



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:28 PM UTC

PDB ID : 3B94 / pdb_00003b94
Title : Crystal structure of human GITRL
Authors : Song, X.M.; Zhou, Z.C.
Deposited on : 2007-11-02
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

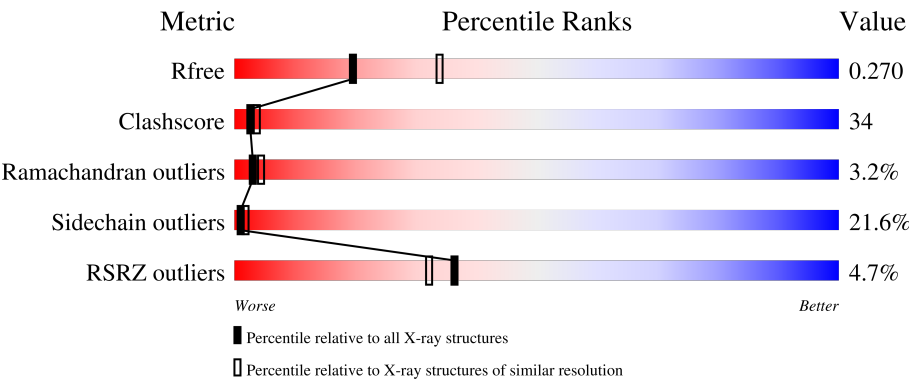
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	133	
1	B	133	
1	C	133	
1	D	133	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3293 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 ligand superfamily member 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			777	500	130	142	5			
1	B	113	Total	C	N	O	S	0	0	0
			859	558	140	156	5			
1	C	100	Total	C	N	O	S	0	0	0
			781	512	125	139	5			
1	D	112	Total	C	N	O	S	0	0	0
			847	550	141	152	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	expression tag	UNP Q9UNG2
A	46	ALA	-	expression tag	UNP Q9UNG2
A	47	MET	-	expression tag	UNP Q9UNG2
A	48	ALA	-	expression tag	UNP Q9UNG2
A	49	SER	-	expression tag	UNP Q9UNG2
B	45	GLY	-	expression tag	UNP Q9UNG2
B	46	ALA	-	expression tag	UNP Q9UNG2
B	47	MET	-	expression tag	UNP Q9UNG2
B	48	ALA	-	expression tag	UNP Q9UNG2
B	49	SER	-	expression tag	UNP Q9UNG2
C	45	GLY	-	expression tag	UNP Q9UNG2
C	46	ALA	-	expression tag	UNP Q9UNG2
C	47	MET	-	expression tag	UNP Q9UNG2
C	48	ALA	-	expression tag	UNP Q9UNG2
C	49	SER	-	expression tag	UNP Q9UNG2
D	45	GLY	-	expression tag	UNP Q9UNG2
D	46	ALA	-	expression tag	UNP Q9UNG2
D	47	MET	-	expression tag	UNP Q9UNG2
D	48	ALA	-	expression tag	UNP Q9UNG2
D	49	SER	-	expression tag	UNP Q9UNG2

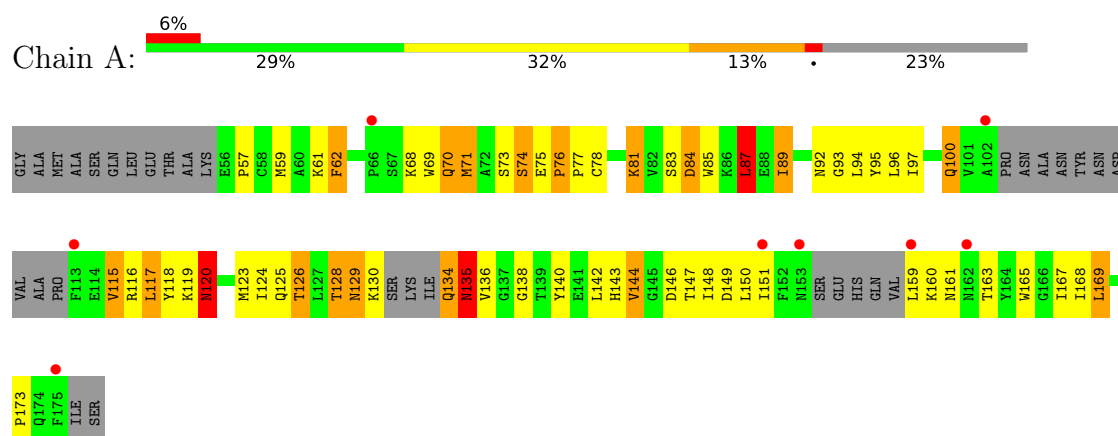
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total 6	O 6	0	0
2	B	8	Total 8	O 8	0	0
2	C	10	Total 10	O 10	0	0
2	D	5	Total 5	O 5	0	0

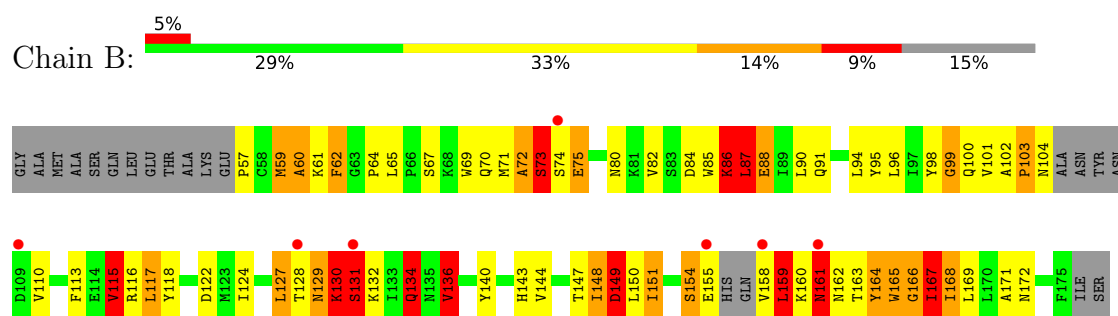
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

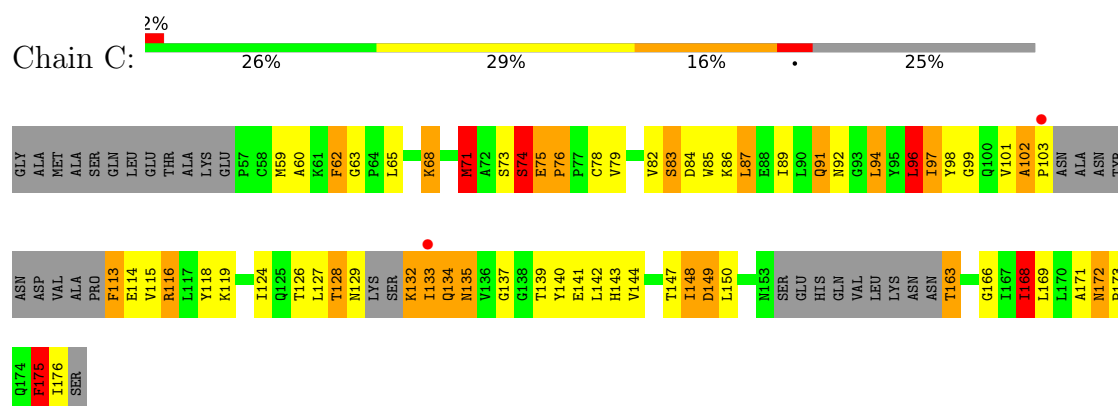
- Molecule 1: Tumor necrosis factor ligand superfamily member 18



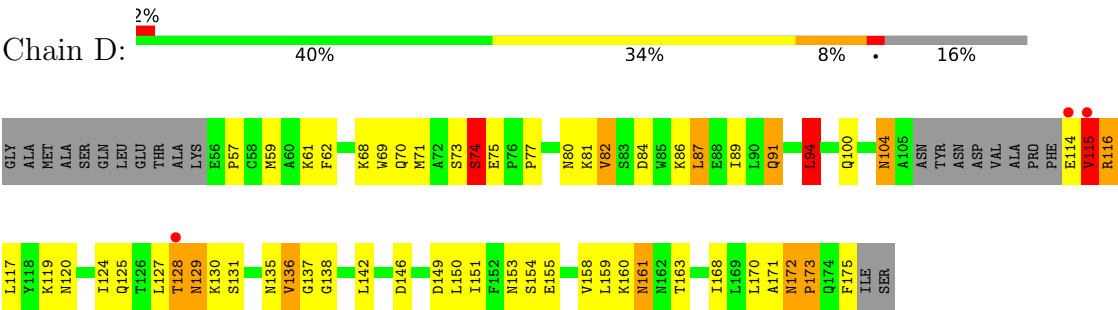
- Molecule 1: Tumor necrosis factor ligand superfamily member 18



- Molecule 1: Tumor necrosis factor ligand superfamily member 18



● Molecule 1: Tumor necrosis factor ligand superfamily member 18



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	141.94Å 141.94Å 47.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-2.50) 95.7 (30.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.276 0.212 , 0.270	Depositor DCC
R_{free} test set	1067 reflections (5.57%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3293	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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	1.52	7/793 (0.9%)	1.47	15/1078 (1.4%)
1	B	2.37	32/880 (3.6%)	2.05	32/1199 (2.7%)
1	C	1.91	17/800 (2.1%)	1.84	17/1087 (1.6%)
1	D	1.83	13/868 (1.5%)	1.80	17/1187 (1.4%)
All	All	1.94	69/3341 (2.1%)	1.81	81/4551 (1.8%)

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	1
1	B	0	5
1	C	0	1
All	All	0	7

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLY	C-O	17.56	1.41	1.23
1	B	60	ALA	C-O	15.97	1.44	1.23
1	B	165	TRP	C-O	14.17	1.41	1.23
1	B	165	TRP	CA-C	-13.32	1.36	1.52
1	B	167	ILE	CA-C	-12.32	1.37	1.52
1	B	72	ALA	CA-CB	-10.94	1.34	1.53
1	B	164	TYR	CA-CB	10.54	1.71	1.53
1	B	159	LEU	N-CA	-10.43	1.33	1.46
1	B	162	ASN	CA-CB	9.20	1.65	1.53
1	C	89	ILE	N-CA	-8.32	1.36	1.46
1	D	89	ILE	N-CA	-7.58	1.36	1.46
1	B	149	ASP	CA-C	-7.43	1.43	1.52
1	B	122	ASP	CA-C	-7.42	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	SER	N-CA	7.31	1.56	1.46
1	B	136	VAL	CA-CB	6.89	1.63	1.54
1	B	59	MET	C-O	-6.71	1.15	1.23
1	C	68	LYS	N-CA	-6.64	1.42	1.46
1	C	124	ILE	C-O	-6.54	1.16	1.24
1	C	148	ILE	CA-CB	6.47	1.62	1.54
1	D	172	ASN	CB-CG	-6.37	1.36	1.52
1	C	115	VAL	CA-CB	-6.34	1.46	1.54
1	B	144	VAL	C-O	6.14	1.30	1.24
1	D	87	LEU	C-O	6.14	1.31	1.23
1	B	129	ASN	CA-C	-6.12	1.44	1.52
1	B	148	ILE	CA-CB	-6.11	1.47	1.54
1	D	171	ALA	C-O	6.07	1.31	1.23
1	A	89	ILE	CA-CB	6.05	1.59	1.53
1	C	149	ASP	CA-C	-6.01	1.45	1.52
1	B	116	ARG	CA-C	-6.00	1.45	1.52
1	B	86	LYS	N-CA	5.97	1.53	1.46
1	B	164	TYR	N-CA	5.94	1.52	1.46
1	C	89	ILE	CA-CB	5.92	1.61	1.54
1	C	140	TYR	CZ-OH	5.90	1.50	1.38
1	B	62	PHE	C-O	5.79	1.31	1.24
1	D	82	VAL	N-CA	-5.79	1.38	1.46
1	C	63	GLY	N-CA	5.70	1.52	1.44
1	D	70	GLN	C-O	5.66	1.30	1.23
1	D	173	PRO	CA-C	5.66	1.60	1.52
1	C	98	TYR	C-O	5.59	1.31	1.23
1	D	59	MET	C-O	-5.59	1.17	1.23
1	A	167	ILE	N-CA	-5.58	1.39	1.46
1	C	166	GLY	C-O	5.58	1.30	1.24
1	B	115	VAL	CA-CB	-5.54	1.47	1.54
1	B	163	THR	CA-CB	-5.51	1.43	1.53
1	B	94	LEU	N-CA	-5.48	1.39	1.46
1	B	87	LEU	N-CA	-5.46	1.38	1.45
1	A	73	SER	CA-C	5.43	1.60	1.52
1	B	159	LEU	CA-C	-5.37	1.46	1.52
1	D	70	GLN	CD-NE2	5.35	1.44	1.33
1	C	168	ILE	N-CA	5.34	1.52	1.46
1	B	143	HIS	N-CA	5.33	1.52	1.45
1	A	128	THR	CA-CB	5.32	1.59	1.52
1	C	147	THR	CA-C	5.30	1.59	1.52
1	D	137	GLY	C-O	-5.29	1.18	1.24
1	D	94	LEU	CA-C	5.22	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	MET	CA-C	-5.21	1.46	1.52
1	C	76	PRO	CA-C	5.21	1.57	1.52
1	C	141	GLU	N-CA	-5.18	1.40	1.46
1	A	167	ILE	CA-CB	-5.18	1.50	1.55
1	D	172	ASN	C-O	-5.17	1.19	1.24
1	A	135	ASN	N-CA	5.16	1.52	1.45
1	C	60	ALA	CA-C	-5.12	1.46	1.52
1	B	99	GLY	N-CA	5.09	1.50	1.45
1	B	134	GLN	N-CA	5.07	1.52	1.45
1	B	150	LEU	CA-CB	5.06	1.60	1.53
1	C	97	ILE	C-O	-5.04	1.18	1.24
1	B	67	SER	CA-C	-5.01	1.46	1.52
1	D	136	VAL	C-O	-5.01	1.19	1.24
1	A	62	PHE	CA-C	-5.00	1.46	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	GLN	N-CA-C	15.15	129.65	108.74
1	D	172	ASN	CB-CA-C	-13.10	93.31	110.34
1	B	130	LYS	N-CA-C	-11.32	97.20	112.03
1	A	138	GLY	N-CA-C	-10.22	96.02	110.63
1	B	165	TRP	O-C-N	-10.15	111.86	123.33
1	B	159	LEU	CB-CG-CD1	-9.90	81.01	110.70
1	C	62	PHE	CA-C-N	-9.31	107.25	121.87
1	C	62	PHE	C-N-CA	-9.31	107.25	121.87
1	B	161	ASN	N-CA-C	9.09	121.35	110.44
1	D	138	GLY	N-CA-C	-8.75	98.12	110.63
1	B	163	THR	CA-C-O	8.56	129.82	120.32
1	B	91	GLN	N-CA-C	8.54	122.40	108.99
1	B	102	ALA	CA-C-N	8.51	130.48	119.84
1	B	102	ALA	C-N-CA	8.51	130.48	119.84
1	B	149	ASP	N-CA-C	8.25	121.69	109.24
1	D	74	SER	N-CA-C	-8.13	103.45	112.72
1	C	168	ILE	CB-CA-C	-7.94	97.99	110.69
1	C	116	ARG	N-CA-C	7.87	122.44	109.06
1	B	60	ALA	CA-C-O	7.76	130.20	121.51
1	B	168	ILE	CB-CA-C	-7.71	97.37	110.71
1	B	168	ILE	N-CA-C	7.59	119.68	108.45
1	B	167	ILE	N-CA-C	7.20	117.85	108.35
1	D	153	ASN	N-CA-C	-7.18	103.45	111.28
1	B	164	TYR	CB-CA-C	-7.13	97.20	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	TRP	N-CA-CB	6.80	124.16	111.52
1	D	128	THR	N-CA-C	-6.78	96.11	108.65
1	C	134	GLN	CA-C-N	6.75	133.15	122.21
1	C	134	GLN	C-N-CA	6.75	133.15	122.21
1	B	162	ASN	N-CA-C	-6.67	101.53	111.81
1	B	110	VAL	N-CA-C	6.59	116.74	110.42
1	B	116	ARG	CB-CG-CD	-6.54	96.25	111.30
1	B	161	ASN	CA-C-N	6.53	132.89	123.17
1	B	161	ASN	C-N-CA	6.53	132.89	123.17
1	C	86	LYS	CA-C-N	-6.35	112.62	122.59
1	C	86	LYS	C-N-CA	-6.35	112.62	122.59
1	A	135	ASN	N-CA-C	6.21	118.73	110.53
1	A	140	TYR	N-CA-C	6.14	118.52	109.24
1	B	60	ALA	N-CA-C	6.06	118.17	109.14
1	B	115	VAL	CA-C-N	-5.99	113.18	122.59
1	B	115	VAL	C-N-CA	-5.99	113.18	122.59
1	D	130	LYS	N-CA-C	-5.90	106.13	113.15
1	A	89	ILE	N-CA-C	5.89	115.73	107.37
1	C	71	MET	N-CA-C	5.86	123.29	110.80
1	B	159	LEU	N-CA-CB	-5.85	102.45	111.46
1	D	87	LEU	CB-CG-CD1	-5.84	93.17	110.70
1	D	115	VAL	N-CA-C	5.82	121.44	109.34
1	A	93	GLY	N-CA-C	5.80	118.98	110.80
1	D	137	GLY	N-CA-C	5.76	119.15	110.97
1	C	171	ALA	CA-C-N	-5.76	117.02	122.37
1	C	171	ALA	C-N-CA	-5.76	117.02	122.37
1	B	59	MET	N-CA-C	5.70	117.73	109.07
1	D	135	ASN	N-CA-C	5.69	118.70	110.28
1	B	166	GLY	O-C-N	-5.65	117.01	123.51
1	A	74	SER	N-CA-C	5.63	119.25	112.38
1	B	166	GLY	CA-C-O	5.62	128.25	121.68
1	A	78	CYS	N-CA-C	-5.60	107.09	114.31
1	A	160	LYS	N-CA-C	5.58	122.68	110.80
1	B	164	TYR	CA-C-O	5.55	127.27	121.38
1	A	75	GLU	CB-CA-C	-5.50	104.07	110.17
1	B	151	ILE	N-CA-C	5.48	115.78	108.11
1	D	61	LYS	CD-CE-NZ	-5.47	94.41	111.90
1	D	150	LEU	CA-C-N	-5.42	115.58	123.06
1	D	150	LEU	C-N-CA	-5.42	115.58	123.06
1	D	59	MET	CG-SD-CE	5.40	112.77	100.90
1	B	144	VAL	N-CA-C	-5.39	102.23	109.30
1	A	76	PRO	CA-C-N	5.39	125.33	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	PRO	C-N-CA	5.39	125.33	119.78
1	C	59	MET	N-CA-C	5.37	116.14	108.74
1	B	136	VAL	CB-CA-C	5.21	118.32	110.98
1	D	115	VAL	CB-CA-C	5.20	119.82	111.29
1	D	161	ASN	CB-CA-C	-5.13	99.71	110.17
1	A	73	SER	CA-C-N	5.06	128.70	120.60
1	A	73	SER	C-N-CA	5.06	128.70	120.60
1	D	82	VAL	CB-CA-C	5.06	117.37	111.55
1	C	148	ILE	CB-CG1-CD1	-5.05	103.20	113.80
1	A	87	LEU	N-CA-C	5.03	116.46	108.96
1	C	96	LEU	CA-C-N	-5.03	116.61	123.10
1	C	96	LEU	C-N-CA	-5.03	116.61	123.10
1	B	149	ASP	O-C-N	5.03	129.25	123.17
1	C	119	LYS	CG-CD-CE	5.02	122.86	111.30
1	A	84	ASP	N-CA-C	-5.01	103.10	110.42

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	LEU	Peptide
1	B	118	TYR	Peptide
1	B	130	LYS	Peptide
1	B	131	SER	Peptide
1	B	161	ASN	Peptide
1	B	167	ILE	Mainchain
1	C	175	PHE	Peptide

5.2 Too-close contacts [i](#)

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	777	0	736	55	0
1	B	859	0	818	64	0
1	C	781	0	754	70	0
1	D	847	0	809	37	0
2	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	0	4	0
2	C	10	0	0	3	0
2	D	5	0	0	0	0
All	All	3293	0	3117	216	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 34.

All (216) 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:59:MET:HE1	1:B:171:ALA:HB1	1.15	1.15
1:C:96:LEU:HB3	1:C:168:ILE:CD1	1.76	1.13
1:C:96:LEU:HG	1:C:168:ILE:HD11	1.35	1.09
1:C:132:LYS:HB2	1:C:133:ILE:HD12	1.25	1.08
1:B:134:GLN:HB2	2:B:21:HOH:O	1.63	0.99
1:C:132:LYS:CB	1:C:133:ILE:HD12	1.93	0.97
1:A:59:MET:HE1	1:B:171:ALA:CB	1.95	0.95
1:B:103:PRO:HG2	1:B:132:LYS:O	1.69	0.92
1:C:96:LEU:HB3	1:C:168:ILE:HD12	1.47	0.92
1:A:57:PRO:HG3	1:A:168:ILE:HD11	1.56	0.86
1:C:113:PHE:C	1:C:113:PHE:HD1	1.83	0.85
1:D:116:ARG:HG3	1:D:116:ARG:HH11	1.42	0.85
1:B:88:GLU:HG2	1:B:147:THR:HG22	1.59	0.84
1:C:113:PHE:HE1	1:C:128:THR:HA	1.43	0.81
1:B:70:GLN:HG2	2:B:24:HOH:O	1.79	0.81
1:B:86:LYS:HG2	1:B:149:ASP:HB3	1.62	0.80
1:C:132:LYS:HB2	1:C:133:ILE:CD1	2.10	0.80
1:C:113:PHE:C	1:C:113:PHE:CD1	2.58	0.80
1:C:113:PHE:CE1	1:C:128:THR:HA	2.18	0.78
1:B:113:PHE:CD1	1:B:129:ASN:CB	2.66	0.78
1:B:103:PRO:CG	1:B:132:LYS:O	2.32	0.78
1:C:75:GLU:CB	1:C:76:PRO:HD3	2.14	0.78
1:A:69:TRP:CD1	1:A:81:LYS:HB2	2.18	0.77
1:C:75:GLU:CB	1:C:76:PRO:CD	2.62	0.77
1:C:96:LEU:CG	1:C:168:ILE:HD11	2.14	0.77
1:A:62:PHE:HB2	1:A:69:TRP:CZ3	2.19	0.76
1:D:115:VAL:O	1:D:151:ILE:O	2.03	0.76
1:A:68:LYS:O	1:A:70:GLN:NE2	2.19	0.76
1:A:87:LEU:CD2	1:A:165:TRP:HH2	1.99	0.75
1:C:134:GLN:HE21	1:C:135:ASN:HD22	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ASN:ND2	1:C:144:VAL:H	1.85	0.75
1:A:59:MET:CE	1:B:171:ALA:HB1	2.09	0.74
1:C:133:ILE:HG22	1:C:133:ILE:O	1.85	0.74
1:C:128:THR:O	1:C:129:ASN:C	2.30	0.73
1:C:96:LEU:HB3	1:C:168:ILE:HD11	1.70	0.73
1:A:87:LEU:HD22	1:A:165:TRP:CH2	2.24	0.73
1:A:92:ASN:OD1	1:A:143:HIS:HA	1.89	0.72
1:D:115:VAL:HG13	1:D:127:LEU:HB2	1.71	0.72
1:D:104:ASN:HB3	1:D:159:LEU:CD2	2.20	0.71
1:D:175:PHE:N	1:D:175:PHE:CD2	2.56	0.71
1:C:96:LEU:CB	1:C:168:ILE:CD1	2.64	0.71
1:C:101:VAL:O	1:C:163:THR:HG23	1.92	0.70
1:D:116:ARG:HH11	1:D:116:ARG:CG	2.04	0.70
1:D:104:ASN:HB3	1:D:159:LEU:HD21	1.74	0.70
1:C:132:LYS:N	2:C:5:HOH:O	2.24	0.70
1:C:84:ASP:O	1:C:85:TRP:HB2	1.92	0.69
1:D:86:LYS:HD2	1:D:149:ASP:OD1	1.93	0.69
1:A:87:LEU:CD2	1:A:165:TRP:CH2	2.76	0.68
1:B:64:PRO:HB2	1:B:161:ASN:OD1	1.93	0.67
1:B:117:LEU:HD13	1:B:124:ILE:HD11	1.77	0.66
1:B:103:PRO:HG2	1:B:132:LYS:C	2.20	0.65
1:A:62:PHE:HB2	1:A:69:TRP:CE3	2.31	0.65
1:B:88:GLU:CG	1:B:147:THR:HG22	2.27	0.65
1:C:149:ASP:N	1:C:149:ASP:OD1	2.29	0.65
1:B:101:VAL:O	1:B:103:PRO:HD3	1.97	0.65
1:A:119:LYS:HA	1:A:148:ILE:HD13	1.78	0.65
1:B:103:PRO:O	1:B:104:ASN:HB3	1.98	0.63
1:A:150:LEU:HD22	1:A:165:TRP:CD1	2.34	0.63
1:B:87:LEU:CD1	1:B:87:LEU:C	2.72	0.63
1:B:65:LEU:H	1:B:161:ASN:HD21	1.47	0.63
1:C:62:PHE:O	1:C:68:LYS:O	2.18	0.61
1:C:176:ILE:N	2:C:17:HOH:O	2.33	0.61
1:C:175:PHE:C	2:C:17:HOH:O	2.44	0.61
1:D:104:ASN:CB	1:D:159:LEU:HD21	2.31	0.60
1:C:82:VAL:O	1:C:83:SER:HB3	1.99	0.60
1:A:125:GLN:HG2	1:A:126:THR:N	2.16	0.60
1:C:92:ASN:ND2	1:C:143:HIS:HA	2.17	0.60
1:B:155:GLU:O	1:B:158:VAL:CB	2.50	0.59
1:A:129:ASN:HD22	1:A:130:LYS:N	2.01	0.59
1:B:72:ALA:HB2	1:C:175:PHE:HE1	1.68	0.59
1:C:96:LEU:CB	1:C:168:ILE:HD11	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PRO:HG2	1:D:168:ILE:HD11	1.84	0.58
1:D:116:ARG:HA	1:D:125:GLN:O	2.03	0.58
1:A:125:GLN:HG2	1:A:126:THR:H	1.69	0.58
1:B:128:THR:O	1:B:129:ASN:CB	2.52	0.58
1:D:158:VAL:HG22	1:D:159:LEU:C	2.28	0.57
1:C:101:VAL:O	1:C:102:ALA:CB	2.52	0.57
1:B:72:ALA:HB2	1:C:175:PHE:CE1	2.39	0.57
1:C:92:ASN:HD22	1:C:143:HIS:HA	1.69	0.57
1:C:127:LEU:C	1:C:128:THR:HG23	2.30	0.57
1:D:68:LYS:HE3	1:D:84:ASP:OD1	2.04	0.57
1:C:135:ASN:HD22	1:C:135:ASN:H	1.52	0.57
1:C:172:ASN:HD22	1:C:172:ASN:N	2.02	0.56
1:A:135:ASN:OD1	1:B:140:TYR:CE2	2.59	0.56
1:B:103:PRO:O	1:B:159:LEU:HA	2.05	0.56
1:B:87:LEU:C	1:B:87:LEU:HD12	2.31	0.56
1:A:126:THR:H	1:C:133:ILE:HG21	1.69	0.56
1:B:57:PRO:O	1:B:73:SER:HB2	2.06	0.56
1:A:95:TYR:CD1	1:A:142:LEU:HD12	2.41	0.56
1:D:173:PRO:HB2	1:D:175:PHE:CZ	2.40	0.56
1:C:127:LEU:O	1:C:128:THR:CG2	2.55	0.55
1:B:101:VAL:HG13	1:B:159:LEU:CD1	2.36	0.55
1:C:132:LYS:C	1:C:133:ILE:HG13	2.31	0.55
1:C:135:ASN:O	1:C:135:ASN:ND2	2.39	0.55
1:A:117:LEU:HD13	1:A:124:ILE:HD11	1.88	0.55
1:D:173:PRO:HB2	1:D:175:PHE:CE2	2.42	0.55
1:B:99:GLY:HA3	1:B:165:TRP:HA	1.88	0.55
1:D:80:ASN:O	1:D:87:LEU:HD12	2.08	0.54
1:A:95:TYR:CE2	1:A:169:LEU:HB2	2.42	0.54
1:B:84:ASP:O	1:B:85:TRP:HB2	2.07	0.54
1:A:57:PRO:CG	1:A:168:ILE:HD11	2.33	0.53
1:B:65:LEU:H	1:B:161:ASN:ND2	2.06	0.53
1:A:129:ASN:HD22	1:A:129:ASN:C	2.16	0.53
1:C:99:GLY:O	1:C:135:ASN:HB2	2.09	0.52
1:D:94:LEU:HD13	1:D:170:LEU:HD12	1.90	0.52
1:B:59:MET:SD	1:C:173:PRO:HG3	2.51	0.51
1:B:70:GLN:NE2	2:B:24:HOH:O	2.31	0.51
1:C:134:GLN:HE21	1:C:135:ASN:ND2	2.03	0.51
1:B:82:VAL:HB	1:B:86:LYS:HB3	1.91	0.51
1:D:116:ARG:CG	1:D:116:ARG:NH1	2.67	0.51
1:B:159:LEU:C	1:B:159:LEU:HD23	2.35	0.51
1:A:85:TRP:CH2	1:A:163:THR:HG22	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASN:HB3	1:A:134:GLN:HE22	1.76	0.50
1:C:134:GLN:NE2	1:C:135:ASN:ND2	2.59	0.50
1:C:142:LEU:HD13	1:C:148:ILE:HD11	1.94	0.50
1:D:125:GLN:HE22	1:D:136:VAL:HA	1.76	0.50
1:A:83:SER:O	1:A:84:ASP:C	2.54	0.50
1:A:120:ASN:HD22	1:A:146:ASP:HA	1.77	0.50
1:C:94:LEU:CD2	1:C:139:THR:HG22	2.40	0.50
1:A:143:HIS:O	1:A:144:VAL:C	2.53	0.50
1:C:94:LEU:HD21	1:C:139:THR:HG22	1.93	0.50
1:C:172:ASN:HD22	1:C:172:ASN:H	1.60	0.50
1:B:101:VAL:HG13	1:B:159:LEU:HD12	1.93	0.50
1:C:74:SER:O	1:C:75:GLU:C	2.55	0.49
1:B:101:VAL:CG1	1:B:159:LEU:HD12	2.43	0.49
1:D:74:SER:O	1:D:77:PRO:HB3	2.13	0.49
1:A:62:PHE:CZ	1:A:84:ASP:HA	2.48	0.49
1:B:104:ASN:HB3	1:B:159:LEU:HA	1.95	0.49
1:A:61:LYS:HG2	1:A:62:PHE:N	2.27	0.49
1:C:135:ASN:ND2	1:C:135:ASN:C	2.71	0.49
1:B:74:SER:O	1:B:75:GLU:C	2.56	0.49
1:D:119:LYS:HB2	1:D:124:ILE:HD13	1.94	0.48
1:A:120:ASN:HA	1:A:147:THR:OG1	2.13	0.48
1:B:159:LEU:HD23	1:B:159:LEU:O	2.13	0.48
1:C:133:ILE:O	1:C:134:GLN:CD	2.56	0.48
1:B:62:PHE:O	1:B:164:TYR:HB2	2.13	0.48
1:B:115:VAL:HA	1:B:151:ILE:O	2.13	0.48
1:C:118:TYR:O	1:C:148:ILE:HA	2.13	0.48
1:A:84:ASP:HB3	1:A:85:TRP:CD1	2.49	0.48
1:B:74:SER:O	1:B:75:GLU:O	2.31	0.47
1:D:158:VAL:HG22	1:D:160:LYS:N	2.28	0.47
1:A:96:LEU:HD12	1:A:97:ILE:N	2.29	0.47
1:A:125:GLN:HE22	1:A:136:VAL:HA	1.79	0.47
1:A:150:LEU:CD2	1:A:165:TRP:CD1	2.98	0.47
1:A:68:LYS:HB2	1:A:68:LYS:HE2	1.57	0.47
1:C:73:SER:C	1:C:74:SER:OG	2.57	0.47
1:B:113:PHE:HD1	1:B:129:ASN:CB	2.23	0.47
1:C:113:PHE:HE1	1:C:128:THR:CA	2.21	0.47
1:C:127:LEU:O	1:C:128:THR:HG23	2.15	0.47
1:C:127:LEU:C	1:C:128:THR:CG2	2.88	0.47
1:D:104:ASN:C	1:D:104:ASN:HD22	2.23	0.47
1:D:158:VAL:CG2	1:D:159:LEU:N	2.78	0.47
1:C:84:ASP:O	1:C:85:TRP:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:VAL:O	1:D:116:ARG:HB2	2.14	0.46
1:A:62:PHE:HE2	1:A:85:TRP:CE2	2.33	0.46
1:B:60:ALA:O	1:B:166:GLY:CA	2.64	0.46
1:B:80:ASN:HB2	1:B:90:LEU:HD11	1.96	0.46
1:B:95:TYR:CZ	1:B:169:LEU:HD13	2.51	0.46
1:C:97:ILE:O	1:C:137:GLY:HA3	2.16	0.46
1:A:143:HIS:N	1:A:146:ASP:OD2	2.45	0.46
1:A:89:ILE:O	1:A:144:VAL:HA	2.17	0.45
1:D:129:ASN:C	1:D:131:SER:H	2.23	0.45
1:B:80:ASN:HD21	1:D:91:GLN:HE21	1.63	0.45
1:A:118:TYR:HB2	1:A:149:ASP:HB3	1.99	0.45
1:D:62:PHE:HB2	1:D:69:TRP:CE2	2.51	0.44
1:B:98:TYR:HA	1:B:136:VAL:O	2.17	0.44
1:A:126:THR:HG22	1:C:133:ILE:HG12	2.00	0.44
1:D:114:GLU:C	1:D:116:ARG:HH12	2.25	0.44
1:B:148:ILE:O	1:B:149:ASP:HB3	2.17	0.44
1:D:104:ASN:HB3	1:D:159:LEU:HD23	1.99	0.44
1:A:85:TRP:HH2	1:A:163:THR:HG22	1.81	0.44
1:B:64:PRO:CB	1:B:161:ASN:OD1	2.62	0.44
1:B:70:GLN:CG	2:B:24:HOH:O	2.51	0.44
1:B:101:VAL:HG21	1:B:115:VAL:HG21	2.00	0.44
1:A:116:ARG:HB3	1:A:123:MET:HG2	1.99	0.44
1:B:103:PRO:O	1:B:158:VAL:O	2.35	0.44
1:C:92:ASN:HD22	1:C:144:VAL:H	1.63	0.44
1:A:116:ARG:HB2	1:A:118:TYR:CE1	2.54	0.43
1:C:134:GLN:NE2	1:C:135:ASN:HD22	2.05	0.43
1:D:120:ASN:HD21	1:D:146:ASP:HA	1.83	0.43
1:C:87:LEU:C	1:C:87:LEU:HD12	2.43	0.43
1:A:125:GLN:CG	1:A:126:THR:N	2.80	0.43
1:C:132:LYS:HB3	1:C:133:ILE:HD12	1.92	0.43
1:D:87:LEU:HD12	1:D:87:LEU:HA	1.75	0.43
1:A:71:MET:HG3	2:A:18:HOH:O	2.19	0.43
1:B:69:TRP:CZ2	1:B:87:LEU:HB3	2.53	0.43
1:B:127:LEU:HG	1:B:134:GLN:HG3	1.99	0.43
1:C:102:ALA:HA	1:C:103:PRO:HD2	1.54	0.43
1:B:86:LYS:HG2	1:B:149:ASP:CB	2.40	0.42
1:B:84:ASP:O	1:B:85:TRP:CB	2.67	0.42
1:C:134:GLN:HE21	1:C:135:ASN:H	1.66	0.42
1:A:125:GLN:CG	1:A:126:THR:H	2.30	0.42
1:A:76:PRO:HA	1:A:77:PRO:HD3	1.90	0.42
1:A:119:LYS:HB2	1:A:124:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:VAL:HG22	1:D:159:LEU:N	2.34	0.42
1:B:172:ASN:OD1	1:B:172:ASN:N	2.52	0.42
1:C:113:PHE:CD1	1:C:114:GLU:N	2.87	0.42
1:D:104:ASN:C	1:D:104:ASN:ND2	2.78	0.42
1:B:167:ILE:CG1	1:B:168:ILE:N	2.83	0.41
1:A:85:TRP:CE3	1:A:150:LEU:HD23	2.55	0.41
1:A:92:ASN:OD1	1:A:143:HIS:CA	2.62	0.41
1:B:127:LEU:CD1	1:B:134:GLN:HG3	2.50	0.41
1:A:115:VAL:HG22	1:A:151:ILE:O	2.21	0.41
1:C:78:CYS:HA	1:C:91:GLN:HG2	2.03	0.41
1:D:159:LEU:C	1:D:161:ASN:N	2.77	0.41
1:C:92:ASN:HD21	1:C:144:VAL:H	1.66	0.41
1:B:60:ALA:O	1:B:167:ILE:N	2.44	0.41
1:C:73:SER:O	1:C:74:SER:CB	2.68	0.41
1:B:99:GLY:C	1:B:136:VAL:HG13	2.46	0.40
1:D:142:LEU:HA	1:D:142:LEU:HD23	1.86	0.40
1:C:91:GLN:HE21	1:C:91:GLN:HB2	1.71	0.40
1:A:100:GLN:O	1:A:163:THR:HA	2.21	0.40
1:D:158:VAL:CG2	1:D:163:THR:OG1	2.69	0.40
1:A:144:VAL:H	1:A:144:VAL:HG23	1.61	0.40
1:B:130:LYS:O	1:B:131:SER:C	2.64	0.40
1:B:154:SER:OG	1:B:155:GLU:N	2.50	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	94/133 (71%)	82 (87%)	10 (11%)	2 (2%)	5	9
1	B	107/133 (80%)	91 (85%)	14 (13%)	2 (2%)	6	11
1	C	92/133 (69%)	77 (84%)	7 (8%)	8 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	108/133 (81%)	98 (91%)	9 (8%)	1 (1%)	14	27
All	All	401/532 (75%)	348 (87%)	40 (10%)	13 (3%)	3	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	SER
1	C	71	MET
1	C	102	ALA
1	C	128	THR
1	A	173	PRO
1	C	75	GLU
1	C	83	SER
1	D	155	GLU
1	A	120	ASN
1	C	175	PHE
1	C	74	SER
1	B	75	GLU
1	C	133	ILE

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	80/116 (69%)	62 (78%)	18 (22%)	1	1
1	B	89/116 (77%)	69 (78%)	20 (22%)	1	1
1	C	82/116 (71%)	64 (78%)	18 (22%)	1	2
1	D	87/116 (75%)	70 (80%)	17 (20%)	1	2
All	All	338/464 (73%)	265 (78%)	73 (22%)	1	2

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLN

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Mol	Chain	Res	Type
1	A	71	MET
1	A	74	SER
1	A	81	LYS
1	A	87	LEU
1	A	94	LEU
1	A	100	GLN
1	A	115	VAL
1	A	117	LEU
1	A	120	ASN
1	A	126	THR
1	A	128	THR
1	A	129	ASN
1	A	134	GLN
1	A	135	ASN
1	A	144	VAL
1	A	161	ASN
1	A	169	LEU
1	B	61	LYS
1	B	71	MET
1	B	73	SER
1	B	86	LYS
1	B	87	LEU
1	B	88	GLU
1	B	96	LEU
1	B	100	GLN
1	B	103	PRO
1	B	115	VAL
1	B	117	LEU
1	B	127	LEU
1	B	130	LYS
1	B	131	SER
1	B	134	GLN
1	B	136	VAL
1	B	149	ASP
1	B	154	SER
1	B	159	LEU
1	B	160	LYS
1	C	65	LEU
1	C	71	MET
1	C	74	SER
1	C	79	VAL
1	C	87	LEU

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Mol	Chain	Res	Type
1	C	91	GLN
1	C	94	LEU
1	C	96	LEU
1	C	113	PHE
1	C	116	ARG
1	C	126	THR
1	C	132	LYS
1	C	135	ASN
1	C	150	LEU
1	C	163	THR
1	C	168	ILE
1	C	169	LEU
1	C	172	ASN
1	D	71	MET
1	D	73	SER
1	D	74	SER
1	D	75	GLU
1	D	81	LYS
1	D	82	VAL
1	D	91	GLN
1	D	94	LEU
1	D	100	GLN
1	D	104	ASN
1	D	115	VAL
1	D	116	ARG
1	D	117	LEU
1	D	128	THR
1	D	129	ASN
1	D	154	SER
1	D	172	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	100	GLN
1	A	125	GLN
1	A	129	ASN
1	A	134	GLN
1	A	135	ASN
1	A	161	ASN
1	A	162	ASN

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Mol	Chain	Res	Type
1	B	135	ASN
1	C	91	GLN
1	C	92	ASN
1	C	134	GLN
1	C	135	ASN
1	C	143	HIS
1	C	172	ASN
1	D	91	GLN
1	D	100	GLN
1	D	104	ASN
1	D	120	ASN
1	D	135	ASN
1	D	162	ASN

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 [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	102/133 (76%)	0.60	8 (7%) 19 17	30, 52, 71, 78	0
1	B	113/133 (84%)	-0.06	7 (6%) 26 23	18, 30, 51, 57	0
1	C	100/133 (75%)	-0.04	2 (2%) 65 61	18, 34, 58, 61	0
1	D	112/133 (84%)	-0.09	3 (2%) 56 51	17, 33, 58, 67	0
All	All	427/532 (80%)	0.10	20 (4%) 36 32	17, 36, 62, 78	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	PHE	4.7
1	A	153	ASN	3.3
1	A	113	PHE	3.2
1	B	131	SER	2.9
1	A	66	PRO	2.8
1	A	159	LEU	2.8
1	B	109	ASP	2.7
1	D	115	VAL	2.5
1	B	128	THR	2.5
1	C	103	PRO	2.5
1	C	133	ILE	2.4
1	A	151	ILE	2.4
1	D	114	GLU	2.3
1	B	158	VAL	2.2
1	A	162	ASN	2.2
1	D	128	THR	2.2
1	B	74	SER	2.2
1	A	102	ALA	2.2
1	B	155	GLU	2.0
1	B	161	ASN	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.