	CD-OE2	6.10	1.32	1.25
1	E	238	GLU	CD-OE1	6.09	1.32	1.25
2	H	34	GLU	CD-OE1	-5.91	1.19	1.25
2	N	72	ARG	CD-NE	-5.43	1.37	1.46

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	72	ARG	NE-CZ-NH1	-13.25	113.68	120.30
2	F	72	ARG	NE-CZ-NH2	9.93	125.27	120.30
2	C	42	ARG	NE-CZ-NH1	-7.84	116.38	120.30
2	B	72	ARG	NE-CZ-NH1	-7.80	116.40	120.30
2	N	72	ARG	NE-CZ-NH2	7.49	124.05	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	LEU	Mainchain
2	B	42	ARG	Mainchain
2	D	73	LEU	Peptide
2	G	74	ARG	Peptide
2	L	70	VAL	Mainchain

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	2034	0	2049	69	0
1	E	2029	0	2044	45	0
1	I	2029	0	2044	59	0
1	M	2029	0	2044	61	0
2	B	605	0	632	33	0
2	C	601	0	629	9	0
2	D	602	0	629	18	0
2	F	605	0	632	28	0
2	G	597	0	626	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	601	0	629	19	0
2	J	605	0	632	21	0
2	K	597	0	626	16	0
2	L	602	0	629	8	0
2	N	609	0	635	33	0
2	O	597	0	626	9	0
2	P	606	0	632	16	0
3	A	73	0	0	8	0
3	B	20	0	0	10	0
3	C	14	0	0	3	0
3	D	5	0	0	6	0
3	E	68	0	0	3	0
3	F	31	0	0	6	0
3	G	8	0	0	3	0
3	H	14	0	0	5	0
3	I	61	0	0	4	0
3	J	26	0	0	5	0
3	K	11	0	0	6	0
3	L	7	0	0	2	0
3	M	89	0	0	11	0
3	N	23	0	0	3	0
3	O	10	0	0	5	0
3	P	16	0	0	5	0
All	All	15824	0	15738	353	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 11.

The worst 5 of 353 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:O:29:LYS:HE2	3:O:108:HOH:O	1.37	1.20
1:A:104:ASP:HB2	3:A:320:HOH:O	1.46	1.12
2:K:40:GLN:NE2	3:K:101:HOH:O	1.83	1.08
2:O:54:ARG:NH1	3:O:101:HOH:O	1.88	1.06
2:L:14:THR:HG23	3:L:106:HOH:O	1.57	1.05

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	257/260 (99%)	249 (97%)	6 (2%)	2 (1%)	19 19
1	E	256/260 (98%)	251 (98%)	5 (2%)	0	100 100
1	I	256/260 (98%)	250 (98%)	6 (2%)	0	100 100
1	M	256/260 (98%)	251 (98%)	5 (2%)	0	100 100
2	B	75/79 (95%)	75 (100%)	0	0	100 100
2	C	74/79 (94%)	73 (99%)	1 (1%)	0	100 100
2	D	74/79 (94%)	73 (99%)	0	1 (1%)	11 8
2	F	75/79 (95%)	75 (100%)	0	0	100 100
2	G	73/79 (92%)	73 (100%)	0	0	100 100
2	H	74/79 (94%)	73 (99%)	1 (1%)	0	100 100
2	J	75/79 (95%)	75 (100%)	0	0	100 100
2	K	73/79 (92%)	73 (100%)	0	0	100 100
2	L	74/79 (94%)	74 (100%)	0	0	100 100
2	N	76/79 (96%)	76 (100%)	0	0	100 100
2	O	73/79 (92%)	72 (99%)	1 (1%)	0	100 100
2	P	75/79 (95%)	75 (100%)	0	0	100 100
All	All	1916/1988 (96%)	1888 (98%)	25 (1%)	3 (0%)	47 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	2	ALA
2	D	74	ARG

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	233/235 (99%)	214 (92%)	19 (8%)	11	11
1	E	233/235 (99%)	211 (91%)	22 (9%)	8	8
1	I	233/235 (99%)	211 (91%)	22 (9%)	8	8
1	M	233/235 (99%)	216 (93%)	17 (7%)	14	15
2	B	68/68 (100%)	58 (85%)	10 (15%)	3	2
2	C	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	D	68/68 (100%)	58 (85%)	10 (15%)	3	2
2	F	68/68 (100%)	55 (81%)	13 (19%)	1	1
2	G	68/68 (100%)	62 (91%)	6 (9%)	10	10
2	H	68/68 (100%)	60 (88%)	8 (12%)	5	4
2	J	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	K	68/68 (100%)	61 (90%)	7 (10%)	7	6
2	L	68/68 (100%)	60 (88%)	8 (12%)	5	4
2	N	68/68 (100%)	58 (85%)	10 (15%)	3	2
2	O	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	P	68/68 (100%)	60 (88%)	8 (12%)	5	4
All	All	1748/1756 (100%)	1561 (89%)	187 (11%)	6	6

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	15	LEU
1	I	83	LYS
2	O	24	GLU
2	G	71	LEU
2	H	71	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	60	ASN
1	I	53	GLN
2	N	68	HIS
2	F	68	HIS
2	H	60	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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	259/260 (99%)	-0.35	1 (0%) 92 91	27, 45, 66, 105	0
1	E	258/260 (99%)	-0.30	1 (0%) 92 91	27, 46, 66, 80	0
1	I	258/260 (99%)	-0.33	1 (0%) 92 91	29, 47, 68, 109	0
1	M	258/260 (99%)	-0.35	2 (0%) 86 85	28, 42, 64, 88	0
2	B	77/79 (97%)	-0.16	0 100 100	27, 46, 68, 81	0
2	C	76/79 (96%)	0.23	1 (1%) 77 75	46, 75, 97, 100	0
2	D	76/79 (96%)	0.74	8 (10%) 6 5	59, 101, 133, 147	0
2	F	77/79 (97%)	-0.18	0 100 100	30, 45, 65, 75	0
2	G	75/79 (94%)	1.28	20 (26%) 0 0	79, 117, 136, 145	0
2	H	76/79 (96%)	0.37	2 (2%) 56 53	51, 72, 91, 101	0
2	J	77/79 (97%)	-0.33	0 100 100	29, 46, 62, 66	0
2	K	75/79 (94%)	0.30	1 (1%) 77 75	49, 81, 104, 116	0
2	L	76/79 (96%)	0.62	3 (3%) 39 37	58, 101, 135, 151	0
2	N	78/79 (98%)	-0.31	0 100 100	30, 43, 57, 65	0
2	O	75/79 (94%)	0.41	4 (5%) 26 25	56, 93, 116, 127	0
2	P	77/79 (97%)	0.17	1 (1%) 77 75	35, 64, 96, 112	0
All	All	1948/1988 (97%)	-0.06	45 (2%) 60 58	27, 51, 112, 151	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	86	MET	6.2
2	P	76	GLY	5.7
2	G	23	ILE	4.8
1	M	2	ALA	4.6
2	G	1	MET	3.6

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.