



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:34 PM EDT

PDB ID : 3IR0 / pdb_00003ir0
Title : Crystal Structure of Human Insulin complexed with Cu+2 metal ion
Authors : Raghavendra, N.; Pattabhi, V.; Rajan, S.S.
Deposited on : 2009-08-21
Resolution : 2.20 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

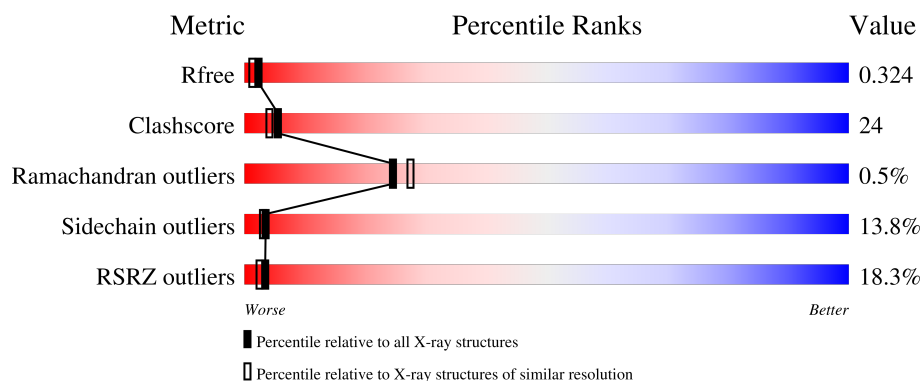
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	21	24% 52% 43% 5%
1	C	21	38% 33% 43% 19% 5%
1	E	21	33% 38% 48% 14%
1	G	21	19% 52% 38% 10%
1	I	21	5% 81% 10% 5% 5%

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Mol	Chain	Length	Quality of chain
1	K	21	
1	M	21	
1	O	21	
1	R	21	
1	T	21	
1	V	21	
1	X	21	
2	B	30	
2	D	30	
2	F	30	
2	H	30	
2	J	30	
2	L	30	
2	N	30	
2	P	30	
2	S	30	
2	U	30	
2	W	30	
2	Y	30	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5143 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 Insulin A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	E	21	Total	C	N	O	S	0	0	0
			162	99	24	35	4			
1	G	21	Total	C	N	O	S	0	0	0
			162	99	25	34	4			
1	I	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	K	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	M	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	O	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	R	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	T	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	V	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	X	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	D	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	H	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	J	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	L	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	N	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	P	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	S	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	U	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	W	30	Total	C	N	O	S	0	0	0
			241	158	39	42	2			
2	Y	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cu	0	0
			1	1		
3	D	1	Total	Cu	0	0
			1	1		
3	F	1	Total	Cu	0	0
			1	1		
3	H	1	Total	Cu	0	0
			1	1		
3	J	1	Total	Cu	0	0
			1	1		
3	L	1	Total	Cu	0	0
			1	1		
3	N	1	Total	Cu	0	0
			1	1		
3	P	1	Total	Cu	0	0
			1	1		
3	S	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	U	1	Total 1	Cu 1	0	0
3	W	1	Total 1	Cu 1	0	0
3	Y	1	Total 1	Cu 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total 9	O 9	0	0
4	B	12	Total 12	O 12	0	0
4	C	9	Total 9	O 9	0	0
4	D	22	Total 22	O 22	0	0
4	E	8	Total 8	O 8	0	0
4	F	13	Total 13	O 13	0	0
4	G	8	Total 8	O 8	0	0
4	H	12	Total 12	O 12	0	0
4	I	12	Total 12	O 12	0	0
4	J	17	Total 17	O 17	0	0
4	K	5	Total 5	O 5	0	0
4	L	19	Total 19	O 19	0	0
4	M	7	Total 7	O 7	0	0
4	N	16	Total 16	O 16	0	0
4	O	11	Total 11	O 11	0	0
4	P	24	Total 24	O 24	0	0

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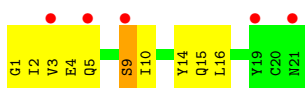
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	4	Total 4	O 4	0	0
4	S	15	Total 15	O 15	0	0
4	T	13	Total 13	O 13	0	0
4	U	10	Total 10	O 10	0	0
4	V	15	Total 15	O 15	0	0
4	W	20	Total 20	O 20	0	0
4	X	9	Total 9	O 9	0	0
4	Y	20	Total 20	O 20	0	0

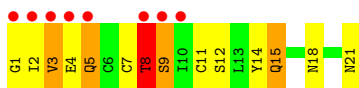
3 Residue-property plots [i](#)

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.

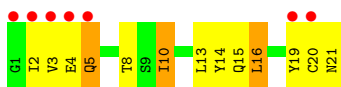
- Molecule 1: Insulin A chain



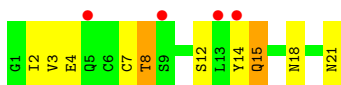
- Molecule 1: Insulin A chain



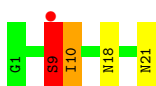
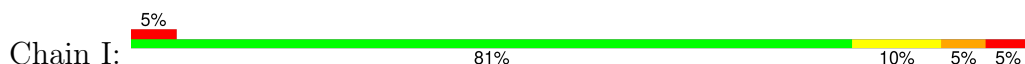
- Molecule 1: Insulin A chain



- Molecule 1: Insulin A chain



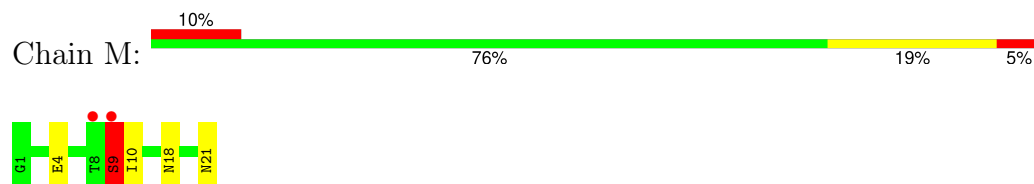
- Molecule 1: Insulin A chain



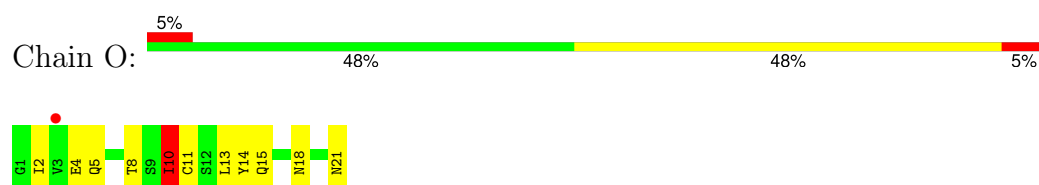
- Molecule 1: Insulin A chain



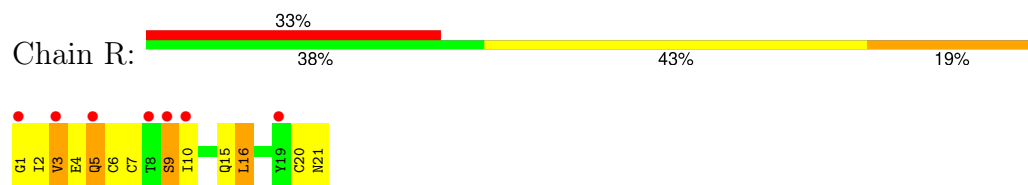
- Molecule 1: Insulin A chain



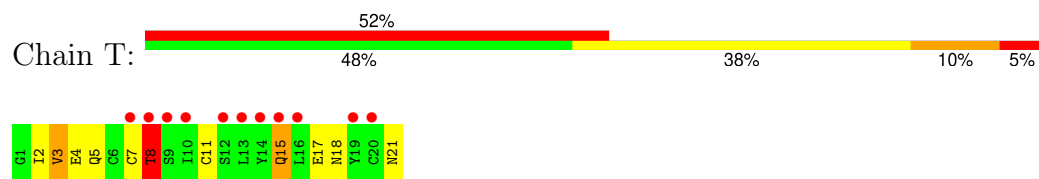
- Molecule 1: Insulin A chain



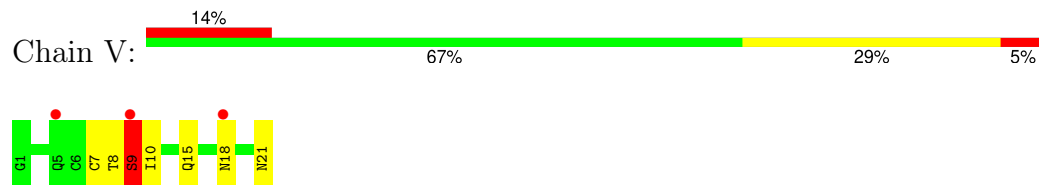
- Molecule 1: Insulin A chain



- Molecule 1: Insulin A chain



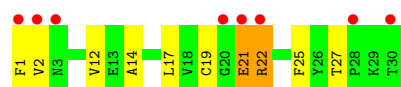
- Molecule 1: Insulin A chain



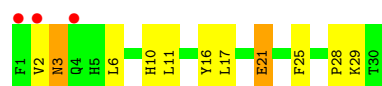
- Molecule 1: Insulin A chain



- Molecule 2: Insulin B chain



● Molecule 2: Insulin B chain



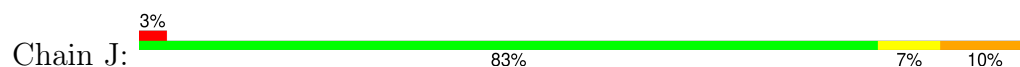
● Molecule 2: Insulin B chain



● Molecule 2: Insulin B chain



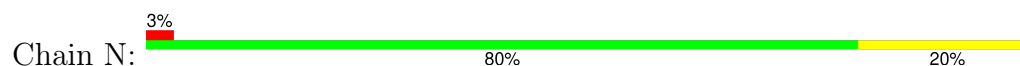
● Molecule 2: Insulin B chain



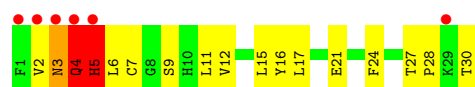
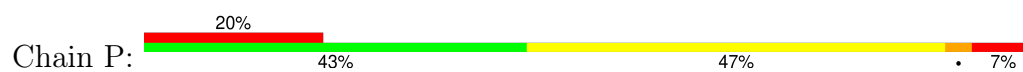
● Molecule 2: Insulin B chain



● Molecule 2: Insulin B chain



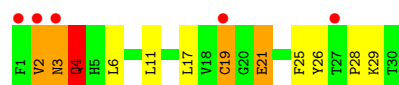
● Molecule 2: Insulin B chain



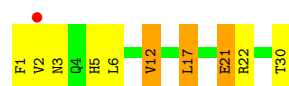
● Molecule 2: Insulin B chain



● Molecule 2: Insulin B chain



● Molecule 2: Insulin B chain



● Molecule 2: Insulin B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	81.56Å 81.56Å 68.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.70 – 2.20 26.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.70-2.20) 99.9 (26.70-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.299 0.301 , 0.324	Depositor DCC
R_{free} test set	1645 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.047 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5143	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9868e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	1.14	0/164	1.46	3/220 (1.4%)
1	C	1.22	0/164	1.43	3/220 (1.4%)
1	E	0.91	0/163	1.93	2/219 (0.9%)
1	G	1.01	0/163	1.24	0/220
1	I	1.08	0/164	1.54	2/220 (0.9%)
1	K	0.97	0/164	1.25	0/220
1	M	1.11	0/164	1.37	1/220 (0.5%)
1	O	1.05	0/164	1.37	2/220 (0.9%)
1	R	1.03	0/164	1.16	0/220
1	T	0.99	0/164	1.49	3/220 (1.4%)
1	V	1.10	0/164	1.34	1/220 (0.5%)
1	X	1.23	2/164 (1.2%)	1.49	2/220 (0.9%)
2	B	0.95	0/249	1.22	1/335 (0.3%)
2	D	1.20	0/242	1.28	0/326
2	F	1.00	0/249	1.21	0/335
2	H	1.05	0/242	1.96	5/326 (1.5%)
2	J	1.07	0/249	0.97	0/335
2	L	1.30	0/242	1.46	4/326 (1.2%)
2	N	1.01	0/249	1.02	0/335
2	P	1.28	0/242	1.62	7/326 (2.1%)
2	S	1.00	0/249	1.12	0/335
2	U	1.09	1/242 (0.4%)	1.96	5/326 (1.5%)
2	W	1.09	0/248	0.99	0/333
2	Y	1.13	0/242	1.38	2/326 (0.6%)
All	All	1.09	3/4911 (0.1%)	1.41	43/6603 (0.7%)

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
2	D	0	1
2	L	0	2
2	P	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	17	LEU	C-N	-6.31	1.26	1.33
1	X	10	ILE	CA-CB	5.38	1.61	1.54
1	X	2	ILE	CA-CB	5.12	1.60	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5	GLN	N-CA-C	19.65	136.90	111.75
2	H	3	ASN	N-CA-CB	-16.57	85.27	110.45
2	U	3	ASN	N-CA-C	16.19	132.40	110.55
2	U	3	ASN	N-CA-CB	-14.18	88.89	110.45
2	U	2	VAL	N-CA-C	-14.08	88.45	108.17
2	H	2	VAL	CB-CA-C	-13.48	90.67	110.63
2	H	3	ASN	N-CA-C	12.58	127.53	110.55
2	H	2	VAL	N-CA-C	-11.74	91.67	108.11
1	I	9	SER	N-CA-C	11.72	127.81	108.48
1	E	5	GLN	CB-CA-C	-11.29	88.56	110.46
1	T	8	THR	CB-CA-C	-10.55	89.47	109.72
2	U	2	VAL	CB-CA-C	-9.17	97.16	110.83
2	P	5	HIS	CB-CA-C	-8.77	97.87	110.06
1	A	9	SER	CB-CA-C	-8.30	100.01	113.37
2	P	4	GLN	CB-CA-C	8.09	127.79	111.60
2	H	4	GLN	N-CA-C	8.06	121.55	109.95
2	P	4	GLN	CA-C-N	7.88	133.79	121.26
2	P	4	GLN	C-N-CA	7.88	133.79	121.26
2	L	4	GLN	CB-CA-C	7.69	124.69	110.24
1	V	9	SER	N-CA-C	7.67	121.14	108.48
2	B	22	ARG	N-CA-C	-7.16	103.41	111.07
1	X	2	ILE	N-CA-C	-6.77	103.25	110.36
1	M	9	SER	N-CA-C	6.68	125.03	110.80
1	X	6	CYS	N-CA-C	-6.58	104.84	114.39
2	U	4	GLN	N-CA-C	6.54	119.75	110.14
1	I	9	SER	CB-CA-C	-6.38	102.98	114.52
1	C	9	SER	N-CA-C	-6.29	99.11	109.80
2	Y	27	THR	CA-C-N	6.25	127.65	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	27	THR	C-N-CA	6.25	127.65	119.84
1	T	11	CYS	N-CA-C	6.04	118.14	109.14
2	L	3	ASN	CB-CA-C	-6.03	100.32	112.99
2	P	4	GLN	N-CA-CB	-5.89	101.03	110.51
1	C	8	THR	N-CA-C	-5.84	104.55	111.03
1	A	14	TYR	N-CA-C	5.70	117.49	111.28
2	P	3	ASN	CB-CA-C	-5.41	98.39	110.19
1	O	10	ILE	CB-CA-C	5.35	118.94	110.81
1	T	3	VAL	N-CA-C	5.22	118.37	111.17
2	P	6	LEU	N-CA-C	5.19	117.36	108.90
1	O	13	LEU	N-CA-C	-5.14	105.76	111.36
2	L	4	GLN	CA-C-N	5.09	128.08	120.90
2	L	4	GLN	C-N-CA	5.09	128.08	120.90
1	C	9	SER	CB-CA-C	-5.02	105.29	113.37
1	A	10	ILE	N-CA-C	-5.00	101.29	108.89

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	ASN	Peptide
2	L	4	GLN	Peptide
2	L	5	HIS	Peptide
2	P	4	GLN	Peptide
2	P	5	HIS	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	163	0	149	8	0
1	C	163	0	149	16	0
1	E	162	0	144	17	0
1	G	162	0	149	8	0
1	I	163	0	149	5	1
1	K	163	0	149	12	0
1	M	163	0	149	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	163	0	149	14	0
1	R	163	0	149	15	0
1	T	163	0	149	9	0
1	V	163	0	149	4	2
1	X	163	0	149	23	0
2	B	242	0	232	10	0
2	D	236	0	225	9	0
2	F	242	0	232	16	0
2	H	236	0	225	9	0
2	J	242	0	232	6	0
2	L	236	0	225	12	1
2	N	242	0	232	3	0
2	P	236	0	225	16	1
2	S	242	0	232	20	1
2	U	236	0	225	14	0
2	W	241	0	228	8	0
2	Y	236	0	225	14	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	U	1	0	0	0	0
3	W	1	0	0	0	0
3	Y	1	0	0	0	0
4	A	9	0	0	2	0
4	B	12	0	0	3	0
4	C	9	0	0	5	0
4	D	22	0	0	5	0
4	E	8	0	0	1	0
4	F	13	0	0	4	0
4	G	8	0	0	2	0
4	H	12	0	0	4	0
4	I	12	0	0	0	0
4	J	17	0	0	4	0
4	K	5	0	0	7	1
4	L	19	0	0	3	0
4	M	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	16	0	0	0	0
4	O	11	0	0	7	0
4	P	24	0	0	7	0
4	R	4	0	0	0	0
4	S	15	0	0	6	0
4	T	13	0	0	1	0
4	U	10	0	0	4	1
4	V	15	0	0	1	0
4	W	20	0	0	6	0
4	X	9	0	0	8	0
4	Y	20	0	0	4	0
All	All	5143	0	4521	222	4

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 24.

All (222) 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:X:4:GLU:HA	1:X:8:THR:OG1	1.40	1.21
2:D:21:GLU:HG2	4:D:199:HOH:O	1.43	1.15
2:S:15:LEU:HA	4:S:192:HOH:O	1.56	1.05
1:K:14:TYR:CD1	4:K:181:HOH:O	2.15	0.98
1:I:9:SER:O	1:I:10:ILE:HG23	1.64	0.98
2:F:15:LEU:HA	4:F:178:HOH:O	1.64	0.98
1:C:7:CYS:HB2	2:D:6:LEU:O	1.63	0.97
2:P:7:CYS:SG	4:P:33:HOH:O	2.23	0.95
2:S:17:LEU:HG	4:S:243:HOH:O	1.65	0.95
1:K:14:TYR:CE1	4:K:181:HOH:O	2.19	0.94
1:X:14:TYR:CD1	4:X:300:HOH:O	2.21	0.93
1:O:14:TYR:CE1	4:O:141:HOH:O	2.23	0.92
2:U:2:VAL:O	2:U:2:VAL:HG23	1.70	0.89
1:O:14:TYR:CD1	4:O:141:HOH:O	2.26	0.89
1:M:9:SER:O	1:M:10:ILE:HG23	1.74	0.88
1:E:5:GLN:HE22	1:E:15:GLN:HE22	1.20	0.87
1:X:4:GLU:CA	1:X:8:THR:OG1	2.24	0.85
2:U:2:VAL:O	2:U:2:VAL:CG2	2.25	0.84
1:E:4:GLU:O	1:E:8:THR:OG1	1.95	0.83
2:U:19:CYS:O	4:U:143:HOH:O	1.96	0.82
1:X:8:THR:HA	4:X:36:HOH:O	1.80	0.81
4:J:32:HOH:O	2:L:29:LYS:HG3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:CYS:HB2	2:H:6:LEU:O	1.82	0.80
1:C:3:VAL:HG22	4:D:164:HOH:O	1.83	0.79
2:P:5:HIS:HB3	4:P:133:HOH:O	1.82	0.78
2:Y:7:CYS:HB2	4:Y:268:HOH:O	1.83	0.77
1:O:5:GLN:O	1:O:11:CYS:HB3	1.85	0.77
1:V:9:SER:O	1:V:10:ILE:HG23	1.85	0.76
2:U:21:GLU:N	4:U:143:HOH:O	2.18	0.76
2:W:6:LEU:HA	4:W:292:HOH:O	1.86	0.76
2:P:4:GLN:O	4:P:67:HOH:O	2.04	0.74
1:E:5:GLN:O	1:E:5:GLN:HG2	1.85	0.74
1:T:2:ILE:HG12	2:U:11:LEU:HD21	1.69	0.74
2:W:22:ARG:NH2	4:W:120:HOH:O	2.20	0.74
2:F:17:LEU:HG	4:F:278:HOH:O	1.88	0.74
2:S:21:GLU:HA	2:U:28:PRO:CG	2.17	0.74
1:G:2:ILE:HG12	2:H:11:LEU:HD21	1.71	0.73
1:X:14:TYR:CE1	4:X:300:HOH:O	2.42	0.72
4:W:61:HOH:O	2:Y:29:LYS:HG3	1.88	0.72
1:T:7:CYS:HB2	2:U:6:LEU:O	1.89	0.72
1:C:5:GLN:O	1:C:11:CYS:HB3	1.90	0.72
4:S:263:HOH:O	2:U:29:LYS:HE2	1.90	0.70
2:H:21:GLU:N	4:H:271:HOH:O	2.24	0.70
1:X:21:ASN:HB3	4:X:37:HOH:O	1.90	0.69
1:K:21:ASN:CB	4:K:49:HOH:O	2.41	0.69
1:E:5:GLN:NE2	1:E:15:GLN:HE22	1.90	0.69
2:S:21:GLU:HA	2:U:28:PRO:HG3	1.75	0.68
1:O:4:GLU:HG3	4:O:48:HOH:O	1.95	0.67
2:Y:7:CYS:SG	4:Y:268:HOH:O	2.52	0.67
1:C:14:TYR:CD2	4:C:154:HOH:O	2.48	0.66
2:W:21:GLU:O	2:Y:28:PRO:HG2	1.95	0.66
1:C:21:ASN:HB3	4:C:92:HOH:O	1.95	0.65
2:S:26:TYR:HE2	4:U:291:HOH:O	1.80	0.65
2:L:5:HIS:H	2:L:5:HIS:CD2	2.14	0.64
1:X:1:GLY:HA3	2:Y:30:THR:O	1.97	0.64
2:L:4:GLN:O	4:L:58:HOH:O	2.15	0.64
1:R:1:GLY:HA3	1:R:4:GLU:OE1	1.97	0.64
2:B:21:GLU:HA	2:D:28:PRO:HG3	1.79	0.64
1:X:4:GLU:HA	1:X:8:THR:HG1	1.58	0.64
1:K:21:ASN:HB3	4:K:49:HOH:O	1.97	0.63
1:O:10:ILE:HG22	2:P:4:GLN:C	2.24	0.63
1:C:1:GLY:N	1:C:4:GLU:OE1	2.27	0.63
1:K:5:GLN:O	1:K:11:CYS:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:21:ASN:HB3	4:O:87:HOH:O	1.98	0.62
2:P:7:CYS:CB	4:P:33:HOH:O	2.47	0.62
2:P:7:CYS:HB2	4:P:33:HOH:O	1.98	0.62
1:O:14:TYR:HD2	4:O:259:HOH:O	1.82	0.62
2:D:21:GLU:N	4:D:199:HOH:O	2.31	0.61
2:N:12:VAL:HG21	2:P:16:TYR:HB2	1.82	0.61
1:X:20:CYS:SG	4:X:100:HOH:O	2.56	0.61
1:E:3:VAL:HG13	4:E:212:HOH:O	2.01	0.60
1:R:20:CYS:HB2	2:S:22:ARG:NH1	2.16	0.60
1:E:4:GLU:C	1:E:8:THR:HG1	2.03	0.60
2:J:12:VAL:HG21	2:L:16:TYR:HB2	1.84	0.60
1:K:5:GLN:OE1	1:K:15:GLN:HG2	2.02	0.59
1:M:9:SER:O	1:M:10:ILE:CG2	2.49	0.59
2:S:21:GLU:HA	2:U:28:PRO:HG2	1.83	0.59
1:R:10:ILE:HB	2:S:3:ASN:HB3	1.83	0.59
2:F:21:GLU:HA	2:H:28:PRO:CG	2.33	0.59
1:K:21:ASN:C	4:K:49:HOH:O	2.44	0.59
2:Y:7:CYS:CB	4:Y:268:HOH:O	2.47	0.59
2:P:5:HIS:CB	4:P:133:HOH:O	2.47	0.58
2:S:25:PHE:CE2	2:U:25:PHE:HB3	2.38	0.58
1:A:5:GLN:O	1:A:9:SER:N	2.34	0.58
2:B:22:ARG:NH1	4:B:316:HOH:O	2.37	0.58
1:G:4:GLU:HA	1:G:8:THR:HG22	1.84	0.58
1:O:21:ASN:CB	4:O:87:HOH:O	2.52	0.57
1:X:21:ASN:C	4:X:37:HOH:O	2.48	0.56
1:R:5:GLN:O	1:R:9:SER:N	2.28	0.56
1:T:4:GLU:HA	1:T:8:THR:OG1	2.05	0.56
1:I:21:ASN:HB3	2:J:22:ARG:O	2.05	0.56
1:X:4:GLU:CA	1:X:8:THR:HG1	2.16	0.56
2:L:5:HIS:HB2	4:L:142:HOH:O	2.06	0.56
1:A:1:GLY:N	1:A:4:GLU:OE1	2.35	0.55
1:X:1:GLY:O	1:X:4:GLU:N	2.37	0.55
2:B:22:ARG:NH1	4:B:227:HOH:O	2.25	0.55
1:T:5:GLN:NE2	1:T:15:GLN:HE21	2.04	0.55
2:Y:14:ALA:O	2:Y:18:VAL:HG23	2.06	0.55
1:C:15:GLN:O	1:C:18:ASN:HB2	2.07	0.55
1:O:14:TYR:HE2	4:O:320:HOH:O	1.89	0.54
1:T:21:ASN:HB3	4:T:22:HOH:O	2.07	0.54
2:B:17:LEU:HG	4:B:297:HOH:O	2.07	0.54
1:K:4:GLU:H	1:K:4:GLU:CD	2.16	0.54
2:W:17:LEU:HG	4:W:302:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:TYR:HD2	4:G:89:HOH:O	1.91	0.53
1:A:5:GLN:HE22	1:A:15:GLN:HE22	1.55	0.53
2:W:3:ASN:HB2	4:W:312:HOH:O	2.07	0.53
1:O:10:ILE:HG22	2:P:4:GLN:O	2.09	0.53
1:X:21:ASN:CB	4:X:37:HOH:O	2.52	0.53
1:T:15:GLN:O	1:T:18:ASN:HB2	2.08	0.53
2:L:5:HIS:H	2:L:5:HIS:HD2	1.57	0.52
1:V:21:ASN:ND2	2:Y:27:THR:HG22	2.24	0.52
2:F:21:GLU:HA	2:H:28:PRO:HG3	1.92	0.52
4:A:330:HOH:O	2:B:19:CYS:SG	2.59	0.52
1:O:15:GLN:O	1:O:18:ASN:HB2	2.10	0.52
1:C:2:ILE:C	1:C:4:GLU:H	2.19	0.51
1:X:4:GLU:C	1:X:8:THR:HG1	2.18	0.51
1:X:21:ASN:HA	4:X:134:HOH:O	2.10	0.51
1:A:2:ILE:HG23	1:A:3:VAL:N	2.26	0.51
4:A:62:HOH:O	2:B:25:PHE:HD1	1.93	0.51
2:B:21:GLU:O	2:D:28:PRO:HG2	2.11	0.51
1:X:4:GLU:C	1:X:8:THR:OG1	2.53	0.51
2:P:28:PRO:C	2:P:30:THR:N	2.67	0.50
1:E:13:LEU:HD12	2:F:1:PHE:CZ	2.46	0.50
2:F:21:GLU:HA	2:H:28:PRO:HG2	1.93	0.50
1:X:1:GLY:N	1:X:4:GLU:OE1	2.43	0.50
1:R:16:LEU:HD11	2:S:14:ALA:CB	2.42	0.49
1:E:5:GLN:HE22	1:E:15:GLN:NE2	2.01	0.49
1:R:21:ASN:HB3	2:S:22:ARG:O	2.13	0.49
1:C:1:GLY:N	1:C:4:GLU:HB2	2.28	0.48
1:G:3:VAL:HG22	4:H:211:HOH:O	2.13	0.48
1:K:21:ASN:HA	4:K:114:HOH:O	2.13	0.48
1:E:16:LEU:HD11	2:F:14:ALA:CB	2.43	0.48
2:P:28:PRO:C	2:P:30:THR:H	2.21	0.48
2:P:5:HIS:CD2	4:P:152:HOH:O	2.66	0.48
1:R:16:LEU:HD21	2:S:11:LEU:HD11	1.95	0.48
1:X:19:TYR:HB2	2:Y:15:LEU:HD21	1.96	0.47
1:C:14:TYR:HD2	4:C:154:HOH:O	1.89	0.47
1:E:16:LEU:HD11	2:F:14:ALA:HB1	1.95	0.47
1:E:20:CYS:HB2	2:F:22:ARG:NH1	2.29	0.47
1:R:16:LEU:HD21	2:S:11:LEU:CD1	2.45	0.47
1:A:4:GLU:H	1:A:4:GLU:CD	2.22	0.47
1:G:14:TYR:CD2	4:G:89:HOH:O	2.56	0.47
2:L:14:ALA:O	2:L:18:VAL:HG23	2.14	0.47
2:J:17:LEU:HD22	4:J:261:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:26:TYR:OH	4:U:33:HOH:O	2.07	0.47
2:F:15:LEU:HD23	4:F:178:HOH:O	2.14	0.47
2:J:21:GLU:O	2:L:28:PRO:HG2	2.15	0.47
1:I:9:SER:O	1:I:10:ILE:CG2	2.51	0.47
2:L:5:HIS:ND1	4:L:69:HOH:O	2.31	0.46
1:M:18:ASN:CG	4:M:132:HOH:O	2.58	0.46
1:R:3:VAL:HG21	2:S:28:PRO:HA	1.97	0.46
2:F:13:GLU:OE2	2:H:9:SER:HB2	2.16	0.46
1:O:11:CYS:HB2	1:O:15:GLN:HB2	1.98	0.46
1:R:2:ILE:O	1:R:6:CYS:HB2	2.16	0.46
2:W:12:VAL:HG21	2:Y:16:TYR:HB2	1.98	0.46
2:H:3:ASN:C	2:H:4:GLN:OE1	2.59	0.45
1:R:3:VAL:HG21	2:S:28:PRO:CA	2.47	0.45
1:C:14:TYR:CD1	4:C:95:HOH:O	2.70	0.45
1:X:21:ASN:ND2	2:Y:24:PHE:N	2.64	0.45
1:V:8:THR:HG21	4:V:24:HOH:O	2.16	0.45
4:W:61:HOH:O	2:Y:29:LYS:HE3	2.16	0.45
1:A:4:GLU:CD	1:A:4:GLU:N	2.75	0.45
1:O:4:GLU:H	1:O:4:GLU:CD	2.25	0.45
2:P:28:PRO:O	2:P:30:THR:N	2.50	0.45
2:W:1:PHE:HB3	2:W:2:VAL:H	1.65	0.45
2:J:13:GLU:HG3	4:J:262:HOH:O	2.17	0.45
2:D:10:HIS:CD2	4:D:298:HOH:O	2.70	0.44
1:E:2:ILE:HG23	1:E:3:VAL:N	2.32	0.44
1:K:2:ILE:HG12	2:L:11:LEU:HD21	2.00	0.44
2:U:26:TYR:CE2	2:U:28:PRO:HD3	2.52	0.44
1:E:2:ILE:HD13	1:E:19:TYR:CD1	2.53	0.44
1:E:21:ASN:O	2:F:22:ARG:HD2	2.18	0.44
1:I:9:SER:HB3	1:I:10:ILE:H	1.54	0.44
1:X:1:GLY:CA	1:X:4:GLU:OE1	2.64	0.44
2:Y:22:ARG:NH1	4:Y:88:HOH:O	2.14	0.43
1:A:16:LEU:HD11	2:B:14:ALA:HB1	2.00	0.43
1:C:11:CYS:N	4:C:94:HOH:O	2.17	0.43
1:T:15:GLN:O	1:T:18:ASN:N	2.50	0.43
2:D:16:TYR:HE1	4:D:304:HOH:O	2.00	0.43
2:S:15:LEU:HD23	4:S:192:HOH:O	2.17	0.43
1:M:9:SER:HB3	1:M:10:ILE:H	1.48	0.43
2:P:15:LEU:HD13	2:P:24:PHE:CD1	2.53	0.43
1:E:4:GLU:CD	1:E:4:GLU:H	2.27	0.43
2:B:1:PHE:HB3	2:B:2:VAL:H	1.59	0.43
1:C:2:ILE:HG12	2:D:11:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:6:LEU:HA	4:S:83:HOH:O	2.18	0.42
1:C:8:THR:HG22	1:C:9:SER:N	2.35	0.42
1:E:10:ILE:HB	2:F:3:ASN:HB3	2.01	0.42
2:H:19:CYS:O	2:H:22:ARG:HG3	2.19	0.42
1:I:21:ASN:ND2	2:L:27:THR:HG22	2.35	0.42
2:J:22:ARG:NH1	4:J:322:HOH:O	2.41	0.42
1:M:21:ASN:HB3	2:N:22:ARG:O	2.20	0.42
1:R:16:LEU:HD11	2:S:14:ALA:HB1	2.01	0.42
1:T:2:ILE:HG23	1:T:3:VAL:H	1.84	0.42
2:Y:5:HIS:H	2:Y:5:HIS:CD2	2.38	0.42
1:C:11:CYS:HB2	1:C:15:GLN:HB2	2.00	0.42
1:E:14:TYR:CE2	2:F:1:PHE:HD2	2.37	0.42
1:G:21:ASN:HB3	4:H:50:HOH:O	2.19	0.42
1:R:21:ASN:O	2:S:22:ARG:HD2	2.20	0.42
1:A:2:ILE:CG2	1:A:3:VAL:N	2.83	0.42
2:F:22:ARG:HG3	4:F:217:HOH:O	2.20	0.42
1:O:2:ILE:HG12	2:P:11:LEU:HD21	2.01	0.42
2:F:26:TYR:HE2	4:H:208:HOH:O	2.03	0.41
1:V:7:CYS:O	2:W:5:HIS:NE2	2.53	0.41
1:K:4:GLU:HG3	4:K:42:HOH:O	2.20	0.41
2:B:25:PHE:CZ	2:D:25:PHE:HB3	2.55	0.41
1:G:15:GLN:O	1:G:18:ASN:HB2	2.20	0.41
1:R:3:VAL:O	1:R:7:CYS:HB3	2.21	0.41
1:M:4:GLU:H	1:M:4:GLU:CD	2.29	0.41
1:T:17:GLU:O	1:T:18:ASN:C	2.63	0.41
1:M:4:GLU:CD	1:M:4:GLU:N	2.79	0.41
1:R:5:GLN:NE2	1:R:15:GLN:OE1	2.53	0.41
1:C:1:GLY:CA	1:C:4:GLU:OE1	2.68	0.41
1:M:10:ILE:HD12	2:N:3:ASN:HB3	2.03	0.41
2:U:3:ASN:C	2:U:4:GLN:OE1	2.64	0.41
1:X:5:GLN:NE2	1:X:15:GLN:HE21	2.19	0.41
2:S:1:PHE:HB3	4:S:325:HOH:O	2.21	0.41
1:X:1:GLY:C	1:X:4:GLU:H	2.26	0.41
1:K:19:TYR:HB2	2:L:15:LEU:HD21	2.02	0.40
2:P:9:SER:HA	2:P:12:VAL:HG22	2.02	0.40
1:X:1:GLY:HA3	1:X:4:GLU:OE1	2.21	0.40

All (4) 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)
2:S:21:GLU:OE1	4:U:324:HOH:O[2_655]	2.14	0.06
2:L:27:THR:CG2	1:V:18:ASN:OD1[2_655]	2.15	0.05
1:V:15:GLN:NE2	4:K:114:HOH:O[3_665]	2.18	0.02
1:I:18:ASN:OD1	2:P:27:THR:CG2[3_675]	2.19	0.01

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	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
1	C	19/21 (90%)	14 (74%)	4 (21%)	1 (5%)	1	0
1	E	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	G	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	I	19/21 (90%)	17 (90%)	1 (5%)	1 (5%)	1	0
1	K	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	M	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	O	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
1	R	19/21 (90%)	16 (84%)	2 (10%)	1 (5%)	1	0
1	T	19/21 (90%)	15 (79%)	4 (21%)	0	100	100
1	V	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	X	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
2	B	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	D	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	F	28/30 (93%)	28 (100%)	0	0	100	100
2	H	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	J	28/30 (93%)	28 (100%)	0	0	100	100
2	L	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	N	28/30 (93%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	S	28/30 (93%)	28 (100%)	0	0	100	100
2	U	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	W	28/30 (93%)	28 (100%)	0	0	100	100
2	Y	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
All	All	564/612 (92%)	520 (92%)	41 (7%)	3 (0%)	24	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	5	GLN
1	C	3	VAL
1	I	10	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	20/20 (100%)	20 (100%)	0	100	100
1	C	20/20 (100%)	16 (80%)	4 (20%)	1	1
1	E	20/20 (100%)	18 (90%)	2 (10%)	7	7
1	G	20/20 (100%)	17 (85%)	3 (15%)	3	2
1	I	20/20 (100%)	19 (95%)	1 (5%)	22	28
1	K	20/20 (100%)	18 (90%)	2 (10%)	7	7
1	M	20/20 (100%)	19 (95%)	1 (5%)	22	28
1	O	20/20 (100%)	18 (90%)	2 (10%)	7	7
1	R	20/20 (100%)	17 (85%)	3 (15%)	3	2
1	T	20/20 (100%)	18 (90%)	2 (10%)	7	7
1	V	20/20 (100%)	19 (95%)	1 (5%)	22	28
1	X	20/20 (100%)	16 (80%)	4 (20%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	26/26 (100%)	23 (88%)	3 (12%)	5	5
2	D	25/26 (96%)	20 (80%)	5 (20%)	1	1
2	F	26/26 (100%)	20 (77%)	6 (23%)	1	0
2	H	25/26 (96%)	23 (92%)	2 (8%)	11	13
2	J	26/26 (100%)	23 (88%)	3 (12%)	5	5
2	L	25/26 (96%)	19 (76%)	6 (24%)	1	0
2	N	26/26 (100%)	23 (88%)	3 (12%)	5	5
2	P	25/26 (96%)	20 (80%)	5 (20%)	1	1
2	S	26/26 (100%)	21 (81%)	5 (19%)	1	1
2	U	25/26 (96%)	22 (88%)	3 (12%)	5	4
2	W	25/26 (96%)	21 (84%)	4 (16%)	2	2
2	Y	25/26 (96%)	20 (80%)	5 (20%)	1	1
All	All	545/552 (99%)	470 (86%)	75 (14%)	3	3

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	12	VAL
2	B	21	GLU
2	B	27	THR
1	C	5	GLN
1	C	8	THR
1	C	12	SER
1	C	15	GLN
2	D	2	VAL
2	D	3	ASN
2	D	17	LEU
2	D	21	GLU
2	D	29	LYS
1	E	10	ILE
1	E	16	LEU
2	F	1	PHE
2	F	2	VAL
2	F	12	VAL
2	F	27	THR
2	F	29	LYS
2	F	30	THR
1	G	8	THR

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Mol	Chain	Res	Type
1	G	12	SER
1	G	15	GLN
2	H	4	GLN
2	H	29	LYS
1	I	9	SER
2	J	12	VAL
2	J	17	LEU
2	J	21	GLU
1	K	8	THR
1	K	10	ILE
2	L	2	VAL
2	L	4	GLN
2	L	5	HIS
2	L	9	SER
2	L	17	LEU
2	L	29	LYS
1	M	9	SER
2	N	17	LEU
2	N	21	GLU
2	N	29	LYS
1	O	8	THR
1	O	10	ILE
2	P	2	VAL
2	P	3	ASN
2	P	4	GLN
2	P	17	LEU
2	P	21	GLU
1	R	3	VAL
1	R	9	SER
1	R	16	LEU
2	S	1	PHE
2	S	12	VAL
2	S	27	THR
2	S	29	LYS
2	S	30	THR
1	T	8	THR
1	T	15	GLN
2	U	4	GLN
2	U	19	CYS
2	U	21	GLU
1	V	9	SER
2	W	12	VAL

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Mol	Chain	Res	Type
2	W	17	LEU
2	W	21	GLU
2	W	30	THR
1	X	2	ILE
1	X	5	GLN
1	X	10	ILE
1	X	13	LEU
2	Y	2	VAL
2	Y	3	ASN
2	Y	4	GLN
2	Y	15	LEU
2	Y	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
2	B	4	GLN
1	C	18	ASN
1	E	15	GLN
2	F	4	GLN
1	G	15	GLN
1	G	18	ASN
1	I	21	ASN
2	J	3	ASN
2	J	4	GLN
1	K	18	ASN
1	M	21	ASN
2	N	4	GLN
1	O	18	ASN
2	P	5	HIS
1	R	5	GLN
2	S	3	ASN
1	T	5	GLN
1	T	18	ASN
1	V	15	GLN
1	V	18	ASN
2	W	3	ASN
2	W	4	GLN
1	X	5	GLN
1	X	18	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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	21/21 (100%)	1.32	5 (23%) 2 1	15, 21, 29, 34	0
1	C	21/21 (100%)	1.77	8 (38%) 1 0	15, 27, 33, 34	0
1	E	21/21 (100%)	2.00	7 (33%) 1 0	23, 28, 39, 40	0
1	G	21/21 (100%)	1.06	4 (19%) 3 2	21, 24, 32, 40	0
1	I	21/21 (100%)	-0.08	1 (4%) 35 32	3, 8, 11, 14	0
1	K	21/21 (100%)	0.61	1 (4%) 35 32	13, 19, 24, 27	0
1	M	21/21 (100%)	0.17	2 (9%) 14 11	7, 11, 13, 17	0
1	O	21/21 (100%)	0.63	1 (4%) 35 32	11, 21, 26, 26	0
1	R	21/21 (100%)	1.85	7 (33%) 1 0	23, 29, 33, 39	0
1	T	21/21 (100%)	1.97	11 (52%) 0 0	22, 32, 42, 47	0
1	V	21/21 (100%)	0.68	3 (14%) 6 4	13, 16, 20, 21	0
1	X	21/21 (100%)	2.67	12 (57%) 0 0	28, 33, 40, 43	0
2	B	30/30 (100%)	1.02	8 (26%) 1 1	3, 19, 39, 41	0
2	D	30/30 (100%)	0.65	3 (10%) 12 10	3, 15, 39, 45	0
2	F	30/30 (100%)	1.08	6 (20%) 3 2	7, 22, 47, 49	0
2	H	30/30 (100%)	0.60	3 (10%) 12 10	7, 19, 37, 38	0
2	J	30/30 (100%)	0.05	1 (3%) 49 46	2, 8, 20, 28	0
2	L	30/30 (100%)	0.48	5 (16%) 4 3	3, 9, 39, 42	0
2	N	30/30 (100%)	0.16	1 (3%) 49 46	2, 9, 24, 30	0
2	P	30/30 (100%)	0.64	6 (20%) 3 2	2, 8, 37, 44	0
2	S	30/30 (100%)	1.09	4 (13%) 7 5	10, 22, 44, 45	0
2	U	30/30 (100%)	1.12	5 (16%) 4 3	8, 22, 39, 41	0
2	W	30/30 (100%)	0.68	1 (3%) 49 46	7, 16, 30, 32	0
2	Y	30/30 (100%)	0.84	7 (23%) 2 1	6, 18, 38, 43	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	612/612 (100%)	0.92	112 (18%) 3 2	2, 20, 39, 49	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	8	THR	6.9
1	C	8	THR	6.8
1	X	1	GLY	6.1
2	F	3	ASN	6.0
1	R	5	GLN	5.9
1	E	5	GLN	5.9
1	X	4	GLU	5.4
1	E	3	VAL	5.1
1	X	2	ILE	4.9
1	X	8	THR	4.9
2	P	1	PHE	4.9
1	C	9	SER	4.7
1	X	5	GLN	4.3
2	D	1	PHE	4.3
2	F	2	VAL	4.2
2	S	2	VAL	4.2
1	E	1	GLY	4.2
2	H	2	VAL	4.1
2	U	2	VAL	4.1
1	C	1	GLY	4.0
2	Y	1	PHE	3.9
2	L	1	PHE	3.9
2	D	2	VAL	3.8
1	R	8	THR	3.8
2	S	3	ASN	3.7
2	L	3	ASN	3.7
2	P	3	ASN	3.7
1	R	10	ILE	3.6
1	A	19	TYR	3.5
2	L	4	GLN	3.5
1	A	3	VAL	3.4
2	P	5	HIS	3.4
1	E	4	GLU	3.4
2	B	22	ARG	3.4
1	X	9	SER	3.3
2	L	2	VAL	3.2
2	P	2	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	9	SER	3.2
2	L	5	HIS	3.2
1	X	10	ILE	3.2
2	B	3	ASN	3.1
2	P	4	GLN	3.0
1	M	9	SER	3.0
1	V	9	SER	3.0
1	E	19	TYR	3.0
1	T	13	LEU	2.9
1	E	20	CYS	2.9
1	T	14	TYR	2.9
2	B	1	PHE	2.9
1	G	9	SER	2.9
1	I	9	SER	2.9
1	T	12	SER	2.9
1	R	9	SER	2.9
2	U	1	PHE	2.9
1	X	3	VAL	2.9
1	A	21	ASN	2.8
2	Y	3	ASN	2.8
2	F	30	THR	2.8
1	C	5	GLN	2.7
2	B	20	GLY	2.7
2	H	4	GLN	2.7
1	C	10	ILE	2.7
1	O	3	VAL	2.6
2	B	2	VAL	2.6
2	F	28	PRO	2.6
2	U	19	CYS	2.6
1	T	10	ILE	2.6
1	C	4	GLU	2.5
1	G	13	LEU	2.5
1	T	20	CYS	2.5
1	T	16	LEU	2.5
1	T	9	SER	2.5
1	R	3	VAL	2.4
1	V	18	ASN	2.4
1	X	18	ASN	2.4
2	J	30	THR	2.4
1	X	6	CYS	2.3
1	X	14	TYR	2.3
1	T	15	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	21	GLU	2.3
2	U	3	ASN	2.3
1	R	19	TYR	2.3
2	S	30	THR	2.3
1	V	5	GLN	2.3
2	F	29	LYS	2.3
2	Y	7	CYS	2.2
1	M	8	THR	2.2
2	D	4	GLN	2.2
2	F	1	PHE	2.2
2	N	30	THR	2.2
1	C	2	ILE	2.2
1	T	7	CYS	2.2
2	B	30	THR	2.2
1	E	2	ILE	2.2
1	C	3	VAL	2.2
1	X	12	SER	2.2
1	G	14	TYR	2.1
2	Y	2	VAL	2.1
2	Y	5	HIS	2.1
1	T	19	TYR	2.1
1	K	10	ILE	2.1
1	G	5	GLN	2.1
2	W	2	VAL	2.1
2	Y	28	PRO	2.1
1	R	1	GLY	2.1
2	H	3	ASN	2.1
2	B	28	PRO	2.1
1	A	5	GLN	2.0
2	U	27	THR	2.0
2	Y	30	THR	2.0
2	S	28	PRO	2.0
2	P	29	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	S	31	1/1	0.70	0.12	35,35,35,35	1
3	CU	Y	31	1/1	0.91	0.05	28,28,28,28	1
3	CU	U	31	1/1	0.93	0.08	31,31,31,31	1
3	CU	L	31	1/1	0.94	0.06	25,25,25,25	1
3	CU	P	31	1/1	0.95	0.06	24,24,24,24	1
3	CU	W	31	1/1	0.97	0.07	21,21,21,21	1
3	CU	B	31	1/1	0.98	0.06	17,17,17,17	1
3	CU	H	31	1/1	0.99	0.04	26,26,26,26	1
3	CU	J	31	1/1	0.99	0.03	12,12,12,12	1
3	CU	D	31	1/1	0.99	0.07	25,25,25,25	1
3	CU	F	31	1/1	0.99	0.03	21,21,21,21	1
3	CU	N	31	1/1	1.00	0.04	14,14,14,14	1

6.5 Other polymers [i](#)

There are no such residues in this entry.