



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:06 PM UTC

PDB ID : 1A8M / pdb_00001a8m
Title : TUMOR NECROSIS FACTOR ALPHA, R31D MUTANT
Authors : Reed, C.; Fu, Z.-Q.; Wu, J.; Xue, Y.-N.; Harrison, R.W.; Chen, M.-J.; Weber, I.T.
Deposited on : 1998-03-27
Resolution : 2.30 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

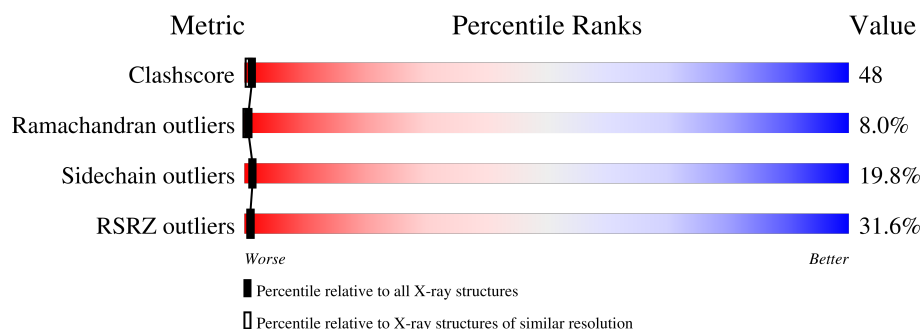
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	157	40% 25% 55% 13% • •
1	B	157	17% 30% 48% 13% 6% •
1	C	157	34% 31% 43% 22% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3630 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 TUMOR NECROSIS FACTOR ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1187	756	204	225	2			
1	B	152	Total	C	N	O	S	0	0	0
			1187	756	204	225	2			
1	C	152	Total	C	N	O	S	0	0	0
			1187	756	204	225	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ASP	ARG	engineered mutation	UNP P01375
B	31	ASP	ARG	engineered mutation	UNP P01375
C	31	ASP	ARG	engineered mutation	UNP P01375

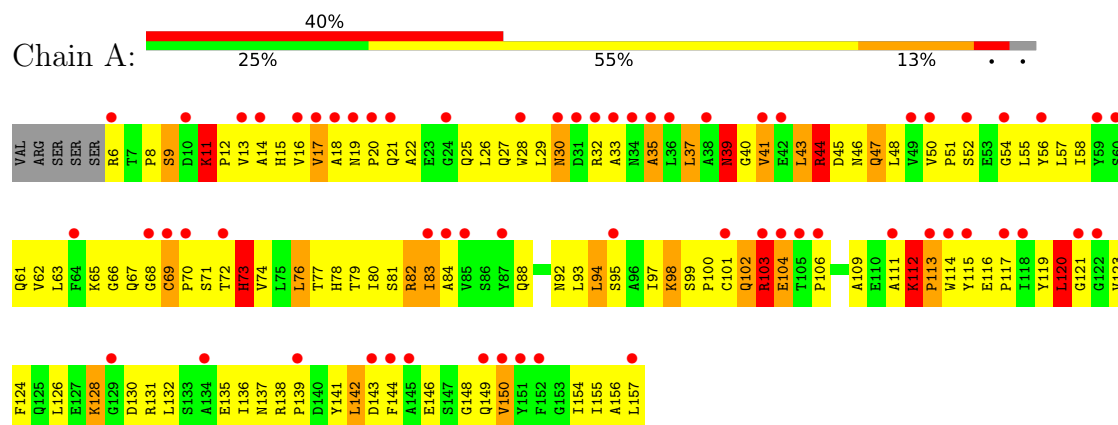
- Molecule 2 is water.

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

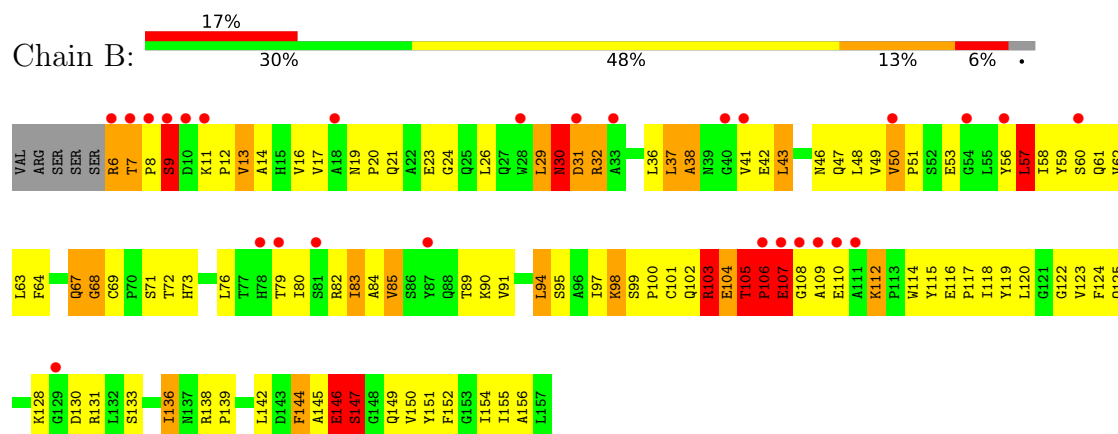
3 Residue-property plots

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.

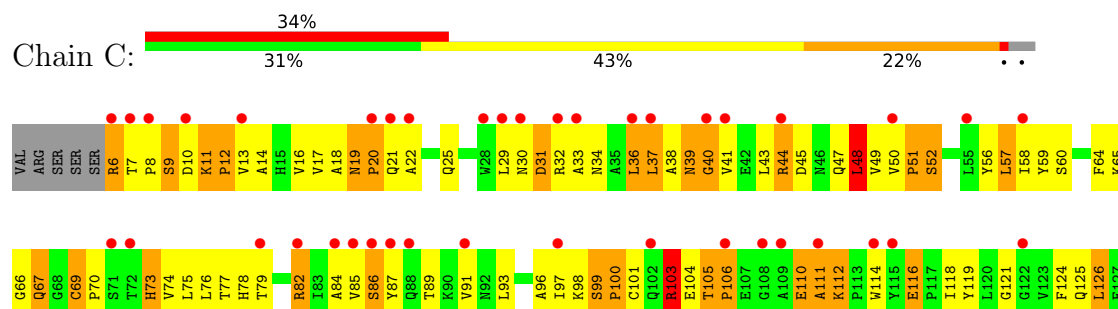
• Molecule 1: TUMOR NECROSIS FACTOR ALPHA

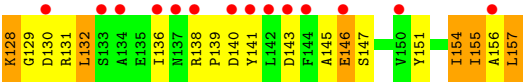


• Molecule 1: TUMOR NECROSIS FACTOR ALPHA



• Molecule 1: TUMOR NECROSIS FACTOR ALPHA





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.70Å 94.70Å 117.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (10.00-2.30) 86.5 (10.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.218 , 0.240 0.349 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 138.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	3630	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 5.15% 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	0.86	0/1214	1.43	22/1653 (1.3%)
1	B	0.84	0/1214	1.43	19/1653 (1.1%)
1	C	0.81	0/1214	1.27	11/1653 (0.7%)
All	All	0.84	0/3642	1.38	52/4959 (1.0%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	PHE	N-CA-C	14.86	132.86	109.83
1	A	112	LYS	CA-C-N	12.66	132.82	119.78
1	A	112	LYS	C-N-CA	12.66	132.82	119.78
1	B	145	ALA	N-CA-C	-11.12	95.80	111.81
1	A	50	VAL	N-CA-C	9.66	116.94	108.63
1	C	145	ALA	N-CA-C	-9.28	100.28	111.69
1	B	105	THR	CA-C-N	9.05	131.16	119.84
1	B	105	THR	C-N-CA	9.05	131.16	119.84
1	A	11	LYS	N-CA-C	8.52	121.74	109.48
1	A	73	HIS	N-CA-C	8.52	122.39	108.26
1	B	50	VAL	N-CA-C	8.41	116.25	107.76
1	B	147	SER	N-CA-C	-8.22	93.30	110.80
1	C	34	ASN	N-CA-C	-8.18	98.33	109.54
1	C	37	LEU	N-CA-C	-8.14	93.46	110.80
1	A	52	SER	N-CA-C	7.83	119.55	108.74
1	C	48	LEU	N-CA-C	-7.71	98.03	110.20
1	A	44	ARG	N-CA-C	7.70	120.36	108.12
1	C	104	GLU	N-CA-C	-7.52	102.04	112.12
1	B	57	LEU	N-CA-C	-7.04	97.78	109.46
1	A	102	GLN	N-CA-C	-6.98	96.23	108.23
1	B	30	ASN	N-CA-C	-6.45	96.57	107.99
1	A	99	SER	CA-C-N	6.43	126.61	120.31
1	A	99	SER	C-N-CA	6.43	126.61	120.31
1	C	40	GLY	N-CA-C	6.39	126.03	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	SER	N-CA-C	-6.38	101.54	110.35
1	C	99	SER	CA-C-N	6.38	127.81	119.84
1	C	99	SER	C-N-CA	6.38	127.81	119.84
1	A	39	ASN	N-CA-C	5.94	123.45	110.80
1	C	147	SER	N-CA-C	-5.88	98.27	110.80
1	B	50	VAL	CA-C-N	5.87	127.17	119.84
1	B	50	VAL	C-N-CA	5.87	127.17	119.84
1	B	38	ALA	N-CA-C	5.80	119.13	110.14
1	B	97	ILE	CB-CA-C	-5.64	101.86	110.95
1	B	67	GLN	N-CA-C	-5.64	99.21	108.41
1	B	146	GLU	N-CA-C	5.60	122.73	110.80
1	A	113	PRO	N-CA-C	5.59	120.10	111.21
1	A	54	GLY	N-CA-C	5.54	117.69	112.04
1	B	151	TYR	N-CA-C	5.49	117.42	109.07
1	A	135	GLU	N-CA-C	5.45	118.28	109.40
1	A	114	TRP	N-CA-C	-5.40	101.15	109.52
1	A	69	CYS	CA-C-N	5.37	126.55	119.84
1	A	69	CYS	C-N-CA	5.37	126.55	119.84
1	C	69	CYS	N-CA-C	5.31	116.34	109.65
1	A	41	VAL	N-CA-C	-5.28	102.27	109.55
1	A	98	LYS	N-CA-C	-5.27	101.52	109.85
1	B	103	ARG	N-CA-C	5.26	122.00	110.80
1	A	43	LEU	N-CA-C	-5.25	101.87	109.59
1	B	46	ASN	N-CA-C	-5.21	106.88	113.23
1	C	16	VAL	N-CA-C	5.18	116.44	108.71
1	A	84	ALA	N-CA-C	5.17	117.53	110.24
1	A	9	SER	N-CA-C	5.04	121.54	110.80
1	B	118	ILE	N-CA-C	-5.01	101.00	108.46

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	1187	0	1178	151	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1187	0	1178	104	2
1	C	1187	0	1178	106	0
2	A	16	0	0	4	1
2	B	25	0	0	5	0
2	C	28	0	0	9	0
All	All	3630	0	3534	334	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 48.

All (334) 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:C:11:LYS:HB2	2:C:266:HOH:O	1.61	1.00
1:A:11:LYS:HD2	1:A:12:PRO:HD2	1.42	0.96
1:A:112:LYS:HZ2	1:A:112:LYS:HB3	1.36	0.91
1:A:112:LYS:HB3	1:A:112:LYS:NZ	1.88	0.88
1:A:149:GLN:HG2	1:A:150:VAL:HG12	1.56	0.87
1:C:19:ASN:HB2	1:C:29:LEU:HD12	1.57	0.87
1:C:58:ILE:HD12	1:C:124:PHE:HD2	1.36	0.87
1:C:52:SER:HA	1:C:128:LYS:HB2	1.55	0.86
1:C:20:PRO:HD3	1:C:32:ARG:NH1	1.93	0.83
1:A:128:LYS:HB2	1:A:128:LYS:NZ	1.91	0.82
1:B:79:THR:HG22	1:B:95:SER:HB2	1.60	0.82
1:A:14:ALA:HB2	1:A:41:VAL:HG11	1.60	0.81
1:C:7:THR:HB	2:C:260:HOH:O	1.80	0.81
1:B:26:LEU:HD22	1:B:136:ILE:HD12	1.65	0.79
1:A:15:HIS:O	1:A:35:ALA:HA	1.83	0.78
1:A:12:PRO:HB3	1:A:39:ASN:O	1.83	0.78
1:B:61:GLN:HA	2:B:224:HOH:O	1.82	0.77
1:A:13:VAL:HG12	1:A:155:ILE:HA	1.64	0.77
2:B:262:HOH:O	1:C:36:LEU:HD23	1.84	0.77
1:C:69:CYS:SG	1:C:101:CYS:CB	2.72	0.77
1:B:146:GLU:O	1:B:147:SER:HB2	1.86	0.76
1:C:58:ILE:HD12	1:C:124:PHE:CD2	2.20	0.76
1:A:63:LEU:HD12	1:A:149:GLN:HG3	1.67	0.76
1:B:12:PRO:HG2	1:B:156:ALA:HB2	1.68	0.75
1:A:76:LEU:HD22	1:A:100:PRO:HD3	1.70	0.73
1:A:112:LYS:HE3	1:C:103:ARG:HB2	1.69	0.73
1:C:82:ARG:HH11	1:C:84:ALA:HB2	1.54	0.73
1:C:76:LEU:HD13	2:C:234:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PRO:HB3	1:B:116:GLU:HG3	1.70	0.72
1:A:98:LYS:HD3	1:A:116:GLU:OE1	1.89	0.72
1:B:47:GLN:HG2	1:B:133:SER:HB3	1.72	0.71
1:B:136:ILE:HD13	1:B:136:ILE:H	1.53	0.71
1:B:124:PHE:HA	2:C:242:HOH:O	1.90	0.71
1:B:69:CYS:CB	1:B:101:CYS:HG	2.04	0.71
1:A:11:LYS:HD2	1:A:12:PRO:CD	2.21	0.71
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.53	0.71
1:C:69:CYS:SG	1:C:101:CYS:HB3	2.32	0.70
1:A:16:VAL:HG11	1:A:43:LEU:HD22	1.73	0.69
1:A:146:GLU:HB2	1:A:149:GLN:HB2	1.74	0.69
1:B:146:GLU:HG3	1:B:147:SER:H	1.57	0.69
1:B:146:GLU:HB3	1:B:149:GLN:HB2	1.73	0.69
1:B:69:CYS:CB	1:B:101:CYS:SG	2.81	0.69
1:A:67:GLN:HA	1:A:113:PRO:HA	1.73	0.69
1:B:26:LEU:HB3	2:B:220:HOH:O	1.91	0.68
1:A:17:VAL:HG12	1:A:35:ALA:HB2	1.75	0.68
1:B:29:LEU:HD23	1:B:32:ARG:HD3	1.74	0.68
1:A:113:PRO:HG2	1:C:73:HIS:HE1	1.58	0.68
1:A:92:ASN:HB2	1:B:147:SER:HB3	1.76	0.67
1:C:103:ARG:HH11	1:C:103:ARG:HB3	1.59	0.67
1:A:32:ARG:HB3	2:A:201:HOH:O	1.94	0.67
1:B:144:PHE:HB2	1:B:146:GLU:HG2	1.75	0.67
1:B:49:VAL:HG22	1:B:131:ARG:HG2	1.76	0.67
1:A:69:CYS:SG	1:A:101:CYS:CB	2.83	0.67
1:A:11:LYS:HB3	1:A:156:ALA:HB3	1.77	0.67
1:A:22:ALA:HB2	1:A:27:GLN:HG3	1.77	0.66
1:C:11:LYS:HB3	1:C:156:ALA:HB3	1.78	0.66
1:C:52:SER:N	1:C:128:LYS:HZ2	1.94	0.66
1:C:77:THR:HG22	1:C:97:ILE:HG23	1.77	0.66
1:A:30:ASN:HB3	1:A:37:LEU:HD23	1.77	0.66
1:A:128:LYS:HB2	1:A:128:LYS:HZ2	1.58	0.65
1:B:19:ASN:HB2	1:B:29:LEU:HD13	1.79	0.65
1:A:149:GLN:HG2	1:A:150:VAL:CG1	2.27	0.65
1:A:112:LYS:HD2	1:C:103:ARG:HG3	1.78	0.65
1:A:18:ALA:HB2	1:A:150:VAL:HG22	1.78	0.64
1:B:59:TYR:HA	1:B:120:LEU:O	1.95	0.64
1:B:144:PHE:C	1:B:146:GLU:H	2.05	0.64
1:C:126:LEU:HD11	1:C:132:LEU:HD21	1.79	0.63
1:A:136:ILE:HD11	1:A:139:PRO:HA	1.80	0.63
1:A:13:VAL:HG12	1:A:155:ILE:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:CYS:HG	1:A:101:CYS:CB	2.10	0.63
1:A:137:ASN:OD1	1:A:138:ARG:HG2	1.99	0.63
1:C:44:ARG:HE	1:C:44:ARG:HA	1.64	0.63
1:A:142:LEU:HD11	1:A:150:VAL:HG11	1.81	0.62
1:A:142:LEU:CD1	1:A:150:VAL:HG11	2.29	0.62
1:A:30:ASN:HA	1:A:35:ALA:HB1	1.82	0.62
1:C:50:VAL:HG12	1:C:130:ASP:O	1.99	0.62
1:A:69:CYS:SG	1:A:101:CYS:HB3	2.40	0.62
1:C:87:TYR:C	1:C:89:THR:H	2.06	0.62
1:A:93:LEU:O	1:A:94:LEU:HG	2.00	0.62
1:B:16:VAL:HG11	1:B:43:LEU:HD21	1.80	0.62
1:C:87:TYR:HB2	1:C:89:THR:HG22	1.80	0.62
1:B:51:PRO:O	1:B:128:LYS:HG3	2.00	0.61
1:B:30:ASN:O	1:B:31:ASP:HB2	1.99	0.61
1:C:20:PRO:HD3	1:C:32:ARG:HH11	1.64	0.61
1:B:73:HIS:CD2	1:C:112:LYS:HD2	2.36	0.61
1:A:67:GLN:HB3	1:A:111:ALA:HA	1.81	0.60
1:A:71:SER:O	1:A:73:HIS:N	2.34	0.60
1:A:13:VAL:CG1	1:A:155:ILE:HG13	2.31	0.60
1:A:73:HIS:CE1	1:B:112:LYS:HG2	2.37	0.60
1:B:13:VAL:HG22	1:B:14:ALA:N	2.17	0.60
1:C:100:PRO:HA	1:C:116:GLU:OE2	2.01	0.60
1:A:146:GLU:CB	1:A:149:GLN:HB2	2.33	0.58
1:B:59:TYR:HD1	1:B:59:TYR:H	1.51	0.58
1:C:143:ASP:O	1:C:146:GLU:HG3	2.03	0.58
1:A:68:GLY:HA2	1:A:106:PRO:HG3	1.86	0.58
1:C:69:CYS:O	1:C:105:THR:HA	2.03	0.58
1:B:62:VAL:HB	1:B:142:LEU:HD21	1.84	0.58
1:B:20:PRO:HA	1:B:144:PHE:CE1	2.39	0.58
1:C:39:ASN:N	1:C:39:ASN:HD22	2.02	0.58
1:B:146:GLU:CB	1:B:149:GLN:HB2	2.34	0.57
1:B:13:VAL:CG2	1:B:14:ALA:N	2.67	0.57
1:A:41:VAL:HA	1:A:51:PRO:HD3	1.85	0.57
1:A:56:TYR:HE2	2:A:206:HOH:O	1.87	0.57
1:A:80:ILE:O	1:A:93:LEU:HB2	2.05	0.57
1:B:53:GLU:HG2	1:C:8:PRO:HG3	1.86	0.57
1:C:36:LEU:HD21	2:C:242:HOH:O	2.03	0.56
1:B:6:ARG:HE	1:B:6:ARG:N	2.02	0.56
1:A:17:VAL:CG1	1:A:32:ARG:HG3	2.35	0.56
1:A:61:GLN:O	1:A:150:VAL:HA	2.05	0.56
1:A:62:VAL:CG1	1:A:142:LEU:HD21	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:O	1:B:104:GLU:HG2	2.06	0.56
1:C:19:ASN:ND2	1:C:22:ALA:HB2	2.21	0.56
1:A:30:ASN:HD22	1:A:37:LEU:HG	1.70	0.56
1:B:146:GLU:HB2	1:B:149:GLN:H	1.71	0.56
1:A:69:CYS:CB	1:A:101:CYS:SG	2.93	0.56
1:B:7:THR:H	1:B:8:PRO:HD2	1.71	0.56
1:A:83:ILE:HG23	1:A:131:ARG:HB2	1.88	0.55
1:A:58:ILE:O	1:A:121:GLY:HA2	2.07	0.55
1:B:144:PHE:CB	1:B:146:GLU:HG2	2.35	0.55
1:A:14:ALA:CB	1:A:41:VAL:HG11	2.35	0.55
1:C:69:CYS:O	1:C:106:PRO:HD2	2.06	0.55
1:A:82:ARG:CB	1:A:93:LEU:HD11	2.36	0.55
1:C:67:GLN:CD	1:C:67:GLN:H	2.14	0.55
1:B:60:SER:HB3	1:B:80:ILE:HD11	1.89	0.55
1:B:83:ILE:HG22	1:B:90:LYS:HG2	1.90	0.54
1:A:30:ASN:ND2	1:A:37:LEU:HG	2.23	0.54
1:A:40:GLY:O	1:A:51:PRO:HB3	2.07	0.54
1:A:131:ARG:O	1:A:132:LEU:HD12	2.08	0.54
1:B:60:SER:CB	1:B:80:ILE:HD11	2.38	0.54
1:C:41:VAL:HG22	1:C:51:PRO:HD3	1.89	0.54
1:C:43:LEU:HD13	1:C:48:LEU:HD13	1.90	0.54
1:A:69:CYS:H	1:A:106:PRO:HD2	1.72	0.54
1:A:18:ALA:CB	1:A:150:VAL:HG22	2.38	0.54
1:B:69:CYS:O	1:B:105:THR:HA	2.07	0.54
1:A:13:VAL:HG12	1:A:155:ILE:CA	2.38	0.54
1:C:98:LYS:CD	1:C:118:ILE:HG12	2.37	0.54
1:C:66:GLY:HA3	1:C:114:TRP:CE2	2.43	0.53
1:A:57:LEU:HB3	1:A:155:ILE:HG23	1.91	0.53
1:A:17:VAL:HG13	1:A:32:ARG:HG3	1.90	0.53
1:A:6:ARG:HH22	1:C:125:GLN:NE2	2.07	0.53
1:B:20:PRO:HA	1:B:144:PHE:CD1	2.43	0.53
1:B:146:GLU:CG	1:B:147:SER:H	2.18	0.53
1:C:57:LEU:O	1:C:154:ILE:HA	2.09	0.53
1:A:12:PRO:HB2	2:A:206:HOH:O	2.08	0.53
1:A:29:LEU:HD12	1:A:32:ARG:HD3	1.90	0.53
1:B:69:CYS:HG	1:B:101:CYS:HG	0.54	0.53
1:B:16:VAL:CG2	1:B:152:PHE:HB3	2.38	0.53
1:A:58:ILE:HD11	1:A:126:LEU:HD11	1.90	0.52
1:A:138:ARG:NH1	1:A:141:TYR:CE2	2.77	0.52
1:B:82:ARG:NH1	1:B:84:ALA:HB2	2.24	0.52
1:A:112:LYS:HZ2	1:A:112:LYS:CB	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:CYS:HB3	1:B:101:CYS:SG	2.49	0.52
1:C:64:PHE:HE2	1:C:118:ILE:HD12	1.73	0.52
1:B:136:ILE:HD13	1:B:136:ILE:N	2.23	0.52
1:A:119:TYR:O	1:A:120:LEU:HB3	2.10	0.52
1:A:16:VAL:CG2	1:A:28:TRP:HB3	2.40	0.52
1:B:107:GLU:C	1:B:109:ALA:H	2.18	0.52
1:B:123:VAL:HG23	1:C:59:TYR:HE2	1.75	0.52
1:B:144:PHE:C	1:B:146:GLU:N	2.68	0.52
1:C:38:ALA:O	1:C:39:ASN:HB2	2.08	0.52
1:A:61:GLN:CD	2:A:236:HOH:O	2.53	0.51
1:A:103:ARG:HA	1:B:112:LYS:CD	2.40	0.51
1:B:58:ILE:HG23	1:B:154:ILE:HG22	1.92	0.51
1:B:69:CYS:O	1:B:106:PRO:HD2	2.10	0.51
1:A:144:PHE:HA	1:A:149:GLN:HE22	1.75	0.51
1:A:92:ASN:CB	1:B:147:SER:HB3	2.39	0.51
1:A:47:GLN:OE1	1:A:131:ARG:HD3	2.10	0.51
1:C:52:SER:H	1:C:128:LYS:HE3	1.75	0.51
1:A:77:THR:HG22	1:A:97:ILE:HG23	1.92	0.51
1:A:6:ARG:HH21	1:A:8:PRO:CG	2.23	0.51
1:C:69:CYS:HG	1:C:101:CYS:HG	0.55	0.51
1:B:82:ARG:NH2	1:B:130:ASP:OD2	2.43	0.51
1:C:52:SER:N	1:C:128:LYS:NZ	2.58	0.51
1:B:13:VAL:HG13	1:B:38:ALA:HB3	1.93	0.50
1:A:16:VAL:HG21	1:A:28:TRP:HB3	1.93	0.50
1:B:123:VAL:HG23	1:C:59:TYR:CE2	2.46	0.50
1:C:64:PHE:HA	1:C:141:TYR:O	2.12	0.50
1:A:65:LYS:HG2	1:A:66:GLY:N	2.25	0.50
1:A:113:PRO:HG2	1:C:73:HIS:CE1	2.45	0.50
1:A:139:PRO:O	1:A:142:LEU:HB2	2.12	0.50
1:C:14:ALA:HA	1:C:36:LEU:O	2.12	0.49
1:A:112:LYS:CE	1:C:103:ARG:HB2	2.42	0.49
1:B:119:TYR:HA	2:B:224:HOH:O	2.12	0.49
1:C:98:LYS:HD2	1:C:118:ILE:HG12	1.93	0.49
1:C:100:PRO:HB3	1:C:114:TRP:CE3	2.48	0.49
1:B:43:LEU:HD22	1:B:48:LEU:HD23	1.93	0.49
1:A:82:ARG:HB2	1:A:93:LEU:HD11	1.95	0.49
1:A:58:ILE:HG21	1:A:80:ILE:HG21	1.93	0.49
1:A:143:ASP:C	1:A:149:GLN:OE1	2.56	0.49
1:A:128:LYS:HB2	1:A:128:LYS:HZ3	1.74	0.49
1:B:37:LEU:HD11	1:B:42:GLU:HA	1.95	0.49
1:B:62:VAL:HA	1:B:150:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HA	1:B:112:LYS:HD2	1.94	0.48
1:A:146:GLU:HB2	1:A:149:GLN:CB	2.42	0.48
1:C:30:ASN:O	1:C:31:ASP:HB2	2.13	0.48
1:B:67:GLN:O	1:B:68:GLY:O	2.32	0.48
1:A:20:PRO:HD3	1:A:32:ARG:HH11	1.77	0.48
1:B:102:GLN:HG2	2:B:245:HOH:O	2.14	0.48
1:A:104:GLU:HA	1:B:103:ARG:HH12	1.78	0.48
1:A:146:GLU:HB2	1:A:149:GLN:CD	2.38	0.48
1:C:60:SER:OG	1:C:78:HIS:HE1	1.97	0.48
1:C:43:LEU:HD12	1:C:47:GLN:C	2.38	0.48
1:A:63:LEU:CD2	1:A:117:PRO:HB3	2.44	0.48
1:C:70:PRO:HG3	2:C:238:HOH:O	2.13	0.48
1:C:77:THR:HA	1:C:96:ALA:O	2.13	0.48
1:A:22:ALA:HB1	1:A:25:GLN:HG3	1.94	0.47
1:B:26:LEU:HD13	1:B:142:LEU:CD1	2.44	0.47
1:C:19:ASN:HB2	1:C:29:LEU:CD1	2.38	0.47
1:C:51:PRO:O	1:C:52:SER:OG	2.25	0.47
1:A:69:CYS:H	1:A:106:PRO:CD	2.27	0.47
1:C:20:PRO:O	1:C:22:ALA:N	2.47	0.47
1:B:83:ILE:C	1:B:83:ILE:HD12	2.40	0.47
1:B:115:TYR:C	1:B:116:GLU:HG2	2.40	0.47
1:A:44:ARG:C	1:A:46:ASN:H	2.22	0.47
1:A:102:GLN:NE2	1:B:114:TRP:HB3	2.30	0.47
1:B:16:VAL:HG22	1:B:152:PHE:O	2.15	0.47
1:B:59:TYR:CD1	1:B:59:TYR:N	2.83	0.47
1:C:77:THR:CG2	1:C:97:ILE:HG23	2.42	0.47
1:C:47:GLN:OE1	1:C:131:ARG:HD3	2.14	0.47
1:B:9:SER:OG	1:B:11:LYS:HG2	2.14	0.47
1:C:155:ILE:HD11	2:C:266:HOH:O	2.13	0.47
1:A:66:GLY:O	1:A:113:PRO:HA	2.15	0.46
1:A:82:ARG:HB3	1:A:93:LEU:HD11	1.97	0.46
1:A:18:ALA:HA	1:A:27:GLN:O	2.14	0.46
1:A:119:TYR:CG	1:A:120:LEU:N	2.83	0.46
1:A:62:VAL:HG12	1:A:63:LEU:N	2.29	0.46
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.69	0.46
1:C:58:ILE:O	1:C:121:GLY:HA2	2.15	0.46
1:B:83:ILE:HG13	1:B:83:ILE:O	2.16	0.46
1:C:65:LYS:NZ	1:C:143:ASP:HA	2.31	0.46
1:A:63:LEU:HD21	1:A:117:PRO:HB3	1.97	0.46
1:A:18:ALA:HB2	1:A:150:VAL:CG2	2.43	0.46
1:A:26:LEU:HD21	1:A:28:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HB3	1:A:155:ILE:CG2	2.46	0.46
1:B:63:LEU:HD13	1:B:117:PRO:HB3	1.96	0.46
1:C:41:VAL:HG12	1:C:41:VAL:O	2.16	0.46
1:C:138:ARG:NH2	1:C:140:ASP:OD2	2.46	0.46
1:B:13:VAL:CG1	1:B:38:ALA:HB3	2.45	0.45
1:A:79:THR:HG22	1:A:95:SER:HB3	1.98	0.45
1:A:102:GLN:O	1:A:104:GLU:N	2.49	0.45
1:B:107:GLU:O	1:B:109:ALA:N	2.49	0.45
1:B:85:VAL:HG23	1:B:130:ASP:OD1	2.16	0.45
1:B:98:LYS:NZ	1:B:117:PRO:O	2.50	0.45
1:A:69:CYS:CB	1:A:101:CYS:HG	2.26	0.45
1:B:138:ARG:HA	1:B:138:ARG:HD2	1.84	0.45
1:C:67:GLN:CD	1:C:67:GLN:N	2.75	0.45
1:A:119:TYR:CE1	1:C:121:GLY:O	2.70	0.44
1:B:85:VAL:HG21	1:B:128:LYS:O	2.17	0.44
1:A:76:LEU:HD22	1:A:100:PRO:CD	2.46	0.44
1:A:144:PHE:C	1:A:146:GLU:H	2.23	0.44
1:C:6:ARG:NH2	1:C:8:PRO:HB3	2.32	0.44
1:B:26:LEU:HD13	1:B:142:LEU:HD13	1.99	0.44
1:C:98:LYS:HD3	1:C:118:ILE:HG12	1.99	0.44
1:A:69:CYS:HB3	1:A:101:CYS:HB3	2.00	0.44
1:B:105:THR:O	1:B:106:PRO:O	2.35	0.44
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.82	0.44
1:C:19:ASN:ND2	1:C:19:ASN:C	2.75	0.44
1:C:44:ARG:N	1:C:47:GLN:O	2.50	0.44
1:C:110:GLU:O	1:C:111:ALA:HB3	2.18	0.44
1:C:30:ASN:HB3	1:C:37:LEU:CD1	2.47	0.43
1:C:82:ARG:NH1	2:C:257:HOH:O	2.50	0.43
1:C:103:ARG:HH11	1:C:103:ARG:CB	2.30	0.43
1:B:50:VAL:HA	1:B:51:PRO:HD2	1.69	0.43
1:A:100:PRO:O	1:A:101:CYS:HB2	2.18	0.43
1:C:85:VAL:HB	1:C:129:GLY:C	2.43	0.43
1:A:65:LYS:CG	1:A:66:GLY:N	2.80	0.43
1:B:30:ASN:CG	1:B:37:LEU:HB2	2.44	0.43
1:C:50:VAL:HG23	1:C:56:TYR:CZ	2.53	0.43
1:A:30:ASN:OD1	1:A:30:ASN:N	2.51	0.43
1:B:144:PHE:O	1:B:146:GLU:HG2	2.18	0.43
1:C:85:VAL:HG11	2:C:258:HOH:O	2.17	0.43
1:C:13:VAL:HB	1:C:155:ILE:HD12	1.99	0.43
1:A:39:ASN:OD1	1:A:39:ASN:N	2.51	0.43
1:A:103:ARG:HB2	1:A:104:GLU:H	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:HA3	1:C:93:LEU:O	2.18	0.43
1:C:64:PHE:HE2	1:C:118:ILE:CD1	2.32	0.43
1:C:86:SER:OG	1:C:87:TYR:N	2.49	0.43
1:A:6:ARG:NH2	1:A:8:PRO:HD3	2.34	0.43
1:B:64:PHE:CD2	1:B:76:LEU:HD13	2.54	0.43
1:A:19:ASN:OD1	1:A:21:GLN:HB3	2.19	0.43
1:A:47:GLN:HB3	1:A:132:LEU:O	2.19	0.43
1:B:58:ILE:HG22	1:B:58:ILE:O	2.17	0.43
1:C:51:PRO:C	1:C:128:LYS:NZ	2.76	0.42
1:C:57:LEU:HB2	1:C:157:LEU:HD22	2.00	0.42
1:A:106:PRO:HB2	1:A:109:ALA:HB3	2.00	0.42
1:C:51:PRO:C	1:C:128:LYS:HZ2	2.26	0.42
1:B:24:GLY:C	1:B:139:PRO:HB2	2.45	0.42
1:B:37:LEU:HD22	1:B:37:LEU:HA	1.87	0.42
1:B:94:LEU:HD23	1:C:151:TYR:CE2	2.55	0.42
1:C:52:SER:CA	1:C:128:LYS:HB2	2.37	0.42
1:A:123:VAL:C	1:A:124:PHE:CD1	2.97	0.42
1:B:37:LEU:HD13	1:B:41:VAL:O	2.20	0.42
1:C:49:VAL:HG22	1:C:131:ARG:HG2	2.01	0.42
1:A:62:VAL:HG11	1:A:136:ILE:HG21	2.02	0.42
1:A:102:GLN:HE22	1:B:114:TRP:HB3	1.84	0.42
1:A:142:LEU:HD22	1:A:142:LEU:HA	1.78	0.42
1:A:22:ALA:CB	1:A:27:GLN:HG3	2.49	0.42
1:A:69:CYS:HB3	1:A:101:CYS:SG	2.60	0.42
1:A:119:TYR:CE2	1:C:119:TYR:HE1	2.37	0.42
1:B:50:VAL:HG13	1:B:56:TYR:OH	2.20	0.42
1:B:103:ARG:HG3	1:B:104:GLU:N	2.33	0.42
1:C:17:VAL:HG12	1:C:18:ALA:N	2.34	0.42
1:C:40:GLY:C	1:C:51:PRO:HG3	2.44	0.42
1:A:137:ASN:O	1:A:138:ARG:HD3	2.20	0.42
1:C:74:VAL:HG23	1:C:74:VAL:O	2.20	0.42
1:C:110:GLU:OE2	1:C:111:ALA:HB2	2.20	0.42
1:A:115:TYR:CE2	1:C:75:LEU:HD22	2.54	0.41
1:C:87:TYR:CB	1:C:89:THR:HG22	2.49	0.41
1:A:16:VAL:CG1	1:A:43:LEU:HD22	2.47	0.41
1:A:82:ARG:HD3	1:A:126:LEU:CD2	2.50	0.41
1:B:13:VAL:CG2	1:B:14:ALA:H	2.33	0.41
1:B:32:ARG:HG3	1:B:32:ARG:NH1	2.29	0.41
1:A:113:PRO:CG	1:C:73:HIS:HE1	2.30	0.41
1:A:67:GLN:HB3	1:A:111:ALA:C	2.45	0.41
1:A:69:CYS:CB	1:A:101:CYS:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PRO:HG2	1:C:114:TRP:CZ3	2.55	0.41
1:A:58:ILE:O	1:A:121:GLY:CA	2.69	0.41
1:A:67:GLN:CB	1:A:111:ALA:HA	2.48	0.41
1:A:82:ARG:NH1	1:A:130:ASP:OD2	2.53	0.41
1:A:48:LEU:HD12	1:A:154:ILE:HG23	2.02	0.41
1:A:136:ILE:CD1	1:A:139:PRO:HA	2.47	0.41
1:B:57:LEU:HA	1:B:122:GLY:O	2.20	0.41
1:A:115:TYR:CD2	1:C:75:LEU:HD22	2.56	0.41
1:A:32:ARG:O	1:A:33:ALA:C	2.63	0.40
1:A:12:PRO:HB2	1:A:51:PRO:HG3	2.03	0.40
1:A:124:PHE:HA	1:B:36:LEU:HD11	2.03	0.40
1:C:10:ASP:CA	1:C:39:ASN:OD1	2.69	0.40
1:C:87:TYR:C	1:C:89:THR:N	2.75	0.40
1:A:131:ARG:C	1:A:132:LEU:HD12	2.46	0.40
1:B:73:HIS:CE1	1:B:99:SER:HB2	2.57	0.40
1:A:62:VAL:HG23	1:A:78:HIS:CE1	2.57	0.40
1:A:103:ARG:CA	1:B:112:LYS:HD2	2.52	0.40
1:B:110:GLU:H	1:B:110:GLU:CD	2.30	0.40
1:C:12:PRO:HB2	1:C:56:TYR:HE2	1.86	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)
1:B:131:ARG:NH2	2:A:212:HOH:O[4_454]	1.82	0.38
1:A:88:GLN:NE2	1:B:31:ASP:O[8_665]	1.90	0.30

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	150/157 (96%)	108 (72%)	34 (23%)	8 (5%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	150/157 (96%)	118 (79%)	19 (13%)	13 (9%)	0	0
1	C	150/157 (96%)	107 (71%)	28 (19%)	15 (10%)	0	0
All	All	450/471 (96%)	333 (74%)	81 (18%)	36 (8%)	1	0

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	39	ASN
1	A	72	THR
1	B	31	ASP
1	B	103	ARG
1	B	106	PRO
1	C	9	SER
1	C	20	PRO
1	C	21	GLN
1	C	33	ALA
1	C	103	ARG
1	C	112	LYS
1	A	70	PRO
1	B	68	GLY
1	B	108	GLY
1	C	31	ASP
1	C	51	PRO
1	C	73	HIS
1	C	111	ALA
1	C	146	GLU
1	A	35	ALA
1	A	103	ARG
1	A	104	GLU
1	B	85	VAL
1	B	146	GLU
1	C	86	SER
1	A	120	LEU
1	B	7	THR
1	B	72	THR
1	B	107	GLU
1	B	9	SER
1	B	105	THR
1	B	112	LYS
1	C	11	LYS

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Mol	Chain	Res	Type
1	C	52	SER
1	C	105	THR

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	128/133 (96%)	105 (82%)	23 (18%)	2	2
1	B	128/133 (96%)	104 (81%)	24 (19%)	1	1
1	C	128/133 (96%)	99 (77%)	29 (23%)	1	1
All	All	384/399 (96%)	308 (80%)	76 (20%)	1	1

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	17	VAL
1	A	30	ASN
1	A	37	LEU
1	A	39	ASN
1	A	44	ARG
1	A	45	ASP
1	A	47	GLN
1	A	55	LEU
1	A	73	HIS
1	A	74	VAL
1	A	76	LEU
1	A	81	SER
1	A	82	ARG
1	A	83	ILE
1	A	94	LEU
1	A	103	ARG
1	A	112	LYS
1	A	120	LEU
1	A	128	LYS

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Mol	Chain	Res	Type
1	A	142	LEU
1	A	150	VAL
1	A	157	LEU
1	B	6	ARG
1	B	9	SER
1	B	13	VAL
1	B	17	VAL
1	B	21	GLN
1	B	23	GLU
1	B	29	LEU
1	B	30	ASN
1	B	32	ARG
1	B	37	LEU
1	B	43	LEU
1	B	57	LEU
1	B	83	ILE
1	B	89	THR
1	B	91	VAL
1	B	94	LEU
1	B	98	LYS
1	B	104	GLU
1	B	106	PRO
1	B	107	GLU
1	B	125	GLN
1	B	136	ILE
1	B	147	SER
1	B	155	ILE
1	C	6	ARG
1	C	9	SER
1	C	12	PRO
1	C	19	ASN
1	C	25	GLN
1	C	36	LEU
1	C	39	ASN
1	C	44	ARG
1	C	45	ASP
1	C	48	LEU
1	C	57	LEU
1	C	67	GLN
1	C	79	THR
1	C	82	ARG
1	C	91	VAL

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Mol	Chain	Res	Type
1	C	99	SER
1	C	100	PRO
1	C	103	ARG
1	C	106	PRO
1	C	110	GLU
1	C	116	GLU
1	C	126	LEU
1	C	128	LYS
1	C	132	LEU
1	C	136	ILE
1	C	139	PRO
1	C	154	ILE
1	C	155	ILE
1	C	157	LEU

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

Mol	Chain	Res	Type
1	A	27	GLN
1	A	46	ASN
1	B	73	HIS
1	B	92	ASN
1	C	27	GLN
1	C	34	ASN
1	C	61	GLN
1	C	73	HIS
1	C	92	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 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	152/157 (96%)	1.89	63 (41%) 0 0	10, 36, 81, 91	0
1	B	152/157 (96%)	1.35	27 (17%) 4 4	12, 31, 77, 108	0
1	C	152/157 (96%)	1.75	54 (35%) 1 1	16, 35, 77, 91	0
All	All	456/471 (96%)	1.66	144 (31%) 1 1	10, 34, 79, 108	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	6.4
1	B	129	GLY	6.3
1	A	32	ARG	5.0
1	B	56	TYR	5.0
1	B	81	SER	4.7
1	C	71	SER	4.6
1	C	8	PRO	4.6
1	B	10	ASP	4.4
1	C	108	GLY	4.3
1	B	111	ALA	4.1
1	A	49	VAL	4.1
1	A	72	THR	4.0
1	C	87	TYR	4.0
1	A	85	VAL	4.0
1	A	69	CYS	4.0
1	B	7	THR	4.0
1	C	85	VAL	3.9
1	A	121	GLY	3.9
1	A	50	VAL	3.9
1	C	86	SER	3.6
1	C	20	PRO	3.6
1	A	70	PRO	3.5
1	A	13	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	21	GLN	3.4
1	A	115	TYR	3.3
1	C	10	ASP	3.3
1	A	83	ILE	3.3
1	A	6	ARG	3.3
1	A	151	TYR	3.2
1	A	139	PRO	3.2
1	A	134	ALA	3.2
1	C	22	ALA	3.2
1	C	97	ILE	3.2
1	A	143	ASP	3.1
1	A	59	TYR	3.1
1	B	8	PRO	3.1
1	A	42	GLU	3.1
1	B	79	THR	3.1
1	B	108	GLY	3.1
1	A	16	VAL	3.1
1	A	122	GLY	3.0
1	C	133	SER	3.0
1	B	110	GLU	3.0
1	A	17	VAL	2.9
1	B	41	VAL	2.9
1	A	18	ALA	2.9
1	C	136	ILE	2.9
1	A	34	ASN	2.9
1	C	21	GLN	2.8
1	C	88	GLN	2.8
1	A	144	PHE	2.8
1	C	79	THR	2.8
1	A	36	LEU	2.8
1	A	52	SER	2.8
1	A	54	GLY	2.7
1	A	33	ALA	2.7
1	A	113	PRO	2.7
1	B	106	PRO	2.7
1	B	107	GLU	2.7
1	C	28	TRP	2.7
1	B	40	GLY	2.7
1	C	102	GLN	2.7
1	C	72	THR	2.7
1	C	130	ASP	2.7
1	B	60	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	38	ALA	2.6
1	A	56	TYR	2.6
1	A	64	PHE	2.6
1	C	144	PHE	2.6
1	C	6	ARG	2.6
1	C	44	ARG	2.6
1	C	106	PRO	2.6
1	A	19	ASN	2.6
1	A	68	GLY	2.6
1	A	111	ALA	2.6
1	C	30	ASN	2.6
1	A	145	ALA	2.5
1	C	111	ALA	2.5
1	A	87	TYR	2.5
1	B	6	ARG	2.5
1	C	40	GLY	2.5
1	C	146	GLU	2.5
1	B	11	LYS	2.5
1	B	9	SER	2.5
1	C	33	ALA	2.5
1	C	134	ALA	2.5
1	A	114	TRP	2.4
1	C	36	LEU	2.4
1	A	84	ALA	2.4
1	C	109	ALA	2.4
1	C	156	ALA	2.4
1	A	157	LEU	2.4
1	B	33	ALA	2.4
1	A	101	CYS	2.4
1	A	129	GLY	2.4
1	C	122	GLY	2.4
1	A	41	VAL	2.4
1	B	50	VAL	2.4
1	A	28	TRP	2.4
1	C	115	TYR	2.3
1	C	84	ALA	2.3
1	A	118	ILE	2.3
1	C	13	VAL	2.3
1	C	142	LEU	2.3
1	B	31	ASP	2.3
1	A	105	THR	2.3
1	A	103	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	31	ASP	2.3
1	C	137	ASN	2.3
1	C	143	ASP	2.3
1	C	141	TYR	2.3
1	C	82	ARG	2.3
1	A	149	GLN	2.3
1	A	14	ALA	2.2
1	A	152	PHE	2.2
1	C	150	VAL	2.2
1	C	7	THR	2.2
1	B	87	TYR	2.2
1	C	58	ILE	2.2
1	C	55	LEU	2.2
1	C	138	ARG	2.2
1	A	106	PRO	2.2
1	C	50	VAL	2.2
1	A	117	PRO	2.2
1	A	60	SER	2.2
1	C	29	LEU	2.1
1	A	150	VAL	2.1
1	B	78	HIS	2.1
1	B	18	ALA	2.1
1	B	109	ALA	2.1
1	A	104	GLU	2.1
1	A	30	ASN	2.1
1	C	91	VAL	2.1
1	B	28	TRP	2.1
1	C	37	LEU	2.1
1	C	140	ASP	2.1
1	A	24	GLY	2.1
1	C	32	ARG	2.1
1	A	95	SER	2.0
1	A	20	PRO	2.0
1	C	41	VAL	2.0
1	B	54	GLY	2.0
1	C	114	TRP	2.0
1	A	10	ASP	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.