



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:08 PM UTC

PDB ID : 9KQ6 / pdb_00009kq6
Title : The structure of the apo-YcfA from Erwinia amylovora
Authors : Zhang, L.; Dou, C.; Zheng, Y.H.; Zhu, X.F.; Cheng, W.
Deposited on : 2024-11-25
Resolution : 2.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

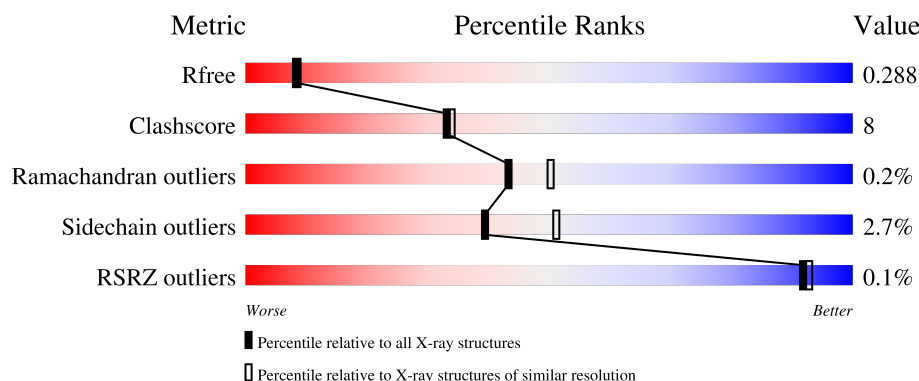
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

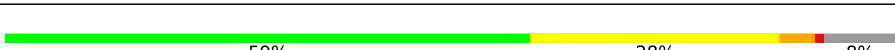
The reported resolution of this entry is 2.34 Å.

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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	234	
1	B	234	
1	C	234	
1	D	234	
1	E	234	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	234	 78%15% • 6%
1	G	234	 78%12% • 7%
1	H	234	 79%14% • •
1	I	234	 76%17% • 6%
1	J	234	 79%12% • 6%
1	K	234	 74%18% • • 6%
1	L	234	 80%14% • 5%
1	M	234	 81%12% • 6%
1	N	234	 80%13% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24736 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 Asparagine synthetase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	222	Total	C	N	O	S	0	0	0
			1750	1115	300	325	10			
1	H	224	Total	C	N	O	S	0	0	0
			1761	1121	303	327	10			
1	D	222	Total	C	N	O	S	0	0	0
			1747	1114	300	323	10			
1	C	222	Total	C	N	O	S	0	0	0
			1750	1115	300	325	10			
1	L	222	Total	C	N	O	S	0	0	0
			1750	1115	300	325	10			
1	A	222	Total	C	N	O	S	0	0	0
			1745	1111	300	324	10			
1	M	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	J	221	Total	C	N	O	S	0	0	0
			1739	1108	299	322	10			
1	F	221	Total	C	N	O	S	0	0	0
			1737	1106	299	322	10			
1	K	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	E	216	Total	C	N	O	S	0	0	0
			1702	1083	293	316	10			
1	I	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	B	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	G	218	Total	C	N	O	S	0	0	0
			1720	1095	295	320	10			

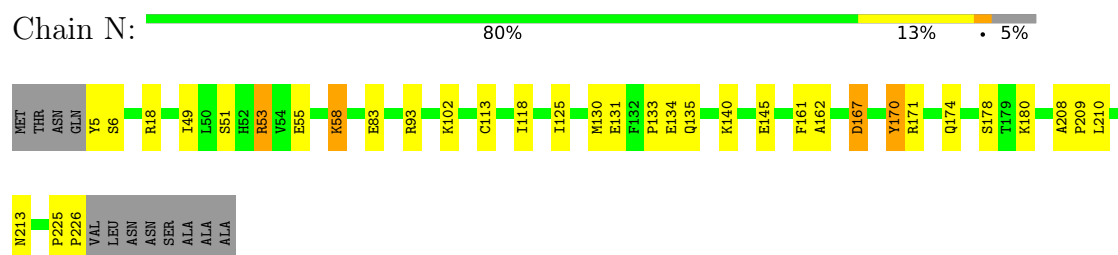
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	32	Total 32	O 32	0	0
2	H	22	Total 22	O 22	0	0
2	D	31	Total 31	O 31	0	0
2	C	32	Total 32	O 32	0	0
2	L	17	Total 17	O 17	0	0
2	A	37	Total 37	O 37	0	0
2	M	32	Total 32	O 32	0	0
2	J	24	Total 24	O 24	0	0
2	F	23	Total 23	O 23	0	0
2	K	10	Total 10	O 10	0	0
2	E	52	Total 52	O 52	0	0
2	I	18	Total 18	O 18	0	0
2	B	30	Total 30	O 30	0	0
2	G	35	Total 35	O 35	0	0

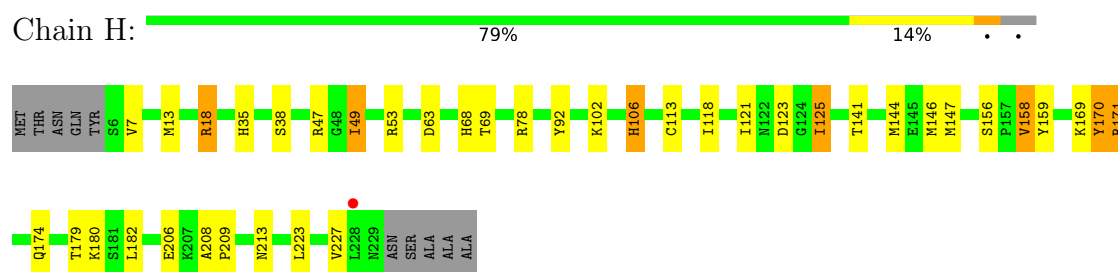
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

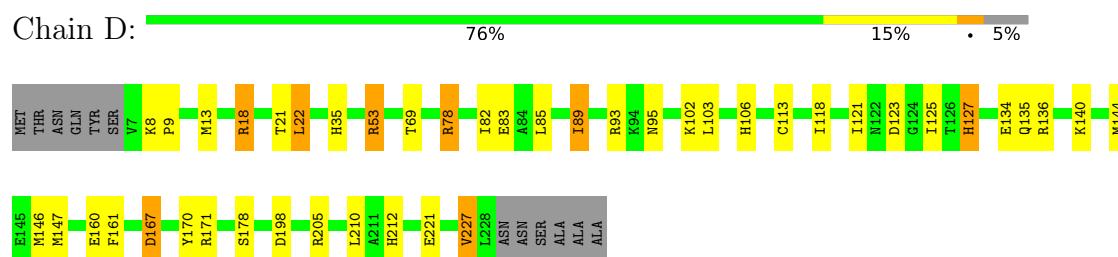
- Molecule 1: Asparagine synthetase domain-containing protein



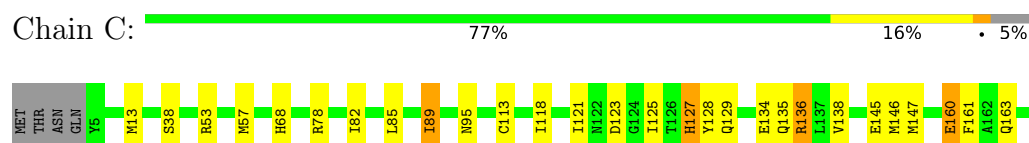
- Molecule 1: Asparagine synthetase domain-containing protein



- Molecule 1: Asparagine synthetase domain-containing protein



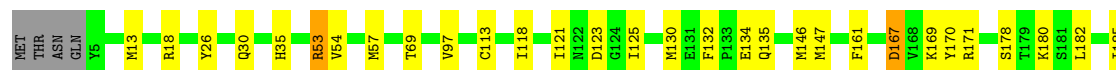
- Molecule 1: Asparagine synthetase domain-containing protein





- Molecule 1: Asparagine synthetase domain-containing protein

Chain L:
80% 14% 5%



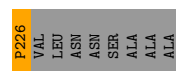
- Molecule 1: Asparagine synthetase domain-containing protein

Chain A:
79% 14% 5%



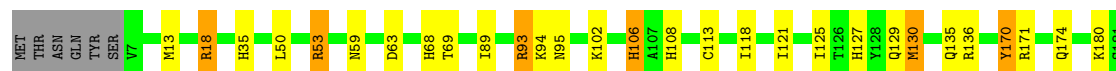
- Molecule 1: Asparagine synthetase domain-containing protein

Chain M:
81% 12% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain J:
79% 12% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain F:
78% 15% 6%





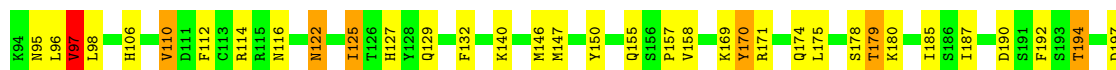
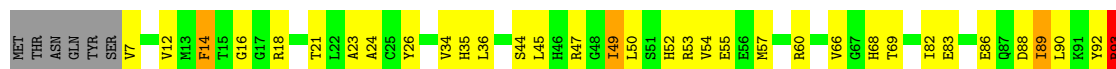
- Molecule 1: Asparagine synthetase domain-containing protein

Chain K: 74% 18% 6%



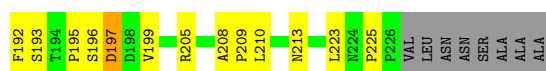
- Molecule 1: Asparagine synthetase domain-containing protein

Chain E: 59% 28% 8%



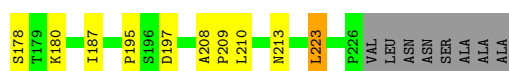
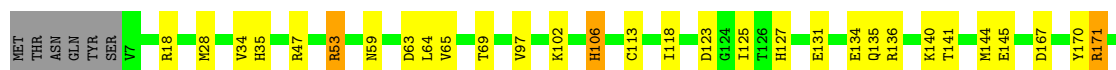
- Molecule 1: Asparagine synthetase domain-containing protein

Chain I: 76% 17% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain B: 77% 15% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

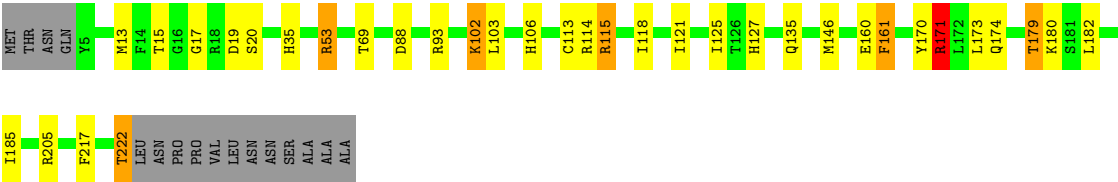
Chain G:

78%

12%

•

7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.76Å 134.92Å 234.27Å 90.00° 98.55° 90.00°	Depositor
Resolution (Å)	48.28 – 2.34 48.28 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.28-2.34) 99.2 (48.28-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.247 , 0.285 0.253 , 0.288	Depositor DCC
R_{free} test set	9081 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.287 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24736	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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	0.92	0/1780	1.27	11/2410 (0.5%)
1	B	0.86	0/1767	1.25	6/2392 (0.3%)
1	C	0.85	0/1786	1.22	6/2418 (0.2%)
1	D	0.83	0/1782	1.25	10/2413 (0.4%)
1	E	0.99	2/1735 (0.1%)	1.66	25/2346 (1.1%)
1	F	0.77	0/1772	1.15	2/2399 (0.1%)
1	G	0.86	0/1754	1.21	7/2372 (0.3%)
1	H	0.75	0/1796	1.16	4/2432 (0.2%)
1	I	0.75	0/1767	1.20	7/2392 (0.3%)
1	J	0.72	0/1774	1.20	9/2402 (0.4%)
1	K	0.72	0/1773	1.14	3/2400 (0.1%)
1	L	0.74	0/1786	1.14	6/2418 (0.2%)
1	M	0.85	0/1773	1.27	5/2400 (0.2%)
1	N	0.90	0/1786	1.26	6/2418 (0.2%)
All	All	0.82	2/24831 (0.0%)	1.25	107/33612 (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	2
1	B	0	2
1	C	0	1
1	D	0	4
1	E	0	1
1	F	0	1
1	G	0	4
1	H	0	1
1	I	0	4
1	J	0	3
1	K	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
1	M	0	2
1	N	0	3
All	All	0	33

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	SER	CA-CB	-5.77	1.44	1.53
1	E	208	ALA	C-O	-5.02	1.20	1.24

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ASP	CA-CB-CG	9.58	122.18	112.60
1	E	197	ASP	CA-CB-CG	9.14	121.74	112.60
1	J	59	ASN	CA-CB-CG	8.67	121.27	112.60
1	B	59	ASN	CA-CB-CG	8.33	120.93	112.60
1	E	194	THR	CA-CB-OG1	-7.61	98.19	109.60
1	F	192	PHE	N-CA-C	-7.52	103.20	112.38
1	A	227	VAL	N-CA-CB	7.37	124.03	111.50
1	C	127	HIS	CA-CB-CG	7.37	121.17	113.80
1	E	88	ASP	CA-CB-CG	7.31	119.91	112.60
1	B	223	LEU	N-CA-C	-7.30	105.30	114.56
1	E	179	THR	CA-CB-OG1	-7.21	98.78	109.60
1	L	223	LEU	N-CA-C	-7.00	104.40	114.12
1	L	30	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	C	167	ASP	CA-CB-CG	6.77	119.37	112.60
1	L	18	ARG	CB-CA-C	-6.67	99.34	110.68
1	H	170	TYR	CB-CA-C	6.64	123.03	109.55
1	D	198	ASP	CA-CB-CG	6.64	119.24	112.60
1	E	26	TYR	CB-CA-C	6.61	122.09	110.85
1	I	145	GLU	CB-CG-CD	6.55	123.73	112.60
1	A	223	LEU	N-CA-C	-6.52	105.90	114.31
1	D	127	HIS	CB-CG-CD2	-6.51	122.74	131.20
1	E	122	ASN	CA-CB-CG	6.39	118.99	112.60
1	E	170	TYR	N-CA-C	-6.29	103.95	111.69
1	N	167	ASP	CA-C-O	-6.27	113.78	120.42
1	E	170	TYR	N-CA-CB	6.25	119.52	110.20
1	G	179	THR	N-CA-C	-6.18	105.69	113.72
1	H	170	TYR	N-CA-CB	-6.16	100.84	110.44
1	E	14	PHE	N-CA-CB	-6.15	100.91	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PRO	CB-CA-C	6.14	119.04	111.12
1	D	227	VAL	N-CA-CB	6.12	120.78	110.56
1	M	170	TYR	CB-CA-C	6.12	122.13	109.95
1	J	127	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	G	102	LYS	CB-CG-CD	6.01	125.12	111.30
1	E	194	THR	OG1-CB-CG2	5.97	121.23	109.30
1	E	26	TYR	N-CA-C	-5.95	104.87	111.36
1	C	194	THR	CA-CB-OG1	-5.94	100.69	109.60
1	E	97	VAL	N-CA-CB	-5.94	101.22	110.54
1	E	90	LEU	N-CA-CB	5.92	118.94	110.06
1	D	167	ASP	CA-CB-CG	5.92	118.52	112.60
1	M	145	GLU	CB-CG-CD	5.91	122.64	112.60
1	B	145	GLU	CB-CG-CD	5.86	122.56	112.60
1	C	145	GLU	CB-CG-CD	5.86	122.55	112.60
1	I	132	PHE	CB-CA-C	5.83	116.35	109.47
1	E	16	GLY	N-CA-C	-5.78	107.35	115.32
1	L	18	ARG	CG-CD-NE	-5.75	99.35	112.00
1	A	106	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	E	110	VAL	N-CA-C	-5.72	104.95	110.72
1	G	19	ASP	CA-CB-CG	5.65	118.25	112.60
1	J	18	ARG	CB-CA-C	-5.64	101.42	110.79
1	N	161	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	18	ARG	CB-CA-C	-5.57	101.20	110.68
1	E	192	PHE	N-CA-CB	-5.56	102.62	111.62
1	B	106	HIS	CB-CG-CD2	-5.54	123.99	131.20
1	D	170	TYR	N-CA-C	-5.54	106.02	112.89
1	G	93	ARG	CB-CA-C	5.54	120.39	111.36
1	E	89	ILE	N-CA-C	-5.51	105.35	110.53
1	F	136	ARG	CG-CD-NE	-5.50	99.89	112.00
1	K	63	ASP	CB-CA-C	-5.49	98.73	110.32
1	E	86	GLU	CB-CA-C	5.49	119.42	110.96
1	H	63	ASP	CB-CA-C	-5.49	98.74	110.32
1	E	98	LEU	N-CA-CB	-5.48	101.85	110.46
1	L	169	LYS	CG-CD-CE	5.47	123.89	111.30
1	N	170	TYR	CB-CA-C	5.44	120.78	109.95
1	J	170	TYR	CB-CA-C	5.44	121.68	110.31
1	B	127	HIS	CA-CB-CG	5.43	119.23	113.80
1	H	106	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	J	129	GLN	CG-CD-NE2	-5.41	108.28	116.40
1	J	106	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	D	170	TYR	CB-CA-C	5.38	121.23	109.99
1	D	83	GLU	CB-CG-CD	-5.37	103.46	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	ARG	N-CA-CB	-5.34	104.44	113.15
1	K	18	ARG	CB-CA-C	-5.32	101.97	110.79
1	D	127	HIS	CB-CG-ND1	5.30	130.65	122.70
1	C	198	ASP	CA-CB-CG	5.28	117.88	112.60
1	I	170	TYR	N-CA-C	-5.26	106.37	112.89
1	E	179	THR	OG1-CB-CG2	5.24	119.78	109.30
1	I	190	ASP	CA-CB-CG	5.22	117.82	112.60
1	G	127	HIS	CB-CG-CD2	5.20	137.95	131.20
1	E	132	PHE	N-CA-CB	5.19	117.89	109.90
1	I	225	PRO	O-C-N	-5.15	115.38	121.46
1	N	83	GLU	CB-CG-CD	-5.15	103.84	112.60
1	M	131	GLU	CG-CD-OE2	-5.15	106.55	118.40
1	D	18	ARG	CA-CB-CG	5.15	124.39	114.10
1	J	63	ASP	CB-CA-C	-5.14	99.48	110.32
1	J	170	TYR	N-CA-CB	-5.14	101.86	110.39
1	C	163	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	170	TYR	N-CA-C	-5.12	106.54	112.89
1	A	180	LYS	CB-CG-CD	5.12	123.06	111.30
1	K	141	THR	OG1-CB-CG2	5.11	119.53	109.30
1	M	185	ILE	N-CA-CB	-5.11	104.86	110.99
1	I	128	TYR	CA-C-N	-5.10	115.58	123.17
1	I	128	TYR	C-N-CA	-5.10	115.58	123.17
1	N	135	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	L	167	ASP	CA-CB-CG	5.09	117.69	112.60
1	E	125	ILE	O-C-N	5.08	127.86	122.62
1	N	145	GLU	CB-CG-CD	5.08	121.23	112.60
1	G	88	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	136	ARG	CG-CD-NE	-5.06	100.87	112.00
1	A	136	ARG	CG-CD-NE	-5.06	100.88	112.00
1	A	106	HIS	CB-CG-ND1	5.04	130.27	122.70
1	A	145	GLU	CB-CG-CD	5.03	121.16	112.60
1	B	106	HIS	CB-CG-ND1	5.03	130.25	122.70
1	E	158	VAL	CA-C-N	5.01	126.96	120.44
1	E	158	VAL	C-N-CA	5.01	126.96	120.44
1	M	167	ASP	CA-C-O	-5.01	115.24	120.55
1	J	127	HIS	CB-CG-ND1	5.01	130.21	122.70
1	G	171	ARG	N-CA-C	-5.00	106.68	112.89

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	18	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	18	ARG	Sidechain
1	C	136	ARG	Sidechain
1	D	18	ARG	Sidechain
1	D	205	ARG	Sidechain
1	D	78	ARG	Sidechain
1	D	93	ARG	Sidechain
1	E	205	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	114	ARG	Sidechain
1	G	115	ARG	Sidechain
1	G	171	ARG	Sidechain
1	G	205	ARG	Sidechain
1	H	18	ARG	Sidechain
1	I	171	ARG	Sidechain
1	I	205	ARG	Sidechain
1	I	78	ARG	Sidechain
1	I	93	ARG	Sidechain
1	J	171	ARG	Sidechain
1	J	18	ARG	Sidechain
1	J	93	ARG	Sidechain
1	K	171	ARG	Sidechain
1	K	18	ARG	Sidechain
1	K	93	ARG	Sidechain
1	L	171	ARG	Sidechain
1	L	205	ARG	Sidechain
1	M	115	ARG	Sidechain
1	M	171	ARG	Sidechain
1	N	171	ARG	Sidechain
1	N	18	ARG	Sidechain
1	N	93	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1745	0	1742	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1732	0	1728	32	0
1	C	1750	0	1742	30	1
1	D	1747	0	1748	25	0
1	E	1702	0	1697	41	1
1	F	1737	0	1730	36	0
1	G	1720	0	1711	23	0
1	H	1761	0	1759	32	0
1	I	1732	0	1728	23	0
1	J	1739	0	1737	26	0
1	K	1738	0	1733	58	0
1	L	1750	0	1742	19	0
1	M	1738	0	1733	22	0
1	N	1750	0	1742	19	0
2	A	37	0	0	1	0
2	B	30	0	0	3	0
2	C	32	0	0	0	0
2	D	31	0	0	1	0
2	E	52	0	0	4	0
2	F	23	0	0	1	0
2	G	35	0	0	0	0
2	H	22	0	0	2	0
2	I	18	0	0	1	0
2	J	24	0	0	2	0
2	K	10	0	0	0	0
2	L	17	0	0	0	0
2	M	32	0	0	0	0
2	N	32	0	0	1	0
All	All	24736	0	24272	379	1

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 (379) 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:B:141:THR:HA	1:B:144:MET:HE3	1.31	1.12
1:K:28:MET:HE3	1:K:34:VAL:CG2	1.80	1.10
1:K:28:MET:CE	1:K:34:VAL:HG22	1.82	1.08
1:M:28:MET:CE	1:M:34:VAL:HG22	1.85	1.06
1:B:28:MET:CE	1:B:34:VAL:HG22	1.87	1.04
1:M:28:MET:HE3	1:M:34:VAL:CG2	1.88	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:MET:HE3	1:B:34:VAL:CG2	1.92	1.00
1:B:28:MET:HE3	1:B:34:VAL:HG22	0.98	0.98
1:J:89:ILE:HD11	1:J:95:ASN:HA	1.49	0.92
1:K:28:MET:HE3	1:K:34:VAL:HG22	0.96	0.91
1:M:28:MET:HE3	1:M:34:VAL:HG22	0.94	0.91
1:K:28:MET:HE1	1:K:65:VAL:HG22	1.53	0.89
1:G:15:THR:HG23	1:G:17:GLY:H	1.36	0.88
1:D:8:LYS:HD2	1:D:9:PRO:HD2	1.56	0.87
1:K:161:PHE:CE2	1:K:162:ALA:HB2	2.10	0.86
1:H:141:THR:HA	1:H:144:MET:HE3	1.59	0.84
1:A:125:ILE:HG22	1:A:135:GLN:HG2	1.60	0.82
1:E:106:HIS:HB3	1:E:147:MET:HE3	1.62	0.81
1:K:26:TYR:CD1	1:I:223:LEU:HD13	2.15	0.81
1:B:125:ILE:HG22	1:B:135:GLN:HG2	1.62	0.81
1:J:89:ILE:CD1	1:J:95:ASN:HA	2.10	0.80
1:M:28:MET:HE1	1:M:65:VAL:HG22	1.62	0.80
1:F:65:VAL:CG1	1:F:65:VAL:O	2.29	0.80
1:H:123:ASP:OD1	1:H:125:ILE:HG22	1.81	0.80
1:B:28:MET:HE1	1:B:65:VAL:HG22	1.63	0.80
1:B:141:THR:HA	1:B:144:MET:CE	2.11	0.80
1:J:89:ILE:HD13	1:J:94:LYS:O	1.82	0.79
1:H:213:ASN:HD21	1:F:171:ARG:HH22	1.26	0.79
1:F:65:VAL:O	1:F:65:VAL:HG13	1.84	0.77
1:F:190:ASP:C	1:F:192:PHE:H	1.93	0.77
1:K:161:PHE:CD2	1:K:162:ALA:HB2	2.19	0.77
1:K:53:ARG:HG3	1:K:57:MET:HE1	1.68	0.76
1:M:26:TYR:HE1	1:G:222:THR:HG23	1.50	0.76
1:F:141:THR:HA	1:F:144:MET:HE3	1.69	0.75
1:C:213:ASN:HD21	1:E:171:ARG:HH22	1.32	0.75
1:K:201:LEU:HG	1:K:205:ARG:NH1	2.01	0.75
1:D:8:LYS:HD2	1:D:9:PRO:CD	2.17	0.74
1:K:201:LEU:HD21	1:K:205:ARG:HH12	1.51	0.74
1:H:141:THR:HA	1:H:144:MET:CE	2.18	0.73
1:D:140:LYS:HE2	1:D:144:MET:HE2	1.69	0.73
1:A:148:ALA:HB3	2:A:301:HOH:O	1.87	0.73
1:H:47:ARG:HD3	2:H:316:HOH:O	1.89	0.72
1:D:171:ARG:HH22	1:B:213:ASN:HD21	1.34	0.72
1:K:53:ARG:HG3	1:K:57:MET:CE	2.19	0.72
1:D:22:LEU:HD11	1:B:223:LEU:HD21	1.72	0.72
1:E:35:HIS:HE1	1:E:69:THR:OG1	1.73	0.71
1:K:162:ALA:O	1:K:163:GLN:HB2	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:TYR:O	1:K:151:ASP:OD1	2.07	0.71
1:N:131:GLU:O	1:N:133:PRO:HD3	1.90	0.71
1:F:94:LYS:NZ	1:F:193:SER:O	2.21	0.71
1:B:47:ARG:HG3	2:B:324:HOH:O	1.91	0.70
1:E:169:LYS:NZ	2:E:301:HOH:O	2.23	0.70
1:G:173:LEU:HG	1:G:179:THR:CG2	2.21	0.70
1:M:131:GLU:O	1:M:133:PRO:HD3	1.93	0.69
1:L:213:ASN:HD21	1:A:171:ARG:HH22	1.40	0.68
1:G:102:LYS:HD2	1:G:106:HIS:CD2	2.29	0.68
1:K:28:MET:HE2	1:K:64:LEU:O	1.94	0.68
1:H:38:SER:OG	1:H:68:HIS:HE1	1.76	0.68
1:F:58:LYS:HG2	1:F:65:VAL:HG11	1.75	0.68
1:E:146:MET:HE2	1:E:147:MET:CE	2.24	0.67
1:K:87:GLN:O	1:K:91:LYS:HG2	1.94	0.67
1:K:127:HIS:ND1	1:K:163:GLN:HG3	2.09	0.66
1:K:94:LYS:HG2	1:K:195:PRO:HB3	1.77	0.66
1:K:201:LEU:CD2	1:K:205:ARG:HH12	2.08	0.66
1:I:191:SER:C	1:I:193:SER:H	2.04	0.65
1:K:201:LEU:CG	1:K:205:ARG:HH12	2.09	0.65
1:F:128:TYR:HE1	1:F:129:GLN:HE21	1.41	0.65
1:C:213:ASN:ND2	1:E:171:ARG:HH22	1.94	0.65
1:B:28:MET:HE2	1:B:64:LEU:C	2.20	0.65
1:J:50:LEU:HD21	1:J:68:HIS:HE1	1.62	0.65
1:E:23:ALA:HB1	1:E:157:PRO:HG2	1.78	0.65
1:C:125:ILE:HG22	1:C:135:GLN:HG2	1.79	0.65
1:H:213:ASN:ND2	1:F:171:ARG:HH22	1.95	0.65
1:J:53:ARG:NH2	1:J:180:LYS:O	2.30	0.64
1:K:162:ALA:HB1	1:K:167:ASP:HB2	1.78	0.64
1:L:53:ARG:NH2	1:L:180:LYS:O	2.30	0.64
1:M:28:MET:HE2	1:M:64:LEU:C	2.23	0.64
1:I:38:SER:OG	1:I:68:HIS:HE1	1.80	0.63
1:N:210:LEU:HD23	1:N:226:PRO:HG3	1.80	0.63
1:K:28:MET:HE1	1:K:65:VAL:CG2	2.25	0.63
1:N:53:ARG:NH2	1:N:180:LYS:O	2.31	0.63
1:H:158:VAL:CG1	1:H:158:VAL:O	2.46	0.63
1:D:21:THR:HG21	1:D:53:ARG:HE	1.64	0.62
1:B:131:GLU:HG2	2:B:303:HOH:O	1.98	0.62
1:B:28:MET:HG2	1:B:64:LEU:HB3	1.82	0.62
1:N:125:ILE:HD12	1:N:140:LYS:HE3	1.82	0.61
1:C:169:LYS:O	1:C:179:THR:HG22	1.99	0.61
1:K:201:LEU:CG	1:K:205:ARG:NH1	2.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:161:PHE:O	1:K:162:ALA:HB3	2.00	0.60
1:M:53:ARG:NH2	1:M:180:LYS:O	2.33	0.60
1:B:140:LYS:HG2	1:B:144:MET:HE2	1.84	0.60
1:C:146:MET:HE2	1:C:147:MET:HE1	1.82	0.60
1:E:96:LEU:HD11	1:E:199:VAL:CG1	2.32	0.60
1:E:14:PHE:HZ	1:E:53:ARG:HG3	1.67	0.60
1:F:192:PHE:O	1:F:193:SER:C	2.43	0.59
1:K:53:ARG:NH2	1:K:180:LYS:O	2.33	0.59
1:K:53:ARG:O	1:K:57:MET:HE3	2.02	0.59
1:M:28:MET:HG2	1:M:64:LEU:HB3	1.85	0.59
1:G:53:ARG:NH2	1:G:180:LYS:O	2.32	0.59
1:F:190:ASP:O	1:F:192:PHE:N	2.35	0.59
1:K:28:MET:HE2	1:K:64:LEU:C	2.28	0.59
1:G:53:ARG:NH1	1:G:182:LEU:HD12	2.18	0.59
1:F:140:LYS:HG2	1:F:144:MET:HE2	1.83	0.59
1:E:150:TYR:HH	1:E:212:HIS:HD1	1.51	0.58
1:I:196:SER:O	1:I:197:ASP:C	2.47	0.58
1:J:50:LEU:HD21	1:J:68:HIS:CE1	2.38	0.58
1:J:130:MET:O	1:J:136:ARG:HG2	2.03	0.58
1:K:141:THR:HA	1:K:144:MET:HE3	1.84	0.58
1:M:167:ASP:O	1:M:171:ARG:HG2	2.03	0.58
1:K:140:LYS:HG2	1:K:144:MET:HE2	1.85	0.58
1:N:102:LYS:HD3	1:N:134:GLU:CB	2.33	0.58
1:B:53:ARG:NH2	1:B:180:LYS:O	2.33	0.58
1:K:201:LEU:HD21	1:K:205:ARG:NH1	2.18	0.58
1:H:125:ILE:HG12	1:H:159:TYR:CD1	2.38	0.58
1:C:38:SER:OG	1:C:68:HIS:HE1	1.86	0.57
1:M:13:MET:HE1	1:M:154:TYR:CE1	2.39	0.57
1:J:89:ILE:HD13	1:J:94:LYS:C	2.28	0.57
1:C:136:ARG:HH22	1:C:195:PRO:HD2	1.68	0.57
1:N:140:LYS:NZ	2:N:302:HOH:O	2.37	0.57
1:C:85:LEU:O	1:C:89:ILE:HG12	2.04	0.57
1:H:146:MET:HE2	1:H:147:MET:HE1	1.86	0.57
1:J:108:HIS:HE1	2:J:310:HOH:O	1.88	0.57
1:A:53:ARG:NH2	1:A:180:LYS:O	2.34	0.57
1:K:28:MET:CE	1:K:65:VAL:HA	2.35	0.57
1:B:136:ARG:NH1	1:B:195:PRO:O	2.35	0.56
1:K:53:ARG:HD2	1:K:57:MET:HE2	1.87	0.56
1:E:34:VAL:CG1	1:E:36:LEU:HD23	2.35	0.56
1:J:210:LEU:HD12	1:J:210:LEU:H	1.70	0.56
1:M:28:MET:HE1	1:M:65:VAL:CG2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:89:ILE:CD1	1:J:95:ASN:CA	2.83	0.56
1:H:53:ARG:NH2	1:H:180:LYS:O	2.36	0.56
1:F:129:GLN:HB3	1:F:135:GLN:OE1	2.06	0.55
1:E:34:VAL:HG12	1:E:36:LEU:HD23	1.88	0.55
1:G:102:LYS:HD2	1:G:106:HIS:HD2	1.72	0.55
1:H:123:ASP:CG	1:H:125:ILE:HG22	2.32	0.55
1:C:171:ARG:HH22	1:A:213:ASN:HD21	1.54	0.55
1:L:54:VAL:HA	1:L:57:MET:HE2	1.89	0.55
1:C:170:TYR:O	1:C:174:GLN:HG3	2.07	0.55
1:D:85:LEU:O	1:D:89:ILE:HG12	2.06	0.54
1:N:102:LYS:HD3	1:N:134:GLU:HG3	1.88	0.54
1:A:35:HIS:HE1	1:A:69:THR:OG1	1.90	0.54
1:N:225:PRO:HD3	2:H:318:HOH:O	2.06	0.54
1:C:128:TYR:HE1	1:C:129:GLN:HE21	1.50	0.53
1:K:167:ASP:HA	1:K:170:TYR:CE2	2.42	0.53
1:L:125:ILE:HG22	1:L:135:GLN:HG2	1.91	0.53
1:F:137:LEU:C	1:F:137:LEU:HD23	2.33	0.53
1:C:53:ARG:NH2	1:C:180:LYS:O	2.35	0.53
1:B:210:LEU:HB2	2:B:323:HOH:O	2.09	0.53
1:G:35:HIS:HE1	1:G:69:THR:OG1	1.92	0.53
1:K:161:PHE:HB3	1:I:223:LEU:HD23	1.90	0.53
1:K:162:ALA:C	1:K:167:ASP:OD2	2.52	0.53
1:K:201:LEU:CD2	1:K:205:ARG:NH1	2.71	0.53
1:F:191:SER:C	1:F:193:SER:N	2.67	0.52
1:K:205:ARG:HG3	1:K:205:ARG:HH11	1.72	0.52
1:D:171:ARG:HH22	1:B:213:ASN:ND2	2.03	0.52
1:H:169:LYS:O	1:H:179:THR:HG22	2.09	0.52
1:B:28:MET:HE1	1:B:65:VAL:CG2	2.36	0.52
1:C:160:GLU:CD	1:C:160:GLU:C	2.77	0.52
1:I:196:SER:O	1:I:199:VAL:N	2.42	0.52
1:K:18:ARG:NH2	1:K:179:THR:O	2.42	0.52
1:E:12:VAL:HG22	1:E:122:ASN:HB2	1.91	0.52
1:C:160:GLU:OE2	1:C:161:PHE:HA	2.10	0.52
1:L:26:TYR:CE1	1:F:223:LEU:HG	2.45	0.52
1:K:28:MET:HE1	1:K:65:VAL:HA	1.92	0.52
1:D:106:HIS:HB3	1:D:147:MET:HE3	1.92	0.51
1:K:201:LEU:HG	1:K:205:ARG:HH11	1.73	0.51
1:H:125:ILE:CG2	1:H:156:SER:OG	2.58	0.51
1:D:134:GLU:HG2	1:D:135:GLN:HG3	1.91	0.51
1:L:123:ASP:OD1	1:L:125:ILE:HG12	2.10	0.51
1:B:123:ASP:OD1	1:B:125:ILE:HG12	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:134:GLU:HG2	1:L:135:GLN:HG3	1.92	0.51
1:K:213:ASN:HD21	1:B:171:ARG:HH12	1.58	0.51
1:A:123:ASP:OD1	1:A:125:ILE:HG12	2.11	0.51
1:M:146:MET:HE3	1:M:147:MET:HE3	1.93	0.51
1:F:194:THR:N	1:F:195:PRO:HD3	2.25	0.51
1:N:49:ILE:HD12	1:N:49:ILE:H	1.76	0.50
1:D:89:ILE:HD13	1:D:95:ASN:HA	1.93	0.50
1:G:113:CYS:HB3	1:G:118:ILE:O	2.10	0.50
1:A:77:PHE:CZ	1:A:97:VAL:HG13	2.46	0.50
1:E:106:HIS:HB3	1:E:147:MET:CE	2.37	0.50
1:B:102:LYS:NZ	1:B:106:HIS:HE1	2.10	0.50
1:K:26:TYR:CE1	1:I:223:LEU:HD13	2.45	0.50
1:B:35:HIS:HE1	1:B:69:THR:OG1	1.94	0.50
1:G:217:PHE:HD1	1:G:222:THR:HG21	1.75	0.50
1:L:146:MET:HE2	1:L:147:MET:HE1	1.94	0.50
1:E:208:ALA:HB3	1:E:209:PRO:HD3	1.94	0.50
1:I:133:PRO:HG3	1:I:195:PRO:HG3	1.93	0.50
1:J:125:ILE:HD12	1:J:135:GLN:HA	1.94	0.49
1:K:14:PHE:CZ	1:K:57:MET:HE1	2.47	0.49
1:F:192:PHE:O	1:F:194:THR:HG23	2.13	0.49
1:G:161:PHE:CD1	1:G:161:PHE:C	2.91	0.49
1:E:12:VAL:HG11	1:E:24:ALA:HB2	1.93	0.49
1:D:123:ASP:OD1	1:D:125:ILE:HG12	2.12	0.49
1:A:145:GLU:CD	1:A:149:GLN:HE21	2.20	0.49
1:J:125:ILE:HD12	1:J:135:GLN:HG2	1.93	0.49
1:D:140:LYS:CE	1:D:144:MET:HE2	2.41	0.49
1:E:114:ARG:NH2	2:E:309:HOH:O	2.46	0.49
1:G:125:ILE:HG23	1:G:135:GLN:HB3	1.95	0.49
1:F:190:ASP:C	1:F:192:PHE:N	2.58	0.49
1:N:102:LYS:HD3	1:N:134:GLU:HB2	1.94	0.48
1:H:78:ARG:HD3	1:F:173:LEU:HD21	1.95	0.48
1:J:207:LYS:HA	1:J:210:LEU:HD13	1.95	0.48
1:E:54:VAL:HA	1:E:57:MET:HE2	1.93	0.48
1:I:53:ARG:NH2	1:I:180:LYS:O	2.38	0.48
1:C:113:CYS:HB3	1:C:118:ILE:O	2.14	0.48
1:A:79:SER:O	1:A:210:LEU:HD21	2.13	0.48
1:N:113:CYS:HB3	1:N:118:ILE:O	2.14	0.48
1:C:123:ASP:OD1	1:C:125:ILE:HG12	2.12	0.48
1:J:108:HIS:CE1	2:J:310:HOH:O	2.64	0.48
1:I:94:LYS:HD2	1:I:193:SER:OG	2.14	0.48
1:H:125:ILE:HG12	1:H:159:TYR:HD1	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:MET:HE2	1:D:212:HIS:CE1	2.48	0.48
1:K:127:HIS:O	1:K:130:MET:HG3	2.14	0.48
1:N:170:TYR:O	1:N:174:GLN:HG3	2.13	0.48
1:J:102:LYS:NZ	1:J:106:HIS:HE1	2.11	0.48
1:G:15:THR:HG23	1:G:17:GLY:N	2.17	0.47
1:G:173:LEU:HG	1:G:179:THR:HG21	1.95	0.47
1:A:102:LYS:NZ	1:A:106:HIS:HE1	2.12	0.47
1:M:113:CYS:HB3	1:M:118:ILE:O	2.13	0.47
1:K:150:TYR:O	1:K:151:ASP:CG	2.58	0.47
1:E:52:HIS:HE1	2:E:307:HOH:O	1.96	0.47
1:I:191:SER:C	1:I:193:SER:N	2.70	0.47
1:H:102:LYS:NZ	1:H:106:HIS:HE1	2.12	0.47
1:C:13:MET:HE2	1:C:121:ILE:HD12	1.96	0.47
1:A:134:GLU:HG2	1:A:135:GLN:HG3	1.96	0.47
1:F:45:LEU:HD11	1:F:187:ILE:HD13	1.97	0.47
1:K:171:ARG:NH2	1:I:213:ASN:HD21	2.13	0.47
1:E:220:GLY:C	1:E:221:GLU:HG2	2.40	0.47
1:H:170:TYR:O	1:H:174:GLN:HG3	2.14	0.47
1:A:113:CYS:HB3	1:A:118:ILE:O	2.15	0.46
1:K:185:ILE:HD11	1:K:189:ALA:CB	2.45	0.46
1:I:167:ASP:HA	1:I:170:TYR:CE2	2.49	0.46
1:H:35:HIS:HE1	1:H:69:THR:OG1	1.99	0.46
1:E:125:ILE:HD11	1:E:140:LYS:HD2	1.96	0.46
1:F:113:CYS:HB3	1:F:118:ILE:O	2.16	0.46
1:F:192:PHE:O	1:F:194:THR:N	2.49	0.46
1:L:167:ASP:HA	1:L:170:TYR:CE2	2.50	0.46
1:D:102:LYS:NZ	1:D:106:HIS:HE1	2.13	0.46
1:D:221:GLU:OE2	2:D:301:HOH:O	2.21	0.46
1:E:35:HIS:CE1	1:E:69:THR:OG1	2.62	0.46
1:E:45:LEU:HD11	1:E:187:ILE:HG13	1.96	0.46
1:A:77:PHE:HZ	1:A:97:VAL:HG13	1.81	0.46
1:F:65:VAL:O	1:F:65:VAL:HG12	2.15	0.46
1:E:95:ASN:OD1	1:E:97:VAL:HB	2.15	0.46
1:C:89:ILE:HD13	1:C:95:ASN:HA	1.97	0.46
1:F:167:ASP:HA	1:F:170:TYR:CE2	2.51	0.46
1:B:134:GLU:HG2	1:B:135:GLN:HG3	1.97	0.46
1:N:210:LEU:CD2	1:N:226:PRO:HG3	2.43	0.46
1:A:28:MET:HG2	1:A:64:LEU:HB3	1.98	0.46
1:K:161:PHE:O	1:K:162:ALA:CB	2.62	0.46
1:H:113:CYS:HB3	1:H:118:ILE:O	2.15	0.46
1:D:146:MET:HG2	1:D:147:MET:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:CYS:HB3	1:K:118:ILE:O	2.15	0.46
1:K:158:VAL:HG23	1:I:223:LEU:HD21	1.97	0.46
1:I:121:ILE:HD13	1:I:147:MET:HE2	1.98	0.46
1:C:213:ASN:HD21	1:E:171:ARG:NH2	2.06	0.45
1:E:60:ARG:HD3	1:E:175:LEU:O	2.16	0.45
1:I:13:MET:HE2	1:I:121:ILE:HD12	1.97	0.45
1:I:113:CYS:HB3	1:I:118:ILE:O	2.16	0.45
1:L:113:CYS:HB3	1:L:118:ILE:O	2.16	0.45
1:J:113:CYS:HB3	1:J:118:ILE:O	2.16	0.45
1:H:146:MET:HE2	1:H:147:MET:CE	2.47	0.45
1:H:158:VAL:O	1:H:158:VAL:HG13	2.15	0.45
1:D:13:MET:HE2	1:D:121:ILE:HD12	1.97	0.45
1:L:130:MET:C	1:L:132:PHE:H	2.24	0.45
1:D:113:CYS:HB3	1:D:118:ILE:O	2.16	0.45
1:M:208:ALA:HB3	1:M:209:PRO:HD3	1.98	0.45
1:E:92:TYR:O	1:E:93:ARG:HB2	2.15	0.45
1:L:53:ARG:NH1	1:L:182:LEU:HD12	2.32	0.45
1:J:136:ARG:HH22	1:J:194:THR:HG22	1.82	0.45
1:K:13:MET:HE2	1:K:121:ILE:HD12	1.98	0.45
1:M:28:MET:HE1	1:M:65:VAL:HA	1.98	0.45
1:K:171:ARG:HH22	1:I:213:ASN:HD21	1.65	0.45
1:A:167:ASP:HA	1:A:170:TYR:CE2	2.52	0.45
1:G:170:TYR:CE1	1:G:171:ARG:HG2	2.52	0.45
1:C:138:VAL:HG22	1:C:201:LEU:HD13	1.97	0.45
1:F:193:SER:O	1:F:194:THR:OG1	2.28	0.45
1:N:102:LYS:HD3	1:N:134:GLU:CG	2.47	0.44
1:M:144:MET:HG2	1:M:154:TYR:HB3	2.00	0.44
1:C:146:MET:HE2	1:C:147:MET:CE	2.48	0.44
1:M:225:PRO:O	1:M:226:PRO:C	2.60	0.44
1:B:167:ASP:HA	1:B:170:TYR:CE2	2.52	0.44
1:G:125:ILE:HD12	1:G:135:GLN:HG2	1.99	0.44
1:J:213:ASN:HD21	1:I:171:ARG:HH22	1.64	0.44
1:L:13:MET:HE2	1:L:121:ILE:HD12	2.00	0.44
1:H:49:ILE:HG13	1:H:182:LEU:HB3	2.00	0.44
1:C:78:ARG:HA	1:C:82:ILE:HB	2.00	0.44
1:F:102:LYS:HG3	1:F:134:GLU:HB2	2.00	0.44
1:N:208:ALA:HB3	1:N:209:PRO:HD3	1.99	0.44
1:B:28:MET:HE2	1:B:65:VAL:N	2.32	0.44
1:H:18:ARG:HE	1:H:169:LYS:HE2	1.82	0.43
1:D:22:LEU:HD11	1:B:223:LEU:CD2	2.45	0.43
1:A:130:MET:HE2	1:A:159:TYR:OH	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:28:MET:CE	1:M:65:VAL:HA	2.49	0.43
1:E:18:ARG:HH21	1:E:180:LYS:HA	1.84	0.43
1:I:210:LEU:HD21	2:I:304:HOH:O	2.18	0.43
1:B:113:CYS:HB3	1:B:118:ILE:O	2.19	0.43
1:I:35:HIS:HE1	1:I:69:THR:OG1	2.02	0.43
1:I:208:ALA:HB3	1:I:209:PRO:HD3	2.01	0.43
1:G:170:TYR:O	1:G:174:GLN:HG3	2.19	0.43
1:G:217:PHE:HA	1:G:222:THR:CG2	2.49	0.43
1:C:160:GLU:CD	1:C:161:PHE:N	2.76	0.43
1:J:35:HIS:HE1	1:J:69:THR:OG1	2.01	0.43
1:K:53:ARG:NH1	1:K:182:LEU:HD12	2.34	0.43
1:C:171:ARG:HH22	1:A:213:ASN:ND2	2.17	0.43
1:N:5:TYR:HB3	1:N:6:SER:H	1.76	0.42
1:L:35:HIS:HE1	1:L:69:THR:OG1	2.02	0.42
1:F:134:GLU:HG2	1:F:135:GLN:HG3	2.01	0.42
1:E:55:GLU:OE1	1:E:55:GLU:HA	2.19	0.42
1:C:161:PHE:CZ	1:C:167:ASP:HB3	2.54	0.42
1:M:140:LYS:NZ	1:M:154:TYR:OH	2.49	0.42
1:F:13:MET:HE2	1:F:121:ILE:HD12	2.01	0.42
1:E:112:PHE:CE1	1:E:116:ASN:ND2	2.87	0.42
1:E:122:ASN:HA	1:E:155:GLN:O	2.19	0.42
1:E:214:ILE:O	1:E:215:VAL:C	2.61	0.42
1:H:213:ASN:HD21	1:F:171:ARG:NH2	2.04	0.42
1:A:97:VAL:HG11	1:A:188:PHE:CD2	2.55	0.42
1:B:28:MET:HE1	1:B:65:VAL:HA	2.00	0.42
1:N:213:ASN:HD21	1:H:171:ARG:NH2	2.18	0.42
1:D:35:HIS:HE1	1:D:69:THR:OG1	2.02	0.42
1:E:21:THR:HG21	1:E:53:ARG:HD2	2.02	0.42
1:E:49:ILE:H	1:E:49:ILE:HG12	1.75	0.42
1:E:219:ALA:HB2	2:E:319:HOH:O	2.20	0.42
1:H:223:LEU:HG	1:F:26:TYR:CE1	2.54	0.42
1:C:128:TYR:CE1	1:C:129:GLN:NE2	2.79	0.42
1:F:208:ALA:HB3	1:F:209:PRO:HD3	2.02	0.42
1:E:208:ALA:O	1:E:209:PRO:C	2.60	0.42
1:D:160:GLU:OE1	1:D:160:GLU:N	2.51	0.42
1:L:130:MET:C	1:L:132:PHE:N	2.77	0.42
1:F:94:LYS:HD2	1:F:193:SER:CB	2.49	0.42
1:G:103:LEU:HD11	1:G:146:MET:HE1	2.02	0.42
1:H:92:TYR:OH	1:H:206:GLU:OE1	2.32	0.42
1:C:38:SER:OG	1:C:68:HIS:CE1	2.71	0.42
1:J:210:LEU:H	1:J:210:LEU:CD1	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:VAL:HG12	1:E:114:ARG:HD2	2.01	0.42
1:J:210:LEU:HD12	1:J:210:LEU:N	2.34	0.42
1:F:35:HIS:HE1	1:F:69:THR:OG1	2.02	0.42
1:E:54:VAL:HA	1:E:57:MET:CE	2.50	0.42
1:D:161:PHE:CZ	1:D:167:ASP:HB3	2.55	0.41
1:M:28:MET:HE2	1:M:65:VAL:N	2.35	0.41
1:L:132:PHE:HB2	1:L:135:GLN:OE1	2.20	0.41
1:B:208:ALA:HB3	1:B:209:PRO:HD3	2.02	0.41
1:N:162:ALA:HB1	1:N:167:ASP:HB2	2.02	0.41
1:J:53:ARG:NH1	1:J:182:LEU:HD12	2.35	0.41
1:N:55:GLU:HA	1:N:58:LYS:HE3	2.03	0.41
1:H:13:MET:HE2	1:H:121:ILE:HD12	2.02	0.41
1:M:26:TYR:CE1	1:G:222:THR:HG23	2.41	0.41
1:I:161:PHE:CZ	1:I:167:ASP:HB3	2.56	0.41
1:K:185:ILE:HD12	1:K:185:ILE:HA	1.90	0.41
1:E:82:ILE:O	1:E:83:GLU:C	2.64	0.41
1:K:28:MET:HE1	1:K:65:VAL:CA	2.50	0.41
1:E:170:TYR:O	1:E:174:GLN:HG3	2.21	0.41
1:B:136:ARG:HD3	1:B:197:ASP:OD1	2.21	0.41
1:H:208:ALA:HB3	1:H:209:PRO:HD3	2.02	0.41
1:D:78:ARG:HA	1:D:82:ILE:HB	2.02	0.41
1:C:134:GLU:HG2	1:C:135:GLN:HG3	2.03	0.41
1:C:208:ALA:HB3	1:C:209:PRO:HD3	2.02	0.41
1:L:223:LEU:HG	1:A:26:TYR:CE1	2.55	0.41
1:F:161:PHE:CZ	1:F:167:ASP:HB3	2.56	0.41
1:K:210:LEU:HD23	1:K:226:PRO:HG2	2.03	0.41
1:E:50:LEU:HD21	1:E:68:HIS:HE1	1.86	0.41
1:C:53:ARG:O	1:C:57:MET:HG3	2.21	0.41
1:A:125:ILE:HD13	1:A:125:ILE:HG21	1.91	0.41
1:J:89:ILE:O	1:J:93:ARG:N	2.51	0.41
1:F:175:LEU:HA	2:F:307:HOH:O	2.21	0.41
1:L:208:ALA:HB3	1:L:209:PRO:HD3	2.02	0.40
1:J:13:MET:HE2	1:J:121:ILE:HD12	2.03	0.40
1:J:170:TYR:O	1:J:174:GLN:HG3	2.20	0.40
1:G:15:THR:HG22	1:G:20:SER:OG	2.21	0.40
1:G:115:ARG:HH11	1:G:115:ARG:HG2	1.86	0.40
1:H:125:ILE:HG23	1:H:156:SER:OG	2.21	0.40
1:K:35:HIS:HE1	1:K:69:THR:OG1	2.03	0.40
1:B:125:ILE:HD13	1:B:125:ILE:HG21	1.94	0.40
1:G:13:MET:HE2	1:G:121:ILE:HD12	2.03	0.40
1:L:161:PHE:CZ	1:L:167:ASP:HB3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:ILE:HD13	1:K:147:MET:HE2	2.02	0.40
1:K:208:ALA:HB3	1:K:209:PRO:HD3	2.03	0.40
1:H:158:VAL:O	1:H:158:VAL:HG12	2.21	0.40
1:D:103:LEU:HD21	1:D:146:MET:HE1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:TYR:OH	1:E:190:ASP:OD2[2_555]	1.81	0.39

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	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
1	B	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
1	C	220/234 (94%)	212 (96%)	8 (4%)	0	100	100
1	D	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
1	E	214/234 (92%)	204 (95%)	8 (4%)	2 (1%)	14	13
1	F	219/234 (94%)	210 (96%)	7 (3%)	2 (1%)	14	13
1	G	216/234 (92%)	212 (98%)	4 (2%)	0	100	100
1	H	222/234 (95%)	218 (98%)	4 (2%)	0	100	100
1	I	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	24	26
1	J	219/234 (94%)	215 (98%)	4 (2%)	0	100	100
1	K	219/234 (94%)	211 (96%)	6 (3%)	2 (1%)	14	13
1	L	220/234 (94%)	214 (97%)	6 (3%)	0	100	100
1	M	219/234 (94%)	212 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	220/234 (94%)	212 (96%)	8 (4%)	0	100	100
All	All	3064/3276 (94%)	2973 (97%)	84 (3%)	7 (0%)	43	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	162	ALA
1	E	221	GLU
1	F	191	SER
1	F	193	SER
1	K	163	GLN
1	E	178	SER
1	I	197	ASP

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	191/200 (96%)	187 (98%)	4 (2%)	47	60
1	B	189/200 (94%)	184 (97%)	5 (3%)	40	53
1	C	191/200 (96%)	188 (98%)	3 (2%)	55	67
1	D	191/200 (96%)	184 (96%)	7 (4%)	30	39
1	E	185/200 (92%)	172 (93%)	13 (7%)	14	15
1	F	189/200 (94%)	188 (100%)	1 (0%)	81	88
1	G	187/200 (94%)	182 (97%)	5 (3%)	39	51
1	H	193/200 (96%)	187 (97%)	6 (3%)	35	45
1	I	189/200 (94%)	183 (97%)	6 (3%)	34	44
1	J	190/200 (95%)	185 (97%)	5 (3%)	40	53
1	K	190/200 (95%)	187 (98%)	3 (2%)	55	67
1	L	191/200 (96%)	187 (98%)	4 (2%)	47	60
1	M	190/200 (95%)	185 (97%)	5 (3%)	40	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	191/200 (96%)	186 (97%)	5 (3%)	40 53
All	All	2657/2800 (95%)	2585 (97%)	72 (3%)	39 51

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	51	SER
1	N	53	ARG
1	N	58	LYS
1	N	130	MET
1	N	178	SER
1	H	7	VAL
1	H	49	ILE
1	H	125	ILE
1	H	158	VAL
1	H	171	ARG
1	H	227	VAL
1	D	22	LEU
1	D	53	ARG
1	D	89	ILE
1	D	127	HIS
1	D	178	SER
1	D	210	LEU
1	D	227	VAL
1	C	89	ILE
1	C	127	HIS
1	C	160	GLU
1	L	53	ARG
1	L	97	VAL
1	L	178	SER
1	L	185	ILE
1	A	97	VAL
1	A	129	GLN
1	A	178	SER
1	A	180	LYS
1	M	44	SER
1	M	58	LYS
1	M	163	GLN
1	M	178	SER
1	M	226	PRO
1	J	53	ARG
1	J	130	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	201	LEU
1	J	210	LEU
1	J	227	VAL
1	F	65	VAL
1	K	53	ARG
1	K	163	GLN
1	K	198	ASP
1	E	7	VAL
1	E	47	ARG
1	E	49	ILE
1	E	66	VAL
1	E	89	ILE
1	E	93	ARG
1	E	97	VAL
1	E	127	HIS
1	E	129	GLN
1	E	179	THR
1	E	185	ILE
1	E	194	THR
1	E	221	GLU
1	I	44	SER
1	I	49	ILE
1	I	51	SER
1	I	97	VAL
1	I	178	SER
1	I	192	PHE
1	B	53	ARG
1	B	63	ASP
1	B	97	VAL
1	B	178	SER
1	B	187	ILE
1	G	53	ARG
1	G	160	GLU
1	G	161	PHE
1	G	185	ILE
1	G	222	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	35	HIS
1	N	149	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	213	ASN
1	H	35	HIS
1	H	68	HIS
1	H	106	HIS
1	H	135	GLN
1	H	155	GLN
1	H	213	ASN
1	D	30	GLN
1	D	35	HIS
1	D	106	HIS
1	D	108	HIS
1	D	129	GLN
1	D	135	GLN
1	D	163	GLN
1	D	212	HIS
1	D	213	ASN
1	C	35	HIS
1	C	68	HIS
1	C	108	HIS
1	C	149	GLN
1	C	213	ASN
1	L	35	HIS
1	L	213	ASN
1	A	35	HIS
1	A	106	HIS
1	A	108	HIS
1	A	127	HIS
1	A	149	GLN
1	A	163	GLN
1	A	213	ASN
1	M	10	GLN
1	M	35	HIS
1	M	106	HIS
1	M	108	HIS
1	M	122	ASN
1	M	155	GLN
1	M	213	ASN
1	J	35	HIS
1	J	106	HIS
1	J	108	HIS
1	J	127	HIS
1	J	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	163	GLN
1	J	213	ASN
1	F	35	HIS
1	F	108	HIS
1	F	127	HIS
1	F	213	ASN
1	K	35	HIS
1	K	46	HIS
1	K	213	ASN
1	E	35	HIS
1	E	52	HIS
1	E	106	HIS
1	E	116	ASN
1	E	135	GLN
1	I	35	HIS
1	I	68	HIS
1	I	149	GLN
1	I	213	ASN
1	B	35	HIS
1	B	106	HIS
1	B	127	HIS
1	B	135	GLN
1	B	163	GLN
1	B	213	ASN
1	G	35	HIS
1	G	135	GLN
1	G	149	GLN
1	G	163	GLN

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	222/234 (94%)	-1.29	0 100 100	30, 42, 62, 96	0
1	B	220/234 (94%)	-1.21	0 100 100	35, 47, 73, 98	0
1	C	222/234 (94%)	-1.25	0 100 100	30, 45, 83, 98	0
1	D	222/234 (94%)	-1.13	0 100 100	35, 51, 99, 127	0
1	E	216/234 (92%)	-1.34	0 100 100	27, 39, 56, 70	0
1	F	221/234 (94%)	-1.21	1 (0%) 87 89	37, 55, 81, 141	0
1	G	218/234 (93%)	-1.21	0 100 100	31, 44, 61, 80	0
1	H	224/234 (95%)	-1.20	1 (0%) 88 90	35, 54, 72, 121	0
1	I	220/234 (94%)	-1.20	0 100 100	44, 58, 86, 113	0
1	J	221/234 (94%)	-1.18	0 100 100	43, 60, 77, 96	0
1	K	221/234 (94%)	-1.14	0 100 100	44, 64, 100, 133	0
1	L	222/234 (94%)	-1.19	0 100 100	30, 58, 88, 121	0
1	M	221/234 (94%)	-1.28	0 100 100	34, 50, 68, 94	0
1	N	222/234 (94%)	-1.29	0 100 100	33, 46, 64, 128	0
All	All	3092/3276 (94%)	-1.22	2 (0%) 92 93	27, 51, 80, 141	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	228	LEU	2.7
1	F	192	PHE	2.3

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.