



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:49 PM UTC

PDB ID : 6UPU / pdb_00006upu
Title : Crystal structure of the Orientia tsutsugamushi OtDUB in complex with three molecules of ubiquitin
Authors : Lim, C.S.; Ronau, J.A.; Xiong, Y.
Deposited on : 2019-10-18
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:

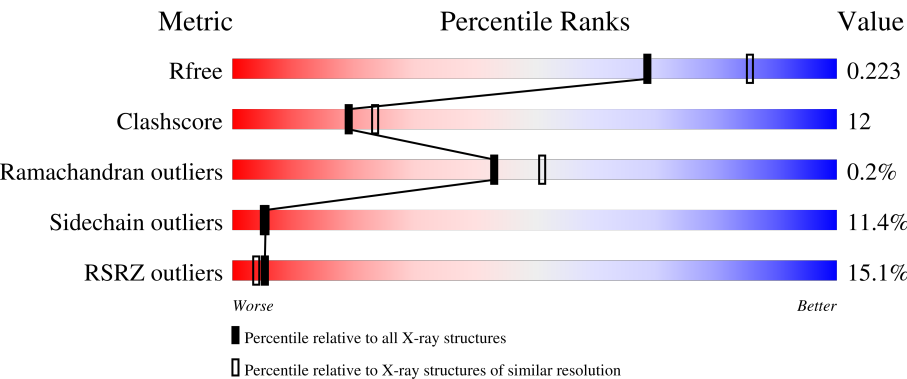
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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	260	4% 73% 20% . .
1	E	260	2% 71% 23% . ..
1	I	260	3% 73% 22% . ..
1	M	260	3% 73% 23% . ..
2	B	79	8% 65% 24% 8% . ..

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Mol	Chain	Length	Quality of chain
2	C	79	14% 75% 18%
2	D	79	53% 72% 16% 8%
2	F	79	66% 20% 10%
2	G	79	76% 78% 15% 5%
2	H	79	28% 70% 23%
2	J	79	73% 19% 5%
2	K	79	32% 72% 22% 5%
2	L	79	66% 78% 14%
2	N	79	4% 65% 23% 9%
2	O	79	35% 76% 15% 5%
2	P	79	22% 71% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15824 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 ULP_PROTEASE domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2034	1269	354	401	10			
1	E	258	Total	C	N	O	S	0	0	0
			2029	1266	353	400	10			
1	I	258	Total	C	N	O	S	0	0	0
			2029	1266	353	400	10			
1	M	258	Total	C	N	O	S	0	0	0
			2029	1266	353	400	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B3CVM3
E	0	GLY	-	expression tag	UNP B3CVM3
I	0	GLY	-	expression tag	UNP B3CVM3
M	0	GLY	-	expression tag	UNP B3CVM3

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	S	0	0	0
			605	380	106	118	1			
2	C	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	D	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			
2	F	77	Total	C	N	O	S	0	0	0
			605	380	106	118	1			
2	G	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	H	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	77	Total	C	N	O	S	0	0	0
			605	380	106	118	1			
2	K	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	L	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			
2	N	78	Total	C	N	O	S	0	0	0
			609	382	107	119	1			
2	O	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	P	77	Total	C	N	O	S	0	0	0
			606	380	106	119	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP F5H388
B	-1	GLY	-	expression tag	UNP F5H388
B	0	GLY	-	expression tag	UNP F5H388
C	-2	GLY	-	expression tag	UNP F5H388
C	-1	GLY	-	expression tag	UNP F5H388
C	0	GLY	-	expression tag	UNP F5H388
D	-2	GLY	-	expression tag	UNP F5H388
D	-1	GLY	-	expression tag	UNP F5H388
D	0	GLY	-	expression tag	UNP F5H388
F	-2	GLY	-	expression tag	UNP F5H388
F	-1	GLY	-	expression tag	UNP F5H388
F	0	GLY	-	expression tag	UNP F5H388
G	-2	GLY	-	expression tag	UNP F5H388
G	-1	GLY	-	expression tag	UNP F5H388
G	0	GLY	-	expression tag	UNP F5H388
H	-2	GLY	-	expression tag	UNP F5H388
H	-1	GLY	-	expression tag	UNP F5H388
H	0	GLY	-	expression tag	UNP F5H388
J	-2	GLY	-	expression tag	UNP F5H388
J	-1	GLY	-	expression tag	UNP F5H388
J	0	GLY	-	expression tag	UNP F5H388
K	-2	GLY	-	expression tag	UNP F5H388
K	-1	GLY	-	expression tag	UNP F5H388
K	0	GLY	-	expression tag	UNP F5H388
L	-2	GLY	-	expression tag	UNP F5H388
L	-1	GLY	-	expression tag	UNP F5H388
L	0	GLY	-	expression tag	UNP F5H388

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-2	GLY	-	expression tag	UNP F5H388
N	-1	GLY	-	expression tag	UNP F5H388
N	0	GLY	-	expression tag	UNP F5H388
O	-2	GLY	-	expression tag	UNP F5H388
O	-1	GLY	-	expression tag	UNP F5H388
O	0	GLY	-	expression tag	UNP F5H388
P	-2	GLY	-	expression tag	UNP F5H388
P	-1	GLY	-	expression tag	UNP F5H388
P	0	GLY	-	expression tag	UNP F5H388

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total O 73 73	0	0
3	B	20	Total O 20 20	0	0
3	C	14	Total O 14 14	0	0
3	D	5	Total O 5 5	0	0
3	E	68	Total O 68 68	0	0
3	F	31	Total O 31 31	0	0
3	G	8	Total O 8 8	0	0
3	H	14	Total O 14 14	0	0
3	I	61	Total O 61 61	0	0
3	J	26	Total O 26 26	0	0
3	K	11	Total O 11 11	0	0
3	L	7	Total O 7 7	0	0
3	M	89	Total O 89 89	0	0
3	N	23	Total O 23 23	0	0
3	O	10	Total O 10 10	0	0

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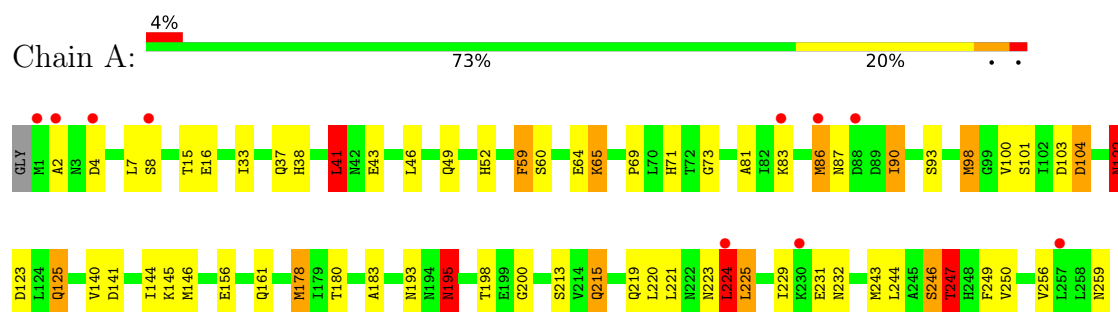
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	16	Total	O	0	0
			16	16		

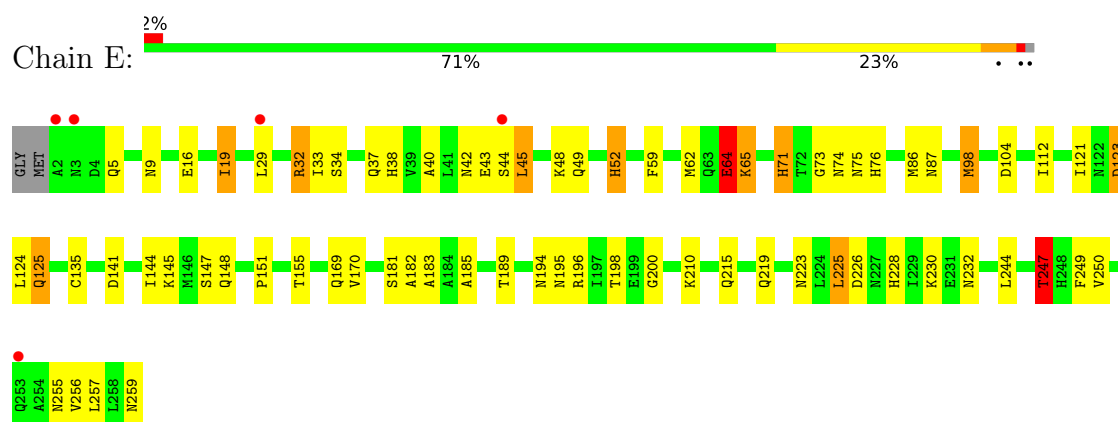
3 Residue-property plots [i](#)

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.

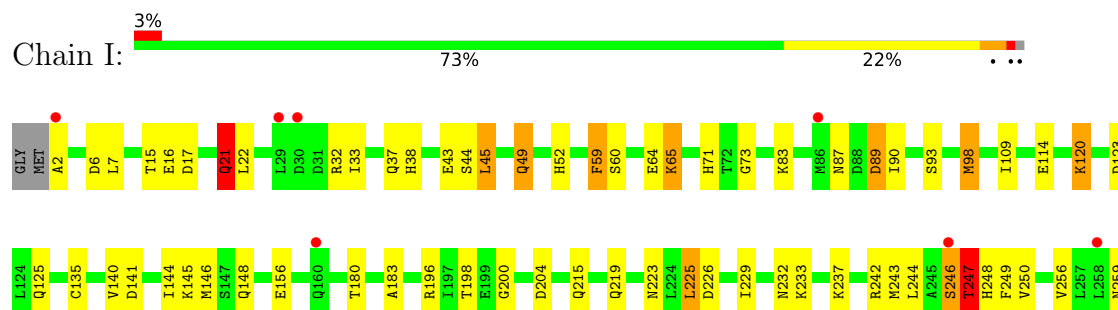
- Molecule 1: ULP_PROTEASE domain-containing protein



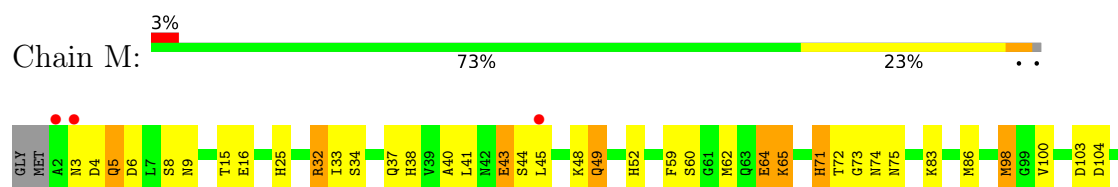
- Molecule 1: ULP_PROTEASE domain-containing protein



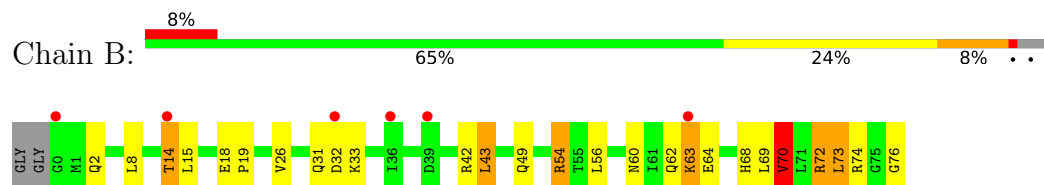
- Molecule 1: ULP_PROTEASE domain-containing protein



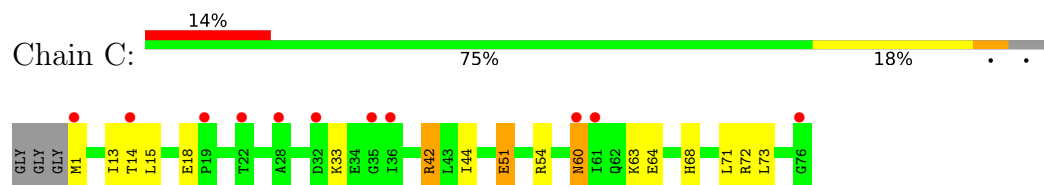
- Molecule 1: ULP_PROTEASE domain-containing protein



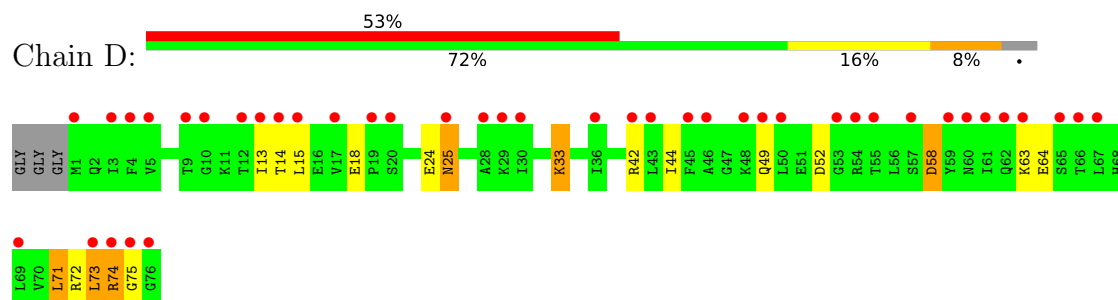
• Molecule 2: Ubiquitin



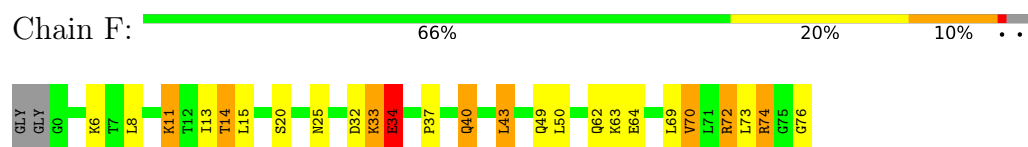
• Molecule 2: Ubiquitin



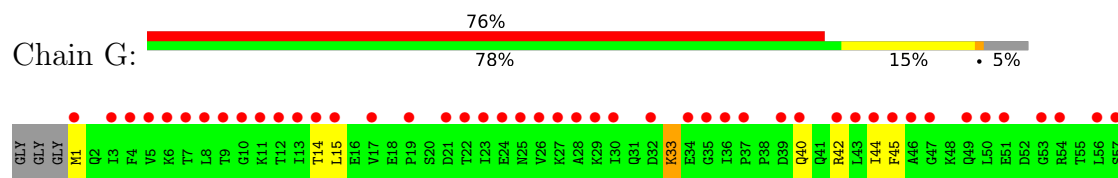
• Molecule 2: Ubiquitin

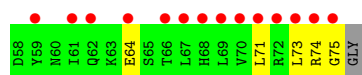


• Molecule 2: Ubiquitin

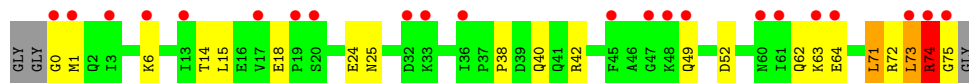


• Molecule 2: Ubiquitin





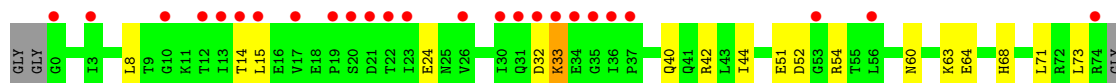
• Molecule 2: Ubiquitin



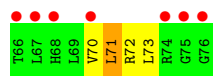
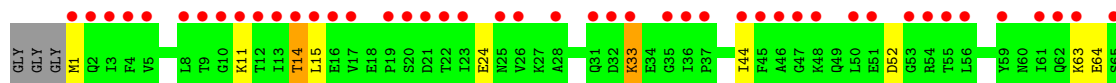
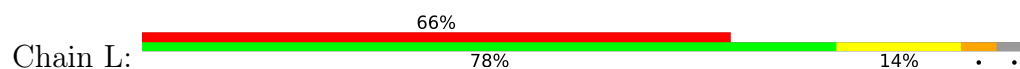
• Molecule 2: Ubiquitin



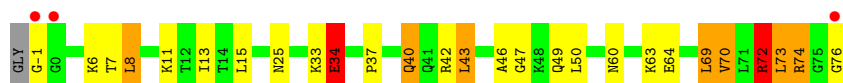
• Molecule 2: Ubiquitin



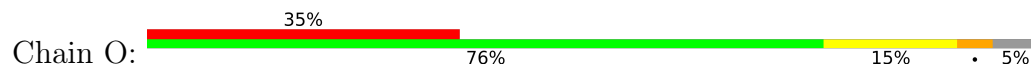
• Molecule 2: Ubiquitin

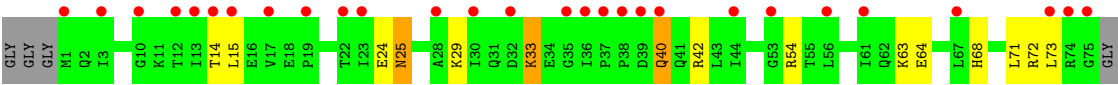


• Molecule 2: Ubiquitin



• Molecule 2: Ubiquitin





● Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.75Å 144.07Å 143.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.70 – 2.20 56.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (56.70-2.20) 98.5 (56.70-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.209 0.198 , 0.223	Depositor DCC
R_{free} test set	6079 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
Reported twinning fraction	0.742 for H, K, L 0.258 for -H, -L, -K	Depositor
Outliers	0 of 124051 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15824	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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	1.17	3/2058 (0.1%)	1.57	16/2788 (0.6%)
1	E	1.26	8/2053 (0.4%)	1.55	11/2781 (0.4%)
1	I	1.15	2/2053 (0.1%)	1.52	7/2781 (0.3%)
1	M	1.25	4/2053 (0.2%)	1.55	10/2781 (0.4%)
2	B	1.17	2/611 (0.3%)	1.58	5/821 (0.6%)
2	C	1.04	0/607	1.42	4/816 (0.5%)
2	D	1.03	0/608	1.33	2/816 (0.2%)
2	F	1.18	0/611	1.56	4/821 (0.5%)
2	G	0.97	0/603	1.30	0/811
2	H	1.10	0/607	1.36	2/816 (0.2%)
2	J	1.17	0/611	1.49	2/821 (0.2%)
2	K	1.03	0/603	1.35	0/811
2	L	1.02	0/608	1.31	0/816
2	N	1.21	1/615 (0.2%)	1.55	7/826 (0.8%)
2	O	1.03	0/603	1.38	1/811 (0.1%)
2	P	1.09	0/612	1.36	1/821 (0.1%)
All	All	1.15	20/15516 (0.1%)	1.49	72/20938 (0.3%)

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
2	B	0	1
2	D	0	1
2	G	0	1
2	L	0	1
All	All	0	5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	52	HIS	CE1-NE2	7.50	1.40	1.32
1	M	100	VAL	C-O	7.02	1.33	1.24
1	M	169	GLN	C-O	-6.90	1.16	1.24
1	E	169	GLN	C-O	-6.65	1.16	1.24
1	A	69	PRO	C-O	-6.45	1.15	1.24
2	N	72	ARG	CD-NE	-6.45	1.37	1.46
2	B	43	LEU	N-CA	5.98	1.53	1.46
1	E	228	HIS	CE1-NE2	5.81	1.38	1.32
1	M	25	HIS	CE1-NE2	5.77	1.38	1.32
1	E	123	ASP	C-O	-5.75	1.17	1.24
1	E	76	HIS	CE1-NE2	5.74	1.38	1.32
1	A	100	VAL	C-O	5.71	1.30	1.24
1	M	71	HIS	CG-ND1	5.54	1.44	1.38
1	A	4	ASP	CG-OD1	5.45	1.35	1.25
1	E	170	VAL	C-O	-5.43	1.17	1.24
1	E	151	PRO	C-O	-5.22	1.18	1.23
1	E	71	HIS	CE1-NE2	5.21	1.37	1.32
2	B	70	VAL	C-O	-5.20	1.18	1.24
1	I	22	LEU	C-O	5.12	1.30	1.24
1	I	237	LYS	C-O	5.04	1.29	1.24

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	CA-C-N	8.85	132.50	120.38
1	A	103	ASP	C-N-CA	8.85	132.50	120.38
1	A	104	ASP	CA-CB-CG	8.80	121.40	112.60
1	M	103	ASP	CA-C-N	8.17	132.31	120.38
1	M	103	ASP	C-N-CA	8.17	132.31	120.38
2	C	51	GLU	CB-CG-CD	7.92	126.07	112.60
2	F	72	ARG	NE-CZ-NH1	-7.82	113.68	121.50
2	P	40	GLN	CB-CG-CD	-7.35	100.10	112.60
1	I	6	ASP	CB-CA-C	7.31	122.03	110.19
1	E	247	THR	N-CA-CB	-7.15	98.65	110.23
2	N	40	GLN	CB-CG-CD	7.13	124.73	112.60
2	C	72	ARG	CG-CD-NE	-7.12	96.34	112.00
2	D	58	ASP	CA-CB-CG	7.10	119.70	112.60
1	I	259	ASN	CA-C-O	-7.09	108.75	120.80
1	E	32	ARG	CG-CD-NE	7.00	127.41	112.00
1	M	175	GLU	CB-CG-CD	6.96	124.42	112.60
1	E	19	ILE	CA-CB-CG2	6.88	122.20	110.50
1	A	247	THR	CB-CA-C	6.78	120.90	109.84
2	F	72	ARG	NE-CZ-NH2	6.74	125.27	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	247	THR	N-CA-CB	-6.73	99.52	109.95
2	N	34	GLU	CB-CG-CD	6.57	123.78	112.60
2	B	14	THR	CA-CB-OG1	-6.54	99.79	109.60
2	D	75	GLY	CA-C-O	-6.53	115.88	121.04
2	O	25	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	247	THR	N-CA-CB	-6.38	100.06	109.95
1	I	21	GLN	CA-CB-CG	6.27	126.64	114.10
1	I	247	THR	CB-CA-C	6.26	120.05	109.84
1	M	156	GLU	CB-CA-C	6.17	120.64	110.90
1	M	180	THR	CA-CB-OG1	-6.16	100.35	109.60
1	A	104	ASP	N-CA-CB	-6.15	100.84	110.06
1	I	21	GLN	N-CA-CB	5.96	118.97	110.16
2	J	36	ILE	CA-C-O	5.92	122.64	119.15
1	A	231	GLU	CB-CG-CD	5.89	122.62	112.60
2	B	76	GLY	CA-C-O	-5.85	108.51	120.80
1	E	64	GLU	CB-CG-CD	5.85	122.54	112.60
1	I	180	THR	CA-CB-OG1	-5.84	100.85	109.60
1	A	195	ASN	N-CA-CB	5.80	119.31	110.44
2	B	54	ARG	CG-CD-NE	-5.79	99.27	112.00
1	E	155	THR	CA-CB-OG1	-5.76	100.97	109.60
1	E	9	ASN	CA-CB-CG	5.71	118.31	112.60
2	J	74	ARG	CA-C-O	-5.67	115.21	121.33
2	C	13	ILE	CB-CA-C	-5.61	103.06	110.98
1	A	104	ASP	CB-CA-C	-5.61	101.14	110.68
2	N	-1	GLY	CA-C-N	5.57	125.26	119.92
2	N	-1	GLY	C-N-CA	5.57	125.26	119.92
2	H	1	MET	N-CA-C	5.53	117.70	108.02
1	M	104	ASP	CB-CA-C	-5.51	99.77	110.46
2	B	14	THR	CB-CA-C	5.50	119.28	109.38
2	F	34	GLU	CB-CG-CD	5.48	121.91	112.60
1	M	43	GLU	CA-C-O	-5.45	115.29	121.39
2	N	25	ASN	CB-CA-C	5.41	120.04	110.85
2	N	72	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	A	180	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	122	ASN	CB-CA-C	5.33	120.40	111.22
2	N	7	THR	CA-C-O	-5.33	115.65	121.89
1	A	224	LEU	N-CA-CB	5.33	118.51	110.30
1	M	211	ILE	O-C-N	5.28	126.68	121.98
1	M	74	ASN	CA-CB-CG	-5.26	107.34	112.60
1	A	125	GLN	CB-CA-C	-5.26	103.80	112.06
1	E	182	ALA	N-CA-C	-5.26	105.63	111.36
2	F	40	GLN	CB-CG-CD	5.25	121.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASN	CB-CA-C	-5.24	100.59	110.01
1	E	195	ASN	N-CA-CB	-5.21	102.20	110.28
2	C	42	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	M	104	ASP	N-CA-CB	-5.12	102.06	110.14
2	B	72	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	E	194	ASN	CA-C-N	5.10	128.06	120.31
1	E	194	ASN	C-N-CA	5.10	128.06	120.31
1	A	41	LEU	CB-CA-C	5.09	119.78	110.11
1	A	49	GLN	CB-CG-CD	-5.03	104.04	112.60
1	E	74	ASN	CA-CB-CG	-5.01	107.59	112.60
2	H	74	ARG	CB-CA-C	5.00	120.38	110.42

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	LEU	Mainchain
2	B	42	ARG	Mainchain
2	D	73	LEU	Peptide
2	G	74	ARG	Peptide
2	L	70	VAL	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2034	0	2049	74	0
1	E	2029	0	2044	49	0
1	I	2029	0	2044	60	0
1	M	2029	0	2044	64	0
2	B	605	0	632	32	0
2	C	601	0	629	8	0
2	D	602	0	629	19	0
2	F	605	0	632	29	0
2	G	597	0	626	6	0
2	H	601	0	629	19	0
2	J	605	0	632	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	597	0	626	17	0
2	L	602	0	629	8	0
2	N	609	0	635	33	0
2	O	597	0	626	9	0
2	P	606	0	632	17	0
3	A	73	0	0	8	0
3	B	20	0	0	9	0
3	C	14	0	0	3	0
3	D	5	0	0	6	0
3	E	68	0	0	3	0
3	F	31	0	0	6	0
3	G	8	0	0	3	0
3	H	14	0	0	5	0
3	I	61	0	0	4	0
3	J	26	0	0	5	0
3	K	11	0	0	7	0
3	L	7	0	0	2	0
3	M	89	0	0	11	0
3	N	23	0	0	3	0
3	O	10	0	0	5	0
3	P	16	0	0	5	0
All	All	15824	0	15738	364	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 12.

All (364) 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)
2:O:29:LYS:HE2	3:O:108:HOH:O	1.37	1.20
1:A:104:ASP:HB2	3:A:320:HOH:O	1.46	1.12
2:K:40:GLN:NE2	3:K:101:HOH:O	1.83	1.08
2:O:54:ARG:NH1	3:O:101:HOH:O	1.88	1.06
2:L:14:THR:HG23	3:L:106:HOH:O	1.57	1.05
2:N:37:PRO:HG2	2:N:40:GLN:HE21	1.22	1.01
1:A:81:ALA:HB3	1:A:146:MET:HE2	1.41	0.99
2:J:60:ASN:HB3	3:J:120:HOH:O	1.61	0.98
3:B:115:HOH:O	1:M:3:ASN:CB	2.11	0.98
1:A:81:ALA:CB	1:A:146:MET:HE2	1.94	0.96
1:A:221:LEU:HA	1:A:224:LEU:CD1	1.98	0.94
2:F:37:PRO:HG2	2:F:40:GLN:HE21	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ASN:HD21	2:D:42:ARG:NH2	1.67	0.90
1:I:15:THR:HB	2:J:72:ARG:HD3	1.53	0.90
1:I:37:GLN:HE22	2:J:49:GLN:NE2	1.72	0.87
1:M:37:GLN:HE22	2:N:49:GLN:NE2	1.74	0.86
1:M:32:ARG:HD3	1:M:64:GLU:OE1	1.75	0.86
1:M:37:GLN:HE22	2:N:49:GLN:HE21	1.21	0.86
1:E:135:CYS:SG	2:F:76:GLY:C	2.59	0.85
1:A:221:LEU:HA	1:A:224:LEU:HD11	1.59	0.84
1:I:37:GLN:HE22	2:J:49:GLN:HE21	1.23	0.84
1:A:161:GLN:HG2	3:A:356:HOH:O	1.76	0.84
2:H:42:ARG:NH1	2:H:49:GLN:OE1	2.10	0.83
1:A:37:GLN:HE22	2:B:49:GLN:NE2	1.76	0.83
2:C:1:MET:N	3:C:101:HOH:O	2.11	0.83
2:G:45:PHE:HA	3:G:101:HOH:O	1.78	0.81
2:K:32:ASP:HA	3:K:107:HOH:O	1.79	0.81
1:E:37:GLN:HE22	2:F:49:GLN:HE21	1.29	0.81
1:I:247:THR:HG22	1:I:250:VAL:H	1.46	0.81
2:N:63:LYS:O	2:P:72:ARG:NH2	2.13	0.80
1:A:247:THR:HG22	1:A:250:VAL:H	1.45	0.80
2:H:62:GLN:HG2	3:H:105:HOH:O	1.82	0.80
1:M:135:CYS:SG	2:N:76:GLY:O	2.40	0.80
1:M:48:LYS:HD3	3:M:363:HOH:O	1.83	0.79
2:P:75:GLY:N	3:P:101:HOH:O	2.06	0.79
2:B:63:LYS:HG3	3:B:111:HOH:O	1.81	0.78
2:D:42:ARG:NH1	2:D:49:GLN:OE1	2.15	0.78
2:D:58:ASP:OD1	3:D:101:HOH:O	2.00	0.78
2:C:18:GLU:HG3	3:C:113:HOH:O	1.84	0.78
2:F:20:SER:HB3	3:F:127:HOH:O	1.83	0.78
2:F:32:ASP:OD2	3:F:101:HOH:O	2.01	0.78
1:A:37:GLN:HE22	2:B:49:GLN:HE21	1.32	0.77
2:L:14:THR:CG2	3:L:106:HOH:O	2.19	0.75
2:B:63:LYS:O	2:D:72:ARG:NH2	2.20	0.74
2:K:60:ASN:HB2	3:K:106:HOH:O	1.84	0.74
1:E:247:THR:HG22	1:E:250:VAL:H	1.52	0.74
3:A:341:HOH:O	2:C:42:ARG:HD3	1.87	0.74
1:I:16:GLU:OE1	1:I:38:HIS:HD2	1.72	0.73
1:M:153:LEU:HD23	3:M:335:HOH:O	1.89	0.73
2:F:62:GLN:CD	2:H:42:ARG:HH21	1.98	0.71
1:E:144:ILE:O	1:E:148:GLN:NE2	2.24	0.71
2:F:13:ILE:HG21	2:F:34:GLU:HG2	1.73	0.70
2:D:13:ILE:HG21	3:D:103:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:GLU:OE1	1:E:38:HIS:HD2	1.74	0.70
2:B:18:GLU:HG3	2:B:19:PRO:HD2	1.72	0.70
1:I:98:MET:HA	1:I:98:MET:CE	2.21	0.70
3:A:341:HOH:O	2:C:42:ARG:CD	2.39	0.70
2:B:54:ARG:CD	3:B:118:HOH:O	2.40	0.69
1:E:244:LEU:O	1:E:247:THR:HB	1.93	0.69
1:A:244:LEU:O	1:A:247:THR:HB	1.93	0.69
1:E:87:ASN:HD22	1:I:120:LYS:HB3	1.57	0.68
2:J:62:GLN:NE2	2:L:72:ARG:HD3	2.08	0.68
1:E:98:MET:CE	1:E:98:MET:HA	2.23	0.68
2:B:72:ARG:H	2:N:40:GLN:HE22	1.40	0.68
1:A:98:MET:HE3	1:A:98:MET:HA	1.75	0.68
1:A:38:HIS:CD2	2:B:70:VAL:HG11	2.29	0.67
1:I:244:LEU:O	1:I:247:THR:HB	1.93	0.67
2:B:72:ARG:H	2:N:40:GLN:NE2	1.92	0.67
1:A:81:ALA:HB3	1:A:146:MET:CE	2.19	0.67
1:M:62:MET:HE1	2:P:42:ARG:HH22	1.59	0.67
1:A:98:MET:HA	1:A:98:MET:CE	2.25	0.67
2:C:60:ASN:N	2:C:60:ASN:HD22	1.93	0.67
2:B:72:ARG:HD2	3:B:107:HOH:O	1.95	0.66
1:I:98:MET:HA	1:I:98:MET:HE3	1.76	0.66
2:D:18:GLU:OE1	2:K:51:GLU:HB3	1.95	0.66
1:A:38:HIS:CD2	2:B:73:LEU:HD22	2.31	0.66
2:D:13:ILE:CG2	3:D:103:HOH:O	2.42	0.66
2:B:54:ARG:HD3	3:B:118:HOH:O	1.95	0.65
1:M:98:MET:HE3	1:M:98:MET:HA	1.78	0.65
1:A:221:LEU:HA	1:A:224:LEU:HD12	1.77	0.65
2:N:74:ARG:HG2	2:N:74:ARG:HH11	1.62	0.65
1:M:178:MET:HE3	1:M:258:LEU:HD21	1.76	0.65
1:A:16:GLU:OE1	1:A:38:HIS:HD2	1.79	0.65
1:E:98:MET:HA	1:E:98:MET:HE3	1.78	0.64
1:M:98:MET:HA	1:M:98:MET:CE	2.27	0.64
1:I:204:ASP:OD1	2:K:68:HIS:HE1	1.80	0.63
2:N:74:ARG:HH11	2:N:74:ARG:CG	2.11	0.63
2:F:63:LYS:O	2:H:72:ARG:NH2	2.24	0.63
1:M:38:HIS:HE1	1:M:43:GLU:OE2	1.82	0.63
1:I:37:GLN:NE2	2:J:49:GLN:HE21	1.97	0.63
1:M:16:GLU:OE1	1:M:38:HIS:HD2	1.82	0.63
1:A:86:MET:HE3	1:A:86:MET:HA	1.79	0.63
2:F:20:SER:CB	3:F:127:HOH:O	2.41	0.63
1:A:243:MET:O	1:A:246:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:PRO:HG2	2:F:40:GLN:NE2	2.12	0.62
1:M:37:GLN:NE2	2:N:49:GLN:HE21	1.93	0.62
2:B:31:GLN:OE1	1:M:5:GLN:NE2	2.32	0.62
1:E:32:ARG:NH1	1:E:64:GLU:OE2	2.31	0.62
1:M:52:HIS:HD2	3:M:346:HOH:O	1.81	0.62
1:A:15:THR:HB	2:B:72:ARG:HD3	1.80	0.62
1:A:193:ASN:ND2	1:M:178:MET:HE1	2.14	0.62
2:F:62:GLN:CD	2:H:42:ARG:NH2	2.58	0.61
1:E:75:ASN:ND2	2:F:74:ARG:HD3	2.16	0.61
1:M:5:GLN:HA	3:M:384:HOH:O	1.99	0.61
1:A:71:HIS:HE1	2:B:74:ARG:O	1.83	0.61
1:E:198:THR:HB	1:E:232:ASN:HD21	1.65	0.61
1:E:87:ASN:ND2	1:I:120:LYS:HB3	2.15	0.61
2:J:0:GLY:CA	3:J:122:HOH:O	2.49	0.61
1:M:73:GLY:HA2	3:M:331:HOH:O	2.01	0.60
1:I:38:HIS:HE1	1:I:43:GLU:OE1	1.85	0.60
1:A:193:ASN:CG	1:M:178:MET:HE1	2.27	0.60
1:I:198:THR:HB	1:I:232:ASN:ND2	2.17	0.59
1:E:75:ASN:HD21	2:F:74:ARG:HD3	1.66	0.59
1:I:243:MET:O	1:I:246:SER:HB2	2.00	0.59
1:E:37:GLN:HE22	2:F:49:GLN:NE2	1.96	0.59
1:E:198:THR:HB	1:E:232:ASN:ND2	2.17	0.59
1:M:71:HIS:HE1	2:N:74:ARG:O	1.85	0.59
1:M:198:THR:HB	1:M:232:ASN:ND2	2.17	0.59
1:M:198:THR:HB	1:M:232:ASN:HD21	1.68	0.59
1:A:81:ALA:HB2	1:A:146:MET:HE2	1.80	0.59
1:E:71:HIS:HE1	2:F:74:ARG:O	1.86	0.58
1:I:38:HIS:CD2	2:J:70:VAL:HG11	2.38	0.58
1:M:135:CYS:SG	2:N:76:GLY:C	2.86	0.58
1:A:198:THR:HB	1:A:232:ASN:ND2	2.18	0.58
2:N:13:ILE:HG21	2:N:34:GLU:HG2	1.86	0.58
1:A:247:THR:CG2	1:A:250:VAL:H	2.14	0.58
1:I:247:THR:CG2	1:I:250:VAL:H	2.14	0.58
2:B:54:ARG:HD2	3:B:118:HOH:O	2.02	0.57
1:I:198:THR:HB	1:I:232:ASN:HD21	1.68	0.57
2:N:43:LEU:HD13	2:N:50:LEU:HD12	1.84	0.57
1:A:225:LEU:HD11	2:C:44:ILE:HD11	1.86	0.57
2:B:32:ASP:CG	3:B:105:HOH:O	2.47	0.57
1:A:223:ASN:ND2	1:A:249:PHE:H	2.03	0.57
2:N:69:LEU:HG	3:N:113:HOH:O	2.05	0.57
1:A:37:GLN:NE2	2:B:49:GLN:HE21	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:MET:HA	1:A:86:MET:CE	2.32	0.57
2:P:48:LYS:HE2	3:P:112:HOH:O	2.05	0.57
2:B:72:ARG:N	2:N:40:GLN:HE22	2.02	0.57
2:P:6:LYS:HD2	3:P:116:HOH:O	2.04	0.56
1:A:178:MET:HE1	1:M:192:LYS:C	2.30	0.56
1:E:52:HIS:HE1	2:H:71:LEU:O	1.88	0.56
3:M:367:HOH:O	2:N:60:ASN:CB	2.54	0.56
1:A:198:THR:HB	1:A:232:ASN:HD21	1.71	0.56
2:J:43:LEU:HD13	2:J:50:LEU:HD12	1.88	0.56
1:M:122:ASN:C	1:M:122:ASN:HD22	2.12	0.56
1:E:247:THR:CG2	1:E:250:VAL:H	2.19	0.56
2:H:75:GLY:HA2	2:P:74:ARG:HH12	1.71	0.56
1:E:42:ASN:HB3	3:E:313:HOH:O	2.06	0.55
1:M:98:MET:HE2	3:M:366:HOH:O	2.05	0.55
1:A:38:HIS:CD2	2:B:70:VAL:CG1	2.89	0.55
1:A:229:ILE:HG22	1:A:229:ILE:O	2.07	0.55
1:E:185:ALA:O	1:E:189:THR:HG23	2.06	0.55
2:F:43:LEU:HD13	2:F:50:LEU:HD12	1.89	0.55
1:E:147:SER:OG	1:E:148:GLN:NE2	2.39	0.54
2:J:60:ASN:CB	3:J:120:HOH:O	2.34	0.54
2:H:0:GLY:HA3	3:H:111:HOH:O	2.07	0.54
1:I:156:GLU:HA	1:I:156:GLU:OE2	2.08	0.54
2:J:62:GLN:HE22	2:L:72:ARG:HD3	1.72	0.54
1:A:38:HIS:HE1	1:A:43:GLU:OE1	1.90	0.54
2:F:13:ILE:HG21	2:F:34:GLU:CG	2.38	0.54
1:A:93:SER:HB2	1:A:146:MET:HE3	1.90	0.54
1:A:140:VAL:O	1:A:144:ILE:HG12	2.08	0.54
2:H:18:GLU:HB3	3:H:102:HOH:O	2.08	0.53
1:I:16:GLU:HG2	2:J:72:ARG:HG2	1.90	0.53
1:I:38:HIS:CD2	2:J:73:LEU:HD22	2.43	0.53
2:H:25:ASN:HB2	3:H:108:HOH:O	2.09	0.53
1:E:247:THR:HG23	1:E:249:PHE:HB3	1.90	0.53
1:I:247:THR:CG2	1:I:250:VAL:HG23	2.39	0.53
1:E:62:MET:HE3	3:E:352:HOH:O	2.07	0.53
1:M:223:ASN:ND2	1:M:249:PHE:H	2.07	0.53
1:A:221:LEU:O	1:A:224:LEU:HD12	2.09	0.52
2:F:62:GLN:OE1	2:H:42:ARG:NH2	2.42	0.52
2:O:72:ARG:HG2	3:O:103:HOH:O	2.09	0.52
1:E:223:ASN:ND2	1:E:249:PHE:H	2.07	0.52
2:D:13:ILE:HB	3:D:103:HOH:O	2.09	0.52
1:I:17:ASP:O	1:I:21:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:ASN:ND2	1:I:249:PHE:H	2.06	0.52
1:M:38:HIS:CD2	2:N:70:VAL:HG11	2.44	0.52
1:E:45:LEU:HD12	1:E:45:LEU:O	2.10	0.52
1:E:226:ASP:OD2	2:G:42:ARG:NH1	2.31	0.52
2:F:63:LYS:HG3	3:F:109:HOH:O	2.09	0.52
2:B:60:ASN:ND2	2:D:42:ARG:NH2	2.48	0.52
1:M:38:HIS:CD2	2:N:73:LEU:HD22	2.45	0.52
1:M:229:ILE:HG22	1:M:229:ILE:O	2.10	0.52
1:M:140:VAL:O	1:M:144:ILE:HG12	2.10	0.52
1:E:86:MET:HE1	1:I:109:ILE:HG23	1.92	0.52
1:E:38:HIS:HE1	1:E:43:GLU:OE1	1.92	0.52
2:F:74:ARG:HG3	2:F:74:ARG:HH11	1.74	0.52
1:A:123:ASP:CG	1:A:125:GLN:HG3	2.35	0.51
1:I:229:ILE:HG22	1:I:229:ILE:O	2.10	0.51
1:A:229:ILE:N	1:A:229:ILE:HD12	2.24	0.51
1:A:259:ASN:C	1:M:210:LYS:NZ	2.68	0.51
1:A:247:THR:CG2	1:A:250:VAL:HG23	2.41	0.51
1:A:247:THR:HG23	1:A:249:PHE:HB3	1.93	0.51
1:E:225:LEU:HD11	2:G:44:ILE:HD11	1.91	0.51
2:H:75:GLY:HA2	2:P:74:ARG:NH1	2.26	0.51
1:I:93:SER:HB3	1:I:146:MET:HE2	1.92	0.51
1:I:2:ALA:HB2	3:I:344:HOH:O	2.10	0.51
1:I:45:LEU:HD12	1:I:45:LEU:O	2.10	0.51
1:M:60:SER:HB2	2:P:44:ILE:HG13	1.94	0.50
2:K:24:GLU:HG3	2:K:52:ASP:HB3	1.94	0.50
2:F:14:THR:HG22	3:F:125:HOH:O	2.10	0.50
1:I:49:GLN:HE21	2:J:46:ALA:H	1.59	0.50
1:M:49:GLN:HE21	2:N:46:ALA:H	1.59	0.50
2:P:25:ASN:HB2	3:P:106:HOH:O	2.11	0.50
2:H:42:ARG:HH11	2:H:49:GLN:CD	2.18	0.49
1:I:52:HIS:HE1	2:L:71:LEU:O	1.95	0.49
1:I:123:ASP:CG	1:I:125:GLN:HG3	2.37	0.49
1:I:229:ILE:HD12	1:I:229:ILE:N	2.27	0.49
2:P:42:ARG:HH21	2:P:49:GLN:NE2	2.10	0.49
1:A:247:THR:HG21	1:A:250:VAL:HG23	1.95	0.49
1:E:33:ILE:HG12	1:E:65:LYS:HG3	1.93	0.49
1:I:247:THR:HG21	1:I:250:VAL:HG23	1.95	0.49
2:K:40:GLN:CD	3:K:101:HOH:O	2.39	0.49
1:A:16:GLU:OE1	1:A:38:HIS:CD2	2.64	0.49
3:M:367:HOH:O	2:N:60:ASN:HB3	2.13	0.49
1:M:229:ILE:N	1:M:229:ILE:HD12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:HIS:HD2	3:I:335:HOH:O	1.95	0.49
1:A:156:GLU:OE2	1:A:156:GLU:HA	2.12	0.48
2:B:32:ASP:CB	3:B:105:HOH:O	2.60	0.48
1:A:60:SER:HB2	2:D:44:ILE:HG13	1.95	0.48
2:J:0:GLY:HA2	3:J:122:HOH:O	2.12	0.48
3:M:314:HOH:O	2:O:42:ARG:HD3	2.14	0.48
1:E:210:LYS:HD2	3:E:325:HOH:O	2.12	0.48
2:G:75:GLY:C	3:G:103:HOH:O	2.56	0.48
1:M:122:ASN:C	1:M:122:ASN:ND2	2.71	0.48
2:P:24:GLU:HG3	2:P:52:ASP:HB3	1.96	0.48
1:I:60:SER:HB2	2:L:44:ILE:HG13	1.96	0.48
1:I:33:ILE:HG12	1:I:65:LYS:HG3	1.95	0.48
1:I:16:GLU:OE1	1:I:38:HIS:CD2	2.59	0.47
1:I:248:HIS:HD2	3:I:308:HOH:O	1.97	0.47
1:M:52:HIS:HE1	2:P:71:LEU:O	1.97	0.47
1:A:33:ILE:HG12	1:A:65:LYS:HG3	1.96	0.47
1:A:178:MET:HE1	1:M:192:LYS:CA	2.45	0.47
1:I:204:ASP:OD1	2:K:68:HIS:CE1	2.65	0.47
1:E:135:CYS:HG	2:F:76:GLY:C	2.22	0.47
1:E:247:THR:CG2	1:E:250:VAL:HG23	2.45	0.47
1:I:247:THR:HG23	1:I:249:PHE:HB3	1.96	0.47
2:K:60:ASN:CB	3:K:106:HOH:O	2.51	0.47
1:I:2:ALA:CB	3:I:344:HOH:O	2.63	0.47
1:I:38:HIS:CD2	2:J:70:VAL:CG1	2.98	0.47
1:I:135:CYS:SG	2:J:76:GLY:C	2.97	0.47
2:K:54:ARG:HG2	2:K:54:ARG:HH11	1.79	0.47
2:H:14:THR:OG1	3:H:101:HOH:O	2.20	0.47
1:A:259:ASN:C	3:A:312:HOH:O	2.57	0.46
1:A:259:ASN:C	1:M:210:LYS:HZ3	2.23	0.46
2:H:73:LEU:HD22	2:H:74:ARG:N	2.29	0.46
1:A:71:HIS:HD2	1:A:73:GLY:H	1.63	0.46
2:H:73:LEU:HD22	2:H:74:ARG:H	1.80	0.46
2:L:33:LYS:HB2	2:L:33:LYS:HE2	1.67	0.46
1:A:223:ASN:HD22	1:A:249:PHE:H	1.64	0.46
2:H:24:GLU:HG3	2:H:52:ASP:HB3	1.97	0.46
1:M:62:MET:HE1	2:P:42:ARG:NH2	2.28	0.46
1:E:200:GLY:H	1:E:232:ASN:ND2	2.14	0.46
1:I:140:VAL:O	1:I:144:ILE:HG12	2.16	0.46
2:D:33:LYS:HB2	2:D:33:LYS:HE2	1.70	0.46
2:K:42:ARG:HD3	3:K:104:HOH:O	2.16	0.46
2:L:24:GLU:HG3	2:L:52:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:200:GLY:H	1:M:232:ASN:ND2	2.14	0.46
1:A:200:GLY:H	1:A:232:ASN:ND2	2.14	0.46
1:M:98:MET:CE	3:M:366:HOH:O	2.62	0.46
1:A:81:ALA:CB	1:A:146:MET:CE	2.82	0.46
1:E:247:THR:HG21	1:E:250:VAL:HG23	1.97	0.46
1:I:71:HIS:HE1	2:J:74:ARG:O	1.99	0.46
1:M:33:ILE:HG12	1:M:65:LYS:HG3	1.97	0.46
2:N:8:LEU:HD22	3:N:112:HOH:O	2.15	0.46
1:I:45:LEU:HD12	1:I:45:LEU:C	2.41	0.45
1:I:141:ASP:O	1:I:145:LYS:HG3	2.16	0.45
2:N:74:ARG:HG2	2:N:74:ARG:NH1	2.29	0.45
2:P:73:LEU:HB2	3:P:102:HOH:O	2.15	0.45
2:J:0:GLY:HA3	3:J:122:HOH:O	2.14	0.45
1:A:259:ASN:CA	3:A:312:HOH:O	2.64	0.45
2:D:13:ILE:CB	3:D:103:HOH:O	2.61	0.45
1:I:49:GLN:NE2	2:J:46:ALA:H	2.15	0.45
2:B:60:ASN:HD21	2:D:42:ARG:HH22	1.56	0.45
3:M:367:HOH:O	2:N:60:ASN:HB2	2.15	0.45
2:O:29:LYS:CE	3:O:108:HOH:O	2.18	0.45
1:A:46:LEU:HD13	2:B:68:HIS:CD2	2.52	0.45
1:E:183:ALA:HB2	1:E:250:VAL:HG11	1.98	0.45
2:F:11:LYS:HE2	2:P:33:LYS:O	2.17	0.44
1:I:200:GLY:H	1:I:232:ASN:ND2	2.15	0.44
1:M:38:HIS:NE2	2:N:70:VAL:HG13	2.32	0.44
2:N:8:LEU:HD22	3:N:113:HOH:O	2.17	0.44
2:G:1:MET:HA	3:G:108:HOH:O	2.17	0.44
2:K:40:GLN:HE21	2:K:40:GLN:HA	1.83	0.44
1:E:38:HIS:NE2	2:F:70:VAL:HG13	2.33	0.44
2:G:33:LYS:HB2	2:G:33:LYS:HE2	1.70	0.44
1:A:71:HIS:CD2	1:A:73:GLY:H	2.35	0.44
1:A:221:LEU:CA	1:A:224:LEU:HD12	2.46	0.44
1:M:32:ARG:NH2	1:M:62:MET:O	2.50	0.44
1:A:141:ASP:O	1:A:145:LYS:HG3	2.17	0.44
2:F:74:ARG:HG3	2:F:74:ARG:NH1	2.33	0.44
1:M:38:HIS:CD2	2:N:70:VAL:CG1	3.00	0.44
1:M:141:ASP:O	1:M:145:LYS:HG3	2.17	0.44
1:E:123:ASP:OD2	1:E:125:GLN:HG3	2.18	0.44
1:M:40:ALA:HA	1:M:71:HIS:O	2.18	0.44
1:A:41:LEU:HD13	3:A:372:HOH:O	2.18	0.43
2:D:24:GLU:HG3	2:D:52:ASP:HB3	2.00	0.43
1:A:178:MET:CE	1:M:192:LYS:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:341:HOH:O	2:C:42:ARG:HD2	2.11	0.43
2:K:33:LYS:HB2	2:K:33:LYS:HE2	1.75	0.43
2:O:25:ASN:HB3	3:O:108:HOH:O	2.18	0.43
1:E:141:ASP:O	1:E:145:LYS:HG3	2.19	0.43
1:I:59:PHE:HB2	1:I:90:ILE:HD11	2.01	0.43
1:A:195:ASN:OD1	1:M:6:ASP:OD2	2.37	0.43
1:I:71:HIS:CD2	1:I:73:GLY:H	2.36	0.43
1:E:32:ARG:HH12	1:E:64:GLU:CD	2.26	0.43
1:E:71:HIS:HD2	1:E:73:GLY:H	1.67	0.43
1:E:40:ALA:HA	1:E:71:HIS:O	2.19	0.43
1:E:71:HIS:CD2	1:E:73:GLY:H	2.36	0.43
1:A:59:PHE:HB2	1:A:90:ILE:HD11	2.01	0.43
1:I:183:ALA:HB2	1:I:250:VAL:HG11	2.01	0.42
1:M:204:ASP:OD1	2:O:68:HIS:HE1	2.01	0.42
1:M:223:ASN:HD22	1:M:249:PHE:H	1.65	0.42
2:O:40:GLN:HA	2:O:40:GLN:HE21	1.82	0.42
1:I:225:LEU:HD11	2:K:44:ILE:HD11	2.02	0.42
1:I:226:ASP:OD2	2:K:42:ARG:NH1	2.38	0.42
1:M:15:THR:HB	2:N:72:ARG:HD3	2.00	0.42
1:M:38:HIS:O	2:N:47:GLY:HA2	2.20	0.42
2:B:26:VAL:HG21	2:B:56:LEU:HD21	2.01	0.42
1:I:87:ASN:HB3	1:I:89:ASP:HB2	2.01	0.42
1:M:60:SER:OG	1:M:62:MET:HG3	2.19	0.42
1:A:38:HIS:NE2	2:B:70:VAL:HG13	2.35	0.42
2:K:60:ASN:CG	3:K:106:HOH:O	2.62	0.42
1:M:41:LEU:HD12	1:M:72:THR:HA	2.01	0.42
2:O:33:LYS:HB2	2:O:33:LYS:HE2	1.67	0.42
2:P:33:LYS:HB2	2:P:33:LYS:HE2	1.69	0.42
1:A:38:HIS:NE2	2:B:70:VAL:CG1	2.83	0.42
1:A:38:HIS:NE2	2:B:73:LEU:HD22	2.33	0.42
1:A:178:MET:HE1	1:M:192:LYS:HA	2.02	0.42
1:I:38:HIS:NE2	2:J:73:LEU:HD22	2.35	0.42
1:A:183:ALA:HB2	1:A:250:VAL:HG11	2.01	0.42
1:E:38:HIS:CD2	2:F:70:VAL:HG11	2.54	0.42
2:F:33:LYS:HD3	3:F:112:HOH:O	2.19	0.41
1:I:71:HIS:HD2	1:I:73:GLY:H	1.66	0.41
1:M:16:GLU:OE1	1:M:38:HIS:CD2	2.67	0.41
1:M:71:HIS:CD2	1:M:73:GLY:H	2.38	0.41
1:A:200:GLY:H	1:A:232:ASN:HD21	1.67	0.41
1:I:200:GLY:H	1:I:232:ASN:HD21	1.69	0.41
1:M:4:ASP:HB3	1:M:9:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:13:ILE:HG21	2:N:34:GLU:CG	2.49	0.41
2:N:42:ARG:HD2	2:N:70:VAL:HG12	2.02	0.41
1:M:49:GLN:NE2	2:N:46:ALA:H	2.17	0.41
2:C:68:HIS:HD2	3:C:110:HOH:O	2.02	0.41
1:E:255:ASN:O	1:E:259:ASN:ND2	2.53	0.41
1:M:62:MET:CE	2:P:42:ARG:HH22	2.29	0.41
2:D:25:ASN:HD22	2:D:25:ASN:HA	1.57	0.41
2:K:8:LEU:HD23	2:K:8:LEU:HA	1.84	0.41
1:A:52:HIS:HE1	2:D:71:LEU:O	2.03	0.41
1:A:122:ASN:OD1	1:A:122:ASN:O	2.38	0.41
2:B:72:ARG:CD	3:B:107:HOH:O	2.62	0.41
2:D:42:ARG:HH11	2:D:49:GLN:CD	2.25	0.41
2:F:25:ASN:HD22	2:F:25:ASN:HA	1.51	0.41
2:F:62:GLN:NE2	2:H:42:ARG:HH21	2.18	0.41
2:B:2:GLN:HE22	1:I:148:GLN:HE22	1.67	0.41
2:B:62:GLN:NE2	2:D:42:ARG:HH21	2.18	0.40
1:E:112:ILE:HG21	1:E:121:ILE:HD11	2.02	0.40
1:E:124:LEU:O	1:E:125:GLN:C	2.63	0.40
1:A:213:SER:HB2	1:A:215:GLN:HE21	1.86	0.40
1:A:220:LEU:O	1:A:224:LEU:CD1	2.69	0.40
2:D:33:LYS:HG2	3:D:103:HOH:O	2.20	0.40
1:E:45:LEU:HD12	1:E:45:LEU:C	2.46	0.40
1:M:75:ASN:ND2	2:N:74:ARG:HH12	2.19	0.40
2:H:74:ARG:HD3	2:H:74:ARG:O	2.22	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	257/260 (99%)	249 (97%)	6 (2%)	2 (1%)	16 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	256/260 (98%)	251 (98%)	5 (2%)	0	100	100
1	I	256/260 (98%)	250 (98%)	6 (2%)	0	100	100
1	M	256/260 (98%)	251 (98%)	5 (2%)	0	100	100
2	B	75/79 (95%)	75 (100%)	0	0	100	100
2	C	74/79 (94%)	73 (99%)	1 (1%)	0	100	100
2	D	74/79 (94%)	73 (99%)	0	1 (1%)	9	7
2	F	75/79 (95%)	75 (100%)	0	0	100	100
2	G	73/79 (92%)	73 (100%)	0	0	100	100
2	H	74/79 (94%)	73 (99%)	1 (1%)	0	100	100
2	J	75/79 (95%)	75 (100%)	0	0	100	100
2	K	73/79 (92%)	73 (100%)	0	0	100	100
2	L	74/79 (94%)	74 (100%)	0	0	100	100
2	N	76/79 (96%)	76 (100%)	0	0	100	100
2	O	73/79 (92%)	72 (99%)	1 (1%)	0	100	100
2	P	75/79 (95%)	75 (100%)	0	0	100	100
All	All	1916/1988 (96%)	1888 (98%)	25 (1%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	2	ALA
2	D	74	ARG

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	233/235 (99%)	212 (91%)	21 (9%)	9	9
1	E	233/235 (99%)	210 (90%)	23 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	233/235 (99%)	210 (90%)	23 (10%)	7	8
1	M	233/235 (99%)	214 (92%)	19 (8%)	10	12
2	B	68/68 (100%)	58 (85%)	10 (15%)	3	2
2	C	68/68 (100%)	58 (85%)	10 (15%)	3	2
2	D	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	F	68/68 (100%)	54 (79%)	14 (21%)	1	1
2	G	68/68 (100%)	61 (90%)	7 (10%)	7	7
2	H	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	J	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	K	68/68 (100%)	61 (90%)	7 (10%)	7	7
2	L	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	N	68/68 (100%)	55 (81%)	13 (19%)	1	1
2	O	68/68 (100%)	59 (87%)	9 (13%)	4	3
2	P	68/68 (100%)	60 (88%)	8 (12%)	5	5
All	All	1748/1756 (100%)	1548 (89%)	200 (11%)	5	5

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	SER
1	A	41	LEU
1	A	59	PHE
1	A	64	GLU
1	A	65	LYS
1	A	83	LYS
1	A	86	MET
1	A	90	ILE
1	A	98	MET
1	A	101	SER
1	A	122	ASN
1	A	178	MET
1	A	195	ASN
1	A	215	GLN
1	A	219	GLN
1	A	224	LEU
1	A	225	LEU

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Mol	Chain	Res	Type
1	A	246	SER
1	A	247	THR
1	A	256	VAL
2	B	8	LEU
2	B	14	THR
2	B	15	LEU
2	B	33	LYS
2	B	43	LEU
2	B	63	LYS
2	B	64	GLU
2	B	69	LEU
2	B	70	VAL
2	B	73	LEU
2	C	14	THR
2	C	15	LEU
2	C	33	LYS
2	C	51	GLU
2	C	54	ARG
2	C	60	ASN
2	C	63	LYS
2	C	64	GLU
2	C	71	LEU
2	C	73	LEU
2	D	14	THR
2	D	15	LEU
2	D	25	ASN
2	D	33	LYS
2	D	63	LYS
2	D	64	GLU
2	D	71	LEU
2	D	73	LEU
2	D	74	ARG
1	E	5	GLN
1	E	19	ILE
1	E	29	LEU
1	E	34	SER
1	E	44	SER
1	E	45	LEU
1	E	48	LYS
1	E	49	GLN
1	E	59	PHE
1	E	64	GLU

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Mol	Chain	Res	Type
1	E	65	LYS
1	E	98	MET
1	E	104	ASP
1	E	125	GLN
1	E	181	SER
1	E	196	ARG
1	E	215	GLN
1	E	219	GLN
1	E	225	LEU
1	E	230	LYS
1	E	247	THR
1	E	256	VAL
1	E	257	LEU
2	F	6	LYS
2	F	8	LEU
2	F	11	LYS
2	F	14	THR
2	F	15	LEU
2	F	33	LYS
2	F	34	GLU
2	F	43	LEU
2	F	64	GLU
2	F	69	LEU
2	F	70	VAL
2	F	72	ARG
2	F	73	LEU
2	F	74	ARG
2	G	14	THR
2	G	15	LEU
2	G	33	LYS
2	G	40	GLN
2	G	64	GLU
2	G	71	LEU
2	G	73	LEU
2	H	6	LYS
2	H	15	LEU
2	H	38	PRO
2	H	40	GLN
2	H	63	LYS
2	H	64	GLU
2	H	71	LEU
2	H	73	LEU

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Mol	Chain	Res	Type
2	H	74	ARG
1	I	7	LEU
1	I	21	GLN
1	I	32	ARG
1	I	44	SER
1	I	45	LEU
1	I	49	GLN
1	I	59	PHE
1	I	64	GLU
1	I	65	LYS
1	I	83	LYS
1	I	89	ASP
1	I	98	MET
1	I	114	GLU
1	I	120	LYS
1	I	196	ARG
1	I	215	GLN
1	I	219	GLN
1	I	225	LEU
1	I	233	LYS
1	I	242	ARG
1	I	246	SER
1	I	247	THR
1	I	256	VAL
2	J	8	LEU
2	J	15	LEU
2	J	33	LYS
2	J	38	PRO
2	J	43	LEU
2	J	64	GLU
2	J	69	LEU
2	J	70	VAL
2	J	73	LEU
2	K	14	THR
2	K	15	LEU
2	K	33	LYS
2	K	63	LYS
2	K	64	GLU
2	K	71	LEU
2	K	73	LEU
2	L	1	MET
2	L	11	LYS

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Mol	Chain	Res	Type
2	L	14	THR
2	L	15	LEU
2	L	33	LYS
2	L	63	LYS
2	L	64	GLU
2	L	71	LEU
2	L	73	LEU
1	M	5	GLN
1	M	8	SER
1	M	32	ARG
1	M	34	SER
1	M	44	SER
1	M	45	LEU
1	M	49	GLN
1	M	59	PHE
1	M	64	GLU
1	M	65	LYS
1	M	83	LYS
1	M	86	MET
1	M	98	MET
1	M	168	SER
1	M	215	GLN
1	M	219	GLN
1	M	225	LEU
1	M	230	LYS
1	M	256	VAL
2	N	6	LYS
2	N	8	LEU
2	N	11	LYS
2	N	15	LEU
2	N	33	LYS
2	N	34	GLU
2	N	43	LEU
2	N	64	GLU
2	N	69	LEU
2	N	70	VAL
2	N	72	ARG
2	N	73	LEU
2	N	74	ARG
2	O	14	THR
2	O	15	LEU
2	O	24	GLU

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Mol	Chain	Res	Type
2	O	33	LYS
2	O	40	GLN
2	O	63	LYS
2	O	64	GLU
2	O	71	LEU
2	O	73	LEU
2	P	11	LYS
2	P	14	THR
2	P	15	LEU
2	P	33	LYS
2	P	38	PRO
2	P	63	LYS
2	P	64	GLU
2	P	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	38	HIS
1	A	52	HIS
1	A	71	HIS
1	A	75	ASN
1	A	128	GLN
1	A	142	ASN
1	A	215	GLN
1	A	218	GLN
1	A	223	ASN
1	A	232	ASN
2	B	2	GLN
2	B	31	GLN
2	B	49	GLN
2	B	60	ASN
2	B	62	GLN
2	C	2	GLN
2	C	60	ASN
2	C	68	HIS
2	D	2	GLN
2	D	25	ASN
2	D	60	ASN
1	E	5	GLN
1	E	38	HIS

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Mol	Chain	Res	Type
1	E	49	GLN
1	E	52	HIS
1	E	71	HIS
1	E	75	ASN
1	E	87	ASN
1	E	122	ASN
1	E	128	GLN
1	E	142	ASN
1	E	215	GLN
1	E	218	GLN
1	E	232	ASN
1	E	253	GLN
1	E	259	ASN
2	F	2	GLN
2	F	25	ASN
2	F	31	GLN
2	F	40	GLN
2	F	49	GLN
2	F	60	ASN
2	F	68	HIS
2	G	2	GLN
2	G	60	ASN
2	G	68	HIS
2	H	2	GLN
2	H	60	ASN
1	I	5	GLN
1	I	38	HIS
1	I	52	HIS
1	I	71	HIS
1	I	75	ASN
1	I	110	ASN
1	I	122	ASN
1	I	128	GLN
1	I	142	ASN
1	I	215	GLN
1	I	223	ASN
1	I	232	ASN
2	J	2	GLN
2	J	40	GLN
2	J	49	GLN
2	J	62	GLN
2	J	68	HIS

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Mol	Chain	Res	Type
2	K	2	GLN
2	K	40	GLN
2	K	60	ASN
2	K	68	HIS
2	L	2	GLN
2	L	49	GLN
2	L	60	ASN
1	M	5	GLN
1	M	21	GLN
1	M	38	HIS
1	M	49	GLN
1	M	52	HIS
1	M	71	HIS
1	M	75	ASN
1	M	122	ASN
1	M	125	GLN
1	M	128	GLN
1	M	142	ASN
1	M	215	GLN
1	M	218	GLN
1	M	223	ASN
1	M	232	ASN
1	M	252	GLN
2	N	2	GLN
2	N	40	GLN
2	N	49	GLN
2	N	60	ASN
2	N	62	GLN
2	N	68	HIS
2	O	2	GLN
2	O	40	GLN
2	O	60	ASN
2	O	62	GLN
2	O	68	HIS
2	P	2	GLN
2	P	49	GLN
2	P	60	ASN

5.3.3 RNA ⓘ

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	259/260 (99%)	0.42	10 (3%) 43 40	27, 45, 66, 105	0
1	E	258/260 (99%)	0.44	5 (1%) 66 63	27, 46, 66, 80	0
1	I	258/260 (99%)	0.39	7 (2%) 56 53	29, 47, 68, 109	0
1	M	258/260 (99%)	0.34	7 (2%) 56 53	28, 42, 64, 88	0
2	B	77/79 (97%)	0.62	6 (7%) 19 16	27, 46, 68, 81	0
2	C	76/79 (96%)	1.31	11 (14%) 6 4	46, 75, 97, 100	0
2	D	76/79 (96%)	2.16	42 (55%) 0 0	59, 101, 133, 147	0
2	F	77/79 (97%)	0.49	0 100 100	30, 45, 65, 75	0
2	G	75/79 (94%)	2.79	60 (80%) 0 0	79, 117, 136, 145	0
2	H	76/79 (96%)	1.66	22 (28%) 1 1	51, 72, 91, 101	0
2	J	77/79 (97%)	0.41	0 100 100	29, 46, 62, 66	0
2	K	75/79 (94%)	1.75	25 (33%) 1 0	49, 81, 104, 116	0
2	L	76/79 (96%)	2.35	52 (68%) 0 0	58, 101, 135, 151	0
2	N	78/79 (98%)	0.35	3 (3%) 44 41	30, 43, 57, 65	0
2	O	75/79 (94%)	1.93	28 (37%) 1 0	56, 93, 116, 127	0
2	P	77/79 (97%)	1.27	17 (22%) 2 1	35, 64, 96, 112	0
All	All	1948/1988 (97%)	0.88	295 (15%) 5 4	27, 51, 112, 151	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	76	GLY	6.9
1	E	2	ALA	6.0
2	L	53	GLY	5.4
1	M	2	ALA	5.2
2	G	36	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
2	G	50	LEU	4.6
2	L	14	THR	4.4
2	K	13	ILE	4.4
2	G	5	VAL	4.3
2	G	13	ILE	4.3
2	B	0	GLY	4.3
2	G	61	ILE	4.1
2	O	73	LEU	4.0
2	G	14	THR	4.0
2	L	4	PHE	4.0
2	D	61	ILE	4.0
2	G	23	ILE	4.0
2	G	30	ILE	4.0
2	L	15	LEU	3.9
2	G	73	LEU	3.9
2	L	20	SER	3.9
2	D	3	ILE	3.9
2	L	76	GLY	3.9
2	G	67	LEU	3.8
2	H	74	ARG	3.8
2	G	15	LEU	3.8
2	L	50	LEU	3.8
2	G	45	PHE	3.7
2	D	46	ALA	3.7
2	L	13	ILE	3.6
2	D	76	GLY	3.6
2	O	15	LEU	3.6
2	O	36	ILE	3.6
2	G	9	THR	3.6
2	L	12	THR	3.6
2	G	56	LEU	3.5
2	C	14	THR	3.5
2	O	14	THR	3.5
2	K	12	THR	3.5
2	O	44	ILE	3.5
2	H	48	LYS	3.4
2	L	56	LEU	3.4
2	G	17	VAL	3.4
2	G	12	THR	3.4
2	H	75	GLY	3.4
2	D	9	THR	3.4
1	M	3	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	257	LEU	3.3
2	G	69	LEU	3.3
2	O	17	VAL	3.3
2	G	8	LEU	3.3
2	G	44	ILE	3.3
2	G	59	TYR	3.3
1	E	3	ASN	3.2
2	D	13	ILE	3.2
2	G	37	PRO	3.2
2	K	30	ILE	3.2
2	D	75	GLY	3.2
2	G	35	GLY	3.2
2	N	0	GLY	3.2
2	L	59	TYR	3.2
2	D	10	GLY	3.2
2	G	3	ILE	3.2
2	G	4	PHE	3.2
2	G	47	GLY	3.2
2	L	75	GLY	3.2
2	O	35	GLY	3.2
2	G	71	LEU	3.2
2	O	13	ILE	3.2
2	D	15	LEU	3.1
2	L	19	PRO	3.1
2	L	3	ILE	3.1
2	P	48	LYS	3.1
2	G	68	HIS	3.1
2	G	40	GLN	3.1
2	L	51	GLU	3.1
1	A	86	MET	3.1
1	I	86	MET	3.1
2	C	32	ASP	3.1
2	D	48	LYS	3.1
1	A	224	LEU	3.1
1	I	29	LEU	3.1
2	G	28	ALA	3.0
2	D	59	TYR	3.0
2	B	36	ILE	3.0
2	K	14	THR	3.0
2	L	22	THR	3.0
2	K	35	GLY	3.0
2	G	19	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	63	LYS	3.0
2	D	4	PHE	3.0
2	G	70	VAL	3.0
2	O	19	PRO	3.0
2	G	46	ALA	2.9
2	D	50	LEU	2.9
2	L	37	PRO	2.9
2	G	43	LEU	2.9
2	D	55	THR	2.9
2	L	25	ASN	2.9
2	N	-1	GLY	2.9
2	D	67	LEU	2.9
2	L	45	PHE	2.9
2	G	54	ARG	2.9
1	M	161	GLN	2.9
2	D	14	THR	2.9
2	D	25	ASN	2.9
2	G	10	GLY	2.9
2	G	26	VAL	2.9
2	P	0	GLY	2.8
2	D	74	ARG	2.8
2	H	13	ILE	2.8
1	A	4	ASP	2.8
2	L	8	LEU	2.8
2	L	17	VAL	2.8
2	D	42	ARG	2.8
2	C	36	ILE	2.8
2	L	61	ILE	2.8
2	O	12	THR	2.8
2	L	35	GLY	2.8
2	P	75	GLY	2.8
2	K	19	PRO	2.8
2	O	37	PRO	2.8
2	D	45	PHE	2.8
2	G	7	THR	2.7
2	G	39	ASP	2.7
1	E	44	SER	2.7
2	L	9	THR	2.7
2	L	66	THR	2.7
2	D	30	ILE	2.7
2	K	36	ILE	2.7
1	I	258	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	5	VAL	2.7
2	D	62	GLN	2.7
2	D	66	THR	2.7
2	G	22	THR	2.7
2	K	3	ILE	2.7
2	G	6	LYS	2.7
2	O	38	PRO	2.7
2	P	19	PRO	2.7
2	O	32	ASP	2.7
2	H	61	ILE	2.7
2	O	10	GLY	2.7
2	D	60	ASN	2.6
2	O	22	THR	2.6
2	G	53	GLY	2.6
2	H	0	GLY	2.6
2	O	23	ILE	2.6
2	H	63	LYS	2.6
2	G	24	GLU	2.6
2	D	1	MET	2.6
2	C	28	ALA	2.6
1	A	88	ASP	2.6
1	A	1	MET	2.6
2	D	12	THR	2.6
2	P	14	THR	2.6
1	A	83	LYS	2.6
2	P	58	ASP	2.6
2	L	10	GLY	2.6
2	K	17	VAL	2.6
2	D	36	ILE	2.6
2	P	59	TYR	2.6
2	D	20	SER	2.5
2	D	57	SER	2.5
2	L	5	VAL	2.5
2	L	23	ILE	2.5
1	E	29	LEU	2.5
2	H	73	LEU	2.5
2	P	60	ASN	2.5
2	C	76	GLY	2.5
2	G	72	ARG	2.5
2	C	1	MET	2.5
2	L	1	MET	2.5
2	O	1	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	63	LYS	2.5
2	G	25	ASN	2.5
2	O	39	ASP	2.5
2	K	0	GLY	2.5
2	L	31	GLN	2.5
2	D	17	VAL	2.5
2	G	34	GLU	2.5
2	L	36	ILE	2.5
2	O	74	ARG	2.5
2	K	33	LYS	2.5
2	L	33	LYS	2.5
2	G	75	GLY	2.5
2	L	2	GLN	2.5
2	N	76	GLY	2.5
2	H	32	ASP	2.4
2	G	64	GLU	2.4
2	K	15	LEU	2.4
2	L	68	HIS	2.4
2	K	32	ASP	2.4
2	L	74	ARG	2.4
1	I	2	ALA	2.4
2	O	53	GLY	2.4
2	O	61	ILE	2.4
2	G	74	ARG	2.4
2	B	32	ASP	2.4
2	G	32	ASP	2.4
2	H	47	GLY	2.4
2	P	55	THR	2.4
2	H	45	PHE	2.4
2	K	23	ILE	2.4
2	L	26	VAL	2.4
2	O	75	GLY	2.3
2	P	53	GLY	2.3
2	K	22	THR	2.3
2	G	57	SER	2.3
2	G	1	MET	2.3
2	C	61	ILE	2.3
2	K	74	ARG	2.3
2	G	51	GLU	2.3
2	H	64	GLU	2.3
1	I	30	ASP	2.3
2	H	60	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	19	PRO	2.3
2	L	28	ALA	2.3
1	A	8	SER	2.3
2	G	42	ARG	2.3
2	G	11	LYS	2.3
2	G	29	LYS	2.3
2	L	48	LYS	2.3
2	K	37	PRO	2.3
2	G	66	THR	2.3
2	P	54	ARG	2.3
2	L	70	VAL	2.3
2	O	56	LEU	2.3
2	B	39	ASP	2.3
2	L	65	SER	2.3
2	L	62	GLN	2.3
2	P	32	ASP	2.2
2	K	34	GLU	2.2
2	L	11	LYS	2.2
2	O	3	ILE	2.2
2	D	69	LEU	2.2
2	L	32	ASP	2.2
2	H	1	MET	2.2
2	L	46	ALA	2.2
2	L	55	THR	2.2
2	D	65	SER	2.2
1	M	259	ASN	2.2
2	K	53	GLY	2.2
2	K	31	GLN	2.2
2	C	22	THR	2.2
2	D	28	ALA	2.2
2	O	28	ALA	2.2
2	K	56	LEU	2.2
2	L	44	ILE	2.2
2	L	67	LEU	2.2
2	P	1	MET	2.2
2	L	16	GLU	2.2
2	G	62	GLN	2.2
1	M	45	LEU	2.1
2	H	36	ILE	2.1
2	O	30	ILE	2.1
2	G	21	ASP	2.1
2	P	51	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	257	LEU	2.1
2	H	6	LYS	2.1
1	M	255	ASN	2.1
2	C	60	ASN	2.1
1	I	160	GLN	2.1
2	D	49	GLN	2.1
2	D	54	ARG	2.1
2	L	54	ARG	2.1
2	P	22	THR	2.1
2	B	63	LYS	2.1
1	E	253	GLN	2.1
2	C	19	PRO	2.1
2	D	19	PRO	2.1
2	K	26	VAL	2.1
2	L	47	GLY	2.1
1	I	246	SER	2.1
2	H	33	LYS	2.1
2	O	67	LEU	2.1
2	L	21	ASP	2.1
2	D	29	LYS	2.0
1	A	2	ALA	2.0
2	G	49	GLN	2.0
2	D	43	LEU	2.0
2	D	73	LEU	2.0
2	P	56	LEU	2.0
2	H	17	VAL	2.0
2	C	35	GLY	2.0
2	D	53	GLY	2.0
2	K	10	GLY	2.0
2	B	14	THR	2.0
2	H	20	SER	2.0
2	K	20	SER	2.0
2	H	49	GLN	2.0
2	O	40	GLN	2.0
2	K	21	ASP	2.0
2	H	3	ILE	2.0
1	A	230	LYS	2.0
2	G	27	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.