



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:40 AM UTC

PDB ID : 7DOV / pdb_00007dov
Title : The crystal structure of zebrafish tumor necrosis factor alpha
Authors : Duan, Y.; Xia, C.
Deposited on : 2020-12-17
Resolution : 2.59 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

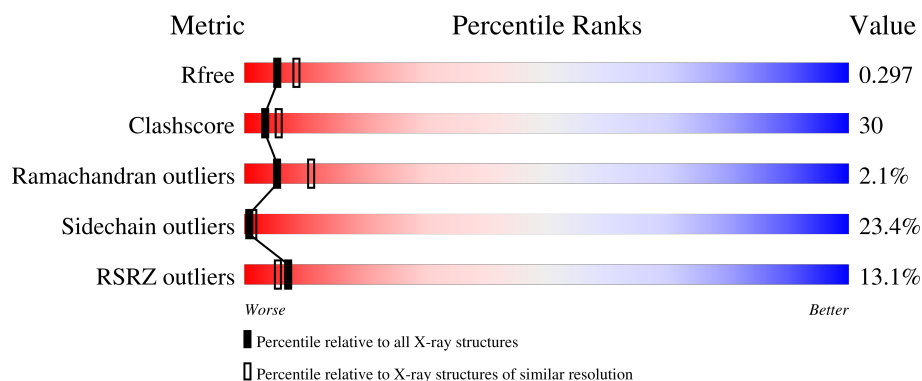
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

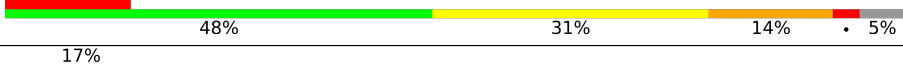
The reported resolution of this entry is 2.59 Å.

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	155	
1	B	155	
1	C	155	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3565 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 Lymphotoxin-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1162	734	192	231	5			
1	B	148	Total	C	N	O	S	0	0	0
			1162	734	192	231	5			
1	C	148	Total	C	N	O	S	0	1	0
			1172	740	195	232	5			

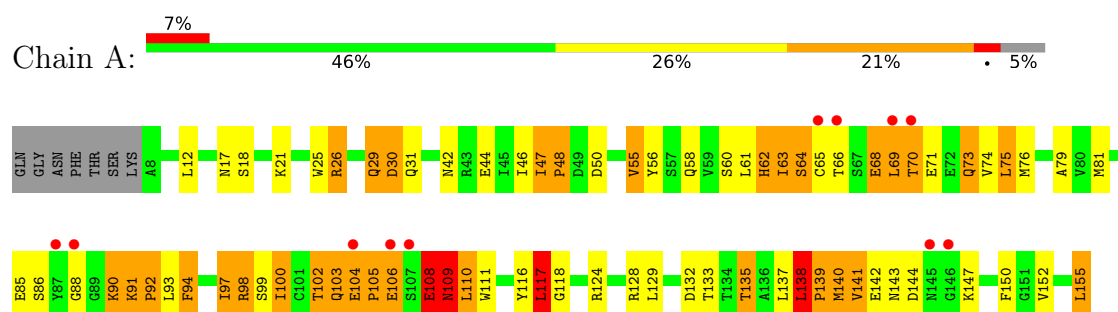
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	28	Total	O	0	0
			28	28		
2	C	25	Total	O	0	0
			25	25		

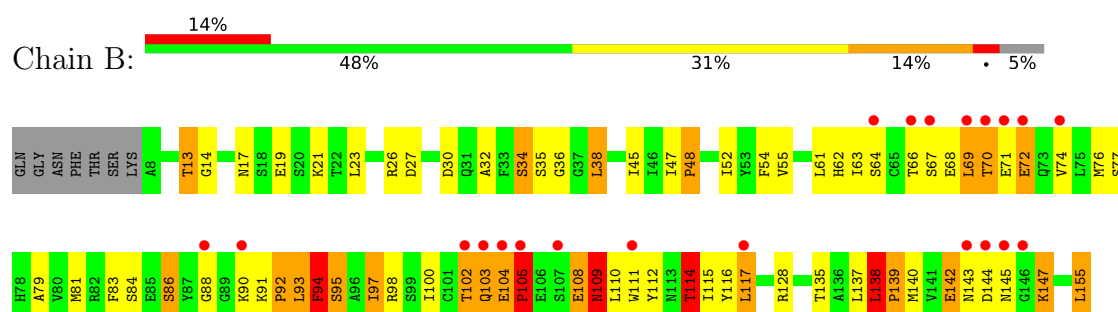
3 Residue-property plots [i](#)

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.

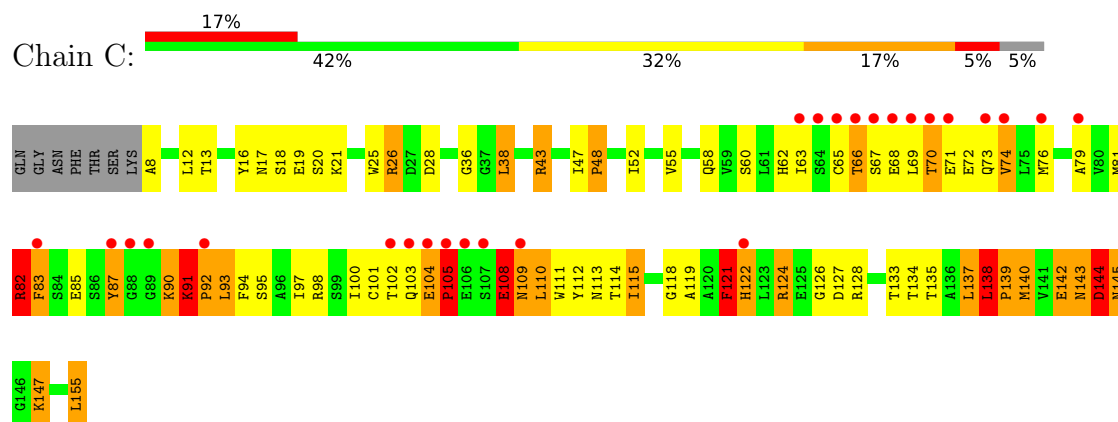
• Molecule 1: Lymphotoxin-alpha



• Molecule 1: Lymphotoxin-alpha



• Molecule 1: Lymphotoxin-alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.33Å 91.02Å 63.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.27 – 2.59 44.27 – 2.59	Depositor EDS
% Data completeness (in resolution range)	93.5 (44.27-2.59) 93.7 (44.27-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.31 (at 2.58Å)	Xtriage
Refinement program	REFMAC 7.0.077, PHENIX 1.19	Depositor
R, R_{free}	0.218 , 0.299 0.221 , 0.297	Depositor DCC
R_{free} test set	682 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3565	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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	1.76	15/1187 (1.3%)	2.06	27/1606 (1.7%)
1	B	1.78	13/1187 (1.1%)	1.92	33/1606 (2.1%)
1	C	1.68	12/1198 (1.0%)	2.19	39/1621 (2.4%)
All	All	1.74	40/3572 (1.1%)	2.06	99/4833 (2.0%)

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	2
1	C	0	7
All	All	0	9

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	PRO	N-CA	18.51	1.71	1.47
1	C	105	PRO	N-CA	17.71	1.70	1.47
1	B	105	PRO	N-CA	17.66	1.70	1.47
1	B	139	PRO	N-CA	17.14	1.69	1.47
1	C	92	PRO	N-CA	16.71	1.68	1.47
1	B	92	PRO	N-CA	16.64	1.68	1.47
1	C	139	PRO	N-CA	16.63	1.68	1.47
1	A	92	PRO	N-CA	16.19	1.68	1.47
1	A	139	PRO	N-CA	15.90	1.68	1.47
1	A	106	GLU	C-N	15.44	1.54	1.33
1	C	48	PRO	N-CA	15.39	1.68	1.47
1	A	48	PRO	N-CA	15.35	1.68	1.47
1	B	48	PRO	N-CA	15.15	1.67	1.47
1	A	17	ASN	C-O	-10.98	1.09	1.23
1	B	114	THR	C-O	-10.50	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	LEU	C-N	9.77	1.44	1.34
1	A	91	LYS	C-N	9.69	1.44	1.33
1	B	91	LYS	C-N	9.64	1.44	1.33
1	A	108	GLU	C-N	-8.93	1.21	1.33
1	C	47	ILE	C-N	7.77	1.44	1.34
1	A	47	ILE	C-N	7.72	1.44	1.34
1	B	47	ILE	C-N	7.61	1.43	1.34
1	A	138	LEU	C-N	7.51	1.44	1.33
1	B	55	VAL	C-O	-7.46	1.16	1.24
1	C	83	PHE	N-CA	6.69	1.54	1.46
1	B	34	SER	C-O	-6.64	1.16	1.24
1	C	82	ARG	C-O	6.51	1.33	1.23
1	B	48	PRO	C-O	-6.14	1.15	1.24
1	B	138	LEU	C-O	-5.97	1.18	1.24
1	C	114	THR	C-O	-5.83	1.17	1.24
1	A	48	PRO	C-O	-5.80	1.16	1.24
1	C	138	LEU	C-O	-5.64	1.19	1.24
1	A	152	VAL	C-O	-5.58	1.18	1.24
1	A	150	PHE	C-O	-5.47	1.17	1.23
1	C	83	PHE	CA-C	5.39	1.58	1.52
1	A	139	PRO	C-O	-5.37	1.17	1.24
1	B	45	ILE	C-O	-5.20	1.18	1.24
1	A	55	VAL	C-O	-5.14	1.18	1.24
1	C	82	ARG	C-N	5.13	1.40	1.33
1	B	54	PHE	C-O	-5.09	1.17	1.24

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	GLU	O-C-N	-25.23	94.51	123.03
1	C	47	ILE	CA-C-N	18.14	137.83	118.97
1	C	47	ILE	C-N-CA	18.14	137.83	118.97
1	A	47	ILE	CA-C-N	18.04	137.74	118.97
1	A	47	ILE	C-N-CA	18.04	137.74	118.97
1	B	47	ILE	CA-C-N	17.70	137.38	118.97
1	B	47	ILE	C-N-CA	17.70	137.38	118.97
1	C	138	LEU	CA-C-N	17.29	136.76	119.82
1	C	138	LEU	C-N-CA	17.29	136.76	119.82
1	A	108	GLU	CA-C-N	17.09	154.18	121.54
1	A	108	GLU	C-N-CA	17.09	154.18	121.54
1	C	104	GLU	CA-C-N	17.00	141.09	119.84
1	C	104	GLU	C-N-CA	17.00	141.09	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLU	CA-C-N	15.62	139.36	119.84
1	A	104	GLU	C-N-CA	15.62	139.36	119.84
1	A	91	LYS	CA-C-N	15.53	137.99	119.98
1	A	91	LYS	C-N-CA	15.53	137.99	119.98
1	A	138	LEU	CA-C-N	15.22	137.13	119.47
1	A	138	LEU	C-N-CA	15.22	137.13	119.47
1	B	104	GLU	CA-C-N	15.07	138.67	119.84
1	B	104	GLU	C-N-CA	15.07	138.67	119.84
1	C	91	LYS	CA-C-N	15.04	138.65	119.84
1	C	91	LYS	C-N-CA	15.04	138.65	119.84
1	A	108	GLU	O-C-N	-15.00	102.64	122.59
1	B	91	LYS	CA-C-N	14.77	137.11	119.98
1	B	91	LYS	C-N-CA	14.77	137.11	119.98
1	B	138	LEU	CA-C-N	14.33	137.75	119.84
1	B	138	LEU	C-N-CA	14.33	137.75	119.84
1	C	109	ASN	CB-CA-C	-10.30	89.92	110.42
1	B	102	THR	CB-CA-C	9.55	126.31	110.17
1	C	83	PHE	CB-CA-C	8.96	125.32	109.65
1	B	147	LYS	N-CA-C	-8.80	102.68	113.50
1	A	93	LEU	N-CA-C	-8.57	102.02	111.36
1	B	139	PRO	CA-N-CD	-8.47	100.14	112.00
1	C	105	PRO	CA-N-CD	-8.44	100.18	112.00
1	C	139	PRO	N-CA-C	-8.04	103.60	113.98
1	A	92	PRO	CA-N-CD	-8.02	100.78	112.00
1	B	105	PRO	CA-N-CD	-8.00	100.79	112.00
1	C	82	ARG	N-CA-C	-7.98	100.60	110.41
1	C	82	ARG	CA-C-N	7.92	135.64	122.33
1	C	82	ARG	C-N-CA	7.92	135.64	122.33
1	A	105	PRO	CA-N-CD	-7.66	101.28	112.00
1	C	121	PHE	CA-C-O	-7.55	112.87	121.40
1	C	139	PRO	CA-N-CD	-7.40	101.64	112.00
1	C	71	GLU	N-CA-C	-7.40	103.15	111.14
1	A	73	GLN	CB-CA-C	7.29	121.62	111.86
1	A	139	PRO	CA-N-CD	-7.28	101.81	112.00
1	B	92	PRO	CA-N-CD	-7.25	101.85	112.00
1	A	139	PRO	N-CA-C	-7.11	103.50	113.81
1	C	92	PRO	CA-N-CD	-7.06	102.12	112.00
1	A	109	ASN	CB-CA-C	7.02	124.40	110.42
1	C	108	GLU	CA-C-N	6.91	134.74	121.54
1	C	108	GLU	C-N-CA	6.91	134.74	121.54
1	C	83	PHE	CA-C-O	-6.78	111.94	120.28
1	C	19	GLU	CB-CA-C	6.78	121.40	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	PRO	CA-N-CD	-6.73	102.57	112.00
1	B	92	PRO	N-CA-C	-6.73	100.04	110.95
1	B	108	GLU	CA-C-N	6.68	134.31	121.54
1	B	108	GLU	C-N-CA	6.68	134.31	121.54
1	B	67	SER	CA-C-N	6.67	132.01	120.68
1	B	67	SER	C-N-CA	6.67	132.01	120.68
1	B	93	LEU	N-CA-C	-6.66	103.50	111.69
1	C	85	GLU	N-CA-C	-6.65	105.16	113.28
1	C	48	PRO	CA-N-CD	-6.65	102.70	112.00
1	C	36	GLY	CA-C-N	-6.59	115.60	123.44
1	C	36	GLY	C-N-CA	-6.59	115.60	123.44
1	C	48	PRO	N-CA-C	-6.54	104.11	113.47
1	A	64	SER	O-C-N	6.54	129.05	122.12
1	A	70	THR	N-CA-C	-6.51	104.52	113.18
1	B	67	SER	O-C-N	6.46	129.87	122.25
1	B	48	PRO	CA-N-CD	-6.37	103.08	112.00
1	A	92	PRO	N-CA-C	-6.13	101.02	110.95
1	B	13	THR	CA-C-N	-5.96	117.02	121.61
1	B	13	THR	C-N-CA	-5.96	117.02	121.61
1	B	64	SER	O-C-N	5.94	128.19	122.07
1	C	93	LEU	N-CA-C	-5.82	104.85	111.07
1	A	68	GLU	CB-CA-C	-5.79	101.23	110.84
1	C	82	ARG	N-CA-CB	-5.67	102.61	110.38
1	C	13	THR	CA-C-N	-5.53	115.65	121.35
1	C	13	THR	C-N-CA	-5.53	115.65	121.35
1	A	117	LEU	N-CA-CB	-5.52	101.02	111.00
1	B	117	LEU	N-CA-CB	-5.42	101.19	111.00
1	A	64	SER	CA-C-N	5.39	131.83	121.54
1	A	64	SER	C-N-CA	5.39	131.83	121.54
1	B	36	GLY	CA-C-N	-5.35	117.07	123.44
1	B	36	GLY	C-N-CA	-5.35	117.07	123.44
1	C	109	ASN	N-CA-C	-5.35	99.40	110.80
1	B	94	PHE	CA-CB-CG	5.27	119.07	113.80
1	C	133	THR	CA-C-O	-5.23	115.25	121.16
1	A	30	ASP	CB-CA-C	-5.17	110.59	116.54
1	B	109	ASN	N-CA-CB	5.16	119.21	110.49
1	C	121	PHE	O-C-N	5.15	129.41	123.17
1	B	108	GLU	O-C-N	5.13	128.40	121.83
1	B	112	TYR	CB-CA-C	-5.08	100.94	109.72
1	C	108	GLU	CA-C-O	-5.06	115.49	121.66
1	C	66	THR	CA-C-N	5.02	128.34	120.82
1	C	66	THR	C-N-CA	5.02	128.34	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	SER	CA-C-N	5.01	131.10	121.54
1	B	64	SER	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	Peptide
1	A	109	ASN	Mainchain
1	C	103	GLN	Mainchain
1	C	108	GLU	Mainchain
1	C	121	PHE	Mainchain
1	C	122[A]	HIS	Mainchain
1	C	122[B]	HIS	Mainchain
1	C	82	ARG	Mainchain

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	1162	0	1108	61	1
1	B	1162	0	1110	64	0
1	C	1172	0	1116	95	1
2	A	16	0	0	1	0
2	B	28	0	0	2	0
2	C	25	0	0	2	0
All	All	3565	0	3334	205	1

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 30.

All (205) 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:48:PRO:N	1:A:48:PRO:CA	1.68	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:PRO:CA	1:C:48:PRO:N	1.68	1.48
1:A:92:PRO:N	1:A:92:PRO:CA	1.68	1.43
1:A:105:PRO:N	1:A:105:PRO:CA	1.71	1.43
1:C:105:PRO:N	1:C:105:PRO:CA	1.70	1.41
1:C:139:PRO:N	1:C:139:PRO:CA	1.68	1.41
1:B:139:PRO:N	1:B:139:PRO:CA	1.69	1.40
1:C:92:PRO:N	1:C:92:PRO:CA	1.68	1.36
1:B:92:PRO:CA	1:B:92:PRO:N	1.68	1.36
1:B:48:PRO:N	1:B:48:PRO:CA	1.67	1.35
1:A:139:PRO:CA	1:A:139:PRO:N	1.68	1.34
1:B:105:PRO:N	1:B:105:PRO:CA	1.69	1.33
1:C:66:THR:N	1:C:108:GLU:OE2	1.77	1.07
1:B:74:VAL:CG1	1:B:100:ILE:HD11	1.85	1.06
1:C:66:THR:H	1:C:108:GLU:CD	1.65	1.05
1:A:58:GLN:HE22	1:B:117:LEU:CD1	1.72	1.02
1:C:74:VAL:HG12	1:C:100:ILE:HD11	1.41	1.00
1:B:74:VAL:HG13	1:B:100:ILE:HD11	1.44	0.99
1:A:75:LEU:HD13	1:A:97:ILE:HD11	1.01	0.98
1:A:137:LEU:HA	1:A:140:MET:HE2	1.45	0.96
1:A:75:LEU:HD13	1:A:97:ILE:CD1	1.94	0.95
1:B:77:SER:HB2	1:B:97:ILE:HD12	1.51	0.89
1:C:66:THR:N	1:C:108:GLU:CD	2.25	0.87
1:A:135:THR:HA	1:A:138:LEU:HD22	1.57	0.86
1:A:144:ASP:OD2	1:A:147:LYS:NZ	2.07	0.86
1:A:58:GLN:NE2	1:B:117:LEU:CD1	2.38	0.86
1:C:60:SER:HB2	1:C:147:LYS:HG2	1.58	0.85
1:A:26:ARG:HE	1:A:29:GLN:HE22	1.24	0.85
1:C:8:ALA:HB1	1:C:38:LEU:HD22	1.56	0.85
1:A:74:VAL:HG13	1:A:100:ILE:HD11	1.61	0.83
1:C:60:SER:CB	1:C:147:LYS:HG2	2.08	0.82
1:A:26:ARG:NE	1:A:29:GLN:HE22	1.78	0.81
1:A:117:LEU:HD12	1:C:58:GLN:HE22	1.44	0.81
1:B:63:ILE:HD12	1:B:111:TRP:HE3	1.42	0.81
1:B:52:ILE:HG22	1:B:155:LEU:HD22	1.63	0.80
1:C:135:THR:HA	1:C:138:LEU:HD22	1.63	0.79
1:A:75:LEU:CD1	1:A:97:ILE:HD11	1.98	0.79
1:B:63:ILE:HD12	1:B:111:TRP:CE3	2.18	0.78
1:A:58:GLN:HE22	1:B:117:LEU:HD13	1.47	0.78
1:B:84:SER:OG	1:B:86:SER:OG	1.98	0.77
1:C:62:HIS:NE2	1:C:142:GLU:OE2	2.18	0.77
1:A:117:LEU:CD1	1:C:58:GLN:HE22	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:CG1	1:C:100:ILE:HD11	2.15	0.76
1:C:16:TYR:OH	1:C:21:LYS:HD2	1.87	0.74
1:B:92:PRO:N	1:B:92:PRO:C	2.46	0.74
1:B:104:GLU:H	1:B:104:GLU:CD	1.97	0.73
1:A:92:PRO:HB2	1:C:145:ASN:HB2	1.71	0.72
1:A:92:PRO:N	1:A:92:PRO:C	2.47	0.71
1:C:98:ARG:NH2	2:C:201:HOH:O	1.82	0.71
1:B:77:SER:HB2	1:B:97:ILE:CD1	2.21	0.71
1:C:108:GLU:HG3	1:C:109:ASN:H	1.56	0.71
1:C:83:PHE:CE1	1:C:90:LYS:HB3	2.25	0.70
1:C:62:HIS:O	1:C:140:MET:HG2	1.91	0.69
1:C:92:PRO:N	1:C:92:PRO:C	2.50	0.69
1:A:46:ILE:HD12	1:A:128:ARG:HG2	1.74	0.68
1:A:81:MET:HG3	1:A:90:LYS:HE3	1.74	0.68
1:B:114:THR:CG2	2:B:203:HOH:O	2.41	0.67
1:B:66:THR:HB	1:B:68:GLU:OE1	1.95	0.67
1:B:142:GLU:O	1:B:142:GLU:HG3	1.92	0.67
1:B:81:MET:HE2	1:B:90:LYS:HE3	1.77	0.67
1:C:48:PRO:N	1:C:48:PRO:C	2.53	0.67
1:A:139:PRO:N	1:A:139:PRO:C	2.52	0.67
1:C:72:GLU:HA	1:C:72:GLU:OE1	1.95	0.67
1:C:60:SER:OG	1:C:147:LYS:HG3	1.95	0.65
1:B:14:GLY:O	1:B:143:ASN:HB2	1.96	0.65
1:C:60:SER:OG	1:C:147:LYS:CG	2.45	0.65
1:B:135:THR:HA	1:B:138:LEU:HD22	1.80	0.64
1:C:82:ARG:NH2	1:C:127:ASP:OD2	2.30	0.63
1:A:31:GLN:HG3	1:B:93:LEU:HD23	1.80	0.63
1:B:145:ASN:ND2	1:C:92:PRO:HB2	2.14	0.62
1:C:139:PRO:N	1:C:139:PRO:C	2.53	0.62
1:B:137:LEU:HA	1:B:140:MET:HE3	1.81	0.62
1:A:62:HIS:HE1	2:A:212:HOH:O	1.81	0.62
1:C:144:ASP:OD1	1:C:144:ASP:N	2.33	0.62
1:B:74:VAL:HG13	1:B:100:ILE:CD1	2.26	0.61
1:C:83:PHE:HB2	1:C:128:ARG:HB2	1.83	0.61
1:B:48:PRO:N	1:B:48:PRO:C	2.58	0.61
1:B:74:VAL:HG12	1:B:100:ILE:HD11	1.81	0.60
1:B:77:SER:CB	1:B:97:ILE:HD12	2.27	0.60
1:A:26:ARG:NE	1:A:29:GLN:NE2	2.50	0.60
1:C:76:MET:HE2	1:C:115:ILE:HG13	1.83	0.60
1:A:106:GLU:HA	1:A:106:GLU:OE1	2.01	0.59
1:C:52:ILE:HG22	1:C:155:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:OE1	1:C:104:GLU:N	2.31	0.59
1:C:74:VAL:O	1:C:100:ILE:HG12	2.03	0.59
1:A:117:LEU:HD12	1:C:58:GLN:NE2	2.17	0.58
1:C:62:HIS:CD2	1:C:142:GLU:OE2	2.56	0.58
1:B:139:PRO:N	1:B:139:PRO:C	2.57	0.57
1:A:58:GLN:NE2	1:B:117:LEU:HD11	2.18	0.57
1:C:62:HIS:HB3	1:C:112:TYR:CE2	2.40	0.57
1:C:126:GLY:C	2:C:205:HOH:O	2.48	0.56
1:B:114:THR:HG21	2:B:203:HOH:O	2.02	0.56
1:C:60:SER:CB	1:C:147:LYS:CG	2.80	0.56
1:B:69:LEU:HD23	1:B:69:LEU:O	2.06	0.56
1:C:102:THR:HG22	1:C:102:THR:O	2.05	0.56
1:A:69:LEU:O	1:A:69:LEU:HD23	2.06	0.55
1:A:63:ILE:HG23	1:A:140:MET:HG3	1.89	0.55
1:C:69:LEU:N	1:C:69:LEU:HD22	2.21	0.55
1:C:104:GLU:H	1:C:104:GLU:CD	2.15	0.54
1:C:52:ILE:CG2	1:C:155:LEU:HD22	2.38	0.54
1:A:74:VAL:HG13	1:A:100:ILE:CD1	2.34	0.53
1:B:105:PRO:N	1:B:105:PRO:C	2.62	0.53
1:C:82:ARG:C	1:C:87:TYR:OH	2.52	0.53
1:C:79:ALA:HB2	1:C:95:SER:HB3	1.91	0.53
1:A:58:GLN:HE22	1:B:117:LEU:HD11	1.68	0.53
1:A:48:PRO:N	1:A:48:PRO:C	2.59	0.52
1:B:81:MET:HE2	1:B:90:LYS:CD	2.39	0.52
1:C:62:HIS:CD2	1:C:142:GLU:CD	2.88	0.52
1:B:66:THR:HB	1:B:68:GLU:CD	2.35	0.52
1:C:63:ILE:O	1:C:110:LEU:HD12	2.10	0.52
1:B:14:GLY:O	1:B:143:ASN:CG	2.53	0.52
1:B:69:LEU:HD23	1:B:69:LEU:C	2.35	0.51
1:C:55:VAL:O	1:C:118:GLY:HA2	2.10	0.51
1:A:55:VAL:O	1:A:118:GLY:HA2	2.10	0.51
1:A:79:ALA:HB3	1:A:81:MET:HE2	1.92	0.51
1:B:81:MET:HE2	1:B:90:LYS:CE	2.41	0.51
1:C:83:PHE:N	1:C:128:ARG:O	2.44	0.51
1:A:98:ARG:HD3	1:C:113:ASN:OD1	2.11	0.51
1:C:98:ARG:HH11	1:C:113:ASN:ND2	2.09	0.50
1:C:74:VAL:HG12	1:C:100:ILE:CD1	2.29	0.50
1:A:56:TYR:HA	1:A:117:LEU:O	2.12	0.50
1:A:61:LEU:HD23	1:A:141:VAL:HA	1.94	0.50
1:A:50:ASP:OD1	1:A:124:ARG:HA	2.13	0.49
1:C:139:PRO:N	1:C:140:MET:N	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:N	1:C:104:GLU:CD	2.71	0.49
1:A:74:VAL:CG1	1:A:100:ILE:HD11	2.39	0.49
1:B:27:ASP:HA	1:B:32:ALA:HB1	1.95	0.49
1:B:145:ASN:HD22	1:C:92:PRO:HB2	1.78	0.49
1:B:98:ARG:NH1	1:B:114:THR:O	2.46	0.48
1:A:79:ALA:CB	1:A:81:MET:HE2	2.44	0.48
1:A:102:THR:HB	1:C:102:THR:O	2.14	0.48
1:C:111:TRP:CZ3	1:C:113:ASN:HB2	2.49	0.48
1:B:14:GLY:O	1:B:143:ASN:CB	2.60	0.48
1:A:58:GLN:NE2	1:B:117:LEU:HD12	2.26	0.48
1:C:87:TYR:CE2	1:C:91:LYS:HD3	2.49	0.48
1:A:73:GLN:O	1:A:73:GLN:NE2	2.47	0.47
1:B:79:ALA:HB2	1:B:95:SER:HB3	1.95	0.47
1:C:76:MET:HB2	1:C:100:ILE:CG2	2.45	0.47
1:C:83:PHE:N	1:C:87:TYR:OH	2.48	0.47
1:A:137:LEU:O	1:A:140:MET:HG2	2.15	0.47
1:B:38:LEU:HD13	1:B:48:PRO:CD	2.45	0.47
1:B:61:LEU:HD12	1:B:76:MET:HE3	1.97	0.46
1:C:76:MET:CE	1:C:115:ILE:HG13	2.46	0.46
1:C:17:ASN:OD1	1:C:20:SER:N	2.48	0.46
1:A:108:GLU:H	1:A:108:GLU:HG3	1.64	0.46
1:C:142:GLU:HG3	1:C:144:ASP:OD1	2.16	0.46
1:C:81:MET:CE	1:C:92:PRO:HA	2.46	0.45
1:C:63:ILE:HG22	1:C:65:CYS:H	1.80	0.45
1:C:93:LEU:HD12	1:C:93:LEU:HA	1.80	0.45
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.76	0.45
1:B:81:MET:CE	1:B:90:LYS:HE3	2.46	0.45
1:B:83:PHE:HB2	1:B:128:ARG:HB2	1.98	0.45
1:C:104:GLU:HA	1:C:105:PRO:HD3	1.58	0.45
1:A:12:LEU:HD13	1:A:25:TRP:HB3	1.99	0.45
1:C:82:ARG:O	1:C:87:TYR:OH	2.33	0.45
1:C:119:ALA:HB3	1:C:121:PHE:CE2	2.52	0.45
1:A:103:GLN:NE2	1:A:111:TRP:HD1	2.15	0.44
1:B:13:THR:HG21	1:B:30:ASP:HB2	2.00	0.44
1:B:104:GLU:CD	1:B:104:GLU:N	2.72	0.44
1:C:87:TYR:CD1	1:C:87:TYR:O	2.70	0.44
1:A:144:ASP:O	1:A:147:LYS:HD2	2.18	0.44
1:C:70:THR:HG21	1:C:101:CYS:HB2	2.00	0.44
1:B:116:TYR:CD2	1:B:116:TYR:C	2.96	0.43
1:C:38:LEU:HD12	1:C:38:LEU:HA	1.91	0.43
1:A:44:GLU:OE1	1:A:128:ARG:NE	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:O	1:A:69:LEU:CG	2.66	0.43
1:A:66:THR:O	1:A:70:THR:OG1	2.37	0.43
1:B:86:SER:H	1:B:86:SER:HG	1.53	0.43
1:B:144:ASP:O	1:B:147:LYS:HD2	2.19	0.43
1:C:134:THR:HG21	1:C:137:LEU:HD22	2.00	0.43
1:A:44:GLU:HA	1:A:129:LEU:O	2.18	0.42
1:A:94:PHE:CD1	1:A:94:PHE:N	2.86	0.42
1:C:147:LYS:HE2	1:C:147:LYS:HB2	1.83	0.42
1:C:26:ARG:HE	1:C:26:ARG:HB3	1.49	0.42
1:C:60:SER:OG	1:C:147:LYS:O	2.37	0.42
1:C:111:TRP:CH2	1:C:113:ASN:HB2	2.54	0.42
1:C:28:ASP:OD1	1:C:28:ASP:N	2.52	0.42
1:C:98:ARG:HH11	1:C:113:ASN:HD21	1.67	0.42
1:C:66:THR:HG22	1:C:108:GLU:HG2	2.00	0.42
1:C:87:TYR:O	1:C:87:TYR:HD1	2.03	0.42
1:C:63:ILE:HD13	1:C:100:ILE:HD12	2.02	0.42
1:A:76:MET:O	1:A:97:ILE:HA	2.19	0.41
1:A:116:TYR:CD2	1:A:116:TYR:C	2.98	0.41
1:B:70:THR:O	1:B:72:GLU:N	2.53	0.41
1:B:103:GLN:HG2	1:B:111:TRP:CD1	2.56	0.41
1:C:66:THR:CG2	1:C:108:GLU:HG2	2.51	0.41
1:C:137:LEU:O	1:C:140:MET:HB2	2.20	0.41
1:C:140:MET:HB2	1:C:140:MET:HE3	1.90	0.41
1:B:94:PHE:CD2	1:B:117:LEU:HG	2.55	0.41
1:B:139:PRO:N	1:B:140:MET:N	2.69	0.41
1:C:12:LEU:HD13	1:C:25:TRP:HB3	2.02	0.41
1:C:79:ALA:CB	1:C:95:SER:HB3	2.50	0.41
1:C:138:LEU:HD12	1:C:138:LEU:HA	1.85	0.41
1:C:79:ALA:CB	1:C:81:MET:HE3	2.51	0.41
1:C:143:ASN:O	1:C:145:ASN:N	2.54	0.41
1:A:62:HIS:HB2	1:A:110:LEU:HD23	2.02	0.40
1:B:69:LEU:O	1:B:69:LEU:HG	2.20	0.40
1:C:74:VAL:CG1	1:C:100:ILE:CD1	2.92	0.40
1:A:73:GLN:O	1:A:73:GLN:CG	2.70	0.40
1:B:72:GLU:O	1:B:72:GLU:CG	2.70	0.40
1:B:17:ASN:O	1:B:21:LYS:N	2.51	0.40
1:A:58:GLN:HE21	1:A:116:TYR:HB2	1.85	0.40
1:C:43:ARG:HE	1:C:43:ARG:HB3	1.71	0.40
1:B:81:MET:HE2	1:B:90:LYS:CG	2.52	0.40
1:C:87:TYR:CD1	1:C:87:TYR:C	3.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLY:O	1:C:124:ARG:NH1[3_556]	2.17	0.03

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	146/155 (94%)	129 (88%)	14 (10%)	3 (2%)	5	11
1	B	146/155 (94%)	129 (88%)	13 (9%)	4 (3%)	4	7
1	C	147/155 (95%)	132 (90%)	13 (9%)	2 (1%)	9	19
All	All	439/465 (94%)	390 (89%)	40 (9%)	9 (2%)	5	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	CYS
1	A	109	ASN
1	B	109	ASN
1	C	144	ASP
1	B	71	GLU
1	B	88	GLY
1	A	42	ASN
1	B	105	PRO
1	C	105	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/133 (96%)	89 (70%)	38 (30%)	0	0
1	B	127/133 (96%)	103 (81%)	24 (19%)	1	2
1	C	128/133 (96%)	100 (78%)	28 (22%)	1	2
All	All	382/399 (96%)	292 (76%)	90 (24%)	1	1

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	21	LYS
1	A	26	ARG
1	A	29	GLN
1	A	30	ASP
1	A	47	ILE
1	A	60	SER
1	A	62	HIS
1	A	63	ILE
1	A	64	SER
1	A	68	GLU
1	A	69	LEU
1	A	71	GLU
1	A	75	LEU
1	A	85	GLU
1	A	86	SER
1	A	90	LYS
1	A	91	LYS
1	A	94	PHE
1	A	97	ILE
1	A	98	ARG
1	A	99	SER
1	A	100	ILE
1	A	102	THR
1	A	103	GLN
1	A	104	GLU
1	A	108	GLU
1	A	110	LEU
1	A	117	LEU
1	A	132	ASP
1	A	133	THR
1	A	135	THR

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Mol	Chain	Res	Type
1	A	138	LEU
1	A	140	MET
1	A	141	VAL
1	A	142	GLU
1	A	143	ASN
1	A	155	LEU
1	B	19	GLU
1	B	23	LEU
1	B	26	ARG
1	B	34	SER
1	B	35	SER
1	B	38	LEU
1	B	62	HIS
1	B	69	LEU
1	B	70	THR
1	B	72	GLU
1	B	86	SER
1	B	94	PHE
1	B	95	SER
1	B	97	ILE
1	B	102	THR
1	B	103	GLN
1	B	108	GLU
1	B	109	ASN
1	B	110	LEU
1	B	114	THR
1	B	115	ILE
1	B	138	LEU
1	B	142	GLU
1	B	155	LEU
1	C	18	SER
1	C	26	ARG
1	C	38	LEU
1	C	43	ARG
1	C	67	SER
1	C	68	GLU
1	C	70	THR
1	C	73	GLN
1	C	74	VAL
1	C	87	TYR
1	C	90	LYS
1	C	91	LYS

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Mol	Chain	Res	Type
1	C	94	PHE
1	C	97	ILE
1	C	110	LEU
1	C	115	ILE
1	C	122[A]	HIS
1	C	122[B]	HIS
1	C	124	ARG
1	C	137	LEU
1	C	138	LEU
1	C	140	MET
1	C	142	GLU
1	C	143	ASN
1	C	144	ASP
1	C	145	ASN
1	C	147	LYS
1	C	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	58	GLN
1	A	103	GLN
1	A	143	ASN
1	B	31	GLN
1	B	143	ASN
1	B	145	ASN
1	C	58	GLN

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 oligosaccharides 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, 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	148/155 (95%)	0.64	11 (7%)	20 16	13, 40, 116, 146	0
1	B	148/155 (95%)	0.69	21 (14%)	6 5	11, 32, 121, 148	0
1	C	148/155 (95%)	0.83	26 (17%)	4 3	12, 45, 135, 224	1 (0%)
All	All	444/465 (95%)	0.72	58 (13%)	7 5	11, 40, 125, 224	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	GLY	5.5
1	C	68	GLU	5.0
1	B	117	LEU	4.9
1	C	67	SER	4.5
1	B	69	LEU	4.2
1	C	69	LEU	4.0
1	B	105	PRO	3.9
1	C	76	MET	3.9
1	C	107	SER	3.8
1	C	66	THR	3.7
1	B	145	ASN	3.6
1	A	107	SER	3.5
1	B	67	SER	3.5
1	C	105	PRO	3.5
1	B	146	GLY	3.5
1	B	102	THR	3.4
1	C	74	VAL	3.4
1	B	70	THR	3.4
1	B	88	GLY	3.2
1	C	88	GLY	3.1
1	C	103	GLN	2.9
1	A	87	TYR	2.9
1	A	106	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	104	GLU	2.8
1	B	103	GLN	2.7
1	B	71	GLU	2.7
1	C	71	GLU	2.7
1	A	69	LEU	2.6
1	A	145	ASN	2.6
1	B	144	ASP	2.6
1	C	87	TYR	2.6
1	B	111	TRP	2.6
1	B	72	GLU	2.6
1	C	70	THR	2.6
1	B	74	VAL	2.5
1	B	143	ASN	2.5
1	B	107	SER	2.5
1	C	83	PHE	2.4
1	C	109	ASN	2.4
1	C	89	GLY	2.4
1	B	66	THR	2.4
1	C	106	GLU	2.4
1	B	90	LYS	2.4
1	C	102	THR	2.3
1	A	104	GLU	2.3
1	B	104	GLU	2.3
1	C	79	ALA	2.2
1	A	88	GLY	2.2
1	C	122[A]	HIS	2.2
1	C	65	CYS	2.2
1	A	66	THR	2.1
1	A	70	THR	2.1
1	C	63	ILE	2.1
1	C	92	PRO	2.1
1	C	73	GLN	2.1
1	B	64	SER	2.1
1	A	65	CYS	2.1
1	C	64	SER	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 [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.