Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:37 PM GMT

PDB ID	:	1L7C
Title	:	alpha-catenin fragment, residues 385-651
Authors	:	Pokutta, S.; Drees, F.; Takai, Y.; Nelson, W.J.; Weis, W.I.
Deposited on	:	2002-03-14
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) 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
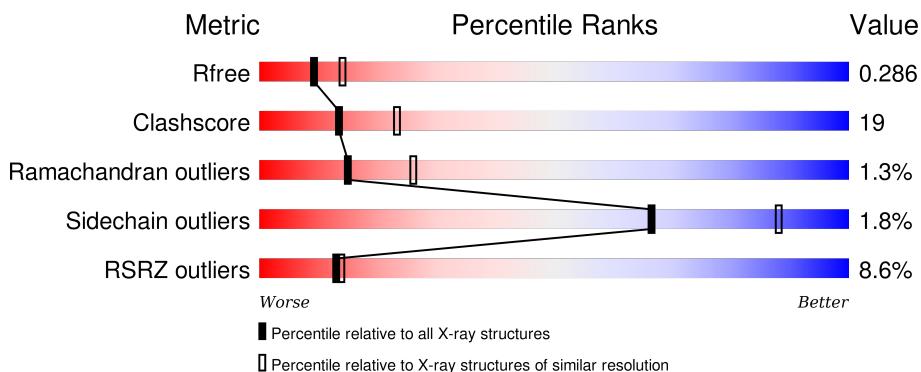
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
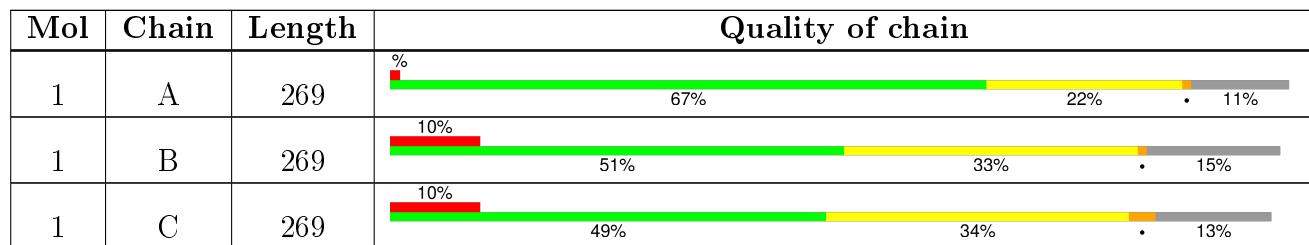
The reported resolution of this entry is 2.50 Å.

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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	269	
1	B	269	
1	C	269	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5544 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 Alpha E-catenin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	Se	0	0	0
			1866	1162	319	376	3	6			
1	B	229	Total	C	N	O	S	Se	0	0	0
			1777	1107	306	356	3	5			
1	C	233	Total	C	N	O	S	Se	0	0	0
			1811	1131	310	362	3	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	GLY	-	CLONING ARTIFACT	UNP P35221
A	384	SER	-	CLONING ARTIFACT	UNP P35221
A	452	MSE	MET	MODIFIED RESIDUE	UNP P35221
A	484	MSE	MET	MODIFIED RESIDUE	UNP P35221
A	560	MSE	MET	MODIFIED RESIDUE	UNP P35221
A	584	MSE	MET	MODIFIED RESIDUE	UNP P35221
A	606	MSE	MET	MODIFIED RESIDUE	UNP P35221
A	631	MSE	MET	MODIFIED RESIDUE	UNP P35221
B	383	GLY	-	CLONING ARTIFACT	UNP P35221
B	384	SER	-	CLONING ARTIFACT	UNP P35221
B	452	MSE	MET	MODIFIED RESIDUE	UNP P35221
B	484	MSE	MET	MODIFIED RESIDUE	UNP P35221
B	560	MSE	MET	MODIFIED RESIDUE	UNP P35221
B	584	MSE	MET	MODIFIED RESIDUE	UNP P35221
B	606	MSE	MET	MODIFIED RESIDUE	UNP P35221
B	631	MSE	MET	MODIFIED RESIDUE	UNP P35221
C	383	GLY	-	CLONING ARTIFACT	UNP P35221
C	384	SER	-	CLONING ARTIFACT	UNP P35221
C	452	MSE	MET	MODIFIED RESIDUE	UNP P35221
C	484	MSE	MET	MODIFIED RESIDUE	UNP P35221
C	560	MSE	MET	MODIFIED RESIDUE	UNP P35221
C	584	MSE	MET	MODIFIED RESIDUE	UNP P35221
C	606	MSE	MET	MODIFIED RESIDUE	UNP P35221

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Chain	Residue	Modelled	Actual	Comment	Reference
C	631	MSE	MET	MODIFIED RESIDUE	UNP P35221
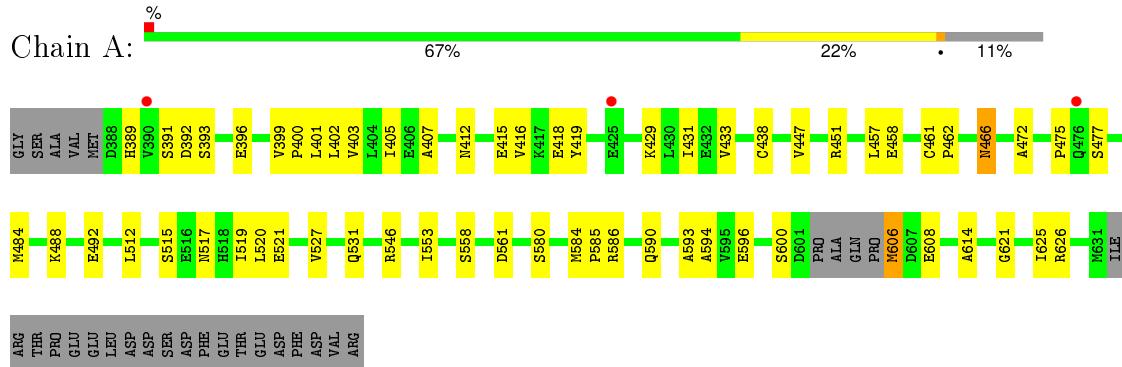
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	43	Total 43	O 43	0	0
2	B	26	Total 26	O 26	0	0
2	C	21	Total 21	O 21	0	0
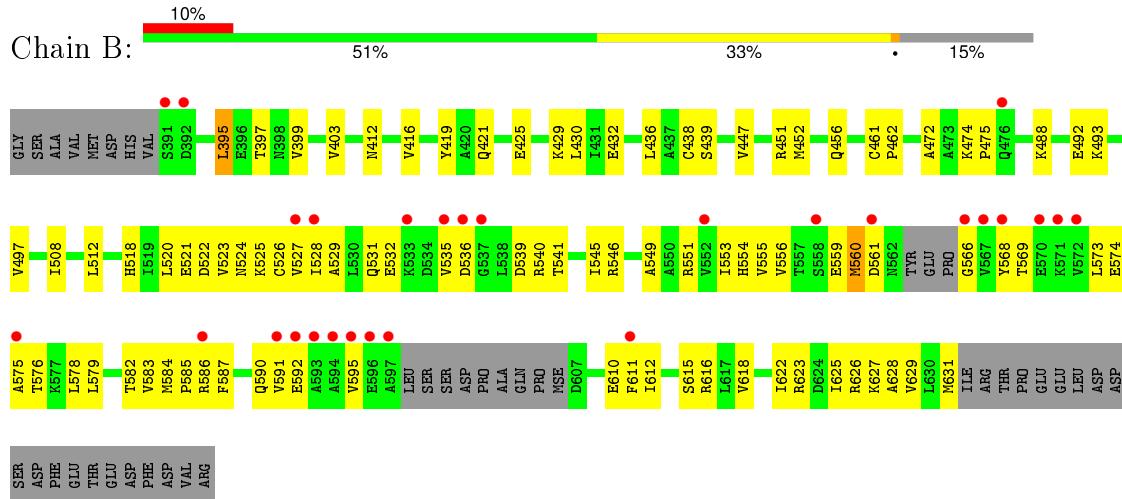
3 Residue-property plots ⓘ

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.
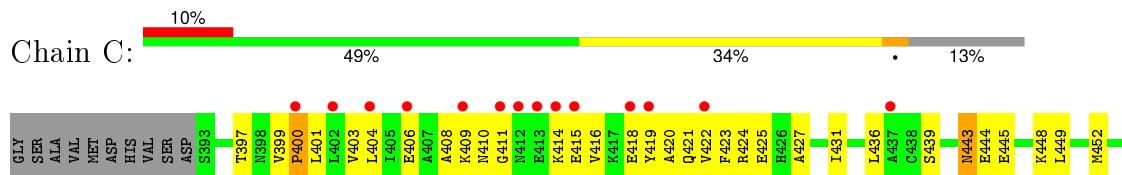
- Molecule 1: Alpha E-catenin
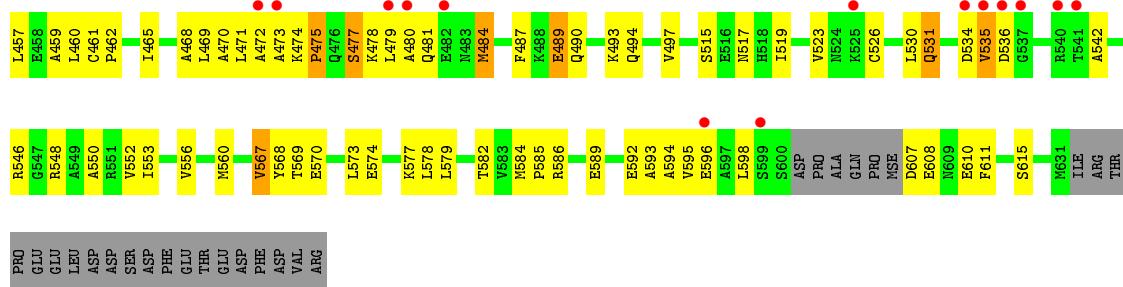
- Molecule 1: Alpha E-catenin

- Molecule 1: Alpha E-catenin

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.78Å 105.29Å 123.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.50 29.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.95-2.50) 98.3 (29.94-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$<I/\sigma(I)>$ [1]	6.43 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.238 , 0.273 0.249 , 0.286	Depositor DCC
R_{free} test set	2919 reflections (9.93%)	DCC
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 56360 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.43	0/1880	0.60	0/2535
1	B	0.36	0/1787	0.53	0/2406
1	C	0.35	0/1824	0.53	0/2459
All	All	0.38	0/5491	0.56	0/7400

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 (i)

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	1866	0	1863	43	0
1	B	1777	0	1786	68	0
1	C	1811	0	1821	96	0
2	A	43	0	0	1	0
2	B	26	0	0	1	0
2	C	21	0	0	1	0
All	All	5544	0	5470	204	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 19.

All (204) 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:560:MSE:HE2	1:C:569:THR:HA	1.42	1.01
1:B:553:ILE:HD11	1:B:579:LEU:HD23	1.47	0.97
1:B:560:MSE:HE2	1:B:569:THR:HG22	1.44	0.97
1:B:628:ALA:HA	1:B:631:MSE:HE2	1.49	0.94
1:C:420:ALA:HB1	1:C:465:ILE:HD11	1.49	0.93
1:C:567:VAL:HG13	1:C:568:TYR:H	1.39	0.86
1:A:461:CYS:HB3	1:A:462:PRO:HD3	1.58	0.84
1:B:591:VAL:O	1:B:595:VAL:HG23	1.85	0.77
1:C:468:ALA:HA	1:C:484:MSE:HE1	1.66	0.76
1:C:542:ALA:O	1:C:546:ARG:HG3	1.86	0.76
1:A:415:GLU:HA	1:A:418:GLU:HG3	1.66	0.75
1:C:461:CYS:HB3	1:C:462:PRO:HD3	1.68	0.75
1:B:586:ARG:O	1:B:590:GLN:HG2	1.85	0.75
1:C:399:VAL:HB	1:C:400:PRO:HD3	1.69	0.73
1:B:549:ALA:O	1:B:553:ILE:HG12	1.89	0.73
1:C:459:ALA:O	1:C:462:PRO:HD2	1.89	0.73
1:B:574:GLU:O	1:B:578:LEU:HG	1.88	0.73
1:C:460:LEU:HD21	1:C:490:GLN:HG3	1.70	0.72
1:A:553:ILE:HD13	1:A:580:SER:HB3	1.71	0.71
1:A:488:LYS:O	1:A:492:GLU:HG3	1.91	0.71
1:C:523:VAL:HG13	1:C:615:SER:HB3	1.72	0.70
1:B:579:LEU:HD12	1:B:583:VAL:HB	1.74	0.70
1:A:447:VAL:O	1:A:451:ARG:HG2	1.91	0.70
1:B:461:CYS:HB3	1:B:462:PRO:HD3	1.74	0.68
1:A:594:ALA:HA	1:A:606:MSE:HE2	1.73	0.68
1:B:421:GLN:O	1:B:425:GLU:HG3	1.93	0.67
1:C:531:GLN:O	1:C:531:GLN:HG2	1.96	0.65
1:C:462:PRO:O	1:C:465:ILE:HG22	1.97	0.64
1:B:520:LEU:O	1:B:523:VAL:HG12	1.95	0.64
1:B:625:ILE:O	1:B:629:VAL:HG23	1.97	0.63
1:B:512:LEU:HD13	1:B:626:ARG:HA	1.79	0.63
1:A:584:MSE:HB2	1:A:585:PRO:HD3	1.80	0.63
1:C:535:VAL:HG13	1:C:595:VAL:HG12	1.80	0.63
1:B:553:ILE:HG23	1:B:576:THR:HG23	1.81	0.62
1:C:422:VAL:HG23	1:C:423:PHE:N	2.13	0.62
1:C:421:GLN:HE22	1:C:424:ARG:HH12	1.48	0.62
1:C:515:SER:O	1:C:519:ILE:HG12	1.99	0.62
1:C:421:GLN:O	1:C:425:GLU:HG3	2.00	0.61
1:B:566:GLY:N	1:B:569:THR:HG1	1.98	0.61
1:C:570:GLU:O	1:C:574:GLU:HG3	2.01	0.60
1:B:560:MSE:HE3	1:B:560:MSE:HA	1.83	0.60
1:B:416:VAL:HG21	1:B:472:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ALA:CB	1:C:465:ILE:HD11	2.27	0.60
1:C:471:LEU:HD11	1:C:481:GLN:HG2	1.84	0.59
1:B:584:MSE:HB2	1:B:585:PRO:HD3	1.84	0.59
1:A:412:ASN:O	1:A:416:VAL:HG23	2.02	0.59
1:B:493:LYS:O	1:B:497:VAL:HG23	2.03	0.58
1:A:621:GLY:O	1:A:625:ILE:HG13	2.03	0.58
1:B:575:ALA:HA	1:B:578:LEU:HD12	1.86	0.58
1:C:419:TYR:O	1:C:422:VAL:HG22	2.03	0.58
1:B:584:MSE:SE	1:B:618:VAL:HG13	2.53	0.57
1:B:541:THR:O	1:B:545:ILE:HG13	2.04	0.57
1:B:574:GLU:OE2	1:B:578:LEU:HD21	2.04	0.57
1:C:465:ILE:O	1:C:469:LEU:HD13	2.04	0.57
1:B:399:VAL:O	1:B:403:VAL:HG23	2.05	0.57
1:B:526:CYS:HG	1:B:611:PHE:HZ	1.52	0.57
1:A:392:ASP:O	1:A:396:GLU:HG2	2.05	0.57
1:B:508:ILE:HD12	1:B:559:GLU:HG3	1.86	0.57
1:B:592:GLU:O	1:B:595:VAL:HB	2.05	0.56
1:C:489:GLU:HG3	1:C:490:GLN:N	2.20	0.56
1:C:560:MSE:HE1	1:C:568:TYR:CE2	2.41	0.56
1:B:518:HIS:HA	1:B:521:GLU:HG2	1.88	0.56
1:B:438:CYS:HA	1:B:447:VAL:HG22	1.87	0.56
1:C:445:GLU:O	1:C:449:LEU:HD23	2.05	0.56
1:A:558:SER:O	1:A:561:ASP:HB2	2.05	0.56
1:A:586:ARG:NH1	2:A:718:HOH:O	2.39	0.56
1:C:567:VAL:HG13	1:C:568:TYR:N	2.15	0.55
1:C:535:VAL:HG12	1:C:535:VAL:O	2.07	0.55
1:C:474:LYS:HG3	1:C:477:SER:HB3	1.88	0.55
1:C:560:MSE:HE2	1:C:569:THR:CA	2.28	0.55
1:C:493:LYS:O	1:C:497:VAL:HG23	2.07	0.55
1:C:530:LEU:CD1	1:C:594:ALA:HB1	2.37	0.55
1:C:397:THR:HG23	1:C:400:PRO:HD2	1.88	0.55
1:C:548:ARG:HD3	2:C:751:HOH:O	2.07	0.54
1:B:628:ALA:HA	1:B:631:MSE:CE	2.32	0.54
1:C:422:VAL:HG23	1:C:423:PHE:H	1.71	0.54
1:C:474:LYS:N	1:C:475:PRO:HD3	2.22	0.54
1:B:578:LEU:O	1:B:582:THR:HB	2.08	0.54
1:A:403:VAL:HG12	1:A:419:TYR:CD1	2.43	0.54
1:C:585:PRO:O	1:C:589:GLU:HG3	2.07	0.54
1:A:517:ASN:O	1:A:521:GLU:HG3	2.08	0.54
1:B:590:GLN:OE1	1:B:610:GLU:HB3	2.08	0.53
1:B:612:ILE:O	1:B:616:ARG:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:VAL:O	1:A:531:GLN:HG3	2.09	0.53
1:A:429:LYS:O	1:A:433:VAL:HG23	2.08	0.53
1:A:399:VAL:HG11	1:B:436:LEU:HD13	1.91	0.53
1:C:478:LYS:HA	1:C:481:GLN:HB2	1.90	0.53
1:C:523:VAL:CG1	1:C:615:SER:HB3	2.39	0.53
1:C:401:LEU:O	1:C:404:LEU:HB3	2.08	0.52
1:C:399:VAL:HG13	1:C:403:VAL:HG21	1.90	0.52
1:A:399:VAL:HB	1:A:400:PRO:HD3	1.92	0.52
1:C:530:LEU:HD13	1:C:594:ALA:HB1	1.91	0.51
1:C:474:LYS:HB2	1:C:477:SER:HB2	1.92	0.51
1:C:550:ALA:HA	1:C:553:ILE:HD12	1.93	0.51
1:C:594:ALA:O	1:C:598:LEU:HG	2.11	0.51
1:A:520:LEU:HD23	1:B:462:PRO:HB2	1.93	0.50
1:A:466:ASN:N	1:A:466:ASN:HD22	2.10	0.50
1:B:524:ASN:O	1:B:528:ILE:HG12	2.11	0.50
1:A:515:SER:O	1:A:519:ILE:HG12	2.11	0.50
1:C:489:GLU:OE2	1:C:493:LYS:HD2	2.12	0.49
1:A:415:GLU:HA	1:A:418:GLU:CG	2.37	0.49
1:C:399:VAL:CB	1:C:400:PRO:HD3	2.39	0.49
1:C:449:LEU:HD13	1:C:452:MSE:HE2	1.93	0.49
1:C:592:GLU:O	1:C:596:GLU:HB2	2.11	0.49
1:A:407:ALA:HB1	1:A:415:GLU:HG3	1.93	0.49
1:A:512:LEU:HD13	1:A:626:ARG:HA	1.94	0.49
1:C:593:ALA:O	1:C:596:GLU:HB3	2.14	0.48
1:A:593:ALA:O	1:A:596:GLU:HB3	2.13	0.48
1:C:478:LYS:HD2	1:C:481:GLN:HB2	1.96	0.48
1:C:448:LYS:O	1:C:452:MSE:HG3	2.14	0.48
1:B:587:PHE:O	1:B:591:VAL:HG23	2.13	0.48
1:A:402:LEU:HD11	1:B:432:GLU:OE2	2.13	0.48
1:B:425:GLU:O	1:B:429:LYS:HG3	2.14	0.48
1:B:582:THR:O	1:B:585:PRO:HD2	2.12	0.48
1:A:461:CYS:HB3	1:A:462:PRO:CD	2.35	0.48
1:B:452:MSE:O	1:B:456:GLN:HG3	2.13	0.48
1:C:415:GLU:O	1:C:419:TYR:HD1	1.96	0.47
1:C:477:SER:OG	1:C:479:LEU:HB3	2.14	0.47
1:B:523:VAL:O	1:B:527:VAL:HG23	2.14	0.47
1:C:560:MSE:HE1	1:C:568:TYR:CD2	2.48	0.47
1:C:427:ALA:O	1:C:431:ILE:HG13	2.14	0.47
1:C:409:LYS:HE3	1:C:410:ASN:OD1	2.13	0.47
1:C:607:ASP:O	1:C:610:GLU:HB3	2.15	0.47
1:C:578:LEU:HD12	1:C:582:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:GLU:HG2	1:C:448:LYS:HE3	1.97	0.47
1:B:536:ASP:O	1:B:540:ARG:HG2	2.15	0.46
1:C:414:LYS:O	1:C:418:GLU:HB2	2.15	0.46
1:C:415:GLU:O	1:C:418:GLU:HB3	2.15	0.46
1:C:474:LYS:HE2	1:C:477:SER:OG	2.15	0.46
1:B:615:SER:O	1:B:618:VAL:HB	2.16	0.46
1:C:582:THR:O	1:C:586:ARG:HG2	2.15	0.46
1:A:403:VAL:CG1	1:A:419:TYR:CE1	2.99	0.46
1:B:579:LEU:HG	1:B:584:MSE:HG2	1.97	0.46
1:C:494:GLN:HA	1:C:494:GLN:NE2	2.31	0.46
1:A:590:GLN:HG3	1:A:614:ALA:CB	2.45	0.46
1:C:471:LEU:C	1:C:473:ALA:H	2.19	0.46
1:C:420:ALA:HB1	1:C:465:ILE:CD1	2.35	0.45
1:C:526:CYS:SG	1:C:611:PHE:HZ	2.39	0.45
1:C:471:LEU:C	1:C:471:LEU:HD23	2.36	0.45
1:A:405:ILE:HG12	1:A:484:MSE:HE2	1.98	0.45
1:B:569:THR:O	1:B:573:LEU:HD12	2.16	0.45
1:C:468:ALA:HA	1:C:484:MSE:CE	2.40	0.45
1:C:552:VAL:O	1:C:556:VAL:HG23	2.15	0.45
1:A:389:HIS:N	1:A:389:HIS:CD2	2.84	0.45
1:C:443:ASN:HD22	1:C:443:ASN:C	2.19	0.45
1:C:399:VAL:HG13	1:C:403:VAL:CG2	2.47	0.45
1:C:406:GLU:O	1:C:406:GLU:HG2	2.17	0.45
1:B:395:LEU:CD2	1:B:430:LEU:HD23	2.47	0.45
1:A:546:ARG:HG3	1:A:546:ARG:HH11	1.80	0.45
1:B:451:ARG:NH2	2:B:743:HOH:O	2.50	0.44
1:C:534:ASP:C	1:C:536:ASP:H	2.21	0.44
1:C:465:ILE:O	1:C:468:ALA:HB3	2.17	0.44
1:A:438:CYS:SG	1:A:447:VAL:HG13	2.58	0.44
1:B:554:HIS:C	1:B:554:HIS:ND1	2.70	0.44
1:C:399:VAL:O	1:C:401:LEU:N	2.50	0.44
1:A:531:GLN:HG2	1:A:608:GLU:OE2	2.18	0.44
1:C:573:LEU:O	1:C:577:LYS:HG3	2.17	0.44
1:C:471:LEU:HD12	1:C:480:ALA:O	2.17	0.44
1:C:471:LEU:HD23	1:C:471:LEU:O	2.18	0.44
1:B:623:ARG:O	1:B:627:LYS:HG3	2.18	0.44
1:C:579:LEU:O	1:C:584:MSE:HG2	2.18	0.43
1:C:408:ALA:HA	1:C:416:VAL:HG21	1.99	0.43
1:B:527:VAL:O	1:B:531:GLN:HG3	2.18	0.43
1:C:477:SER:C	1:C:479:LEU:H	2.21	0.43
1:A:431:ILE:HD13	1:A:458:GLU:HG3	1.99	0.43

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:LEU:O	1:C:439:SER:HB3	2.18	0.43
1:B:551:ARG:O	1:B:555:VAL:HG23	2.18	0.43
1:B:474:LYS:N	1:B:475:PRO:HD3	2.33	0.43
1:A:457:LEU:HA	1:A:457:LEU:HD23	1.87	0.43
1:A:594:ALA:CA	1:A:606:MSE:HE2	2.47	0.43
1:C:470:ALA:O	1:C:473:ALA:HB3	2.18	0.43
1:B:546:ARG:HA	1:B:584:MSE:CE	2.49	0.42
1:C:421:GLN:NE2	1:C:424:ARG:HH12	2.14	0.42
1:B:529:ALA:HA	1:B:532:GLU:HG2	1.99	0.42
1:B:579:LEU:HD21	1:B:622:ILE:CD1	2.49	0.42
1:C:546:ARG:HA	1:C:584:MSE:HE2	2.01	0.42
1:A:407:ALA:CB	1:A:415:GLU:HG3	2.49	0.42
1:B:488:LYS:O	1:B:492:GLU:HG3	2.20	0.42
1:C:584:MSE:HB2	1:C:585:PRO:HD3	2.01	0.42
1:B:579:LEU:HD21	1:B:622:ILE:HD13	2.02	0.42
1:C:457:LEU:HD13	1:C:494:GLN:HG3	2.02	0.42
1:A:391:SER:OG	1:A:393:SER:HB3	2.20	0.42
1:B:535:VAL:O	1:B:539:ASP:OD2	2.38	0.42
1:C:517:ASN:N	1:C:517:ASN:ND2	2.68	0.42
1:B:556:VAL:O	1:B:560:MSE:HB2	2.20	0.42
1:B:403:VAL:HG12	1:B:419:TYR:CE1	2.55	0.42
1:B:436:LEU:O	1:B:439:SER:HB3	2.20	0.42
1:A:472:ALA:O	1:A:475:PRO:HD3	2.20	0.42
1:A:594:ALA:HA	1:A:606:MSE:CE	2.44	0.41
1:A:466:ASN:H	1:A:466:ASN:HD22	1.66	0.41
1:B:582:THR:HG23	1:B:586:ARG:CZ	2.51	0.41
1:B:522:ASP:O	1:B:526:CYS:HB2	2.21	0.41
1:B:403:VAL:HG12	1:B:419:TYR:CD1	2.56	0.41
1:C:523:VAL:O	1:C:526:CYS:HB3	2.21	0.41
1:C:608:GLU:O	1:C:611:PHE:HB3	2.21	0.41
1:C:416:VAL:HG21	1:C:472:ALA:HB2	2.02	0.41
1:C:449:LEU:HA	1:C:452:MSE:HE2	2.03	0.41
1:C:409:LYS:HE2	1:C:409:LYS:HB3	1.91	0.40
1:B:395:LEU:C	1:B:395:LEU:CD2	2.89	0.40
1:C:408:ALA:HA	1:C:416:VAL:CG2	2.51	0.40
1:B:525:LYS:O	1:B:529:ALA:HB2	2.22	0.40
1:C:569:THR:O	1:C:573:LEU:HG	2.22	0.40
1:A:401:LEU:HD21	1:A:488:LYS:HG3	2.03	0.40
1:B:559:GLU:O	1:B:561:ASP:N	2.54	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	236/269 (88%)	221 (94%)	14 (6%)	1 (0%)	39	61
1	B	223/269 (83%)	206 (92%)	16 (7%)	1 (0%)	39	61
1	C	229/269 (85%)	197 (86%)	25 (11%)	7 (3%)	5	7
All	All	688/807 (85%)	624 (91%)	55 (8%)	9 (1%)	15	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	411	GLY
1	B	560	MSE
1	C	477	SER
1	A	477	SER
1	C	531	GLN
1	C	535	VAL
1	C	567	VAL
1	C	475	PRO
1	C	400	PRO

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	206/226 (91%)	203 (98%)	3 (2%)	72	91
1	B	195/226 (86%)	191 (98%)	4 (2%)	61	85
1	C	199/226 (88%)	195 (98%)	4 (2%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	600/678 (88%)	589 (98%)	11 (2%)	66 88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	466	ASN
1	A	600	SER
1	A	606	MSE
1	B	395	LEU
1	B	397	THR
1	B	412	ASN
1	B	568	TYR
1	C	443	ASN
1	C	484	MSE
1	C	487	PHE
1	C	489	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	HIS
1	A	442	ASN
1	A	466	ASN
1	A	494	GLN
1	B	412	ASN
1	B	494	GLN
1	B	524	ASN
1	B	609	ASN
1	C	421	GLN
1	C	435	ASN
1	C	443	ASN
1	C	456	GLN
1	C	463	GLN
1	C	466	ASN
1	C	481	GLN
1	C	517	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 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	234/269 (86%)	0.21	3 (1%)	79	82	25, 43, 71, 84	0
1	B	224/269 (83%)	0.68	28 (12%)	5	5	27, 57, 105, 111	0
1	C	228/269 (84%)	0.75	28 (12%)	5	5	27, 64, 100, 112	0
All	All	686/807 (85%)	0.54	59 (8%)	13	14	25, 54, 100, 112	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	595	VAL	8.8
1	C	419	TYR	6.7
1	C	414	LYS	6.5
1	C	479	LEU	6.3
1	B	567	VAL	5.3
1	C	480	ALA	5.3
1	C	537	GLY	5.3
1	C	536	ASP	4.5
1	B	594	ALA	4.4
1	B	568	TYR	4.3
1	C	402	LEU	4.2
1	C	400	PRO	4.2
1	B	570	GLU	4.1
1	C	418	GLU	4.0
1	C	412	ASN	3.8
1	B	527	VAL	3.7
1	C	525	LYS	3.7
1	C	473	ALA	3.7
1	B	591	VAL	3.6
1	C	413	GLU	3.5
1	B	593	ALA	3.4
1	B	592	GLU	3.4
1	B	596	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	409	LYS	3.4
1	C	541	THR	3.4
1	B	597	ALA	3.2
1	A	425	GLU	3.1
1	C	406	GLU	3.1
1	B	561	ASP	3.1
1	B	391	SER	3.0
1	B	537	GLY	3.0
1	C	534	ASP	3.0
1	C	596	GLU	2.9
1	B	535	VAL	2.8
1	C	422	VAL	2.6
1	B	611	PHE	2.6
1	C	535	VAL	2.6
1	C	404	LEU	2.5
1	B	571	LYS	2.5
1	B	558	SER	2.5
1	C	415	GLU	2.5
1	B	536	ASP	2.5
1	B	566	GLY	2.4
1	B	572	VAL	2.4
1	B	528	ILE	2.4
1	C	482	GLU	2.4
1	C	411	GLY	2.3
1	B	552	VAL	2.3
1	B	476	GLN	2.2
1	C	599	SER	2.2
1	B	586	ARG	2.2
1	A	390	VAL	2.2
1	C	472	ALA	2.2
1	C	540	ARG	2.2
1	B	575	ALA	2.1
1	C	437	ALA	2.1
1	B	533	LYS	2.1
1	B	392	ASP	2.1
1	A	476	GLN	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.