



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:43 AM UTC

PDB ID : 3WAO / pdb_00003wao
Title : Crystal structure of Atg13 LIR-fused human LC3B_2-119
Authors : Suzuki, H.; Tabata, K.; Morita, E.; Kawasaki, M.; Kato, R.; Dobson, R.C.J.;
Yoshimori, T.; Wakatsuki, S.
Deposited on : 2013-05-06
Resolution : 2.60 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

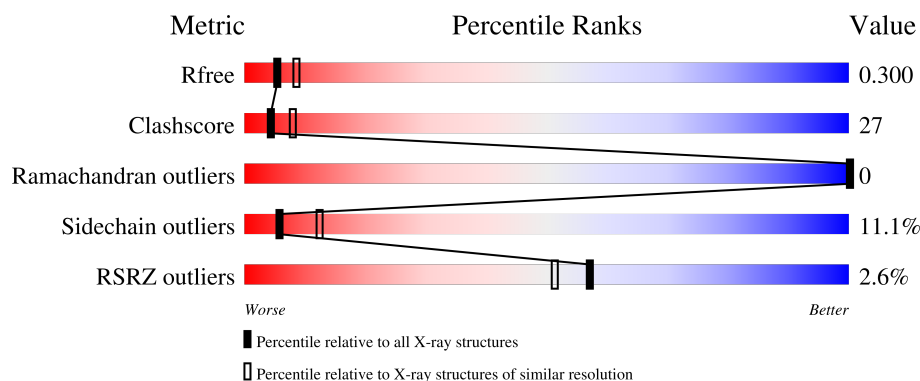
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	134	
1	B	134	
1	C	134	
1	D	134	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4113 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, Microtubule-associated proteins 1A/1B light chain 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1042	665	179	194	4			
1	B	124	Total	C	N	O	S	0	0	0
			1024	652	177	191	4			
1	C	124	Total	C	N	O	S	0	0	0
			1024	652	177	191	4			
1	D	124	Total	C	N	O	S	0	0	0
			1023	652	177	190	4			

There are 16 discrepancies between the modelled and reference sequences:

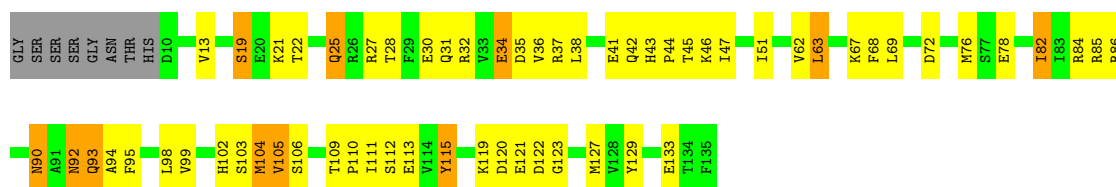
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP O75143
A	3	SER	-	expression tag	UNP O75143
A	16	GLY	-	linker	UNP O75143
A	17	SER	-	linker	UNP O75143
B	2	GLY	-	expression tag	UNP O75143
B	3	SER	-	expression tag	UNP O75143
B	16	GLY	-	linker	UNP O75143
B	17	SER	-	linker	UNP O75143
C	2	GLY	-	expression tag	UNP O75143
C	3	SER	-	expression tag	UNP O75143
C	16	GLY	-	linker	UNP O75143
C	17	SER	-	linker	UNP O75143
D	2	GLY	-	expression tag	UNP O75143
D	3	SER	-	expression tag	UNP O75143
D	16	GLY	-	linker	UNP O75143
D	17	SER	-	linker	UNP O75143

3 Residue-property plots

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.

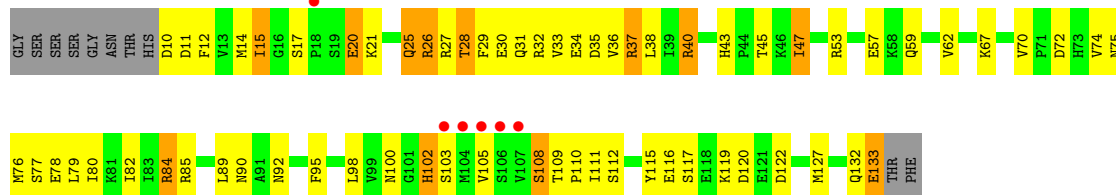
- Molecule 1: Autophagy-related protein 13, Microtubule-associated proteins 1A/1B light chain 3B

Chain A: 



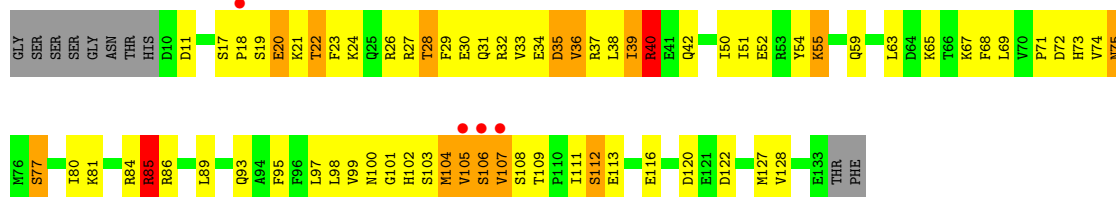
- Molecule 1: Autophagy-related protein 13, Microtubule-associated proteins 1A/1B light chain 3B

Chain B: 



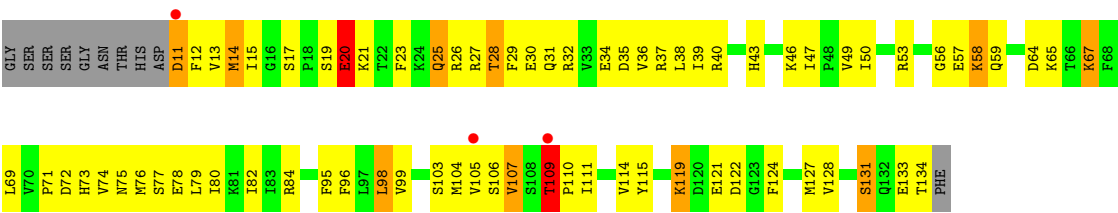
- Molecule 1: Autophagy-related protein 13, Microtubule-associated proteins 1A/1B light chain 3B

Chain C: 



- Molecule 1: Autophagy-related protein 13, Microtubule-associated proteins 1A/1B light chain 3B

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	64.57Å 64.57Å 130.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 2.60 43.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.44-2.60) 99.8 (43.44-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.294 0.228 , 0.300	Depositor DCC
R_{free} test set	827 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4113	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.80	0/1062	1.24	6/1430 (0.4%)
1	B	0.84	0/1043	1.42	20/1404 (1.4%)
1	C	0.82	0/1043	1.45	25/1404 (1.8%)
1	D	0.99	1/1042 (0.1%)	1.26	6/1403 (0.4%)
All	All	0.87	1/4190 (0.0%)	1.35	57/5641 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	109	THR	CA-C	5.64	1.59	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	SER	N-CA-C	-12.15	84.00	107.44
1	C	107	VAL	N-CA-C	-11.11	86.83	106.61
1	B	25	GLN	N-CA-C	10.94	126.45	112.89
1	A	19	SER	N-CA-C	-10.86	92.01	108.52
1	C	20	GLU	N-CA-C	-9.05	96.47	109.96
1	C	65	LYS	CB-CA-C	-8.94	90.41	110.07
1	B	105	VAL	CB-CA-C	8.84	119.45	110.70
1	A	115	TYR	N-CA-C	8.66	120.72	111.28
1	D	119	LYS	N-CA-C	8.31	122.28	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	MET	CA-C-N	8.12	131.40	120.77
1	C	104	MET	C-N-CA	8.12	131.40	120.77
1	C	108	SER	N-CA-C	-7.76	92.09	107.69
1	B	43	HIS	CA-C-N	7.76	127.94	119.87
1	B	43	HIS	C-N-CA	7.76	127.94	119.87
1	B	102	HIS	N-CA-C	7.73	124.54	113.02
1	B	15	ILE	N-CA-C	-7.35	97.69	108.87
1	B	59	GLN	CB-CA-C	-7.22	98.15	109.34
1	C	36	VAL	CB-CA-C	-7.17	102.70	111.88
1	B	15	ILE	CB-CA-C	7.08	120.90	111.21
1	B	27	ARG	N-CA-C	-7.03	99.53	110.42
1	D	20	GLU	CB-CA-C	-6.99	101.20	109.80
1	C	112	SER	N-CA-C	6.98	120.69	111.75
1	C	106	SER	CA-C-N	6.93	132.04	123.17
1	C	106	SER	C-N-CA	6.93	132.04	123.17
1	A	115	TYR	CB-CA-C	-6.89	99.34	110.79
1	A	34	GLU	N-CA-C	6.80	120.80	112.23
1	B	37	ARG	N-CA-C	6.73	119.19	111.11
1	C	105	VAL	N-CA-C	6.61	117.11	110.23
1	C	39	ILE	CB-CA-C	-6.60	101.57	112.26
1	C	40	ARG	CB-CA-C	-6.43	98.74	110.63
1	B	20	GLU	N-CA-C	6.30	118.28	110.91
1	D	19	SER	N-CA-C	6.25	119.99	111.17
1	C	40	ARG	N-CA-C	6.19	118.83	111.71
1	C	39	ILE	N-CA-C	6.17	118.80	111.09
1	D	119	LYS	CB-CA-C	-6.05	99.67	109.72
1	A	104	MET	N-CA-C	6.01	119.67	112.93
1	C	106	SER	N-CA-C	-5.95	98.21	108.56
1	B	132	GLN	CB-CA-C	-5.93	99.68	111.91
1	D	49	VAL	N-CA-C	5.92	116.53	107.77
1	B	37	ARG	CB-CA-C	-5.89	101.38	110.81
1	C	54	TYR	CB-CA-C	-5.88	101.01	109.84
1	C	39	ILE	CA-C-N	5.87	128.73	120.28
1	C	39	ILE	C-N-CA	5.87	128.73	120.28
1	C	104	MET	CB-CA-C	-5.84	97.63	111.65
1	D	109	THR	CB-CA-C	5.73	121.45	110.17
1	B	38	LEU	N-CA-C	5.72	117.51	111.28
1	C	101	GLY	N-CA-C	5.65	123.61	114.90
1	C	77	SER	N-CA-C	5.63	118.96	111.75
1	C	77	SER	CB-CA-C	-5.63	99.53	110.46
1	B	28	THR	N-CA-C	-5.53	103.24	110.53
1	A	51	ILE	N-CA-C	5.51	115.79	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	GLN	N-CA-C	5.50	120.48	113.55
1	C	85	ARG	N-CA-C	-5.42	105.45	111.36
1	B	47	ILE	N-CA-C	5.39	113.87	107.73
1	C	112	SER	CB-CA-C	-5.28	100.21	110.46
1	B	26	ARG	CA-C-N	-5.28	113.13	122.74
1	B	26	ARG	C-N-CA	-5.28	113.13	122.74

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	106	SER	Peptide
1	D	109	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1042	0	1051	64	0
1	B	1024	0	1035	51	0
1	C	1024	0	1035	61	0
1	D	1023	0	1038	57	0
All	All	4113	0	4159	222	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 27.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:HG12	1:D:105:VAL:O	1.39	1.17
1:D:75:ASN:HB2	1:D:109:THR:HA	1.25	1.12
1:C:85:ARG:HH11	1:C:85:ARG:HG2	1.03	1.12
1:D:103:SER:OG	1:D:105:VAL:HG23	1.47	1.11
1:A:78:GLU:O	1:A:82:ILE:HG13	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HH11	1:A:37:ARG:HB3	1.23	1.03
1:C:36:VAL:O	1:C:40:ARG:HB2	1.57	1.03
1:B:98:LEU:HD23	1:B:103:SER:O	1.57	1.02
1:C:20:GLU:H	1:C:55:LYS:HZ3	1.06	1.00
1:C:85:ARG:HG2	1:C:85:ARG:NH1	1.75	0.95
1:D:105:VAL:O	1:D:105:VAL:CG1	2.10	0.94
1:C:99:VAL:HG22	1:C:127:MET:HE2	1.53	0.88
1:A:37:ARG:HB3	1:A:37:ARG:NH1	1.87	0.87
1:A:46:LYS:HB3	1:A:69:LEU:HB3	1.56	0.86
1:B:133:GLU:C	1:B:133:GLU:CD	2.45	0.84
1:B:100:ASN:HB2	1:B:102:HIS:CE1	2.11	0.84
1:A:19:SER:OG	1:A:21:LYS:HE3	1.78	0.84
1:D:21:LYS:HG3	1:D:25:GLN:HE21	1.44	0.82
1:D:75:ASN:CB	1:D:109:THR:HA	2.08	0.82
1:A:72:ASP:HB2	1:A:112:SER:HB3	1.59	0.82
1:B:115:TYR:O	1:B:119:LYS:HG2	1.78	0.82
1:C:99:VAL:H	1:C:103:SER:HB3	1.47	0.80
1:C:104:MET:O	1:C:107:VAL:HG23	1.82	0.80
1:C:59:GLN:HB3	1:C:93:GLN:HE22	1.46	0.79
1:B:20:GLU:O	1:B:20:GLU:HG3	1.82	0.79
1:B:109:THR:HB	1:B:110:PRO:HD2	1.64	0.79
1:C:85:ARG:HH11	1:C:85:ARG:CG	1.89	0.77
1:D:75:ASN:HA	1:D:110:PRO:HA	1.67	0.76
1:D:103:SER:HG	1:D:105:VAL:HG23	1.48	0.75
1:C:24:LYS:HG2	1:C:32:ARG:NH1	2.01	0.75
1:C:28:THR:HG22	1:C:31:GLN:CG	2.17	0.75
1:D:39:ILE:HG12	1:D:69:LEU:HD11	1.69	0.74
1:A:99:VAL:HG22	1:A:127:MET:HE2	1.68	0.74
1:A:34:GLU:O	1:A:34:GLU:HG3	1.89	0.73
1:C:28:THR:HG22	1:C:31:GLN:HG3	1.68	0.72
1:C:98:LEU:HA	1:C:103:SER:O	1.90	0.72
1:A:99:VAL:CG2	1:A:127:MET:HE2	2.20	0.71
1:C:34:GLU:OE2	1:C:37:ARG:NH1	2.23	0.70
1:B:72:ASP:HB2	1:B:112:SER:HB3	1.73	0.69
1:C:98:LEU:HD23	1:C:103:SER:O	1.92	0.69
1:A:90:ASN:HB3	1:A:92:ASN:ND2	2.08	0.69
1:B:79:LEU:HA	1:B:82:ILE:HD12	1.75	0.69
1:A:115:TYR:O	1:A:119:LYS:HB3	1.92	0.69
1:D:36:VAL:O	1:D:40:ARG:HB2	1.94	0.68
1:B:85:ARG:HD3	1:D:121:GLU:CD	2.19	0.67
1:D:34:GLU:OE2	1:D:37:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:NH1	1:A:35:ASP:OD2	2.27	0.67
1:C:72:ASP:HB2	1:C:112:SER:OG	1.94	0.67
1:C:84:ARG:HG2	1:C:89:LEU:HD12	1.76	0.67
1:D:84:ARG:NH1	1:D:95:PHE:HB3	2.10	0.67
1:C:50:ILE:HD11	1:C:67:LYS:HG2	1.77	0.67
1:D:75:ASN:OD1	1:D:78:GLU:HG3	1.95	0.66
1:D:75:ASN:HB2	1:D:109:THR:CA	2.15	0.66
1:D:34:GLU:O	1:D:38:LEU:HB2	1.95	0.66
1:A:28:THR:HG23	1:A:30:GLU:H	1.61	0.65
1:B:20:GLU:O	1:B:20:GLU:CG	2.45	0.65
1:D:25:GLN:O	1:D:25:GLN:HG3	1.96	0.64
1:A:63:LEU:HD11	1:A:86:ARG:HG2	1.78	0.64
1:A:92:ASN:ND2	1:A:92:ASN:H	1.95	0.64
1:D:110:PRO:O	1:D:114:VAL:HG23	1.96	0.64
1:D:122:ASP:OD1	1:D:124:PHE:HB2	1.98	0.64
1:B:78:GLU:O	1:B:82:ILE:HG13	1.98	0.64
1:A:42:GLN:C	1:A:44:PRO:HD3	2.23	0.63
1:C:77:SER:O	1:C:81:LYS:HG2	1.99	0.63
1:A:90:ASN:HB2	1:A:93:GLN:HB2	1.81	0.63
1:D:28:THR:O	1:D:32:ARG:HG3	1.99	0.62
1:B:80:ILE:O	1:B:84:ARG:HB2	1.99	0.62
1:A:36:VAL:HG11	1:A:123:GLY:HA3	1.82	0.62
1:D:39:ILE:CG1	1:D:69:LEU:HD11	2.29	0.61
1:B:133:GLU:CD	1:B:133:GLU:O	2.44	0.61
1:A:92:ASN:H	1:A:92:ASN:HD22	1.48	0.61
1:A:120:ASP:OD1	1:A:121:GLU:N	2.34	0.60
1:A:22:THR:H	1:A:25:GLN:NE2	2.00	0.60
1:B:100:ASN:HB2	1:B:102:HIS:HE1	1.66	0.59
1:B:28:THR:HG23	1:B:31:GLN:H	1.66	0.59
1:A:67:LYS:HD3	1:D:11:ASP:O	2.02	0.59
1:A:37:ARG:HH11	1:A:37:ARG:CB	2.07	0.59
1:D:50:ILE:HG12	1:D:124:PHE:CD1	2.38	0.59
1:B:34:GLU:OE2	1:B:37:ARG:NH1	2.35	0.59
1:B:29:PHE:O	1:B:33:VAL:HG22	2.03	0.58
1:A:90:ASN:HB3	1:A:92:ASN:HD21	1.66	0.58
1:B:133:GLU:C	1:B:133:GLU:OE1	2.45	0.58
1:C:63:LEU:HD11	1:C:86:ARG:HD3	1.85	0.58
1:C:52:GLU:O	1:C:128:VAL:HA	2.04	0.58
1:C:26:ARG:O	1:C:26:ARG:HG2	2.04	0.57
1:D:56:GLY:O	1:D:58:LYS:HE2	2.04	0.57
1:B:36:VAL:O	1:B:40:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:O	1:C:102:HIS:CE1	2.57	0.57
1:C:112:SER:O	1:C:116:GLU:HG2	2.05	0.56
1:B:20:GLU:C	1:B:20:GLU:OE2	2.47	0.56
1:C:29:PHE:O	1:C:33:VAL:HG13	2.05	0.56
1:A:19:SER:OG	1:A:21:LYS:CE	2.51	0.56
1:B:90:ASN:HB3	1:B:92:ASN:ND2	2.21	0.56
1:C:50:ILE:CD1	1:C:67:LYS:HG2	2.36	0.56
1:B:11:ASP:OD1	1:B:12:PHE:N	2.36	0.55
1:C:30:GLU:H	1:C:30:GLU:CD	2.14	0.55
1:D:115:TYR:O	1:D:119:LYS:HB3	2.07	0.55
1:D:30:GLU:CD	1:D:30:GLU:H	2.15	0.55
1:A:34:GLU:O	1:A:34:GLU:CG	2.55	0.55
1:B:92:ASN:HD22	1:D:128:VAL:HG21	1.72	0.55
1:B:109:THR:HB	1:B:110:PRO:CD	2.36	0.54
1:C:32:ARG:HD2	1:C:122:ASP:OD2	2.07	0.54
1:C:38:LEU:HG	1:C:42:GLN:HE21	1.73	0.54
1:D:77:SER:HA	1:D:107:VAL:HG12	1.88	0.54
1:D:98:LEU:O	1:D:127:MET:HA	2.07	0.54
1:D:71:PRO:HB2	1:D:74:VAL:HG23	1.90	0.54
1:C:27:ARG:HH12	1:C:67:LYS:NZ	2.06	0.53
1:B:47:ILE:N	1:B:70:VAL:O	2.31	0.53
1:A:84:ARG:NH1	1:A:95:PHE:HB3	2.24	0.53
1:B:17:SER:HB2	1:C:73:HIS:CE1	2.44	0.53
1:B:85:ARG:O	1:B:85:ARG:HG2	2.09	0.53
1:B:98:LEU:HD23	1:B:103:SER:C	2.30	0.53
1:D:27:ARG:NH1	1:D:67:LYS:HE3	2.23	0.52
1:D:99:VAL:HG22	1:D:127:MET:HG2	1.90	0.52
1:B:53:ARG:HD2	1:B:57:GLU:HB3	1.92	0.52
1:B:74:VAL:HG13	1:B:78:GLU:HB2	1.90	0.52
1:B:75:ASN:HB2	1:B:109:THR:O	2.10	0.52
1:C:97:LEU:O	1:C:103:SER:O	2.27	0.52
1:A:38:LEU:O	1:A:41:GLU:HB3	2.10	0.51
1:B:84:ARG:HG2	1:B:89:LEU:HD12	1.93	0.51
1:C:20:GLU:H	1:C:55:LYS:NZ	1.93	0.51
1:D:43:HIS:HB3	1:D:46:LYS:HD2	1.93	0.51
1:D:12:PHE:O	1:D:13:VAL:HG23	2.11	0.51
1:D:96:PHE:HD1	1:D:105:VAL:CG2	2.23	0.51
1:C:32:ARG:O	1:C:35:ASP:HB2	2.11	0.50
1:C:27:ARG:HH12	1:C:67:LYS:HZ2	1.57	0.50
1:C:39:ILE:CG2	1:C:40:ARG:N	2.72	0.50
1:A:90:ASN:H	1:A:90:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLU:CD	1:D:37:ARG:NH1	2.70	0.50
1:A:99:VAL:HG22	1:A:127:MET:HB3	1.94	0.50
1:C:28:THR:CG2	1:C:31:GLN:HG3	2.38	0.50
1:A:27:ARG:NH1	1:A:31:GLN:HB3	2.27	0.49
1:A:47:ILE:HG23	1:A:115:TYR:CD1	2.47	0.49
1:B:20:GLU:O	1:B:21:LYS:C	2.54	0.49
1:B:80:ILE:HG23	1:B:95:PHE:HE1	1.76	0.49
1:C:17:SER:C	1:C:18:PRO:O	2.54	0.49
1:A:110:PRO:HD2	1:A:113:GLU:HG3	1.93	0.49
1:C:22:THR:OG1	1:C:23:PHE:N	2.45	0.48
1:B:108:SER:O	1:B:108:SER:OG	2.28	0.48
1:B:29:PHE:CD1	1:B:29:PHE:C	2.91	0.48
1:C:80:ILE:HG23	1:C:95:PHE:CE2	2.48	0.48
1:A:27:ARG:HH11	1:A:31:GLN:HB3	1.78	0.48
1:A:95:PHE:CE2	1:A:129:TYR:HB2	2.49	0.48
1:A:69:LEU:HD12	1:D:14:MET:HE2	1.96	0.48
1:C:74:VAL:O	1:C:111:ILE:N	2.42	0.48
1:A:43:HIS:N	1:A:44:PRO:HD3	2.28	0.48
1:A:92:ASN:HD22	1:A:92:ASN:N	2.12	0.47
1:A:93:GLN:OE1	1:A:94:ALA:N	2.46	0.47
1:A:34:GLU:O	1:A:38:LEU:HB2	2.14	0.47
1:B:17:SER:HB2	1:C:73:HIS:HE1	1.80	0.47
1:C:38:LEU:O	1:C:42:GLN:HG3	2.13	0.47
1:A:32:ARG:HD2	1:A:122:ASP:OD2	2.14	0.47
1:D:80:ILE:HD11	1:D:104:MET:O	2.15	0.47
1:B:17:SER:HB3	1:C:71:PRO:HG2	1.97	0.47
1:A:45:THR:HG21	1:D:53:ARG:HH22	1.80	0.47
1:D:57:GLU:OE2	1:D:131:SER:OG	2.32	0.47
1:D:64:ASP:OD1	1:D:65:LYS:HG2	2.15	0.46
1:B:80:ILE:HG23	1:B:95:PHE:CE1	2.51	0.46
1:B:116:GLU:OE1	1:B:116:GLU:HA	2.16	0.46
1:A:115:TYR:O	1:A:115:TYR:CG	2.66	0.46
1:A:127:MET:HE2	1:A:127:MET:HB3	1.73	0.46
1:B:74:VAL:O	1:B:111:ILE:HG22	2.16	0.46
1:A:46:LYS:HE2	1:D:14:MET:HG2	1.97	0.46
1:D:79:LEU:HD22	1:D:111:ILE:HD12	1.97	0.46
1:A:62:VAL:HG12	1:A:63:LEU:O	2.15	0.45
1:C:51:ILE:HG13	1:C:68:PHE:HD2	1.80	0.45
1:A:19:SER:HG	1:A:21:LYS:HE3	1.78	0.45
1:A:28:THR:HG22	1:A:31:GLN:CG	2.46	0.45
1:D:47:ILE:HG13	1:D:111:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:THR:HG22	1:C:31:GLN:CD	2.41	0.45
1:B:98:LEU:HA	1:B:103:SER:O	2.17	0.45
1:A:72:ASP:O	1:A:110:PRO:HB2	2.17	0.44
1:A:92:ASN:ND2	1:A:92:ASN:N	2.62	0.44
1:C:59:GLN:HB3	1:C:93:GLN:NE2	2.24	0.44
1:A:28:THR:CG2	1:A:31:GLN:H	2.30	0.44
1:C:38:LEU:HG	1:C:42:GLN:NE2	2.32	0.44
1:A:103:SER:OG	1:A:105:VAL:HG22	2.18	0.44
1:C:39:ILE:CG1	1:C:69:LEU:HD11	2.48	0.44
1:C:50:ILE:CD1	1:C:67:LYS:CG	2.96	0.44
1:C:80:ILE:HD11	1:C:105:VAL:HA	1.99	0.44
1:C:81:LYS:O	1:C:85:ARG:HG3	2.18	0.44
1:C:100:ASN:HB2	1:C:102:HIS:CE1	2.53	0.44
1:D:69:LEU:HD23	1:D:69:LEU:HA	1.70	0.43
1:A:47:ILE:HG13	1:A:111:ILE:HG23	2.00	0.43
1:C:23:PHE:HA	1:C:26:ARG:NH1	2.33	0.43
1:A:21:LYS:HA	1:A:25:GLN:NE2	2.32	0.43
1:D:21:LYS:HB3	1:D:25:GLN:HB3	1.99	0.43
1:A:99:VAL:HG21	1:A:127:MET:HE2	2.01	0.43
1:B:31:GLN:O	1:B:35:ASP:HB2	2.18	0.43
1:D:28:THR:O	1:D:29:PHE:C	2.60	0.43
1:B:120:ASP:HB3	1:B:122:ASP:OD1	2.19	0.43
1:C:77:SER:HA	1:C:80:ILE:HD12	2.00	0.43
1:D:23:PHE:HA	1:D:26:ARG:HG3	2.00	0.43
1:A:76:MET:HA	1:A:76:MET:HE2	2.01	0.42
1:B:40:ARG:HD2	1:B:40:ARG:HA	1.80	0.42
1:A:22:THR:H	1:A:25:GLN:HE21	1.64	0.42
1:A:85:ARG:HB2	1:A:85:ARG:CZ	2.49	0.42
1:A:68:PHE:CD1	1:D:15:ILE:HD11	2.55	0.42
1:A:76:MET:HE1	1:A:111:ILE:HB	2.01	0.42
1:D:71:PRO:O	1:D:74:VAL:HG23	2.20	0.42
1:D:28:THR:HG23	1:D:31:GLN:HG3	2.02	0.42
1:B:76:MET:O	1:B:80:ILE:HG13	2.20	0.41
1:C:30:GLU:CD	1:C:30:GLU:N	2.78	0.41
1:D:20:GLU:H	1:D:20:GLU:HG3	1.73	0.41
1:B:115:TYR:O	1:B:119:LYS:CG	2.59	0.41
1:C:39:ILE:HG23	1:C:40:ARG:N	2.35	0.41
1:C:120:ASP:HB3	1:C:122:ASP:OD1	2.21	0.41
1:B:10:ASP:OD1	1:C:27:ARG:NH2	2.54	0.41
1:D:72:ASP:OD1	1:D:73:HIS:N	2.54	0.41
1:D:133:GLU:O	1:D:133:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:O	1:A:82:ILE:CG1	2.48	0.41
1:D:27:ARG:HH12	1:D:67:LYS:HE3	1.86	0.41
1:C:75:ASN:HB3	1:C:109:THR:C	2.45	0.41
1:A:98:LEU:HA	1:A:102:HIS:O	2.21	0.41
1:A:72:ASP:HA	1:A:111:ILE:CG2	2.52	0.40
1:D:21:LYS:HD3	1:D:21:LYS:HA	1.87	0.40
1:B:28:THR:O	1:B:32:ARG:HG3	2.20	0.40
1:D:76:MET:CE	1:D:111:ILE:HG13	2.51	0.40
1:B:120:ASP:OD2	1:B:122:ASP:OD1	2.38	0.40
1:A:99:VAL:HG23	1:A:104:MET:HG3	2.03	0.40
1:B:84:ARG:NH2	1:B:90:ASN:O	2.55	0.40
1:C:100:ASN:HB2	1:C:102:HIS:HE1	1.86	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	124/134 (92%)	121 (98%)	3 (2%)	0	100	100
1	B	122/134 (91%)	113 (93%)	9 (7%)	0	100	100
1	C	122/134 (91%)	118 (97%)	4 (3%)	0	100	100
1	D	122/134 (91%)	114 (93%)	8 (7%)	0	100	100
All	All	490/536 (91%)	466 (95%)	24 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	119/125 (95%)	108 (91%)	11 (9%)	8	19
1	B	117/125 (94%)	103 (88%)	14 (12%)	5	10
1	C	117/125 (94%)	106 (91%)	11 (9%)	8	18
1	D	117/125 (94%)	101 (86%)	16 (14%)	3	7
All	All	470/500 (94%)	418 (89%)	52 (11%)	6	12

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	25	GLN
1	A	63	LEU
1	A	82	ILE
1	A	90	ASN
1	A	92	ASN
1	A	93	GLN
1	A	105	VAL
1	A	106	SER
1	A	109	THR
1	A	133	GLU
1	B	14	MET
1	B	15	ILE
1	B	25	GLN
1	B	26	ARG
1	B	30	GLU
1	B	40	ARG
1	B	45	THR
1	B	62	VAL
1	B	67	LYS
1	B	77	SER
1	B	84	ARG
1	B	117	SER
1	B	127	MET
1	B	133	GLU
1	C	11	ASP
1	C	19	SER
1	C	21	LYS

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Mol	Chain	Res	Type
1	C	22	THR
1	C	28	THR
1	C	35	ASP
1	C	40	ARG
1	C	55	LYS
1	C	75	ASN
1	C	85	ARG
1	C	113	GLU
1	D	11	ASP
1	D	14	MET
1	D	17	SER
1	D	20	GLU
1	D	25	GLN
1	D	28	THR
1	D	35	ASP
1	D	58	LYS
1	D	59	GLN
1	D	67	LYS
1	D	82	ILE
1	D	98	LEU
1	D	106	SER
1	D	107	VAL
1	D	131	SER
1	D	134	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	59	GLN
1	A	73	HIS
1	A	90	ASN
1	A	92	ASN
1	A	100	ASN
1	B	90	ASN
1	B	92	ASN
1	C	42	GLN
1	C	59	GLN
1	C	73	HIS
1	C	90	ASN
1	C	93	GLN
1	C	102	HIS

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Mol	Chain	Res	Type
1	D	25	GLN
1	D	92	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	126/134 (94%)	0.07	0 100 100	37, 61, 90, 124	0
1	B	124/134 (92%)	0.07	6 (4%) 35 30	39, 59, 100, 131	0
1	C	124/134 (92%)	0.16	4 (3%) 50 44	39, 60, 101, 132	0
1	D	124/134 (92%)	-0.17	3 (2%) 59 54	32, 51, 83, 111	0
All	All	498/536 (92%)	0.04	13 (2%) 57 51	32, 59, 97, 132	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	VAL	4.3
1	D	105	VAL	3.4
1	C	18	PRO	2.8
1	B	107	VAL	2.7
1	C	107	VAL	2.5
1	B	106	SER	2.3
1	C	106	SER	2.3
1	B	103	SER	2.3
1	D	11	ASP	2.2
1	B	105	VAL	2.1
1	B	18	PRO	2.1
1	B	104	MET	2.0
1	D	109	THR	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.