



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:50 PM UTC

PDB ID : 2NZI / pdb_00002nzi
Title : Crystal structure of domains A168-A170 from titin
Authors : Mrosek, M.C.; Labeit, D.; Labeit, S.; Mayans, O.
Deposited on : 2006-11-23
Resolution : 2.90 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

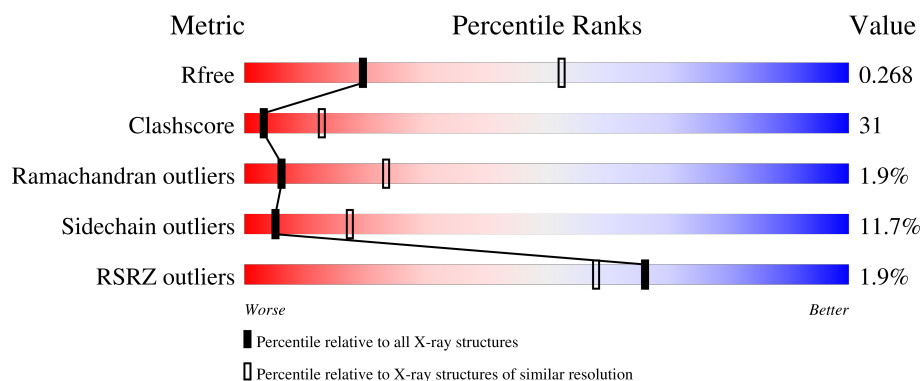
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	305	2% 46% 41% 9% .
1	B	305	2% 45% 44% 7% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4596 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 Titin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2276	1440	401	431	4			
1	B	292	Total	C	N	O	S	0	0	0
			2276	1440	401	431	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q8WZ42
A	-1	ALA	-	cloning artifact	UNP Q8WZ42
A	0	MET	-	cloning artifact	UNP Q8WZ42
B	-2	GLY	-	cloning artifact	UNP Q8WZ42
B	-1	ALA	-	cloning artifact	UNP Q8WZ42
B	0	MET	-	cloning artifact	UNP Q8WZ42

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	23	Total	O	0	0
			23	23		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.89Å 125.89Å 134.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (15.00-2.90) 96.6 (15.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.274 0.215 , 0.268	Depositor DCC
R_{free} test set	1205 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4596	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/2325	1.15	14/3157 (0.4%)
1	B	0.65	0/2325	1.12	11/3157 (0.3%)
All	All	0.64	0/4650	1.13	25/6314 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASP	CA-C-N	10.32	130.42	119.89
1	A	130	ASP	C-N-CA	10.32	130.42	119.89
1	A	185	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	B	185	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	B	197	ASP	CA-C-N	-8.54	111.58	120.38
1	B	197	ASP	C-N-CA	-8.54	111.58	120.38
1	A	259	PHE	N-CA-C	8.29	120.40	111.36
1	A	161	PHE	CA-C-N	8.20	128.67	119.32
1	A	161	PHE	C-N-CA	8.20	128.67	119.32
1	A	11	LEU	N-CA-C	7.96	121.34	108.76
1	B	278	LYS	CA-C-N	-7.94	112.66	120.52
1	B	278	LYS	C-N-CA	-7.94	112.66	120.52
1	B	259	PHE	N-CA-C	7.35	122.01	112.89
1	B	185	GLN	CG-CD-NE2	6.67	126.41	116.40
1	A	122	LYS	CA-C-N	-6.23	117.43	122.85
1	A	122	LYS	C-N-CA	-6.23	117.43	122.85
1	A	185	GLN	CG-CD-NE2	6.00	125.40	116.40
1	B	111	VAL	N-CA-C	-5.99	99.72	108.11
1	B	5	LYS	N-CA-C	-5.53	104.94	110.97
1	A	199	PRO	N-CA-C	-5.44	103.60	111.22
1	B	73	VAL	N-CA-C	5.37	116.72	108.71
1	A	0	MET	N-CA-C	5.35	117.78	110.55
1	A	7	GLU	N-CA-C	5.26	117.65	109.60
1	A	17	SER	N-CA-C	-5.21	102.28	110.36
1	B	0	MET	N-CA-C	5.15	118.12	110.14

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	2276	0	2275	136	0
1	B	2276	0	2275	146	0
2	A	21	0	0	10	0
2	B	23	0	0	9	0
All	All	4596	0	4550	282	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 31.

All (282) 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:260:GLY:HA2	1:A:288:THR:HB	1.38	1.03
1:B:14:ARG:O	1:B:17:SER:HB2	1.62	0.99
1:B:144:ASN:HD21	1:B:150:VAL:H	0.95	0.92
1:B:260:GLY:HA2	1:B:288:THR:HB	1.50	0.91
1:B:75:GLN:HG3	1:B:88:THR:HG22	1.55	0.88
1:B:244:ARG:HH11	1:B:244:ARG:HB3	1.39	0.88
1:A:199:PRO:HG3	1:A:268:VAL:HG12	1.54	0.87
1:B:228:THR:HG23	1:B:229:ASN:OD1	1.76	0.85
1:B:144:ASN:ND2	1:B:150:VAL:H	1.75	0.85
1:B:45:ASP:HA	2:B:306:HOH:O	1.77	0.85
1:B:103:LYS:HD3	1:B:106:GLU:OE2	1.76	0.84
1:A:134:THR:HG22	1:A:176:CYS:HB3	1.60	0.83
1:B:79:THR:HG22	1:B:84:SER:CB	2.08	0.82
1:A:209:ARG:H	1:A:209:ARG:HD2	1.44	0.81
1:B:144:ASN:HD21	1:B:150:VAL:N	1.78	0.81
1:B:79:THR:HG22	1:B:84:SER:HB2	1.63	0.79
1:A:13:VAL:CG1	1:A:17:SER:HB3	2.14	0.78
1:B:166:GLU:HG3	1:B:167:ARG:CZ	2.13	0.77
1:B:167:ARG:NE	1:B:167:ARG:H	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLY:CA	1:A:288:THR:HB	2.13	0.76
1:B:3:HIS:HB2	1:B:26:THR:HG22	1.68	0.75
1:A:11:LEU:HD13	1:A:91:LEU:HD12	1.69	0.74
1:A:1:ALA:HB1	1:A:2:PRO:HD2	1.69	0.74
1:B:166:GLU:HG3	1:B:167:ARG:NH2	2.03	0.74
1:A:245:VAL:HG11	1:A:255:VAL:HG13	1.69	0.73
1:B:199:PRO:HG3	1:B:268:VAL:HG12	1.69	0.73
1:A:13:VAL:HG12	1:A:17:SER:HB3	1.70	0.72
1:A:209:ARG:H	1:A:209:ARG:CD	2.02	0.72
1:A:260:GLY:HA2	1:A:288:THR:CB	2.17	0.71
1:A:144:ASN:ND2	1:A:150:VAL:H	1.86	0.71
1:B:79:THR:HG22	1:B:84:SER:OG	1.91	0.71
1:A:2:PRO:HD3	1:A:80:ASN:OD1	1.90	0.71
1:B:178:LYS:HG2	1:B:183:ILE:HG23	1.73	0.71
1:A:55:LYS:CE	2:A:321:HOH:O	2.39	0.70
1:B:107:GLY:C	1:B:109:GLY:H	1.99	0.70
1:A:207:VAL:HG12	1:A:208:SER:N	2.06	0.69
1:B:55:LYS:HG3	2:B:314:HOH:O	1.92	0.69
1:A:98:LYS:HD3	1:A:100:HIS:HE1	1.56	0.69
1:A:211:SER:O	1:A:212:VAL:HG23	1.94	0.68
1:B:199:PRO:HG2	1:B:280:SER:HB3	1.75	0.68
1:A:123:ILE:CD1	1:A:175:VAL:HG11	2.24	0.67
1:B:216:TRP:CD1	1:B:251:THR:HG22	2.29	0.67
1:B:242:TRP:CE3	1:B:267:ARG:HD2	2.30	0.67
1:A:228:THR:HG23	1:A:229:ASN:OD1	1.95	0.67
1:B:105:LEU:HD11	1:B:111:VAL:HG12	1.77	0.66
1:A:112:HIS:CD2	2:A:323:HOH:O	2.48	0.66
1:A:11:LEU:HD13	1:A:91:LEU:CD1	2.25	0.66
1:A:18:ASN:ND2	1:A:65:SER:H	1.94	0.66
1:A:242:TRP:O	1:A:243:LEU:HD23	1.96	0.66
1:B:134:THR:CG2	1:B:176:CYS:HB3	2.25	0.66
1:A:79:THR:HG22	1:A:84:SER:OG	1.95	0.65
1:A:96:PRO:HB3	1:A:181:PHE:O	1.96	0.65
1:B:209:ARG:H	1:B:209:ARG:NE	1.94	0.65
1:A:11:LEU:N	1:A:11:LEU:HD12	2.11	0.65
1:B:242:TRP:CZ3	1:B:267:ARG:HD2	2.32	0.65
1:B:260:GLY:HA2	1:B:288:THR:CB	2.25	0.65
1:A:193:ALA:HB3	1:A:274:PHE:CE2	2.32	0.65
1:A:195:VAL:CG1	1:A:277:SER:HA	2.27	0.65
1:B:13:VAL:HG12	1:B:17:SER:HB3	1.79	0.64
1:A:242:TRP:CZ3	1:A:267:ARG:HD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLN:O	1:B:186:LYS:HE2	1.99	0.63
1:B:258:LEU:HD22	1:B:264:TYR:CZ	2.33	0.63
1:A:242:TRP:CE3	1:A:267:ARG:HD2	2.32	0.63
1:B:1:ALA:HB1	1:B:2:PRO:HD2	1.79	0.63
1:B:237:THR:HG21	1:B:285:PRO:HB3	1.81	0.62
1:A:195:VAL:HG13	1:A:196:PRO:HD2	1.82	0.62
1:B:3:HIS:HB2	1:B:26:THR:CG2	2.29	0.62
1:B:209:ARG:H	1:B:209:ARG:CD	2.12	0.62
1:A:123:ILE:HD13	1:A:175:VAL:HG11	1.80	0.61
1:B:2:PRO:HD3	1:B:80:ASN:OD1	2.01	0.61
1:A:166:GLU:OE1	1:A:168:LYS:HE2	2.01	0.61
1:A:3:HIS:O	1:A:26:THR:HG22	2.01	0.61
1:A:202:VAL:HG23	2:A:322:HOH:O	2.01	0.61
1:A:258:LEU:HD22	1:A:264:TYR:CE1	2.36	0.61
1:B:207:VAL:HG12	1:B:208:SER:N	2.15	0.60
1:A:128:LYS:HA	1:A:129:PRO:C	2.25	0.60
1:A:250:GLU:OE1	1:A:250:GLU:HA	2.01	0.60
1:B:208:SER:HB2	1:B:209:ARG:NH1	2.15	0.60
1:B:207:VAL:CG1	1:B:208:SER:N	2.65	0.59
1:B:262:THR:O	1:B:287:ILE:HA	2.02	0.59
1:A:55:LYS:HD2	2:A:321:HOH:O	2.02	0.59
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.66	0.59
1:B:11:LEU:HD23	2:B:304:HOH:O	2.03	0.58
1:B:112:HIS:CB	2:B:322:HOH:O	2.52	0.58
1:A:22:VAL:HG22	1:A:23:CYS:N	2.19	0.57
1:A:204:VAL:HG13	1:A:212:VAL:CG1	2.34	0.57
1:B:13:VAL:CG1	1:B:17:SER:HB3	2.33	0.57
1:B:107:GLY:O	1:B:109:GLY:N	2.37	0.57
1:B:210:ASP:O	1:B:258:LEU:HB2	2.04	0.57
1:A:19:ALA:HB2	1:A:66:VAL:HG21	1.87	0.57
1:A:207:VAL:HG12	1:A:208:SER:H	1.69	0.57
1:B:185:GLN:O	1:B:186:LYS:CE	2.52	0.57
1:B:166:GLU:OE2	1:B:168:LYS:HE2	2.05	0.56
1:A:115:ARG:NH2	1:A:167:ARG:HE	2.03	0.56
1:A:98:LYS:HD3	1:A:100:HIS:CE1	2.40	0.56
1:B:11:LEU:N	1:B:11:LEU:CD1	2.69	0.56
1:B:258:LEU:HD22	1:B:264:TYR:CE1	2.40	0.55
1:A:100:HIS:HE2	1:A:126:SER:HG	1.48	0.55
1:B:204:VAL:HG13	1:B:212:VAL:CG1	2.36	0.55
1:A:55:LYS:HG3	2:A:306:HOH:O	2.07	0.55
1:A:100:HIS:NE2	1:A:126:SER:OG	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HD3	1:A:24:LYS:HD3	1.89	0.55
1:A:111:VAL:HG13	1:A:189:GLU:O	2.07	0.55
1:B:75:GLN:CG	1:B:88:THR:HG22	2.34	0.55
1:B:70:ASP:O	1:B:91:LEU:HD23	2.07	0.54
1:B:115:ARG:HG2	1:B:116:GLY:N	2.21	0.54
1:A:55:LYS:HE3	2:A:321:HOH:O	2.02	0.54
1:B:112:HIS:N	2:B:322:HOH:O	2.27	0.54
1:A:111:VAL:HG22	1:A:190:LEU:HD12	1.88	0.54
1:B:134:THR:HG23	1:B:176:CYS:HB3	1.88	0.54
1:A:207:VAL:CG1	1:A:208:SER:N	2.72	0.53
1:A:236:ALA:HB1	1:A:238:THR:HG23	1.89	0.53
1:B:103:LYS:HA	1:B:106:GLU:OE2	2.07	0.53
1:A:115:ARG:HH21	1:A:167:ARG:NE	2.06	0.53
1:B:24:LYS:HE3	1:B:58:TYR:CZ	2.44	0.53
1:A:256:ILE:HG13	1:A:257:ASN:OD1	2.07	0.53
1:B:19:ALA:HB3	1:B:63:ILE:HB	1.91	0.53
1:B:2:PRO:HA	1:B:26:THR:O	2.09	0.53
1:B:242:TRP:O	1:B:243:LEU:HD23	2.08	0.53
1:A:112:HIS:HB3	1:A:274:PHE:CE1	2.44	0.53
1:A:114:LEU:HB3	1:A:117:GLU:HG3	1.89	0.53
1:B:73:VAL:HG12	1:B:75:GLN:NE2	2.24	0.53
1:B:13:VAL:HG12	1:B:14:ARG:H	1.74	0.52
1:B:235:CYS:HB2	1:B:242:TRP:CE3	2.44	0.52
1:A:75:GLN:HG3	1:A:88:THR:HG22	1.90	0.52
1:B:111:VAL:HG22	1:B:190:LEU:CD1	2.39	0.52
1:A:153:THR:HG21	1:A:156:PHE:CE2	2.45	0.52
1:A:195:VAL:HG11	1:A:276:LEU:O	2.09	0.52
1:A:55:LYS:CD	2:A:321:HOH:O	2.58	0.51
1:B:55:LYS:HD3	1:B:55:LYS:N	2.25	0.51
1:B:102:PRO:HG2	1:B:105:LEU:HB2	1.93	0.51
1:A:222:ASP:HB3	1:A:227:ILE:HG13	1.92	0.51
1:B:237:THR:CG2	1:B:265:GLN:HG3	2.41	0.51
1:A:154:ARG:NH1	2:A:311:HOH:O	2.43	0.51
1:A:216:TRP:CE3	1:A:268:VAL:HG21	2.46	0.51
1:B:11:LEU:HD22	1:B:13:VAL:HG22	1.92	0.51
1:A:12:ASN:HA	1:A:92:GLU:O	2.11	0.50
1:A:107:GLY:C	1:A:109:GLY:H	2.18	0.50
1:A:18:ASN:HD21	1:A:65:SER:H	1.59	0.50
1:B:11:LEU:N	1:B:11:LEU:HD12	2.26	0.50
1:A:149:GLN:HB3	1:A:160:VAL:HB	1.94	0.50
1:B:128:LYS:HA	1:B:129:PRO:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:THR:OG1	1:A:263:SER:HB3	2.11	0.50
1:A:193:ALA:HB1	1:A:224:GLY:HA3	1.94	0.50
1:B:112:HIS:HB2	2:B:322:HOH:O	2.10	0.50
1:B:211:SER:HB2	1:B:256:ILE:HG22	1.95	0.49
1:B:237:THR:OG1	1:B:263:SER:HB3	2.12	0.49
1:A:55:LYS:O	1:A:55:LYS:HD3	2.12	0.49
1:A:180:ARG:NH2	2:A:320:HOH:O	2.44	0.49
1:B:16:GLN:NE2	1:B:65:SER:HB2	2.28	0.49
1:B:193:ALA:HB3	1:B:274:PHE:CZ	2.46	0.49
1:A:195:VAL:HG11	1:A:277:SER:HA	1.94	0.49
1:A:212:VAL:HG12	1:A:213:ASN:N	2.27	0.49
1:A:195:VAL:HG13	1:A:196:PRO:CD	2.42	0.49
1:B:33:VAL:HG21	1:B:59:HIS:CD2	2.48	0.49
1:B:11:LEU:HD13	1:B:11:LEU:O	2.13	0.49
1:A:45:ASP:OD2	1:A:47:LEU:HB2	2.13	0.48
1:A:250:GLU:HB3	1:A:252:ARG:HG2	1.94	0.48
1:A:115:ARG:HH21	1:A:167:ARG:HE	1.61	0.48
1:A:130:ASP:HA	1:A:131:PRO:HD3	1.62	0.48
1:B:271:GLU:HG2	1:B:272:ASN:N	2.28	0.48
1:A:159:LEU:HD11	1:A:173:TYR:CD1	2.49	0.48
1:B:193:ALA:HB3	1:B:274:PHE:CE2	2.49	0.48
1:B:230:TYR:O	1:B:247:GLN:HA	2.13	0.48
1:A:102:PRO:HG2	1:A:105:LEU:HB2	1.96	0.48
1:A:117:GLU:OE1	1:A:117:GLU:HA	2.14	0.48
1:A:2:PRO:HA	1:A:26:THR:O	2.14	0.48
1:A:131:PRO:HA	1:A:178:LYS:O	2.13	0.48
1:B:112:HIS:CA	2:B:322:HOH:O	2.61	0.48
1:B:205:SER:O	1:B:207:VAL:N	2.46	0.48
1:A:13:VAL:HG12	1:A:14:ARG:N	2.29	0.47
1:A:114:LEU:HB3	1:A:117:GLU:CG	2.45	0.47
1:A:207:VAL:CG1	1:A:208:SER:H	2.26	0.47
1:A:85:VAL:HG22	1:A:86:SER:N	2.29	0.47
1:B:154:ARG:HG3	1:B:154:ARG:NH1	2.30	0.47
1:B:196:PRO:O	1:B:277:SER:CB	2.63	0.47
1:A:1:ALA:HB1	1:A:2:PRO:CD	2.41	0.47
1:A:22:VAL:CG2	1:A:23:CYS:N	2.78	0.47
1:A:114:LEU:O	1:A:115:ARG:C	2.57	0.47
1:B:107:GLY:C	1:B:109:GLY:N	2.62	0.47
1:A:28:HIS:HA	1:A:29:PRO:C	2.40	0.47
1:A:228:THR:HG22	1:A:271:GLU:O	2.15	0.47
1:A:204:VAL:HG13	1:A:212:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLU:C	1:A:252:ARG:H	2.23	0.46
1:B:179:ASN:OD1	1:B:179:ASN:C	2.58	0.46
1:A:119:VAL:HG12	1:A:120:SER:N	2.30	0.46
1:A:0:MET:O	1:A:28:HIS:O	2.34	0.46
1:B:122:LYS:HE3	1:B:156:PHE:CD1	2.50	0.46
1:B:196:PRO:O	1:B:277:SER:HB3	2.16	0.46
1:B:200:ARG:HH12	1:B:220:ALA:HA	1.80	0.46
1:B:235:CYS:HB2	1:B:242:TRP:CD2	2.51	0.46
1:B:262:THR:HG23	2:B:324:HOH:O	2.15	0.46
1:A:144:ASN:HD22	1:A:150:VAL:H	1.64	0.46
1:B:167:ARG:H	1:B:167:ARG:CD	2.28	0.46
1:B:216:TRP:NE1	1:B:251:THR:HG22	2.31	0.46
1:B:8:LEU:HD22	1:B:76:VAL:HG12	1.97	0.46
1:A:115:ARG:HH21	1:A:167:ARG:CD	2.29	0.45
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.80	0.45
1:B:2:PRO:O	1:B:85:VAL:HG13	2.16	0.45
1:A:233:GLU:OE1	1:A:267:ARG:NH1	2.48	0.45
1:A:54:PHE:O	1:A:55:LYS:C	2.59	0.45
1:A:261:LYS:N	1:A:288:THR:HB	2.32	0.45
1:B:103:LYS:C	1:B:105:LEU:H	2.24	0.45
1:B:290:GLU:O	1:B:290:GLU:HG2	2.17	0.45
1:A:112:HIS:HD2	2:A:323:HOH:O	1.96	0.45
1:B:77:ARG:NH1	1:B:84:SER:OG	2.50	0.45
1:B:98:LYS:CD	1:B:100:HIS:HE1	2.30	0.45
1:A:15:TYR:O	1:A:16:GLN:HB2	2.17	0.44
1:B:112:HIS:CD2	2:B:322:HOH:O	2.69	0.44
1:B:114:LEU:O	1:B:115:ARG:C	2.57	0.44
1:B:204:VAL:HG13	1:B:212:VAL:HG11	1.98	0.44
1:A:199:PRO:HG2	1:A:280:SER:HB3	1.98	0.44
1:A:111:VAL:HG22	1:A:190:LEU:CD1	2.48	0.44
1:B:237:THR:OG1	1:B:263:SER:CB	2.66	0.44
1:B:167:ARG:H	1:B:167:ARG:HE	1.63	0.44
1:B:53:GLU:HA	1:B:58:TYR:O	2.18	0.43
1:A:199:PRO:CG	1:A:268:VAL:O	2.66	0.43
1:B:8:LEU:CD1	1:B:23:CYS:HB3	2.48	0.43
1:B:103:LYS:C	1:B:105:LEU:N	2.76	0.43
1:A:114:LEU:HD12	1:A:117:GLU:HG2	1.98	0.43
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.80	0.43
1:B:209:ARG:CD	1:B:209:ARG:N	2.79	0.43
1:A:115:ARG:HG2	1:A:116:GLY:N	2.32	0.43
1:A:205:SER:O	1:A:206:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HD12	1:B:135:TRP:CH2	2.54	0.43
1:B:271:GLU:HG3	1:B:276:LEU:HD23	2.00	0.43
1:A:11:LEU:CD1	1:A:91:LEU:CD1	2.96	0.43
1:A:33:VAL:HA	1:A:77:ARG:O	2.18	0.43
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.79	0.43
1:B:111:VAL:HG22	1:B:190:LEU:HD12	1.99	0.43
1:B:258:LEU:HD23	1:B:258:LEU:HA	1.77	0.43
1:A:37:ARG:HG3	1:A:37:ARG:HH11	1.84	0.43
1:A:11:LEU:CD1	1:A:91:LEU:HD13	2.50	0.42
1:B:13:VAL:HG12	1:B:17:SER:CB	2.48	0.42
1:B:98:LYS:HD3	1:B:100:HIS:HE1	1.84	0.42
1:A:166:GLU:OE1	1:A:168:LYS:CE	2.67	0.42
1:B:228:THR:HG22	1:B:272:ASN:HA	2.01	0.42
1:B:219:PRO:HD2	1:B:227:ILE:HD11	2.00	0.42
1:B:142:ILE:HG23	1:B:148:TYR:CD2	2.55	0.42
1:B:256:ILE:HG13	1:B:257:ASN:OD1	2.19	0.42
1:B:36:TYR:CD1	1:B:41:GLU:HA	2.55	0.42
1:B:263:SER:HA	1:B:286:THR:O	2.20	0.42
1:A:211:SER:O	1:A:212:VAL:CG2	2.64	0.42
1:B:14:ARG:HE	1:B:14:ARG:HB3	1.69	0.42
1:B:208:SER:O	1:B:288:THR:HG22	2.20	0.42
1:B:247:GLN:HE21	1:B:247:GLN:HB2	1.56	0.42
1:B:173:TYR:O	1:B:187:THR:HA	2.20	0.42
1:B:233:GLU:OE1	1:B:267:ARG:NH1	2.52	0.42
1:B:274:PHE:N	1:B:274:PHE:CD2	2.87	0.42
1:A:136:GLN:HA	1:A:142:ILE:HG13	2.02	0.41
1:A:209:ARG:HD2	1:A:209:ARG:N	2.24	0.41
1:B:241:ARG:O	1:B:241:ARG:HG2	2.20	0.41
1:A:11:LEU:HD12	1:A:11:LEU:H	1.83	0.41
1:B:11:LEU:HD11	1:B:91:LEU:HD13	2.01	0.41
1:B:262:THR:C	1:B:287:ILE:HG23	2.45	0.41
1:A:124:PRO:HA	1:A:156:PHE:HA	2.01	0.41
1:A:212:VAL:CG1	1:A:213:ASN:N	2.84	0.41
1:A:34:LYS:HD3	1:A:41:GLU:CD	2.45	0.41
1:A:260:GLY:O	1:A:261:LYS:C	2.62	0.41
1:A:260:GLY:CA	1:A:288:THR:CB	2.89	0.41
1:A:290:GLU:OE2	1:A:290:GLU:O	2.39	0.41
1:B:209:ARG:O	1:B:260:GLY:CA	2.69	0.41
1:B:24:LYS:HE3	1:B:58:TYR:CE2	2.55	0.41
1:B:99:ILE:HD13	1:B:175:VAL:HG13	2.02	0.41
1:B:237:THR:HG23	1:B:265:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:VAL:HG13	1:B:212:VAL:HG13	2.02	0.41
1:B:226:LYS:O	1:B:272:ASN:HB2	2.21	0.41
1:B:255:VAL:HG12	1:B:256:ILE:N	2.35	0.41
1:A:134:THR:O	1:A:134:THR:CG2	2.69	0.41
1:A:165:VAL:HG22	1:A:169:ASP:HB2	2.03	0.41
1:B:11:LEU:CD2	1:B:13:VAL:HG22	2.51	0.41
1:B:113:ALA:CB	1:B:119:VAL:HG21	2.51	0.41
1:B:114:LEU:HB3	1:B:117:GLU:HG3	2.02	0.41
1:B:231:ILE:HB	1:B:269:ILE:HB	2.03	0.41
1:A:225:SER:HB2	1:A:274:PHE:CE2	2.57	0.40
1:B:112:HIS:HA	1:B:191:ASP:O	2.21	0.40
1:A:210:ASP:O	1:A:258:LEU:HB2	2.21	0.40
1:B:54:PHE:O	1:B:55:LYS:C	2.64	0.40
1:A:21:LEU:O	1:A:60:GLN:HG3	2.22	0.40
1:A:91:LEU:HD12	1:A:91:LEU:HA	1.88	0.40
1:B:22:VAL:HA	1:B:59:HIS:O	2.21	0.40
1:A:128:LYS:CA	1:A:129:PRO:C	2.93	0.40

There are no symmetry-related clashes.

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	290/305 (95%)	262 (90%)	22 (8%)	6 (2%)	5	21
1	B	290/305 (95%)	255 (88%)	30 (10%)	5 (2%)	7	26
All	All	580/610 (95%)	517 (89%)	52 (9%)	11 (2%)	6	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	MET

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Mol	Chain	Res	Type
1	A	108	MET
1	A	206	ASP
1	B	206	ASP
1	B	207	VAL
1	A	237	THR
1	B	104	THR
1	A	7	GLU
1	B	15	TYR
1	A	207	VAL
1	A	164	GLY

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	248/261 (95%)	221 (89%)	27 (11%)	6	20
1	B	248/261 (95%)	217 (88%)	31 (12%)	4	15
All	All	496/522 (95%)	438 (88%)	58 (12%)	5	17

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	20	THR
1	A	40	LYS
1	A	55	LYS
1	A	61	LEU
1	A	86	SER
1	A	90	SER
1	A	105	LEU
1	A	111	VAL
1	A	114	LEU
1	A	118	VAL
1	A	123	ILE
1	A	134	THR

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Mol	Chain	Res	Type
1	A	140	ASP
1	A	143	ASP
1	A	144	ASN
1	A	159	LEU
1	A	185	GLN
1	A	195	VAL
1	A	208	SER
1	A	209	ARG
1	A	218	GLU
1	A	238	THR
1	A	250	GLU
1	A	267	ARG
1	A	276	LEU
1	A	288	THR
1	B	8	LEU
1	B	11	LEU
1	B	13	VAL
1	B	17	SER
1	B	20	THR
1	B	26	THR
1	B	37	ARG
1	B	40	LYS
1	B	55	LYS
1	B	61	LEU
1	B	77	ARG
1	B	105	LEU
1	B	111	VAL
1	B	114	LEU
1	B	121	ILE
1	B	141	LEU
1	B	159	LEU
1	B	167	ARG
1	B	195	VAL
1	B	208	SER
1	B	209	ARG
1	B	211	SER
1	B	221	SER
1	B	234	LYS
1	B	238	THR
1	B	244	ARG
1	B	250	GLU
1	B	251	THR

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Mol	Chain	Res	Type
1	B	267	ARG
1	B	281	GLU
1	B	288	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	144	ASN
1	A	163	ASN
1	A	247	GLN
1	B	16	GLN
1	B	38	GLN
1	B	60	GLN
1	B	144	ASN
1	B	149	GLN
1	B	247	GLN

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 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 ⓘ

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	292/305 (95%)	-0.21	6 (2%) 63 54	15, 51, 96, 132	0
1	B	292/305 (95%)	-0.19	5 (1%) 69 61	20, 50, 91, 124	0
All	All	584/610 (95%)	-0.20	11 (1%) 66 58	15, 51, 93, 132	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	3.4
1	B	108	MET	3.4
1	A	185	GLN	3.3
1	A	139	GLN	3.2
1	A	1	ALA	3.0
1	B	209	ARG	2.7
1	A	209	ARG	2.6
1	B	239	ALA	2.5
1	B	0	MET	2.5
1	B	40	LYS	2.1
1	A	28	HIS	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.