



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:43 PM UTC

PDB ID : 1SJ8 / pdb_00001sj8
Title : Solution Structure of the R1R2 Domains of Talin
Authors : Papagrigoriou, E.; Gingras, A.R.; Barsukov, I.L.; Critchley, D.R.; Emsley, J.
Deposited on : 2004-03-03
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

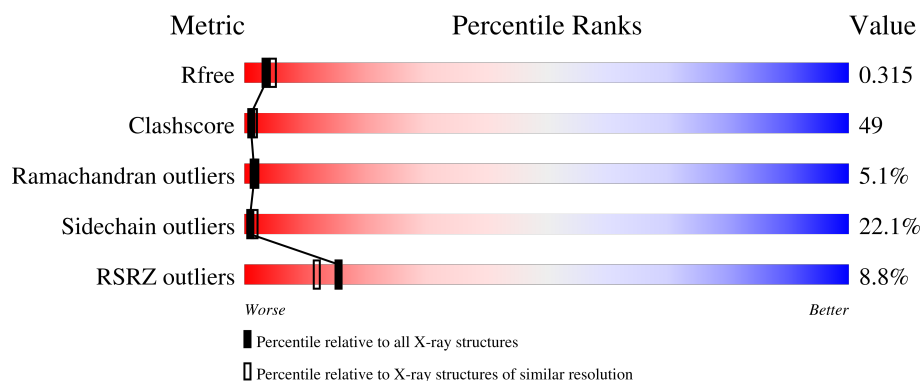
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	308	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2199 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	297	Total	C	N	O	S	0	0	0
			2113	1291	373	440	9			

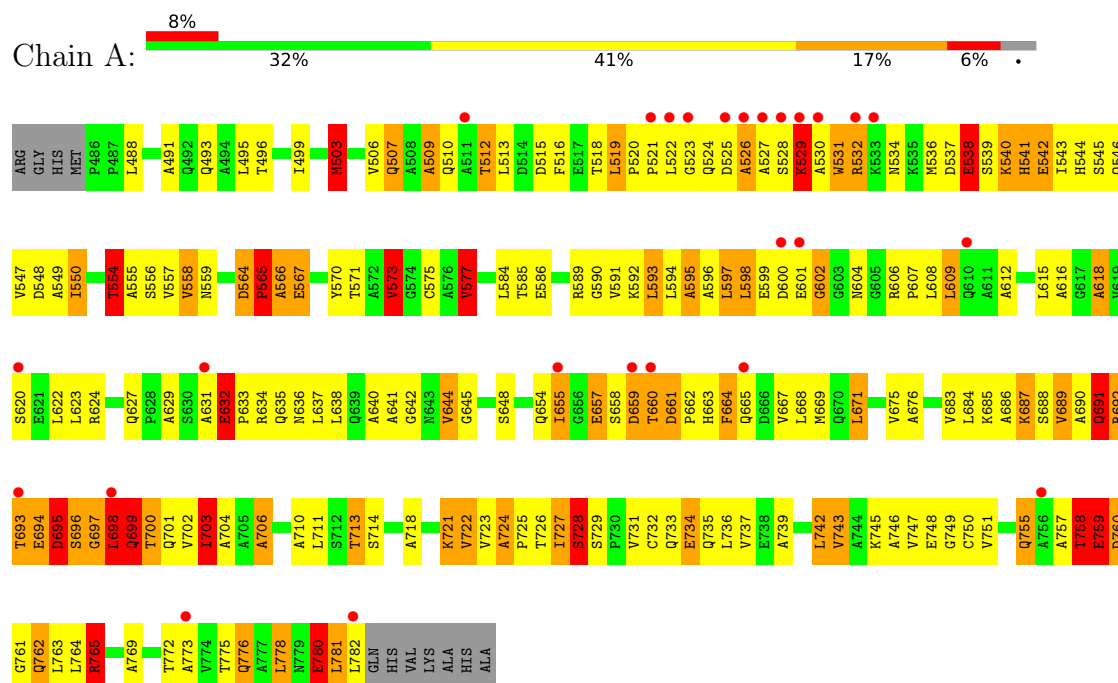
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		

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 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: Talin 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	105.81Å 105.81Å 173.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 99.3 (20.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.258 , 0.297 0.294 , 0.315	Depositor DCC
R_{free} test set	579 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2199	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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	1.90	42/2131 (2.0%)	1.92	65/2902 (2.2%)

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	3	2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	550	ILE	C-O	-11.57	1.11	1.24
1	A	573	VAL	CA-CB	10.93	1.68	1.54
1	A	618	ALA	CA-CB	-8.69	1.39	1.53
1	A	703	ILE	CA-CB	8.66	1.64	1.54
1	A	693	THR	CA-C	-8.46	1.41	1.52
1	A	690	ALA	CA-C	-7.97	1.41	1.52
1	A	702	VAL	CA-CB	-7.78	1.44	1.54
1	A	696	SER	CA-C	-7.67	1.43	1.53
1	A	577	VAL	CA-CB	7.01	1.63	1.54
1	A	638	LEU	C-O	-6.73	1.16	1.24
1	A	660	THR	CA-C	-6.68	1.44	1.53
1	A	694	GLU	N-CA	-6.63	1.37	1.46
1	A	640	ALA	C-O	-6.54	1.16	1.24
1	A	750	CYS	N-CA	-6.43	1.38	1.46
1	A	710	ALA	CA-CB	6.40	1.63	1.53
1	A	491	ALA	CA-CB	-6.26	1.43	1.53
1	A	549	ALA	CA-CB	-6.17	1.43	1.53
1	A	755	GLN	C-O	-6.13	1.16	1.24
1	A	575	CYS	N-CA	-6.12	1.38	1.46
1	A	776	GLN	CA-C	-6.12	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	LEU	C-O	-6.09	1.16	1.24
1	A	718	ALA	C-O	-6.07	1.17	1.24
1	A	724	ALA	CA-C	6.01	1.59	1.52
1	A	644	VAL	CA-C	-5.99	1.44	1.52
1	A	565	PRO	C-O	5.95	1.31	1.24
1	A	550	ILE	CG1-CD1	-5.87	1.28	1.51
1	A	654	GLN	C-O	-5.85	1.16	1.24
1	A	714	SER	C-O	-5.72	1.17	1.24
1	A	499	ILE	N-CA	-5.64	1.39	1.46
1	A	699	GLN	CA-C	-5.61	1.45	1.52
1	A	503	MET	CG-SD	-5.46	1.67	1.80
1	A	631	ALA	CA-C	5.40	1.59	1.52
1	A	632	GLU	CA-CB	-5.28	1.45	1.53
1	A	595	ALA	CA-CB	-5.27	1.44	1.53
1	A	675	VAL	CA-CB	-5.27	1.47	1.54
1	A	636	ASN	C-O	-5.24	1.17	1.24
1	A	706	ALA	CA-CB	-5.24	1.45	1.53
1	A	703	ILE	C-O	-5.22	1.18	1.24
1	A	509	ALA	CA-CB	-5.19	1.45	1.53
1	A	758	THR	CA-CB	5.17	1.62	1.53
1	A	540	LYS	CA-C	5.12	1.59	1.52
1	A	590	GLY	C-O	-5.11	1.17	1.23

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	GLY	CA-C-N	-12.91	96.88	121.54
1	A	697	GLY	C-N-CA	-12.91	96.88	121.54
1	A	698	LEU	O-C-N	-12.52	105.94	122.59
1	A	659	ASP	CA-C-N	-12.09	104.25	123.23
1	A	659	ASP	C-N-CA	-12.09	104.25	123.23
1	A	690	ALA	CA-C-N	-9.82	106.66	122.66
1	A	690	ALA	C-N-CA	-9.82	106.66	122.66
1	A	699	GLN	N-CA-C	9.04	130.05	110.80
1	A	659	ASP	CB-CA-C	-8.68	93.15	110.42
1	A	698	LEU	CB-CA-C	8.41	127.16	110.42
1	A	689	VAL	N-CA-C	-8.17	101.78	110.36
1	A	689	VAL	CA-C-N	-8.06	107.78	122.38
1	A	689	VAL	C-N-CA	-8.06	107.78	122.38
1	A	687	LYS	N-CA-C	-8.06	102.58	111.36
1	A	658	SER	N-CA-C	7.77	127.35	110.80
1	A	531	TRP	N-CA-C	-7.73	103.46	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	689	VAL	CB-CA-C	-7.56	102.21	111.88
1	A	698	LEU	CA-C-N	7.24	135.37	121.54
1	A	698	LEU	C-N-CA	7.24	135.37	121.54
1	A	499	ILE	N-CA-C	-7.23	103.25	110.62
1	A	657	GLU	CA-C-N	7.12	135.14	121.54
1	A	657	GLU	C-N-CA	7.12	135.14	121.54
1	A	664	PHE	N-CA-C	-6.94	103.92	112.38
1	A	506	VAL	N-CA-C	-6.90	102.62	112.35
1	A	555	ALA	N-CA-C	-6.87	103.90	112.90
1	A	691	GLN	N-CA-CB	6.83	120.35	110.65
1	A	538	GLU	N-CA-C	-6.66	103.72	110.97
1	A	697	GLY	N-CA-C	-6.58	97.59	113.18
1	A	567	GLU	N-CA-C	-6.40	104.72	113.30
1	A	609	LEU	N-CA-C	-6.38	104.42	111.82
1	A	659	ASP	N-CA-C	6.36	124.34	110.80
1	A	554	THR	N-CA-C	-6.32	105.54	113.18
1	A	620	SER	CB-CA-C	-6.22	100.10	110.68
1	A	702	VAL	CB-CA-C	-6.21	103.75	112.14
1	A	691	GLN	N-CA-C	-6.07	106.54	112.97
1	A	631	ALA	O-C-N	-6.03	116.17	123.16
1	A	695	ASP	N-CA-C	6.02	123.62	110.80
1	A	573	VAL	N-CA-CB	5.91	118.58	110.54
1	A	780	GLU	CB-CA-C	5.91	122.65	110.31
1	A	749	GLY	N-CA-C	-5.81	107.71	115.32
1	A	493	GLN	N-CA-C	-5.79	105.05	111.36
1	A	745	LYS	CA-C-N	-5.76	111.56	120.31
1	A	745	LYS	C-N-CA	-5.76	111.56	120.31
1	A	746	ALA	N-CA-C	-5.68	105.23	111.82
1	A	507	GLN	CA-C-N	5.65	128.12	120.44
1	A	507	GLN	C-N-CA	5.65	128.12	120.44
1	A	728	SER	N-CA-C	-5.58	105.20	112.23
1	A	693	THR	O-C-N	5.56	129.99	122.59
1	A	573	VAL	CA-C-N	-5.54	113.83	119.98
1	A	573	VAL	C-N-CA	-5.54	113.83	119.98
1	A	739	ALA	N-CA-C	-5.50	106.07	112.89
1	A	757	ALA	CA-C-N	5.43	131.91	121.54
1	A	757	ALA	C-N-CA	5.43	131.91	121.54
1	A	758	THR	N-CA-C	5.42	122.35	110.80
1	A	743	VAL	N-CA-C	5.35	115.56	110.53
1	A	765	ARG	CB-CA-C	5.34	120.47	110.70
1	A	697	GLY	O-C-N	-5.30	115.81	122.70
1	A	558	VAL	CB-CA-C	-5.28	105.21	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	692	ARG	N-CA-C	-5.26	105.18	113.02
1	A	554	THR	N-CA-CB	5.25	119.23	110.41
1	A	616	ALA	N-CA-C	-5.22	104.65	111.02
1	A	742	LEU	N-CA-C	-5.03	105.80	111.28
1	A	722	VAL	CB-CA-C	-5.02	104.12	112.26
1	A	693	THR	N-CA-CB	5.02	118.98	110.49
1	A	530	ALA	N-CA-C	-5.00	105.66	112.26

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	695	ASP	CA
1	A	698	LEU	CA
1	A	699	GLN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	698	LEU	Mainchain,Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2113	0	2127	209	0
2	A	86	0	0	3	0
All	All	2199	0	2127	209	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 49.

All (209) 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:769:ALA:O	1:A:772:THR:HG22	1.31	1.24
1:A:598:LEU:HD12	1:A:598:LEU:H	1.23	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ARG:HD3	1:A:762:GLN:HE22	1.29	0.97
1:A:664:PHE:O	1:A:667:VAL:HG12	1.67	0.94
1:A:541:HIS:HD2	1:A:542:GLU:N	1.66	0.93
1:A:598:LEU:HD12	1:A:598:LEU:N	1.81	0.93
1:A:761:GLY:HA2	1:A:764:LEU:HD13	1.51	0.92
1:A:697:GLY:O	1:A:698:LEU:C	2.03	0.90
1:A:660:THR:O	1:A:661:ASP:C	2.14	0.89
1:A:632:GLU:HB3	1:A:633:PRO:O	1.74	0.87
1:A:759:GLU:O	1:A:760:ASP:HB2	1.72	0.87
1:A:755:GLN:O	1:A:758:THR:HG23	1.74	0.87
1:A:726:THR:O	1:A:728:SER:N	2.07	0.87
1:A:541:HIS:CD2	1:A:542:GLU:N	2.42	0.86
1:A:769:ALA:O	1:A:772:THR:CG2	2.23	0.85
1:A:721:LYS:C	1:A:721:LYS:HD3	2.00	0.85
1:A:726:THR:O	1:A:727:ILE:HG13	1.77	0.84
1:A:559:ASN:ND2	1:A:735:GLN:HE21	1.77	0.83
1:A:726:THR:HG22	1:A:727:ILE:N	1.94	0.83
1:A:496:THR:HG23	1:A:627:GLN:HE22	1.46	0.81
1:A:554:THR:HG21	1:A:644:VAL:HG11	1.62	0.81
1:A:727:ILE:C	1:A:727:ILE:HD12	2.08	0.79
1:A:693:THR:HB	1:A:699:GLN:HB2	1.64	0.79
1:A:532:ARG:O	1:A:536:MET:HB2	1.82	0.79
1:A:726:THR:CG2	1:A:729:SER:HB3	2.17	0.75
1:A:769:ALA:C	1:A:772:THR:HG22	2.11	0.75
1:A:559:ASN:HD22	1:A:735:GLN:HE21	1.32	0.74
1:A:697:GLY:C	1:A:698:LEU:HD23	2.12	0.74
1:A:698:LEU:CB	1:A:701:GLN:H	2.00	0.74
1:A:529:LYS:HA	1:A:532:ARG:NE	2.04	0.73
1:A:726:THR:HG21	1:A:729:SER:HB3	1.68	0.73
1:A:564:ASP:N	1:A:564:ASP:OD1	2.21	0.73
1:A:684:LEU:C	1:A:684:LEU:HD23	2.14	0.73
1:A:539:SER:O	1:A:543:ILE:HG12	1.88	0.72
1:A:676:ALA:HA	1:A:713:THR:HG21	1.73	0.71
1:A:721:LYS:HD3	1:A:721:LYS:O	1.90	0.71
1:A:565:PRO:O	1:A:566:ALA:HB2	1.91	0.71
1:A:523:GLY:O	1:A:532:ARG:NH2	2.23	0.70
1:A:660:THR:HG22	1:A:664:PHE:HD2	1.55	0.70
1:A:755:GLN:CA	1:A:758:THR:HG23	2.22	0.70
1:A:698:LEU:HB2	1:A:701:GLN:N	2.06	0.70
1:A:541:HIS:CD2	1:A:541:HIS:C	2.69	0.70
1:A:598:LEU:H	1:A:598:LEU:CD1	2.02	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:PRO:O	1:A:566:ALA:CB	2.39	0.69
1:A:726:THR:C	1:A:728:SER:H	1.99	0.69
1:A:559:ASN:HD22	1:A:735:GLN:NE2	1.91	0.68
1:A:641:ALA:O	1:A:722:VAL:HG22	1.93	0.68
1:A:697:GLY:CA	1:A:698:LEU:HD23	2.24	0.68
1:A:512:THR:HG23	1:A:592:LYS:HD2	1.74	0.68
1:A:541:HIS:HD2	1:A:542:GLU:H	1.40	0.67
1:A:698:LEU:HB2	1:A:701:GLN:H	1.57	0.67
1:A:657:GLU:HA	1:A:657:GLU:OE2	1.93	0.67
1:A:703:ILE:HG13	1:A:704:ALA:N	2.10	0.67
1:A:758:THR:HG22	1:A:763:LEU:HD11	1.77	0.66
1:A:697:GLY:HA2	1:A:698:LEU:HD23	1.78	0.66
1:A:737:VAL:HG12	1:A:781:LEU:HD13	1.78	0.66
1:A:529:LYS:HA	1:A:532:ARG:CZ	2.25	0.66
1:A:585:THR:HG22	1:A:589:ARG:NH1	2.11	0.66
1:A:698:LEU:HD23	1:A:698:LEU:N	2.10	0.65
1:A:726:THR:HG21	1:A:732:CYS:SG	2.36	0.65
1:A:532:ARG:H	1:A:532:ARG:HD2	1.61	0.65
1:A:546:GLN:O	1:A:550:ILE:HG12	1.96	0.65
1:A:698:LEU:HB2	1:A:701:GLN:CB	2.27	0.65
1:A:755:GLN:HA	1:A:758:THR:HG23	1.79	0.65
1:A:698:LEU:CB	1:A:701:GLN:N	2.60	0.65
1:A:697:GLY:O	1:A:699:GLN:N	2.31	0.64
1:A:698:LEU:HD22	1:A:700:THR:HG23	1.80	0.64
1:A:755:GLN:C	1:A:758:THR:HG23	2.22	0.64
1:A:655:ILE:HG13	1:A:657:GLU:HB2	1.79	0.64
1:A:661:ASP:O	1:A:664:PHE:HB3	1.97	0.64
1:A:762:GLN:HA	1:A:765:ARG:HD2	1.80	0.63
1:A:637:LEU:C	1:A:637:LEU:HD23	2.24	0.63
1:A:516:PHE:CZ	1:A:606:ARG:HD2	2.34	0.63
1:A:520:PRO:HG2	1:A:520:PRO:O	1.98	0.62
1:A:559:ASN:ND2	1:A:735:GLN:NE2	2.45	0.61
1:A:698:LEU:HB3	1:A:700:THR:HG23	1.81	0.61
1:A:519:LEU:HD21	1:A:597:LEU:HD13	1.81	0.61
1:A:683:VAL:HG22	1:A:706:ALA:O	2.01	0.61
1:A:698:LEU:HB3	1:A:700:THR:N	2.15	0.61
1:A:759:GLU:O	1:A:760:ASP:CB	2.48	0.60
1:A:645:GLY:HA3	1:A:722:VAL:HA	1.82	0.60
1:A:542:GLU:O	1:A:543:ILE:C	2.41	0.60
1:A:755:GLN:O	1:A:758:THR:CG2	2.49	0.60
1:A:550:ILE:O	1:A:554:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:PRO:O	1:A:521:PRO:C	2.42	0.60
1:A:594:LEU:O	1:A:598:LEU:CD1	2.50	0.59
1:A:595:ALA:HB2	1:A:608:LEU:HB3	1.84	0.59
1:A:723:VAL:O	1:A:727:ILE:HG23	2.03	0.58
1:A:536:MET:HG3	1:A:594:LEU:CD1	2.34	0.58
1:A:693:THR:CB	1:A:699:GLN:HB2	2.32	0.58
1:A:593:LEU:C	1:A:593:LEU:HD13	2.29	0.58
1:A:525:ASP:O	1:A:526:ALA:C	2.47	0.57
1:A:733:GLN:O	1:A:734:GLU:C	2.45	0.57
1:A:685:LYS:HD2	1:A:769:ALA:HB2	1.87	0.57
1:A:698:LEU:HB3	1:A:700:THR:H	1.69	0.57
1:A:762:GLN:O	1:A:765:ARG:HG2	2.05	0.57
1:A:692:ARG:O	1:A:694:GLU:N	2.37	0.56
1:A:536:MET:O	1:A:540:LYS:HB2	2.06	0.56
1:A:778:LEU:HD22	1:A:778:LEU:O	2.06	0.56
1:A:509:ALA:O	1:A:512:THR:HB	2.06	0.56
1:A:503:MET:HE1	1:A:624:ARG:HH11	1.71	0.55
1:A:634:ARG:HG2	1:A:711:LEU:HD11	1.89	0.55
1:A:545:SER:O	1:A:548:ASP:HB2	2.05	0.55
1:A:665:GLN:O	1:A:669:MET:HG2	2.07	0.54
1:A:692:ARG:HH12	1:A:760:ASP:CG	2.15	0.54
1:A:593:LEU:HD13	1:A:597:LEU:CD2	2.38	0.54
1:A:662:PRO:C	1:A:664:PHE:H	2.16	0.54
1:A:528:SER:O	1:A:531:TRP:N	2.37	0.54
1:A:543:ILE:HD12	1:A:591:VAL:HG23	1.91	0.53
1:A:669:MET:HE1	1:A:721:LYS:HG2	1.89	0.53
1:A:696:SER:C	1:A:697:GLY:O	2.45	0.53
1:A:534:ASN:O	1:A:538:GLU:HG2	2.09	0.53
1:A:632:GLU:CB	1:A:633:PRO:CA	2.86	0.53
1:A:595:ALA:HA	1:A:598:LEU:HD13	1.91	0.53
1:A:573:VAL:O	1:A:577:VAL:HG13	2.08	0.52
1:A:564:ASP:HB2	1:A:567:GLU:OE1	2.10	0.52
1:A:671:LEU:HB3	1:A:780:GLU:HB2	1.91	0.52
1:A:687:LYS:O	1:A:691:GLN:HG3	2.10	0.52
1:A:723:VAL:HB	1:A:732:CYS:HB3	1.92	0.52
1:A:532:ARG:HG2	1:A:601:GLU:CD	2.35	0.52
1:A:667:VAL:O	1:A:671:LEU:HB2	2.10	0.52
1:A:525:ASP:O	1:A:526:ALA:O	2.27	0.51
1:A:529:LYS:O	1:A:529:LYS:HD3	2.10	0.51
1:A:541:HIS:CE1	2:A:87:HOH:O	2.63	0.51
1:A:546:GLN:NE2	1:A:586:GLU:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:GLU:HB3	1:A:633:PRO:C	2.35	0.51
1:A:761:GLY:HA2	1:A:764:LEU:CD1	2.33	0.51
1:A:600:ASP:O	1:A:601:GLU:C	2.50	0.51
1:A:726:THR:C	1:A:727:ILE:HG13	2.35	0.50
1:A:495:LEU:HD11	1:A:573:VAL:HG22	1.93	0.50
1:A:724:ALA:N	1:A:725:PRO:HD2	2.26	0.50
1:A:743:VAL:O	1:A:747:VAL:HG23	2.12	0.50
1:A:772:THR:HG23	1:A:773:ALA:N	2.26	0.50
1:A:547:VAL:CG1	1:A:648:SER:HB3	2.42	0.50
1:A:684:LEU:HD23	1:A:685:LYS:N	2.27	0.50
1:A:724:ALA:C	1:A:726:THR:H	2.19	0.49
1:A:554:THR:O	1:A:558:VAL:HG23	2.13	0.49
1:A:513:LEU:HD13	1:A:612:ALA:HB3	1.94	0.49
1:A:758:THR:HG22	1:A:763:LEU:CD1	2.42	0.49
1:A:541:HIS:ND1	2:A:87:HOH:O	2.35	0.48
1:A:540:LYS:O	1:A:657:GLU:HG2	2.14	0.48
1:A:660:THR:CG2	1:A:727:ILE:HD11	2.44	0.48
1:A:698:LEU:HB2	1:A:701:GLN:HB2	1.96	0.48
1:A:660:THR:CG2	1:A:664:PHE:HD2	2.23	0.48
1:A:513:LEU:HD13	1:A:612:ALA:CB	2.44	0.47
1:A:698:LEU:HB3	1:A:701:GLN:N	2.29	0.47
1:A:536:MET:HE2	1:A:597:LEU:HB3	1.95	0.47
1:A:532:ARG:O	1:A:536:MET:HE3	2.14	0.47
1:A:688:SER:O	1:A:689:VAL:C	2.58	0.47
1:A:692:ARG:HD3	1:A:762:GLN:NE2	2.13	0.47
1:A:698:LEU:HB3	1:A:701:GLN:H	1.78	0.47
1:A:594:LEU:O	1:A:598:LEU:HD12	2.14	0.47
1:A:609:LEU:N	1:A:609:LEU:HD22	2.31	0.46
1:A:727:ILE:C	1:A:727:ILE:CD1	2.77	0.46
1:A:601:GLU:O	1:A:602:GLY:O	2.34	0.46
1:A:684:LEU:C	1:A:684:LEU:CD2	2.88	0.46
1:A:523:GLY:C	1:A:525:ASP:H	2.24	0.45
1:A:735:GLN:NE2	1:A:735:GLN:HA	2.30	0.45
1:A:759:GLU:H	1:A:763:LEU:HD12	1.81	0.45
1:A:660:THR:HG21	1:A:727:ILE:HD11	1.99	0.45
1:A:676:ALA:HA	1:A:713:THR:CG2	2.44	0.45
1:A:724:ALA:O	1:A:726:THR:N	2.49	0.45
1:A:518:THR:O	1:A:518:THR:HG23	2.16	0.45
1:A:723:VAL:CG1	1:A:732:CYS:HB3	2.46	0.45
1:A:608:LEU:HA	1:A:608:LEU:HD12	1.58	0.45
1:A:724:ALA:C	1:A:726:THR:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:GLN:O	1:A:699:GLN:HG2	2.11	0.45
1:A:495:LEU:HD22	1:A:570:TYR:HD1	1.82	0.45
1:A:632:GLU:CB	1:A:633:PRO:C	2.90	0.45
1:A:503:MET:HE1	1:A:624:ARG:NH1	2.33	0.44
1:A:632:GLU:CB	1:A:633:PRO:HA	2.47	0.44
1:A:556:SER:O	1:A:557:VAL:C	2.58	0.44
1:A:564:ASP:HA	1:A:565:PRO:HD2	1.86	0.44
1:A:599:GLU:OE1	1:A:604:ASN:HA	2.18	0.44
1:A:516:PHE:HB3	1:A:596:ALA:HB2	2.00	0.44
1:A:660:THR:O	1:A:661:ASP:O	2.34	0.44
1:A:607:PRO:HG3	2:A:99:HOH:O	2.17	0.43
1:A:634:ARG:CG	1:A:711:LEU:HD11	2.47	0.43
1:A:615:LEU:O	1:A:618:ALA:HB3	2.19	0.43
1:A:527:ALA:O	1:A:528:SER:C	2.61	0.43
1:A:660:THR:CG2	1:A:664:PHE:CD2	3.01	0.43
1:A:662:PRO:C	1:A:664:PHE:N	2.77	0.43
1:A:544:HIS:CD2	1:A:657:GLU:HG3	2.54	0.43
1:A:635:GLN:O	1:A:635:GLN:HG3	2.18	0.43
1:A:684:LEU:O	1:A:687:LYS:N	2.47	0.42
1:A:762:GLN:HA	1:A:765:ARG:CD	2.48	0.42
1:A:727:ILE:HD12	1:A:728:SER:N	2.34	0.42
1:A:782:LEU:HA	1:A:782:LEU:HD13	1.22	0.42
1:A:632:GLU:HB2	1:A:633:PRO:HA	2.02	0.42
1:A:488:LEU:HD11	1:A:629:ALA:HB2	2.01	0.42
1:A:781:LEU:HD22	1:A:781:LEU:HA	1.89	0.42
1:A:693:THR:HB	1:A:699:GLN:CB	2.44	0.42
1:A:593:LEU:O	1:A:597:LEU:HD22	2.19	0.42
1:A:698:LEU:HD22	1:A:700:THR:CG2	2.47	0.42
1:A:586:GLU:HG2	1:A:589:ARG:NH2	2.35	0.42
1:A:532:ARG:H	1:A:532:ARG:CD	2.25	0.42
1:A:543:ILE:CD1	1:A:591:VAL:HG23	2.50	0.42
1:A:662:PRO:O	1:A:664:PHE:N	2.51	0.42
1:A:694:GLU:O	1:A:695:ASP:C	2.62	0.42
1:A:585:THR:HG22	1:A:589:ARG:HH12	1.83	0.41
1:A:684:LEU:C	1:A:686:ALA:N	2.76	0.41
1:A:661:ASP:HA	1:A:662:PRO:HD2	1.81	0.41
1:A:515:ASP:CG	1:A:516:PHE:H	2.29	0.41
1:A:642:GLY:HA2	1:A:722:VAL:HG23	2.03	0.41
1:A:655:ILE:HG21	1:A:655:ILE:HD13	1.76	0.41
1:A:606:ARG:N	1:A:607:PRO:CD	2.84	0.41
1:A:772:THR:CG2	1:A:773:ALA:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:ILE:O	1:A:733:GLN:NE2	2.54	0.40
1:A:727:ILE:HD12	1:A:727:ILE:O	2.20	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	295/308 (96%)	247 (84%)	33 (11%)	15 (5%)	1 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	ALA
1	A	659	ASP
1	A	699	GLN
1	A	727	ILE
1	A	758	THR
1	A	760	ASP
1	A	565	PRO
1	A	566	ALA
1	A	695	ASP
1	A	632	GLU
1	A	529	LYS
1	A	661	ASP
1	A	602	GLY
1	A	655	ILE
1	A	759	GLU

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	222/230 (96%)	173 (78%)	49 (22%)	1 2

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	MET
1	A	507	GLN
1	A	510	GLN
1	A	512	THR
1	A	519	LEU
1	A	522	LEU
1	A	524	GLN
1	A	529	LYS
1	A	532	ARG
1	A	537	ASP
1	A	538	GLU
1	A	541	HIS
1	A	542	GLU
1	A	554	THR
1	A	564	ASP
1	A	571	THR
1	A	573	VAL
1	A	577	VAL
1	A	584	LEU
1	A	593	LEU
1	A	597	LEU
1	A	598	LEU
1	A	623	LEU
1	A	663	HIS
1	A	668	LEU
1	A	671	LEU
1	A	691	GLN
1	A	695	ASP
1	A	698	LEU
1	A	700	THR

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Mol	Chain	Res	Type
1	A	703	ILE
1	A	713	THR
1	A	721	LYS
1	A	728	SER
1	A	731	VAL
1	A	734	GLU
1	A	736	LEU
1	A	742	LEU
1	A	748	GLU
1	A	751	VAL
1	A	758	THR
1	A	759	GLU
1	A	762	GLN
1	A	765	ARG
1	A	775	THR
1	A	776	GLN
1	A	778	LEU
1	A	780	GLU
1	A	781	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	GLN
1	A	510	GLN
1	A	534	ASN
1	A	541	HIS
1	A	610	GLN
1	A	627	GLN
1	A	653	GLN
1	A	715	GLN
1	A	733	GLN
1	A	735	GLN
1	A	762	GLN
1	A	776	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/308 (96%)	0.75	26 (8%) 15 12	18, 41, 45, 66	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	LYS	5.1
1	A	523	GLY	4.2
1	A	660	THR	4.0
1	A	659	ASP	4.0
1	A	782	LEU	3.9
1	A	530	ALA	3.7
1	A	532	ARG	3.4
1	A	600	ASP	3.2
1	A	693	THR	2.8
1	A	522	LEU	2.7
1	A	756	ALA	2.6
1	A	526	ALA	2.6
1	A	631	ALA	2.5
1	A	525	ASP	2.5
1	A	601	GLU	2.5
1	A	665	GLN	2.4
1	A	773	ALA	2.4
1	A	528	SER	2.3
1	A	511	ALA	2.3
1	A	698	LEU	2.3
1	A	529	LYS	2.3
1	A	521	PRO	2.3
1	A	620	SER	2.2
1	A	610	GLN	2.2
1	A	527	ALA	2.1
1	A	655	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.