



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:15 pm BST

PDB ID : 6O3E  
Title : mouse aE-catenin 82-883  
Authors : Pokutta, S.; Weis, W.I.  
Deposited on : 2019-02-26  
Resolution : 4.00 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

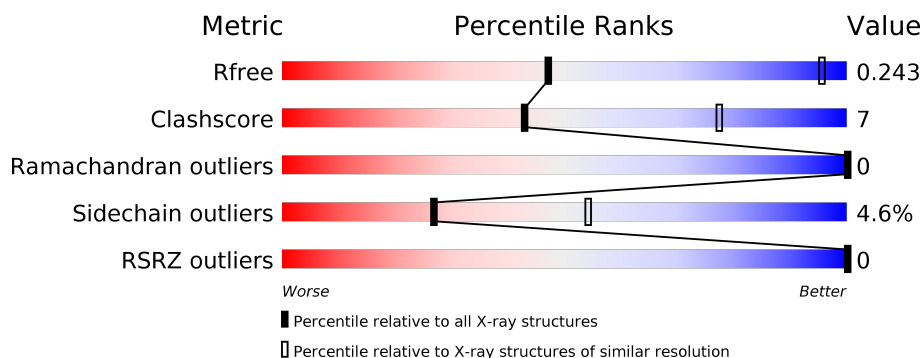
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	806	
1	B	806	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8070 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 Catenin alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4004	2485	707	793	19			
1	B	541	Total	C	N	O	S	0	0	0
			4066	2515	724	807	20			

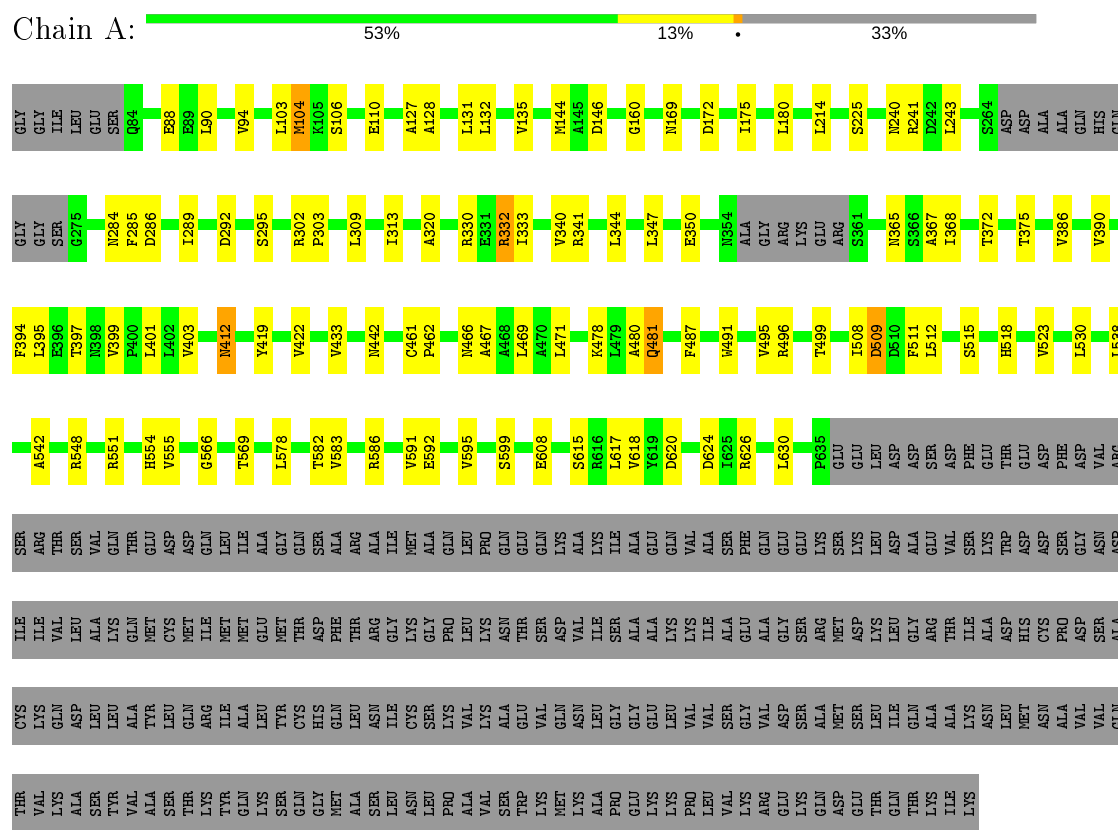
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	expression tag	UNP P26231
A	79	GLY	-	expression tag	UNP P26231
A	80	ILE	-	expression tag	UNP P26231
A	81	LEU	-	expression tag	UNP P26231
A	116	SER	CYS	engineered mutation	UNP P26231
B	78	GLY	-	expression tag	UNP P26231
B	79	GLY	-	expression tag	UNP P26231
B	80	ILE	-	expression tag	UNP P26231
B	81	LEU	-	expression tag	UNP P26231
B	116	SER	CYS	engineered mutation	UNP P26231

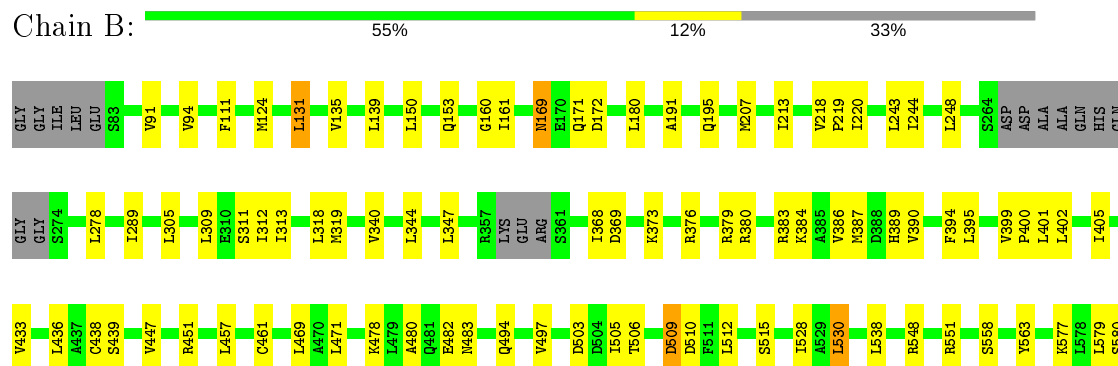
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Catenin alpha-1



#### • Molecule 1: Catenin alpha-1



LYS	LYS	VAL	SER	GLN	V583
MET	GLN	ASN	ASP	LYS	
LYS	ASN	VAL	VAL	ALA	P605
ALA	LEU	ILE	ILE	LYS	
PRO	GLY	SER	SER	ILE	F611
GLU	GLY	ALA	ALA	ALA	
LYS	GLU	LYS	LYS	GLN	L617
LYS	LYS	VAL	LYS	VAL	
PRO	VAL	VAL	ILE	ALA	G621
LEU	VAL	VAL	ILE	ALA	
VAL	VAL	SER	ALA	SER	R626
VAL	SER	GLY	GLU	PHE	
LYS	GLY	VAL	GLU	GLN	R633
ARG	GLU	ASP	GLY	GLU	T634
GLU	GLU	ASP	SER	GLU	P635
LYS	LYS	GLN	SER	LYS	
ASN	ALA	MET	ARG	LYS	GLU
ASP	ALA	ALA	MET	SER	
ASP	ASP	VAL	MET	SER	GLU
GLU	SER	SER	ASP	LYS	GLU
THR	LEU	LEU	LYS	LEU	LEU
GLN	ILE	ILE	LEU	ASP	ASP
THR	GLN	GLN	GLY	ALA	ASP
LYS	LYS	ALA	THR	GLU	SER
ILE	ALA	ALA	ARG	ALA	ASP
ILE	ALA	ALA	THR	VAL	ASP
LYS	LYS	LYS	ILE	SER	PHE
LYS	ASN	ASN	ALA	LYS	GLU
ASN	LEU	LEU	ALA	LYS	GLU
ASN	MET	MET	HIS	ASP	THR
ASN	MET	LYS	ASP	TRP	THR
ALA	ASN	ASN	CYS	ASP	ASP
VAL	ALA	ALA	PRO	SER	PHE
VAL	VAL	VAL	ASP	GLY	ASP
VAL	VAL	VAL	SER	ASN	VAL
LYS	GLN	GLN	ALA	ASP	ARG
ALA	THR	THR	CYS	ILE	SER
ALA	VAL	VAL	LYS	ILE	ARG
ALA	LYS	LYS	GLN	VAL	THR
ALA	ALA	ASP	LEU	VAL	SER
ALA	ALA	LEU	ASP	ALA	VAL
ALA	THR	LEU	LEU	ALA	VAL
ALA	THR	LEU	LEU	GLN	GLN
ALA	VAL	ALA	ALA	THR	THR
ALA	VAL	ALA	LYS	GLU	GLU
ALA	VAL	ALA	THR	MET	ASP
ALA	VAL	ALA	LYS	CYS	ASP
ALA	VAL	ALA	LYS	GLN	GLN
ALA	VAL	ALA	THR	THR	GLN
ALA	VAL	ALA	CYS	THR	SER
ALA	VAL	ALA	HIS	ASP	GLN
ALA	VAL	ALA	GLN	PHE	ALA
ALA	VAL	ALA	LEU	THR	ARG
ALA	VAL	ALA	ASN	ARG	ALA
ALA	VAL	ALA	ILE	GLY	ILE
ALA	VAL	ALA	CYS	LYS	MET
ALA	VAL	ALA	SER	GLY	ALA
ALA	VAL	ALA	LYS	PRO	GLN
ALA	VAL	ALA	VAL	LEU	LEU
ALA	VAL	ALA	LYS	LYS	PRO
ALA	VAL	ALA	LYS	ASN	GLN
ALA	VAL	ALA	THR	THR	GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.26Å 145.26Å 136.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 4.00 19.97 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.97-4.00) 97.9 (19.97-4.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 4.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.213 , 0.243 0.213 , 0.243	Depositor DCC
$R_{free}$ test set	1324 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	200.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 126.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l 0.053 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.25	0/4043	0.41	0/5486
1	B	0.25	0/4105	0.40	0/5566
All	All	0.25	0/8148	0.41	0/11052

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

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	4004	0	3922	62	0
1	B	4066	0	3988	50	0
All	All	8070	0	7910	109	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 7.

All (109) 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:B:376:ARG:HE	1:B:380:ARG:HH11	1.24	0.84
1:B:195:GLN:HB2	1:B:207:MET:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:TYR:OH	1:B:633:ARG:NH2	2.29	0.65
1:B:278:LEU:HD13	1:B:439:SER:HB3	1.78	0.64
1:A:243:LEU:HD21	1:A:462:PRO:HB2	1.81	0.61
1:A:467:ALA:HB2	1:A:487:PHE:HD2	1.66	0.60
1:A:509:ASP:N	1:A:509:ASP:OD1	2.33	0.60
1:A:530:LEU:HD12	1:A:538:LEU:HD21	1.85	0.59
1:A:160:GLY:HA3	1:A:180:LEU:HD11	1.88	0.56
1:A:530:LEU:HD21	1:A:608:GLU:HG2	1.86	0.56
1:B:389:HIS:HB3	1:B:433:VAL:HG13	1.86	0.56
1:B:509:ASP:N	1:B:509:ASP:OD1	2.38	0.55
1:A:592:GLU:HA	1:A:595:VAL:HG22	1.89	0.55
1:B:309:LEU:O	1:B:313:ILE:HG12	2.06	0.55
1:B:503:ASP:OD1	1:B:551:ARG:NH2	2.40	0.54
1:B:577:LYS:HA	1:B:580:SER:HB3	1.90	0.54
1:B:220:ILE:HG22	1:B:244:ILE:HG12	1.89	0.54
1:B:512:LEU:HD13	1:B:626:ARG:HA	1.90	0.54
1:B:379:ARG:O	1:B:383:ARG:HG3	2.09	0.53
1:A:511:PHE:HZ	1:A:551:ARG:HG3	1.73	0.53
1:A:542:ALA:HB2	1:A:591:VAL:HG21	1.89	0.53
1:A:135:VAL:HG11	1:B:131:LEU:HD21	1.91	0.53
1:B:218:VAL:HB	1:B:219:PRO:HD3	1.92	0.51
1:B:169:ASN:ND2	1:B:172:ASP:H	2.08	0.51
1:A:523:VAL:HG13	1:A:615:SER:HB3	1.93	0.51
1:A:401:LEU:HD22	1:A:491:TRP:CD1	2.46	0.50
1:B:150:LEU:HD11	1:B:191:ALA:HA	1.93	0.50
1:B:457:LEU:HD12	1:B:494:GLN:HB3	1.94	0.50
1:A:397:THR:HB	1:A:495:VAL:HG11	1.94	0.50
1:A:399:VAL:O	1:A:403:VAL:HG23	2.12	0.50
1:B:538:LEU:HD11	1:B:611:PHE:CZ	2.47	0.49
1:A:478:LYS:O	1:A:481:GLN:NE2	2.46	0.49
1:B:478:LYS:O	1:B:482:GLU:HG2	2.14	0.48
1:A:225:SER:HA	1:A:241:ARG:HD3	1.96	0.47
1:A:394:PHE:HD2	1:A:499:THR:HG23	1.79	0.47
1:A:412:ASN:OD1	1:A:412:ASN:N	2.46	0.47
1:A:478:LYS:HA	1:A:481:GLN:HE22	1.78	0.47
1:A:320:ALA:HB2	1:A:333:ILE:HG21	1.95	0.47
1:A:332:ARG:HD2	1:A:332:ARG:HA	1.50	0.47
1:B:438:CYS:SG	1:B:447:VAL:HG13	2.55	0.47
1:B:319:MET:HE2	1:B:436:LEU:HD22	1.97	0.46
1:A:372:THR:HA	1:A:375:THR:HG22	1.95	0.46
1:A:578:LEU:O	1:A:582:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:HG22	1:B:305:LEU:HD13	1.96	0.46
1:B:169:ASN:HD22	1:B:171:GLN:H	1.63	0.46
1:A:466:ASN:HA	1:A:469:LEU:HB2	1.98	0.46
1:B:309:LEU:HD11	1:B:340:VAL:HG13	1.98	0.46
1:B:634:THR:H	1:B:635:PRO:HD2	1.80	0.46
1:A:471:LEU:HD11	1:A:480:ALA:O	2.16	0.46
1:B:161:ILE:HD11	1:B:218:VAL:HG22	1.97	0.46
1:A:508:ILE:O	1:A:512:LEU:HG	2.15	0.46
1:A:309:LEU:HD11	1:A:340:VAL:HG13	1.98	0.45
1:B:579:LEU:HD12	1:B:621:GLY:HA3	1.98	0.45
1:A:394:PHE:HE1	1:A:433:VAL:HG11	1.81	0.45
1:B:399:VAL:H	1:B:400:PRO:HD2	1.81	0.45
1:A:309:LEU:O	1:A:313:ILE:HG12	2.16	0.45
1:A:582:THR:O	1:A:586:ARG:HG2	2.17	0.45
1:A:320:ALA:HB1	1:A:330:ARG:HB2	2.00	0.44
1:B:471:LEU:HA	1:B:480:ALA:HB1	2.00	0.44
1:A:419:TYR:HA	1:A:422:VAL:HG12	1.98	0.44
1:B:583:VAL:HG13	1:B:617:LEU:HG	2.00	0.44
1:A:620:ASP:O	1:A:624:ASP:HB2	2.18	0.44
1:A:286:ASP:OD1	1:A:375:THR:HG21	2.18	0.44
1:A:313:ILE:HG13	1:A:341:ARG:HH11	1.82	0.43
1:A:350:GLU:HG3	1:A:367:ALA:HB2	2.00	0.43
1:B:373:LYS:HD3	1:B:373:LYS:HA	1.68	0.43
1:B:161:ILE:HD13	1:B:180:LEU:HD21	1.99	0.43
1:A:615:SER:O	1:A:618:VAL:HG12	2.18	0.43
1:B:387:MET:HG3	1:B:510:ASP:HB3	2.00	0.43
1:B:530:LEU:HD13	1:B:611:PHE:CD2	2.54	0.43
1:A:88:GLU:HG2	1:A:88:GLU:H	1.61	0.43
1:A:285:PHE:HZ	1:A:344:LEU:HD12	1.84	0.43
1:A:386:VAL:O	1:A:390:VAL:HG23	2.19	0.43
1:A:467:ALA:HB2	1:A:487:PHE:CD2	2.51	0.43
1:A:496:ARG:HD2	1:A:554:HIS:NE2	2.34	0.43
1:A:104:MET:HA	1:A:127:ALA:HB1	2.01	0.42
1:A:313:ILE:HG13	1:A:341:ARG:NH1	2.33	0.42
1:B:494:GLN:HA	1:B:497:VAL:HG12	2.01	0.42
1:A:347:LEU:HD11	1:A:368:ILE:HG12	2.01	0.42
1:A:583:VAL:HG13	1:A:617:LEU:HB3	2.01	0.42
1:B:160:GLY:HA3	1:B:180:LEU:HD13	2.02	0.42
1:A:131:LEU:O	1:A:135:VAL:HG13	2.20	0.42
1:B:505:ILE:HG23	1:B:506:THR:HG23	2.01	0.42
1:A:292:ASP:OD2	1:A:295:SER:OG	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ARG:O	1:A:630:LEU:HG	2.19	0.42
1:A:285:PHE:O	1:A:289:ILE:HG23	2.20	0.42
1:A:128:ALA:HB3	1:B:139:LEU:HD21	2.00	0.42
1:B:401:LEU:O	1:B:405:ILE:HG23	2.20	0.42
1:A:106:SER:O	1:A:110:GLU:HG2	2.19	0.41
1:A:132:LEU:HB2	1:B:135:VAL:HG11	2.02	0.41
1:B:528:ILE:HA	1:B:528:ILE:HD13	1.85	0.41
1:A:169:ASN:HB2	1:A:172:ASP:H	1.84	0.41
1:B:451:ARG:HD2	1:B:451:ARG:HA	1.89	0.41
1:A:461:CYS:HB3	1:A:462:PRO:HD3	2.03	0.41
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.84	0.41
1:A:309:LEU:HB2	1:A:344:LEU:HD13	2.03	0.41
1:A:240:ASN:HA	1:A:466:ASN:HD22	1.84	0.41
1:B:111:PHE:HB3	1:B:124:MET:HE3	2.01	0.41
1:B:213:ILE:HD13	1:B:213:ILE:HA	1.95	0.41
1:A:90:LEU:O	1:A:94:VAL:HG23	2.20	0.41
1:B:390:VAL:O	1:B:394:PHE:HB2	2.21	0.41
1:B:402:LEU:HA	1:B:405:ILE:HG12	2.03	0.41
1:B:91:VAL:O	1:B:94:VAL:HG12	2.20	0.41
1:B:309:LEU:HD22	1:B:344:LEU:HD22	2.03	0.41
1:A:511:PHE:CE2	1:A:555:VAL:HG11	2.55	0.41
1:A:595:VAL:O	1:A:599:SER:HB3	2.21	0.40
1:A:566:GLY:H	1:A:569:THR:HB	1.86	0.40
1:B:395:LEU:HD11	1:B:548:ARG:HG3	2.03	0.40
1:A:302:ARG:N	1:A:303:PRO:HD2	2.37	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	530/806 (66%)	508 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	535/806 (66%)	511 (96%)	24 (4%)	0	100	100
All	All	1065/1612 (66%)	1019 (96%)	46 (4%)	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	413/675 (61%)	396 (96%)	17 (4%)	30	57
1	B	422/675 (62%)	401 (95%)	21 (5%)	24	52
All	All	835/1350 (62%)	797 (95%)	38 (5%)	27	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	104	MET
1	A	144	MET
1	A	146	ASP
1	A	175	ILE
1	A	214	LEU
1	A	284	ASN
1	A	332	ARG
1	A	365	ASN
1	A	395	LEU
1	A	412	ASN
1	A	442	ASN
1	A	481	GLN
1	A	509	ASP
1	A	515	SER
1	A	518	HIS
1	A	548	ARG
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	153	GLN
1	B	169	ASN
1	B	243	LEU
1	B	248	LEU
1	B	311	SER
1	B	312	ILE
1	B	318	LEU
1	B	347	LEU
1	B	368	ILE
1	B	369	ASP
1	B	384	LYS
1	B	386	VAL
1	B	461	CYS
1	B	469	LEU
1	B	483	ASN
1	B	509	ASP
1	B	515	SER
1	B	530	LEU
1	B	558	SER
1	B	605	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	230	GLN
1	A	381	GLN
1	A	481	GLN
1	A	483	ASN
1	A	490	GLN
1	B	153	GLN
1	B	169	ASN
1	B	230	GLN
1	B	481	GLN
1	B	490	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	536/806 (66%)	-0.71	0 100 100	153, 204, 280, 494	0
1	B	541/806 (67%)	-0.68	0 100 100	147, 202, 269, 461	0
All	All	1077/1612 (66%)	-0.69	0 100 100	147, 203, 273, 494	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 carbohydrates 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.