



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:15 PM UTC

PDB ID : 4RAU / pdb_00004rau
Title : crystal structure of RTOFab in complex with human PF4
Authors : Cai, Z.; Zhu, Z.; Liu, Q.; Greene, M.I.
Deposited on : 2014-09-11
Resolution : 3.74 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

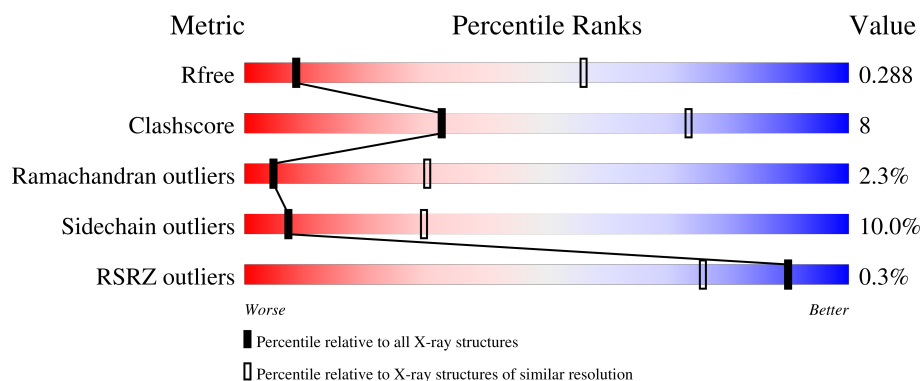
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 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	1234 (3.88-3.60)
Clashscore	190562	1274 (3.88-3.60)
Ramachandran outliers	187476	1226 (3.88-3.60)
Sidechain outliers	187428	1221 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	212	 75% 23% .
1	D	212	 75% 21% .
1	G	212	 80% 17% .
1	J	212	 80% 17% .
1	M	212	 81% 17% .

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Mol	Chain	Length	Quality of chain
1	P	212	 78% 20% .
1	S	212	 77% 20% .
1	V	212	 84% 14% .
2	B	219	 83% 14% .
2	E	219	 83% 14% .
2	H	219	 83% 14% .
2	K	219	 80% 14% 5% .
2	N	219	 82% 14% .
2	Q	219	 82% 15% .
2	T	219	 83% 12% 5%
2	W	219	 82% 14% .
3	C	70	 64% 23% 6% 7%
3	F	70	 59% 29% 6% 7%
3	I	70	 69% 19% 6% 6%
3	L	70	 61% 23% 7% 7%
3	O	70	 57% 30% 6% 7%
3	R	70	 61% 26% . 7%
3	U	70	 63% 23% 7% 7%
3	X	70	 60% 30% . 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30074 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 RTOFab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	D	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	G	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	J	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	M	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	P	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	S	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	V	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			

- Molecule 2 is a protein called RTOFab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	E	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	H	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	K	219	Total	C	N	O	S	0	0	0
			1620	1021	268	322	9			
2	N	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	Q	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	W	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			

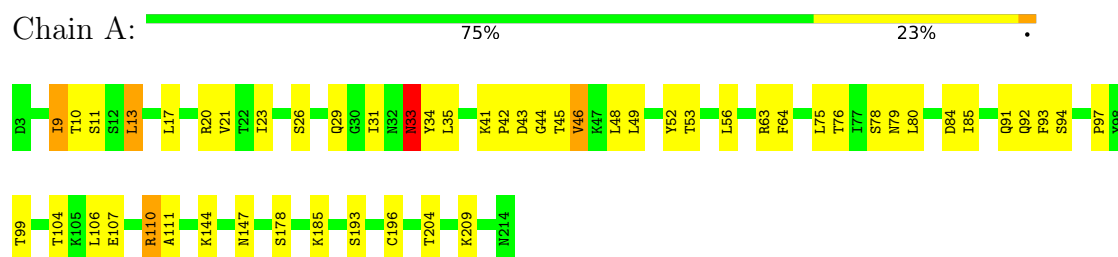
- Molecule 3 is a protein called Platelet factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	F	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	I	66	Total	C	N	O	S	0	0	0
			508	323	92	89	4			
3	L	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	O	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	R	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	U	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	X	66	Total	C	N	O	S	0	0	0
			504	321	92	87	4			

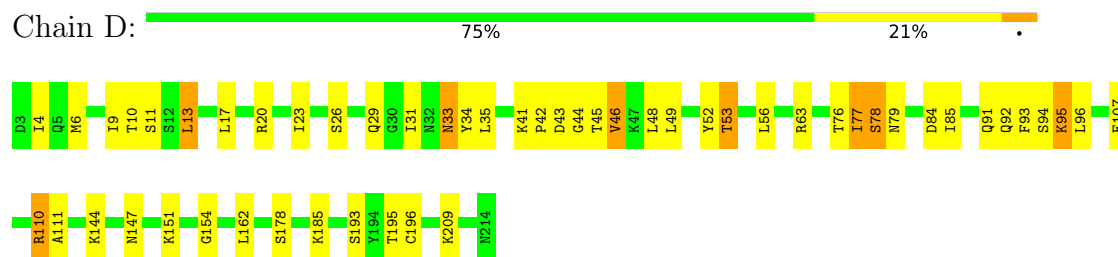
3 Residue-property plots [i](#)

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.

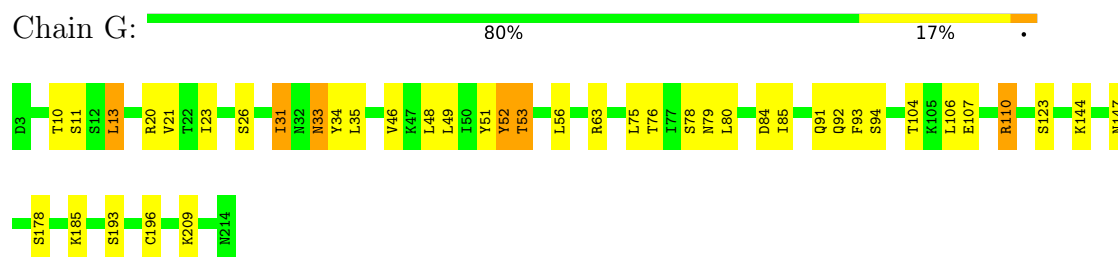
• Molecule 1: RTOFab light chain



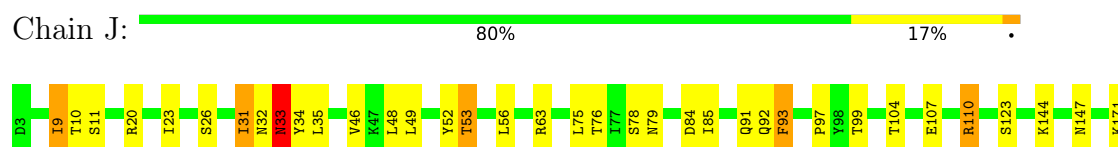
• Molecule 1: RTOFab light chain



• Molecule 1: RTOFab light chain

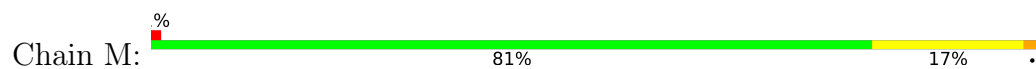


• Molecule 1: RTOFab light chain

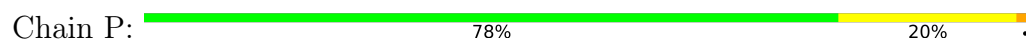




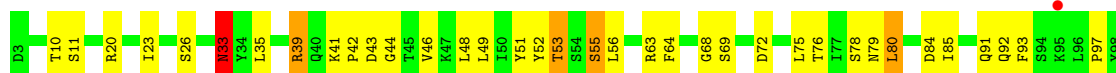
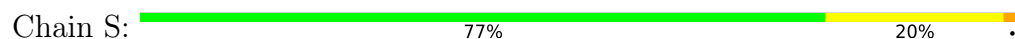
- Molecule 1: RTOFab light chain



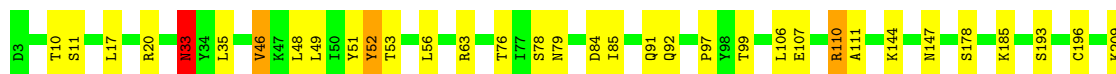
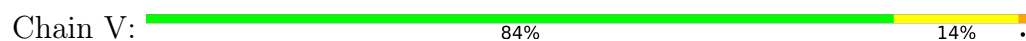
- Molecule 1: RTOFab light chain



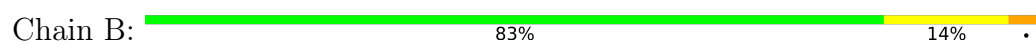
- Molecule 1: RTOFab light chain

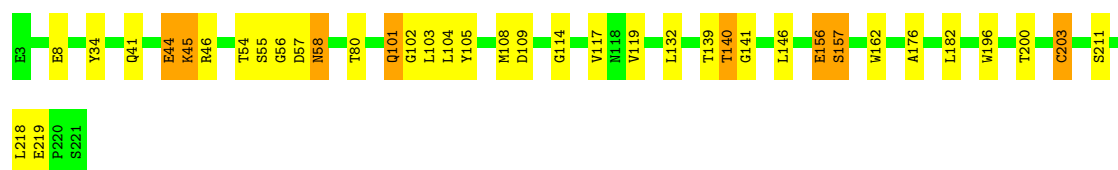


- Molecule 1: RTOFab light chain



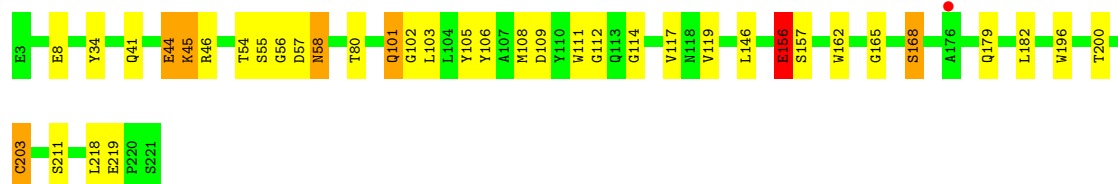
- Molecule 2: RTOFab heavy chain





- Molecule 2: RTOFab heavy chain

Chain E: 83% 14% •



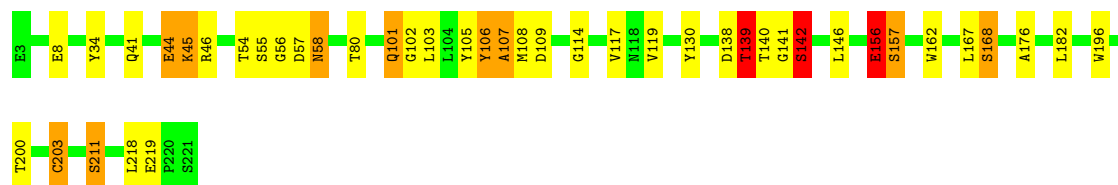
- Molecule 2: RTOFab heavy chain

Chain H: 83% 14% •



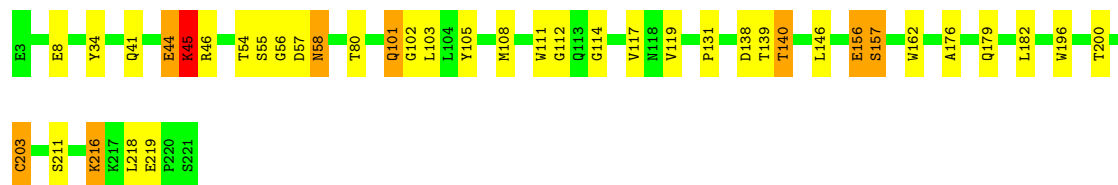
- Molecule 2: RTOFab heavy chain

Chain K: 80% 14% 5% •



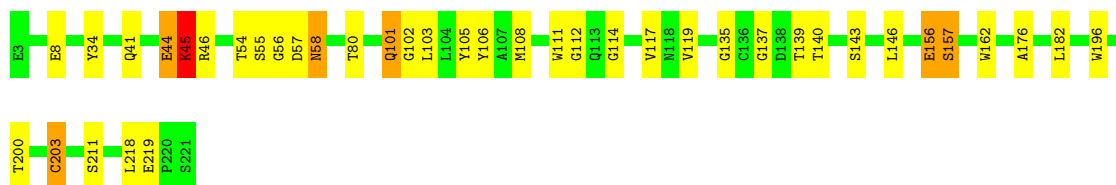
- Molecule 2: RTOFab heavy chain

Chain N: 82% 14% •



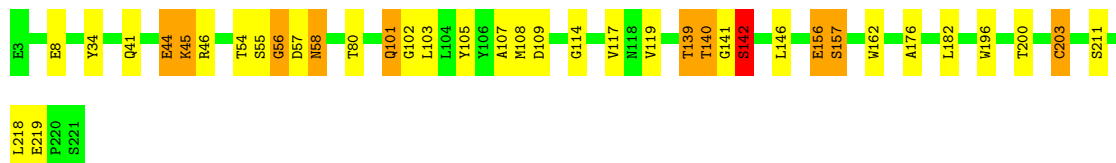
- Molecule 2: RTOFab heavy chain

Chain Q: 82% 15% •



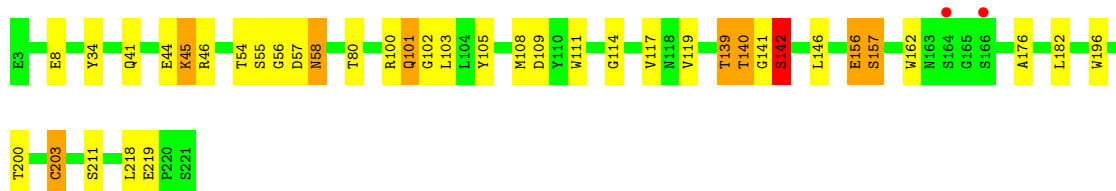
• Molecule 2: RTOFab heavy chain

Chain T: 83% 12% 5%



• Molecule 2: RTOFab heavy chain

Chain W: 82% 14% 2%



• Molecule 3: Platelet factor 4

Chain C: 64% 23% 6% 7%



• Molecule 3: Platelet factor 4

Chain F: 59% 29% 6% 7%

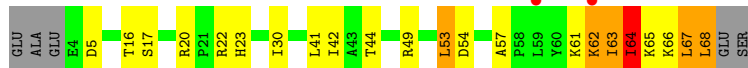


• Molecule 3: Platelet factor 4

Chain I: 69% 19% 6% 6%



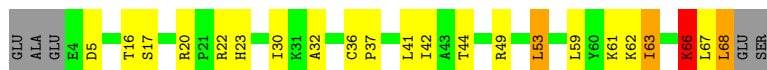
• Molecule 3: Platelet factor 4



• Molecule 3: Platelet factor 4



• Molecule 3: Platelet factor 4



• Molecule 3: Platelet factor 4



• Molecule 3: Platelet factor 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	161.42Å 171.87Å 208.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74 50.00 – 3.74	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.74) 99.2 (50.00-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.243 , 0.284 0.246 , 0.288	Depositor DCC
R_{free} test set	3030 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	118.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 103.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30074	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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	0.47	0/1671	0.75	1/2270 (0.0%)
1	D	0.49	0/1671	0.77	2/2270 (0.1%)
1	G	0.49	0/1671	0.76	2/2270 (0.1%)
1	J	0.49	0/1671	0.78	2/2270 (0.1%)
1	M	0.47	0/1671	0.75	1/2270 (0.0%)
1	P	0.52	0/1671	0.78	1/2270 (0.0%)
1	S	0.48	0/1671	0.77	1/2270 (0.0%)
1	V	0.52	0/1671	0.76	1/2270 (0.0%)
2	B	0.51	0/1666	0.77	1/2274 (0.0%)
2	E	0.50	1/1666 (0.1%)	0.86	4/2274 (0.2%)
2	H	0.48	0/1666	0.76	1/2274 (0.0%)
2	K	0.56	2/1662 (0.1%)	0.86	6/2268 (0.3%)
2	N	0.54	0/1666	0.80	3/2274 (0.1%)
2	Q	0.55	1/1666 (0.1%)	0.83	5/2274 (0.2%)
2	T	0.59	3/1666 (0.2%)	0.88	4/2274 (0.2%)
2	W	0.54	2/1666 (0.1%)	0.78	3/2274 (0.1%)
3	C	0.54	0/505	0.88	0/681
3	F	0.56	0/505	0.90	0/681
3	I	0.63	0/514	1.06	5/693 (0.7%)
3	L	0.64	0/505	0.95	0/681
3	O	0.57	0/505	0.91	0/681
3	R	0.57	0/505	0.91	0/681
3	U	0.61	0/505	1.00	1/681 (0.1%)
3	X	0.61	0/510	0.94	0/688
All	All	0.52	9/30746 (0.0%)	0.81	44/41813 (0.1%)

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	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	H	0	1
2	K	0	1
2	N	0	1
2	Q	0	1
2	T	0	1
2	W	0	1
All	All	0	8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	56	GLY	C-O	-7.91	1.17	1.24
2	W	142	SER	N-CA	7.37	1.55	1.46
2	K	142	SER	N-CA	7.22	1.55	1.46
2	T	142	SER	N-CA	7.16	1.55	1.46
2	T	139	THR	N-CA	6.05	1.53	1.46
2	W	139	THR	N-CA	5.80	1.53	1.46
2	Q	140	THR	N-CA	5.64	1.53	1.46
2	E	156	GLU	N-CA	5.31	1.53	1.46
2	K	106	TYR	C-O	5.09	1.30	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	56	GLY	N-CA-C	-16.08	85.89	110.97
2	E	156	GLU	N-CA-C	10.64	133.47	110.80
2	K	106	TYR	CB-CA-C	10.45	131.21	110.42
2	T	56	GLY	CA-C-O	-9.59	112.34	120.30
1	J	31	ILE	CB-CA-C	-9.44	97.61	111.68
3	U	67	LEU	N-CA-C	9.23	130.46	110.80
2	Q	137	GLY	N-CA-C	9.07	125.91	114.66
2	Q	45	LYS	CA-CB-CG	8.35	130.79	114.10
2	E	157	SER	N-CA-C	8.18	122.89	113.15
2	K	167	LEU	N-CA-C	-7.75	96.93	109.96
2	K	106	TYR	N-CA-C	-7.63	94.55	110.80
3	I	59	LEU	N-CA-CB	7.54	122.06	110.46
2	T	102	GLY	N-CA-C	7.51	120.26	111.63
2	K	102	GLY	N-CA-C	7.47	120.22	111.63
2	W	140	THR	N-CA-C	7.29	121.30	111.24
2	W	102	GLY	N-CA-C	7.24	119.96	111.63
2	N	102	GLY	N-CA-C	7.21	119.92	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	GLY	N-CA-C	7.18	119.88	111.63
2	T	140	THR	N-CA-C	7.14	121.09	111.24
1	M	23	ILE	CB-CA-C	7.14	118.55	110.41
2	Q	102	GLY	N-CA-C	7.12	119.81	111.63
2	E	102	GLY	N-CA-C	7.09	119.78	111.63
2	H	102	GLY	N-CA-C	7.00	119.69	111.63
2	K	156	GLU	CB-CG-CD	6.57	123.77	112.60
3	I	66	LYS	CA-C-N	6.46	129.58	120.28
3	I	66	LYS	C-N-CA	6.46	129.58	120.28
1	S	55	SER	CB-CA-C	-6.35	100.74	110.26
2	N	45	LYS	CB-CG-CD	6.28	125.75	111.30
1	G	31	ILE	CB-CA-C	-6.18	102.47	111.68
2	E	157	SER	N-CA-CB	-6.16	100.98	110.46
3	I	59	LEU	CA-CB-CG	5.88	136.88	116.30
2	Q	135	GLY	N-CA-C	5.85	127.05	113.18
1	G	52	TYR	N-CA-C	-5.84	98.57	109.32
1	V	52	TYR	N-CA-C	-5.84	98.58	109.32
1	P	81	GLU	CB-CA-C	5.68	117.41	108.84
3	I	67	LEU	CA-CB-CG	5.64	136.06	116.30
2	N	138	ASP	N-CA-C	5.54	117.94	109.62
1	A	9	ILE	N-CA-C	5.52	116.30	110.72
1	J	9	ILE	N-CA-C	5.44	116.22	110.72
2	K	139	THR	N-CA-C	5.25	121.99	110.80
2	W	139	THR	N-CA-C	5.07	121.60	110.80
2	Q	139	THR	N-CA-C	5.07	116.88	111.36
1	D	23	ILE	CB-CA-C	-5.04	104.73	110.73
1	D	77	ILE	N-CA-C	5.03	119.81	109.34

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	101	GLN	Peptide
2	E	101	GLN	Peptide
2	H	101	GLN	Peptide
2	K	101	GLN	Peptide
2	N	101	GLN	Peptide
2	Q	101	GLN	Peptide
2	T	101	GLN	Peptide
2	W	101	GLN	Peptide

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	1635	0	1559	34	0
1	D	1635	0	1559	45	0
1	G	1635	0	1559	31	0
1	J	1635	0	1559	40	0
1	M	1635	0	1559	23	0
1	P	1635	0	1559	38	0
1	S	1635	0	1559	39	0
1	V	1635	0	1559	18	0
2	B	1624	0	1525	28	0
2	E	1624	0	1525	29	0
2	H	1624	0	1525	24	0
2	K	1620	0	1515	29	0
2	N	1624	0	1525	28	0
2	Q	1624	0	1525	25	0
2	T	1624	0	1525	23	0
2	W	1624	0	1525	23	0
3	C	499	0	544	10	0
3	F	499	0	544	13	0
3	I	508	0	550	5	0
3	L	499	0	544	10	0
3	O	499	0	544	14	0
3	R	499	0	544	13	0
3	U	499	0	544	9	0
3	X	504	0	546	9	0
All	All	30074	0	29022	466	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 8.

All (466) 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:D:6:MET:HE3	1:D:92:GLN:HG2	1.18	1.17
1:D:6:MET:HE3	1:D:92:GLN:CG	1.79	1.11
1:D:154:GLY:O	1:S:68:GLY:HA2	1.51	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:55:SER:OG	3:O:31:LYS:NZ	1.92	1.01
1:D:6:MET:CE	1:D:92:GLN:HG2	1.97	0.94
1:D:6:MET:HE3	1:D:92:GLN:CB	2.03	0.88
1:S:51:TYR:CE1	1:S:55:SER:OG	2.27	0.87
1:G:31:ILE:HG23	1:G:94:SER:OG	1.76	0.86
1:J:34:TYR:HB3	1:J:93:PHE:CE1	2.14	0.81
1:J:34:TYR:HB3	1:J:93:PHE:CD1	2.14	0.81
1:D:195:THR:OG1	1:S:72:ASP:OD1	1.97	0.80
1:D:4:ILE:HG21	1:D:6:MET:HE2	1.62	0.80
1:J:34:TYR:O	1:J:93:PHE:CD1	2.35	0.79
2:Q:44:GLU:O	2:Q:45:LYS:HB2	1.81	0.79
2:E:55:SER:OG	3:F:31:LYS:NZ	2.17	0.77
1:S:51:TYR:CD1	1:S:55:SER:OG	2.36	0.77
1:G:52:TYR:CD1	2:H:105:TYR:HE2	2.03	0.77
1:P:35:LEU:CD2	1:P:73:TYR:CD1	2.68	0.76
2:N:44:GLU:O	2:N:45:LYS:HB2	1.87	0.75
3:X:41:LEU:HD13	3:X:63:ILE:HD11	1.67	0.74
1:D:6:MET:HE3	1:D:92:GLN:HB3	1.66	0.74
1:D:154:GLY:C	1:S:68:GLY:HA2	2.13	0.73
1:P:35:LEU:CD2	1:P:73:TYR:CG	2.71	0.73
1:P:52:TYR:CD1	2:Q:105:TYR:HE2	2.06	0.73
1:D:52:TYR:CD1	2:E:105:TYR:HE2	2.07	0.72
1:M:52:TYR:CD1	2:N:105:TYR:HE2	2.08	0.72
2:H:55:SER:OG	3:I:31:LYS:NZ	2.23	0.71
2:B:104:LEU:HD23	2:B:104:LEU:H	1.55	0.71
1:A:52:TYR:CD1	2:B:105:TYR:HE2	2.10	0.69
1:J:34:TYR:O	1:J:93:PHE:CE1	2.46	0.69
1:D:151:LYS:HE3	1:S:69:SER:O	1.92	0.69
1:D:95:LYS:HG2	1:D:96:LEU:O	1.95	0.67
1:J:34:TYR:CA	1:J:93:PHE:HE1	2.08	0.67
2:K:138:ASP:O	2:K:139:THR:CB	2.43	0.67
1:P:35:LEU:HD22	1:P:73:TYR:CG	2.29	0.66
1:G:13:LEU:C	1:G:13:LEU:HD12	2.21	0.66
1:D:13:LEU:C	1:D:13:LEU:HD12	2.21	0.66
1:D:4:ILE:CG2	1:D:6:MET:HE2	2.26	0.66
1:A:13:LEU:C	1:A:13:LEU:HD12	2.21	0.65
1:G:52:TYR:CD1	2:H:105:TYR:CE2	2.84	0.65
2:W:55:SER:OG	3:X:31:LYS:NZ	2.31	0.63
3:L:63:ILE:O	3:L:64:ILE:C	2.41	0.63
3:L:67:LEU:O	3:L:67:LEU:HD12	1.99	0.63
1:J:171:LYS:HG2	1:J:172:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:LEU:HD22	3:F:68:LEU:HG	1.82	0.62
1:V:52:TYR:CD1	2:W:105:TYR:HE2	2.16	0.62
1:J:34:TYR:CB	1:J:93:PHE:HE1	2.12	0.62
2:Q:103:LEU:HD22	3:R:68:LEU:HB3	1.81	0.62
1:J:34:TYR:CB	1:J:93:PHE:CE1	2.83	0.62
1:P:110:ARG:HG2	1:P:110:ARG:HH11	1.65	0.62
1:P:52:TYR:CD1	2:Q:105:TYR:CE2	2.86	0.61
2:W:56:GLY:O	2:W:58:ASN:N	2.33	0.61
1:G:110:ARG:HG2	1:G:110:ARG:HH11	1.65	0.61
1:V:110:ARG:HH11	1:V:110:ARG:HG2	1.66	0.61
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.64	0.61
1:A:204:THR:OG1	3:O:54:ASP:OD1	2.17	0.61
1:D:110:ARG:HG2	1:D:110:ARG:HH11	1.65	0.61
1:M:110:ARG:HH11	1:M:110:ARG:HG2	1.66	0.61
2:Q:56:GLY:O	2:Q:58:ASN:N	2.34	0.61
1:J:31:ILE:HG22	1:J:34:TYR:H	1.66	0.60
1:A:33:ASN:OD1	1:A:33:ASN:N	2.34	0.60
1:P:13:LEU:C	1:P:13:LEU:HD23	2.27	0.60
2:H:56:GLY:O	2:H:58:ASN:N	2.34	0.60
2:K:56:GLY:O	2:K:58:ASN:N	2.33	0.60
1:S:33:ASN:N	1:S:33:ASN:OD1	2.33	0.60
2:B:56:GLY:O	2:B:58:ASN:N	2.34	0.60
2:E:56:GLY:O	2:E:58:ASN:N	2.33	0.60
1:S:110:ARG:HG2	1:S:110:ARG:HH11	1.66	0.60
1:J:110:ARG:HH11	1:J:110:ARG:HG2	1.66	0.60
2:N:56:GLY:O	2:N:58:ASN:N	2.33	0.59
1:S:55:SER:OG	1:S:55:SER:O	2.18	0.59
1:V:33:ASN:OD1	1:V:33:ASN:N	2.33	0.59
1:A:52:TYR:CD1	2:B:105:TYR:CE2	2.90	0.59
1:D:154:GLY:O	1:S:68:GLY:CA	2.39	0.59
1:D:52:TYR:CD1	2:E:105:TYR:CE2	2.89	0.59
1:S:56:LEU:HD21	1:S:64:PHE:O	2.03	0.59
1:A:56:LEU:HD21	1:A:64:PHE:O	2.03	0.58
1:M:56:LEU:HD21	1:M:64:PHE:O	2.03	0.58
1:P:56:LEU:HD21	1:P:64:PHE:O	2.03	0.58
1:M:52:TYR:CD1	2:N:105:TYR:CE2	2.90	0.58
1:J:52:TYR:CD1	2:K:105:TYR:HE2	2.22	0.58
1:S:52:TYR:CD1	2:T:105:TYR:HE2	2.22	0.58
2:E:101:GLN:HE22	2:E:108:MET:HE2	1.70	0.57
3:F:62:LYS:HB2	3:R:62:LYS:HB2	1.85	0.57
2:N:101:GLN:HE22	2:N:108:MET:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:67:LEU:HB3	3:O:68:LEU:HD22	1.87	0.57
2:Q:101:GLN:HE22	2:Q:108:MET:HE2	1.69	0.57
2:W:101:GLN:HE22	2:W:108:MET:HE2	1.69	0.57
3:R:67:LEU:HB3	3:R:68:LEU:HD22	1.87	0.57
1:G:31:ILE:HG22	1:G:34:TYR:H	1.68	0.57
1:M:95:LYS:HE2	3:O:7:ASP:HB3	1.86	0.57
3:F:67:LEU:HB3	3:F:68:LEU:HD22	1.87	0.57
2:K:101:GLN:HE22	2:K:108:MET:HE2	1.70	0.57
1:J:34:TYR:CA	1:J:93:PHE:CE1	2.88	0.57
1:J:34:TYR:C	1:J:93:PHE:CE1	2.83	0.57
2:B:101:GLN:HE22	2:B:108:MET:HE2	1.69	0.56
2:T:101:GLN:HE22	2:T:108:MET:HE2	1.69	0.56
3:C:67:LEU:HB3	3:C:68:LEU:HD22	1.86	0.56
2:N:103:LEU:HD22	3:O:68:LEU:HG	1.86	0.56
1:D:151:LYS:HD3	1:S:69:SER:OG	2.05	0.56
1:J:93:PHE:CE2	2:K:107:ALA:HB2	2.40	0.56
2:H:101:GLN:HE22	2:H:108:MET:HE2	1.70	0.56
1:D:6:MET:CE	1:D:92:GLN:HB3	2.35	0.56
1:P:35:LEU:HD21	1:P:73:TYR:CD1	2.39	0.56
1:D:77:ILE:O	1:D:78:SER:C	2.49	0.56
1:G:91:GLN:OE1	2:H:108:MET:HE3	2.06	0.55
1:P:85:ILE:HD12	1:P:85:ILE:O	2.07	0.55
3:X:59:LEU:HD12	3:X:62:LYS:HD2	1.89	0.55
3:F:59:LEU:HD12	3:F:62:LYS:HD2	1.88	0.55
3:I:41:LEU:HG	3:I:53:LEU:CD1	2.37	0.55
1:M:162:LEU:HD11	2:N:179:GLN:HB3	1.89	0.55
3:R:59:LEU:HD12	3:R:62:LYS:HD2	1.89	0.55
1:D:45:THR:HG23	2:E:112:GLY:O	2.07	0.55
1:D:85:ILE:HD12	1:D:85:ILE:O	2.06	0.55
2:E:56:GLY:C	2:E:58:ASN:H	2.15	0.55
3:C:59:LEU:HD12	3:C:62:LYS:HD2	1.89	0.55
3:O:59:LEU:HD12	3:O:62:LYS:HD2	1.88	0.55
3:U:41:LEU:HG	3:U:53:LEU:CD1	2.37	0.55
1:J:23:ILE:HD11	1:J:104:THR:HB	1.89	0.55
2:K:56:GLY:C	2:K:58:ASN:H	2.15	0.55
1:P:23:ILE:HD11	1:P:104:THR:HB	1.89	0.55
3:U:59:LEU:HD12	3:U:62:LYS:HD2	1.88	0.55
3:X:41:LEU:HG	3:X:53:LEU:CD1	2.37	0.55
2:W:56:GLY:C	2:W:58:ASN:H	2.15	0.55
1:G:23:ILE:HD11	1:G:104:THR:HB	1.89	0.54
1:J:85:ILE:O	1:J:85:ILE:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:41:LEU:HG	3:O:53:LEU:CD1	2.37	0.54
1:A:85:ILE:HD12	1:A:85:ILE:O	2.07	0.54
1:A:91:GLN:OE1	2:B:108:MET:HE3	2.08	0.54
3:C:41:LEU:HG	3:C:53:LEU:CD1	2.38	0.54
3:F:41:LEU:HG	3:F:53:LEU:CD1	2.37	0.54
3:L:41:LEU:HG	3:L:53:LEU:CD1	2.37	0.54
1:A:34:TYR:CZ	3:C:37:PRO:HG2	2.42	0.54
1:P:91:GLN:OE1	2:Q:108:MET:HE3	2.07	0.54
1:A:23:ILE:HD11	1:A:104:THR:HB	1.88	0.54
1:J:34:TYR:HB3	1:J:93:PHE:HD1	1.69	0.54
1:J:171:LYS:HG2	1:J:172:ASP:N	2.22	0.54
1:S:23:ILE:HD11	1:S:104:THR:HB	1.89	0.54
2:H:56:GLY:C	2:H:58:ASN:H	2.15	0.53
3:R:41:LEU:HG	3:R:53:LEU:CD1	2.38	0.53
2:B:56:GLY:C	2:B:58:ASN:H	2.16	0.53
2:N:56:GLY:C	2:N:58:ASN:H	2.15	0.53
1:D:162:LEU:HD11	2:E:179:GLN:HB3	1.90	0.53
2:T:41:GLN:HG3	2:T:45:LYS:O	2.09	0.53
1:V:51:TYR:C	1:V:52:TYR:O	2.52	0.53
1:D:110:ARG:HH11	1:D:110:ARG:CG	2.22	0.53
2:N:41:GLN:HG3	2:N:45:LYS:O	2.09	0.53
1:G:31:ILE:HG23	1:G:94:SER:HG	1.74	0.53
2:Q:56:GLY:C	2:Q:58:ASN:H	2.16	0.53
2:H:41:GLN:HG3	2:H:45:LYS:O	2.09	0.52
1:M:34:TYR:CZ	3:O:37:PRO:HG2	2.45	0.52
2:N:131:PRO:HD3	2:N:216:LYS:HZ3	1.73	0.52
1:P:35:LEU:HD12	1:P:36:SER:O	2.09	0.52
2:K:41:GLN:HG3	2:K:45:LYS:O	2.09	0.52
2:E:41:GLN:HG3	2:E:45:LYS:O	2.09	0.52
3:U:67:LEU:HB3	3:U:68:LEU:HD22	1.91	0.52
1:J:48:LEU:HD22	2:K:109:ASP:HA	1.91	0.52
1:J:110:ARG:HH11	1:J:110:ARG:CG	2.23	0.52
1:P:110:ARG:HH11	1:P:110:ARG:CG	2.22	0.52
1:S:48:LEU:HD22	2:T:109:ASP:HA	1.92	0.52
1:V:52:TYR:CD1	2:W:105:TYR:CE2	2.98	0.52
2:W:41:GLN:HG3	2:W:45:LYS:O	2.09	0.52
1:G:110:ARG:HH11	1:G:110:ARG:CG	2.22	0.52
2:B:41:GLN:HG3	2:B:45:LYS:O	2.09	0.52
1:D:151:LYS:CE	1:S:69:SER:O	2.57	0.51
1:V:35:LEU:O	1:V:52:TYR:O	2.29	0.51
1:M:110:ARG:HH11	1:M:110:ARG:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:TRP:CZ3	2:B:203:CYS:HB3	2.46	0.51
1:A:110:ARG:HH11	1:A:110:ARG:CG	2.22	0.51
1:D:91:GLN:OE1	2:E:108:MET:HE3	2.11	0.51
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.46	0.51
1:S:52:TYR:CD1	2:T:105:TYR:CE2	2.98	0.51
2:K:162:TRP:CZ3	2:K:203:CYS:HB3	2.46	0.51
2:Q:41:GLN:HG3	2:Q:45:LYS:O	2.11	0.51
1:G:51:TYR:C	1:G:52:TYR:O	2.51	0.51
1:G:35:LEU:O	1:G:52:TYR:O	2.29	0.51
1:G:48:LEU:HD22	2:H:109:ASP:HA	1.93	0.50
2:H:162:TRP:CZ3	2:H:203:CYS:HB3	2.46	0.50
2:N:162:TRP:CZ3	2:N:203:CYS:HB3	2.46	0.50
2:Q:162:TRP:CZ3	2:Q:203:CYS:HB3	2.45	0.50
1:D:20:ARG:HG3	1:D:78:SER:HA	1.92	0.50
2:W:162:TRP:CZ3	2:W:203:CYS:HB3	2.46	0.50
1:G:93:PHE:CE1	2:H:105:TYR:O	2.65	0.50
2:E:165:GLY:O	2:E:168:SER:OG	2.30	0.50
2:T:162:TRP:CZ3	2:T:203:CYS:HB3	2.46	0.50
1:V:110:ARG:HH11	1:V:110:ARG:CG	2.23	0.50
1:M:43:ASP:CG	1:M:44:GLY:N	2.70	0.50
1:S:110:ARG:HH11	1:S:110:ARG:CG	2.24	0.50
1:P:43:ASP:CG	1:P:44:GLY:N	2.70	0.50
1:G:20:ARG:HG3	1:G:78:SER:HA	1.94	0.50
1:S:39:ARG:NH2	1:S:84:ASP:OD1	2.43	0.50
1:P:45:THR:HG23	2:Q:112:GLY:O	2.12	0.49
1:P:93:PHE:CE1	2:Q:105:TYR:O	2.65	0.49
1:S:35:LEU:O	1:S:52:TYR:O	2.30	0.49
1:G:52:TYR:CG	2:H:105:TYR:CE2	3.00	0.49
1:J:20:ARG:HG3	1:J:78:SER:HA	1.94	0.49
1:G:52:TYR:CG	2:H:105:TYR:HE2	2.30	0.49
1:J:35:LEU:O	1:J:52:TYR:O	2.31	0.49
1:V:20:ARG:HG3	1:V:78:SER:HA	1.95	0.49
1:A:43:ASP:CG	1:A:44:GLY:N	2.69	0.49
1:D:45:THR:HG22	1:D:46:VAL:N	2.28	0.49
1:J:93:PHE:CD2	2:K:107:ALA:N	2.81	0.49
1:P:46:VAL:CG2	2:Q:111:TRP:CD2	2.95	0.49
1:A:35:LEU:O	1:A:52:TYR:O	2.31	0.49
1:D:110:ARG:HD3	1:D:110:ARG:C	2.38	0.49
1:A:93:PHE:CE1	2:B:105:TYR:O	2.65	0.49
1:D:35:LEU:O	1:D:52:TYR:O	2.31	0.49
1:J:31:ILE:CG2	1:J:34:TYR:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:TYR:CD1	2:K:105:TYR:CE2	3.00	0.49
2:N:55:SER:HG	3:O:31:LYS:NZ	2.05	0.49
1:S:20:ARG:HG3	1:S:78:SER:HA	1.94	0.49
3:I:41:LEU:HD22	3:I:63:ILE:HD11	1.95	0.49
1:G:51:TYR:O	1:G:52:TYR:C	2.56	0.48
1:S:110:ARG:C	1:S:110:ARG:HD3	2.39	0.48
1:V:110:ARG:HD3	1:V:110:ARG:C	2.38	0.48
2:H:8:GLU:OE1	2:H:114:GLY:N	2.46	0.48
1:M:110:ARG:HD3	1:M:110:ARG:C	2.38	0.48
3:U:41:LEU:HD22	3:U:63:ILE:HD11	1.95	0.48
3:X:54:ASP:OD2	3:X:57:ALA:HB2	2.14	0.48
1:A:91:GLN:HG2	1:A:92:GLN:N	2.28	0.48
1:A:110:ARG:HD3	1:A:110:ARG:C	2.39	0.48
1:J:123:SER:OG	2:K:130:TYR:HB3	2.13	0.48
1:P:110:ARG:HD3	1:P:110:ARG:C	2.39	0.48
1:A:20:ARG:HG3	1:A:78:SER:HA	1.94	0.48
1:D:43:ASP:CG	1:D:44:GLY:N	2.70	0.48
3:O:41:LEU:HD22	3:O:63:ILE:HD11	1.96	0.48
1:S:33:ASN:HB2	1:S:53:THR:HG22	1.95	0.48
1:S:43:ASP:CG	1:S:44:GLY:N	2.71	0.48
2:E:8:GLU:OE1	2:E:114:GLY:N	2.47	0.48
1:J:31:ILE:HG22	1:J:32:ASN:N	2.28	0.48
1:P:45:THR:HG22	1:P:46:VAL:N	2.29	0.48
2:Q:103:LEU:HD22	3:R:68:LEU:HG	1.96	0.48
2:W:8:GLU:OE1	2:W:114:GLY:N	2.47	0.48
1:A:45:THR:HG22	1:A:46:VAL:N	2.29	0.48
1:J:91:GLN:HG2	1:J:92:GLN:N	2.29	0.48
1:D:91:GLN:HG2	1:D:92:GLN:N	2.28	0.48
1:M:45:THR:HG23	2:N:112:GLY:O	2.14	0.48
2:T:56:GLY:O	2:T:58:ASN:N	2.46	0.48
1:V:48:LEU:HD22	2:W:109:ASP:HA	1.96	0.48
1:J:110:ARG:HD3	1:J:110:ARG:C	2.39	0.48
3:L:62:LYS:O	3:L:66:LYS:HB2	2.14	0.48
1:G:110:ARG:C	1:G:110:ARG:HD3	2.39	0.48
1:M:45:THR:HG22	1:M:46:VAL:N	2.29	0.48
2:N:34:TYR:CE1	2:N:103:LEU:HD21	2.49	0.48
1:S:33:ASN:HB2	1:S:53:THR:CG2	2.44	0.48
1:A:63:ARG:NH1	1:A:84:ASP:OD2	2.47	0.47
3:C:41:LEU:HD22	3:C:63:ILE:HD11	1.96	0.47
1:M:20:ARG:HG3	1:M:78:SER:HA	1.95	0.47
1:M:63:ARG:NH1	1:M:84:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:8:GLU:OE1	2:N:114:GLY:N	2.47	0.47
1:P:35:LEU:O	1:P:52:TYR:O	2.31	0.47
1:M:35:LEU:O	1:M:52:TYR:O	2.31	0.47
2:T:56:GLY:C	2:T:58:ASN:H	2.20	0.47
2:B:139:THR:O	2:B:141:GLY:N	2.47	0.47
1:D:63:ARG:NH1	1:D:84:ASP:OD2	2.48	0.47
1:D:93:PHE:CE1	2:E:105:TYR:O	2.67	0.47
2:B:8:GLU:OE1	2:B:114:GLY:N	2.47	0.47
1:P:91:GLN:HG2	1:P:92:GLN:N	2.29	0.47
2:E:103:LEU:HD22	3:F:68:LEU:HB3	1.95	0.47
1:G:31:ILE:CG2	1:G:34:TYR:H	2.27	0.47
1:G:91:GLN:HG2	1:G:92:GLN:N	2.30	0.47
2:K:8:GLU:OE1	2:K:114:GLY:N	2.47	0.47
2:K:34:TYR:CE1	2:K:103:LEU:HD21	2.49	0.47
1:P:20:ARG:HG3	1:P:78:SER:HA	1.95	0.47
2:Q:8:GLU:OE1	2:Q:114:GLY:N	2.48	0.47
3:R:41:LEU:HD22	3:R:63:ILE:HD11	1.95	0.47
1:J:63:ARG:NH1	1:J:84:ASP:OD2	2.48	0.47
1:M:93:PHE:CE1	2:N:105:TYR:O	2.68	0.47
2:Q:34:TYR:CE1	2:Q:103:LEU:HD21	2.49	0.47
1:S:91:GLN:HG2	1:S:92:GLN:N	2.30	0.47
1:A:48:LEU:HD22	2:B:109:ASP:HA	1.97	0.47
1:G:63:ARG:NH1	1:G:84:ASP:OD2	2.48	0.47
1:M:91:GLN:OE1	2:N:108:MET:HE3	2.15	0.47
1:V:91:GLN:HG2	1:V:92:GLN:N	2.30	0.47
2:E:34:TYR:CE1	2:E:103:LEU:HD21	2.51	0.46
3:L:54:ASP:OD2	3:L:57:ALA:HB2	2.14	0.46
1:M:33:ASN:HB3	1:M:53:THR:CG2	2.46	0.46
1:S:63:ARG:NH1	1:S:84:ASP:OD2	2.48	0.46
1:V:63:ARG:NH1	1:V:84:ASP:OD2	2.48	0.46
1:P:63:ARG:NH1	1:P:84:ASP:OD2	2.48	0.46
3:L:41:LEU:HD22	3:L:63:ILE:HD11	1.96	0.46
3:O:11:LEU:HD23	3:X:8:LEU:HD21	1.97	0.46
1:J:93:PHE:HD2	2:K:107:ALA:N	2.13	0.46
1:M:91:GLN:HG2	1:M:92:GLN:N	2.29	0.46
1:P:33:ASN:HB3	1:P:53:THR:CG2	2.46	0.46
1:J:34:TYR:HA	1:J:93:PHE:HE1	1.77	0.46
2:T:8:GLU:OE1	2:T:114:GLY:N	2.47	0.46
3:C:67:LEU:HB3	3:C:68:LEU:CD2	2.46	0.46
3:F:41:LEU:HD22	3:F:63:ILE:HD11	1.96	0.46
1:G:33:ASN:HB3	1:G:53:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:35:LEU:HD22	1:P:73:TYR:CD2	2.51	0.46
2:H:34:TYR:CE1	2:H:103:LEU:HD21	2.51	0.46
1:J:171:LYS:CG	1:J:172:ASP:N	2.78	0.46
3:O:67:LEU:HB3	3:O:68:LEU:CD2	2.46	0.46
2:T:34:TYR:CE1	2:T:103:LEU:HD21	2.51	0.46
2:B:34:TYR:CE1	2:B:103:LEU:HD21	2.51	0.45
3:R:67:LEU:HB3	3:R:68:LEU:CD2	2.46	0.45
2:T:141:GLY:O	2:T:142:SER:CB	2.64	0.45
1:V:51:TYR:O	1:V:52:TYR:C	2.56	0.45
3:F:67:LEU:HB3	3:F:68:LEU:CD2	2.46	0.45
1:A:31:ILE:HG22	1:A:94:SER:HB3	1.98	0.45
1:M:21:VAL:HG21	1:M:80:LEU:HD12	1.99	0.45
2:K:34:TYR:CZ	2:K:103:LEU:HD21	2.51	0.45
1:A:23:ILE:HG22	1:A:75:LEU:O	2.17	0.45
1:G:23:ILE:CG2	1:G:75:LEU:HB3	2.47	0.45
1:M:46:VAL:CG2	2:N:111:TRP:CD2	3.00	0.45
1:D:48:LEU:HD22	2:E:109:ASP:HA	1.99	0.45
1:G:23:ILE:O	1:G:23:ILE:HG23	2.17	0.45
1:J:23:ILE:HG22	1:J:75:LEU:O	2.16	0.45
1:J:33:ASN:HB3	1:J:53:THR:CG2	2.47	0.45
1:J:91:GLN:OE1	2:K:108:MET:HE3	2.16	0.45
2:N:34:TYR:CZ	2:N:103:LEU:HD21	2.51	0.45
1:A:21:VAL:HG21	1:A:80:LEU:HD12	1.99	0.45
2:K:141:GLY:O	2:K:142:SER:CB	2.64	0.45
1:S:23:ILE:HG22	1:S:75:LEU:O	2.17	0.45
1:S:93:PHE:CE1	2:T:105:TYR:O	2.69	0.45
1:D:33:ASN:HB3	1:D:53:THR:CG2	2.46	0.45
2:H:146:LEU:HB3	2:H:218:LEU:HD13	1.99	0.45
3:I:31:LYS:HG2	3:I:67:LEU:HD21	1.99	0.45
1:P:21:VAL:HG21	1:P:80:LEU:HD12	1.99	0.45
2:B:104:LEU:H	2:B:104:LEU:CD2	2.26	0.45
1:G:21:VAL:HG21	1:G:80:LEU:HD12	1.99	0.45
1:J:23:ILE:CG2	1:J:75:LEU:HB3	2.47	0.45
1:P:23:ILE:CG2	1:P:75:LEU:HB3	2.47	0.45
2:Q:146:LEU:HB3	2:Q:218:LEU:HD13	1.99	0.45
2:B:146:LEU:HB3	2:B:218:LEU:HD13	1.99	0.44
1:P:23:ILE:HG22	1:P:75:LEU:O	2.17	0.44
2:W:34:TYR:CE1	2:W:103:LEU:HD21	2.52	0.44
2:W:141:GLY:O	2:W:142:SER:CB	2.65	0.44
1:S:23:ILE:HG23	1:S:23:ILE:O	2.18	0.44
1:A:23:ILE:HG23	1:A:23:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:CG2	2:E:111:TRP:CD2	3.00	0.44
1:G:23:ILE:HG22	1:G:75:LEU:O	2.17	0.44
2:K:146:LEU:HB3	2:K:218:LEU:HD13	1.99	0.44
1:D:31:ILE:HG22	1:D:94:SER:HB3	1.99	0.44
2:T:34:TYR:CZ	2:T:103:LEU:HD21	2.53	0.44
3:L:67:LEU:HB3	3:L:68:LEU:HD22	1.99	0.44
2:H:117:VAL:HG12	2:H:119:VAL:HG23	2.00	0.44
2:B:104:LEU:HD23	2:B:104:LEU:N	2.29	0.44
3:L:67:LEU:O	3:L:67:LEU:CD1	2.65	0.44
1:P:13:LEU:HD23	1:P:14:SER:N	2.32	0.44
1:P:23:ILE:HG23	1:P:23:ILE:O	2.18	0.44
1:D:34:TYR:CZ	3:F:37:PRO:HG2	2.52	0.43
2:E:146:LEU:HB3	2:E:218:LEU:HD13	2.00	0.43
2:T:117:VAL:HG12	2:T:119:VAL:HG23	2.00	0.43
2:W:34:TYR:C	2:W:55:SER:HB3	2.43	0.43
2:W:117:VAL:HG12	2:W:119:VAL:HG23	2.00	0.43
2:W:146:LEU:HB3	2:W:218:LEU:HD13	1.99	0.43
2:B:34:TYR:CZ	2:B:103:LEU:HD21	2.53	0.43
2:H:34:TYR:CZ	2:H:103:LEU:HD21	2.53	0.43
2:N:117:VAL:HG12	2:N:119:VAL:HG23	2.00	0.43
2:N:146:LEU:HB3	2:N:218:LEU:HD13	2.00	0.43
1:S:33:ASN:CB	1:S:53:THR:CG2	2.96	0.43
1:A:23:ILE:CG2	1:A:75:LEU:HB3	2.48	0.43
2:K:34:TYR:C	2:K:55:SER:HB3	2.44	0.43
1:P:38:TYR:HE1	2:Q:108:MET:O	2.01	0.43
2:H:217:LYS:HB2	2:K:211:SER:OG	2.19	0.43
2:Q:34:TYR:C	2:Q:55:SER:HB3	2.44	0.43
2:E:117:VAL:HG12	2:E:119:VAL:HG23	1.99	0.43
2:Q:117:VAL:HG12	2:Q:119:VAL:HG23	1.99	0.43
1:S:23:ILE:CG2	1:S:75:LEU:HB3	2.48	0.43
1:S:80:LEU:HD12	1:S:80:LEU:C	2.44	0.43
1:A:34:TYR:CD2	3:C:37:PRO:HB2	2.53	0.43
2:H:156:GLU:OE1	2:H:176:ALA:HB3	2.19	0.43
2:T:34:TYR:C	2:T:55:SER:HB3	2.43	0.43
2:B:117:VAL:HG12	2:B:119:VAL:HG23	1.99	0.43
2:E:34:TYR:CZ	2:E:103:LEU:HD21	2.54	0.43
1:G:33:ASN:HB3	1:G:53:THR:HB	2.01	0.43
1:S:93:PHE:CE2	2:T:107:ALA:HB2	2.54	0.43
1:V:46:VAL:CG2	2:W:111:TRP:CD2	3.01	0.43
3:F:65:LYS:HD2	3:R:66:LYS:HE3	2.00	0.43
1:P:35:LEU:HD21	1:P:73:TYR:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:146:LEU:HB3	2:T:218:LEU:HD13	1.99	0.43
1:D:52:TYR:CG	2:E:105:TYR:HE2	2.37	0.42
2:K:156:GLU:OE1	2:K:176:ALA:HB3	2.19	0.42
2:N:156:GLU:OE1	2:N:176:ALA:HB3	2.19	0.42
2:B:34:TYR:C	2:B:55:SER:HB3	2.44	0.42
3:X:67:LEU:O	3:X:68:LEU:C	2.62	0.42
1:A:52:TYR:CG	2:B:105:TYR:CE2	3.07	0.42
2:K:156:GLU:O	2:K:157:SER:HB3	2.20	0.42
2:Q:34:TYR:CZ	2:Q:103:LEU:HD21	2.53	0.42
1:A:52:TYR:CG	2:B:105:TYR:HE2	2.37	0.42
2:N:34:TYR:C	2:N:55:SER:HB3	2.44	0.42
2:Q:156:GLU:OE1	2:Q:176:ALA:HB3	2.20	0.42
2:B:103:LEU:HD22	3:C:68:LEU:HB3	2.01	0.42
2:E:34:TYR:C	2:E:55:SER:HB3	2.44	0.42
1:S:91:GLN:OE1	2:T:108:MET:HE3	2.20	0.42
2:B:156:GLU:OE1	2:B:176:ALA:HB3	2.19	0.42
2:E:106:TYR:HB2	3:F:32:ALA:HB1	2.02	0.42
2:B:156:GLU:O	2:B:157:SER:HB3	2.19	0.42
1:G:34:TYR:CZ	3:I:37:PRO:HG2	2.55	0.42
2:N:139:THR:OG1	2:N:140:THR:N	2.52	0.42
3:O:20:ARG:HB2	3:O:23:HIS:CD2	2.55	0.42
3:R:36:CYS:HA	3:R:37:PRO:HD2	1.93	0.42
1:D:77:ILE:O	1:D:77:ILE:HG22	2.20	0.42
1:J:23:ILE:HG23	1:J:23:ILE:O	2.18	0.42
2:N:156:GLU:O	2:N:157:SER:HB3	2.20	0.42
2:W:34:TYR:CZ	2:W:103:LEU:HD21	2.54	0.42
2:W:56:GLY:C	2:W:58:ASN:N	2.78	0.42
1:G:85:ILE:HG23	1:G:106:LEU:O	2.20	0.42
2:Q:156:GLU:O	2:Q:157:SER:HB3	2.20	0.42
2:B:44:GLU:O	2:B:45:LYS:HB2	2.19	0.42
2:H:156:GLU:O	2:H:157:SER:HB3	2.20	0.42
1:M:33:ASN:HB3	1:M:53:THR:HB	2.02	0.42
1:P:33:ASN:HB3	1:P:53:THR:HB	2.02	0.42
3:X:20:ARG:HB2	3:X:23:HIS:CD2	2.55	0.42
2:H:34:TYR:C	2:H:55:SER:HB3	2.44	0.41
1:P:34:TYR:CZ	3:R:37:PRO:HG2	2.55	0.41
2:Q:106:TYR:HB2	3:R:32:ALA:HB1	2.01	0.41
3:R:20:ARG:HB2	3:R:23:HIS:CD2	2.55	0.41
2:T:44:GLU:O	2:T:45:LYS:HB2	2.21	0.41
2:T:156:GLU:OE1	2:T:176:ALA:HB3	2.19	0.41
3:U:65:LYS:HD2	3:U:65:LYS:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:52:TYR:CG	2:Q:105:TYR:CE2	3.08	0.41
2:T:156:GLU:O	2:T:157:SER:HB3	2.20	0.41
3:C:20:ARG:HB2	3:C:23:HIS:CD2	2.55	0.41
2:E:44:GLU:O	2:E:45:LYS:HB2	2.20	0.41
1:J:93:PHE:HD2	2:K:107:ALA:H	1.68	0.41
1:S:41:LYS:O	1:S:42:PRO:C	2.64	0.41
2:W:34:TYR:CE1	2:W:100:ARG:CZ	3.03	0.41
1:A:34:TYR:CE1	3:C:37:PRO:HG2	2.55	0.41
1:D:52:TYR:CG	2:E:105:TYR:CE2	3.08	0.41
2:K:117:VAL:HG12	2:K:119:VAL:HG23	2.01	0.41
3:L:20:ARG:HB2	3:L:23:HIS:CD2	2.56	0.41
2:N:56:GLY:O	2:N:58:ASN:CG	2.63	0.41
1:A:41:LYS:O	1:A:42:PRO:C	2.64	0.41
3:L:63:ILE:O	3:L:64:ILE:O	2.37	0.41
1:V:91:GLN:OE1	2:W:108:MET:HE3	2.20	0.41
2:W:156:GLU:OE1	2:W:176:ALA:HB3	2.19	0.41
1:M:85:ILE:HG23	1:M:106:LEU:O	2.21	0.41
2:N:56:GLY:C	2:N:58:ASN:N	2.78	0.41
1:P:35:LEU:HD23	1:P:73:TYR:CD1	2.51	0.41
3:O:36:CYS:HA	3:O:37:PRO:HD2	1.93	0.41
1:A:110:ARG:HD3	1:A:111:ALA:N	2.36	0.41
1:D:110:ARG:HD3	1:D:111:ALA:N	2.36	0.41
2:E:44:GLU:O	2:E:45:LYS:CB	2.69	0.41
1:G:123:SER:OG	2:H:130:TYR:HB3	2.21	0.41
2:H:44:GLU:O	2:H:45:LYS:HB2	2.21	0.41
1:S:85:ILE:HG23	1:S:106:LEU:O	2.21	0.41
1:D:33:ASN:HB3	1:D:53:THR:HB	2.02	0.41
2:K:44:GLU:O	2:K:45:LYS:CB	2.69	0.41
1:P:110:ARG:HD3	1:P:111:ALA:N	2.36	0.41
3:U:20:ARG:HB2	3:U:23:HIS:CD2	2.56	0.41
1:A:97:PRO:O	1:A:99:THR:HG23	2.21	0.40
2:K:56:GLY:C	2:K:58:ASN:N	2.78	0.40
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.95	0.40
2:B:104:LEU:HG	2:B:105:TYR:HD1	1.86	0.40
1:D:41:LYS:O	1:D:42:PRO:C	2.63	0.40
2:E:56:GLY:C	2:E:58:ASN:N	2.78	0.40
3:F:20:ARG:HB2	3:F:23:HIS:CD2	2.56	0.40
2:T:44:GLU:O	2:T:45:LYS:CB	2.69	0.40
1:V:97:PRO:O	1:V:99:THR:HG23	2.22	0.40
2:W:156:GLU:O	2:W:157:SER:HB3	2.20	0.40
2:B:44:GLU:O	2:B:45:LYS:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:44:GLU:O	2:K:45:LYS:HB2	2.21	0.40
3:U:5:ASP:N	3:U:5:ASP:OD2	2.55	0.40
1:V:110:ARG:HD3	1:V:111:ALA:N	2.37	0.40
2:W:56:GLY:O	2:W:58:ASN:CG	2.65	0.40
2:K:56:GLY:O	2:K:58:ASN:CG	2.64	0.40
1:S:52:TYR:CE1	2:T:105:TYR:HE2	2.39	0.40
3:U:67:LEU:HB3	3:U:68:LEU:CD2	2.51	0.40
1:J:97:PRO:O	1:J:99:THR:HG23	2.22	0.40
1:S:97:PRO:O	1:S:99:THR:HG23	2.21	0.40
3:U:29:VAL:HG21	3:U:66:LYS:HD3	2.04	0.40
1:V:85:ILE:HG23	1:V:106:LEU:O	2.21	0.40
3:X:67:LEU:O	3:X:69:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/212 (99%)	197 (94%)	11 (5%)	2 (1%)	12	43
1	D	210/212 (99%)	193 (92%)	14 (7%)	3 (1%)	9	37
1	G	210/212 (99%)	196 (93%)	12 (6%)	2 (1%)	12	43
1	J	210/212 (99%)	196 (93%)	12 (6%)	2 (1%)	12	43
1	M	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	12	43
1	P	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	12	43
1	S	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	12	43
1	V	210/212 (99%)	196 (93%)	12 (6%)	2 (1%)	12	43
2	B	217/219 (99%)	196 (90%)	14 (6%)	7 (3%)	3	25
2	E	217/219 (99%)	197 (91%)	14 (6%)	6 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	217/219 (99%)	196 (90%)	15 (7%)	6 (3%)	4	27
2	K	217/219 (99%)	190 (88%)	15 (7%)	12 (6%)	1	16
2	N	217/219 (99%)	197 (91%)	14 (6%)	6 (3%)	4	27
2	Q	217/219 (99%)	195 (90%)	15 (7%)	7 (3%)	3	25
2	T	217/219 (99%)	193 (89%)	16 (7%)	8 (4%)	2	22
2	W	217/219 (99%)	194 (89%)	15 (7%)	8 (4%)	2	22
3	C	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	3	25
3	F	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	3	25
3	I	64/70 (91%)	55 (86%)	8 (12%)	1 (2%)	7	35
3	L	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	3	25
3	O	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	3	25
3	R	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	3	25
3	U	63/70 (90%)	55 (87%)	8 (13%)	0	100	100
3	X	64/70 (91%)	55 (86%)	7 (11%)	2 (3%)	3	26
All	All	3922/4008 (98%)	3561 (91%)	271 (7%)	90 (2%)	5	30

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	46	ARG
2	B	57	ASP
2	B	58	ASN
2	B	157	SER
1	D	78	SER
2	E	46	ARG
2	E	57	ASP
2	E	58	ASN
2	E	156	GLU
2	H	46	ARG
2	H	57	ASP
2	H	58	ASN
2	H	157	SER
2	K	46	ARG
2	K	57	ASP
2	K	58	ASN
2	K	142	SER
2	K	157	SER

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Mol	Chain	Res	Type
2	N	46	ARG
2	N	57	ASP
2	N	58	ASN
2	N	157	SER
2	Q	46	ARG
2	Q	57	ASP
2	Q	58	ASN
2	Q	157	SER
2	T	46	ARG
2	T	57	ASP
2	T	58	ASN
2	T	142	SER
2	T	157	SER
2	W	46	ARG
2	W	57	ASP
2	W	58	ASN
2	W	142	SER
2	W	157	SER
2	B	45	LYS
2	E	45	LYS
2	H	45	LYS
2	K	45	LYS
2	K	168	SER
3	L	64	ILE
2	N	45	LYS
2	Q	45	LYS
2	T	45	LYS
2	W	45	LYS
3	X	68	LEU
1	A	33	ASN
1	A	79	ASN
2	B	140	THR
3	C	5	ASP
1	D	33	ASN
1	D	79	ASN
3	F	5	ASP
1	G	33	ASN
1	G	79	ASN
3	I	5	ASP
1	J	33	ASN
1	J	79	ASN
2	K	107	ALA

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Mol	Chain	Res	Type
2	K	139	THR
1	M	33	ASN
1	M	79	ASN
3	O	5	ASP
1	P	33	ASN
1	P	79	ASN
1	S	33	ASN
1	S	79	ASN
1	V	33	ASN
1	V	79	ASN
2	W	139	THR
3	X	5	ASP
2	K	106	TYR
3	L	5	ASP
3	R	5	ASP
2	T	139	THR
3	C	66	LYS
3	F	66	LYS
2	K	140	THR
3	O	66	LYS
2	Q	143	SER
3	R	66	LYS
2	B	196	TRP
2	K	196	TRP
2	N	196	TRP
2	Q	196	TRP
2	T	196	TRP
2	W	196	TRP
2	E	196	TRP
2	H	196	TRP

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	188/190 (99%)	167 (89%)	21 (11%)	6 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	188/190 (99%)	166 (88%)	22 (12%)	5	24
1	G	188/190 (99%)	170 (90%)	18 (10%)	8	31
1	J	188/190 (99%)	168 (89%)	20 (11%)	6	27
1	M	188/190 (99%)	171 (91%)	17 (9%)	9	33
1	P	188/190 (99%)	170 (90%)	18 (10%)	8	31
1	S	188/190 (99%)	169 (90%)	19 (10%)	7	29
1	V	188/190 (99%)	170 (90%)	18 (10%)	8	31
2	B	179/189 (95%)	168 (94%)	11 (6%)	17	43
2	E	179/189 (95%)	169 (94%)	10 (6%)	19	45
2	H	179/189 (95%)	168 (94%)	11 (6%)	17	43
2	K	177/189 (94%)	167 (94%)	10 (6%)	19	45
2	N	179/189 (95%)	167 (93%)	12 (7%)	15	42
2	Q	179/189 (95%)	169 (94%)	10 (6%)	19	45
2	T	179/189 (95%)	169 (94%)	10 (6%)	19	45
2	W	179/189 (95%)	169 (94%)	10 (6%)	19	45
3	C	57/62 (92%)	45 (79%)	12 (21%)	1	7
3	F	57/62 (92%)	44 (77%)	13 (23%)	1	6
3	I	58/62 (94%)	44 (76%)	14 (24%)	1	5
3	L	57/62 (92%)	42 (74%)	15 (26%)	0	4
3	O	57/62 (92%)	45 (79%)	12 (21%)	1	7
3	R	57/62 (92%)	45 (79%)	12 (21%)	1	7
3	U	57/62 (92%)	45 (79%)	12 (21%)	1	7
3	X	57/62 (92%)	45 (79%)	12 (21%)	1	7
All	All	3391/3528 (96%)	3052 (90%)	339 (10%)	7	30

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	10	THR
1	A	11	SER
1	A	13	LEU
1	A	17	LEU
1	A	26	SER

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Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	ASN
1	A	46	VAL
1	A	49	LEU
1	A	53	THR
1	A	76	THR
1	A	107	GLU
1	A	110	ARG
1	A	144	LYS
1	A	147	ASN
1	A	178	SER
1	A	185	LYS
1	A	193	SER
1	A	196	CYS
1	A	209	LYS
2	B	44	GLU
2	B	54	THR
2	B	80	THR
2	B	132	LEU
2	B	140	THR
2	B	156	GLU
2	B	182	LEU
2	B	200	THR
2	B	203	CYS
2	B	211	SER
2	B	219	GLU
3	C	16	THR
3	C	17	SER
3	C	22	ARG
3	C	30	ILE
3	C	42	ILE
3	C	44	THR
3	C	49	ARG
3	C	53	LEU
3	C	61	LYS
3	C	63	ILE
3	C	66	LYS
3	C	68	LEU
1	D	9	ILE
1	D	10	THR
1	D	11	SER
1	D	13	LEU

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Mol	Chain	Res	Type
1	D	17	LEU
1	D	26	SER
1	D	29	GLN
1	D	46	VAL
1	D	49	LEU
1	D	53	THR
1	D	56	LEU
1	D	76	THR
1	D	95	LYS
1	D	107	GLU
1	D	110	ARG
1	D	144	LYS
1	D	147	ASN
1	D	178	SER
1	D	185	LYS
1	D	193	SER
1	D	196	CYS
1	D	209	LYS
2	E	44	GLU
2	E	54	THR
2	E	80	THR
2	E	156	GLU
2	E	168	SER
2	E	182	LEU
2	E	200	THR
2	E	203	CYS
2	E	211	SER
2	E	219	GLU
3	F	16	THR
3	F	17	SER
3	F	22	ARG
3	F	30	ILE
3	F	42	ILE
3	F	44	THR
3	F	49	ARG
3	F	53	LEU
3	F	56	GLN
3	F	61	LYS
3	F	63	ILE
3	F	66	LYS
3	F	68	LEU
1	G	10	THR

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Mol	Chain	Res	Type
1	G	11	SER
1	G	13	LEU
1	G	26	SER
1	G	46	VAL
1	G	49	LEU
1	G	53	THR
1	G	56	LEU
1	G	76	THR
1	G	107	GLU
1	G	110	ARG
1	G	144	LYS
1	G	147	ASN
1	G	178	SER
1	G	185	LYS
1	G	193	SER
1	G	196	CYS
1	G	209	LYS
2	H	44	GLU
2	H	54	THR
2	H	80	THR
2	H	132	LEU
2	H	140	THR
2	H	156	GLU
2	H	182	LEU
2	H	200	THR
2	H	203	CYS
2	H	211	SER
2	H	219	GLU
3	I	16	THR
3	I	17	SER
3	I	22	ARG
3	I	30	ILE
3	I	42	ILE
3	I	44	THR
3	I	49	ARG
3	I	53	LEU
3	I	59	LEU
3	I	61	LYS
3	I	63	ILE
3	I	66	LYS
3	I	67	LEU
3	I	68	LEU

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Mol	Chain	Res	Type
1	J	9	ILE
1	J	10	THR
1	J	11	SER
1	J	26	SER
1	J	33	ASN
1	J	46	VAL
1	J	49	LEU
1	J	53	THR
1	J	56	LEU
1	J	76	THR
1	J	93	PHE
1	J	107	GLU
1	J	110	ARG
1	J	144	LYS
1	J	147	ASN
1	J	178	SER
1	J	185	LYS
1	J	193	SER
1	J	196	CYS
1	J	209	LYS
2	K	44	GLU
2	K	54	THR
2	K	80	THR
2	K	156	GLU
2	K	168	SER
2	K	182	LEU
2	K	200	THR
2	K	203	CYS
2	K	211	SER
2	K	219	GLU
3	L	16	THR
3	L	17	SER
3	L	22	ARG
3	L	30	ILE
3	L	42	ILE
3	L	44	THR
3	L	49	ARG
3	L	53	LEU
3	L	61	LYS
3	L	62	LYS
3	L	63	ILE
3	L	64	ILE

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Mol	Chain	Res	Type
3	L	65	LYS
3	L	67	LEU
3	L	68	LEU
1	M	9	ILE
1	M	10	THR
1	M	11	SER
1	M	17	LEU
1	M	26	SER
1	M	46	VAL
1	M	49	LEU
1	M	53	THR
1	M	76	THR
1	M	107	GLU
1	M	110	ARG
1	M	147	ASN
1	M	178	SER
1	M	185	LYS
1	M	193	SER
1	M	196	CYS
1	M	209	LYS
2	N	44	GLU
2	N	45	LYS
2	N	54	THR
2	N	80	THR
2	N	140	THR
2	N	156	GLU
2	N	182	LEU
2	N	200	THR
2	N	203	CYS
2	N	211	SER
2	N	216	LYS
2	N	219	GLU
3	O	16	THR
3	O	17	SER
3	O	22	ARG
3	O	30	ILE
3	O	42	ILE
3	O	44	THR
3	O	49	ARG
3	O	53	LEU
3	O	61	LYS
3	O	63	ILE

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Mol	Chain	Res	Type
3	O	66	LYS
3	O	68	LEU
1	P	10	THR
1	P	11	SER
1	P	26	SER
1	P	29	GLN
1	P	35	LEU
1	P	46	VAL
1	P	49	LEU
1	P	53	THR
1	P	76	THR
1	P	107	GLU
1	P	110	ARG
1	P	144	LYS
1	P	147	ASN
1	P	178	SER
1	P	185	LYS
1	P	193	SER
1	P	196	CYS
1	P	209	LYS
2	Q	44	GLU
2	Q	45	LYS
2	Q	54	THR
2	Q	80	THR
2	Q	156	GLU
2	Q	182	LEU
2	Q	200	THR
2	Q	203	CYS
2	Q	211	SER
2	Q	219	GLU
3	R	16	THR
3	R	17	SER
3	R	22	ARG
3	R	30	ILE
3	R	42	ILE
3	R	44	THR
3	R	49	ARG
3	R	53	LEU
3	R	61	LYS
3	R	63	ILE
3	R	66	LYS
3	R	68	LEU

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Mol	Chain	Res	Type
1	S	10	THR
1	S	11	SER
1	S	26	SER
1	S	33	ASN
1	S	39	ARG
1	S	46	VAL
1	S	49	LEU
1	S	53	THR
1	S	76	THR
1	S	80	LEU
1	S	107	GLU
1	S	110	ARG
1	S	144	LYS
1	S	147	ASN
1	S	178	SER
1	S	185	LYS
1	S	193	SER
1	S	196	CYS
1	S	209	LYS
2	T	44	GLU
2	T	54	THR
2	T	80	THR
2	T	140	THR
2	T	156	GLU
2	T	182	LEU
2	T	200	THR
2	T	203	CYS
2	T	211	SER
2	T	219	GLU
3	U	16	THR
3	U	17	SER
3	U	22	ARG
3	U	30	ILE
3	U	42	ILE
3	U	44	THR
3	U	49	ARG
3	U	53	LEU
3	U	61	LYS
3	U	63	ILE
3	U	66	LYS
3	U	68	LEU
1	V	10	THR

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Mol	Chain	Res	Type
1	V	11	SER
1	V	17	LEU
1	V	33	ASN
1	V	46	VAL
1	V	49	LEU
1	V	53	THR
1	V	56	LEU
1	V	76	THR
1	V	107	GLU
1	V	110	ARG
1	V	144	LYS
1	V	147	ASN
1	V	178	SER
1	V	185	LYS
1	V	193	SER
1	V	196	CYS
1	V	209	LYS
2	W	44	GLU
2	W	54	THR
2	W	80	THR
2	W	140	THR
2	W	156	GLU
2	W	182	LEU
2	W	200	THR
2	W	203	CYS
2	W	211	SER
2	W	219	GLU
3	X	16	THR
3	X	17	SER
3	X	22	ARG
3	X	30	ILE
3	X	42	ILE
3	X	44	THR
3	X	49	ARG
3	X	53	LEU
3	X	61	LYS
3	X	63	ILE
3	X	66	LYS
3	X	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	79	ASN
1	A	212	ASN
2	B	41	GLN
2	B	101	GLN
2	B	179	GLN
3	C	9	GLN
3	C	23	HIS
1	D	57	HIS
1	D	79	ASN
1	D	212	ASN
2	E	101	GLN
3	F	9	GLN
3	F	23	HIS
1	G	40	GLN
1	G	57	HIS
1	G	79	ASN
1	G	212	ASN
2	H	41	GLN
2	H	101	GLN
2	H	179	GLN
3	I	9	GLN
3	I	23	HIS
1	J	40	GLN
1	J	57	HIS
1	J	79	ASN
1	J	212	ASN
2	K	41	GLN
2	K	101	GLN
2	K	179	GLN
3	L	9	GLN
3	L	23	HIS
1	M	40	GLN
1	M	79	ASN
1	M	212	ASN
2	N	41	GLN
2	N	101	GLN
3	O	9	GLN
3	O	23	HIS
1	P	40	GLN
1	P	79	ASN
1	P	212	ASN
2	Q	41	GLN

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Mol	Chain	Res	Type
2	Q	101	GLN
3	R	9	GLN
3	R	23	HIS
1	S	40	GLN
1	S	57	HIS
1	S	79	ASN
1	S	212	ASN
2	T	41	GLN
2	T	101	GLN
3	U	9	GLN
3	U	23	HIS
1	V	40	GLN
1	V	79	ASN
1	V	212	ASN
2	W	41	GLN
2	W	101	GLN
2	W	179	GLN
3	X	23	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	212/212 (100%)	-0.38	0 100 100	78, 118, 159, 182	0
1	D	212/212 (100%)	-0.48	0 100 100	88, 122, 157, 182	0
1	G	212/212 (100%)	-0.31	0 100 100	80, 141, 202, 235	0
1	J	212/212 (100%)	-0.35	0 100 100	96, 144, 187, 212	0
1	M	212/212 (100%)	-0.26	2 (0%) 81 58	85, 123, 179, 198	0
1	P	212/212 (100%)	-0.35	0 100 100	97, 141, 177, 193	0
1	S	212/212 (100%)	-0.34	1 (0%) 87 69	90, 154, 210, 229	0
1	V	212/212 (100%)	-0.38	0 100 100	91, 160, 211, 229	0
2	B	219/219 (100%)	-0.43	0 100 100	87, 124, 169, 206	0
2	E	219/219 (100%)	-0.45	1 (0%) 87 69	93, 132, 170, 211	0
2	H	219/219 (100%)	-0.35	0 100 100	76, 127, 184, 230	0
2	K	219/219 (100%)	-0.36	0 100 100	95, 136, 181, 196	0
2	N	219/219 (100%)	-0.27	0 100 100	90, 145, 195, 254	0
2	Q	219/219 (100%)	-0.37	0 100 100	94, 152, 204, 231	0
2	T	219/219 (100%)	-0.30	0 100 100	87, 144, 192, 249	0
2	W	219/219 (100%)	-0.27	2 (0%) 81 58	90, 145, 207, 244	0
3	C	65/70 (92%)	-0.12	0 100 100	75, 117, 187, 196	0
3	F	65/70 (92%)	-0.00	0 100 100	89, 120, 204, 230	0
3	I	66/70 (94%)	0.01	1 (1%) 72 47	95, 128, 197, 203	0
3	L	65/70 (92%)	0.15	2 (3%) 51 32	104, 141, 232, 265	0
3	O	65/70 (92%)	-0.01	0 100 100	81, 122, 184, 220	0
3	R	65/70 (92%)	-0.22	0 100 100	82, 116, 189, 237	0
3	U	65/70 (92%)	0.05	3 (4%) 37 25	105, 138, 202, 219	0
3	X	66/70 (94%)	-0.11	0 100 100	95, 132, 204, 211	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	3970/4008 (99%)	-0.31	12 (0%)	90 76	75, 136, 196, 265	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	62	LYS	7.1
3	U	62	LYS	5.0
3	U	66	LYS	3.0
2	W	164	SER	2.7
3	L	59	LEU	2.4
2	W	166	SER	2.2
3	U	68	LEU	2.2
1	M	163	ASN	2.1
1	M	145	ASP	2.1
3	I	62	LYS	2.0
1	S	95	LYS	2.0
2	E	176	ALA	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.