Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:18 am BST

PDB ID	:	2FH4
Title	:	C-terminal half of gelsolin soaked in EGTA at pH 8
Authors	:	Chumnarnsilpa, S.; Loonchanta, A.; Xue, B.; Choe, H.; Urosev, D.; Wang, H.; Burtnick, L.D.; Robinson, R.C.
Deposited on	:	2005-12-23
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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:

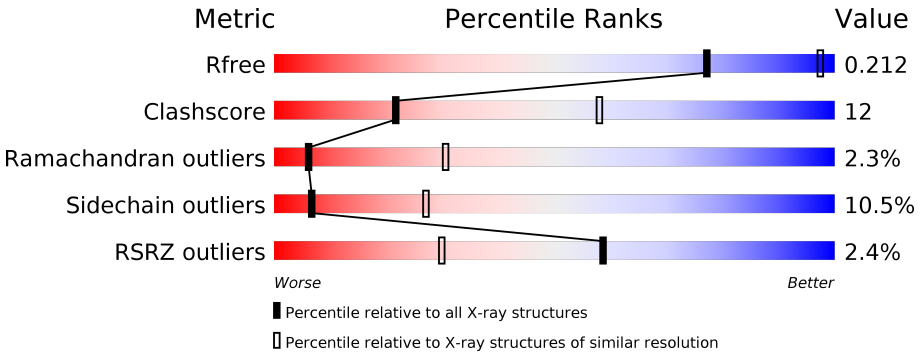
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	344	4% 62% 24% • 11%
1	B	344	% 66% 23% • 7%
1	C	344	% 62% 25% • • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7392 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 Gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2377	1504	403	463	7			
1	B	319	Total	C	N	O	S	0	0	0
			2481	1569	425	481	6			
1	C	318	Total	C	N	O	S	0	0	0
			2467	1561	420	480	6			

- Molecule 2 is water.

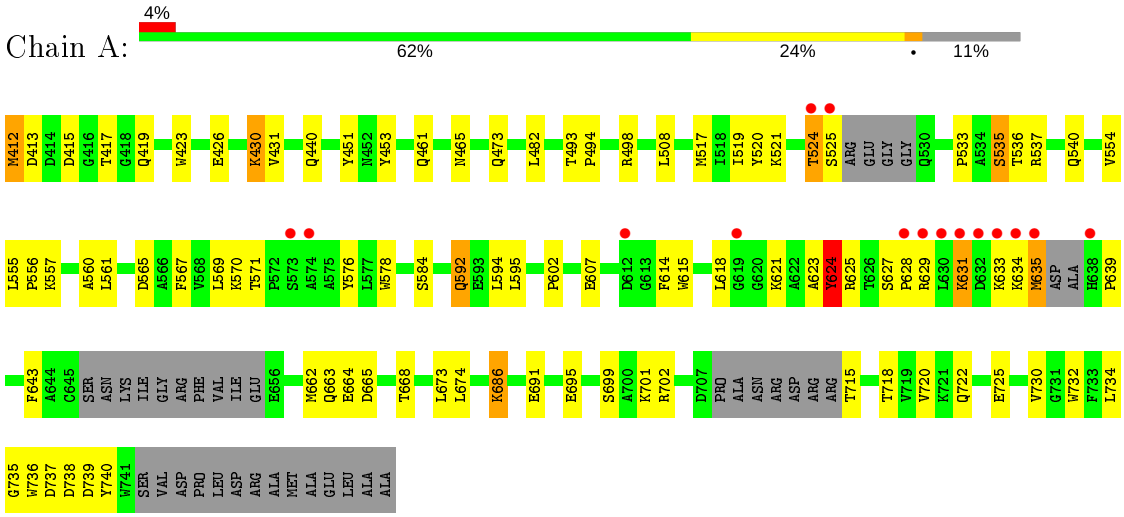
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total	O	0	0
			28	28		
2	B	25	Total	O	0	0
			25	25		
2	C	14	Total	O	0	0
			14	14		

3 Residue-property plots (i)

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.

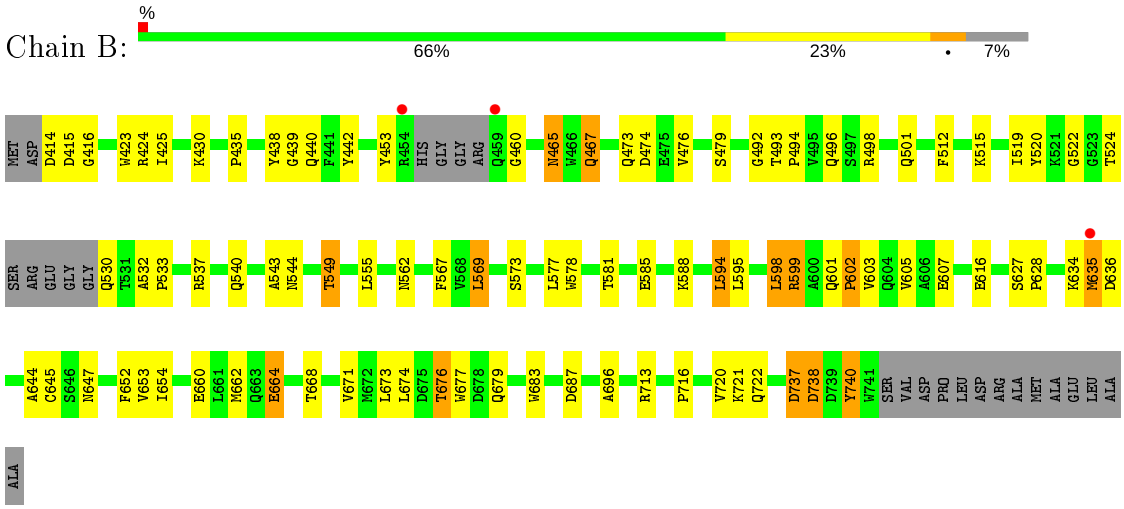
- Molecule 1: Gelsolin

Chain A:



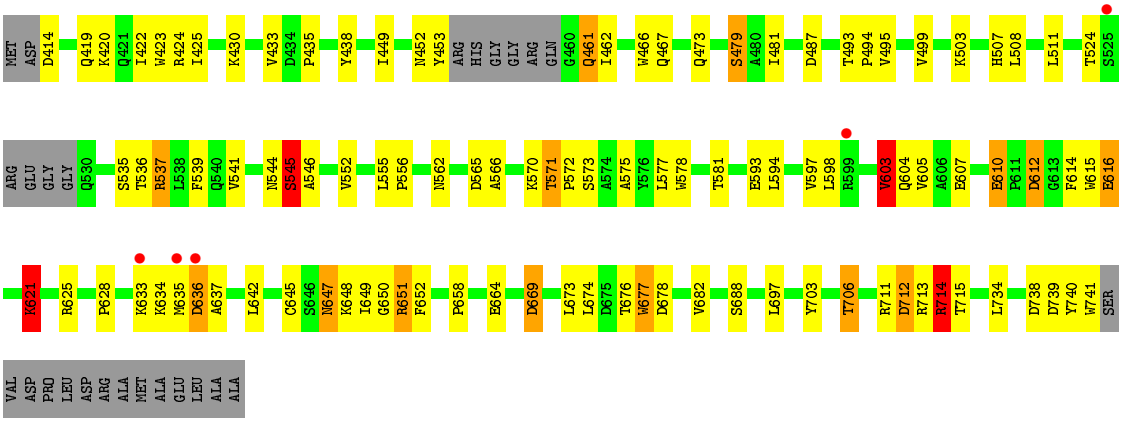
- Molecule 1: Gelsolin

Chain B:



- Molecule 1: Gelsolin

Chain C:


MET ASP D414 Q419 K420 Q421 I422 W423 R424 I425 K430 V433 D434 P435 Y438 I449 N452 Y453 ARG HIS GLY GLY ARG GLN G460 Q461 I462 W466 Q467 Q473 S479 A480 I481 D487 T493 P494 V495 V499 K503 H507 L508 L511 T524 S525
ARG GLU GLY GLY Q530 S535 T536 R537 L538 F539 Q540 V541 N544 S545 A546 V552 L555 P556 N562 D565 A566 K570 T571 P572 S573 A574 A575 Y576 L577 W578 T581 E593 L594 V597 L598 R599 V603 Q604 V605 A606 E607 E610 P611 D612 G613 F614 W615 E616
K621 R625 P628 K633 K634 M635 D636 A637 L642 C645 S646 N647 K648 I649 G650 R651 F652 P658 E664 D669 L673 L674 D675 T676 W677 D678 V682 S688 L697 Y703 T706 R711 D712 R713 R714 T715 L734 D738 D739 Y740 W741 SER
VAL ASP PRO LEU ASP ARG ALA MET ALA GLU LEU ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.11Å 87.78Å 155.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 3.00 29.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.36-3.00) 99.5 (29.36-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.42 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.310 0.217 , 0.212	Depositor DCC
R_{free} test set	1219 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7392	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	0/2431	0.66	0/3298
1	B	0.61	0/2538	0.70	0/3446
1	C	0.58	1/2524 (0.0%)	0.67	0/3428
All	All	0.58	1/7493 (0.0%)	0.68	0/10172

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	565	ASP	CG-OD1	7.09	1.41	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	535	SER	Peptide
1	B	602	PRO	Peptide

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	2377	0	2292	55	0
1	B	2481	0	2406	50	0
1	C	2467	0	2390	66	0
2	A	28	0	0	2	0
2	B	25	0	0	2	0
2	C	14	0	0	1	0
All	All	7392	0	7088	171	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 12.

All (171) 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:426:GLU:OE2	1:A:431:VAL:HB	1.69	0.91
1:C:712:ASP:HB3	1:C:714:ARG:HD2	1.54	0.89
1:B:652:PHE:HE2	1:B:654:ILE:HD11	1.36	0.89
1:B:635:MET:HB3	2:B:758:HOH:O	1.77	0.85
1:C:714:ARG:H	1:C:714:ARG:HD2	1.42	0.85
1:C:712:ASP:HB3	1:C:714:ARG:CD	2.10	0.81
1:A:662:MET:HE1	1:A:734:LEU:HD23	1.64	0.79
1:B:652:PHE:CE2	1:B:654:ILE:HD11	2.18	0.77
1:A:451:TYR:CE2	1:A:453:TYR:HB3	2.21	0.75
1:C:645:CYS:HB3	1:C:652:PHE:CZ	2.24	0.72
1:A:627:SER:HB2	1:A:628:PRO:HD2	1.71	0.71
1:C:435:PRO:HA	1:C:438:TYR:CD2	2.26	0.70
1:A:560:ALA:HA	1:A:625:ARG:CZ	2.21	0.70
1:C:713:ARG:H	1:C:714:ARG:NH1	1.90	0.69
1:C:578:TRP:HZ2	1:C:607:GLU:HG3	1.60	0.67
1:C:433:VAL:O	1:C:438:TYR:HE2	1.77	0.67
1:A:629:ARG:HG3	1:A:732:TRP:HH2	1.59	0.67
1:B:664:GLU:HG2	1:B:740:TYR:OH	1.95	0.66
1:B:599:ARG:HH11	1:B:599:ARG:HB2	1.59	0.66
1:B:738:ASP:N	1:B:738:ASP:OD1	2.25	0.65
1:A:430:LYS:HG2	1:A:482:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:ILE:HG12	1:C:449:ILE:HG12	1.81	0.63
1:A:493:THR:N	1:A:494:PRO:HD2	2.13	0.63
1:C:578:TRP:CZ2	1:C:607:GLU:HG3	2.34	0.62
1:B:493:THR:N	1:B:494:PRO:HD2	2.15	0.61
1:B:524:THR:HB	1:B:530:GLN:OE1	2.00	0.61
1:C:713:ARG:H	1:C:714:ARG:HH11	1.46	0.61
1:A:578:TRP:CZ2	1:A:607:GLU:HG3	2.36	0.61
1:A:561:LEU:O	1:A:625:ARG:HB2	2.02	0.59
1:C:544:ASN:O	1:C:545:SER:C	2.41	0.59
1:A:461:GLN:HB2	1:A:494:PRO:HB3	1.86	0.58
1:C:424:ARG:NH2	1:C:524:THR:OG1	2.35	0.58
1:A:536:THR:HA	1:A:570:LYS:O	2.03	0.57
1:C:649:ILE:HG13	1:C:651:ARG:HB3	1.86	0.57
1:B:423:TRP:CD1	1:B:430:LYS:HG3	2.39	0.57
1:B:465:ASN:HD22	1:B:465:ASN:C	2.08	0.57
1:B:435:PRO:HA	1:B:438:TYR:CD2	2.40	0.57
1:C:605:VAL:HG11	1:C:610:GLU:HB3	1.87	0.56
1:C:615:TRP:CG	1:C:621:LYS:HB2	2.41	0.56
1:A:662:MET:O	1:A:665:ASP:HB2	2.06	0.56
1:C:682:VAL:HG21	1:C:697:LEU:HD23	1.87	0.55
1:B:645:CYS:HB3	1:B:652:PHE:CE1	2.41	0.55
1:B:603:VAL:O	1:B:605:VAL:HG23	2.06	0.55
1:B:671:VAL:HG11	1:B:696:ALA:CB	2.37	0.55
1:C:712:ASP:HB3	1:C:714:ARG:HD3	1.89	0.55
1:B:532:ALA:HB1	1:B:533:PRO:CD	2.37	0.55
1:B:578:TRP:HZ2	1:B:607:GLU:HG3	1.72	0.55
1:A:535:SER:O	1:A:571:THR:HA	2.07	0.54
1:C:739:ASP:O	1:C:741:TRP:N	2.41	0.54
1:C:615:TRP:HB3	1:C:621:LYS:HB2	1.89	0.54
1:A:493:THR:H	1:A:494:PRO:HD2	1.73	0.54
1:C:433:VAL:O	1:C:438:TYR:CE2	2.60	0.53
1:C:612:ASP:HB2	2:C:765:HOH:O	2.09	0.53
1:C:423:TRP:HB3	1:C:430:LYS:HB2	1.89	0.53
1:A:555:LEU:HD23	1:A:557:LYS:HG3	1.91	0.53
1:A:625:ARG:HD3	2:A:774:HOH:O	2.08	0.53
1:B:442:TYR:HB3	1:B:522:GLY:O	2.09	0.53
1:B:737:ASP:O	1:B:740:TYR:HB2	2.10	0.52
1:A:508:LEU:HD12	1:A:508:LEU:O	2.10	0.51
1:B:578:TRP:CZ2	1:B:607:GLU:HG3	2.45	0.51
1:C:712:ASP:OD1	1:C:712:ASP:N	2.38	0.51
1:B:668:THR:HG22	1:B:722:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:ARG:N	1:C:714:ARG:HD2	2.21	0.51
1:B:425:ILE:HG12	1:B:479:SER:HB2	1.92	0.51
1:B:540:GLN:HG3	1:B:567:PHE:CZ	2.45	0.51
1:C:648:LYS:C	1:C:650:GLY:H	2.13	0.50
1:C:676:THR:O	1:C:678:ASP:N	2.40	0.50
1:A:663:GLN:NE2	1:A:736:TRP:CE2	2.79	0.50
1:C:581:THR:O	1:C:633:LYS:HE3	2.11	0.50
1:A:662:MET:CE	1:A:734:LEU:HB3	2.41	0.50
1:C:571:THR:HG22	1:C:573:SER:H	1.76	0.50
1:B:493:THR:H	1:B:494:PRO:HD2	1.76	0.50
1:A:737:ASP:HB3	1:A:740:TYR:HB2	1.94	0.50
1:B:652:PHE:HE2	1:B:654:ILE:CD1	2.17	0.50
1:C:647:ASN:C	1:C:647:ASN:HD22	2.14	0.50
1:A:578:TRP:CD1	1:A:614:PHE:CZ	3.00	0.49
1:A:592:GLN:HA	1:A:595:LEU:HD12	1.93	0.49
1:C:493:THR:N	1:C:494:PRO:CD	2.75	0.49
1:A:561:LEU:HD12	1:A:624:TYR:CD2	2.48	0.49
1:B:453:TYR:N	1:B:460:GLY:O	2.42	0.49
1:C:535:SER:O	1:C:572:PRO:HD3	2.12	0.49
1:A:440:GLN:HG2	1:A:520:TYR:OH	2.13	0.49
1:C:634:LYS:HZ3	1:C:637:ALA:H	1.60	0.49
1:C:612:ASP:O	1:C:616:GLU:HB2	2.13	0.49
1:A:524:THR:CG2	1:A:525:SER:N	2.77	0.48
1:A:557:LYS:O	1:A:618:LEU:HD22	2.13	0.48
1:B:679:GLN:HG3	1:B:716:PRO:HG2	1.94	0.48
1:C:571:THR:HG22	1:C:573:SER:N	2.28	0.48
1:C:462:ILE:HG13	1:C:495:VAL:O	2.13	0.48
1:A:595:LEU:HD13	1:A:602:PRO:HB3	1.96	0.48
1:B:435:PRO:HA	1:B:438:TYR:CE2	2.48	0.48
1:A:423:TRP:HB3	1:A:430:LYS:HB2	1.94	0.48
1:A:629:ARG:CG	1:A:732:TRP:HH2	2.26	0.48
1:B:585:GLU:OE2	1:B:588:LYS:NZ	2.46	0.48
1:B:627:SER:O	1:B:628:PRO:C	2.49	0.48
1:C:452:ASN:HD22	1:C:461:GLN:HG2	1.76	0.48
1:C:577:LEU:HB3	1:C:604:GLN:HA	1.96	0.47
1:C:677:TRP:HA	1:C:711:ARG:NH1	2.29	0.47
1:A:493:THR:N	1:A:494:PRO:CD	2.76	0.47
1:A:686:LYS:HB3	1:A:722:GLN:OE1	2.13	0.47
1:B:524:THR:O	1:B:524:THR:HG23	2.13	0.47
1:A:412:MET:HE1	2:A:757:HOH:O	2.14	0.47
1:C:503:LYS:NZ	1:C:658:PRO:O	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ASP:C	1:B:416:GLY:H	2.18	0.47
1:C:625:ARG:H	1:C:625:ARG:HD2	1.79	0.47
1:A:643:PHE:HB2	1:A:673:LEU:HB2	1.97	0.46
1:B:595:LEU:HD13	1:B:602:PRO:HD3	1.96	0.46
1:C:466:TRP:HA	1:C:499:VAL:O	2.14	0.46
1:C:577:LEU:HD23	1:C:578:TRP:N	2.30	0.46
1:C:714:ARG:O	1:C:715:THR:C	2.53	0.46
1:A:540:GLN:NE2	1:A:565:ASP:OD2	2.39	0.46
1:A:737:ASP:OD2	1:A:738:ASP:N	2.49	0.46
1:B:501:GLN:NE2	1:B:519:ILE:HG21	2.30	0.46
1:C:642:LEU:HD12	1:C:673:LEU:O	2.15	0.46
1:C:712:ASP:CB	1:C:714:ARG:HD2	2.37	0.46
1:A:415:ASP:OD1	1:A:417:THR:OG1	2.28	0.46
1:A:524:THR:HG23	1:A:525:SER:N	2.32	0.46
1:B:636:ASP:HA	2:B:756:HOH:O	2.15	0.46
1:B:671:VAL:HG11	1:B:696:ALA:HB2	1.99	0.45
1:A:629:ARG:HH22	1:A:639:PRO:HA	1.82	0.45
1:C:678:ASP:O	1:C:715:THR:HA	2.17	0.45
1:B:543:ALA:HB2	1:B:549:THR:HG23	1.99	0.45
1:B:644:ALA:O	1:B:654:ILE:HA	2.16	0.45
1:C:414:ASP:OD1	1:C:453:TYR:HB3	2.16	0.45
1:A:554:VAL:HG12	1:A:735:GLY:HA2	1.98	0.45
1:A:662:MET:HE2	1:A:734:LEU:HB3	1.98	0.45
1:B:653:VAL:HG12	1:B:654:ILE:N	2.32	0.45
1:C:493:THR:N	1:C:494:PRO:HD2	2.32	0.45
1:C:645:CYS:HB3	1:C:652:PHE:CE1	2.52	0.45
1:A:615:TRP:CE3	1:A:621:LYS:HA	2.51	0.44
1:B:439:GLY:HA2	1:B:512:PHE:CD2	2.51	0.44
1:B:660:GLU:O	1:B:662:MET:HG3	2.16	0.44
1:C:541:VAL:HB	1:C:566:ALA:HB3	1.99	0.44
1:B:683:TRP:HA	1:B:720:VAL:O	2.17	0.44
1:A:533:PRO:HB2	1:A:537:ARG:NH1	2.32	0.44
1:A:540:GLN:HG3	1:A:567:PHE:CZ	2.52	0.44
1:A:725:GLU:HB3	1:A:730:VAL:HG23	1.99	0.44
1:B:537:ARG:O	1:B:569:LEU:HD23	2.17	0.44
1:C:537:ARG:HG3	1:C:539:PHE:HE1	1.83	0.44
1:C:594:LEU:O	1:C:598:LEU:HB2	2.17	0.44
1:C:669:ASP:O	1:C:688:SER:HA	2.17	0.44
1:A:465:ASN:HB3	1:A:498:ARG:HA	2.00	0.44
1:B:577:LEU:C	1:B:577:LEU:HD23	2.38	0.44
1:B:440:GLN:HB3	1:B:520:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:HD21	1:A:618:LEU:HD23	1.99	0.43
1:B:676:THR:O	1:B:677:TRP:HB3	2.17	0.43
1:C:508:LEU:O	1:C:511:LEU:HB2	2.18	0.43
1:C:552:VAL:HG21	1:C:734:LEU:HD21	2.00	0.43
1:C:578:TRP:CD1	1:C:614:PHE:CZ	3.06	0.43
1:B:594:LEU:HD22	1:B:598:LEU:HD22	2.00	0.43
1:C:703:TYR:O	1:C:706:THR:HB	2.19	0.42
1:A:737:ASP:OD2	1:A:739:ASP:N	2.51	0.42
1:B:532:ALA:HB1	1:B:533:PRO:HD3	2.00	0.42
1:C:593:GLU:O	1:C:597:VAL:HG23	2.19	0.42
1:A:423:TRP:CG	1:A:430:LYS:HD2	2.54	0.42
1:A:578:TRP:HZ2	1:A:607:GLU:HG3	1.84	0.42
1:A:691:GLU:O	1:A:695:GLU:HG2	2.19	0.42
1:C:425:ILE:HG12	1:C:479:SER:HB2	2.02	0.42
1:A:465:ASN:HB3	1:A:498:ARG:HG2	2.02	0.42
1:C:634:LYS:NZ	1:C:637:ALA:H	2.18	0.42
1:C:487:ASP:OD2	1:C:494:PRO:HG2	2.20	0.42
1:A:633:LYS:O	1:A:635:MET:N	2.53	0.41
1:A:627:SER:O	1:A:631:LYS:HB2	2.21	0.41
1:B:467:GLN:HG3	1:B:476:VAL:HG13	2.03	0.41
1:C:575:ALA:O	1:C:603:VAL:HG22	2.21	0.41
1:A:517:MET:HE2	1:A:519:ILE:HD11	2.02	0.41
1:C:555:LEU:HA	1:C:556:PRO:HD3	1.95	0.41
1:C:610:GLU:HG3	1:C:615:TRP:CZ2	2.56	0.41
1:C:648:LYS:C	1:C:650:GLY:N	2.75	0.41
1:B:544:ASN:C	1:B:544:ASN:OD1	2.59	0.40
1:B:493:THR:N	1:B:494:PRO:CD	2.83	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	297/344 (86%)	262 (88%)	31 (10%)	4 (1%)	12 45
1	B	313/344 (91%)	276 (88%)	33 (10%)	4 (1%)	12 45
1	C	312/344 (91%)	268 (86%)	31 (10%)	13 (4%)	3 16
All	All	922/1032 (89%)	806 (87%)	95 (10%)	21 (2%)	6 30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	740	TYR
1	C	603	VAL
1	C	621	LYS
1	C	636	ASP
1	C	677	TRP
1	C	714	ARG
1	C	740	TYR
1	B	492	GLY
1	C	473	GLN
1	C	545	SER
1	A	623	ALA
1	A	634	LYS
1	B	415	ASP
1	C	507	HIS
1	C	546	ALA
1	C	635	MET
1	A	556	PRO
1	B	635	MET
1	C	628	PRO
1	C	651	ARG
1	A	624	TYR

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	246/274 (90%)	222 (90%)	24 (10%)	8 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	257/274 (94%)	227 (88%)	30 (12%)	5 22
1	C	256/274 (93%)	230 (90%)	26 (10%)	7 28
All	All	759/822 (92%)	679 (90%)	80 (10%)	7 27

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	MET
1	A	413	ASP
1	A	419	GLN
1	A	430	LYS
1	A	473	GLN
1	A	521	LYS
1	A	524	THR
1	A	576	TYR
1	A	584	SER
1	A	592	GLN
1	A	594	LEU
1	A	624	TYR
1	A	631	LYS
1	A	635	MET
1	A	664	GLU
1	A	668	THR
1	A	674	LEU
1	A	686	LYS
1	A	699	SER
1	A	701	LYS
1	A	702	ARG
1	A	715	THR
1	A	718	THR
1	A	720	VAL
1	B	424	ARG
1	B	465	ASN
1	B	467	GLN
1	B	473	GLN
1	B	474	ASP
1	B	496	GLN
1	B	498	ARG
1	B	515	LYS
1	B	549	THR
1	B	555	LEU

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Mol	Chain	Res	Type
1	B	562	ASN
1	B	569	LEU
1	B	573	SER
1	B	581	THR
1	B	594	LEU
1	B	598	LEU
1	B	599	ARG
1	B	601	GLN
1	B	616	GLU
1	B	634	LYS
1	B	647	ASN
1	B	664	GLU
1	B	673	LEU
1	B	674	LEU
1	B	676	THR
1	B	687	ASP
1	B	713	ARG
1	B	721	LYS
1	B	737	ASP
1	B	738	ASP
1	C	419	GLN
1	C	420	LYS
1	C	461	GLN
1	C	467	GLN
1	C	479	SER
1	C	481	ILE
1	C	536	THR
1	C	537	ARG
1	C	545	SER
1	C	562	ASN
1	C	570	LYS
1	C	571	THR
1	C	603	VAL
1	C	610	GLU
1	C	612	ASP
1	C	616	GLU
1	C	621	LYS
1	C	636	ASP
1	C	647	ASN
1	C	664	GLU
1	C	669	ASP
1	C	674	LEU

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Mol	Chain	Res	Type
1	C	706	THR
1	C	712	ASP
1	C	714	ARG
1	C	738	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	GLN
1	B	465	ASN
1	B	647	ASN
1	C	421	GLN
1	C	440	GLN
1	C	452	ASN
1	C	507	HIS
1	C	564	ASN
1	C	647	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, 95^{th} 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	307/344 (89%)	-0.01	15 (4%)	29	11	29, 60, 109, 137	0
1	B	319/344 (92%)	-0.34	3 (0%)	84	63	28, 47, 78, 93	0
1	C	318/344 (92%)	-0.18	5 (1%)	72	44	33, 69, 97, 102	0
All	All	944/1032 (91%)	-0.18	23 (2%)	59	30	28, 60, 96, 137	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	ARG	5.2
1	A	525	SER	5.0
1	A	635	MET	4.9
1	A	632	ASP	4.3
1	A	634	LYS	4.1
1	A	633	LYS	4.0
1	A	619	GLY	3.7
1	A	612	ASP	3.6
1	A	524	THR	3.5
1	C	633	LYS	3.3
1	C	599	ARG	3.1
1	A	573	SER	2.8
1	B	459	GLN	2.7
1	C	525	SER	2.7
1	A	630	LEU	2.5
1	C	635	MET	2.4
1	A	628	PRO	2.3
1	A	574	ALA	2.3
1	A	631	LYS	2.2
1	A	638	HIS	2.1
1	C	636	ASP	2.1
1	B	635	MET	2.1
1	B	454	ARG	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.