



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:41 PM GMT

PDB ID : 4MFU
Title : Crystal structure of human CTNNBL1(residues 77 563)
Authors : Ahn, J.W.; Kim, S.; Kim, K.J.
Deposited on : 2013-08-28
Resolution : 2.74 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

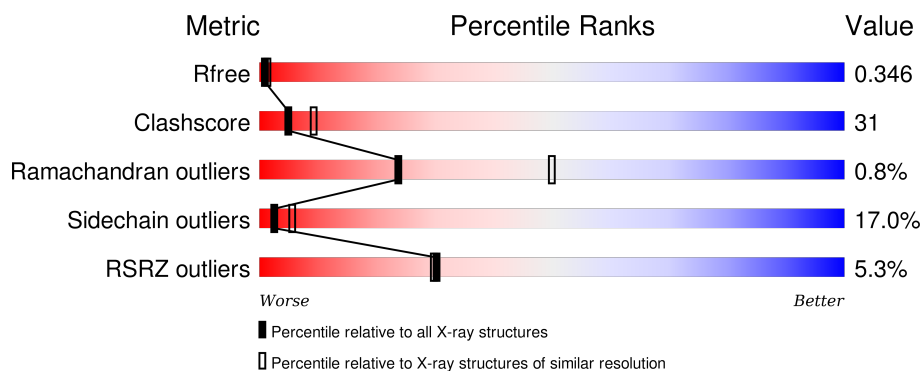
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.74 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}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	490	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3917 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.

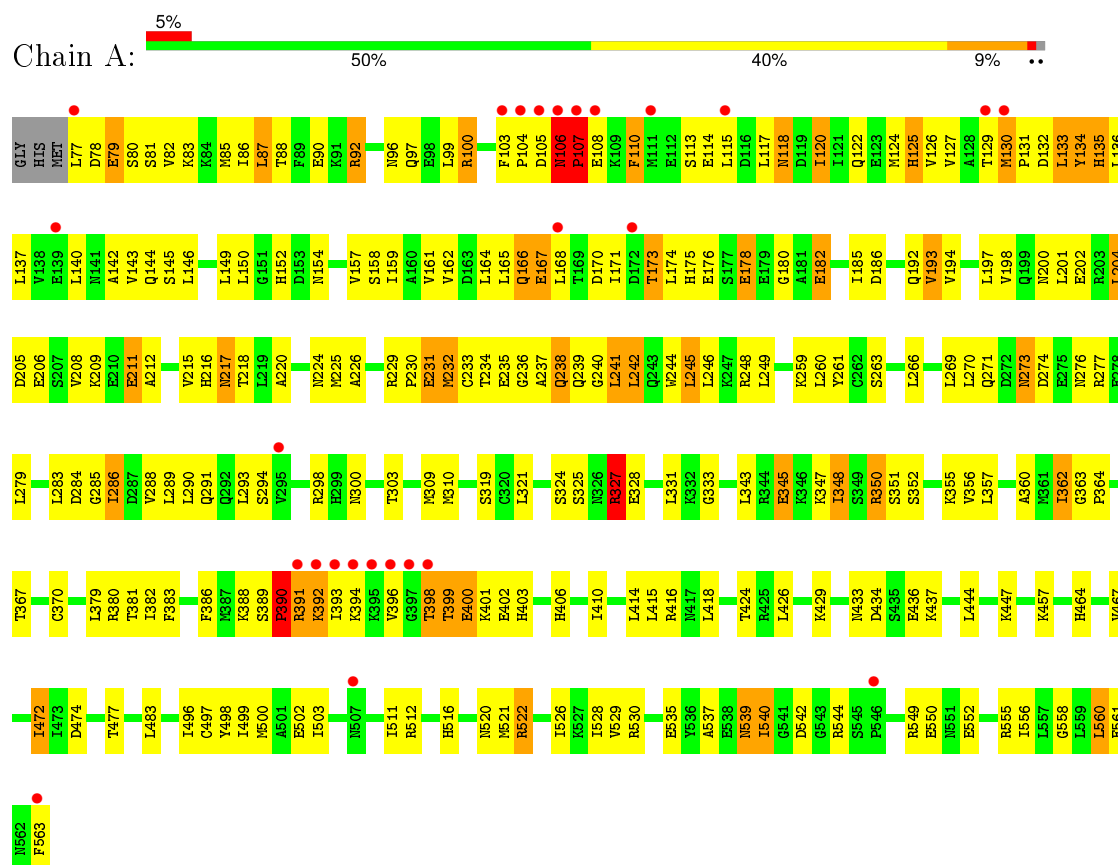
- Molecule 1 is a protein called Beta-catenin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3917	2456	684	750	27	0	0	0

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 errors 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: Beta-catenin-like protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.15Å 90.15Å 178.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.33 – 2.74 47.33 – 2.74	Depositor EDS
% Data completeness (in resolution range)	95.9 (47.33-2.74) 95.9 (47.33-2.74)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.247 , 0.319 0.295 , 0.346	Depositor DCC
R_{free} test set	1114 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.8	EDS
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 21745 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3917	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.60	1/3968 (0.0%)	0.79	4/5334 (0.1%)

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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	PRO	N-CD	5.40	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ASN	C-N-CD	6.36	141.75	128.40
1	A	389	SER	C-N-CD	5.54	140.04	128.40
1	A	327	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	107	PRO	CA-N-CD	-5.05	104.43	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	LYS	Peptide
1	A	539	ASN	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	3917	0	3959	246	0
All	All	3917	0	3959	246	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 31.

All (246) 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:A:135:HIS:NE2	1:A:136:LEU:HD13	1.56	1.18
1:A:521:MET:HA	1:A:522:ARG:CG	1.79	1.12
1:A:392:LYS:HA	1:A:393:ILE:HG13	1.26	1.11
1:A:135:HIS:CD2	1:A:136:LEU:H	1.69	1.10
1:A:103:PHE:HD2	1:A:110:PHE:HB3	1.10	1.10
1:A:230:PRO:C	1:A:231:GLU:OE1	1.90	1.09
1:A:135:HIS:CD2	1:A:136:LEU:HD13	1.89	1.08
1:A:103:PHE:CD2	1:A:110:PHE:HB3	1.89	1.07
1:A:135:HIS:NE2	1:A:136:LEU:CD1	2.18	1.05
1:A:231:GLU:OE1	1:A:231:GLU:N	1.91	1.04
1:A:279:LEU:O	1:A:283:LEU:HD12	1.58	1.03
1:A:135:HIS:CD2	1:A:136:LEU:N	2.25	1.03
1:A:521:MET:CA	1:A:522:ARG:HG3	1.89	1.01
1:A:135:HIS:HD2	1:A:136:LEU:N	1.58	0.98
1:A:178:GLU:OE2	1:A:178:GLU:N	1.98	0.95
1:A:244:TRP:CH2	1:A:248:ARG:HG3	2.04	0.93
1:A:135:HIS:CD2	1:A:136:LEU:CD1	2.54	0.90
1:A:537:ALA:O	1:A:540:ILE:HB	1.73	0.89
1:A:521:MET:HA	1:A:522:ARG:HG3	0.94	0.88
1:A:392:LYS:HA	1:A:393:ILE:CG1	2.08	0.84
1:A:135:HIS:HD2	1:A:136:LEU:H	0.83	0.83
1:A:392:LYS:CA	1:A:393:ILE:HG13	2.07	0.81
1:A:158:SER:HB3	1:A:200:ASN:HD21	1.44	0.81
1:A:82:VAL:O	1:A:85:MET:HB2	1.81	0.81
1:A:390:PRO:HB2	1:A:391:ARG:HA	1.63	0.80
1:A:105:ASP:O	1:A:106:ASN:HB2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:CYS:O	1:A:237:ALA:HB2	1.81	0.79
1:A:289:LEU:O	1:A:293:LEU:HD12	1.83	0.79
1:A:520:ASN:O	1:A:522:ARG:HA	1.80	0.78
1:A:103:PHE:HD2	1:A:110:PHE:CB	1.93	0.78
1:A:540:ILE:HD11	1:A:552:GLU:HB3	1.63	0.78
1:A:244:TRP:CZ3	1:A:248:ARG:HG3	2.19	0.77
1:A:392:LYS:N	1:A:393:ILE:HA	1.98	0.76
1:A:232:MET:SD	1:A:233:CYS:N	2.59	0.76
1:A:406:HIS:O	1:A:410:ILE:HG13	1.85	0.76
1:A:298:ARG:HG2	1:A:345:GLU:OE1	1.87	0.75
1:A:472:ILE:H	1:A:472:ILE:HD13	1.52	0.74
1:A:390:PRO:HB2	1:A:391:ARG:CA	2.17	0.74
1:A:503:ILE:HB	1:A:511:ILE:HD12	1.71	0.73
1:A:134:TYR:HB2	1:A:180:GLY:CA	2.19	0.73
1:A:170:ASP:O	1:A:173:THR:HB	1.90	0.72
1:A:242:LEU:O	1:A:242:LEU:HD12	1.90	0.71
1:A:291:GLN:O	1:A:294:SER:HB3	1.92	0.70
1:A:232:MET:HE2	1:A:233:CYS:HA	1.74	0.70
1:A:520:ASN:C	1:A:522:ARG:HA	2.12	0.69
1:A:537:ALA:O	1:A:540:ILE:CG2	2.39	0.69
1:A:390:PRO:HB2	1:A:391:ARG:CG	2.21	0.69
1:A:192:GLN:OE1	1:A:239:GLN:NE2	2.25	0.69
1:A:152:HIS:CG	1:A:157:VAL:HG11	2.28	0.68
1:A:399:THR:HG22	1:A:400:GLU:HA	1.75	0.68
1:A:232:MET:CE	1:A:233:CYS:HA	2.24	0.67
1:A:126:VAL:O	1:A:129:THR:HG22	1.94	0.67
1:A:540:ILE:O	1:A:540:ILE:HD13	1.95	0.67
1:A:364:PRO:O	1:A:367:THR:HB	1.95	0.67
1:A:124:MET:HA	1:A:127:VAL:HG23	1.77	0.67
1:A:537:ALA:O	1:A:540:ILE:CB	2.42	0.67
1:A:197:LEU:HD22	1:A:218:THR:HG23	1.76	0.67
1:A:348:ILE:O	1:A:348:ILE:HD13	1.96	0.66
1:A:83:LYS:O	1:A:86:ILE:HG22	1.94	0.66
1:A:415:LEU:HB3	1:A:502:GLU:HG2	1.78	0.66
1:A:401:LYS:O	1:A:402:GLU:C	2.33	0.65
1:A:204:LEU:HD23	1:A:211:GLU:HG3	1.78	0.65
1:A:226:ALA:O	1:A:230:PRO:HG3	1.97	0.65
1:A:110:PHE:H	1:A:110:PHE:HD1	1.42	0.64
1:A:540:ILE:CD1	1:A:552:GLU:HB3	2.26	0.64
1:A:164:LEU:O	1:A:168:LEU:HD12	1.97	0.64
1:A:350:ARG:HH22	1:A:390:PRO:HG3	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:CYS:O	1:A:237:ALA:CB	2.45	0.64
1:A:152:HIS:ND1	1:A:157:VAL:HG11	2.13	0.63
1:A:348:ILE:HD13	1:A:348:ILE:C	2.18	0.63
1:A:92:ARG:O	1:A:117:LEU:HD13	1.99	0.63
1:A:235:GLU:O	1:A:239:GLN:HG3	1.99	0.63
1:A:92:ARG:O	1:A:117:LEU:CD1	2.46	0.62
1:A:496:ILE:HA	1:A:499:ILE:HD12	1.81	0.62
1:A:390:PRO:CB	1:A:391:ARG:HA	2.23	0.62
1:A:145:SER:O	1:A:149:LEU:HD13	1.99	0.61
1:A:194:VAL:O	1:A:198:VAL:HG23	1.99	0.61
1:A:273:ASN:ND2	1:A:276:ASN:HD22	1.98	0.61
1:A:122:GLN:O	1:A:125:HIS:HB2	2.00	0.60
1:A:530:ARG:HD3	1:A:560:LEU:HD21	1.82	0.60
1:A:164:LEU:CD2	1:A:168:LEU:HD11	2.33	0.59
1:A:92:ARG:C	1:A:117:LEU:HD13	2.23	0.59
1:A:540:ILE:HD11	1:A:552:GLU:CB	2.32	0.59
1:A:96:ASN:ND2	1:A:114:GLU:HA	2.18	0.59
1:A:118:ASN:OD1	1:A:118:ASN:C	2.41	0.58
1:A:274:ASP:HA	1:A:277:ARG:HD2	1.86	0.58
1:A:170:ASP:O	1:A:173:THR:CB	2.51	0.58
1:A:208:VAL:HB	1:A:211:GLU:HB2	1.85	0.58
1:A:105:ASP:O	1:A:106:ASN:CB	2.52	0.58
1:A:540:ILE:HG13	1:A:556:ILE:HD12	1.86	0.58
1:A:327:ARG:NH2	1:A:362:ILE:HG22	2.19	0.57
1:A:279:LEU:O	1:A:283:LEU:CD1	2.45	0.57
1:A:135:HIS:CD2	1:A:136:LEU:HD12	2.40	0.57
1:A:231:GLU:O	1:A:234:THR:HG22	2.05	0.56
1:A:429:LYS:O	1:A:437:LYS:HG3	2.05	0.55
1:A:383:PHE:O	1:A:386:PHE:HB3	2.05	0.55
1:A:540:ILE:HD11	1:A:552:GLU:HG2	1.89	0.55
1:A:234:THR:HB	1:A:273:ASN:OD1	2.07	0.55
1:A:220:ALA:O	1:A:224:ASN:OD1	2.25	0.55
1:A:286:ILE:HD12	1:A:286:ILE:N	2.22	0.55
1:A:134:TYR:HB2	1:A:180:GLY:HA2	1.87	0.54
1:A:390:PRO:HB2	1:A:391:ARG:HG3	1.87	0.54
1:A:232:MET:CE	1:A:233:CYS:CA	2.86	0.54
1:A:260:LEU:O	1:A:263:SER:HB3	2.07	0.54
1:A:143:VAL:O	1:A:146:LEU:HB2	2.08	0.54
1:A:154:ASN:O	1:A:157:VAL:CG1	2.56	0.53
1:A:158:SER:HB3	1:A:200:ASN:ND2	2.18	0.53
1:A:244:TRP:CH2	1:A:248:ARG:CG	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:O	1:A:429:LYS:HB2	2.08	0.53
1:A:107:PRO:O	1:A:110:PHE:CE1	2.62	0.53
1:A:327:ARG:HH22	1:A:362:ILE:HG22	1.73	0.53
1:A:474:ASP:HB3	1:A:477:THR:OG1	2.09	0.53
1:A:96:ASN:HB2	1:A:117:LEU:HD12	1.91	0.53
1:A:537:ALA:C	1:A:540:ILE:HB	2.29	0.53
1:A:79:GLU:O	1:A:80:SER:HB2	2.08	0.53
1:A:204:LEU:HD23	1:A:211:GLU:CG	2.39	0.53
1:A:540:ILE:HD11	1:A:552:GLU:CG	2.38	0.52
1:A:171:ILE:O	1:A:174:LEU:HB2	2.10	0.52
1:A:503:ILE:O	1:A:511:ILE:HD11	2.10	0.52
1:A:130:MET:O	1:A:131:PRO:C	2.47	0.51
1:A:146:LEU:HD22	1:A:161:VAL:HG13	1.92	0.51
1:A:178:GLU:O	1:A:182:GLU:HB2	2.10	0.51
1:A:521:MET:N	1:A:522:ARG:HA	2.24	0.51
1:A:233:CYS:SG	1:A:234:THR:N	2.84	0.51
1:A:212:ALA:O	1:A:215:VAL:HG22	2.11	0.51
1:A:225:MET:HE1	1:A:232:MET:HG3	1.92	0.51
1:A:331:LEU:O	1:A:331:LEU:HD23	2.10	0.51
1:A:393:ILE:HG22	1:A:394:LYS:N	2.26	0.51
1:A:436:GLU:HG3	1:A:437:LYS:HD3	1.92	0.51
1:A:234:THR:HG23	1:A:235:GLU:H	1.74	0.50
1:A:327:ARG:NH2	1:A:363:GLY:H	2.09	0.50
1:A:117:LEU:N	1:A:117:LEU:HD23	2.26	0.50
1:A:110:PHE:N	1:A:110:PHE:CD1	2.74	0.50
1:A:150:LEU:CD1	1:A:161:VAL:HG11	2.41	0.50
1:A:229:ARG:O	1:A:231:GLU:N	2.41	0.49
1:A:379:LEU:HA	1:A:382:ILE:HG22	1.94	0.49
1:A:134:TYR:CB	1:A:180:GLY:O	2.60	0.49
1:A:194:VAL:HG11	1:A:236:GLY:O	2.13	0.48
1:A:526:ILE:O	1:A:529:VAL:HB	2.13	0.48
1:A:289:LEU:C	1:A:293:LEU:HD12	2.34	0.48
1:A:415:LEU:HD11	1:A:499:ILE:HG23	1.94	0.48
1:A:414:LEU:HD22	1:A:418:LEU:HD11	1.95	0.48
1:A:208:VAL:O	1:A:211:GLU:N	2.47	0.48
1:A:270:LEU:O	1:A:271:GLN:C	2.52	0.48
1:A:122:GLN:O	1:A:125:HIS:CB	2.61	0.48
1:A:321:LEU:HD21	1:A:360:ALA:HB2	1.96	0.47
1:A:154:ASN:O	1:A:157:VAL:HG12	2.15	0.47
1:A:343:LEU:HD23	1:A:381:THR:HG22	1.96	0.47
1:A:96:ASN:HB2	1:A:117:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:HG23	1:A:235:GLU:N	2.28	0.47
1:A:500:MET:O	1:A:503:ILE:HG12	2.15	0.47
1:A:415:LEU:CD1	1:A:499:ILE:HG23	2.44	0.47
1:A:233:CYS:O	1:A:237:ALA:N	2.47	0.47
1:A:351:SER:OG	1:A:398:THR:HB	2.15	0.47
1:A:146:LEU:CD2	1:A:161:VAL:HG13	2.44	0.47
1:A:164:LEU:HD23	1:A:168:LEU:HD11	1.97	0.47
1:A:78:ASP:HB3	1:A:81:SER:OG	2.14	0.47
1:A:100:ARG:HD2	1:A:110:PHE:HE2	1.80	0.47
1:A:82:VAL:HA	1:A:85:MET:HG3	1.96	0.47
1:A:193:VAL:HG22	1:A:197:LEU:HD12	1.97	0.47
1:A:133:LEU:O	1:A:135:HIS:HD2	1.97	0.47
1:A:104:PRO:O	1:A:107:PRO:HG3	2.14	0.47
1:A:208:VAL:O	1:A:209:LYS:C	2.54	0.47
1:A:143:VAL:HG13	1:A:144:GLN:N	2.30	0.47
1:A:472:ILE:H	1:A:472:ILE:CD1	2.26	0.47
1:A:288:VAL:O	1:A:289:LEU:C	2.53	0.46
1:A:234:THR:HA	1:A:276:ASN:HD21	1.81	0.46
1:A:464:HIS:O	1:A:467:VAL:HG22	2.14	0.46
1:A:393:ILE:CG2	1:A:394:LYS:N	2.79	0.46
1:A:232:MET:C	1:A:232:MET:SD	2.94	0.46
1:A:242:LEU:C	1:A:242:LEU:HD12	2.36	0.46
1:A:158:SER:O	1:A:161:VAL:N	2.47	0.46
1:A:193:VAL:HG13	1:A:194:VAL:N	2.32	0.45
1:A:82:VAL:O	1:A:85:MET:N	2.49	0.45
1:A:198:VAL:O	1:A:202:GLU:N	2.49	0.45
1:A:390:PRO:HB2	1:A:391:ARG:CB	2.46	0.45
1:A:217:ASN:HD22	1:A:217:ASN:N	2.15	0.45
1:A:399:THR:CG2	1:A:400:GLU:HA	2.46	0.45
1:A:124:MET:CA	1:A:127:VAL:HG23	2.45	0.45
1:A:300:ASN:CG	1:A:348:ILE:HG22	2.37	0.45
1:A:537:ALA:O	1:A:540:ILE:HG21	2.15	0.45
1:A:97:GLN:NE2	1:A:97:GLN:HA	2.31	0.45
1:A:238:GLN:HE21	1:A:238:GLN:HB2	1.65	0.44
1:A:82:VAL:O	1:A:85:MET:CB	2.61	0.44
1:A:300:ASN:OD1	1:A:348:ILE:HG22	2.17	0.44
1:A:165:LEU:HA	1:A:168:LEU:HD13	1.99	0.44
1:A:185:ILE:O	1:A:186:ASP:C	2.56	0.44
1:A:157:VAL:O	1:A:161:VAL:HG23	2.18	0.44
1:A:331:LEU:C	1:A:331:LEU:HD23	2.38	0.44
1:A:140:LEU:N	1:A:140:LEU:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PHE:CD2	1:A:110:PHE:CB	2.79	0.44
1:A:215:VAL:HG23	1:A:216:HIS:N	2.33	0.44
1:A:309:MET:O	1:A:310:MET:C	2.56	0.44
1:A:133:LEU:O	1:A:135:HIS:CD2	2.70	0.44
1:A:416:ARG:CB	1:A:498:TYR:OH	2.66	0.43
1:A:497:CYS:O	1:A:500:MET:HB3	2.18	0.43
1:A:331:LEU:O	1:A:333:GLY:O	2.36	0.43
1:A:394:LYS:O	1:A:396:VAL:O	2.36	0.43
1:A:539:ASN:C	1:A:540:ILE:HG22	2.38	0.43
1:A:159:ILE:HA	1:A:162:VAL:CG1	2.49	0.43
1:A:104:PRO:O	1:A:107:PRO:HD3	2.18	0.43
1:A:238:GLN:HG3	1:A:239:GLN:N	2.32	0.43
1:A:540:ILE:O	1:A:540:ILE:HG23	2.18	0.43
1:A:558:GLY:O	1:A:561:GLU:HG2	2.19	0.43
1:A:392:LYS:N	1:A:393:ILE:CA	2.78	0.43
1:A:124:MET:O	1:A:127:VAL:HG23	2.19	0.43
1:A:124:MET:O	1:A:127:VAL:N	2.32	0.43
1:A:236:GLY:HA2	1:A:239:GLN:HG3	2.00	0.42
1:A:552:GLU:O	1:A:555:ARG:N	2.52	0.42
1:A:512:ARG:O	1:A:516:HIS:HD2	2.01	0.42
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.74	0.42
1:A:193:VAL:HG22	1:A:197:LEU:CD1	2.49	0.42
1:A:241:LEU:HD12	1:A:245:LEU:HD13	2.00	0.42
1:A:159:ILE:HA	1:A:162:VAL:HG12	2.01	0.42
1:A:520:ASN:O	1:A:522:ARG:CG	2.67	0.42
1:A:92:ARG:HE	1:A:120:ILE:HD12	1.85	0.42
1:A:215:VAL:CG2	1:A:216:HIS:N	2.83	0.42
1:A:416:ARG:NH1	1:A:552:GLU:OE1	2.45	0.42
1:A:170:ASP:O	1:A:173:THR:HG22	2.19	0.42
1:A:134:TYR:HB2	1:A:180:GLY:C	2.39	0.41
1:A:521:MET:HA	1:A:522:ARG:CB	2.41	0.41
1:A:238:GLN:O	1:A:239:GLN:C	2.58	0.41
1:A:530:ARG:NH2	1:A:563:PHE:O	2.53	0.41
1:A:170:ASP:O	1:A:173:THR:CG2	2.68	0.41
1:A:249:LEU:O	1:A:259:LYS:NZ	2.53	0.41
1:A:433:ASN:O	1:A:434:ASP:CB	2.68	0.41
1:A:166:GLN:CG	1:A:167:GLU:N	2.83	0.41
1:A:401:LYS:O	1:A:403:HIS:N	2.53	0.41
1:A:436:GLU:HG3	1:A:437:LYS:N	2.34	0.41
1:A:83:LYS:O	1:A:87:LEU:HD12	2.20	0.41
1:A:88:THR:HG22	1:A:92:ARG:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD12	1:A:215:VAL:HG12	2.03	0.41
1:A:290:LEU:O	1:A:294:SER:N	2.53	0.41
1:A:291:GLN:HA	1:A:294:SER:HB2	2.02	0.41
1:A:530:ARG:CD	1:A:560:LEU:HD21	2.50	0.41
1:A:560:LEU:O	1:A:560:LEU:HD23	2.20	0.41
1:A:356:VAL:O	1:A:357:LEU:C	2.57	0.41
1:A:352:SER:O	1:A:355:LYS:N	2.53	0.41
1:A:392:LYS:C	1:A:393:ILE:HG13	2.41	0.41
1:A:100:ARG:NE	1:A:114:GLU:OE2	2.54	0.41
1:A:198:VAL:HG21	1:A:241:LEU:N	2.36	0.41
1:A:370:CYS:HB3	1:A:414:LEU:HD23	2.02	0.41
1:A:154:ASN:O	1:A:157:VAL:HG13	2.21	0.40
1:A:285:GLY:O	1:A:288:VAL:HB	2.21	0.40
1:A:77:LEU:HA	1:A:78:ASP:HA	1.89	0.40
1:A:137:LEU:O	1:A:142:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	485/490 (99%)	433 (89%)	48 (10%)	4 (1%)	24	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	240	GLY
1	A	107	PRO
1	A	193	VAL

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	440/442 (100%)	365 (83%)	75 (17%)	2 5

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	87	LEU
1	A	90	GLU
1	A	92	ARG
1	A	99	LEU
1	A	100	ARG
1	A	108	GLU
1	A	110	PHE
1	A	113	SER
1	A	115	LEU
1	A	118	ASN
1	A	120	ILE
1	A	125	HIS
1	A	130	MET
1	A	132	ASP
1	A	133	LEU
1	A	134	TYR
1	A	135	HIS
1	A	166	GLN
1	A	167	GLU
1	A	173	THR
1	A	175	HIS
1	A	176	GLU
1	A	178	GLU
1	A	182	GLU
1	A	204	LEU
1	A	205	ASP
1	A	206	GLU
1	A	211	GLU
1	A	217	ASN

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Mol	Chain	Res	Type
1	A	231	GLU
1	A	232	MET
1	A	238	GLN
1	A	241	LEU
1	A	242	LEU
1	A	245	LEU
1	A	261	TYR
1	A	266	LEU
1	A	269	LEU
1	A	273	ASN
1	A	284	ASP
1	A	286	ILE
1	A	303	THR
1	A	319	SER
1	A	324	SER
1	A	325	SER
1	A	327	ARG
1	A	328	GLU
1	A	345	GLU
1	A	348	ILE
1	A	350	ARG
1	A	362	ILE
1	A	380	ARG
1	A	388	LYS
1	A	390	PRO
1	A	391	ARG
1	A	392	LYS
1	A	398	THR
1	A	399	THR
1	A	400	GLU
1	A	424	THR
1	A	444	LEU
1	A	447	LYS
1	A	457	LYS
1	A	472	ILE
1	A	483	LEU
1	A	522	ARG
1	A	528	ILE
1	A	535	GLU
1	A	540	ILE
1	A	542	ASP
1	A	544	ARG

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Mol	Chain	Res	Type
1	A	549	ARG
1	A	550	GLU
1	A	560	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	97	GLN
1	A	122	GLN
1	A	135	HIS
1	A	166	GLN
1	A	200	ASN
1	A	217	ASN
1	A	238	GLN
1	A	273	ASN
1	A	513	GLN
1	A	516	HIS
1	A	539	ASN
1	A	562	ASN

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 carbohydrates 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	487/490 (99%)	0.30	26 (5%) 30 30	24, 81, 129, 182	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	VAL	7.3
1	A	395	LYS	7.1
1	A	105	ASP	6.9
1	A	106	ASN	5.3
1	A	393	ILE	5.0
1	A	129	THR	4.1
1	A	398	THR	3.8
1	A	130	MET	3.7
1	A	107	PRO	3.4
1	A	397	GLY	3.3
1	A	108	GLU	3.0
1	A	295	VAL	2.8
1	A	563	PHE	2.8
1	A	172	ASP	2.8
1	A	77	LEU	2.4
1	A	139	GLU	2.4
1	A	104	PRO	2.4
1	A	115	LEU	2.3
1	A	391	ARG	2.3
1	A	168	LEU	2.3
1	A	392	LYS	2.3
1	A	103	PHE	2.1
1	A	507	ASN	2.1
1	A	394	LYS	2.1
1	A	546	PRO	2.1
1	A	111	MET	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 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.