



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:02 PM UTC

PDB ID : 5XV4 / pdb_00005xv4
Title : Crystal structure of ATG101-ATG13HORMA
Authors : Kim, B.-W.; Song, H.K.
Deposited on : 2017-06-26
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

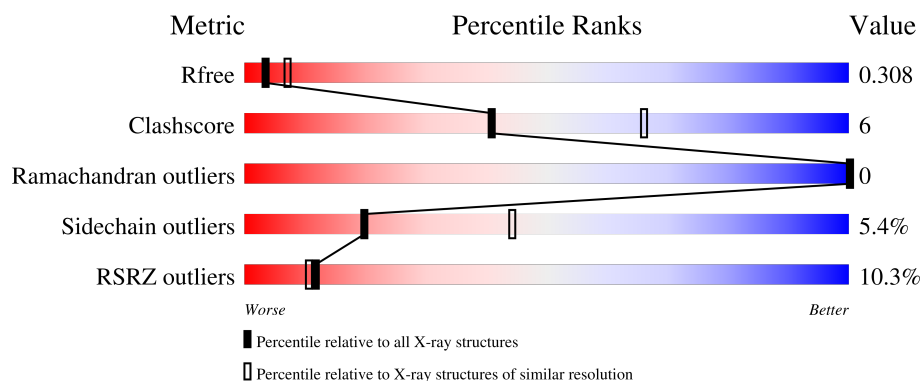
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	11% 82% 13% ..
1	C	190	11% 78% 18% ..
1	E	190	8% 76% 18% ..
1	G	190	11% 77% 17% ..
1	I	190	14% 72% 23% ..

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Mol	Chain	Length	Quality of chain
1	K	190	
1	M	190	
1	O	190	
2	B	218	
2	D	218	
2	F	218	
2	H	218	
2	J	218	
2	L	218	
2	N	218	
2	P	218	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23827 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 Autophagy-related protein 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1356	865	231	252	8			
1	C	183	Total	C	N	O	S	0	0	0
			1358	865	233	253	7			
1	E	182	Total	C	N	O	S	0	0	0
			1357	868	228	253	8			
1	G	182	Total	C	N	O	S	0	0	0
			1357	866	232	252	7			
1	I	182	Total	C	N	O	S	0	0	0
			1363	871	231	253	8			
1	K	182	Total	C	N	O	S	0	0	0
			1365	872	233	252	8			
1	M	183	Total	C	N	O	S	0	0	0
			1375	878	233	256	8			
1	O	182	Total	C	N	O	S	0	0	0
			1354	863	231	252	8			

- Molecule 2 is a protein called Autophagy-related protein 101.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1613	1020	275	309	9			
2	D	207	Total	C	N	O	S	0	0	0
			1610	1018	275	309	8			
2	F	207	Total	C	N	O	S	0	0	0
			1607	1017	272	309	9			
2	H	210	Total	C	N	O	S	0	0	0
			1627	1028	277	312	10			
2	J	207	Total	C	N	O	S	0	0	0
			1613	1020	275	309	9			
2	L	209	Total	C	N	O	S	0	0	0
			1626	1028	277	311	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	212	Total	C	N	O	S	0	0	0
			1636	1036	279	312	9			
2	P	207	Total	C	N	O	S	0	0	0
			1610	1018	275	309	8			

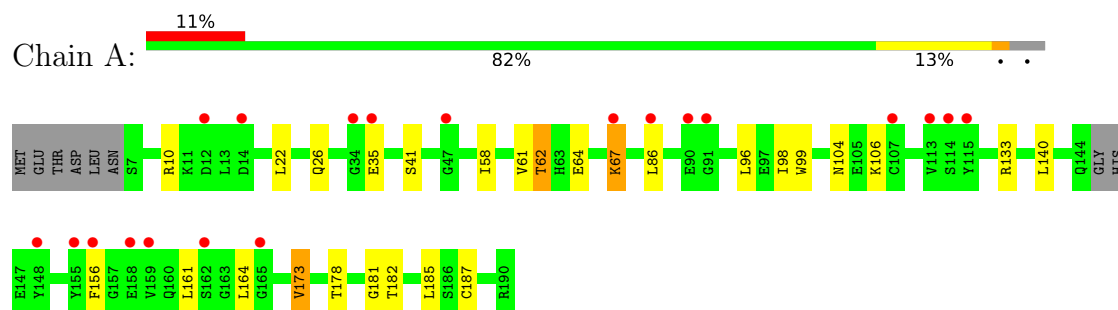
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	40	ALA	LYS	engineered mutation	UNP Q9BSB4
B	41	ALA	LYS	engineered mutation	UNP Q9BSB4
B	42	ALA	GLU	engineered mutation	UNP Q9BSB4
D	40	ALA	LYS	engineered mutation	UNP Q9BSB4
D	41	ALA	LYS	engineered mutation	UNP Q9BSB4
D	42	ALA	GLU	engineered mutation	UNP Q9BSB4
F	40	ALA	LYS	engineered mutation	UNP Q9BSB4
F	41	ALA	LYS	engineered mutation	UNP Q9BSB4
F	42	ALA	GLU	engineered mutation	UNP Q9BSB4
H	40	ALA	LYS	engineered mutation	UNP Q9BSB4
H	41	ALA	LYS	engineered mutation	UNP Q9BSB4
H	42	ALA	GLU	engineered mutation	UNP Q9BSB4
J	40	ALA	LYS	engineered mutation	UNP Q9BSB4
J	41	ALA	LYS	engineered mutation	UNP Q9BSB4
J	42	ALA	GLU	engineered mutation	UNP Q9BSB4
L	40	ALA	LYS	engineered mutation	UNP Q9BSB4
L	41	ALA	LYS	engineered mutation	UNP Q9BSB4
L	42	ALA	GLU	engineered mutation	UNP Q9BSB4
N	40	ALA	LYS	engineered mutation	UNP Q9BSB4
N	41	ALA	LYS	engineered mutation	UNP Q9BSB4
N	42	ALA	GLU	engineered mutation	UNP Q9BSB4
P	40	ALA	LYS	engineered mutation	UNP Q9BSB4
P	41	ALA	LYS	engineered mutation	UNP Q9BSB4
P	42	ALA	GLU	engineered mutation	UNP Q9BSB4

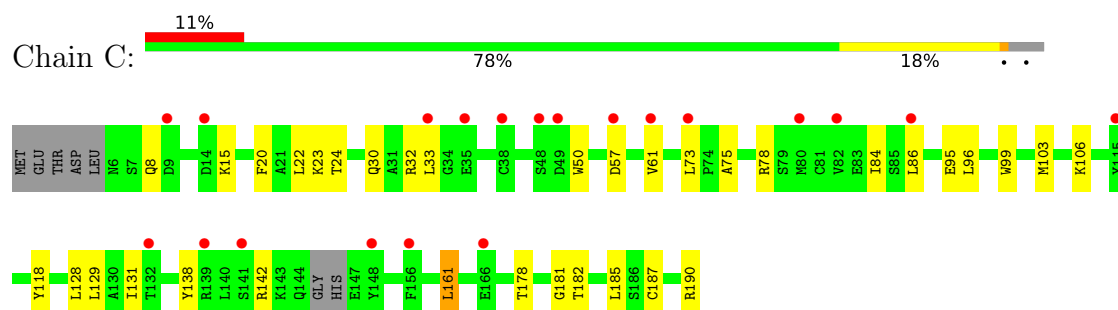
3 Residue-property plots [i](#)

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.

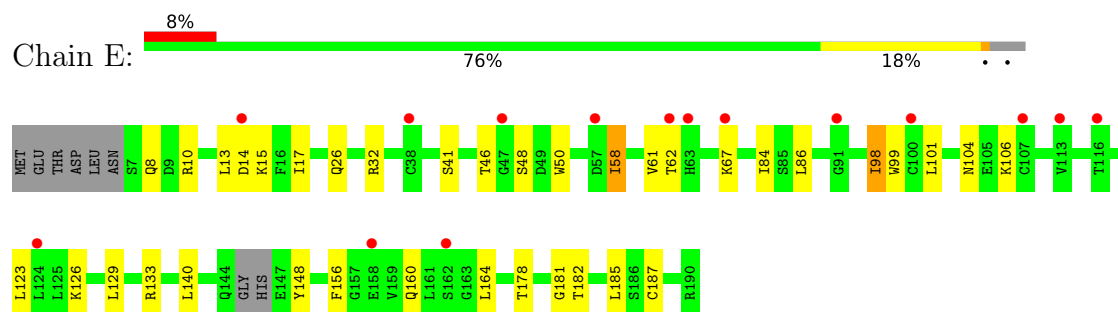
• Molecule 1: Autophagy-related protein 13



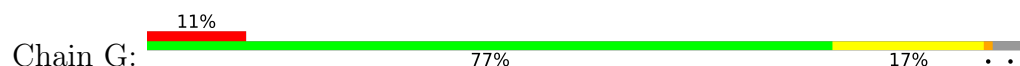
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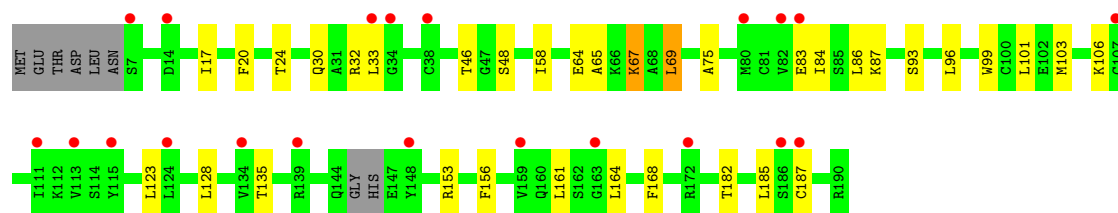


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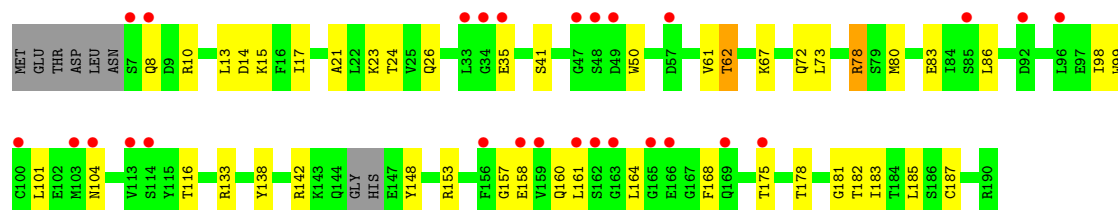
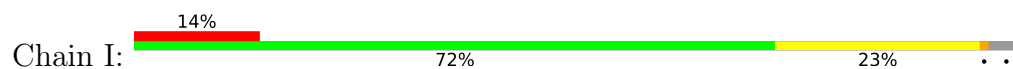


• Molecule 1: Autophagy-related protein 13

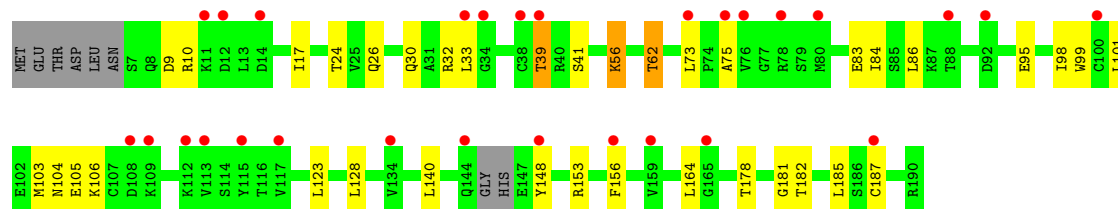
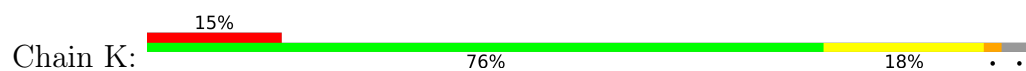




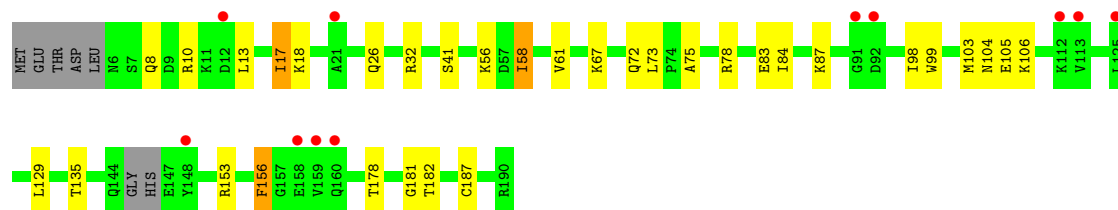
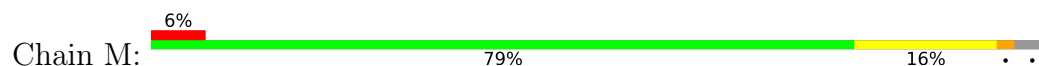
• Molecule 1: Autophagy-related protein 13



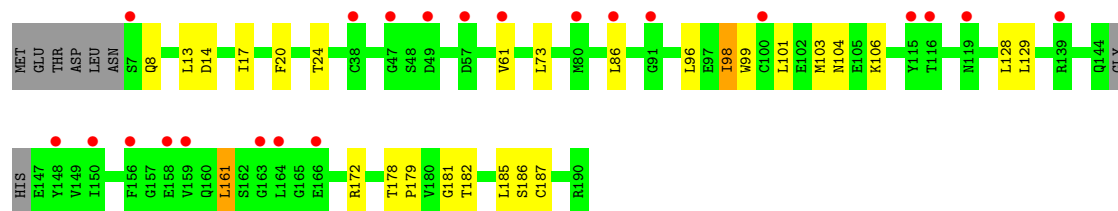
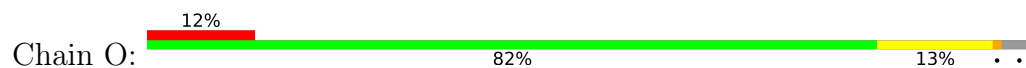
• Molecule 1: Autophagy-related protein 13



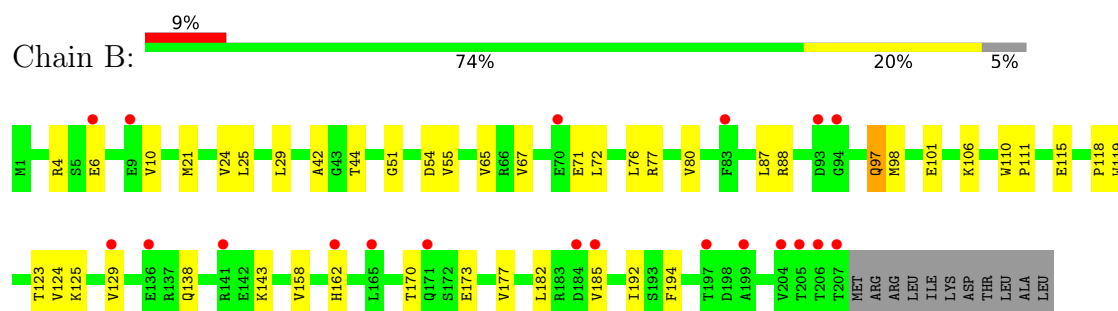
• Molecule 1: Autophagy-related protein 13



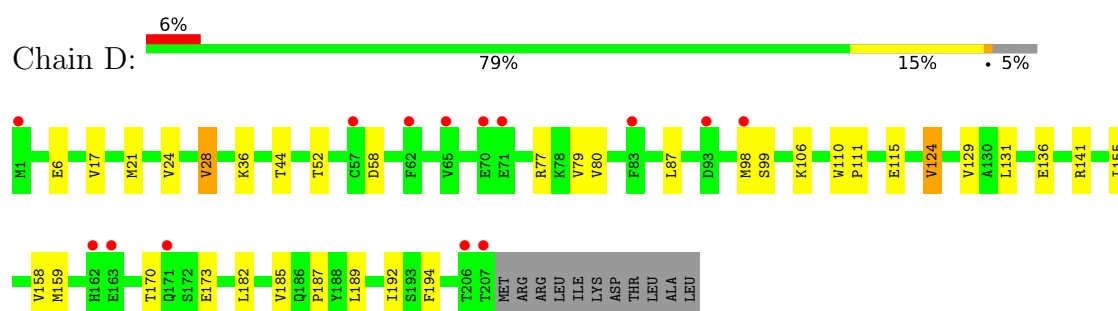
• Molecule 1: Autophagy-related protein 13



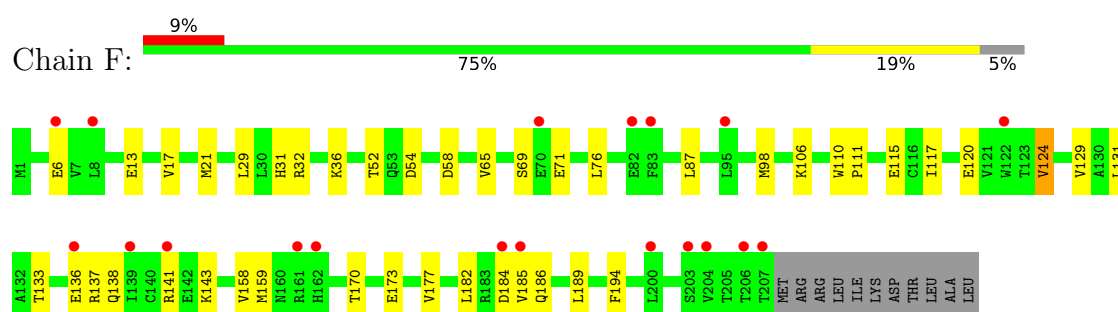
- Molecule 2: Autophagy-related protein 101



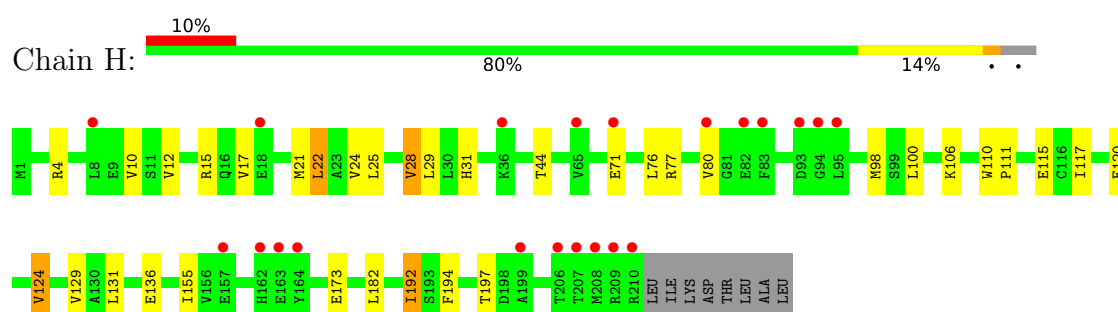
- Molecule 2: Autophagy-related protein 101



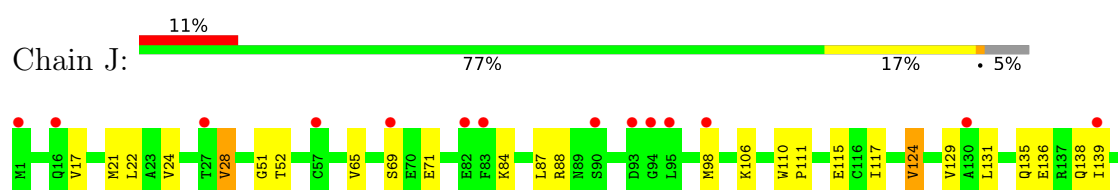
- Molecule 2: Autophagy-related protein 101



- Molecule 2: Autophagy-related protein 101

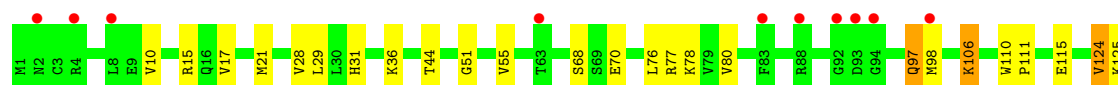
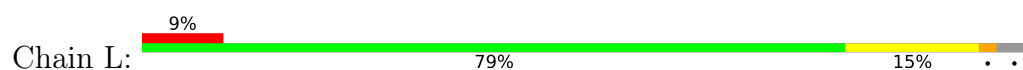


- Molecule 2: Autophagy-related protein 101

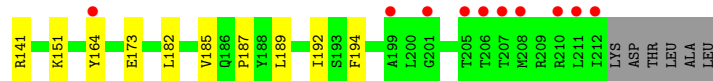
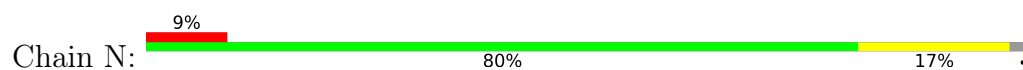




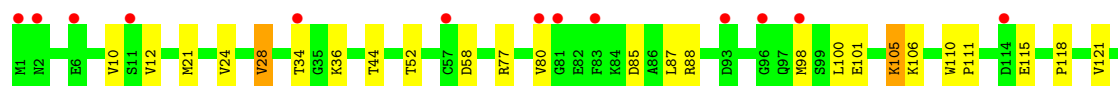
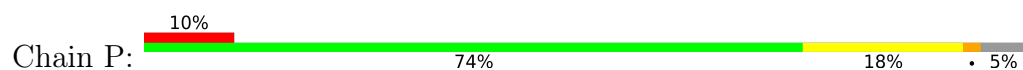
• Molecule 2: Autophagy-related protein 101



• Molecule 2: Autophagy-related protein 101



• Molecule 2: Autophagy-related protein 101



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.29Å 125.36Å 174.62Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	35.78 – 2.95 35.78 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.3 (35.78-2.95) 95.5 (35.78-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.95Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.286 , 0.313 0.285 , 0.308	Depositor DCC
R_{free} test set	1959 reflections (2.13%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtrriage
Anisotropy	0.554	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23827	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.85 % 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 5.6577e-06. 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](#)

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	0.16	0/1376	0.40	0/1867
1	C	0.16	0/1378	0.38	0/1870
1	E	0.17	0/1378	0.37	0/1871
1	G	0.17	0/1377	0.39	0/1868
1	I	0.17	0/1384	0.38	0/1878
1	K	0.17	0/1386	0.39	0/1880
1	M	0.16	0/1396	0.37	0/1893
1	O	0.16	0/1374	0.38	0/1863
2	B	0.17	0/1643	0.35	0/2228
2	D	0.15	0/1640	0.38	0/2225
2	F	0.15	0/1637	0.37	0/2221
2	H	0.16	0/1657	0.36	0/2248
2	J	0.15	0/1643	0.36	0/2228
2	L	0.15	0/1656	0.37	0/2245
2	N	0.17	0/1666	0.36	0/2262
2	P	0.16	0/1640	0.40	0/2225
All	All	0.16	0/24231	0.38	0/32872

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1356	0	1336	15	0
1	C	1358	0	1331	18	0
1	E	1357	0	1332	21	0
1	G	1357	0	1340	19	0
1	I	1363	0	1343	22	0
1	K	1365	0	1348	19	0
1	M	1375	0	1358	18	0
1	O	1354	0	1335	14	0
2	B	1613	0	1563	28	0
2	D	1610	0	1556	20	0
2	F	1607	0	1552	26	0
2	H	1627	0	1565	19	0
2	J	1613	0	1563	23	0
2	L	1626	0	1574	19	0
2	N	1636	0	1576	21	0
2	P	1610	0	1556	26	0
All	All	23827	0	23228	306	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 6.

All (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)
2:J:131:LEU:HD11	2:J:136:GLU:HB3	1.60	0.84
1:O:104:ASN:ND2	1:O:182:THR:OG1	2.16	0.78
2:P:106:LYS:HB3	2:P:115:GLU:HG3	1.68	0.75
2:D:106:LYS:HB3	2:D:115:GLU:HG3	1.69	0.74
2:N:4:ARG:NH2	2:N:120:GLU:OE1	2.21	0.74
2:H:106:LYS:HB3	2:H:115:GLU:HG3	1.68	0.73
1:C:86:LEU:HB2	1:C:96:LEU:HD11	1.67	0.73
1:I:72:GLN:HB3	1:I:78:ARG:HH21	1.53	0.71
2:N:106:LYS:HB3	2:N:115:GLU:HG3	1.70	0.71
1:A:104:ASN:ND2	1:A:182:THR:OG1	2.23	0.71
2:L:106:LYS:HB3	2:L:115:GLU:HG3	1.72	0.70
1:E:104:ASN:ND2	1:E:182:THR:OG1	2.26	0.69
1:M:17:ILE:HD11	1:M:73:LEU:HB3	1.74	0.67
2:J:106:LYS:HB3	2:J:115:GLU:HG3	1.75	0.67
1:K:178:THR:OG1	1:K:181:GLY:O	2.13	0.67
1:G:86:LEU:HB2	1:G:96:LEU:HD11	1.78	0.66
2:N:4:ARG:NH1	2:N:164:TYR:O	2.30	0.65
2:B:98:MET:HE2	2:B:192:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:ASN:ND2	1:I:182:THR:OG1	2.29	0.65
1:A:26:GLN:HE22	1:A:62:THR:HG22	1.62	0.64
1:I:26:GLN:NE2	1:I:62:THR:HG22	2.13	0.64
2:H:100:LEU:HD13	2:H:192:ILE:HG22	1.78	0.64
1:A:26:GLN:NE2	1:A:62:THR:HG22	2.13	0.64
1:E:178:THR:OG1	1:E:181:GLY:O	2.14	0.63
2:P:58:ASP:O	2:P:141:ARG:NH1	2.32	0.62
2:P:100:LEU:HD13	2:P:192:ILE:HG22	1.81	0.62
2:B:106:LYS:HB3	2:B:115:GLU:HG3	1.83	0.61
1:O:86:LEU:HB2	1:O:96:LEU:HD11	1.83	0.61
2:L:28:VAL:HA	2:L:159:MET:HE1	1.81	0.60
2:D:185:VAL:HG13	2:D:187:PRO:HD3	1.83	0.60
2:P:133:THR:HG23	2:P:136:GLU:H	1.67	0.59
2:N:185:VAL:HG13	2:N:187:PRO:HD3	1.84	0.59
1:M:26:GLN:HE22	1:M:58:ILE:HG13	1.67	0.59
2:D:98:MET:HE2	2:D:192:ILE:HD11	1.84	0.59
2:H:4:ARG:NH1	2:H:120:GLU:OE1	2.34	0.59
2:F:106:LYS:HB3	2:F:115:GLU:HG3	1.85	0.59
1:M:178:THR:OG1	1:M:181:GLY:O	2.14	0.59
2:B:6:GLU:CD	2:B:158:VAL:HG11	2.28	0.59
2:J:69:SER:HB2	2:J:185:VAL:HG23	1.86	0.58
2:L:131:LEU:HD23	2:L:136:GLU:HB3	1.86	0.58
1:O:14:ASP:HB2	1:O:73:LEU:HD11	1.85	0.58
1:E:46:THR:HG23	1:E:48:SER:H	1.68	0.58
1:G:87:LYS:NZ	1:G:93:SER:OG	2.36	0.58
1:K:26:GLN:HE21	1:K:62:THR:HG23	1.69	0.57
1:C:178:THR:OG1	1:C:181:GLY:O	2.18	0.57
2:N:7:VAL:HG12	2:N:123:THR:HB	1.86	0.57
1:A:173:VAL:HG22	1:A:185:LEU:HB3	1.86	0.57
1:A:178:THR:OG1	1:A:181:GLY:O	2.20	0.56
1:O:178:THR:OG1	1:O:181:GLY:O	2.19	0.56
1:M:104:ASN:OD1	1:M:105:GLU:N	2.39	0.55
2:L:21:MET:HE2	2:L:98:MET:SD	2.47	0.55
1:I:178:THR:OG1	1:I:181:GLY:O	2.19	0.55
2:B:6:GLU:OE1	2:B:158:VAL:HG11	2.07	0.55
2:L:185:VAL:HG13	2:L:187:PRO:HD3	1.89	0.54
1:C:15:LYS:HE3	1:C:50:TRP:HH2	1.72	0.54
2:J:21:MET:HE2	2:J:98:MET:SD	2.46	0.54
2:D:21:MET:HE2	2:D:98:MET:SD	2.47	0.54
2:F:170:THR:OG1	2:F:173:GLU:OE2	2.25	0.54
2:F:21:MET:HE2	2:F:98:MET:SD	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:GLN:HE22	1:E:58:ILE:HG22	1.73	0.53
2:F:69:SER:HB2	2:F:185:VAL:HG23	1.90	0.53
2:L:98:MET:HG2	2:L:194:PHE:HB3	1.90	0.53
1:K:99:TRP:CE3	1:K:187:CYS:HB2	2.44	0.53
2:N:21:MET:HE2	2:N:98:MET:SD	2.49	0.53
1:I:164:LEU:HD13	1:I:168:PHE:HB3	1.90	0.53
1:A:86:LEU:HB2	1:A:96:LEU:HD11	1.90	0.53
1:I:101:LEU:HD13	1:I:185:LEU:HD13	1.90	0.53
1:O:20:PHE:O	1:O:24:THR:OG1	2.23	0.53
2:B:71:GLU:HB2	2:B:182:LEU:HD23	1.90	0.52
1:G:164:LEU:HD13	1:G:168:PHE:HB3	1.91	0.52
2:P:105:LYS:HB2	2:P:176:ASN:HA	1.92	0.52
1:G:64:GLU:O	1:G:67:LYS:HG3	2.09	0.52
1:E:10:ARG:NH1	1:E:14:ASP:OD1	2.42	0.52
2:F:6:GLU:OE1	2:F:158:VAL:HG21	2.10	0.52
1:A:99:TRP:CE3	1:A:187:CYS:HB2	2.45	0.52
1:E:101:LEU:HD13	1:E:185:LEU:HD13	1.92	0.52
1:E:123:LEU:HA	1:E:126:LYS:HE2	1.92	0.52
1:K:104:ASN:OD1	1:K:105:GLU:N	2.43	0.51
1:O:101:LEU:HD13	1:O:185:LEU:HD13	1.92	0.51
1:G:75:ALA:HA	1:G:103:MET:HG2	1.93	0.51
1:G:99:TRP:CE3	1:G:187:CYS:HB2	2.46	0.51
2:B:4:ARG:NH2	2:B:162:HIS:HB3	2.26	0.51
1:I:26:GLN:HE22	1:I:62:THR:HG22	1.72	0.51
2:P:21:MET:HE2	2:P:98:MET:SD	2.51	0.51
2:F:29:LEU:HD12	2:F:76:LEU:HD11	1.94	0.50
1:C:30:GLN:HA	1:C:33:LEU:HG	1.93	0.50
1:C:32:ARG:HG2	1:C:84:ILE:HG21	1.91	0.50
2:P:98:MET:HG2	2:P:194:PHE:HB3	1.93	0.50
1:I:99:TRP:CE3	1:I:187:CYS:HB2	2.47	0.50
2:N:4:ARG:HH11	2:N:164:TYR:HD2	1.59	0.50
1:I:83:GLU:HG2	1:I:98:ILE:HG13	1.93	0.49
2:H:21:MET:HE2	2:H:98:MET:SD	2.52	0.49
1:M:99:TRP:CE3	1:M:187:CYS:HB2	2.47	0.49
1:I:14:ASP:HB2	1:I:73:LEU:HD11	1.93	0.49
2:P:170:THR:OG1	2:P:173:GLU:OE2	2.22	0.49
1:K:32:ARG:HG2	1:K:84:ILE:HG21	1.94	0.49
2:N:29:LEU:HD12	2:N:76:LEU:HD11	1.94	0.49
2:B:77:ARG:HA	2:B:80:VAL:HG12	1.94	0.49
1:G:101:LEU:HD13	1:G:185:LEU:HD13	1.94	0.49
2:B:4:ARG:HH21	2:B:162:HIS:HB3	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:MET:HE1	2:B:124:VAL:HB	1.95	0.48
2:B:97:GLN:HG3	2:B:123:THR:HG23	1.95	0.48
1:K:17:ILE:HD13	1:K:103:MET:HE1	1.95	0.48
2:B:97:GLN:HB2	2:B:125:LYS:HA	1.95	0.48
2:J:28:VAL:HG12	2:J:155:ILE:HG21	1.95	0.48
2:P:147:LYS:O	2:P:151:LYS:HG2	2.12	0.48
1:E:99:TRP:CE3	1:E:187:CYS:HB2	2.49	0.48
2:J:17:VAL:HG11	2:J:88:ARG:HH22	1.77	0.48
2:J:69:SER:HB2	2:J:184:ASP:HB3	1.95	0.48
2:H:77:ARG:HA	2:H:80:VAL:HG12	1.95	0.48
2:F:36:LYS:HA	2:F:186:GLN:HG2	1.96	0.48
1:G:65:ALA:O	1:G:69:LEU:HD12	2.13	0.48
1:O:99:TRP:CE3	1:O:187:CYS:HB2	2.49	0.48
1:C:99:TRP:CE3	1:C:187:CYS:HB2	2.48	0.48
2:F:31:HIS:HB2	2:F:159:MET:HE3	1.95	0.48
2:H:24:VAL:O	2:H:28:VAL:HG13	2.14	0.48
1:K:75:ALA:HA	1:K:103:MET:HG2	1.96	0.48
1:M:75:ALA:HA	1:M:103:MET:HG2	1.96	0.48
1:M:129:LEU:HD13	2:N:52:THR:HG21	1.96	0.48
2:B:29:LEU:HD12	2:B:76:LEU:HD11	1.95	0.47
2:D:98:MET:HG2	2:D:194:PHE:HB3	1.95	0.47
2:J:84:LYS:HG3	2:J:88:ARG:NH2	2.29	0.47
2:L:97:GLN:HB2	2:L:125:LYS:HA	1.96	0.47
1:K:86:LEU:HD11	1:K:148:TYR:HB3	1.96	0.47
2:N:98:MET:HG2	2:N:194:PHE:HB3	1.97	0.47
2:H:10:VAL:HG12	2:H:12:VAL:HG13	1.96	0.47
2:H:192:ILE:HG13	2:H:192:ILE:O	2.14	0.47
2:L:29:LEU:HD12	2:L:76:LEU:HD11	1.97	0.47
2:B:21:MET:HE2	2:B:98:MET:SD	2.54	0.47
2:F:58:ASP:O	2:F:141:ARG:NH2	2.41	0.47
2:P:87:LEU:HA	2:P:87:LEU:HD23	1.79	0.47
2:D:87:LEU:HD23	2:D:87:LEU:HA	1.81	0.47
1:E:26:GLN:HE22	1:E:58:ILE:CG2	2.28	0.47
1:K:101:LEU:HD13	1:K:185:LEU:HD13	1.96	0.47
2:J:24:VAL:O	2:J:28:VAL:HG13	2.14	0.47
1:M:83:GLU:OE1	1:M:153:ARG:NH1	2.48	0.47
2:D:77:ARG:HA	2:D:80:VAL:HG12	1.97	0.47
2:J:84:LYS:HE2	2:J:88:ARG:NH1	2.30	0.47
2:J:160:ASN:OD1	2:J:160:ASN:N	2.48	0.46
2:H:98:MET:HG2	2:H:194:PHE:HB3	1.98	0.46
2:D:36:LYS:HB2	2:D:36:LYS:HE3	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:VAL:O	2:D:28:VAL:HG13	2.15	0.46
1:G:17:ILE:HD13	1:G:103:MET:HE1	1.98	0.46
2:N:71:GLU:HB2	2:N:182:LEU:HD23	1.96	0.46
2:N:103:TYR:CE2	2:N:189:LEU:HD23	2.50	0.46
1:E:98:ILE:HD12	1:E:164:LEU:HD21	1.98	0.46
2:L:110:TRP:CG	2:L:111:PRO:HA	2.51	0.46
2:L:192:ILE:O	2:L:192:ILE:HG13	2.16	0.46
2:N:110:TRP:CG	2:N:111:PRO:HA	2.51	0.46
2:B:170:THR:OG1	2:B:173:GLU:OE2	2.26	0.46
1:K:39:THR:O	2:L:68:SER:OG	2.29	0.45
1:O:129:LEU:HD13	2:P:52:THR:HG21	1.97	0.45
1:C:78:ARG:NH2	2:F:131:LEU:O	2.49	0.45
2:P:24:VAL:O	2:P:28:VAL:HG13	2.15	0.45
2:F:137:ARG:O	2:F:141:ARG:HG3	2.16	0.45
1:G:32:ARG:HG2	1:G:84:ILE:HG21	1.98	0.45
1:I:15:LYS:HE2	1:I:50:TRP:HH2	1.80	0.45
1:K:83:GLU:OE1	1:K:153:ARG:NH2	2.45	0.45
1:C:138:TYR:OH	1:C:142:ARG:NH1	2.48	0.45
1:O:17:ILE:HD13	1:O:103:MET:HE1	1.98	0.45
1:C:129:LEU:HD13	2:D:52:THR:HG21	1.97	0.45
2:H:28:VAL:HG12	2:H:155:ILE:HG21	1.98	0.45
2:L:15:ARG:NH1	2:L:137:ARG:HD3	2.31	0.45
2:F:110:TRP:CG	2:F:111:PRO:HA	2.51	0.45
2:D:58:ASP:O	2:D:141:ARG:NH2	2.50	0.45
2:J:71:GLU:HB2	2:J:182:LEU:HD23	1.99	0.45
1:M:41:SER:HG	2:N:51:GLY:H	1.61	0.45
2:P:143:LYS:HD2	2:P:143:LYS:HA	1.77	0.45
2:P:192:ILE:O	2:P:192:ILE:HG13	2.16	0.45
2:D:110:TRP:CG	2:D:111:PRO:HA	2.51	0.45
2:J:110:TRP:CG	2:J:111:PRO:HA	2.52	0.45
2:H:71:GLU:HB2	2:H:182:LEU:HD22	1.98	0.45
2:J:21:MET:HE1	2:J:124:VAL:CG1	2.47	0.45
1:K:30:GLN:HA	1:K:33:LEU:HG	1.98	0.45
1:E:15:LYS:HE2	1:E:50:TRP:HH2	1.82	0.44
2:F:69:SER:HB2	2:F:184:ASP:HB3	1.99	0.44
2:H:131:LEU:HD22	2:H:136:GLU:HB3	1.99	0.44
1:O:98:ILE:HD11	1:O:161:LEU:HD23	1.99	0.44
2:P:85:ASP:HA	2:P:88:ARG:HE	1.82	0.44
1:A:133:ARG:HG3	2:B:65:VAL:HG23	1.99	0.44
2:H:15:ARG:H	2:H:15:ARG:HD2	1.81	0.44
1:G:83:GLU:OE1	1:G:153:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:O	1:A:67:LYS:HD3	2.17	0.44
2:B:110:TRP:CG	2:B:111:PRO:HA	2.53	0.44
2:J:87:LEU:HD23	2:J:87:LEU:HA	1.80	0.44
2:L:77:ARG:HA	2:L:80:VAL:HG12	2.00	0.44
1:E:13:LEU:O	1:E:17:ILE:HG12	2.17	0.44
2:F:17:VAL:O	2:F:21:MET:HG2	2.18	0.44
2:J:170:THR:OG1	2:J:173:GLU:OE1	2.29	0.44
1:O:128:LEU:HD13	1:O:185:LEU:HD21	2.00	0.44
2:P:77:ARG:HA	2:P:80:VAL:HG12	2.00	0.44
2:B:24:VAL:HG11	2:B:124:VAL:HG21	2.00	0.44
2:F:32:ARG:NH1	2:F:120:GLU:OE2	2.50	0.44
2:H:110:TRP:CG	2:H:111:PRO:HA	2.53	0.44
1:C:95:GLU:O	1:C:190:ARG:NH1	2.50	0.43
1:E:133:ARG:HG3	2:F:65:VAL:HG23	1.99	0.43
1:M:72:GLN:HB3	1:M:78:ARG:HH12	1.83	0.43
2:B:98:MET:HG2	2:B:194:PHE:HB3	2.00	0.43
2:F:143:LYS:HD2	2:F:143:LYS:HA	1.72	0.43
1:G:123:LEU:HD11	2:H:31:HIS:HB3	2.00	0.43
2:J:98:MET:HG2	2:J:194:PHE:HB3	1.99	0.43
2:P:28:VAL:HG12	2:P:155:ILE:HG21	1.99	0.43
1:E:86:LEU:HD11	1:E:148:TYR:HB3	2.00	0.43
1:G:46:THR:HG23	1:G:48:SER:H	1.83	0.43
2:H:17:VAL:O	2:H:21:MET:HG2	2.17	0.43
1:E:41:SER:HB2	2:F:184:ASP:OD2	2.18	0.43
2:L:17:VAL:O	2:L:21:MET:HG2	2.18	0.43
1:A:22:LEU:O	1:A:26:GLN:HG2	2.19	0.43
2:F:71:GLU:HB2	2:F:182:LEU:HD23	2.00	0.43
1:G:32:ARG:NH2	1:G:135:THR:OG1	2.52	0.43
2:P:10:VAL:HG12	2:P:12:VAL:HG13	1.99	0.43
2:P:101:GLU:OE2	2:P:118:PRO:HB3	2.19	0.43
1:E:32:ARG:HG2	1:E:84:ILE:HG21	2.01	0.43
1:G:128:LEU:HD13	1:G:185:LEU:HD21	2.00	0.43
1:I:41:SER:OG	2:J:51:GLY:N	2.41	0.43
1:I:86:LEU:HD11	1:I:148:TYR:HB3	1.99	0.43
1:K:106:LYS:O	1:K:182:THR:HG23	2.18	0.43
2:P:21:MET:HE1	2:P:124:VAL:CG1	2.48	0.43
1:I:133:ARG:HG3	2:J:65:VAL:HG23	2.01	0.43
1:O:13:LEU:HD11	1:O:179:PRO:HD2	2.01	0.43
1:A:86:LEU:HD22	1:A:140:LEU:HD21	2.00	0.43
1:C:24:THR:HG23	1:C:128:LEU:HD22	2.01	0.43
1:E:86:LEU:HD22	1:E:140:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:56:LYS:HD3	1:M:56:LYS:HA	1.91	0.43
1:E:67:LYS:HD3	1:E:67:LYS:HA	1.86	0.42
1:E:106:LYS:O	1:E:182:THR:HG23	2.19	0.42
1:I:80:MET:HE2	1:I:101:LEU:HD23	2.00	0.42
1:I:138:TYR:OH	1:I:142:ARG:NH1	2.51	0.42
2:B:67:VAL:HG21	2:B:185:VAL:HG11	2.01	0.42
1:C:23:LYS:NZ	1:C:57:ASP:OD2	2.48	0.42
2:F:133:THR:HG23	2:F:136:GLU:H	1.84	0.42
1:G:30:GLN:HA	1:G:33:LEU:HG	2.01	0.42
2:H:29:LEU:HD12	2:H:76:LEU:HD21	2.01	0.42
1:M:13:LEU:O	1:M:17:ILE:HG23	2.20	0.42
2:D:21:MET:HE1	2:D:124:VAL:CG1	2.49	0.42
2:N:17:VAL:O	2:N:21:MET:HG2	2.20	0.42
2:N:58:ASP:O	2:N:141:ARG:NH1	2.35	0.42
2:P:110:TRP:CG	2:P:111:PRO:HA	2.53	0.42
1:G:20:PHE:O	1:G:24:THR:OG1	2.29	0.42
2:J:17:VAL:O	2:J:21:MET:HG2	2.20	0.42
1:K:123:LEU:HD11	2:L:31:HIS:HB3	2.00	0.42
2:P:185:VAL:HG12	2:P:187:PRO:HD3	2.02	0.42
2:F:98:MET:HG2	2:F:194:PHE:HB3	2.01	0.42
1:M:32:ARG:HG2	1:M:84:ILE:HG21	2.00	0.42
1:M:32:ARG:NH2	1:M:135:THR:OG1	2.53	0.42
2:P:134:GLU:O	2:P:138:GLN:HG2	2.20	0.42
2:N:21:MET:HE1	2:N:124:VAL:CG1	2.49	0.42
1:A:133:ARG:NH1	2:B:54:ASP:OD2	2.53	0.42
1:C:106:LYS:O	1:C:182:THR:HG23	2.20	0.42
2:D:6:GLU:HG3	2:D:158:VAL:HG11	2.02	0.42
2:B:143:LYS:HA	2:B:143:LYS:HD2	1.76	0.42
2:D:28:VAL:HA	2:D:159:MET:HE1	2.00	0.42
1:I:41:SER:HB2	2:J:184:ASP:OD2	2.20	0.42
2:H:22:LEU:H	2:H:22:LEU:HG	1.69	0.42
1:A:41:SER:OG	2:B:51:GLY:N	2.44	0.41
2:D:99:SER:O	2:D:192:ILE:HD12	2.19	0.41
1:O:106:LYS:O	1:O:182:THR:HG23	2.20	0.41
1:C:20:PHE:O	1:C:24:THR:OG1	2.32	0.41
1:C:75:ALA:HA	1:C:103:MET:HG2	2.03	0.41
1:C:128:LEU:HD13	1:C:185:LEU:HD21	2.01	0.41
1:G:33:LEU:HD23	1:G:33:LEU:HA	1.92	0.41
2:L:21:MET:HE1	2:L:124:VAL:CG1	2.50	0.41
1:M:106:LYS:O	1:M:182:THR:HG23	2.20	0.41
1:A:41:SER:HG	2:B:51:GLY:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ALA:HB2	1:C:118:TYR:CZ	2.55	0.41
2:D:170:THR:OG1	2:D:173:GLU:OE1	2.31	0.41
1:A:106:LYS:O	1:A:182:THR:HG23	2.21	0.41
2:D:131:LEU:HD22	2:D:136:GLU:HB3	2.02	0.41
1:E:133:ARG:NH1	2:F:54:ASP:OD2	2.53	0.41
2:J:135:GLN:O	2:J:139:ILE:HG12	2.20	0.41
2:L:15:ARG:HH11	2:L:137:ARG:HD3	1.85	0.41
1:M:156:PHE:HD1	1:M:156:PHE:HA	1.74	0.41
2:B:4:ARG:NH1	2:B:119:TRP:HE3	2.18	0.41
2:B:29:LEU:HD13	2:B:72:LEU:HD21	2.02	0.41
2:F:21:MET:HE1	2:F:124:VAL:CG1	2.50	0.41
2:J:161:ARG:HG3	2:J:162:HIS:CD2	2.56	0.41
1:I:21:ALA:O	1:I:24:THR:OG1	2.31	0.41
1:K:24:THR:HG23	1:K:128:LEU:HD22	2.03	0.41
1:K:56:LYS:HA	1:K:56:LYS:HD3	1.89	0.41
2:N:9:GLU:O	2:N:151:LYS:NZ	2.43	0.41
2:B:87:LEU:HD23	2:B:87:LEU:HA	1.76	0.41
1:C:161:LEU:HD12	1:C:161:LEU:H	1.86	0.41
1:G:106:LYS:O	1:G:182:THR:HG23	2.21	0.41
1:I:157:GLY:HA3	1:I:158:GLU:C	2.46	0.41
1:O:186:SER:OG	1:O:187:CYS:N	2.53	0.41
2:F:87:LEU:HD23	2:F:87:LEU:HA	1.79	0.41
1:K:9:ASP:OD2	1:K:10:ARG:N	2.54	0.41
2:P:143:LYS:O	2:P:147:LYS:HG3	2.20	0.41
2:H:21:MET:HE1	2:H:124:VAL:CG1	2.51	0.40
2:N:7:VAL:HA	2:N:123:THR:O	2.21	0.40
1:I:13:LEU:O	1:I:17:ILE:HG12	2.22	0.40
2:L:78:LYS:HA	2:L:78:LYS:HD3	1.92	0.40
2:P:131:LEU:HD23	2:P:136:GLU:HB3	2.04	0.40
1:K:41:SER:HG	2:L:51:GLY:H	1.66	0.40
1:M:41:SER:OG	2:N:51:GLY:N	2.40	0.40
1:E:129:LEU:HD13	2:F:52:THR:HG21	2.02	0.40
2:F:13:GLU:CD	2:F:131:LEU:HD12	2.46	0.40
1:I:67:LYS:HA	1:I:67:LYS:HD3	1.92	0.40
1:I:175:THR:HA	1:I:183:ILE:O	2.22	0.40
2:P:36:LYS:HE3	2:P:36:LYS:HB3	1.94	0.40
2:B:101:GLU:OE1	2:B:118:PRO:HB3	2.21	0.40
2:D:17:VAL:O	2:D:21:MET:HG2	2.21	0.40
2:D:28:VAL:HG12	2:D:155:ILE:HG21	2.03	0.40
1:K:95:GLU:O	1:K:164:LEU:HD23	2.22	0.40
1:M:17:ILE:HG13	1:M:18:LYS:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:103:TYR:CD2	2:N:116:CYS:HB3	2.56	0.40

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	178/190 (94%)	173 (97%)	5 (3%)	0	100	100
1	C	179/190 (94%)	173 (97%)	6 (3%)	0	100	100
1	E	178/190 (94%)	172 (97%)	6 (3%)	0	100	100
1	G	178/190 (94%)	172 (97%)	6 (3%)	0	100	100
1	I	178/190 (94%)	171 (96%)	7 (4%)	0	100	100
1	K	178/190 (94%)	173 (97%)	5 (3%)	0	100	100
1	M	179/190 (94%)	174 (97%)	5 (3%)	0	100	100
1	O	178/190 (94%)	173 (97%)	5 (3%)	0	100	100
2	B	205/218 (94%)	197 (96%)	8 (4%)	0	100	100
2	D	205/218 (94%)	198 (97%)	7 (3%)	0	100	100
2	F	205/218 (94%)	198 (97%)	7 (3%)	0	100	100
2	H	208/218 (95%)	202 (97%)	6 (3%)	0	100	100
2	J	205/218 (94%)	197 (96%)	8 (4%)	0	100	100
2	L	207/218 (95%)	199 (96%)	8 (4%)	0	100	100
2	N	210/218 (96%)	203 (97%)	7 (3%)	0	100	100
2	P	205/218 (94%)	199 (97%)	6 (3%)	0	100	100
All	All	3076/3264 (94%)	2974 (97%)	102 (3%)	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	140/167 (84%)	129 (92%)	11 (8%)	11	29
1	C	139/167 (83%)	133 (96%)	6 (4%)	26	52
1	E	140/167 (84%)	133 (95%)	7 (5%)	22	47
1	G	140/167 (84%)	135 (96%)	5 (4%)	31	56
1	I	141/167 (84%)	130 (92%)	11 (8%)	11	30
1	K	141/167 (84%)	134 (95%)	7 (5%)	22	47
1	M	143/167 (86%)	134 (94%)	9 (6%)	16	38
1	O	140/167 (84%)	135 (96%)	5 (4%)	31	56
2	B	173/194 (89%)	164 (95%)	9 (5%)	21	46
2	D	172/194 (89%)	165 (96%)	7 (4%)	27	53
2	F	172/194 (89%)	166 (96%)	6 (4%)	32	57
2	H	173/194 (89%)	163 (94%)	10 (6%)	18	41
2	J	173/194 (89%)	162 (94%)	11 (6%)	16	38
2	L	174/194 (90%)	161 (92%)	13 (8%)	12	31
2	N	173/194 (89%)	164 (95%)	9 (5%)	21	46
2	P	172/194 (89%)	162 (94%)	10 (6%)	18	41
All	All	2506/2888 (87%)	2370 (95%)	136 (5%)	20	44

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	35	GLU
1	A	58	ILE
1	A	61	VAL
1	A	62	THR
1	A	67	LYS
1	A	98	ILE
1	A	156	PHE

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Mol	Chain	Res	Type
1	A	161	LEU
1	A	164	LEU
1	A	173	VAL
2	B	10	VAL
2	B	25	LEU
2	B	44	THR
2	B	55	VAL
2	B	88	ARG
2	B	97	GLN
2	B	129	VAL
2	B	138	GLN
2	B	177	VAL
1	C	8	GLN
1	C	22	LEU
1	C	61	VAL
1	C	73	LEU
1	C	131	ILE
1	C	161	LEU
2	D	28	VAL
2	D	44	THR
2	D	79	VAL
2	D	124	VAL
2	D	129	VAL
2	D	182	LEU
2	D	189	LEU
1	E	8	GLN
1	E	58	ILE
1	E	61	VAL
1	E	62	THR
1	E	98	ILE
1	E	156	PHE
1	E	160	GLN
2	F	117	ILE
2	F	124	VAL
2	F	129	VAL
2	F	138	GLN
2	F	177	VAL
2	F	189	LEU
1	G	58	ILE
1	G	67	LYS
1	G	69	LEU
1	G	156	PHE

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Mol	Chain	Res	Type
1	G	161	LEU
2	H	22	LEU
2	H	25	LEU
2	H	28	VAL
2	H	44	THR
2	H	117	ILE
2	H	124	VAL
2	H	129	VAL
2	H	173	GLU
2	H	192	ILE
2	H	197	THR
1	I	8	GLN
1	I	10	ARG
1	I	23	LYS
1	I	35	GLU
1	I	61	VAL
1	I	62	THR
1	I	78	ARG
1	I	116	THR
1	I	153	ARG
1	I	160	GLN
1	I	161	LEU
2	J	22	LEU
2	J	28	VAL
2	J	52	THR
2	J	117	ILE
2	J	124	VAL
2	J	129	VAL
2	J	138	GLN
2	J	143	LYS
2	J	160	ASN
2	J	177	VAL
2	J	189	LEU
1	K	39	THR
1	K	56	LYS
1	K	62	THR
1	K	73	LEU
1	K	98	ILE
1	K	140	LEU
1	K	156	PHE
2	L	10	VAL
2	L	36	LYS

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Mol	Chain	Res	Type
2	L	44	THR
2	L	55	VAL
2	L	70	GLU
2	L	97	GLN
2	L	106	LYS
2	L	124	VAL
2	L	133	THR
2	L	138	GLN
2	L	173	GLU
2	L	192	ILE
2	L	197	THR
1	M	8	GLN
1	M	10	ARG
1	M	17	ILE
1	M	58	ILE
1	M	61	VAL
1	M	67	LYS
1	M	87	LYS
1	M	98	ILE
1	M	156	PHE
2	N	10	VAL
2	N	44	THR
2	N	53	GLN
2	N	97	GLN
2	N	121	VAL
2	N	124	VAL
2	N	129	VAL
2	N	173	GLU
2	N	192	ILE
1	O	8	GLN
1	O	61	VAL
1	O	98	ILE
1	O	161	LEU
1	O	172	ARG
2	P	28	VAL
2	P	34	THR
2	P	44	THR
2	P	105	LYS
2	P	121	VAL
2	P	124	VAL
2	P	129	VAL
2	P	147	LYS

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Mol	Chain	Res	Type
2	P	192	ILE
2	P	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	GLN
1	C	26	GLN
1	C	30	GLN
2	D	53	GLN
2	D	89	ASN
2	D	160	ASN
1	E	26	GLN
1	E	52	ASN
1	G	52	ASN
2	H	89	ASN
1	I	26	GLN
1	I	52	ASN
2	J	97	GLN
2	L	89	ASN
2	L	127	HIS
1	M	26	GLN
1	M	52	ASN
1	M	144	GLN
1	O	26	GLN
1	O	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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, 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	182/190 (95%)	0.81	20 (10%) 10 9	49, 75, 105, 141	0
1	C	183/190 (96%)	0.97	20 (10%) 10 9	48, 85, 119, 145	0
1	E	182/190 (95%)	0.78	15 (8%) 17 15	43, 71, 101, 129	0
1	G	182/190 (95%)	1.00	21 (11%) 9 9	56, 86, 121, 147	0
1	I	182/190 (95%)	1.01	27 (14%) 5 5	50, 77, 109, 146	0
1	K	182/190 (95%)	1.10	28 (15%) 5 5	47, 72, 103, 115	0
1	M	183/190 (96%)	0.80	11 (6%) 27 23	42, 69, 102, 122	0
1	O	182/190 (95%)	0.96	22 (12%) 8 8	48, 79, 109, 139	0
2	B	207/218 (94%)	0.94	20 (9%) 13 12	53, 78, 116, 136	0
2	D	207/218 (94%)	0.76	14 (6%) 23 20	51, 76, 107, 117	0
2	F	207/218 (94%)	0.76	19 (9%) 14 13	47, 74, 108, 124	0
2	H	210/218 (96%)	0.87	21 (10%) 12 11	52, 76, 109, 137	0
2	J	207/218 (94%)	0.93	23 (11%) 10 9	50, 73, 109, 123	0
2	L	209/218 (95%)	0.94	19 (9%) 15 13	45, 71, 99, 135	0
2	N	212/218 (97%)	0.94	20 (9%) 14 12	45, 70, 106, 135	0
2	P	207/218 (94%)	1.02	22 (10%) 11 10	48, 74, 112, 123	0
All	All	3124/3264 (95%)	0.91	322 (10%) 12 11	42, 75, 110, 147	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	207	THR	9.2
2	F	207	THR	7.8
2	J	207	THR	7.8
2	P	207	THR	6.9
2	H	207	THR	6.0

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Mol	Chain	Res	Type	RSRZ
2	P	162	HIS	5.6
2	F	162	HIS	5.5
2	J	162	HIS	5.4
2	P	202	THR	5.3
2	P	206	THR	4.9
2	B	6	GLU	4.7
2	N	136	GLU	4.5
1	E	47	GLY	4.3
1	O	119	ASN	4.1
1	I	100	CYS	4.0
1	G	159	VAL	4.0
1	G	80	MET	4.0
1	I	159	VAL	3.9
2	N	208	MET	3.9
2	B	162	HIS	3.9
2	L	206	THR	3.9
2	J	205	THR	3.9
2	F	6	GLU	3.8
1	K	38	CYS	3.8
2	B	205	THR	3.8
2	H	206	THR	3.8
2	P	2	ASN	3.8
2	N	211	LEU	3.7
2	N	210	ARG	3.7
1	I	156	PHE	3.6
2	P	34	THR	3.6
2	H	162	HIS	3.6
1	M	113	VAL	3.6
1	K	148	TYR	3.6
2	J	206	THR	3.5
1	C	80	MET	3.5
2	J	98	MET	3.5
1	O	148	TYR	3.5
2	D	207	THR	3.5
2	L	208	MET	3.5
2	J	204	VAL	3.4
2	L	4	ARG	3.4
2	H	208	MET	3.4
2	B	204	VAL	3.4
2	N	207	THR	3.4
2	P	200	LEU	3.4
1	I	8	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	67	LYS	3.3
1	K	112	LYS	3.3
1	K	14	ASP	3.3
2	F	136	GLU	3.3
1	A	107	CYS	3.3
1	G	148	TYR	3.2
2	P	93	ASP	3.2
1	M	112	LYS	3.2
2	L	93	ASP	3.2
2	H	83	PHE	3.2
1	A	91	GLY	3.2
2	N	94	GLY	3.2
2	P	98	MET	3.2
2	N	83	PHE	3.1
1	C	57	ASP	3.1
1	G	82	VAL	3.1
1	K	159	VAL	3.1
1	O	91	GLY	3.1
1	I	166	GLU	3.1
1	I	48	SER	3.1
2	B	83	PHE	3.1
2	B	184	ASP	3.1
2	H	93	ASP	3.1
1	G	107	CYS	3.0
1	A	34	GLY	3.0
1	C	33	LEU	3.0
1	A	148	TYR	3.0
1	O	139	ARG	3.0
2	J	200	LEU	3.0
1	E	162	SER	3.0
1	I	92	ASP	3.0
1	E	158	GLU	3.0
2	N	6	GLU	3.0
1	M	12	ASP	3.0
1	C	156	PHE	3.0
1	G	115	TYR	2.9
1	A	158	GLU	2.9
1	K	33	LEU	2.9
1	O	86	LEU	2.9
1	I	163	GLY	2.9
1	A	159	VAL	2.9
2	P	205	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	161	LEU	2.9
2	L	207	THR	2.9
2	B	70	GLU	2.9
2	N	70	GLU	2.9
2	P	1	MET	2.9
2	B	206	THR	2.9
2	D	206	THR	2.9
1	I	165	GLY	2.8
2	P	6	GLU	2.8
1	I	104	ASN	2.8
2	L	83	PHE	2.8
1	E	100	CYS	2.8
1	K	165	GLY	2.8
1	A	47	GLY	2.8
1	G	14	ASP	2.8
1	I	49	ASP	2.8
1	I	47	GLY	2.8
2	F	82	GLU	2.8
1	K	78	ARG	2.8
1	I	7	SER	2.8
2	H	80	VAL	2.7
1	C	38	CYS	2.7
1	G	38	CYS	2.7
2	J	194	PHE	2.7
1	I	158	GLU	2.7
2	D	65	VAL	2.7
2	F	139	ILE	2.7
2	J	57	CYS	2.7
2	D	162	HIS	2.7
2	L	164	TYR	2.7
2	N	7	VAL	2.7
2	B	199	ALA	2.7
2	L	209	ARG	2.7
1	M	91	GLY	2.7
2	F	122	TRP	2.6
1	K	39	THR	2.6
2	H	95	LEU	2.6
2	D	57	CYS	2.6
1	I	113	VAL	2.6
2	H	163	GLU	2.6
1	K	12	ASP	2.6
1	O	156	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	115	TYR	2.6
1	I	175	THR	2.6
2	F	83	PHE	2.6
1	K	108	ASP	2.6
2	F	200	LEU	2.6
1	K	88	THR	2.6
2	F	206	THR	2.6
2	L	157	GLU	2.6
2	H	199	ALA	2.6
2	N	93	ASP	2.6
1	G	172	ARG	2.5
2	P	203	SER	2.5
1	G	33	LEU	2.5
2	J	95	LEU	2.5
2	L	165	LEU	2.5
1	M	159	VAL	2.5
1	K	144	GLN	2.5
2	D	163	GLU	2.5
1	K	187	CYS	2.5
1	O	57	ASP	2.5
2	B	141	ARG	2.5
1	I	162	SER	2.5
2	P	193	SER	2.5
2	N	8	LEU	2.5
1	C	82	VAL	2.5
1	K	115	TYR	2.5
2	N	164	TYR	2.5
1	M	160	GLN	2.5
2	H	210	ARG	2.5
2	H	36	LYS	2.5
1	E	124	LEU	2.5
2	B	165	LEU	2.5
1	G	34	GLY	2.5
1	O	150	ILE	2.5
1	C	148	TYR	2.5
2	L	205	THR	2.5
1	I	57	ASP	2.5
2	D	93	ASP	2.5
2	F	184	ASP	2.5
1	A	86	LEU	2.5
1	O	164	LEU	2.5
1	C	115	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	158	GLU	2.5
2	L	88	ARG	2.5
1	O	38	CYS	2.5
1	G	163	GLY	2.4
2	F	204	VAL	2.4
2	J	27	THR	2.4
2	F	8	LEU	2.4
2	F	95	LEU	2.4
1	C	61	VAL	2.4
1	I	85	SER	2.4
2	N	12	VAL	2.4
2	D	71	GLU	2.4
2	P	83	PHE	2.4
2	J	1	MET	2.4
1	G	124	LEU	2.4
1	K	34	GLY	2.4
1	O	47	GLY	2.4
2	B	94	GLY	2.4
2	J	184	ASP	2.4
2	N	199	ALA	2.4
1	E	116	THR	2.4
1	M	148	TYR	2.4
2	J	139	ILE	2.4
1	K	113	VAL	2.3
1	I	34	GLY	2.3
1	C	49	ASP	2.3
1	K	92	ASP	2.3
1	O	166	GLU	2.3
2	F	70	GLU	2.3
1	C	48	SER	2.3
1	I	114	SER	2.3
1	A	113	VAL	2.3
1	A	165	GLY	2.3
1	E	38	CYS	2.3
1	E	107	CYS	2.3
2	D	98	MET	2.3
2	J	16	GLN	2.3
1	C	86	LEU	2.3
2	H	8	LEU	2.3
2	N	205	THR	2.3
2	L	94	GLY	2.3
2	H	71	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	157	GLU	2.3
1	K	100	CYS	2.3
2	B	171	GLN	2.3
1	G	186	SER	2.3
1	C	139	ARG	2.3
1	G	113	VAL	2.3
1	I	103	MET	2.3
1	M	158	GLU	2.3
1	A	14	ASP	2.3
1	C	14	ASP	2.3
1	I	169	GLN	2.3
1	K	73	LEU	2.3
1	O	49	ASP	2.3
2	J	93	ASP	2.3
2	L	8	LEU	2.3
1	O	100	CYS	2.3
2	F	161	ARG	2.3
2	L	2	ASN	2.2
2	N	212	ILE	2.2
1	A	156	PHE	2.2
1	O	80	MET	2.2
2	J	83	PHE	2.2
1	A	35	GLU	2.2
1	A	90	GLU	2.2
2	D	70	GLU	2.2
2	J	82	GLU	2.2
1	G	111	ILE	2.2
1	M	92	ASP	2.2
2	F	141	ARG	2.2
2	B	197	THR	2.2
1	O	7	SER	2.2
2	N	201	GLY	2.2
2	P	81	GLY	2.2
1	G	139	ARG	2.2
1	E	57	ASP	2.2
1	O	61	VAL	2.2
2	L	185	VAL	2.2
1	A	162	SER	2.2
1	O	163	GLY	2.2
2	H	164	TYR	2.2
2	D	62	PHE	2.2
1	E	14	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	113	VAL	2.2
2	F	185	VAL	2.2
1	E	62	THR	2.2
2	J	90	SER	2.2
2	J	203	SER	2.2
2	B	9	GLU	2.2
1	E	63	HIS	2.1
1	K	117	VAL	2.1
2	B	93	ASP	2.1
1	K	109	LYS	2.1
2	H	94	GLY	2.1
1	I	33	LEU	2.1
1	K	75	ALA	2.1
1	C	166	GLU	2.1
1	G	83	GLU	2.1
1	K	11	LYS	2.1
1	E	91	GLY	2.1
2	L	92	GLY	2.1
1	C	73	LEU	2.1
1	M	21	ALA	2.1
1	G	187	CYS	2.1
2	P	149	CYS	2.1
2	H	65	VAL	2.1
2	P	80	VAL	2.1
1	C	9	ASP	2.1
2	J	94	GLY	2.1
2	N	206	THR	2.1
2	H	209	ARG	2.1
2	J	130	ALA	2.1
2	H	82	GLU	2.1
1	E	67	LYS	2.1
1	K	76	VAL	2.1
1	A	12	ASP	2.1
2	L	63	THR	2.1
2	P	114	ASP	2.1
1	I	35	GLU	2.1
1	A	115	TYR	2.1
1	G	7	SER	2.0
2	F	203	SER	2.0
2	J	69	SER	2.0
1	G	134	VAL	2.0
2	B	129	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	185	VAL	2.0
1	K	156	PHE	2.0
2	P	96	GLY	2.0
1	C	132	THR	2.0
1	O	116	THR	2.0
2	N	114	ASP	2.0
2	B	136	GLU	2.0
2	H	18	GLU	2.0
2	D	1	MET	2.0
1	A	114	SER	2.0
1	C	141	SER	2.0
1	O	159	VAL	2.0
2	D	171	GLN	2.0
2	P	11	SER	2.0
2	P	57	CYS	2.0
1	I	96	LEU	2.0
1	M	125	LEU	2.0
2	D	83	PHE	2.0
1	C	35	GLU	2.0
1	K	80	MET	2.0
2	L	98	MET	2.0
1	A	155	TYR	2.0
1	K	134	VAL	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 oligosaccharides 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.