



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:42 pm BST

PDB ID : 3OUW
Title : Structure of beta-catenin with Lef-1
Authors : Weis, W.I.; Sun, J.
Deposited on : 2010-09-15
Resolution : 2.91 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 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

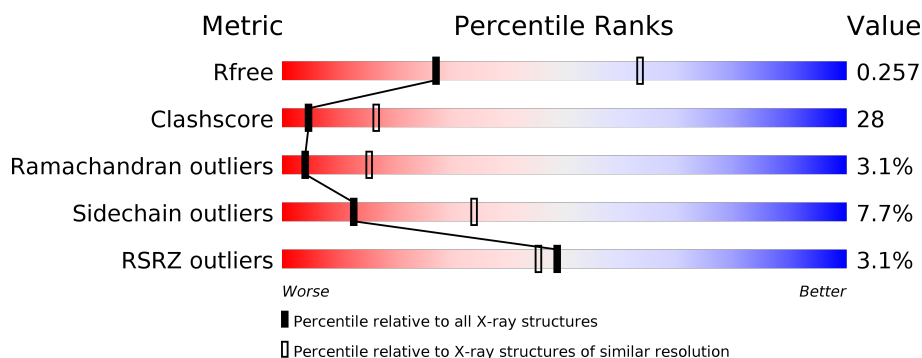
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	540	<div> <div>3%</div> <div> <div></div> <div>44%</div> <div>42%</div> <div>6%</div> <div>8%</div> </div> </div>
2	B	65	<div> <div>3%</div> <div> <div></div> <div>25%</div> <div>18%</div> <div>57%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3963 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 beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3752	2359	681	686	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	GLY	-	EXPRESSION TAG	UNP Q02248
A	133	SER	-	EXPRESSION TAG	UNP Q02248

- Molecule 2 is a protein called Lymphoid enhancer-binding factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	28	Total	C	N	O	S	0	0	0
			211	131	31	47	2			

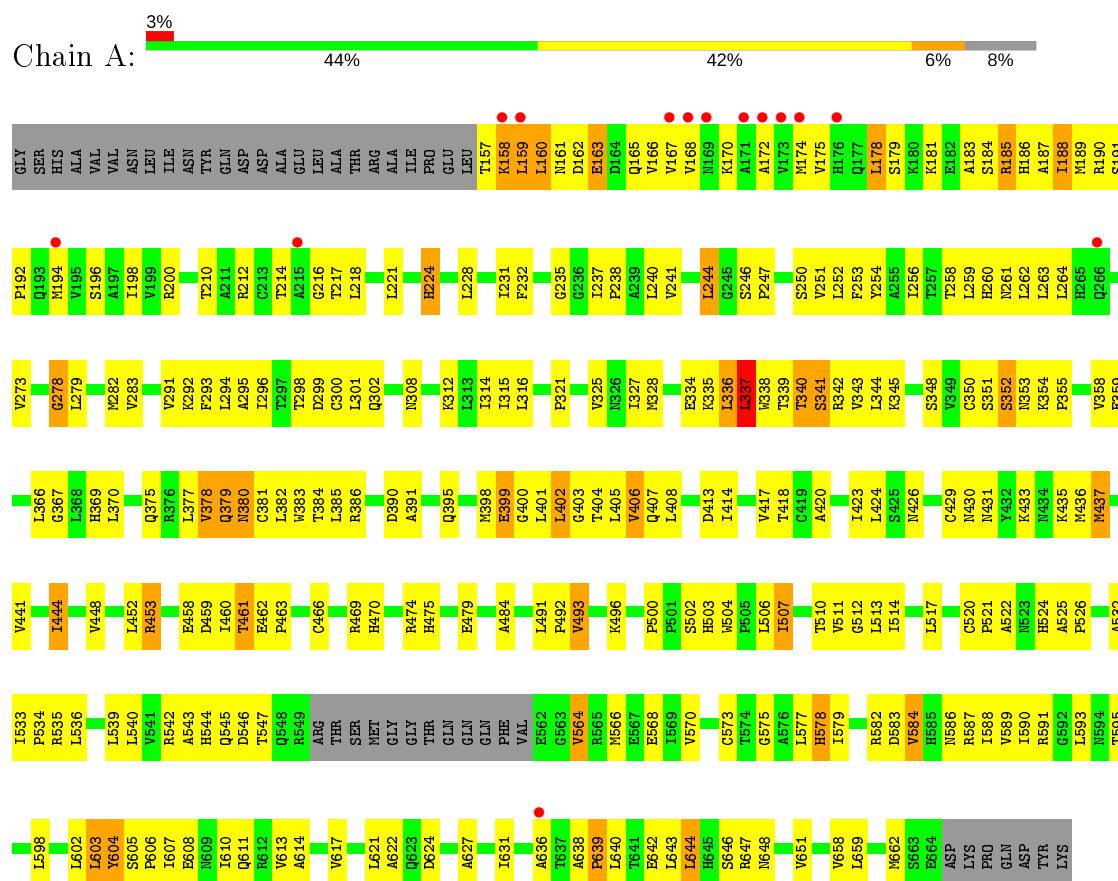
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP P27782
B	0	ALA	-	EXPRESSION TAG	UNP P27782

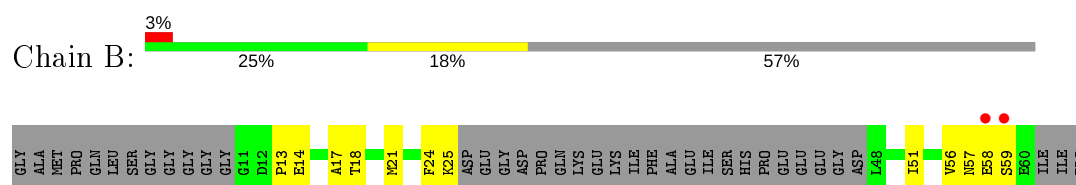
3 Residue-property plots

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 beta-1



• Molecule 2: Lymphoid enhancer-binding factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.93Å 116.93Å 214.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.94 – 2.91 102.63 – 2.91	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.94-2.91) 95.2 (102.63-2.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.203 , 0.256 0.201 , 0.257	Depositor DCC
R_{free} test set	633 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3963	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.40	0/3804	0.61	0/5163
2	B	0.46	0/212	0.62	0/284
All	All	0.41	0/4016	0.61	0/5447

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	3752	0	3880	220	0
2	B	211	0	202	10	0
All	All	3963	0	4082	226	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 28.

All (226) 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:352:SER:O	1:A:355:PRO:HD2	1.62	0.99
1:A:241:VAL:HA	1:A:244:LEU:HD12	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLY:HA2	1:A:254:TYR:CE2	2.06	0.91
1:A:218:LEU:HA	1:A:221:LEU:HD12	1.54	0.89
1:A:279:LEU:O	1:A:283:VAL:HG23	1.76	0.85
1:A:525:ALA:HB3	1:A:526:PRO:HD3	1.59	0.84
2:B:24:PHE:O	2:B:25:LYS:HG3	1.78	0.84
1:A:566:MET:O	1:A:570:VAL:HG23	1.81	0.80
1:A:453:ARG:O	1:A:453:ARG:HG3	1.81	0.78
1:A:535:ARG:HH12	1:A:542:ARG:HH12	1.31	0.78
1:A:413:ASP:O	1:A:417:VAL:HG23	1.85	0.77
1:A:402:LEU:HD23	1:A:437:MET:HB3	1.64	0.77
1:A:335:LYS:O	1:A:339:THR:HG23	1.85	0.77
1:A:354:LYS:HB2	1:A:355:PRO:HD3	1.68	0.75
1:A:607:ILE:O	1:A:611:GLN:HG3	1.86	0.75
1:A:282:MET:HB2	1:A:301:LEU:HD21	1.68	0.75
2:B:57:ASN:C	2:B:59:SER:H	1.90	0.74
1:A:658:VAL:O	1:A:662:MET:HG3	1.88	0.72
1:A:507:ILE:O	1:A:511:VAL:HG23	1.91	0.71
1:A:188:ILE:HB	1:A:194:MET:HG2	1.73	0.70
1:A:260:HIS:CD2	1:A:264:LEU:HD11	2.25	0.70
1:A:302:GLN:HB2	1:A:343:VAL:HG22	1.72	0.70
1:A:345:LYS:HB2	1:A:384:THR:OG1	1.94	0.68
1:A:607:ILE:HB	1:A:610:ILE:HD12	1.76	0.68
1:A:404:THR:HG22	1:A:408:LEU:HD11	1.77	0.67
1:A:328:MET:SD	1:A:340:THR:HG22	2.35	0.66
1:A:586:ASN:O	1:A:590:ILE:HD12	1.96	0.66
1:A:216:GLY:HA2	1:A:254:TYR:CD2	2.29	0.65
1:A:522:ALA:O	1:A:526:PRO:HD2	1.95	0.65
1:A:381:CYS:O	1:A:385:LEU:HD12	1.96	0.65
1:A:157:THR:HA	1:A:160:LEU:HD12	1.79	0.64
1:A:379:GLN:HG2	1:A:383:TRP:CZ3	2.33	0.64
1:A:350:CYS:O	1:A:354:LYS:HG3	1.97	0.64
1:A:418:THR:HG22	1:A:460:ILE:CG1	2.29	0.63
1:A:327:ILE:HG23	1:A:336:LEU:HD21	1.79	0.63
1:A:444:ILE:O	1:A:448:VAL:HG23	1.97	0.63
1:A:237:ILE:O	1:A:241:VAL:HG23	1.99	0.63
1:A:404:THR:O	1:A:408:LEU:HD12	1.98	0.62
1:A:186:HIS:HB3	1:A:190:ARG:CZ	2.29	0.62
1:A:429:CYS:SG	2:B:21:MET:HG3	2.38	0.62
1:A:261:ASN:HA	1:A:264:LEU:HD12	1.81	0.62
1:A:638:ALA:HB3	1:A:639:PRO:HD3	1.82	0.62
1:A:166:VAL:O	1:A:170:LYS:HE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:CB	1:A:168:VAL:HB	2.30	0.62
1:A:186:HIS:HB3	1:A:190:ARG:NH2	2.14	0.62
1:A:458:GLU:HA	1:A:461:THR:OG1	2.00	0.61
1:A:228:LEU:HD22	1:A:262:LEU:HD13	1.82	0.61
1:A:504:TRP:HA	1:A:507:ILE:HG13	1.81	0.61
1:A:510:THR:O	1:A:514:ILE:HG13	2.01	0.61
1:A:604:TYR:OH	1:A:639:PRO:HG3	2.01	0.61
1:A:198:ILE:HG23	1:A:214:THR:HB	1.83	0.60
1:A:282:MET:CB	1:A:301:LEU:HD21	2.31	0.60
1:A:235:GLY:O	1:A:238:PRO:HD2	2.02	0.60
2:B:56:VAL:HA	2:B:59:SER:HB2	1.84	0.60
1:A:260:HIS:HE1	1:A:299:ASP:OD2	1.85	0.59
1:A:513:LEU:O	1:A:517:LEU:HG	2.02	0.59
1:A:444:ILE:HG21	1:A:484:ALA:HB3	1.85	0.59
1:A:385:LEU:HD22	1:A:401:LEU:HD21	1.84	0.59
2:B:13:PRO:HB2	2:B:14:GLU:HG2	1.83	0.58
1:A:294:LEU:HB2	1:A:336:LEU:CD1	2.33	0.57
1:A:403:GLY:O	1:A:407:GLN:HG3	2.04	0.57
1:A:604:TYR:CZ	1:A:639:PRO:HG3	2.39	0.57
1:A:196:SER:O	1:A:200:ARG:HG3	2.04	0.57
1:A:622:ALA:HB2	1:A:631:ILE:HD12	1.87	0.57
1:A:444:ILE:HG21	1:A:484:ALA:CB	2.35	0.56
1:A:588:ILE:HA	1:A:591:ARG:HH22	1.71	0.56
1:A:418:THR:HG22	1:A:460:ILE:HG12	1.88	0.56
1:A:533:ILE:HB	1:A:534:PRO:HD3	1.86	0.56
1:A:402:LEU:HD23	1:A:437:MET:CB	2.33	0.55
1:A:584:VAL:HA	1:A:587:ARG:NH1	2.20	0.55
1:A:627:ALA:O	1:A:631:ILE:HG13	2.05	0.55
1:A:316:LEU:CD2	1:A:352:SER:HB2	2.37	0.55
1:A:418:THR:HG22	1:A:460:ILE:HG13	1.88	0.55
1:A:350:CYS:HB3	1:A:353:ASN:HB2	1.88	0.55
1:A:351:SER:OG	1:A:352:SER:N	2.39	0.55
1:A:607:ILE:N	1:A:607:ILE:HD12	2.22	0.55
1:A:186:HIS:HB3	1:A:190:ARG:NH1	2.21	0.55
1:A:260:HIS:HD2	1:A:264:LEU:HD11	1.71	0.55
1:A:522:ALA:O	1:A:526:PRO:CD	2.56	0.54
1:A:607:ILE:HG22	1:A:610:ILE:H	1.73	0.54
1:A:175:VAL:HG13	1:A:178:LEU:HD12	1.88	0.54
2:B:56:VAL:HG12	2:B:56:VAL:O	2.07	0.54
1:A:179:SER:HB3	1:A:217:THR:HG23	1.89	0.54
1:A:545:GLN:C	1:A:547:THR:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HB3	1:A:259:LEU:HD21	1.90	0.54
1:A:337:LEU:HD11	1:A:369:HIS:CE1	2.42	0.54
1:A:431:ASN:C	1:A:431:ASN:OD1	2.46	0.54
2:B:57:ASN:C	2:B:59:SER:N	2.59	0.54
1:A:466:CYS:O	1:A:469:ARG:HB3	2.07	0.54
1:A:375:GLN:C	1:A:377:LEU:H	2.12	0.54
1:A:184:SER:O	1:A:187:ALA:HB3	2.07	0.53
1:A:595:THR:O	1:A:598:LEU:N	2.33	0.53
1:A:573:CYS:O	1:A:577:LEU:HG	2.08	0.53
1:A:260:HIS:O	1:A:264:LEU:HG	2.08	0.53
1:A:355:PRO:O	1:A:359:GLU:HG2	2.09	0.53
1:A:636:ALA:O	1:A:639:PRO:HD2	2.09	0.53
1:A:178:LEU:O	1:A:184:SER:HB2	2.08	0.53
1:A:312:LYS:O	1:A:353:ASN:ND2	2.41	0.53
1:A:535:ARG:O	1:A:539:LEU:HG	2.09	0.53
1:A:435:LYS:CD	1:A:475:HIS:HD2	2.22	0.52
1:A:244:LEU:HD11	1:A:259:LEU:HD11	1.90	0.52
1:A:543:ALA:HA	1:A:566:MET:HE2	1.91	0.52
1:A:640:LEU:HD13	1:A:659:LEU:HG	1.92	0.52
1:A:328:MET:SD	1:A:340:THR:CG2	2.99	0.51
1:A:469:ARG:NE	1:A:512:GLY:HA3	2.26	0.51
1:A:263:LEU:HD21	1:A:273:VAL:HG21	1.92	0.51
1:A:159:LEU:O	1:A:160:LEU:C	2.48	0.51
1:A:327:ILE:CG2	1:A:336:LEU:HD21	2.41	0.51
1:A:401:LEU:O	1:A:401:LEU:HD12	2.10	0.50
1:A:426:ASN:O	1:A:429:CYS:HB2	2.10	0.50
1:A:354:LYS:O	1:A:358:VAL:HG23	2.10	0.50
1:A:358:VAL:HG12	1:A:395:GLN:HE21	1.76	0.50
1:A:575:GLY:O	1:A:578:HIS:HB3	2.11	0.50
1:A:278:GLY:O	1:A:282:MET:HG3	2.12	0.50
1:A:359:GLU:HA	1:A:395:GLN:NE2	2.27	0.50
1:A:404:THR:HG22	1:A:408:LEU:CD1	2.40	0.50
1:A:545:GLN:C	1:A:547:THR:H	2.13	0.50
1:A:321:PRO:O	1:A:325:VAL:HG23	2.12	0.50
1:A:377:LEU:O	1:A:379:GLN:N	2.45	0.50
1:A:279:LEU:CD2	1:A:315:ILE:HD11	2.42	0.49
1:A:513:LEU:HD11	1:A:517:LEU:HD21	1.94	0.49
1:A:524:HIS:ND1	1:A:583:ASP:HB2	2.27	0.49
1:A:337:LEU:O	1:A:341:SER:HB2	2.12	0.49
1:A:260:HIS:CE1	1:A:299:ASP:OD2	2.65	0.49
1:A:535:ARG:HH12	1:A:542:ARG:NH1	2.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:CD1	1:A:385:LEU:HG	2.42	0.49
1:A:386:ARG:HA	1:A:423:ILE:HG12	1.93	0.49
1:A:433:LYS:O	1:A:436:MET:N	2.44	0.49
1:A:345:LYS:O	1:A:348:SER:HB3	2.13	0.49
1:A:525:ALA:HB3	1:A:526:PRO:CD	2.39	0.48
1:A:183:ALA:HA	1:A:186:HIS:HB2	1.96	0.48
1:A:210:THR:O	1:A:214:THR:HG23	2.13	0.48
1:A:398:MET:O	1:A:399:GLU:C	2.52	0.48
1:A:406:VAL:HG12	1:A:406:VAL:O	2.13	0.48
1:A:452:LEU:HD21	1:A:493:VAL:HG11	1.96	0.48
1:A:506:LEU:O	1:A:506:LEU:HD12	2.13	0.48
1:A:420:ALA:O	1:A:424:LEU:HD12	2.14	0.48
1:A:162:ASP:O	1:A:163:GLU:CB	2.62	0.47
1:A:183:ALA:O	1:A:187:ALA:HB2	2.15	0.47
1:A:212:ARG:HG3	1:A:250:SER:OG	2.13	0.47
1:A:405:LEU:O	1:A:407:GLN:N	2.48	0.47
1:A:544:HIS:ND1	1:A:598:LEU:HD11	2.30	0.47
1:A:366:LEU:HD13	1:A:385:LEU:HG	1.97	0.47
1:A:642:GLU:OE1	1:A:642:GLU:HA	2.14	0.47
1:A:414:ILE:HG13	1:A:460:ILE:HD11	1.97	0.46
1:A:390:ASP:OD1	1:A:391:ALA:N	2.49	0.46
1:A:414:ILE:O	1:A:418:THR:HG23	2.14	0.46
1:A:586:ASN:C	1:A:590:ILE:HD12	2.36	0.46
1:A:165:GLN:C	1:A:167:VAL:H	2.18	0.46
1:A:260:HIS:HE1	1:A:299:ASP:HB3	1.81	0.46
1:A:429:CYS:O	1:A:430:ASN:HB2	2.15	0.46
1:A:587:ARG:HG2	1:A:621:LEU:HD23	1.97	0.46
1:A:181:LYS:HB2	1:A:184:SER:OG	2.16	0.46
1:A:258:THR:O	1:A:261:ASN:HB2	2.15	0.46
1:A:337:LEU:CD1	1:A:369:HIS:CE1	2.99	0.46
1:A:540:LEU:HD12	1:A:570:VAL:HG13	1.98	0.45
1:A:613:VAL:HG23	1:A:614:ALA:N	2.30	0.45
1:A:429:CYS:SG	1:A:470:HIS:CE1	3.10	0.45
1:A:435:LYS:HB3	1:A:475:HIS:CD2	2.51	0.45
1:A:544:HIS:O	1:A:544:HIS:CG	2.69	0.45
1:A:291:VAL:HG23	1:A:292:LYS:N	2.31	0.45
1:A:398:MET:O	1:A:400:GLY:N	2.48	0.45
1:A:188:ILE:HG22	1:A:194:MET:HE3	1.98	0.45
1:A:216:GLY:HA2	1:A:254:TYR:CZ	2.48	0.45
1:A:545:GLN:O	1:A:547:THR:N	2.50	0.45
1:A:358:VAL:O	1:A:395:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ARG:HD2	1:A:624:ASP:OD2	2.17	0.45
1:A:591:ARG:NH2	1:A:591:ARG:HB3	2.33	0.44
1:A:648:ASN:OD1	1:A:651:VAL:HG23	2.18	0.44
1:A:260:HIS:CE1	1:A:299:ASP:HB3	2.52	0.44
1:A:606:PRO:HB2	1:A:607:ILE:HD12	2.00	0.44
1:A:386:ARG:HG2	2:B:24:PHE:CD1	2.53	0.44
1:A:579:ILE:O	1:A:582:ARG:HG3	2.17	0.44
1:A:644:LEU:HD23	1:A:644:LEU:O	2.17	0.44
1:A:295:ALA:N	1:A:336:LEU:HD12	2.32	0.43
1:A:308:ASN:C	1:A:308:ASN:OD1	2.56	0.43
1:A:540:LEU:CD1	1:A:570:VAL:HG13	2.48	0.43
1:A:231:ILE:HG22	1:A:232:PHE:N	2.32	0.43
1:A:314:ILE:O	1:A:314:ILE:HG22	2.19	0.43
1:A:178:LEU:N	1:A:178:LEU:HD23	2.33	0.43
1:A:224:HIS:ND1	1:A:224:HIS:N	2.66	0.43
1:A:246:SER:HA	1:A:247:PRO:HD3	1.86	0.43
1:A:299:ASP:O	1:A:300:CYS:C	2.55	0.43
1:A:520:CYS:HA	1:A:521:PRO:HD3	1.74	0.43
1:A:595:THR:O	1:A:598:LEU:HB3	2.18	0.43
1:A:462:GLU:HB3	1:A:463:PRO:HD2	2.00	0.43
1:A:186:HIS:O	1:A:190:ARG:HD2	2.18	0.43
1:A:379:GLN:O	1:A:383:TRP:HE3	2.01	0.43
1:A:377:LEU:O	1:A:378:VAL:C	2.57	0.43
1:A:367:GLY:HA2	1:A:370:LEU:HG	2.01	0.42
1:A:429:CYS:SG	2:B:21:MET:CG	3.07	0.42
1:A:544:HIS:CD2	1:A:602:LEU:HD21	2.53	0.42
1:A:491:LEU:HB2	1:A:492:PRO:HD3	2.01	0.42
1:A:279:LEU:HD22	1:A:315:ILE:HD11	2.01	0.42
1:A:336:LEU:HD23	1:A:337:LEU:HD23	2.00	0.42
1:A:564:VAL:HG22	1:A:568:GLU:OE1	2.19	0.42
1:A:341:SER:HB3	1:A:380:ASN:HD22	1.84	0.42
1:A:500:PRO:HA	1:A:502:SER:N	2.34	0.42
1:A:157:THR:O	1:A:158:LYS:C	2.59	0.41
1:A:240:LEU:HD13	1:A:259:LEU:HD23	2.02	0.41
1:A:377:LEU:C	1:A:379:GLN:N	2.74	0.41
1:A:253:PHE:CD1	1:A:253:PHE:N	2.88	0.41
1:A:235:GLY:C	1:A:238:PRO:HD2	2.41	0.41
1:A:296:ILE:HA	1:A:296:ILE:HD13	1.85	0.41
1:A:532:ALA:O	1:A:536:LEU:HG	2.19	0.41
1:A:603:LEU:CD1	1:A:603:LEU:N	2.83	0.41
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:C	1:A:338:TRP:N	2.74	0.41
1:A:535:ARG:NE	1:A:539:LEU:HD21	2.36	0.41
1:A:603:LEU:C	1:A:605:SER:H	2.24	0.41
1:A:474:ARG:CZ	2:B:17:ALA:O	2.69	0.41
1:A:191:SER:HA	1:A:192:PRO:HD3	1.81	0.41
1:A:172:ALA:C	1:A:174:MET:H	2.24	0.41
1:A:251:VAL:O	1:A:252:LEU:C	2.59	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.77	0.41
1:A:298:THR:HG21	1:A:340:THR:OG1	2.21	0.40
1:A:435:LYS:HD3	1:A:475:HIS:HD2	1.86	0.40
1:A:589:VAL:HG12	1:A:593:LEU:HD11	2.02	0.40
1:A:334:GLU:O	1:A:335:LYS:C	2.58	0.40
1:A:613:VAL:HG23	1:A:614:ALA:H	1.86	0.40
1:A:643:LEU:O	1:A:646:SER:N	2.53	0.40
1:A:343:VAL:O	1:A:344:LEU:C	2.59	0.40
1:A:241:VAL:HA	1:A:244:LEU:CD1	2.36	0.40
1:A:256:ILE:HG21	1:A:293:PHE:CE1	2.57	0.40
1:A:379:GLN:O	1:A:382:LEU:N	2.54	0.40
1:A:185:ARG:O	1:A:189:MET:HG3	2.22	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	492/540 (91%)	415 (84%)	62 (13%)	15 (3%)	4	16
2	B	24/65 (37%)	21 (88%)	2 (8%)	1 (4%)	3	9
All	All	516/605 (85%)	436 (84%)	64 (12%)	16 (3%)	4	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	LYS
1	A	160	LEU
1	A	163	GLU
1	A	337	LEU
2	B	58	GLU
1	A	159	LEU
1	A	378	VAL
1	A	379	GLN
1	A	380	ASN
1	A	399	GLU
1	A	546	ASP
1	A	604	TYR
1	A	441	VAL
1	A	278	GLY
1	A	639	PRO
1	A	406	VAL

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	404/448 (90%)	373 (92%)	31 (8%)	13	34
2	B	25/52 (48%)	23 (92%)	2 (8%)	12	32
All	All	429/500 (86%)	396 (92%)	33 (8%)	13	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	178	LEU
1	A	185	ARG
1	A	188	ILE
1	A	224	HIS
1	A	244	LEU
1	A	336	LEU
1	A	337	LEU

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Mol	Chain	Res	Type
1	A	340	THR
1	A	341	SER
1	A	342	ARG
1	A	352	SER
1	A	402	LEU
1	A	437	MET
1	A	444	ILE
1	A	453	ARG
1	A	459	ASP
1	A	461	THR
1	A	479	GLU
1	A	493	VAL
1	A	496	LYS
1	A	503	HIS
1	A	507	ILE
1	A	564	VAL
1	A	578	HIS
1	A	584	VAL
1	A	603	LEU
1	A	608	GLU
1	A	617	VAL
1	A	644	LEU
1	A	647	ARG
2	B	18	THR
2	B	51	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	HIS
1	A	375	GLN
1	A	395	GLN
1	A	470	HIS
1	A	545	GLN
1	A	611	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, 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	496/540 (91%)	0.22	14 (2%) 53 50	30, 69, 141, 188	0
2	B	28/65 (43%)	0.61	2 (7%) 16 13	52, 77, 149, 162	0
All	All	524/605 (86%)	0.24	16 (3%) 49 45	30, 70, 144, 188	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	59	SER	4.8
2	B	58	GLU	4.2
1	A	169	ASN	3.9
1	A	174	MET	3.8
1	A	159	LEU	3.7
1	A	172	ALA	3.2
1	A	158	LYS	2.9
1	A	636	ALA	2.9
1	A	194	MET	2.4
1	A	173	VAL	2.4
1	A	176	HIS	2.3
1	A	171	ALA	2.3
1	A	168	VAL	2.2
1	A	266	GLN	2.1
1	A	215	ALA	2.1
1	A	167	VAL	2.1

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.