



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:47 AM UTC

PDB ID : 4MFU / pdb_00004mfu
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

<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

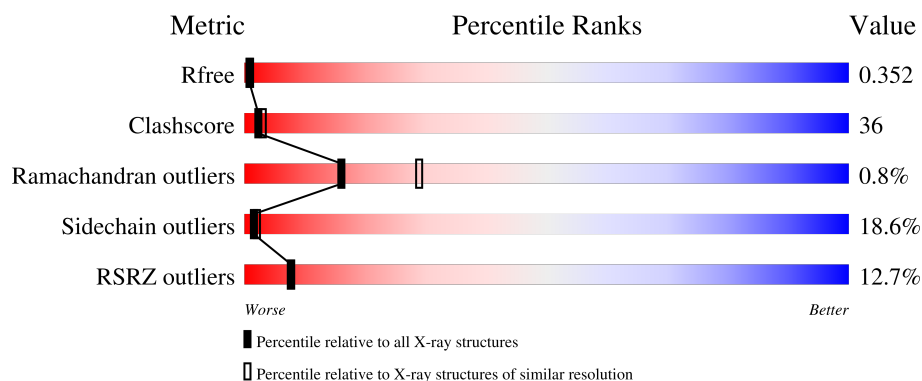
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	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 [i](#)

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: 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	Depositor
R, R_{free}	0.247 , 0.319 0.295 , 0.352	Depositor DCC
R_{free} test set	1114 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	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, 0.333 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	0.82	1/3968 (0.0%)	1.12	21/5334 (0.4%)

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	5.47	1.55	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	MET	N-CA-C	8.77	120.84	111.28
1	A	247	LYS	N-CA-C	7.47	119.07	111.07
1	A	247	LYS	CA-C-N	6.79	129.69	120.38
1	A	247	LYS	C-N-CA	6.79	129.69	120.38
1	A	221	ILE	CB-CA-C	-6.76	103.23	111.88
1	A	218	THR	N-CA-C	-6.60	103.78	110.97
1	A	287	ASP	N-CA-C	-5.97	104.68	111.07
1	A	81	SER	N-CA-C	-5.95	104.87	111.71
1	A	372	LYS	N-CA-C	-5.79	105.05	111.36
1	A	133	LEU	N-CA-C	-5.72	103.56	110.88
1	A	242	LEU	N-CA-C	-5.65	105.12	111.28
1	A	333	GLY	N-CA-C	-5.42	105.15	112.14
1	A	107	PRO	CA-N-CD	-5.41	104.43	112.00
1	A	242	LEU	CA-C-N	-5.41	113.41	120.44
1	A	242	LEU	C-N-CA	-5.41	113.41	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	GLU	N-CA-C	-5.36	105.44	111.28
1	A	127	VAL	CB-CA-C	-5.29	104.99	112.14
1	A	305	GLU	N-CA-C	-5.23	104.50	112.04
1	A	106	ASN	CA-C-N	-5.06	113.52	119.84
1	A	106	ASN	C-N-CA	-5.06	113.52	119.84
1	A	362	ILE	N-CA-C	5.00	115.22	110.42

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	283	0
All	All	3917	0	3959	283	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 36.

All (283) 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:230:PRO:C	1:A:231:GLU:OE1	1.90	1.14
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:178:GLU:OE2	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:232:MET:HE2	1:A:233:CYS:HA	1.62	0.82
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:225:MET:HE2	1:A:232:MET:HG3	1.62	0.79
1:A:105:ASP:O	1:A:106:ASN:HB2	1.81	0.79
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:442:MET:HE1	1:A:500:MET:HE2	1.67	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:520:ASN:C	1:A:522:ARG:HA	2.12	0.74
1:A:472:ILE:HD13	1:A:472:ILE:H	1.52	0.74
1:A:390:PRO:HB2	1:A:391:ARG:CA	2.17	0.74
1:A:134:TYR:HB2	1:A:180:GLY:CA	2.19	0.73
1:A:503:ILE:HB	1:A:511:ILE:HD12	1.71	0.73
1:A:170:ASP:O	1:A:173:THR:HB	1.90	0.72
1:A:242:LEU:HD12	1:A:242:LEU:O	1.90	0.71
1:A:291:GLN:O	1:A:294:SER:HB3	1.92	0.70
1:A:401:LYS:O	1:A:402:GLU:C	2.33	0.70
1:A:537:ALA:O	1:A:540:ILE:CG2	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:452:MET:HE1	1:A:485:ARG:HG2	1.74	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:126:VAL:O	1:A:129:THR:HG22	1.94	0.67
1:A:232:MET:CE	1:A:233:CYS:HA	2.24	0.67
1:A:348:ILE:C	1:A:348:ILE:HD13	2.18	0.67
1:A:364:PRO:O	1:A:367:THR:HB	1.95	0.67
1:A:540:ILE:HD13	1:A:540:ILE:O	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:HD13	1:A:348:ILE:O	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: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
1:A:92:ARG:C	1:A:117:LEU:HD13	2.23	0.64
1:A:233:CYS:O	1:A:237:ALA:CB	2.45	0.64
1:A:118:ASN:C	1:A:118:ASN:OD1	2.41	0.63
1:A:152:HIS:ND1	1:A:157:VAL:HG11	2.13	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:HB	1:A:211:GLU:HB2	1.85	0.58
1:A:78:ASP:H	1:A:130:MET:HE1	1.69	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:537:ALA:C	1:A:540:ILE:HB	2.29	0.57
1:A:327:ARG:NH2	1:A:362:ILE:HG22	2.19	0.57
1:A:466:MET:HE1	1:A:477:THR:HG21	1.86	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:130:MET:O	1:A:131:PRO:C	2.47	0.56
1:A:383:PHE:O	1:A:386:PHE:HB3	2.05	0.55
1:A:429:LYS:O	1:A:437:LYS:HG3	2.05	0.55
1:A:540:ILE:HD11	1:A:552:GLU:HG2	1.89	0.55
1:A:220:ALA:O	1:A:224:ASN:OD1	2.25	0.55
1:A:234:THR:HB	1:A:273:ASN:OD1	2.07	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
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:79:GLU:O	1:A:80:SER:HB2	2.08	0.53
1:A:96:ASN:HB2	1:A:117:LEU:HD12	1.91	0.53
1:A:204:LEU:HD23	1:A:211:GLU:CG	2.39	0.53
1:A:289:LEU:C	1:A:293:LEU:HD12	2.34	0.53
1:A:270:LEU:O	1:A:271:GLN:C	2.52	0.52
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:146:LEU:HD22	1:A:161:VAL:HG13	1.92	0.51
1:A:208:VAL:O	1:A:209:LYS:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:CYS:SG	1:A:234:THR:N	2.84	0.51
1:A:288:VAL:O	1:A:289:LEU:C	2.53	0.51
1:A:212:ALA:O	1:A:215:VAL:HG22	2.11	0.51
1:A:232:MET:SD	1:A:232:MET:C	2.94	0.51
1:A:242:LEU:HD12	1:A:242:LEU:C	2.36	0.51
1:A:331:LEU:HD23	1:A:331:LEU:O	2.10	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:300:ASN:CG	1:A:348:ILE:HG22	2.37	0.50
1:A:327:ARG:NH2	1:A:363:GLY:H	2.09	0.50
1:A:117:LEU:HD23	1:A:117:LEU:N	2.26	0.50
1:A:232:MET:HE2	1:A:233:CYS:CA	2.36	0.50
1:A:110:PHE:CD1	1:A:110:PHE:N	2.74	0.50
1:A:361:MET:HE1	1:A:373:PHE:CG	2.47	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:185:ILE:O	1:A:186:ASP:C	2.56	0.49
1:A:379:LEU:HA	1:A:382:ILE:HG22	1.94	0.49
1:A:539:ASN:C	1:A:540:ILE:HG22	2.38	0.49
1:A:134:TYR:CB	1:A:180:GLY:O	2.60	0.49
1:A:393:ILE:HG22	1:A:394:LYS:N	2.26	0.49
1:A:309:MET:O	1:A:310:MET:C	2.56	0.48
1:A:194:VAL:HG11	1:A:236:GLY:O	2.13	0.48
1:A:331:LEU:HD23	1:A:331:LEU:C	2.38	0.48
1:A:526:ILE:O	1:A:529:VAL:HB	2.13	0.48
1:A:414:LEU:HD22	1:A:418:LEU:HD11	1.95	0.48
1:A:415:LEU:HD11	1:A:499:ILE:HG23	1.94	0.48
1:A:208:VAL:O	1:A:211:GLU:N	2.47	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:452:MET:HE1	1:A:485:ARG:NH1	2.29	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
1:A:234:THR:HG23	1:A:235:GLU:N	2.28	0.47
1:A:415:LEU:CD1	1:A:499:ILE:HG23	2.44	0.47
1:A:500:MET:O	1:A:503:ILE:HG12	2.15	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:78:ASP:HB3	1:A:81:SER:OG	2.14	0.47
1:A:146:LEU:CD2	1:A:161:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD23	1:A:168:LEU:HD11	1.97	0.47
1:A:82:VAL:HA	1:A:85:MET:HG3	1.96	0.47
1:A:100:ARG:HD2	1:A:110:PHE:HE2	1.80	0.47
1:A:85:MET:HE1	1:A:123:GLU:C	2.40	0.47
1:A:193:VAL:HG22	1:A:197:LEU:HD12	1.97	0.47
1:A:104:PRO:O	1:A:107:PRO:HG3	2.14	0.47
1:A:133:LEU:O	1:A:135:HIS:HD2	1.97	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:134:TYR:HB2	1:A:180:GLY:C	2.39	0.46
1:A:234:THR:HA	1:A:276:ASN:HD21	1.81	0.46
1:A:238:GLN:O	1:A:239:GLN:C	2.58	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:158:SER:O	1:A:161:VAL:N	2.47	0.46
1:A:82:VAL:O	1:A:85:MET:N	2.49	0.45
1:A:193:VAL:HG13	1:A:194:VAL:N	2.32	0.45
1:A:356:VAL:O	1:A:357:LEU:C	2.57	0.45
1:A:198:VAL:O	1:A:202:GLU:N	2.49	0.45
1:A:392:LYS:C	1:A:393:ILE:HG13	2.41	0.45
1:A:217:ASN:N	1:A:217:ASN:HD22	2.15	0.45
1:A:390:PRO:HB2	1:A:391:ARG:CB	2.46	0.45
1:A:124:MET:CA	1:A:127:VAL:HG23	2.45	0.45
1:A:399:THR:CG2	1:A:400:GLU:HA	2.46	0.45
1:A:537:ALA:O	1:A:540:ILE:HG21	2.15	0.45
1:A:219:LEU:O	1:A:220:ALA:C	2.59	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:537:ALA:O	1:A:538:GLU:C	2.60	0.44
1:A:82:VAL:O	1:A:85:MET:CB	2.61	0.44
1:A:206:GLU:O	1:A:207:SER:C	2.59	0.44
1:A:165:LEU:HA	1:A:168:LEU:HD13	1.99	0.44
1:A:300:ASN:OD1	1:A:348:ILE:HG22	2.17	0.44
1:A:215:VAL:O	1:A:216:HIS:C	2.58	0.44
1:A:280:LEU:HD23	1:A:280:LEU:C	2.43	0.44
1:A:157:VAL:O	1:A:161:VAL:HG23	2.18	0.44
1:A:140:LEU:N	1:A:140:LEU:HD12	2.33	0.44
1:A:103:PHE:CD2	1:A:110:PHE:CB	2.79	0.44
1:A:442:MET:CE	1:A:500:MET:HE2	2.43	0.44
1:A:452:MET:O	1:A:453:GLN:C	2.60	0.44
1:A:133:LEU:O	1:A:135:HIS:CD2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:THR:O	1:A:398:THR:OG1	2.34	0.44
1:A:248:ARG:NH1	1:A:253:MET:HE1	2.32	0.43
1:A:459:ILE:O	1:A:460:GLU:C	2.59	0.43
1:A:192:GLN:O	1:A:193:VAL:C	2.61	0.43
1:A:331:LEU:O	1:A:333:GLY:O	2.36	0.43
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:394:LYS:O	1:A:396:VAL:O	2.36	0.43
1:A:159:ILE:HA	1:A:162:VAL:CG1	2.49	0.43
1:A:225:MET:HE2	1:A:225:MET:HB3	1.88	0.43
1:A:104:PRO:O	1:A:107:PRO:HD3	2.18	0.43
1:A:215:VAL:HG23	1:A:216:HIS:N	2.33	0.43
1:A:238:GLN:HG3	1:A:239:GLN:N	2.32	0.43
1:A:558:GLY:O	1:A:561:GLU:HG2	2.19	0.43
1:A:289:LEU:O	1:A:290:LEU:C	2.61	0.43
1:A:338:LEU:O	1:A:339:MET:C	2.61	0.43
1:A:228:PHE:C	1:A:230:PRO:HD3	2.44	0.43
1:A:392:LYS:N	1:A:393:ILE:CA	2.78	0.43
1:A:124:MET:O	1:A:125:HIS:C	2.61	0.43
1:A:124:MET:O	1:A:127:VAL:N	2.32	0.43
1:A:124:MET:O	1:A:127:VAL:HG23	2.19	0.43
1:A:452:MET:HE3	1:A:452:MET:HB3	1.88	0.43
1:A:236:GLY:HA2	1:A:239:GLN:HG3	2.00	0.42
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.74	0.42
1:A:512:ARG:O	1:A:516:HIS:HD2	2.01	0.42
1:A:552:GLU:O	1:A:555:ARG:N	2.52	0.42
1:A:159:ILE:HA	1:A:162:VAL:HG12	2.01	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:357:LEU:O	1:A:358:ASP:C	2.61	0.42
1:A:499:ILE:O	1:A:500:MET:C	2.61	0.42
1:A:520:ASN:O	1:A:522:ARG:CG	2.67	0.42
1:A:540:ILE:O	1:A:540:ILE:HG23	2.18	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:200:ASN:O	1:A:201:LEU:C	2.63	0.42
1:A:468:ARG:O	1:A:469:ARG:C	2.62	0.42
1:A:554:LYS:O	1:A:555:ARG:C	2.62	0.42
1:A:135:HIS:CD2	1:A:135:HIS:C	2.90	0.42
1:A:416:ARG:NH1	1:A:552:GLU:OE1	2.45	0.42
1:A:450:GLY:O	1:A:451:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:O	1:A:173:THR:HG22	2.19	0.42
1:A:135:HIS:O	1:A:136:LEU:C	2.61	0.41
1:A:521:MET:HA	1:A:522:ARG:CB	2.41	0.41
1:A:78:ASP:N	1:A:130:MET:HE1	2.32	0.41
1:A:512:ARG:HH12	1:A:563:PHE:C	2.28	0.41
1:A:530:ARG:NH2	1:A:563:PHE:O	2.53	0.41
1:A:166:GLN:CG	1:A:167:GLU:N	2.83	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: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
1:A:201:LEU:HD12	1:A:215:VAL:HG12	2.03	0.41
1:A:507:ASN:O	1:A:507:ASN:CG	2.63	0.41
1:A:184:LEU:O	1:A:185:ILE:C	2.64	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:352:SER:O	1:A:355:LYS:N	2.53	0.41
1:A:530:ARG:CD	1:A:560:LEU:HD21	2.50	0.41
1:A:560:LEU:HD23	1:A:560:LEU:O	2.20	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:77:LEU:HA	1:A:78:ASP:HA	1.89	0.40
1:A:285:GLY:O	1:A:288:VAL:HB	2.21	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%)	16	29

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%)	358 (81%)	82 (19%)	1	2

All (82) 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	99	LEU
1	A	100	ARG
1	A	108	GLU
1	A	110	PHE
1	A	112	GLU
1	A	113	SER
1	A	115	LEU
1	A	117	LEU
1	A	120	ILE
1	A	125	HIS
1	A	130	MET
1	A	132	ASP
1	A	133	LEU
1	A	134	TYR

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Mol	Chain	Res	Type
1	A	157	VAL
1	A	162	VAL
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
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	266	LEU
1	A	269	LEU
1	A	273	ASN
1	A	284	ASP
1	A	286	ILE
1	A	293	LEU
1	A	303	THR
1	A	305	GLU
1	A	319	SER
1	A	325	SER
1	A	327	ARG
1	A	328	GLU
1	A	332	LYS
1	A	345	GLU
1	A	348	ILE
1	A	350	ARG
1	A	355	LYS
1	A	362	ILE
1	A	380	ARG
1	A	388	LYS
1	A	390	PRO
1	A	391	ARG

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Mol	Chain	Res	Type
1	A	392	LYS
1	A	398	THR
1	A	399	THR
1	A	400	GLU
1	A	419	ARG
1	A	424	THR
1	A	444	LEU
1	A	447	LYS
1	A	457	LYS
1	A	467	VAL
1	A	472	ILE
1	A	480	GLU
1	A	483	LEU
1	A	492	VAL
1	A	522	ARG
1	A	528	ILE
1	A	535	GLU
1	A	540	ILE
1	A	544	ARG
1	A	549	ARG
1	A	550	GLU
1	A	560	LEU
1	A	561	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
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	276	ASN
1	A	300	ASN
1	A	433	ASN
1	A	445	HIS
1	A	513	GLN
1	A	531	HIS
1	A	562	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

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%)	0.90	62 (12%) 8 8	24, 81, 129, 182	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ASP	7.8
1	A	106	ASN	6.4
1	A	172	ASP	6.1
1	A	398	THR	5.5
1	A	107	PRO	5.3
1	A	108	GLU	5.3
1	A	237	ALA	4.8
1	A	113	SER	4.8
1	A	171	ILE	4.6
1	A	112	GLU	4.5
1	A	111	MET	4.4
1	A	103	PHE	4.4
1	A	129	THR	4.3
1	A	117	LEU	4.3
1	A	396	VAL	4.0
1	A	233	CYS	4.0
1	A	235	GLU	3.8
1	A	397	GLY	3.7
1	A	110	PHE	3.5
1	A	231	GLU	3.5
1	A	236	GLY	3.4
1	A	507	ASN	3.4
1	A	104	PRO	3.4
1	A	174	LEU	3.3
1	A	238	GLN	3.2
1	A	393	ILE	3.2
1	A	473	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	99	LEU	3.2
1	A	232	MET	3.1
1	A	115	LEU	3.1
1	A	300	ASN	3.0
1	A	394	LYS	3.0
1	A	302	SER	2.9
1	A	93	SER	2.9
1	A	116	ASP	2.8
1	A	109	LYS	2.7
1	A	229	ARG	2.7
1	A	90	GLU	2.7
1	A	239	GLN	2.6
1	A	230	PRO	2.6
1	A	244	TRP	2.5
1	A	89	PHE	2.5
1	A	248	ARG	2.4
1	A	126	VAL	2.4
1	A	120	ILE	2.3
1	A	144	GLN	2.3
1	A	286	ILE	2.3
1	A	296	PHE	2.2
1	A	469	ARG	2.2
1	A	177	SER	2.2
1	A	82	VAL	2.2
1	A	97	GLN	2.2
1	A	255	PHE	2.2
1	A	307	GLN	2.1
1	A	204	LEU	2.1
1	A	242	LEU	2.1
1	A	240	GLY	2.1
1	A	540	ILE	2.1
1	A	92	ARG	2.1
1	A	367	THR	2.0
1	A	295	VAL	2.0
1	A	541	GLY	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 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.