Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 05:19 AM JST

PDB ID	:	7EU4
Title	:	Crystal structure of plant ATG12 complexed with the AIM12 of ATG3
Authors	:	Matoba, K.; Noda, N.N.
Deposited on	:	2021-05-16
Resolution	:	3.20 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:

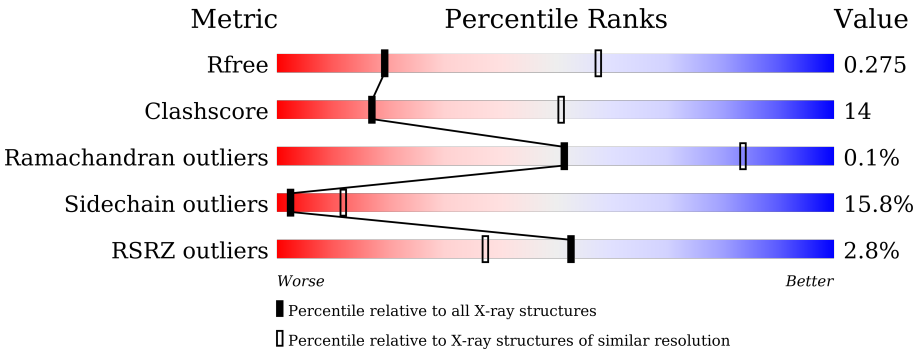
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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 <=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	96	3% 61% 20% • 15%
1	B	96	2% 61% 25% • 11%
1	C	96	67% 25% 6% •
1	D	96	% 56% 29% • 11%
1	E	96	2% 64% 27% 6% • •
1	F	96	2% 56% 31% • 11%

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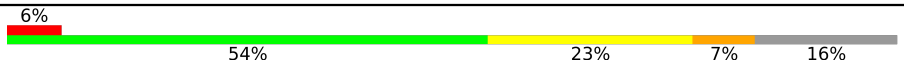
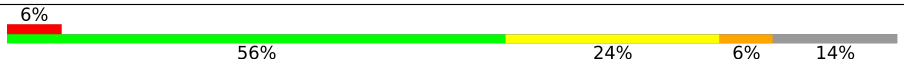
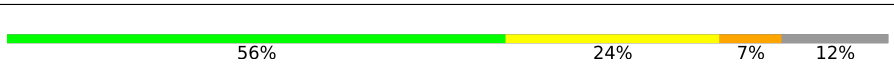
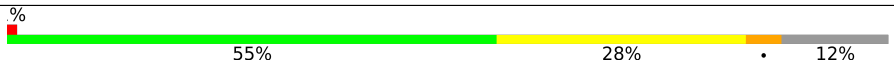
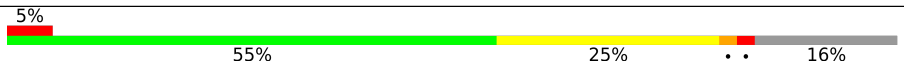
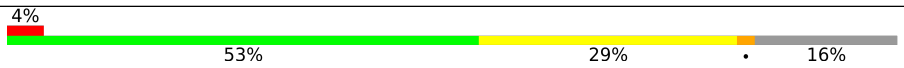
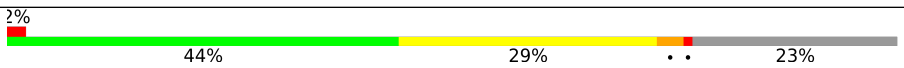
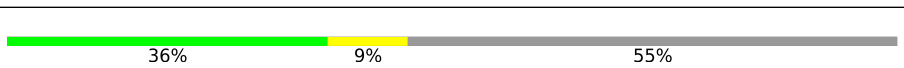
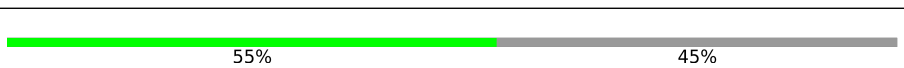
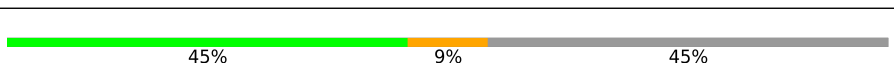
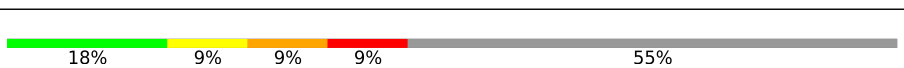
Mol	Chain	Length	Quality of chain
1	G	96	
1	H	96	
1	I	96	
1	J	96	
1	K	96	
1	L	96	
1	M	96	
1	N	96	
2	O	11	
2	P	11	
2	Q	11	
2	R	11	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9301 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-like protein ATG12B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	0	0	0
			644	414	110	118	2			
1	B	85	Total	C	N	O	S	0	0	0
			664	428	113	121	2			
1	C	94	Total	C	N	O	S	0	0	0
			726	465	124	134	3			
1	D	85	Total	C	N	O	S	0	0	0
			661	427	113	119	2			
1	E	94	Total	C	N	O	S	0	0	0
			726	465	124	134	3			
1	F	85	Total	C	N	O	S	0	0	0
			660	425	112	121	2			
1	G	81	Total	C	N	O	S	0	0	0
			606	383	106	115	2			
1	H	83	Total	C	N	O	S	0	0	0
			648	417	110	119	2			
1	I	84	Total	C	N	O	S	0	0	0
			663	428	113	120	2			
1	J	84	Total	C	N	O	S	0	0	0
			659	426	112	119	2			
1	K	83	Total	C	N	O	S	0	0	0
			649	417	111	119	2			
1	L	81	Total	C	N	O	S	0	0	0
			617	395	106	114	2			
1	M	81	Total	C	N	O	S	0	0	0
			630	406	106	117	1			
1	N	74	Total	C	N	O	S	0	0	0
			572	366	97	107	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9LVK3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP Q9LVK3
B	-1	GLY	-	expression tag	UNP Q9LVK3
B	0	PRO	-	expression tag	UNP Q9LVK3
C	-1	GLY	-	expression tag	UNP Q9LVK3
C	0	PRO	-	expression tag	UNP Q9LVK3
D	-1	GLY	-	expression tag	UNP Q9LVK3
D	0	PRO	-	expression tag	UNP Q9LVK3
E	-1	GLY	-	expression tag	UNP Q9LVK3
E	0	PRO	-	expression tag	UNP Q9LVK3
F	-1	GLY	-	expression tag	UNP Q9LVK3
F	0	PRO	-	expression tag	UNP Q9LVK3
G	-1	GLY	-	expression tag	UNP Q9LVK3
G	0	PRO	-	expression tag	UNP Q9LVK3
H	-1	GLY	-	expression tag	UNP Q9LVK3
H	0	PRO	-	expression tag	UNP Q9LVK3
I	-1	GLY	-	expression tag	UNP Q9LVK3
I	0	PRO	-	expression tag	UNP Q9LVK3
J	-1	GLY	-	expression tag	UNP Q9LVK3
J	0	PRO	-	expression tag	UNP Q9LVK3
K	-1	GLY	-	expression tag	UNP Q9LVK3
K	0	PRO	-	expression tag	UNP Q9LVK3
L	-1	GLY	-	expression tag	UNP Q9LVK3
L	0	PRO	-	expression tag	UNP Q9LVK3
M	-1	GLY	-	expression tag	UNP Q9LVK3
M	0	PRO	-	expression tag	UNP Q9LVK3
N	-1	GLY	-	expression tag	UNP Q9LVK3
N	0	PRO	-	expression tag	UNP Q9LVK3

- Molecule 2 is a protein called AIM12 from Autophagy-related protein 3.

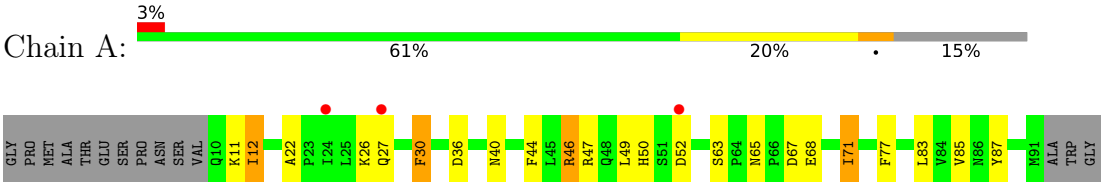
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	5	Total	C	N	O	S	0	0	0
			40	25	5	9	1			
2	P	6	Total	C	N	O	S	0	0	0
			48	29	6	12	1			
2	Q	6	Total	C	N	O	S	0	0	0
			48	29	6	12	1			
2	R	5	Total	C	N	O	S	0	0	0
			40	25	5	9	1			

3 Residue-property plots (i)

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.

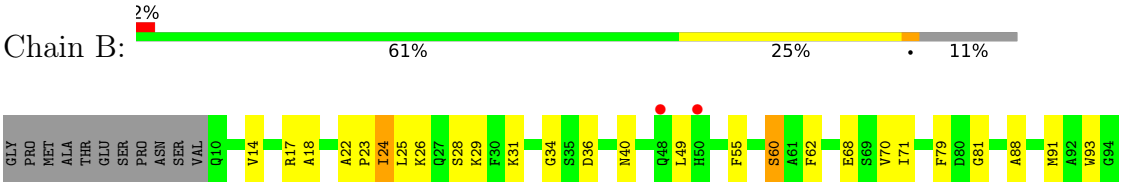
• Molecule 1: Ubiquitin-like protein ATG12B

Chain A:



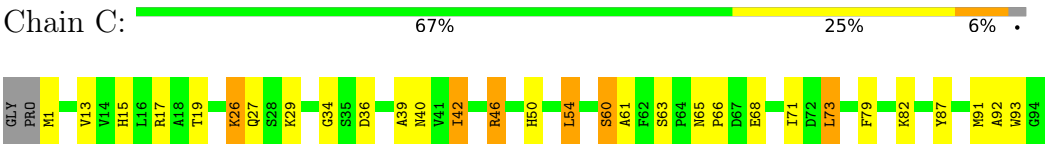
• Molecule 1: Ubiquitin-like protein ATG12B

Chain B:



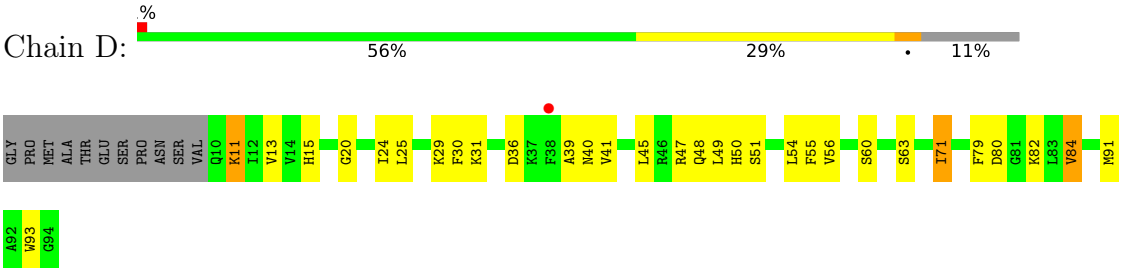
• Molecule 1: Ubiquitin-like protein ATG12B

Chain C:



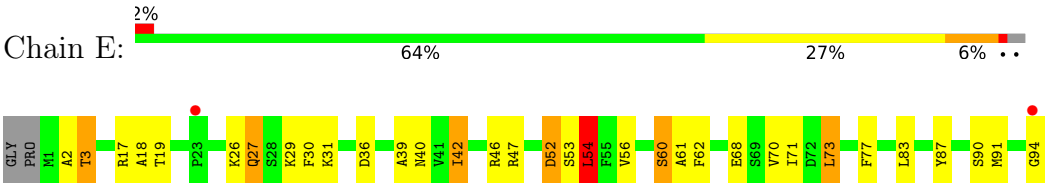
• Molecule 1: Ubiquitin-like protein ATG12B

Chain D:



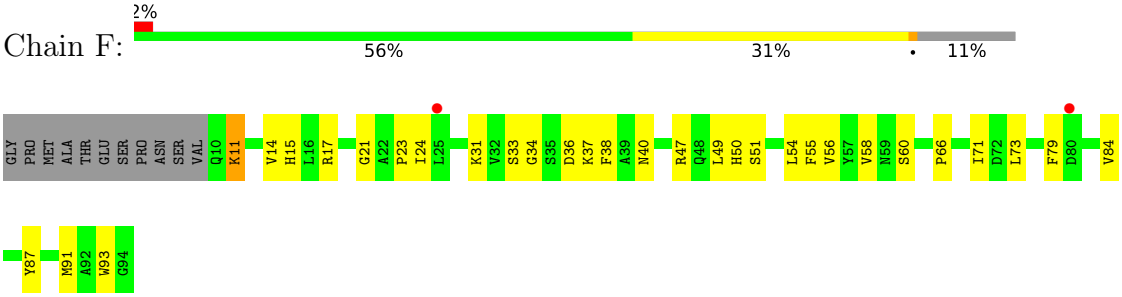
• Molecule 1: Ubiquitin-like protein ATG12B

Chain E:



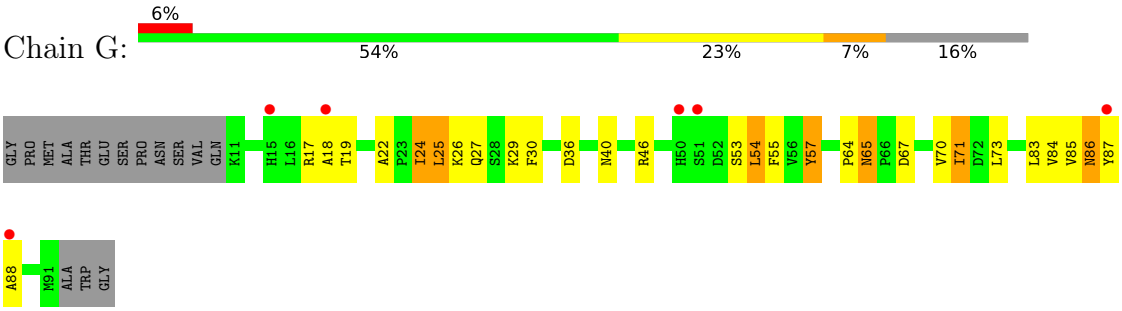
• Molecule 1: Ubiquitin-like protein ATG12B

Chain F:



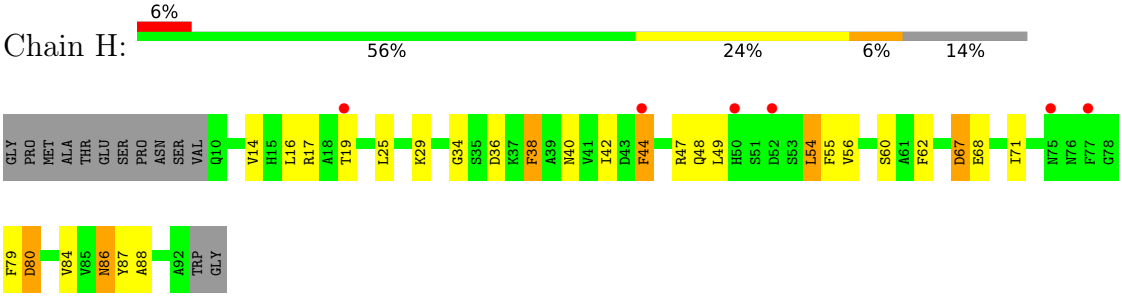
• Molecule 1: Ubiquitin-like protein ATG12B

Chain G:



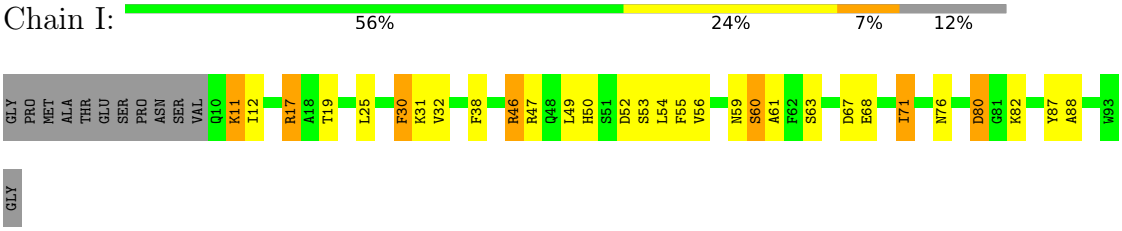
• Molecule 1: Ubiquitin-like protein ATG12B

Chain H:



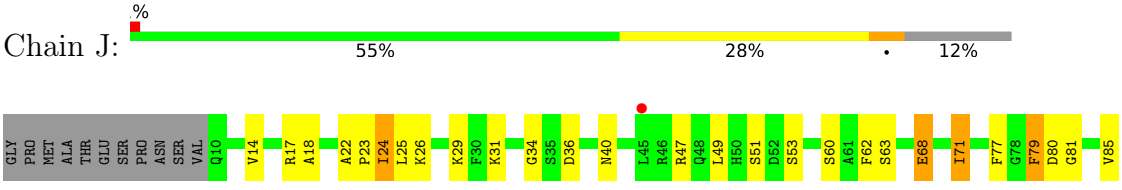
• Molecule 1: Ubiquitin-like protein ATG12B

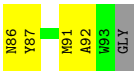
Chain I:



• Molecule 1: Ubiquitin-like protein ATG12B

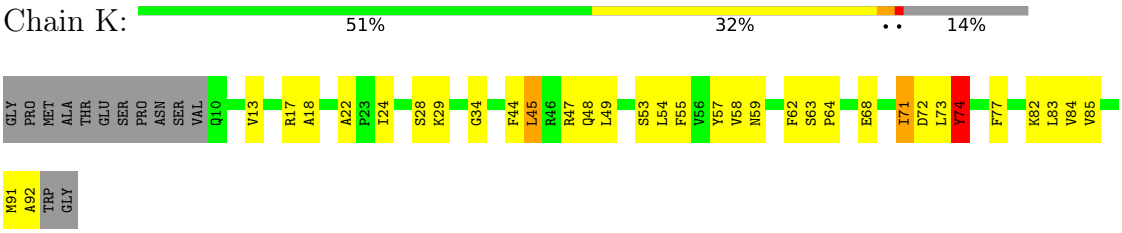
Chain J:





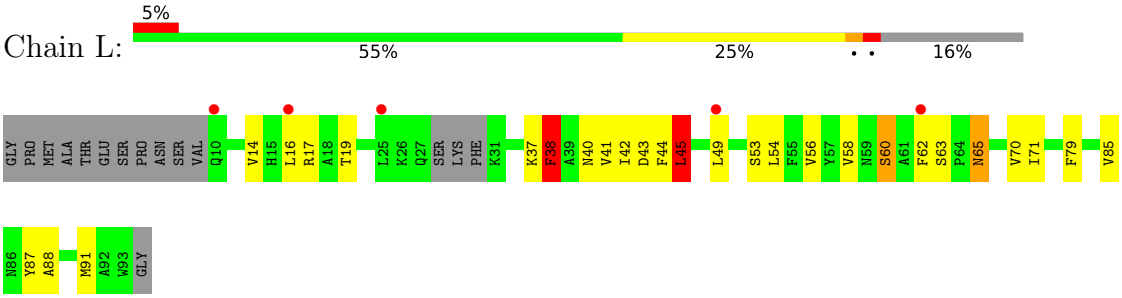
• Molecule 1: Ubiquitin-like protein ATG12B

Chain K:



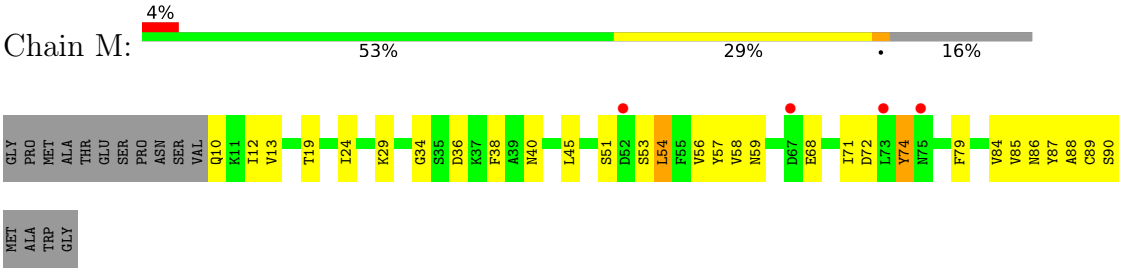
• Molecule 1: Ubiquitin-like protein ATG12B

Chain L:



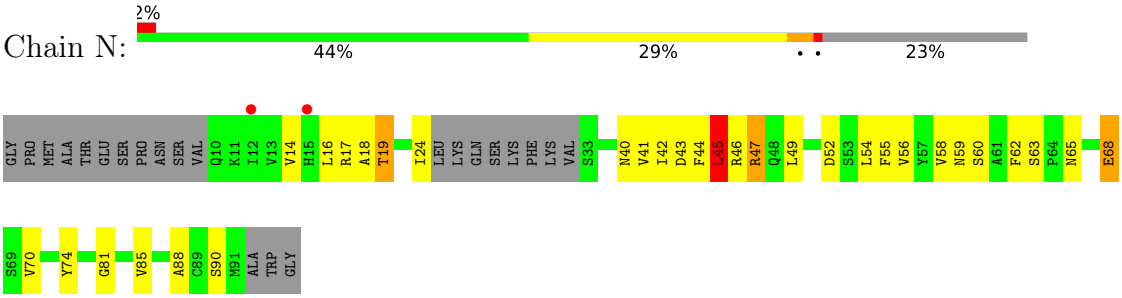
• Molecule 1: Ubiquitin-like protein ATG12B

Chain M:



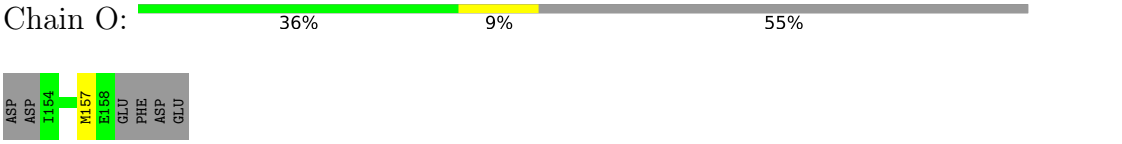
• Molecule 1: Ubiquitin-like protein ATG12B

Chain N:



• Molecule 2: AIM12 from Autophagy-related protein 3

Chain O:

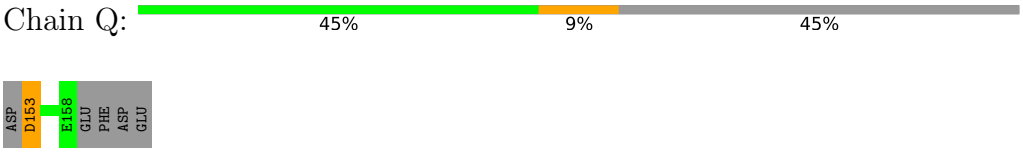


• Molecule 2: AIM12 from Autophagy-related protein 3

Chain P:

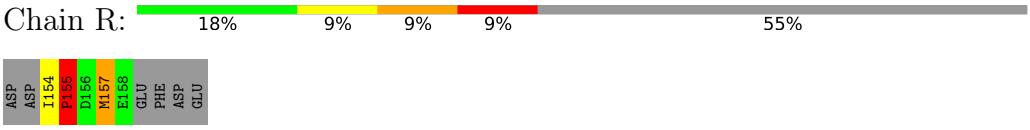
• Molecule 2: AIM12 from Autophagy-related protein 3

Chain Q:



• Molecule 2: AIM12 from Autophagy-related protein 3

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	128.47Å 128.47Å 163.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.96 – 3.20 45.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (45.96-3.20) 99.1 (45.96-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.238 , 0.285 0.240 , 0.275	Depositor DCC
R_{free} test set	1269 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.430 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9301	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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	0.54	0/658	0.78	0/888
1	B	0.52	0/680	0.78	0/918
1	C	0.54	0/743	0.83	0/1005
1	D	0.45	0/677	0.71	0/914
1	E	0.54	0/743	0.86	2/1005 (0.2%)
1	F	0.45	0/676	0.73	0/914
1	G	0.51	0/618	0.78	0/837
1	H	0.50	0/662	0.83	1/893 (0.1%)
1	I	0.49	0/679	0.77	0/918
1	J	0.48	0/675	0.76	2/913 (0.2%)
1	K	0.53	0/663	0.79	1/895 (0.1%)
1	L	0.53	0/629	0.87	2/851 (0.2%)
1	M	0.59	0/644	0.78	2/871 (0.2%)
1	N	0.60	0/584	0.94	1/790 (0.1%)
2	O	0.61	0/40	0.67	0/53
2	P	0.37	0/48	0.61	0/64
2	Q	0.55	0/48	0.63	0/64
2	R	0.57	0/40	0.69	0/53
All	All	0.52	0/9507	0.80	11/12846 (0.1%)

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	C	0	1
1	H	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	N	0	1
All	All	0	6

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	79	PHE	CB-CG-CD1	6.20	125.14	120.80
1	E	52	ASP	CB-CA-C	6.19	122.77	110.40
1	L	38	PHE	CB-CG-CD1	5.70	124.79	120.80
1	M	74	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	J	79	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	E	54	LEU	CB-CG-CD1	5.50	120.35	111.00
1	N	45	LEU	CA-CB-CG	5.26	127.41	115.30
1	H	80	ASP	CB-CA-C	-5.26	99.89	110.40
1	M	74	TYR	CB-CG-CD2	5.22	124.14	121.00
1	L	45	LEU	CA-CB-CG	5.22	127.31	115.30
1	K	74	TYR	CB-CG-CD1	-5.09	117.94	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	46	ARG	Sidechain
1	H	47	ARG	Sidechain
1	J	47	ARG	Sidechain
1	K	47	ARG	Sidechain
1	L	91	MET	Peptide
1	N	47	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	644	0	639	21	0
1	B	664	0	651	24	1
1	C	726	0	712	25	0
1	D	661	0	649	26	1
1	E	726	0	712	36	1
1	F	660	0	640	24	0
1	G	606	0	570	37	0
1	H	648	0	643	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	663	0	654	28	0
1	J	659	0	648	32	1
1	K	649	0	644	31	0
1	L	617	0	591	34	0
1	M	630	0	619	26	0
1	N	572	0	551	29	0
2	O	40	0	36	1	0
2	P	48	0	40	0	0
2	Q	48	0	40	1	0
2	R	40	0	36	4	0
All	All	9301	0	9075	258	2

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 14.

All (258) 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:G:71:ILE:HG23	1:H:34:GLY:O	1.59	1.03
1:L:40:ASN:O	1:L:43:ASP:OD1	1.77	1.02
1:M:34:GLY:HA2	1:N:70:VAL:HG23	1.40	1.02
1:N:40:ASN:O	1:N:43:ASP:OD1	1.78	1.01
1:E:54:LEU:HD13	1:E:56:VAL:HG23	1.45	0.95
1:E:26:LYS:HB2	1:J:24:ILE:HG21	1.51	0.93
1:G:53:SER:HB2	1:L:62:PHE:CD1	2.07	0.89
1:E:70:VAL:HG13	1:F:34:GLY:HA2	1.54	0.88
1:M:34:GLY:HA2	1:N:70:VAL:CG2	2.03	0.88
1:C:34:GLY:HA3	1:D:71:ILE:HD12	1.55	0.87
1:G:53:SER:HB2	1:L:62:PHE:HD1	1.43	0.83
1:E:70:VAL:CG1	1:F:34:GLY:HA2	2.07	0.83
1:B:81:GLY:HA3	1:M:24:ILE:HD11	1.59	0.83
1:B:81:GLY:CA	1:M:24:ILE:HD11	2.12	0.80
1:A:12:ILE:HD12	1:B:70:VAL:HG12	1.64	0.79
1:C:68:GLU:OE2	1:I:52:ASP:OD2	2.02	0.78
1:M:36:ASP:HB3	1:M:40:ASN:HD22	1.48	0.78
2:R:154:ILE:HB	2:R:155:PRO:HD3	1.64	0.77
1:B:36:ASP:HB3	1:B:40:ASN:HD22	1.51	0.75
1:H:36:ASP:HB3	1:H:40:ASN:HD22	1.53	0.74
1:A:12:ILE:CD1	1:B:70:VAL:HG12	2.18	0.73
1:A:71:ILE:HB	1:B:34:GLY:O	1.88	0.73
1:K:64:PRO:HG2	1:L:38:PHE:CE2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:SER:CB	1:L:62:PHE:HD1	2.02	0.72
1:M:19:THR:OG1	1:N:88:ALA:HB2	1.88	0.72
1:G:36:ASP:HB3	1:G:40:ASN:HD22	1.55	0.71
1:E:60:SER:OG	1:E:62:PHE:CE1	2.43	0.71
1:I:12:ILE:HD11	1:J:71:ILE:HA	1.73	0.71
1:J:53:SER:OG	1:K:63:SER:N	2.25	0.70
1:G:19:THR:HG22	1:H:86:ASN:HB3	1.74	0.69
1:J:36:ASP:HB3	1:J:40:ASN:HD22	1.56	0.69
1:F:36:ASP:HB3	1:F:40:ASN:HD22	1.59	0.68
1:F:11:LYS:HB2	1:F:31:LYS:HE2	1.76	0.68
1:G:85:VAL:CG2	1:H:16:LEU:HD23	2.24	0.67
1:C:36:ASP:HB3	1:C:40:ASN:HD22	1.60	0.67
1:K:45:LEU:CD1	1:K:49:LEU:HG	2.25	0.66
1:G:85:VAL:HG22	1:H:16:LEU:HD23	1.77	0.66
1:E:36:ASP:HB3	1:E:40:ASN:HD22	1.60	0.66
1:F:11:LYS:HD3	1:F:11:LYS:N	2.11	0.66
1:E:26:LYS:HB2	1:J:24:ILE:CG2	2.24	0.66
1:D:36:ASP:HB3	1:D:40:ASN:HD22	1.60	0.66
1:C:63:SER:O	1:I:53:SER:HA	1.95	0.65
1:G:71:ILE:HG23	1:H:34:GLY:C	2.16	0.65
1:I:87:TYR:CZ	1:J:18:ALA:HB2	2.31	0.65
1:D:20:GLY:HA2	1:I:76:ASN:ND2	2.11	0.65
1:E:18:ALA:HB2	1:F:87:TYR:CZ	2.31	0.64
1:F:24:ILE:O	1:F:24:ILE:HD12	1.96	0.64
1:E:26:LYS:CB	1:J:24:ILE:HG21	2.25	0.64
1:M:85:VAL:CG2	1:N:16:LEU:HD23	2.28	0.63
1:G:24:ILE:HD13	1:G:25:LEU:N	2.14	0.62
1:G:65:ASN:HD22	1:G:65:ASN:H	1.44	0.62
1:K:85:VAL:CG2	1:L:16:LEU:HD23	2.29	0.62
1:C:61:ALA:HB3	1:J:91:MET:HB2	1.82	0.61
1:D:11:LYS:HD3	1:D:11:LYS:N	2.15	0.61
1:D:24:ILE:HD12	1:D:24:ILE:O	2.01	0.61
1:E:39:ALA:HA	1:E:42:ILE:HG13	1.81	0.61
1:J:80:ASP:HA	1:K:28:SER:HB2	1.83	0.61
1:C:82:LYS:HB2	1:D:13:VAL:O	2.01	0.61
1:H:48:GLN:HE21	1:H:49:LEU:HG	1.65	0.61
1:L:38:PHE:HD1	1:L:38:PHE:O	1.84	0.61
1:I:87:TYR:OH	1:J:18:ALA:HB2	2.00	0.60
1:B:18:ALA:HB1	1:B:22:ALA:HB3	1.82	0.60
1:D:79:PHE:HD2	1:J:92:ALA:CB	2.14	0.60
1:E:18:ALA:HB2	1:F:87:TYR:OH	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LYS:CB	1:J:24:ILE:CG2	2.80	0.59
1:L:42:ILE:HA	1:L:45:LEU:CD1	2.33	0.59
1:M:59:ASN:OD1	1:N:59:ASN:OD1	2.21	0.59
1:G:64:PRO:HG2	1:H:38:PHE:CE2	2.38	0.59
1:M:85:VAL:HG22	1:N:16:LEU:HD23	1.85	0.59
1:C:39:ALA:HA	1:C:42:ILE:HG13	1.84	0.58
1:M:87:TYR:OH	1:N:18:ALA:HB2	2.03	0.58
1:N:42:ILE:HA	1:N:45:LEU:CD1	2.34	0.58
1:E:83:LEU:O	1:F:14:VAL:HA	2.04	0.58
1:E:26:LYS:CG	1:J:24:ILE:HG22	2.33	0.58
1:M:89:CYS:O	1:M:90:SER:C	2.41	0.58
1:M:85:VAL:CG2	1:N:16:LEU:CD2	2.82	0.57
1:M:12:ILE:HD12	1:N:74:TYR:CG	2.39	0.57
1:E:3:THR:HB	1:I:19:THR:HB	1.86	0.57
1:B:23:PRO:HG2	1:B:49:LEU:HD22	1.86	0.57
1:K:59:ASN:OD1	1:L:60:SER:O	2.22	0.57
1:I:88:ALA:HA	1:J:22:ALA:HB2	1.86	0.57
1:F:21:GLY:O	1:N:52:ASP:OD2	2.22	0.57
1:G:19:THR:HG21	1:G:57:TYR:CE2	2.40	0.57
1:G:65:ASN:H	1:G:65:ASN:ND2	2.03	0.56
1:G:86:ASN:OD1	1:H:17:ARG:CZ	2.52	0.56
1:G:18:ALA:HB2	1:H:87:TYR:CZ	2.41	0.56
1:G:71:ILE:CG2	1:H:34:GLY:O	2.46	0.56
1:I:17:ARG:HB3	1:J:86:ASN:HD22	1.70	0.56
1:N:41:VAL:O	1:N:45:LEU:HG	2.06	0.56
1:D:79:PHE:CD2	1:J:92:ALA:CB	2.90	0.55
1:B:24:ILE:HG22	1:C:26:LYS:HG3	1.88	0.55
1:J:81:GLY:HA2	1:K:24:ILE:HD11	1.87	0.55
1:L:41:VAL:O	1:L:45:LEU:HG	2.06	0.55
1:M:13:VAL:HG12	1:N:81:GLY:O	2.07	0.55
1:L:43:ASP:OD1	1:L:44:PHE:N	2.39	0.55
1:G:73:LEU:HD11	1:H:38:PHE:HD2	1.72	0.55
1:N:43:ASP:OD1	1:N:44:PHE:N	2.39	0.55
1:I:12:ILE:HD11	1:J:71:ILE:HD13	1.88	0.54
1:A:83:LEU:CD1	1:A:85:VAL:HG23	2.38	0.54
1:K:58:VAL:CG1	1:L:85:VAL:HG22	2.37	0.54
1:C:34:GLY:CA	1:D:71:ILE:HD12	2.33	0.54
1:G:30:PHE:CB	2:R:157:MET:SD	2.96	0.54
1:D:11:LYS:HB2	1:D:31:LYS:HE2	1.90	0.54
1:E:2:ALA:HB1	1:E:3:THR:OG1	2.08	0.54
1:G:53:SER:CB	1:L:62:PHE:CD1	2.83	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:LEU:HD11	1:H:38:PHE:CD2	2.43	0.54
1:C:15:HIS:HB3	1:D:84:VAL:HG12	1.90	0.53
1:A:77:PHE:CE1	1:B:60:SER:HB2	2.43	0.53
1:B:81:GLY:HA2	1:M:24:ILE:HD11	1.90	0.53
1:F:54:LEU:HD13	1:F:56:VAL:HG23	1.91	0.53
1:K:85:VAL:HG22	1:L:16:LEU:HD23	1.89	0.53
1:B:24:ILE:CG2	1:C:26:LYS:HB2	2.39	0.52
1:C:46:ARG:HG2	1:C:54:LEU:HD21	1.90	0.52
1:M:85:VAL:HA	1:N:58:VAL:HG22	1.91	0.52
1:G:18:ALA:HB2	1:H:87:TYR:OH	2.09	0.52
1:M:38:PHE:HB2	1:N:68:GLU:O	2.09	0.52
1:B:91:MET:HB2	1:E:61:ALA:HB3	1.90	0.52
1:E:77:PHE:CD2	1:F:58:VAL:HG21	2.45	0.52
1:H:38:PHE:HD1	1:H:38:PHE:O	1.92	0.51
1:E:26:LYS:CD	1:J:24:ILE:HG22	2.41	0.51
1:A:46:ARG:HG3	1:A:47:ARG:N	2.24	0.51
1:I:63:SER:O	1:L:53:SER:HA	2.11	0.51
1:A:63:SER:HB2	1:N:55:PHE:CE2	2.45	0.51
1:E:26:LYS:HD3	1:J:24:ILE:HG22	1.91	0.51
1:E:54:LEU:HD13	1:E:56:VAL:CG2	2.31	0.51
1:G:24:ILE:HD13	1:G:25:LEU:O	2.11	0.51
1:D:54:LEU:HD13	1:D:56:VAL:HG23	1.93	0.51
1:K:18:ALA:HB2	1:L:87:TYR:CZ	2.46	0.51
1:A:65:ASN:HA	1:N:46:ARG:NH2	2.26	0.51
1:K:71:ILE:CD1	1:K:74:TYR:CD1	2.94	0.51
1:G:73:LEU:CD1	1:H:38:PHE:CD2	2.93	0.50
1:G:87:TYR:HA	1:H:55:PHE:O	2.11	0.50
1:I:12:ILE:CD1	1:J:71:ILE:HA	2.40	0.50
1:M:54:LEU:CD1	1:M:56:VAL:HG23	2.41	0.50
1:G:85:VAL:CG2	1:H:16:LEU:CD2	2.88	0.50
1:N:88:ALA:HB1	1:N:90:SER:HB3	1.92	0.50
1:H:25:LEU:HD22	1:H:48:GLN:CD	2.32	0.50
1:I:46:ARG:HG3	1:I:47:ARG:N	2.27	0.50
1:J:53:SER:OG	1:K:62:PHE:HA	2.12	0.50
1:K:18:ALA:HB2	1:L:87:TYR:OH	2.11	0.49
1:K:85:VAL:CG2	1:L:16:LEU:CD2	2.90	0.49
1:G:88:ALA:HB2	1:H:19:THR:OG1	2.13	0.49
1:M:51:SER:O	1:M:53:SER:N	2.43	0.49
1:C:93:TRP:HZ2	1:I:59:ASN:HA	1.78	0.49
1:M:85:VAL:HG12	1:N:58:VAL:CG2	2.42	0.49
1:K:55:PHE:O	1:L:87:TYR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:LEU:HD12	1:L:56:VAL:HG23	1.93	0.49
1:C:68:GLU:OE2	1:I:52:ASP:CG	2.51	0.48
1:K:34:GLY:HA2	1:L:70:VAL:CG2	2.43	0.48
1:N:54:LEU:CD1	1:N:56:VAL:HG23	2.43	0.48
1:G:54:LEU:O	1:L:63:SER:HB2	2.13	0.48
1:N:45:LEU:CD1	1:N:56:VAL:HG21	2.43	0.48
1:K:57:TYR:HB2	1:L:62:PHE:O	2.14	0.48
1:E:61:ALA:C	1:E:62:PHE:CD1	2.87	0.48
1:J:23:PRO:HG2	1:J:49:LEU:HD22	1.94	0.48
1:E:87:TYR:HA	1:F:55:PHE:O	2.14	0.48
1:H:62:PHE:CE2	1:K:53:SER:HB2	2.49	0.48
1:M:54:LEU:HD13	1:M:56:VAL:HG23	1.95	0.48
1:H:54:LEU:HD13	1:H:56:VAL:HG23	1.96	0.48
1:K:71:ILE:HD12	1:K:74:TYR:HD1	1.79	0.48
1:B:23:PRO:CG	1:B:49:LEU:HD22	2.43	0.47
1:D:47:ARG:O	1:D:50:HIS:NE2	2.48	0.47
1:F:47:ARG:O	1:F:50:HIS:NE2	2.48	0.47
1:A:77:PHE:HE1	1:E:90:SER:HB2	1.79	0.47
1:G:64:PRO:HG2	1:H:38:PHE:HE2	1.76	0.47
1:B:28:SER:CB	1:C:26:LYS:HZ2	2.28	0.47
1:C:66:PRO:HB3	1:D:39:ALA:HB2	1.97	0.47
1:D:93:TRP:HA	1:D:93:TRP:CE3	2.50	0.47
1:E:94:GLY:HA3	1:F:79:PHE:HD2	1.79	0.47
1:G:46:ARG:CZ	1:L:65:ASN:HB2	2.44	0.47
1:I:80:ASP:OD1	1:I:80:ASP:N	2.48	0.47
1:B:23:PRO:HG2	1:B:49:LEU:CD2	2.44	0.47
1:K:34:GLY:HA2	1:L:70:VAL:HG23	1.96	0.47
1:K:44:PHE:CZ	1:K:48:GLN:NE2	2.83	0.47
1:C:65:ASN:OD1	1:I:52:ASP:OD1	2.34	0.46
1:F:54:LEU:CD1	1:F:56:VAL:HG23	2.45	0.46
1:H:25:LEU:HD22	1:H:48:GLN:OE1	2.16	0.46
1:A:87:TYR:CZ	1:B:18:ALA:HB2	2.51	0.46
1:D:41:VAL:O	1:D:45:LEU:HD23	2.15	0.46
1:I:38:PHE:N	1:J:68:GLU:O	2.49	0.46
1:A:30:PHE:CZ	1:A:44:PHE:HZ	2.34	0.46
1:K:83:LEU:O	1:L:14:VAL:HA	2.15	0.46
1:I:11:LYS:HB3	1:I:31:LYS:HG2	1.97	0.45
1:I:55:PHE:O	1:J:87:TYR:HA	2.15	0.45
1:I:63:SER:N	1:L:53:SER:OG	2.40	0.45
1:K:22:ALA:HB2	1:L:88:ALA:HA	1.96	0.45
1:F:91:MET:HA	1:F:91:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:17:ARG:NH1	2:Q:153:ASP:O	2.49	0.45
1:A:22:ALA:HB2	1:B:88:ALA:HA	1.98	0.45
1:D:25:LEU:HD11	1:D:45:LEU:CD1	2.46	0.45
1:N:42:ILE:HA	1:N:45:LEU:HD11	1.98	0.45
1:A:83:LEU:HD13	1:A:85:VAL:HG23	1.98	0.45
1:L:42:ILE:HA	1:L:45:LEU:HD11	1.98	0.45
1:E:47:ARG:NH2	1:K:13:VAL:HG12	2.32	0.45
1:B:24:ILE:HG22	1:C:26:LYS:CG	2.47	0.45
1:E:68:GLU:OE1	1:E:73:LEU:HD13	2.16	0.45
1:F:23:PRO:HG2	1:F:49:LEU:HD11	1.99	0.45
1:H:44:PHE:CD1	1:H:44:PHE:C	2.90	0.45
1:I:61:ALA:HB3	1:K:91:MET:HB2	1.99	0.45
1:D:79:PHE:HD2	1:J:92:ALA:HB2	1.82	0.45
1:K:62:PHE:CE2	1:K:77:PHE:CE1	3.05	0.45
1:D:55:PHE:CE1	1:J:63:SER:HB2	2.52	0.45
1:H:80:ASP:OD1	1:H:80:ASP:N	2.49	0.45
1:C:87:TYR:HA	1:D:55:PHE:O	2.18	0.44
1:C:34:GLY:O	1:D:71:ILE:HB	2.17	0.44
1:A:87:TYR:OH	1:B:18:ALA:HB2	2.18	0.44
1:A:87:TYR:HA	1:B:55:PHE:O	2.17	0.44
1:E:39:ALA:HB2	1:F:66:PRO:HB3	1.99	0.44
1:G:22:ALA:HB2	1:H:88:ALA:HA	1.98	0.44
1:A:36:ASP:O	1:B:70:VAL:HG23	2.18	0.44
1:G:73:LEU:HD23	1:G:73:LEU:HA	1.90	0.44
1:I:71:ILE:HB	1:J:34:GLY:O	2.17	0.44
1:C:68:GLU:OE1	1:C:73:LEU:HD13	2.19	0.43
1:G:73:LEU:CD1	1:H:38:PHE:HD2	2.31	0.43
1:K:45:LEU:HD13	1:K:49:LEU:HG	1.99	0.43
2:R:154:ILE:CB	2:R:155:PRO:HD3	2.42	0.43
1:G:29:LYS:O	2:R:155:PRO:HG2	2.18	0.43
1:G:70:VAL:HG23	1:H:36:ASP:O	2.18	0.43
1:J:77:PHE:HA	1:K:92:ALA:HB2	2.00	0.43
1:M:57:TYR:HA	1:N:62:PHE:O	2.19	0.43
1:C:92:ALA:HB2	1:I:76:ASN:O	2.18	0.43
1:F:49:LEU:HD12	1:F:49:LEU:HA	1.89	0.43
1:D:25:LEU:HD22	1:D:48:GLN:OE1	2.18	0.43
1:E:46:ARG:NE	1:E:52:ASP:O	2.52	0.43
1:E:70:VAL:HG11	1:F:33:SER:O	2.19	0.43
1:A:36:ASP:HB2	1:A:40:ASN:HD22	1.83	0.43
1:E:68:GLU:O	1:F:38:PHE:N	2.45	0.43
1:E:94:GLY:HA3	1:F:79:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:88:ALA:HB2	1:N:19:THR:HB	2.00	0.43
1:B:81:GLY:HA2	1:M:24:ILE:CD1	2.49	0.42
1:M:87:TYR:CZ	1:N:18:ALA:HB2	2.54	0.42
1:G:55:PHE:CE1	1:L:63:SER:OG	2.73	0.42
1:I:25:LEU:HD12	1:I:25:LEU:HA	1.92	0.42
1:A:26:LYS:HG3	1:A:27:GLN:HG2	2.01	0.42
1:H:38:PHE:O	1:H:38:PHE:CD1	2.70	0.42
1:H:67:ASP:N	1:H:67:ASP:OD1	2.53	0.42
1:D:80:ASP:OD1	1:E:31:LYS:NZ	2.50	0.42
1:D:36:ASP:HB3	1:D:40:ASN:ND2	2.31	0.42
1:I:56:VAL:HG13	1:J:85:VAL:CG1	2.50	0.42
1:C:13:VAL:HB	1:D:82:LYS:HG2	2.02	0.41
1:F:73:LEU:HD23	1:F:73:LEU:HA	1.91	0.41
1:L:14:VAL:O	1:L:14:VAL:HG13	2.20	0.41
1:C:60:SER:HA	1:J:91:MET:O	2.21	0.41
1:N:54:LEU:HD13	1:N:56:VAL:HG23	2.03	0.41
1:A:30:PHE:HB2	2:O:157:MET:HB2	2.03	0.41
1:I:60:SER:HA	1:K:91:MET:O	2.20	0.41
1:L:38:PHE:O	1:L:38:PHE:CD1	2.70	0.41
1:M:58:VAL:CG1	1:N:85:VAL:HG22	2.50	0.41
1:G:83:LEU:O	1:H:14:VAL:HA	2.21	0.41
1:K:57:TYR:CB	1:L:62:PHE:O	2.69	0.41
1:A:12:ILE:HD12	1:B:70:VAL:CG1	2.42	0.40
1:K:73:LEU:HD21	1:L:58:VAL:HG21	2.02	0.40
1:E:54:LEU:O	1:E:54:LEU:HD12	2.21	0.40
1:C:46:ARG:CG	1:C:54:LEU:HD21	2.51	0.40
1:A:52:ASP:OD1	1:E:68:GLU:OE2	2.38	0.40
1:E:27:GLN:O	1:E:30:PHE:CE2	2.74	0.40
1:D:93:TRP:HA	1:D:93:TRP:HE3	1.87	0.40
1:I:30:PHE:CD1	1:I:30:PHE:N	2.89	0.40

All (2) 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:D:63:SER:O	1:E:53:SER:OG[2_565]	2.00	0.20
1:B:40:ASN:OD1	1:J:40:ASN:OD1[4_565]	2.13	0.07

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	80/96 (83%)	80 (100%)	0	0	100	100
1	B	83/96 (86%)	83 (100%)	0	0	100	100
1	C	92/96 (96%)	88 (96%)	4 (4%)	0	100	100
1	D	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
1	E	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
1	F	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
1	G	79/96 (82%)	77 (98%)	2 (2%)	0	100	100
1	H	81/96 (84%)	80 (99%)	1 (1%)	0	100	100
1	I	82/96 (85%)	82 (100%)	0	0	100	100
1	J	82/96 (85%)	82 (100%)	0	0	100	100
1	K	81/96 (84%)	79 (98%)	2 (2%)	0	100	100
1	L	77/96 (80%)	75 (97%)	2 (3%)	0	100	100
1	M	79/96 (82%)	76 (96%)	3 (4%)	0	100	100
1	N	70/96 (73%)	67 (96%)	3 (4%)	0	100	100
2	O	3/11 (27%)	2 (67%)	1 (33%)	0	100	100
2	P	4/11 (36%)	4 (100%)	0	0	100	100
2	Q	4/11 (36%)	4 (100%)	0	0	100	100
2	R	3/11 (27%)	2 (67%)	0	1 (33%)	0	0
All	All	1158/1388 (83%)	1134 (98%)	23 (2%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	155	PRO

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	72/82 (88%)	63 (88%)	9 (12%)	4 21
1	B	72/82 (88%)	59 (82%)	13 (18%)	1 8
1	C	79/82 (96%)	65 (82%)	14 (18%)	2 9
1	D	71/82 (87%)	61 (86%)	10 (14%)	3 16
1	E	79/82 (96%)	68 (86%)	11 (14%)	3 16
1	F	71/82 (87%)	62 (87%)	9 (13%)	4 20
1	G	64/82 (78%)	52 (81%)	12 (19%)	1 8
1	H	71/82 (87%)	59 (83%)	12 (17%)	2 10
1	I	73/82 (89%)	59 (81%)	14 (19%)	1 8
1	J	72/82 (88%)	60 (83%)	12 (17%)	2 10
1	K	72/82 (88%)	62 (86%)	10 (14%)	3 16
1	L	65/82 (79%)	55 (85%)	10 (15%)	2 13
1	M	70/82 (85%)	59 (84%)	11 (16%)	2 12
1	N	63/82 (77%)	52 (82%)	11 (18%)	2 9
2	O	5/11 (46%)	5 (100%)	0	100 100
2	P	6/11 (54%)	6 (100%)	0	100 100
2	Q	6/11 (54%)	5 (83%)	1 (17%)	2 10
2	R	5/11 (46%)	3 (60%)	2 (40%)	0 0
All	All	1016/1192 (85%)	855 (84%)	161 (16%)	2 12

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	12	ILE
1	A	30	PHE
1	A	46	ARG
1	A	49	LEU
1	A	50	HIS

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Mol	Chain	Res	Type
1	A	67	ASP
1	A	68	GLU
1	A	71	ILE
1	B	14	VAL
1	B	17	ARG
1	B	24	ILE
1	B	25	LEU
1	B	26	LYS
1	B	29	LYS
1	B	31	LYS
1	B	60	SER
1	B	62	PHE
1	B	68	GLU
1	B	71	ILE
1	B	79	PHE
1	B	93	TRP
1	C	1	MET
1	C	17	ARG
1	C	19	THR
1	C	26	LYS
1	C	27	GLN
1	C	29	LYS
1	C	42	ILE
1	C	50	HIS
1	C	54	LEU
1	C	60	SER
1	C	71	ILE
1	C	73	LEU
1	C	79	PHE
1	C	91	MET
1	D	11	LYS
1	D	15	HIS
1	D	29	LYS
1	D	30	PHE
1	D	49	LEU
1	D	51	SER
1	D	60	SER
1	D	71	ILE
1	D	84	VAL
1	D	91	MET
1	E	3	THR
1	E	17	ARG

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Mol	Chain	Res	Type
1	E	19	THR
1	E	27	GLN
1	E	29	LYS
1	E	42	ILE
1	E	54	LEU
1	E	60	SER
1	E	71	ILE
1	E	73	LEU
1	E	91	MET
1	F	11	LYS
1	F	15	HIS
1	F	17	ARG
1	F	37	LYS
1	F	51	SER
1	F	60	SER
1	F	71	ILE
1	F	84	VAL
1	F	93	TRP
1	G	17	ARG
1	G	24	ILE
1	G	25	LEU
1	G	26	LYS
1	G	27	GLN
1	G	54	LEU
1	G	57	TYR
1	G	65	ASN
1	G	67	ASP
1	G	71	ILE
1	G	84	VAL
1	G	86	ASN
1	H	29	LYS
1	H	38	PHE
1	H	42	ILE
1	H	44	PHE
1	H	54	LEU
1	H	60	SER
1	H	67	ASP
1	H	68	GLU
1	H	71	ILE
1	H	79	PHE
1	H	84	VAL
1	H	86	ASN

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Mol	Chain	Res	Type
1	I	11	LYS
1	I	17	ARG
1	I	30	PHE
1	I	32	VAL
1	I	46	ARG
1	I	49	LEU
1	I	50	HIS
1	I	54	LEU
1	I	60	SER
1	I	67	ASP
1	I	68	GLU
1	I	71	ILE
1	I	80	ASP
1	I	82	LYS
1	J	14	VAL
1	J	24	ILE
1	J	25	LEU
1	J	26	LYS
1	J	29	LYS
1	J	31	LYS
1	J	51	SER
1	J	60	SER
1	J	62	PHE
1	J	68	GLU
1	J	71	ILE
1	J	79	PHE
1	K	17	ARG
1	K	29	LYS
1	K	45	LEU
1	K	54	LEU
1	K	68	GLU
1	K	71	ILE
1	K	72	ASP
1	K	74	TYR
1	K	82	LYS
1	K	84	VAL
1	L	17	ARG
1	L	19	THR
1	L	37	LYS
1	L	38	PHE
1	L	45	LEU
1	L	49	LEU

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Mol	Chain	Res	Type
1	L	60	SER
1	L	65	ASN
1	L	71	ILE
1	L	79	PHE
1	M	10	GLN
1	M	29	LYS
1	M	45	LEU
1	M	54	LEU
1	M	68	GLU
1	M	71	ILE
1	M	72	ASP
1	M	74	TYR
1	M	79	PHE
1	M	84	VAL
1	M	86	ASN
1	N	14	VAL
1	N	17	ARG
1	N	19	THR
1	N	24	ILE
1	N	45	LEU
1	N	47	ARG
1	N	49	LEU
1	N	60	SER
1	N	63	SER
1	N	65	ASN
1	N	68	GLU
2	Q	153	ASP
2	R	155	PRO
2	R	157	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	86	ASN
1	B	40	ASN
1	B	86	ASN
1	C	40	ASN
1	C	86	ASN
1	D	40	ASN
1	D	86	ASN
1	E	7	ASN

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Mol	Chain	Res	Type
1	E	15	HIS
1	E	40	ASN
1	E	86	ASN
1	F	40	ASN
1	G	40	ASN
1	G	65	ASN
1	H	40	ASN
1	H	48	GLN
1	I	76	ASN
1	J	40	ASN
1	J	86	ASN
1	L	15	HIS
1	M	40	ASN
1	M	86	ASN
1	N	15	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 monosaccharides 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	82/96 (85%)	0.01	3 (3%) 41 26	44, 76, 97, 130	0
1	B	85/96 (88%)	0.01	2 (2%) 59 44	40, 73, 101, 122	0
1	C	94/96 (97%)	-0.06	0 100 100	39, 61, 104, 119	0
1	D	85/96 (88%)	0.15	1 (1%) 79 67	39, 75, 115, 146	0
1	E	94/96 (97%)	0.01	2 (2%) 63 49	35, 67, 94, 119	0
1	F	85/96 (88%)	0.03	2 (2%) 59 44	40, 73, 114, 122	0
1	G	81/96 (84%)	0.38	6 (7%) 14 8	66, 96, 122, 139	0
1	H	83/96 (86%)	0.33	6 (7%) 15 9	49, 94, 124, 138	0
1	I	84/96 (87%)	0.00	0 100 100	41, 73, 99, 120	0
1	J	84/96 (87%)	-0.01	1 (1%) 79 67	49, 70, 92, 115	0
1	K	83/96 (86%)	0.19	0 100 100	47, 84, 117, 136	0
1	L	81/96 (84%)	0.17	5 (6%) 20 11	51, 87, 111, 126	0
1	M	81/96 (84%)	0.19	4 (4%) 29 17	51, 88, 126, 148	0
1	N	74/96 (77%)	0.04	2 (2%) 54 39	49, 88, 127, 147	0
2	O	5/11 (45%)	-0.30	0 100 100	68, 72, 89, 100	0
2	P	6/11 (54%)	0.42	0 100 100	62, 70, 87, 89	0
2	Q	6/11 (54%)	-0.35	0 100 100	56, 60, 62, 64	0
2	R	5/11 (45%)	0.07	0 100 100	65, 72, 88, 94	0
All	All	1198/1388 (86%)	0.10	34 (2%) 53 37	35, 78, 118, 148	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	52	ASP	6.1
1	G	50	HIS	5.9
1	B	50	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	51	SER	3.9
1	M	52	ASP	3.5
1	G	88	ALA	3.3
1	L	10	GLN	3.2
1	L	16	LEU	3.1
1	M	75	ASN	3.1
1	A	24	ILE	3.0
1	N	15	HIS	2.9
1	D	38	PHE	2.6
1	J	45	LEU	2.5
1	E	94	GLY	2.5
1	H	19	THR	2.4
1	H	44	PHE	2.3
1	E	23	PRO	2.3
1	M	67	ASP	2.3
1	A	27	GLN	2.3
1	H	75	ASN	2.2
1	G	87	TYR	2.2
1	L	49	LEU	2.2
1	H	77	PHE	2.2
1	N	12	ILE	2.2
1	B	48	GLN	2.2
1	G	15	HIS	2.2
1	M	73	LEU	2.1
1	G	18	ALA	2.1
1	F	25	LEU	2.1
1	L	62	PHE	2.1
1	H	50	HIS	2.1
1	A	52	ASP	2.1
1	F	80	ASP	2.1
1	L	25	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.