Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 09:52 PM EST

PDB ID	:	1SJ7
Title	:	Crystal Structure of Talin Rod 482-655
Authors	:	Papagrigoriou, E.; Gingras, A.R.; Barsukov, I.L.; Critchley, D.R.; Emsley, J.
Deposited on	:	2004-03-03
Resolution	:	2.50 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:

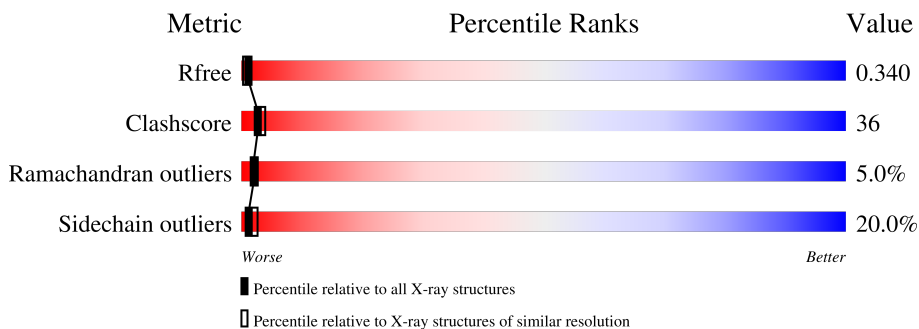|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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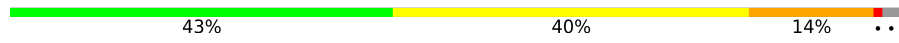*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.340
Clashscore		36
Ramachandran outliers		5.0%
Sidechain outliers		20.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	174	46% 37% 11%
1	B	174	43% 40% 14%
1	C	174	46% 33% 14% 5%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3731 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 Talin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total 1195	C 727	N 214	O 252	S 2	0	0	0
1	B	170	Total 1213	C 739	N 217	O 255	S 2	0	0	0
1	C	166	Total 1186	C 720	N 213	O 251	S 2	0	0	0

- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Pt 2	0	0
2	B	3	Total 3	Pt 3	0	0
2	C	2	Total 2	Pt 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	42	Total 42	O 42	0	0
3	C	39	Total 39	O 39	0	0

3 Residue-property plots ⓘ

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. 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. 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.
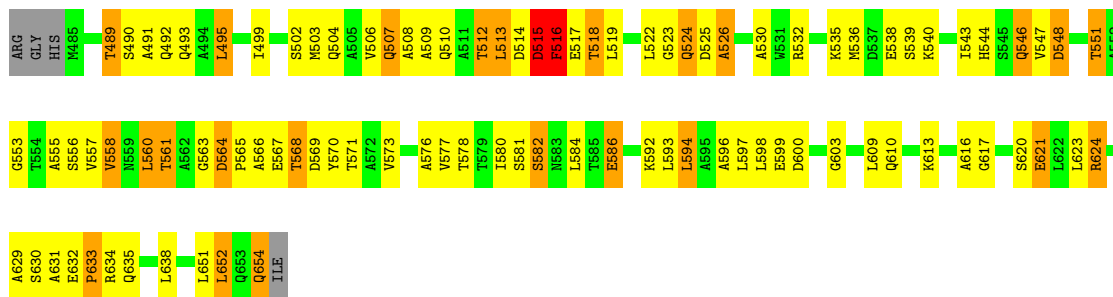
- Molecule 1: Talin 1
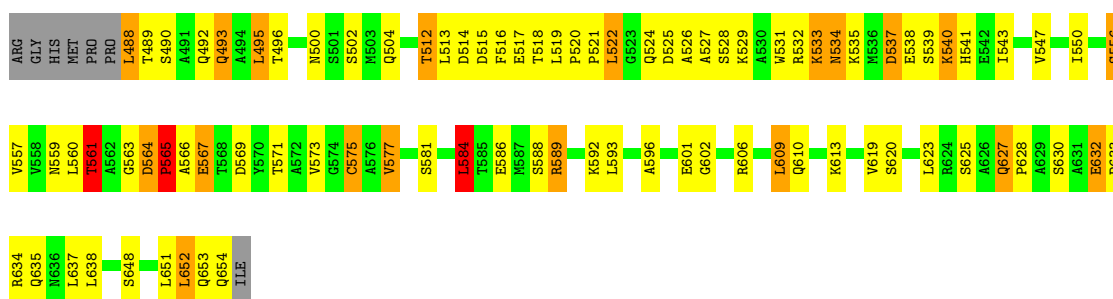
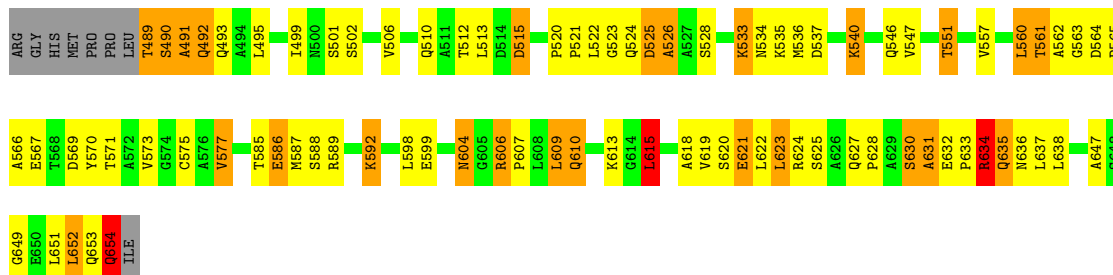- Molecule 1: Talin 1

- Molecule 1: Talin 1

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	95.66Å 95.66Å 115.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.16 – 2.50 47.30 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.16-2.50) 99.8 (47.30-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.241 , 0.286 0.322 , 0.340	Depositor DCC
R_{free} test set	1122 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 11.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	3731	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PT

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	1.24	2/1206 (0.2%)	1.29	8/1640 (0.5%)
1	B	1.18	3/1226 (0.2%)	1.35	10/1670 (0.6%)
1	C	1.21	3/1197 (0.3%)	1.33	11/1628 (0.7%)
All	All	1.21	8/3629 (0.2%)	1.32	29/4938 (0.6%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	GLU	CD-OE2	9.37	1.35	1.25
1	A	575	CYS	CB-SG	6.85	1.93	1.82
1	C	621	GLU	CD-OE2	6.67	1.32	1.25
1	B	654	GLN	CG-CD	6.48	1.66	1.51
1	C	540	LYS	CD-CE	5.81	1.65	1.51
1	C	654	GLN	CA-C	-5.68	1.38	1.52
1	B	621	GLU	CD-OE1	5.45	1.31	1.25
1	B	530	ALA	CA-CB	5.30	1.63	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	515	ASP	CB-CG-OD2	11.23	128.40	118.30
1	B	624	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	B	624	ARG	NE-CZ-NH2	-10.59	115.01	120.30
1	A	514	ASP	CB-CG-OD2	8.33	125.80	118.30
1	B	548	ASP	CB-CG-OD2	8.20	125.68	118.30
1	B	594	LEU	CA-CB-CG	7.92	133.53	115.30
1	C	598	LEU	CB-CG-CD2	-7.91	97.55	111.00
1	C	515	ASP	CB-CG-OD2	7.39	124.95	118.30
1	C	569	ASP	CB-CG-OD2	6.97	124.58	118.30
1	C	606	ARG	CG-CD-NE	-6.83	97.46	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	THR	OG1-CB-CG2	-6.60	94.81	110.00
1	C	615	LEU	CB-CG-CD2	6.60	122.22	111.00
1	C	604	ASN	C-N-CA	-6.50	108.64	122.30
1	C	615	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	515	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	652	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	564	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	623	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	A	584	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	B	594	LEU	CB-CG-CD2	5.63	120.58	111.00
1	A	522	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	B	516	PHE	N-CA-C	-5.50	96.16	111.00
1	A	565	PRO	N-CD-CG	-5.37	95.14	103.20
1	A	589	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	600	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	606	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	540	LYS	CD-CE-NZ	5.11	123.45	111.70
1	A	537	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	532	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	1195	0	1180	92	0
1	B	1213	0	1193	104	0
1	C	1186	0	1167	74	1
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
3	A	49	0	0	3	0
3	B	42	0	0	3	1
3	C	39	0	0	6	1
All	All	3731	0	3540	258	2

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 (258) 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:B:512:THR:CG2	1:B:592:LYS:HE2	1.55	1.37
1:A:632:GLU:CB	1:A:633:PRO:HA	1.62	1.25
1:B:516:PHE:CZ	1:B:599:GLU:HG3	1.75	1.20
1:B:512:THR:HG22	1:B:592:LYS:CE	1.70	1.19
1:B:516:PHE:HZ	1:B:599:GLU:HG3	1.00	1.14
1:A:632:GLU:HB3	1:A:633:PRO:HA	1.14	1.09
1:B:515:ASP:O	1:B:516:PHE:HB2	1.48	1.07
1:C:557:VAL:O	1:C:561:THR:HG22	1.52	1.07
1:C:561:THR:HG23	1:C:634:ARG:HH22	1.16	1.06
1:A:632:GLU:HB3	1:A:633:PRO:CA	1.84	1.06
1:C:586:GLU:HG3	3:C:117:HOH:O	1.55	1.06
1:B:503:MET:O	1:B:506:VAL:HG12	1.57	1.03
1:A:557:VAL:O	1:A:561:THR:HG22	1.61	1.00
1:B:516:PHE:CE2	1:B:596:ALA:HA	1.97	0.99
1:A:550:ILE:HD13	1:A:584:LEU:HD23	1.45	0.97
1:C:523:GLY:O	1:C:525:ASP:N	1.96	0.97
1:C:610:GLN:NE2	1:C:610:GLN:HA	1.79	0.97
1:A:490:SER:O	1:A:493:GLN:HG2	1.65	0.96
1:A:550:ILE:CD1	1:A:584:LEU:HD23	1.96	0.95
1:B:502:SER:HB3	1:B:581:SER:CB	1.96	0.95
1:A:569:ASP:HB2	1:B:568:THR:HG21	1.50	0.94
1:A:632:GLU:CB	1:A:633:PRO:CA	2.40	0.94
1:B:632:GLU:HB3	1:B:633:PRO:HD2	1.51	0.92
1:B:632:GLU:O	1:B:633:PRO:O	1.88	0.90
1:A:632:GLU:HB2	1:A:633:PRO:HA	1.50	0.90
1:B:489:THR:HB	1:B:492:GLN:HG3	1.51	0.90
1:A:569:ASP:CB	1:B:568:THR:HG21	2.03	0.89
1:C:610:GLN:HA	1:C:610:GLN:HE21	1.39	0.88
1:A:517:GLU:OE2	1:B:535:LYS:NZ	2.07	0.87
1:A:561:THR:HG23	1:A:634:ARG:HH22	1.36	0.87
1:B:561:THR:HG23	1:B:561:THR:O	1.74	0.86
1:A:637:LEU:C	1:A:637:LEU:HD23	1.97	0.84
1:C:525:ASP:O	1:C:526:ALA:HB2	1.78	0.82
1:C:561:THR:CG2	1:C:634:ARG:HH22	1.93	0.82
1:A:488:LEU:O	1:A:488:LEU:HG	1.79	0.81
1:B:516:PHE:HZ	1:B:599:GLU:CG	1.89	0.80
1:C:610:GLN:HE21	1:C:610:GLN:CA	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LYS:NZ	1:B:538:GLU:OE2	2.15	0.80
1:B:563:GLY:H	1:B:634:ARG:HH21	1.31	0.79
1:A:652:LEU:C	1:A:654:GLN:H	1.87	0.78
1:B:576:ALA:O	1:B:580:ILE:HG13	1.84	0.78
1:A:637:LEU:HD23	1:A:637:LEU:O	1.83	0.78
1:B:523:GLY:O	1:B:525:ASP:N	2.19	0.76
1:C:495:LEU:HG	1:C:499:ILE:HD12	1.69	0.75
1:B:502:SER:HB3	1:B:581:SER:HB3	1.68	0.74
1:C:565:PRO:C	1:C:567:GLU:H	1.90	0.74
1:B:561:THR:O	1:B:561:THR:CG2	2.36	0.73
1:B:525:ASP:O	1:B:526:ALA:HB3	1.87	0.73
1:C:565:PRO:O	1:C:567:GLU:N	2.21	0.73
1:B:524:GLN:NE2	3:B:121:HOH:O	2.23	0.72
1:A:564:ASP:O	1:A:565:PRO:O	2.07	0.71
1:C:493:GLN:HA	1:C:493:GLN:OE1	1.90	0.71
1:C:502:SER:O	1:C:506:VAL:HG13	1.89	0.71
1:A:540:LYS:NZ	1:A:654:GLN:NE2	2.39	0.71
1:C:525:ASP:O	1:C:526:ALA:CB	2.37	0.71
1:B:632:GLU:CB	1:B:633:PRO:HD2	2.20	0.70
1:C:628:PRO:O	1:C:630:SER:HB2	1.91	0.70
1:A:565:PRO:O	1:A:567:GLU:N	2.24	0.70
1:B:512:THR:CG2	1:B:592:LYS:CE	2.48	0.69
1:A:569:ASP:OD1	1:B:568:THR:CG2	2.41	0.69
1:C:547:VAL:HG11	1:C:652:LEU:HD21	1.75	0.68
1:B:506:VAL:HG13	1:B:507:GLN:N	2.06	0.68
1:C:561:THR:HG23	1:C:634:ARG:NH2	2.00	0.68
1:A:529:LYS:HD3	1:A:532:ARG:NH1	2.09	0.68
1:A:588:SER:O	1:A:592:LYS:HG2	1.93	0.68
1:B:573:VAL:O	1:B:577:VAL:HG13	1.94	0.68
1:C:490:SER:N	3:C:132:HOH:O	2.26	0.68
1:C:533:LYS:HE2	1:C:537:ASP:OD2	1.93	0.68
1:C:546:GLN:NE2	1:C:587:MET:HA	2.08	0.68
1:C:630:SER:O	1:C:631:ALA:CB	2.42	0.67
1:A:527:ALA:O	1:A:528:SER:C	2.31	0.67
1:B:489:THR:CB	1:B:492:GLN:HG3	2.23	0.66
1:A:637:LEU:HB2	3:A:65:HOH:O	1.94	0.66
1:A:586:GLU:OE1	1:B:586:GLU:HG2	1.96	0.66
1:B:510:GLN:HG3	1:B:616:ALA:HB3	1.78	0.66
1:A:512:THR:HG23	1:A:592:LYS:HD3	1.78	0.65
1:B:517:GLU:HG3	1:B:518:THR:N	2.11	0.65
1:B:510:GLN:HG3	1:B:616:ALA:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:SER:HB3	1:B:581:SER:OG	1.97	0.64
1:A:534:ASN:C	1:A:534:ASN:OD1	2.36	0.64
1:A:550:ILE:HD11	1:A:584:LEU:HD23	1.76	0.64
1:B:512:THR:HG22	1:B:592:LYS:HE2	0.75	0.64
1:C:630:SER:O	1:C:631:ALA:HB2	1.99	0.63
1:A:563:GLY:O	1:A:564:ASP:HB3	1.98	0.63
1:C:633:PRO:O	1:C:634:ARG:C	2.35	0.63
1:B:489:THR:HG22	1:B:491:ALA:H	1.65	0.62
1:B:489:THR:HB	1:B:492:GLN:CG	2.26	0.62
1:B:489:THR:HG22	1:B:492:GLN:H	1.63	0.62
1:C:491:ALA:O	1:C:492:GLN:HB2	2.00	0.62
1:B:503:MET:O	1:B:506:VAL:CG1	2.43	0.61
1:B:504:GLN:NE2	3:B:120:HOH:O	2.34	0.60
1:A:652:LEU:C	1:A:654:GLN:N	2.55	0.60
1:A:519:LEU:HB3	1:A:520:PRO:HD2	1.82	0.60
1:C:492:GLN:NE2	3:C:136:HOH:O	2.34	0.60
1:B:547:VAL:O	1:B:551:THR:HG22	2.02	0.60
1:C:606:ARG:N	1:C:607:PRO:CD	2.65	0.59
1:C:637:LEU:HD23	1:C:637:LEU:C	2.22	0.59
1:A:517:GLU:OE2	1:B:535:LYS:CE	2.51	0.59
1:B:632:GLU:HB3	1:B:633:PRO:CD	2.29	0.59
1:A:526:ALA:O	1:A:529:LYS:N	2.36	0.59
1:C:512:THR:O	1:C:592:LYS:HD2	2.02	0.59
1:A:490:SER:O	1:A:493:GLN:CG	2.47	0.59
1:C:633:PRO:O	1:C:635:GLN:N	2.35	0.58
1:B:566:ALA:O	1:B:569:ASP:HB2	2.03	0.58
1:B:631:ALA:O	1:B:632:GLU:HB2	2.03	0.58
1:A:651:LEU:C	1:A:651:LEU:HD13	2.23	0.58
1:B:557:VAL:O	1:B:561:THR:HB	2.04	0.58
1:A:540:LYS:HZ2	1:A:654:GLN:NE2	2.01	0.58
1:A:651:LEU:HD13	1:A:651:LEU:O	2.04	0.58
1:A:537:ASP:HB3	3:A:23:HOH:O	2.04	0.57
1:A:556:SER:O	1:A:560:LEU:HB2	2.03	0.57
1:B:566:ALA:O	1:B:569:ASP:N	2.36	0.57
1:A:557:VAL:O	1:A:561:THR:CG2	2.44	0.57
1:B:544:HIS:HE1	3:B:17:HOH:O	1.87	0.57
1:B:506:VAL:CG1	1:B:507:GLN:N	2.67	0.57
1:B:632:GLU:N	1:B:632:GLU:OE1	2.37	0.57
1:A:517:GLU:OE2	1:B:535:LYS:HE3	2.05	0.57
1:C:615:LEU:HA	1:C:647:ALA:HB1	1.85	0.57
1:B:525:ASP:O	1:B:526:ALA:CB	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:GLY:O	1:C:653:GLN:HG3	2.05	0.56
1:A:632:GLU:HB3	1:A:633:PRO:C	2.24	0.56
1:B:621:GLU:O	1:B:621:GLU:HG3	2.05	0.56
1:C:634:ARG:O	1:C:636:ASN:N	2.39	0.56
1:C:621:GLU:OE2	1:C:624:ARG:NH2	2.37	0.56
1:B:503:MET:C	1:B:506:VAL:HG12	2.25	0.55
1:C:627:GLN:HA	1:C:627:GLN:OE1	2.07	0.55
1:C:615:LEU:HA	1:C:647:ALA:CB	2.36	0.55
1:B:495:LEU:HD22	1:B:499:ILE:HG13	1.89	0.55
1:B:512:THR:C	1:B:514:ASP:H	2.11	0.54
1:B:515:ASP:O	1:B:516:PHE:CB	2.37	0.54
1:C:599:GLU:OE2	1:C:604:ASN:O	2.25	0.54
1:C:610:GLN:HE22	1:C:613:LYS:HE2	1.71	0.54
1:B:578:THR:O	1:B:582:SER:HB3	2.07	0.54
1:C:502:SER:O	1:C:506:VAL:CG1	2.54	0.53
1:C:575:CYS:O	1:C:575:CYS:SG	2.66	0.53
1:A:565:PRO:C	1:A:567:GLU:H	2.11	0.53
1:A:569:ASP:CB	1:B:568:THR:CG2	2.82	0.53
1:C:565:PRO:C	1:C:567:GLU:N	2.57	0.52
1:B:489:THR:HG21	1:B:567:GLU:OE1	2.09	0.52
1:C:520:PRO:HG2	1:C:522:LEU:HD21	1.92	0.52
1:A:495:LEU:HD12	1:A:628:PRO:HG3	1.90	0.52
1:B:507:GLN:HG3	1:B:508:ALA:N	2.24	0.52
1:C:606:ARG:N	1:C:607:PRO:HD2	2.25	0.52
1:A:495:LEU:HD13	1:A:628:PRO:HD3	1.91	0.52
1:A:539:SER:O	1:A:543:ILE:HG13	2.10	0.52
1:A:569:ASP:OD1	1:B:568:THR:HG21	2.09	0.52
1:C:547:VAL:O	1:C:551:THR:HG22	2.11	0.51
1:A:521:PRO:HG2	1:B:522:LEU:HD23	1.92	0.51
1:A:565:PRO:C	1:A:567:GLU:N	2.64	0.51
1:A:550:ILE:HD13	1:A:584:LEU:CD2	2.31	0.50
1:A:516:PHE:CE2	1:A:609:LEU:HD22	2.47	0.50
1:C:491:ALA:O	1:C:492:GLN:CB	2.58	0.50
1:C:534:ASN:OD1	3:C:44:HOH:O	2.20	0.50
1:B:489:THR:HG22	1:B:491:ALA:N	2.27	0.50
1:C:610:GLN:NE2	1:C:613:LYS:HE2	2.27	0.49
1:B:504:GLN:HA	1:B:507:GLN:HG2	1.94	0.49
1:C:489:THR:N	3:C:132:HOH:O	2.45	0.49
1:B:565:PRO:HG2	1:B:570:TYR:OH	2.11	0.49
1:A:496:THR:HG23	1:A:627:GLN:OE1	2.12	0.49
1:C:513:LEU:O	1:C:609:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:MET:O	1:C:540:LYS:HG3	2.11	0.49
1:A:529:LYS:HD3	1:A:532:ARG:HH11	1.76	0.49
1:A:637:LEU:C	1:A:637:LEU:CD2	2.75	0.49
1:B:632:GLU:O	1:B:633:PRO:C	2.51	0.49
1:C:490:SER:O	1:C:491:ALA:HB2	2.13	0.49
1:B:489:THR:CG2	1:B:492:GLN:HG3	2.43	0.49
1:A:531:TRP:O	1:A:532:ARG:C	2.50	0.48
1:B:491:ALA:HB3	1:B:567:GLU:OE1	2.13	0.48
1:C:651:LEU:O	1:C:654:GLN:HA	2.13	0.48
1:C:557:VAL:O	1:C:561:THR:CG2	2.42	0.48
1:B:489:THR:CG2	1:B:567:GLU:OE1	2.62	0.48
1:C:495:LEU:HD11	1:C:573:VAL:HG12	1.96	0.47
1:A:561:THR:O	1:A:561:THR:OG1	2.32	0.47
1:C:622:LEU:O	1:C:622:LEU:HG	2.15	0.47
1:B:652:LEU:C	1:B:654:GLN:N	2.67	0.47
1:B:539:SER:O	1:B:540:LYS:C	2.53	0.47
1:A:569:ASP:CG	1:B:568:THR:HG21	2.34	0.47
1:B:556:SER:O	1:B:560:LEU:HB2	2.14	0.47
1:B:593:LEU:O	1:B:597:LEU:HG	2.14	0.47
1:B:543:ILE:HA	1:B:546:GLN:HE21	1.79	0.47
1:B:548:ASP:HA	1:B:551:THR:HG23	1.97	0.47
1:A:516:PHE:CE2	1:A:609:LEU:CD2	2.99	0.46
1:B:509:ALA:O	1:B:513:LEU:HD22	2.14	0.46
1:C:618:ALA:O	1:C:619:VAL:C	2.53	0.46
1:C:621:GLU:CD	1:C:624:ARG:NH2	2.69	0.46
1:C:586:GLU:CG	3:C:117:HOH:O	2.32	0.46
1:A:547:VAL:O	1:A:550:ILE:N	2.48	0.46
1:A:535:LYS:HA	1:A:535:LYS:HD3	1.71	0.46
1:A:652:LEU:O	1:A:654:GLN:N	2.49	0.46
1:A:495:LEU:CD1	1:A:628:PRO:HD3	2.46	0.46
1:B:489:THR:CG2	1:B:491:ALA:H	2.29	0.46
1:B:553:GLY:O	1:B:557:VAL:N	2.47	0.45
1:B:506:VAL:HG23	1:B:584:LEU:CD2	2.46	0.45
1:C:525:ASP:HB3	1:C:528:SER:HB2	1.98	0.45
1:C:577:VAL:HB	1:C:623:LEU:CD2	2.47	0.45
1:A:561:THR:CG2	1:A:634:ARG:HH22	2.18	0.45
1:A:502:SER:HB3	1:A:581:SER:HB3	1.99	0.45
1:A:564:ASP:OD2	1:A:564:ASP:C	2.55	0.45
1:B:599:GLU:HA	1:B:603:GLY:O	2.17	0.45
1:A:504:GLN:HE21	1:A:504:GLN:HB2	1.53	0.45
1:B:512:THR:C	1:B:514:ASP:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASP:C	1:A:565:PRO:O	2.54	0.45
1:B:507:GLN:HG3	1:B:508:ALA:H	1.81	0.45
1:B:543:ILE:HA	1:B:546:GLN:NE2	2.32	0.44
1:B:652:LEU:C	1:B:654:GLN:H	2.19	0.44
1:B:516:PHE:HE2	1:B:596:ALA:HA	1.71	0.44
1:C:606:ARG:HB2	1:C:607:PRO:HD3	1.99	0.44
1:A:593:LEU:O	1:A:596:ALA:HB3	2.17	0.44
1:B:512:THR:O	1:B:592:LYS:HD3	2.18	0.43
1:C:585:THR:O	1:C:588:SER:HB2	2.18	0.43
1:C:562:ALA:O	1:C:564:ASP:N	2.51	0.43
1:B:513:LEU:HD12	1:B:513:LEU:HA	1.70	0.43
1:B:632:GLU:CB	1:B:633:PRO:CD	2.94	0.43
1:B:512:THR:HG21	1:B:592:LYS:HE2	1.79	0.43
1:C:635:GLN:OE1	1:C:638:LEU:HB2	2.18	0.43
1:A:619:VAL:O	1:A:623:LEU:HD22	2.19	0.43
1:A:637:LEU:CB	3:A:65:HOH:O	2.60	0.43
1:A:588:SER:O	1:A:592:LYS:CG	2.64	0.42
1:C:560:LEU:HD12	1:C:560:LEU:HA	1.64	0.42
1:C:495:LEU:HD22	1:C:570:TYR:HD1	1.84	0.42
1:C:634:ARG:HD2	1:C:634:ARG:HA	1.71	0.42
1:A:490:SER:C	1:A:492:GLN:H	2.22	0.42
1:A:495:LEU:HD12	1:A:628:PRO:CG	2.49	0.42
1:A:560:LEU:HD12	1:A:560:LEU:HA	1.80	0.42
1:B:563:GLY:N	1:B:634:ARG:HH21	2.09	0.42
1:B:617:GLY:O	1:B:620:SER:N	2.52	0.42
1:A:488:LEU:HD12	1:A:489:THR:N	2.34	0.42
1:A:512:THR:HG22	1:A:513:LEU:HG	2.02	0.42
1:A:520:PRO:HB2	1:A:521:PRO:HD2	2.00	0.42
1:B:523:GLY:C	1:B:525:ASP:H	2.22	0.42
1:B:617:GLY:O	1:B:621:GLU:N	2.51	0.42
1:B:564:ASP:HA	1:B:565:PRO:HD2	1.75	0.42
1:B:623:LEU:HA	1:B:623:LEU:HD23	1.75	0.42
1:C:523:GLY:C	1:C:525:ASP:N	2.69	0.42
1:B:616:ALA:O	1:B:617:GLY:C	2.54	0.42
1:C:625:SER:OG	1:C:637:LEU:HG	2.20	0.42
1:A:524:GLN:HE22	1:A:529:LYS:HE2	1.85	0.41
1:C:535:LYS:HA	1:C:535:LYS:HD3	1.96	0.41
1:A:500:ASN:HD22	1:A:500:ASN:HA	1.59	0.41
1:A:569:ASP:OD1	1:B:568:THR:HG22	2.17	0.41
1:B:555:ALA:HA	1:B:558:VAL:HG13	2.02	0.41
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HE3	1:A:533:LYS:HB3	1.77	0.41
1:A:533:LYS:NZ	1:A:537:ASP:OD1	2.51	0.41
1:A:540:LYS:HZ3	1:A:654:GLN:NE2	2.15	0.41
1:C:521:PRO:O	1:C:521:PRO:HG2	2.20	0.41
1:B:633:PRO:C	1:B:635:GLN:N	2.70	0.41
1:A:573:VAL:O	1:A:577:VAL:HG13	2.20	0.41
1:A:630:SER:C	1:A:632:GLU:H	2.25	0.41
1:C:506:VAL:O	1:C:510:GLN:HB2	2.21	0.41
1:C:561:THR:O	1:C:561:THR:OG1	2.39	0.41
1:B:510:GLN:HG3	1:B:616:ALA:HB1	1.99	0.41
1:A:525:ASP:O	1:A:528:SER:HB2	2.21	0.40
1:A:625:SER:OG	1:A:637:LEU:HG	2.22	0.40
1:A:635:GLN:O	1:A:635:GLN:HG3	2.20	0.40
1:B:536:MET:O	1:B:540:LYS:HG3	2.21	0.40
1:C:652:LEU:C	1:C:654:GLN:N	2.74	0.40
1:A:584:LEU:HD22	1:A:584:LEU:HA	1.98	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:73:HOH:O	3:C:10:HOH:O[4_456]	2.03	0.17
1:C:575:CYS:SG	1:C:575:CYS:SG[5_676]	2.16	0.04

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	165/174 (95%)	147 (89%)	12 (7%)	6 (4%)	3	4
1	B	168/174 (97%)	154 (92%)	6 (4%)	8 (5%)	2	2
1	C	164/174 (94%)	146 (89%)	7 (4%)	11 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	497/522 (95%)	447 (90%)	25 (5%)	25 (5%)	2 2

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	PRO
1	A	566	ALA
1	A	632	GLU
1	B	516	PHE
1	B	524	GLN
1	B	526	ALA
1	B	630	SER
1	B	633	PRO
1	C	491	ALA
1	C	525	ASP
1	C	566	ALA
1	C	634	ARG
1	C	490	SER
1	C	492	GLN
1	C	524	GLN
1	C	526	ALA
1	C	563	GLY
1	C	631	ALA
1	C	635	GLN
1	A	602	GLY
1	A	653	GLN
1	B	515	ASP
1	A	564	ASP
1	B	629	ALA
1	B	519	LEU

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	123/131 (94%)	95 (77%)	28 (23%)	1 1

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	125/131 (95%)	99 (79%)	26 (21%)	1	2
1	C	122/131 (93%)	102 (84%)	20 (16%)	2	4
All	All	370/393 (94%)	296 (80%)	74 (20%)	1	2

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	488	LEU
1	A	493	GLN
1	A	495	LEU
1	A	512	THR
1	A	518	THR
1	A	533	LYS
1	A	534	ASN
1	A	540	LYS
1	A	541	HIS
1	A	556	SER
1	A	559	ASN
1	A	561	THR
1	A	567	GLU
1	A	571	THR
1	A	575	CYS
1	A	577	VAL
1	A	584	LEU
1	A	589	ARG
1	A	601	GLU
1	A	606	ARG
1	A	609	LEU
1	A	610	GLN
1	A	613	LYS
1	A	620	SER
1	A	627	GLN
1	A	638	LEU
1	A	648	SER
1	A	652	LEU
1	B	489	THR
1	B	490	SER
1	B	493	GLN
1	B	495	LEU
1	B	507	GLN
1	B	512	THR

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Mol	Chain	Res	Type
1	B	513	LEU
1	B	518	THR
1	B	546	GLN
1	B	551	THR
1	B	558	VAL
1	B	560	LEU
1	B	561	THR
1	B	568	THR
1	B	571	THR
1	B	582	SER
1	B	586	GLU
1	B	594	LEU
1	B	598	LEU
1	B	609	LEU
1	B	610	GLN
1	B	613	LYS
1	B	624	ARG
1	B	638	LEU
1	B	651	LEU
1	B	652	LEU
1	C	489	THR
1	C	501	SER
1	C	515	ASP
1	C	533	LYS
1	C	551	THR
1	C	560	LEU
1	C	561	THR
1	C	571	THR
1	C	577	VAL
1	C	586	GLU
1	C	589	ARG
1	C	592	LYS
1	C	609	LEU
1	C	610	GLN
1	C	615	LEU
1	C	620	SER
1	C	630	SER
1	C	632	GLU
1	C	634	ARG
1	C	654	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	493	GLN
1	A	500	ASN
1	A	504	GLN
1	A	524	GLN
1	A	546	GLN
1	A	635	GLN
1	A	643	ASN
1	A	654	GLN
1	B	493	GLN
1	B	500	ASN
1	B	507	GLN
1	B	546	GLN
1	B	635	GLN
1	B	636	ASN
1	B	639	GLN
1	B	643	ASN
1	C	492	GLN
1	C	500	ASN
1	C	524	GLN
1	C	534	ASN
1	C	546	GLN
1	C	559	ASN
1	C	610	GLN
1	C	639	GLN
1	C	643	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.