



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:29 PM EDT

PDB ID : 3WAO
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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

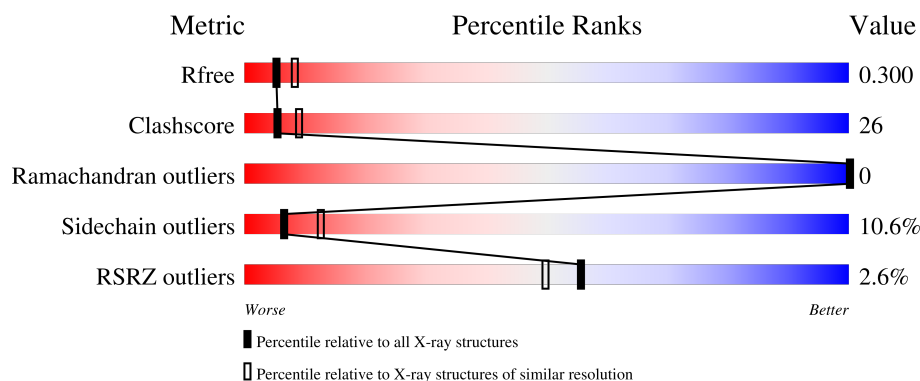
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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.

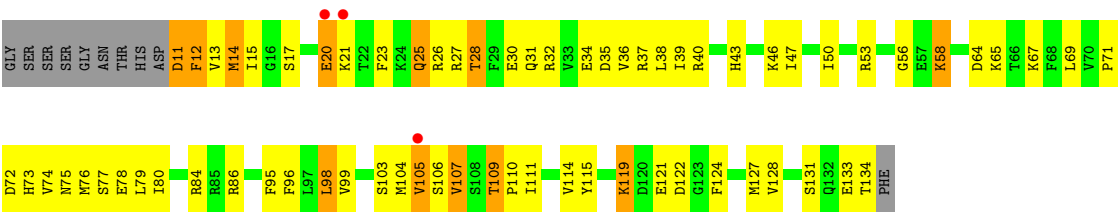
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1042	665	179	194	4			
1	B	124	Total	C	N	O	S	0	0	0
			1024	652	177	191	4			
1	C	124	Total	C	N	O	S	0	0	0
			1024	652	177	191	4			
1	D	124	Total	C	N	O	S	0	0	0
			1023	652	177	190	4			

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

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





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 43.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.44-2.60) 99.9 (43.09-2.60)	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 , 28.6	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	0.60	0/1062	0.91	3/1430 (0.2%)
1	B	0.60	0/1043	0.96	5/1404 (0.4%)
1	C	0.57	0/1043	1.01	9/1404 (0.6%)
1	D	0.69	0/1042	0.92	2/1403 (0.1%)
All	All	0.61	0/4190	0.95	19/5641 (0.3%)

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

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	SER	N-CA-C	-10.00	84.00	111.00
1	C	65	LYS	CB-CA-C	-9.99	90.41	110.40
1	C	107	VAL	N-CA-C	-8.95	86.83	111.00
1	A	105	VAL	CB-CA-C	-8.55	95.16	111.40
1	A	19	SER	N-CA-C	-7.04	92.01	111.00
1	C	108	SER	N-CA-C	-7.00	92.09	111.00
1	D	105	VAL	CB-CA-C	-7.00	98.10	111.40
1	C	104	MET	CB-CA-C	-6.38	97.63	110.40
1	B	59	GLN	CB-CA-C	-6.13	98.15	110.40
1	C	40	ARG	CB-CA-C	-5.83	98.74	110.40
1	B	25	GLN	N-CA-C	5.72	126.45	111.00
1	C	77	SER	CB-CA-C	-5.56	99.53	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	TYR	CB-CA-C	-5.53	99.34	110.40
1	C	20	GLU	N-CA-C	-5.38	96.47	111.00
1	D	119	LYS	CB-CA-C	-5.37	99.67	110.40
1	B	132	GLN	CB-CA-C	-5.36	99.68	110.40
1	C	112	SER	CB-CA-C	-5.21	100.21	110.10
1	B	102	HIS	N-CA-C	5.01	124.54	111.00
1	C	39	ILE	CB-CA-C	-5.01	101.57	111.60

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 [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	1042	0	1051	60	0
1	B	1024	0	1035	52	0
1	C	1024	0	1035	60	0
1	D	1023	0	1038	54	0
All	All	4113	0	4159	216	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 26.

All (216) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:O	1:A:82:ILE:HG13	1.57	1.04
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: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: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: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:20:GLU:H	1:C:55:LYS:HZ1	1.27	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:B:133:GLU:C	1:B:133:GLU:CD	2.45	0.75
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: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: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:D:34:GLU:OE2	1:D:37:ARG:NH1	2.27	0.67
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:20:GLU:H	1:C:55:LYS:NZ	1.93	0.66
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:A:99:VAL:CG2	1:A:127:MET:HE2	2.27	0.64
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: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:B:85:ARG:HD3	1:D:121:GLU:CD	2.19	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: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:C:63:LEU:HD11	1:C:86:ARG:HD3	1.85	0.58
1:A:42:GLN:C	1:A:44:PRO:HD3	2.23	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLU:CD	1:B:133:GLU:O	2.44	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:D:115:TYR:O	1:D:119:LYS:HB3	2.07	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:B:133:GLU:C	1:B:133:GLU:OE1	2.45	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:D:27:ARG:NH1	1:D:67:LYS:HE3	2.23	0.52
1:A:99:VAL:HG21	1:A:127:MET:HE2	1.91	0.52
1:C:39:ILE:CG2	1:C:40:ARG:N	2.72	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:20:GLU:C	1:B:20:GLU:OE2	2.47	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: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:30:GLU:H	1:C:30:GLU:CD	2.14	0.50
1:C:32:ARG:O	1:C:35:ASP:HB2	2.11	0.50
1:C:99:VAL:HG22	1:C:127:MET:CE	2.42	0.50
1:D:30:GLU:CD	1:D:30:GLU:H	2.15	0.50
1:A:90:ASN:H	1:A:90:ASN:ND2	2.09	0.50
1:A:99:VAL:HG22	1:A:127:MET:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:ILE:HG23	1:B:95:PHE:HE1	1.76	0.49
1:A:99:VAL:HG22	1:A:127:MET:HE2	1.95	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: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:C:74:VAL:O	1:C:111:ILE:N	2.42	0.48
1:B:98:LEU:HD23	1:B:103:SER:C	2.30	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: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: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
1:D:34:GLU:CD	1:D:37:ARG:NH1	2.70	0.45
1:C:17:SER:C	1:C:18:PRO:O	2.54	0.45
1:B:20:GLU:O	1:B:21:LYS:C	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:29:PHE:CD1	1:B:29:PHE:C	2.91	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:B:31:GLN:O	1:B:35:ASP:HB2	2.18	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: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:C:99:VAL:HG22	1:C:127:MET:HE1	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: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:27:ARG:HH12	1:C:67:LYS:HZ2	1.68	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:HA	1:B:30:GLU:OE1	2.21	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:C:28:THR:HG22	1:C:31:GLN:CD	2.41	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%)	109 (92%)	10 (8%)	11	21
1	B	117/125 (94%)	104 (89%)	13 (11%)	6	11
1	C	117/125 (94%)	105 (90%)	12 (10%)	7	13
1	D	117/125 (94%)	102 (87%)	15 (13%)	4	8
All	All	470/500 (94%)	420 (89%)	50 (11%)	6	12

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	25	GLN
1	A	63	LEU
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	35	ASP
1	B	40	ARG
1	B	62	VAL
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	12	PHE
1	C	19	SER
1	C	22	THR
1	C	28	THR
1	C	35	ASP
1	C	40	ARG
1	C	58	LYS
1	C	75	ASN
1	C	85	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	113	GLU
1	C	133	GLU
1	D	11	ASP
1	D	12	PHE
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	86	ARG
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	73	HIS
1	A	90	ASN
1	A	92	ASN
1	A	100	ASN
1	B	90	ASN
1	B	92	ASN
1	B	93	GLN
1	B	100	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
1	D	25	GLN

5.3.3 RNA ⓘ

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 monosaccharides 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

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	126/134 (94%)	-0.32	1 (0%) 86 84	37, 61, 90, 124	0
1	B	124/134 (92%)	-0.18	4 (3%) 47 40	39, 59, 100, 131	0
1	C	124/134 (92%)	-0.20	5 (4%) 38 31	39, 60, 101, 132	0
1	D	124/134 (92%)	-0.32	3 (2%) 59 53	32, 51, 83, 111	0
All	All	498/536 (92%)	-0.25	13 (2%) 56 50	32, 59, 97, 132	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	SER	7.6
1	B	105	VAL	6.3
1	D	105	VAL	4.3
1	C	18	PRO	3.5
1	C	106	SER	3.4
1	C	105	VAL	2.7
1	C	19	SER	2.6
1	D	21	LYS	2.4
1	B	107	VAL	2.2
1	C	104	MET	2.1
1	B	104	MET	2.1
1	D	20	GLU	2.1
1	A	105	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.