



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 11:13 PM UTC

PDB ID : 5C6H / pdb_00005c6h
Title : Mcl-1 complexed with Mule
Authors : Song, T.; Wang, Z.; Ji, F.; Chai, G.; Liu, Y.; Li, X.; Li, Z.; Fan, Y.; Zhang, Z.
Deposited on : 2015-06-23
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

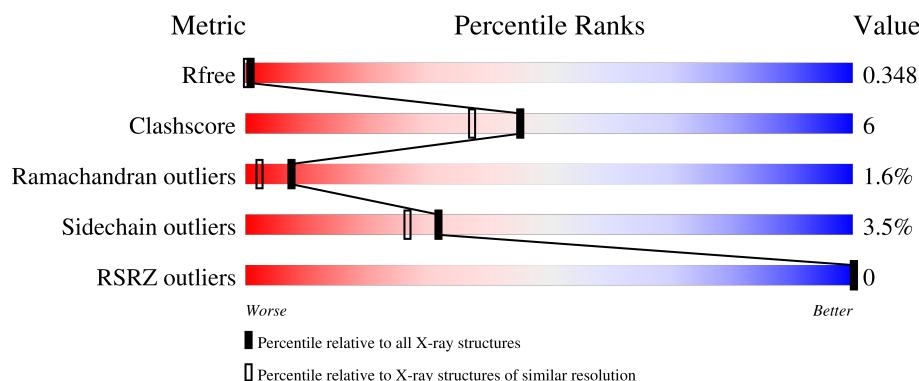
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

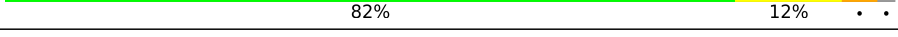
The reported resolution of this entry is 2.05 Å.

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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	157	 75% 22% ..
1	C	157	 85% 11% ..
1	E	157	 82% 15% ...
1	G	157	 82% 12% . .
1	I	157	 78% 19% ..

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Mol	Chain	Length	Quality of chain
1	K	157	
1	M	157	
1	O	157	
1	Q	157	
1	S	157	
1	U	157	
1	W	157	
2	B	26	
2	D	26	
2	F	26	
2	H	26	
2	J	26	
2	L	26	
2	N	26	
2	P	26	
2	R	26	
2	T	26	
2	V	26	
2	X	26	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17481 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1251	784	228	235	4			
1	C	155	Total	C	N	O	S	0	0	0
			1251	784	228	235	4			
1	E	154	Total	C	N	O	S	0	0	0
			1242	779	227	232	4			
1	G	154	Total	C	N	O	S	0	0	0
			1242	779	227	232	4			
1	I	155	Total	C	N	O	S	0	0	0
			1251	784	228	235	4			
1	K	153	Total	C	N	O	S	0	0	0
			1234	773	226	231	4			
1	M	155	Total	C	N	O	S	0	0	0
			1251	784	228	235	4			
1	O	155	Total	C	N	O	S	0	0	0
			1251	784	228	235	4			
1	Q	154	Total	C	N	O	S	0	0	0
			1242	779	227	232	4			
1	S	154	Total	C	N	O	S	0	0	0
			1241	779	227	231	4			
1	U	151	Total	C	N	O	S	0	0	0
			1217	764	224	225	4			
1	W	153	Total	C	N	O	S	0	0	0
			1231	772	226	229	4			

- Molecule 2 is a protein called Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	25	Total	C	N	O	S	0	0	0
			198	121	33	42	2			
2	D	26	Total	C	N	O	S	0	0	0
			206	127	34	43	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	26	Total	C	N	O	S	0	0	0
			206	127	34	43	2			
2	H	26	Total	C	N	O	S	0	0	0
			206	127	34	43	2			
2	J	24	Total	C	N	O	S	0	0	0
			192	118	32	40	2			
2	L	26	Total	C	N	O	S	0	0	0
			206	127	34	43	2			
2	N	26	Total	C	N	O	S	0	0	0
			204	125	34	43	2			
2	P	26	Total	C	N	O	S	0	0	0
			206	127	34	43	2			
2	R	24	Total	C	N	O	S	0	0	0
			192	118	32	40	2			
2	T	26	Total	C	N	O	S	0	0	0
			206	127	34	43	2			
2	V	23	Total	C	N	O	S	0	0	0
			185	113	31	39	2			
2	X	25	Total	C	N	O	S	0	0	0
			198	121	33	42	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	1	Total	O	0	0
			1	1		
3	C	11	Total	O	0	0
			11	11		
3	D	1	Total	O	0	0
			1	1		
3	E	1	Total	O	0	0
			1	1		
3	G	12	Total	O	0	0
			12	12		
3	H	1	Total	O	0	0
			1	1		
3	I	10	Total	O	0	0
			10	10		
3	J	2	Total	O	0	0
			2	2		

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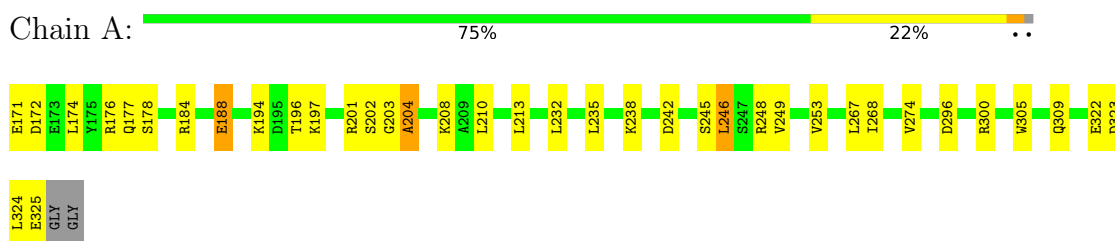
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	7	Total 7	O 7	0	0
3	L	1	Total 1	O 1	0	0
3	M	20	Total 20	O 20	0	0
3	N	4	Total 4	O 4	0	0
3	O	33	Total 33	O 33	0	0
3	P	6	Total 6	O 6	0	0
3	Q	14	Total 14	O 14	0	0
3	R	5	Total 5	O 5	0	0
3	S	12	Total 12	O 12	0	0
3	T	7	Total 7	O 7	0	0
3	U	9	Total 9	O 9	0	0
3	V	2	Total 2	O 2	0	0
3	W	5	Total 5	O 5	0	0
3	X	2	Total 2	O 2	0	0

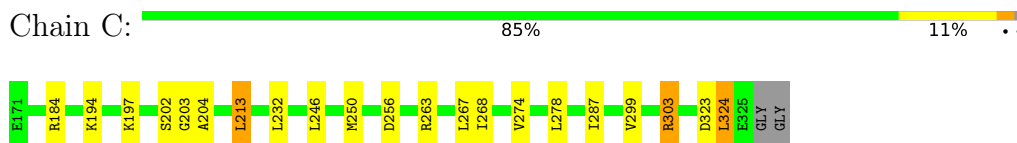
3 Residue-property plots

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.

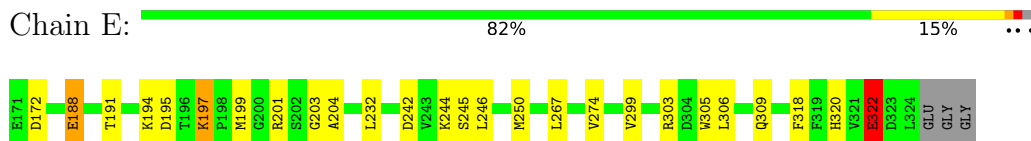
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



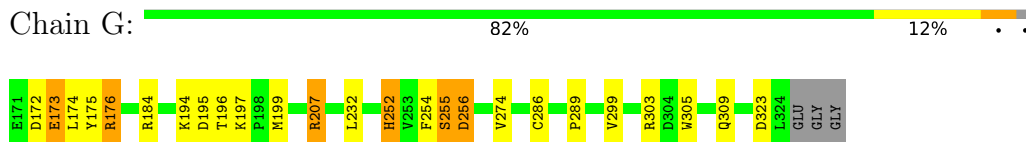
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



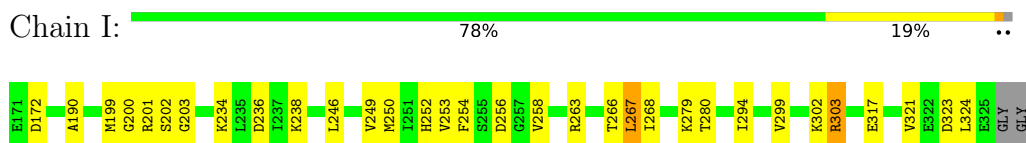
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain K:  85% 10% . .



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain M:  84% 14% ..



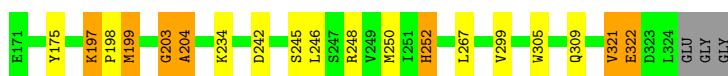
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain O:  83% 12% . .



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain Q:  86% 8% . .



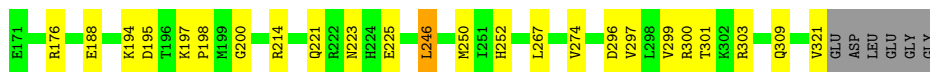
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain S:  82% 14% . .



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain U:  81% 15% . .



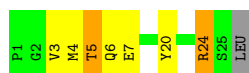
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain W:  82% 13% . . .



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain B:  69% 19% 8% .



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain D:  85% 15%



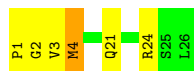
- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain F:  65% 27% 8%



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain H:  77% 19% .



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain J:  81% 12% 8%



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain L:  77% 23%



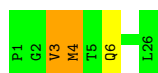
- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain N:  85% 15%



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain P:  88% . 8%



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain R:  73% 19% 8%



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain T:  69% 23% 8%



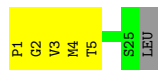
- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain V:  73% 15% 12%



- Molecule 2: Mule BH3 peptide from E3 ubiquitin-protein ligase HUWE1

Chain X:  77% 19% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	31.79Å 114.24Å 135.98Å 90.12° 92.32° 90.01°	Depositor
Resolution (Å)	35.45 – 2.05 35.45 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.6 (35.45-2.05) 95.7 (35.45-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.295 , 0.346 0.296 , 0.348	Depositor DCC
R_{free} test set	5809 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 12.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l 0.299 for -h,k,-l 0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17481	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.04 % 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 7.5113e-07. 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	0.29	0/1271	0.75	1/1709 (0.1%)
1	C	0.30	0/1271	0.71	0/1709
1	E	0.45	1/1262 (0.1%)	0.73	0/1697
1	G	0.30	0/1262	0.77	0/1697
1	I	0.56	4/1271 (0.3%)	0.76	0/1709
1	K	0.31	0/1254	0.69	0/1686
1	M	0.32	0/1271	0.72	0/1709
1	O	0.35	0/1271	0.77	2/1709 (0.1%)
1	Q	0.30	0/1262	0.73	0/1697
1	S	0.31	0/1261	0.75	0/1695
1	U	0.42	0/1237	0.71	0/1663
1	W	0.29	0/1251	0.68	0/1682
2	B	0.26	0/200	0.72	1/268 (0.4%)
2	D	0.27	0/208	0.62	0/279
2	F	0.25	0/208	0.76	1/279 (0.4%)
2	H	0.26	0/208	0.60	0/279
2	J	0.26	0/194	0.70	0/260
2	L	0.23	0/208	0.66	0/279
2	N	0.26	0/206	0.63	0/276
2	P	0.29	0/208	0.63	0/279
2	R	0.25	0/194	0.62	0/260
2	T	0.30	0/208	0.59	0/279
2	V	0.28	0/186	0.69	0/249
2	X	0.28	0/200	0.78	0/268
All	All	0.35	5/17572 (0.0%)	0.72	5/23617 (0.0%)

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	O	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	317	GLU	C-O	-7.86	1.15	1.24
1	I	267	LEU	C-O	-7.15	1.15	1.24
1	E	188	GLU	C-O	-5.33	1.17	1.24
1	I	266	THR	C-O	-5.26	1.17	1.24
1	I	268	ILE	C-O	-5.06	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	24	ARG	N-CA-C	-7.04	103.68	112.90
1	O	321	VAL	N-CA-C	-6.23	99.24	108.45
1	O	320	HIS	N-CA-C	6.21	118.76	109.25
1	A	204	ALA	N-CA-C	-5.56	105.12	111.07
2	B	3	VAL	N-CA-C	-5.13	108.29	113.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	320	HIS	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	1251	0	1253	23	0
1	C	1251	0	1253	12	0
1	E	1242	0	1247	16	0
1	G	1242	0	1247	16	0
1	I	1251	0	1253	15	0
1	K	1234	0	1236	10	0
1	M	1251	0	1253	13	0
1	O	1251	0	1253	17	0
1	Q	1242	0	1247	15	0
1	S	1241	0	1247	12	0
1	U	1217	0	1226	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1231	0	1228	13	0
2	B	198	0	186	5	0
2	D	206	0	197	3	0
2	F	206	0	197	6	0
2	H	206	0	197	3	0
2	J	192	0	181	3	0
2	L	206	0	197	3	0
2	N	204	0	190	2	0
2	P	206	0	197	3	0
2	R	192	0	181	3	0
2	T	206	0	197	5	0
2	V	185	0	171	1	0
2	X	198	0	186	3	0
3	A	6	0	0	0	0
3	B	1	0	0	0	0
3	C	11	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	G	12	0	0	0	0
3	H	1	0	0	0	0
3	I	10	0	0	0	0
3	J	2	0	0	0	0
3	K	7	0	0	0	0
3	L	1	0	0	0	0
3	M	20	0	0	0	0
3	N	4	0	0	0	0
3	O	33	0	0	1	0
3	P	6	0	0	0	0
3	Q	14	0	0	0	0
3	R	5	0	0	0	0
3	S	12	0	0	0	0
3	T	7	0	0	0	0
3	U	9	0	0	0	0
3	V	2	0	0	0	0
3	W	5	0	0	0	0
3	X	2	0	0	0	0
All	All	17481	0	17220	203	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.

The worst 5 of 203 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:C:250:MET:HG2	1:C:267:LEU:HD11	1.40	1.03
1:I:250:MET:HG2	1:I:267:LEU:HD11	1.52	0.92
1:U:250:MET:HG2	1:U:267:LEU:HD11	1.67	0.77
1:A:253:VAL:HG21	1:A:267:LEU:HD21	1.68	0.75
1:E:188:GLU:HB2	1:E:194:LYS:HA	1.67	0.74

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	153/157 (98%)	141 (92%)	11 (7%)	1 (1%)	18	10
1	C	153/157 (98%)	141 (92%)	9 (6%)	3 (2%)	6	1
1	E	152/157 (97%)	144 (95%)	6 (4%)	2 (1%)	9	3
1	G	152/157 (97%)	142 (93%)	7 (5%)	3 (2%)	6	1
1	I	153/157 (98%)	148 (97%)	2 (1%)	3 (2%)	6	1
1	K	151/157 (96%)	142 (94%)	8 (5%)	1 (1%)	18	10
1	M	153/157 (98%)	142 (93%)	9 (6%)	2 (1%)	9	3
1	O	153/157 (98%)	148 (97%)	4 (3%)	1 (1%)	18	10
1	Q	152/157 (97%)	146 (96%)	2 (1%)	4 (3%)	4	0
1	S	152/157 (97%)	146 (96%)	5 (3%)	1 (1%)	18	10
1	U	149/157 (95%)	144 (97%)	5 (3%)	0	100	100
1	W	151/157 (96%)	144 (95%)	5 (3%)	2 (1%)	9	3
2	B	23/26 (88%)	19 (83%)	2 (9%)	2 (9%)	0	0
2	D	24/26 (92%)	22 (92%)	2 (8%)	0	100	100
2	F	24/26 (92%)	22 (92%)	1 (4%)	1 (4%)	2	0
2	H	24/26 (92%)	22 (92%)	1 (4%)	1 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	22/26 (85%)	20 (91%)	2 (9%)	0	100	100
2	L	24/26 (92%)	22 (92%)	1 (4%)	1 (4%)	2	0
2	N	24/26 (92%)	23 (96%)	0	1 (4%)	2	0
2	P	24/26 (92%)	22 (92%)	1 (4%)	1 (4%)	2	0
2	R	22/26 (85%)	22 (100%)	0	0	100	100
2	T	24/26 (92%)	22 (92%)	1 (4%)	1 (4%)	2	0
2	V	21/26 (81%)	19 (90%)	1 (5%)	1 (5%)	2	0
2	X	23/26 (88%)	21 (91%)	1 (4%)	1 (4%)	2	0
All	All	2103/2196 (96%)	1984 (94%)	86 (4%)	33 (2%)	7	2

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	323	ASP
1	M	197	LYS
2	N	3	VAL
1	Q	204	ALA
2	B	5	THR

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	136/136 (100%)	130 (96%)	6 (4%)	25	19
1	C	136/136 (100%)	134 (98%)	2 (2%)	57	58
1	E	135/136 (99%)	131 (97%)	4 (3%)	36	32
1	G	135/136 (99%)	131 (97%)	4 (3%)	36	32
1	I	136/136 (100%)	131 (96%)	5 (4%)	30	25
1	K	134/136 (98%)	129 (96%)	5 (4%)	30	25
1	M	136/136 (100%)	133 (98%)	3 (2%)	45	44
1	O	136/136 (100%)	131 (96%)	5 (4%)	30	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	135/136 (99%)	132 (98%)	3 (2%)	45	44
1	S	135/136 (99%)	130 (96%)	5 (4%)	30	25
1	U	132/136 (97%)	127 (96%)	5 (4%)	29	24
1	W	132/136 (97%)	127 (96%)	5 (4%)	29	24
2	B	22/23 (96%)	21 (96%)	1 (4%)	24	18
2	D	23/23 (100%)	23 (100%)	0	100	100
2	F	23/23 (100%)	20 (87%)	3 (13%)	4	1
2	H	23/23 (100%)	22 (96%)	1 (4%)	26	20
2	J	21/23 (91%)	20 (95%)	1 (5%)	23	16
2	L	23/23 (100%)	23 (100%)	0	100	100
2	N	22/23 (96%)	22 (100%)	0	100	100
2	P	23/23 (100%)	21 (91%)	2 (9%)	9	4
2	R	21/23 (91%)	19 (90%)	2 (10%)	8	3
2	T	23/23 (100%)	21 (91%)	2 (9%)	9	4
2	V	20/23 (87%)	19 (95%)	1 (5%)	22	15
2	X	22/23 (96%)	21 (96%)	1 (4%)	24	18
All	All	1884/1908 (99%)	1818 (96%)	66 (4%)	32	27

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	309	GLN
2	V	22	GLN
2	X	4	MET
1	I	323	ASP
1	I	321	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	223	ASN
1	Q	229	GLN
1	U	320	HIS
1	U	189	GLN
1	G	229	GLN

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	155/157 (98%)	-0.86	0 100 100	16, 31, 62, 79	0
1	C	155/157 (98%)	-0.94	0 100 100	15, 29, 60, 79	0
1	E	154/157 (98%)	-1.05	0 100 100	10, 26, 59, 72	0
1	G	154/157 (98%)	-1.10	0 100 100	9, 24, 51, 67	0
1	I	155/157 (98%)	-1.16	0 100 100	9, 24, 45, 69	0
1	K	153/157 (97%)	-1.13	0 100 100	10, 23, 57, 76	0
1	M	155/157 (98%)	-1.29	0 100 100	7, 16, 46, 71	0
1	O	155/157 (98%)	-1.28	0 100 100	6, 15, 40, 78	0
1	Q	154/157 (98%)	-1.17	0 100 100	9, 20, 51, 70	0
1	S	154/157 (98%)	-1.16	0 100 100	7, 19, 52, 73	0
1	U	151/157 (96%)	-1.11	0 100 100	9, 23, 54, 70	0
1	W	153/157 (97%)	-1.11	0 100 100	9, 24, 48, 66	0
2	B	25/26 (96%)	-0.70	0 100 100	21, 29, 69, 78	0
2	D	26/26 (100%)	-0.75	0 100 100	17, 28, 60, 72	0
2	F	26/26 (100%)	-0.40	0 100 100	17, 34, 73, 82	0
2	H	26/26 (100%)	-0.79	0 100 100	14, 26, 61, 66	0
2	J	24/26 (92%)	-0.89	0 100 100	15, 26, 62, 70	0
2	L	26/26 (100%)	-0.64	0 100 100	14, 29, 74, 79	0
2	N	26/26 (100%)	-0.98	0 100 100	8, 17, 77, 88	0
2	P	26/26 (100%)	-1.04	0 100 100	7, 13, 56, 62	0
2	R	24/26 (92%)	-0.92	0 100 100	13, 23, 58, 72	0
2	T	26/26 (100%)	-0.96	0 100 100	8, 21, 60, 71	0
2	V	23/26 (88%)	-0.85	0 100 100	16, 28, 48, 66	0
2	X	25/26 (96%)	-0.91	0 100 100	17, 25, 68, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2151/2196 (97%)	-1.07	0 100 100	6, 24, 59, 88	0

There are no RSRZ outliers to report.

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.