



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:40 am BST

PDB ID : 1Q52
Title : Crystal Structure of Mycobacterium tuberculosis MenB, a Key Enzyme in Vitamin K2 Biosynthesis
Authors : Truglio, J.J.; Theis, K.; Feng, Y.; Gajda, R.; Machutta, C.; Tonge, P.J.; Kisker, C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-08-05
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

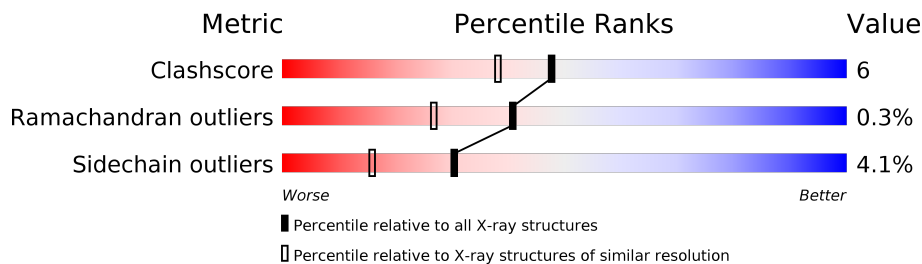
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)





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 on 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	72% (green), 12% (yellow), 14% (grey), 0% (orange), 0% (red)
1	B	314	70% (green), 16% (yellow), 11% (grey), 0% (orange), 0% (red)
1	C	314	71% (green), 12% (yellow), 14% (grey), 0% (orange), 0% (red)
1	D	314	71% (green), 14% (yellow), 14% (grey), 0% (orange), 0% (red)
1	E	314	71% (green), 12% (yellow), 14% (grey), 0% (orange), 0% (red)
1	F	314	71% (green), 13% (yellow), 14% (grey), 0% (orange), 0% (red)
1	G	314	69% (green), 15% (yellow), 14% (grey), 0% (orange), 0% (red)
1	H	314	73% (green), 11% (yellow), 14% (grey), 0% (orange), 0% (red)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	314	 72% 11% • 14%
1	J	314	 70% 12% • 14%
1	K	314	 70% 15% • 14%
1	L	314	 72% 13% • 14%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 28487 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 menB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	B	279	Total 2191	C 1388	N 396	O 398	S 9	0	0	0
1	C	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	D	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	E	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	F	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	G	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	H	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	I	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	J	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0
1	K	271	Total 2132	C 1351	N 382	O 390	S 9	0	0	0
1	L	269	Total 2118	C 1344	N 380	O 385	S 9	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	231	Total 231	O 231	0	0
2	B	244	Total 244	O 244	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	253	Total 253	O 253	0	0
2	D	223	Total 223	O 223	0	0
2	E	264	Total 264	O 264	0	0
2	F	237	Total 237	O 237	0	0
2	G	246	Total 246	O 246	0	0
2	H	242	Total 242	O 242	0	0
2	I	214	Total 214	O 214	0	0
2	J	270	Total 270	O 270	0	0
2	K	275	Total 275	O 275	0	0
2	L	285	Total 285	O 285	0	0

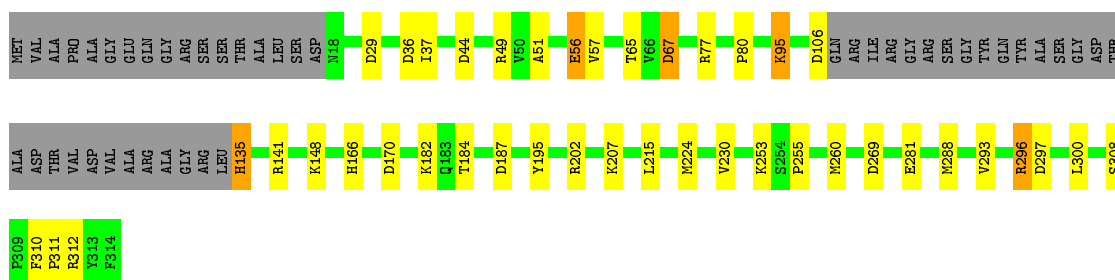
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

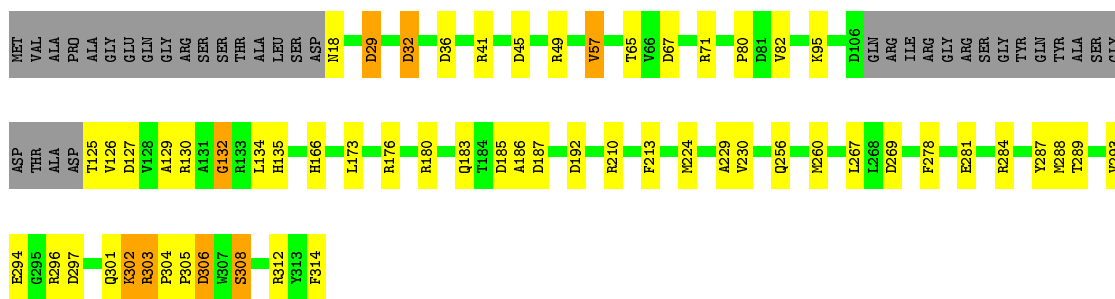
- Molecule 1: menB

Chain A: 



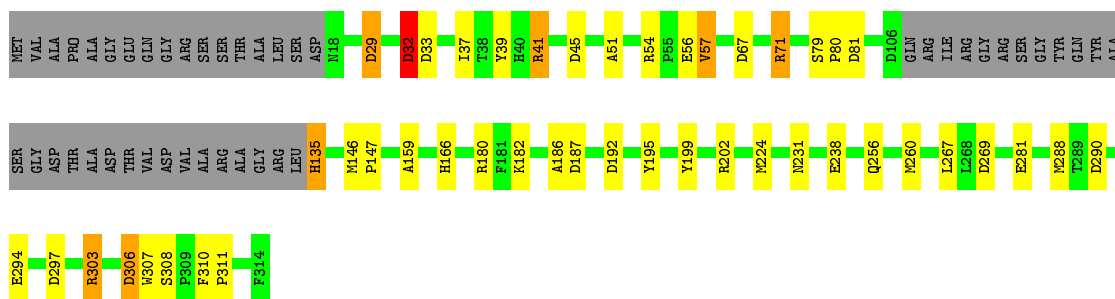
- Molecule 1: menB

Chain B: 



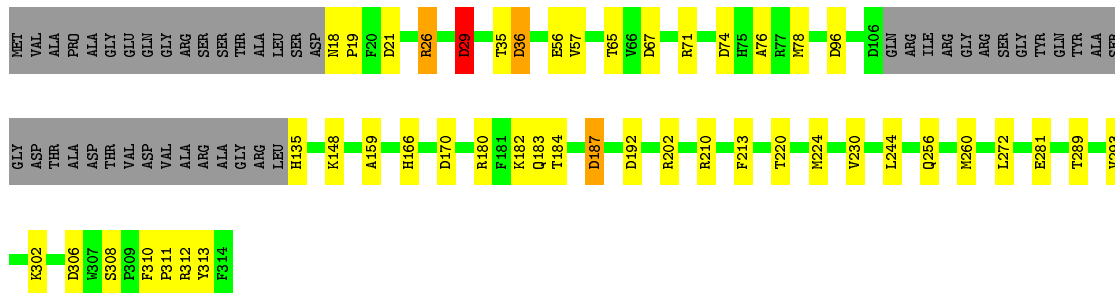
- Molecule 1: menB

Chain C: 



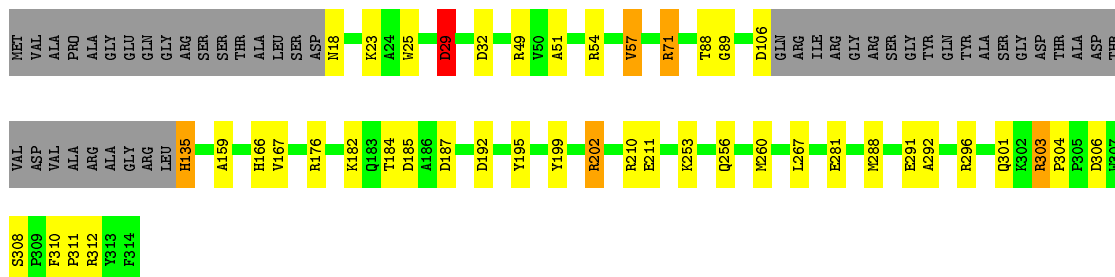
- Molecule 1: menB

Chain D: 



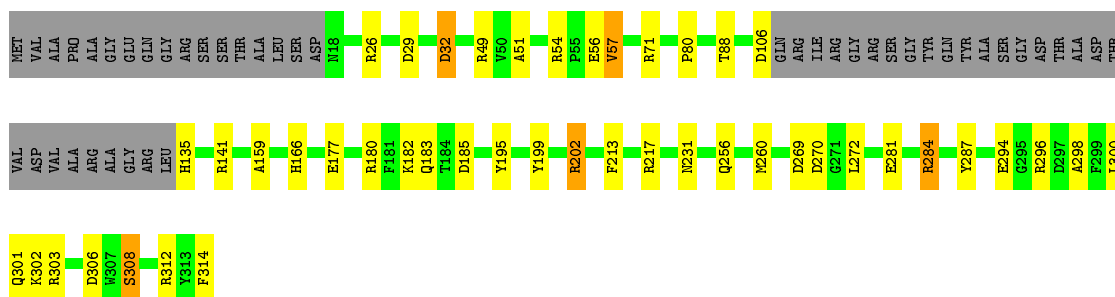
- Molecule 1: menB

Chain E: 



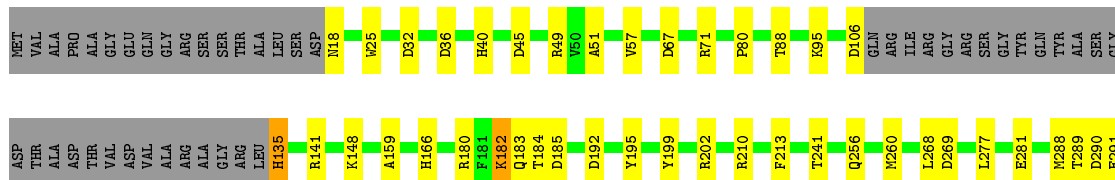
- Molecule 1: menB

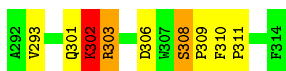
Chain F: 



- Molecule 1: menB

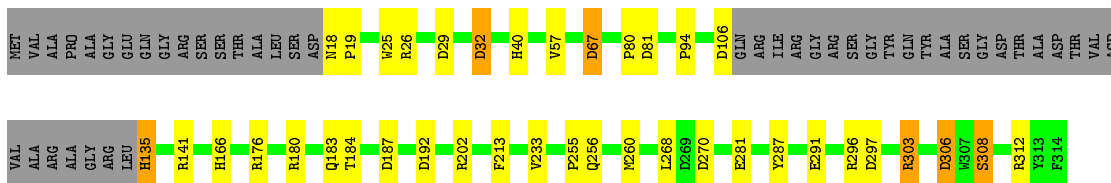
Chain G: 





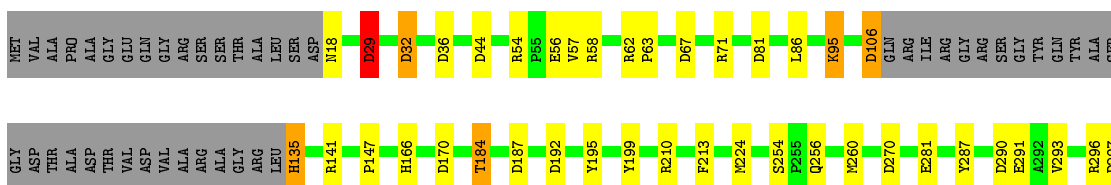
- Molecule 1: menB

Chain H: 73% 11% 14%



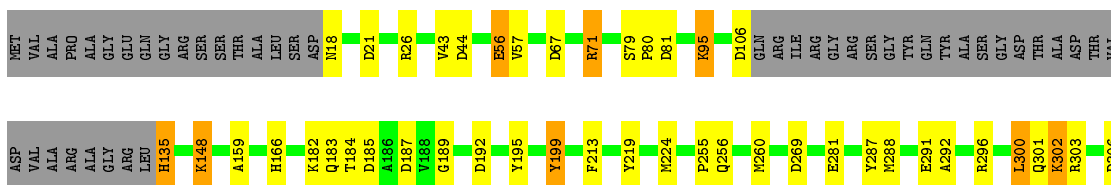
- Molecule 1: menB

Chain I: 72% 11% 14%



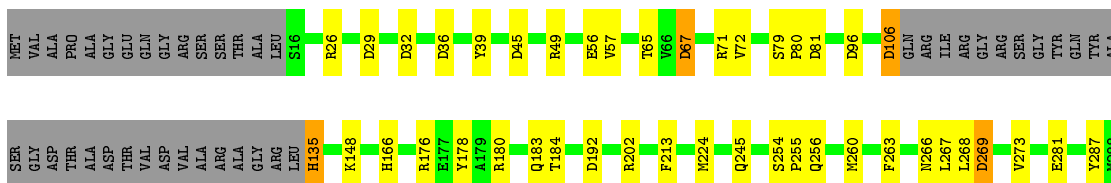
- Molecule 1: menB

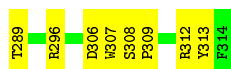
Chain J: 70% 12% 14%



- Molecule 1: menB

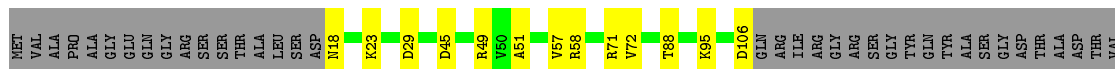
Chain K: 70% 15% 14%





- Molecule 1: menB

Chain L: 72% 13% 14%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.38Å 139.43Å 142.03Å 90.00° 97.29° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	97.4 (50.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.195 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	28487	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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	1.05	1/2172 (0.0%)	1.06	9/2945 (0.3%)
1	B	1.09	3/2245 (0.1%)	1.09	14/3044 (0.5%)
1	C	1.01	2/2172 (0.1%)	1.01	8/2945 (0.3%)
1	D	1.02	0/2172	1.00	10/2945 (0.3%)
1	E	1.05	1/2172 (0.0%)	1.06	12/2945 (0.4%)
1	F	1.03	0/2172	1.04	12/2945 (0.4%)
1	G	1.08	1/2172 (0.0%)	1.06	10/2945 (0.3%)
1	H	1.06	0/2172	1.05	13/2945 (0.4%)
1	I	1.01	2/2172 (0.1%)	1.05	16/2945 (0.5%)
1	J	1.04	2/2172 (0.1%)	1.03	9/2945 (0.3%)
1	K	1.13	3/2186 (0.1%)	1.10	13/2964 (0.4%)
1	L	1.09	1/2172 (0.0%)	1.10	11/2945 (0.4%)
All	All	1.06	16/26151 (0.1%)	1.06	137/35458 (0.4%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	178	TYR	CD2-CE2	6.76	1.49	1.39
1	K	273	VAL	CB-CG1	6.44	1.66	1.52
1	I	141	ARG	CG-CD	5.96	1.66	1.51
1	B	229	ALA	CA-CB	5.96	1.65	1.52
1	C	146	MET	CG-SD	5.86	1.96	1.81
1	B	278	PHE	CE2-CZ	5.81	1.48	1.37
1	I	210	ARG	CZ-NH2	5.58	1.40	1.33
1	J	199	TYR	CD2-CE2	5.52	1.47	1.39
1	L	72	VAL	CB-CG2	5.44	1.64	1.52
1	B	57	VAL	CB-CG2	5.40	1.64	1.52
1	G	182	LYS	CD-CE	5.37	1.64	1.51
1	A	195	TYR	CD2-CE2	5.20	1.47	1.39
1	K	263	PHE	CD2-CE2	5.18	1.49	1.39
1	E	167	VAL	CB-CG2	5.17	1.63	1.52
1	C	39	TYR	CD1-CE1	5.17	1.47	1.39
1	J	219	TYR	CD1-CE1	5.08	1.47	1.39

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	180	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	G	192	ASP	CB-CG-OD2	11.44	128.60	118.30
1	E	192	ASP	CB-CG-OD2	9.32	126.69	118.30
1	B	224	MET	CG-SD-CE	-9.16	85.54	100.20
1	H	192	ASP	CB-CG-OD2	9.11	126.50	118.30
1	K	180	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	G	141	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	H	141	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	K	49	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	B	192	ASP	CB-CG-OD2	8.53	125.98	118.30
1	F	141	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	B	180	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	L	187	ASP	CB-CG-OD2	8.15	125.63	118.30
1	L	192	ASP	CB-CG-OD2	8.13	125.61	118.30
1	I	210	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	H	29	ASP	CB-CG-OD2	7.77	125.29	118.30
1	L	49	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	H	106	ASP	CB-CG-OD2	7.62	125.16	118.30
1	F	54	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	K	192	ASP	CB-CG-OD2	7.35	124.91	118.30
1	C	192	ASP	CB-CG-OD2	7.33	124.89	118.30
1	K	49	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	187	ASP	CB-CG-OD2	7.28	124.85	118.30
1	E	210	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	I	192	ASP	CB-CG-OD2	7.14	124.72	118.30
1	D	192	ASP	CB-CG-OD2	7.13	124.72	118.30
1	F	141	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	187	ASP	CB-CG-OD2	7.09	124.68	118.30
1	D	36	ASP	CB-CG-OD2	7.04	124.64	118.30
1	C	54	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	J	192	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	32	ASP	CB-CG-OD2	6.98	124.58	118.30
1	L	180	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	E	32	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	141	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	E	210	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	L	180	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	J	44	ASP	CB-CG-OD2	6.63	124.27	118.30
1	B	49	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	187	ASP	CB-CG-OD2	6.57	124.22	118.30
1	K	224	MET	CG-SD-CE	-6.57	89.70	100.20
1	I	32	ASP	CB-CG-OD2	6.47	124.13	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	29	ASP	CB-CG-OD2	6.42	124.08	118.30
1	J	269	ASP	CB-CG-OD2	6.41	124.07	118.30
1	L	170	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	49	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	I	210	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	K	32	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	306	ASP	CB-CG-OD2	6.29	123.97	118.30
1	F	202	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	32	ASP	CB-CG-OD2	6.26	123.93	118.30
1	J	306	ASP	CB-CG-OD2	6.24	123.91	118.30
1	H	81	ASP	CB-CG-OD2	6.19	123.87	118.30
1	I	297	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	180	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	G	269	ASP	CB-CG-OD2	6.09	123.78	118.30
1	I	36	ASP	CB-CG-OD2	6.06	123.76	118.30
1	I	187	ASP	CB-CG-OD2	6.02	123.72	118.30
1	I	290	ASP	CB-CG-OD2	6.02	123.71	118.30
1	D	29	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	173	LEU	CB-CG-CD2	-5.97	100.85	111.00
1	H	32	ASP	CB-CG-OD2	5.96	123.67	118.30
1	E	306	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	297	ASP	CB-CG-OD2	5.95	123.65	118.30
1	E	106	ASP	CB-CG-OD2	5.94	123.65	118.30
1	G	277	LEU	CA-CB-CG	-5.94	101.64	115.30
1	H	67	ASP	CB-CG-OD2	5.90	123.61	118.30
1	E	187	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	141	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	K	67	ASP	CB-CG-OD2	5.87	123.58	118.30
1	L	71	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	L	29	ASP	CB-CG-OD2	5.84	123.55	118.30
1	G	210	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	J	106	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	170	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	44	ASP	CB-CG-OD2	5.75	123.48	118.30
1	I	29	ASP	CB-CG-OD2	5.74	123.46	118.30
1	D	67	ASP	CB-CG-OD2	5.73	123.46	118.30
1	I	54	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	29	ASP	CB-CG-OD2	5.70	123.43	118.30
1	I	224	MET	CG-SD-CE	-5.70	91.08	100.20
1	E	202	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	176	ARG	NE-CZ-NH2	-5.66	117.47	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	270	ASP	CB-CG-OD2	5.64	123.37	118.30
1	E	71	ARG	CG-CD-NE	5.63	123.63	111.80
1	L	49	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	G	202	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	297	ASP	CB-CG-OD2	5.56	123.31	118.30
1	G	106	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	45	ASP	CB-CG-OD2	5.53	123.28	118.30
1	H	270	ASP	CB-CG-OD2	5.52	123.27	118.30
1	J	185	ASP	CB-CG-OD2	5.49	123.24	118.30
1	I	44	ASP	CB-CG-OD2	5.47	123.22	118.30
1	L	144	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	F	54	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	F	217	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	L	106	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	306	ASP	CB-CG-OD2	5.39	123.16	118.30
1	D	96	ASP	CB-CG-OD2	5.38	123.14	118.30
1	G	49	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	33	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	57	VAL	CB-CA-C	5.32	121.51	111.40
1	K	106	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	210	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	D	170	ASP	CB-CG-OD2	5.29	123.06	118.30
1	J	187	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	202	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	E	29	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	187	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	21	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	106	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	77	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	K	96	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	202	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	F	32	ASP	CB-CG-OD2	5.16	122.95	118.30
1	H	202	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	I	81	ASP	CB-CG-OD2	5.14	122.93	118.30
1	K	266	ASN	CB-CA-C	-5.14	100.12	110.40
1	D	210	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	K	269	ASP	CB-CG-OD2	5.12	122.91	118.30
1	I	170	ASP	CB-CG-OD2	5.11	122.90	118.30
1	K	176	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	G	36	ASP	CB-CG-OD1	5.11	122.90	118.30
1	F	71	ARG	CG-CD-NE	5.10	122.51	111.80
1	A	67	ASP	CB-CG-OD2	5.10	122.89	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	26	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	I	86	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	H	141	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	J	67	ASP	CB-CG-OD2	5.04	122.83	118.30
1	G	290	ASP	CB-CG-OD2	5.02	122.82	118.30
1	D	74	ASP	CB-CG-OD2	5.02	122.82	118.30
1	H	187	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	230	VAL	CA-CB-CG2	-5.02	103.37	110.90
1	F	49	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	J	21	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	270	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2118	0	2036	24	0
1	B	2191	0	2115	35	0
1	C	2118	0	2036	35	0
1	D	2118	0	2036	26	0
1	E	2118	0	2036	29	0
1	F	2118	0	2036	24	0
1	G	2118	0	2036	34	0
1	H	2118	0	2036	23	0
1	I	2118	0	2036	21	0
1	J	2118	0	2036	27	0
1	K	2132	0	2045	35	0
1	L	2118	0	2036	23	0
2	A	231	0	0	5	2
2	B	244	0	0	8	0
2	C	253	0	0	13	0
2	D	223	0	0	5	0
2	E	264	0	0	15	0
2	F	237	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	246	0	0	12	0
2	H	242	0	0	4	0
2	I	214	0	0	8	0
2	J	270	0	0	6	0
2	K	275	0	0	8	0
2	L	285	0	0	8	2
All	All	28487	0	24520	304	2

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 6.

All (304) 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:E:18:ASN:N	2:E:567:HOH:O	1.84	1.08
1:B:18:ASN:N	2:B:542:HOH:O	1.90	1.04
1:F:185:ASP:HB2	2:F:542:HOH:O	1.56	1.03
1:H:135:HIS:N	2:H:548:HOH:O	1.93	1.00
1:I:18:ASN:N	2:I:521:HOH:O	2.03	0.91
1:C:135:HIS:HB2	2:C:566:HOH:O	1.70	0.90
1:G:288:MET:CE	1:K:289:THR:HG22	2.02	0.89
1:I:287:TYR:O	1:I:296:ARG:NH2	2.04	0.89
1:B:297:ASP:HB3	1:B:303:ARG:NH2	1.88	0.89
1:J:18:ASN:N	2:J:574:HOH:O	2.06	0.88
1:L:226:GLN:HG3	2:L:474:HOH:O	1.74	0.86
1:B:57:VAL:HG12	1:B:57:VAL:O	1.77	0.84
1:B:306:ASP:OD1	1:B:308:SER:OG	1.97	0.82
1:A:182:LYS:HG2	1:A:184:THR:HG23	1.62	0.81
1:L:18:ASN:N	2:L:587:HOH:O	2.14	0.81
1:I:184:THR:HA	2:I:519:HOH:O	1.79	0.80
1:L:57:VAL:O	1:L:57:VAL:HG12	1.81	0.79
1:C:290:ASP:HB2	2:C:561:HOH:O	1.83	0.79
1:G:185:ASP:HB2	2:G:349:HOH:O	1.83	0.78
1:B:297:ASP:HB3	1:B:303:ARG:HH21	1.47	0.78
1:G:288:MET:HE1	1:K:289:THR:CG2	2.15	0.77
1:I:67:ASP:O	1:I:71:ARG:HG3	1.85	0.77
1:B:71:ARG:HD2	2:B:545:HOH:O	1.84	0.77
1:C:45:ASP:HB3	2:C:326:HOH:O	1.84	0.77
1:G:301:GLN:O	1:G:302:LYS:HB2	1.83	0.76
1:G:57:VAL:O	1:G:57:VAL:HG12	1.82	0.76
1:H:80:PRO:O	1:J:312:ARG:HB2	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:287:TYR:O	1:J:296:ARG:NH2	2.18	0.75
1:B:185:ASP:OD1	2:B:540:HOH:O	2.05	0.74
1:G:288:MET:HE3	1:K:289:THR:HG22	1.67	0.74
1:G:45:ASP:HB3	2:G:336:HOH:O	1.88	0.73
1:L:287:TYR:O	1:L:296:ARG:NH2	2.20	0.73
1:E:29:ASP:OD2	2:E:550:HOH:O	2.06	0.73
1:A:135:HIS:N	2:A:529:HOH:O	2.21	0.73
1:C:41:ARG:HH22	1:C:81:ASP:CG	1.92	0.72
1:D:57:VAL:HG11	2:D:387:HOH:O	1.89	0.72
1:J:135:HIS:N	2:J:570:HOH:O	2.22	0.72
1:E:71:ARG:NH1	2:E:564:HOH:O	2.20	0.70
1:B:57:VAL:CG1	1:B:57:VAL:O	2.38	0.70
1:A:260:MET:SD	1:A:281:GLU:HB3	2.31	0.70
1:G:288:MET:HE1	1:K:289:THR:HG21	1.72	0.69
1:K:57:VAL:O	1:K:57:VAL:HG12	1.93	0.69
1:H:287:TYR:O	1:H:296:ARG:NH2	2.25	0.68
1:G:288:MET:CE	1:K:289:THR:CG2	2.69	0.68
1:C:41:ARG:NH2	1:C:81:ASP:CG	2.48	0.67
1:I:213:PHE:O	2:I:518:HOH:O	2.12	0.67
1:G:80:PRO:O	1:K:312:ARG:HB2	1.93	0.67
1:K:67:ASP:O	1:K:71:ARG:HG3	1.96	0.66
1:F:287:TYR:O	1:F:296:ARG:NH2	2.29	0.65
1:L:57:VAL:O	1:L:57:VAL:CG1	2.45	0.65
1:A:207:LYS:HE3	2:B:556:HOH:O	1.97	0.64
1:G:289:THR:O	1:G:293:VAL:HG23	1.98	0.64
1:C:202:ARG:NH1	1:C:269:ASP:OD1	2.31	0.63
1:J:135:HIS:HD2	2:J:372:HOH:O	1.80	0.63
1:I:106:ASP:C	2:I:523:HOH:O	2.37	0.62
1:K:287:TYR:O	1:K:296:ARG:NH2	2.33	0.61
1:D:76:ALA:O	1:D:148:LYS:NZ	2.32	0.61
1:B:260:MET:SD	1:B:281:GLU:HB3	2.41	0.61
1:H:260:MET:SD	1:H:281:GLU:HB3	2.40	0.61
1:B:301:GLN:NE2	2:B:553:HOH:O	2.34	0.61
1:L:135:HIS:HD2	2:L:353:HOH:O	1.83	0.60
1:A:57:VAL:HG12	2:A:419:HOH:O	2.02	0.60
1:C:135:HIS:N	2:C:549:HOH:O	2.34	0.60
1:G:241:THR:HG23	2:G:504:HOH:O	2.00	0.60
1:H:297:ASP:HB3	1:H:303:ARG:HH21	1.66	0.60
1:L:135:HIS:N	2:L:583:HOH:O	2.34	0.60
1:D:306:ASP:OD1	1:D:308:SER:OG	2.19	0.59
1:G:180:ARG:NH2	2:G:552:HOH:O	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:HB3	2:B:544:HOH:O	2.03	0.59
1:C:238:GLU:HG3	2:C:398:HOH:O	2.02	0.59
1:D:35:THR:HG21	2:D:413:HOH:O	2.02	0.59
1:G:303:ARG:HB2	2:G:557:HOH:O	2.02	0.58
1:I:135:HIS:N	2:I:512:HOH:O	2.35	0.58
1:F:202:ARG:NH1	1:F:269:ASP:OD1	2.36	0.58
1:D:57:VAL:O	1:D:57:VAL:HG12	2.03	0.58
1:I:57:VAL:O	1:I:57:VAL:HG12	2.04	0.58
1:B:132:GLY:O	1:F:284:ARG:NH1	2.37	0.57
1:A:56:GLU:H	1:A:56:GLU:CD	2.08	0.57
1:E:159:ALA:HA	1:E:182:LYS:O	2.04	0.56
1:E:292:ALA:HB1	1:E:296:ARG:NH2	2.20	0.56
1:C:303:ARG:HD2	2:C:507:HOH:O	2.06	0.56
1:A:182:LYS:HG2	1:A:184:THR:CG2	2.35	0.55
1:H:57:VAL:HG12	1:H:57:VAL:O	2.05	0.55
1:I:95:LYS:HD2	2:I:485:HOH:O	2.05	0.55
1:C:260:MET:SD	1:C:281:GLU:HB3	2.46	0.55
1:I:29:ASP:OD2	1:I:29:ASP:N	2.30	0.55
1:E:23:LYS:HD2	2:E:508:HOH:O	2.05	0.55
1:K:306:ASP:HB3	2:K:579:HOH:O	2.05	0.55
1:A:67:ASP:OD1	1:A:135:HIS:CD2	2.59	0.55
1:A:288:MET:HE1	2:E:341:HOH:O	2.06	0.55
1:C:41:ARG:NH2	1:C:81:ASP:OD2	2.40	0.55
1:K:260:MET:SD	1:K:281:GLU:HB3	2.47	0.55
1:F:312:ARG:HG3	1:F:312:ARG:HH11	1.73	0.54
1:J:57:VAL:HG12	1:J:57:VAL:O	2.08	0.54
1:H:312:ARG:HG3	1:H:312:ARG:HH11	1.72	0.54
1:E:304:PRO:HA	2:E:578:HOH:O	2.07	0.54
1:F:306:ASP:OD1	1:F:308:SER:OG	2.26	0.54
1:H:297:ASP:CB	1:H:303:ARG:HH21	2.20	0.54
1:D:187:ASP:OD1	1:E:253:LYS:HD3	2.08	0.53
1:B:301:GLN:O	1:B:302:LYS:HB2	2.09	0.53
1:K:26:ARG:HG3	2:K:528:HOH:O	2.08	0.53
1:C:71:ARG:NH1	2:C:546:HOH:O	2.41	0.53
1:J:71:ARG:HH11	1:J:71:ARG:HG2	1.74	0.53
1:B:67:ASP:OD1	1:B:135:HIS:CE1	2.62	0.53
1:C:135:HIS:N	2:C:543:HOH:O	2.41	0.53
1:C:159:ALA:HA	1:C:182:LYS:O	2.08	0.53
1:E:135:HIS:HD2	2:E:375:HOH:O	1.91	0.53
1:L:135:HIS:N	2:L:552:HOH:O	2.43	0.53
1:F:180:ARG:NH2	2:F:522:HOH:O	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ASP:OD1	1:C:308:SER:OG	2.26	0.52
1:C:256:GLN:O	1:C:260:MET:HG2	2.09	0.52
1:F:26:ARG:HD3	2:F:517:HOH:O	2.10	0.52
1:K:309:PRO:HD3	2:K:579:HOH:O	2.08	0.52
1:E:260:MET:SD	1:E:281:GLU:HB3	2.49	0.52
1:B:289:THR:O	1:B:293:VAL:HG23	2.09	0.52
1:C:67:ASP:O	1:C:71:ARG:CG	2.58	0.52
1:H:256:GLN:O	1:H:260:MET:HG2	2.11	0.52
1:K:135:HIS:HD2	2:K:444:HOH:O	1.93	0.52
1:J:256:GLN:O	1:J:260:MET:HG2	2.10	0.51
1:A:135:HIS:HD2	2:A:406:HOH:O	1.93	0.51
1:J:260:MET:SD	1:J:281:GLU:HB3	2.51	0.51
1:C:288:MET:HE2	2:F:355:HOH:O	2.10	0.51
1:G:57:VAL:O	1:G:57:VAL:CG1	2.54	0.51
1:K:256:GLN:O	1:K:260:MET:HG2	2.11	0.51
1:H:135:HIS:HD2	2:H:362:HOH:O	1.93	0.51
1:L:58:ARG:NH1	2:L:432:HOH:O	2.44	0.51
1:E:256:GLN:O	1:E:260:MET:HG2	2.11	0.51
1:D:224:MET:HB3	1:D:230:VAL:HG23	1.92	0.50
1:C:67:ASP:O	1:C:71:ARG:HG3	2.12	0.50
1:F:300:LEU:O	1:F:302:LYS:N	2.44	0.50
1:G:306:ASP:C	1:G:308:SER:H	2.15	0.50
1:H:291:GLU:OE1	1:J:255:PRO:HD2	2.12	0.50
1:G:183:GLN:HG2	1:G:213:PHE:CE2	2.47	0.50
1:K:45:ASP:HB3	2:K:342:HOH:O	2.12	0.50
1:F:159:ALA:HA	1:F:182:LYS:O	2.12	0.49
1:G:268:LEU:HD23	1:K:268:LEU:HD23	1.94	0.49
1:J:184:THR:HA	2:J:495:HOH:O	2.11	0.49
2:J:520:HOH:O	1:K:245:GLN:HG2	2.12	0.49
1:D:260:MET:SD	1:D:281:GLU:HB3	2.51	0.49
1:D:29:ASP:N	1:D:29:ASP:OD2	2.40	0.49
1:D:289:THR:O	1:D:293:VAL:HG23	2.11	0.49
1:I:256:GLN:O	1:I:260:MET:HG2	2.12	0.49
1:K:36:ASP:HB3	1:K:65:THR:HG23	1.94	0.49
1:E:303:ARG:HD2	2:E:557:HOH:O	2.12	0.49
1:K:202:ARG:NH1	1:K:269:ASP:OD1	2.44	0.49
1:H:183:GLN:HG2	1:H:213:PHE:CE2	2.48	0.49
1:I:62:ARG:HB2	1:I:63:PRO:HD2	1.93	0.49
1:B:41:ARG:HG2	2:B:558:HOH:O	2.12	0.48
1:G:256:GLN:O	1:G:260:MET:HG2	2.13	0.48
2:H:418:HOH:O	1:J:288:MET:HE1	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:GLN:HG2	1:H:213:PHE:CZ	2.49	0.48
1:G:18:ASN:N	2:G:344:HOH:O	2.46	0.48
1:K:106:ASP:C	2:K:562:HOH:O	2.51	0.48
1:I:260:MET:SD	1:I:281:GLU:HB3	2.54	0.48
1:A:36:ASP:HB3	1:A:65:THR:HG23	1.94	0.48
1:B:294:GLU:O	1:B:297:ASP:HB2	2.13	0.48
1:D:26:ARG:HD3	2:D:457:HOH:O	2.13	0.47
1:F:312:ARG:HG3	1:F:312:ARG:NH1	2.29	0.47
1:J:159:ALA:HA	1:J:182:LYS:O	2.14	0.47
1:J:292:ALA:HB1	1:J:296:ARG:HH21	1.80	0.47
1:I:291:GLU:OE1	1:L:255:PRO:HD2	2.14	0.47
1:F:260:MET:SD	1:F:281:GLU:HB3	2.54	0.47
1:K:79:SER:O	1:K:148:LYS:NZ	2.46	0.47
1:B:126:VAL:HG13	1:B:130:ARG:HE	1.79	0.47
1:D:159:ALA:HA	1:D:182:LYS:O	2.15	0.47
1:G:260:MET:SD	1:G:281:GLU:HB3	2.55	0.47
1:E:211:GLU:HB2	1:F:231:ASN:ND2	2.30	0.47
1:G:71:ARG:HG3	2:G:430:HOH:O	2.15	0.47
1:D:180:ARG:HH21	1:D:220:THR:HG22	1.80	0.47
1:B:82:VAL:O	1:D:312:ARG:HD3	2.15	0.46
2:G:420:HOH:O	1:H:268:LEU:HD13	2.15	0.46
1:D:256:GLN:O	1:D:260:MET:HG2	2.14	0.46
1:D:71:ARG:HD2	2:D:534:HOH:O	2.14	0.46
1:A:80:PRO:O	1:E:312:ARG:HB2	2.15	0.46
1:G:306:ASP:O	1:G:309:PRO:HD2	2.15	0.46
1:E:185:ASP:HA	2:E:549:HOH:O	2.15	0.46
1:A:224:MET:HB3	1:A:230:VAL:HG23	1.98	0.46
1:E:176:ARG:HD3	2:E:502:HOH:O	2.16	0.46
1:F:51:ALA:HA	1:F:88:THR:O	2.15	0.46
1:K:135:HIS:N	2:K:530:HOH:O	2.48	0.46
1:E:310:PHE:HA	1:E:311:PRO:HD3	1.70	0.46
1:C:180:ARG:NH2	2:C:406:HOH:O	2.41	0.46
1:A:255:PRO:HD2	1:E:291:GLU:OE1	2.16	0.46
1:J:310:PHE:HA	1:J:311:PRO:HD3	1.79	0.46
2:I:348:HOH:O	1:L:288:MET:HE2	2.15	0.46
2:A:342:HOH:O	1:E:288:MET:HE1	2.17	0.45
1:A:312:ARG:NH2	2:A:446:HOH:O	2.49	0.45
1:C:57:VAL:O	1:C:57:VAL:CG1	2.65	0.45
1:G:135:HIS:CE1	2:G:426:HOH:O	2.69	0.45
1:C:231:ASN:N	2:C:562:HOH:O	2.48	0.45
1:B:269:ASP:HB3	1:F:272:LEU:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:MET:HE2	2:D:532:HOH:O	2.16	0.45
1:C:310:PHE:HA	1:C:311:PRO:HD3	1.74	0.45
1:H:94:PRO:HG3	2:H:554:HOH:O	2.16	0.45
1:J:26:ARG:HG2	1:J:43:VAL:HG12	1.98	0.45
1:J:56:GLU:H	1:J:56:GLU:CD	2.20	0.45
1:H:25:TRP:HB3	1:H:40:HIS:HB3	1.98	0.45
1:B:67:ASP:OD1	1:B:135:HIS:HE1	1.99	0.44
1:E:292:ALA:HB1	1:E:296:ARG:HH21	1.81	0.44
1:B:126:VAL:HG22	1:F:80:PRO:HG2	1.99	0.44
1:E:25:TRP:CH2	1:E:49:ARG:HB2	2.51	0.44
1:E:88:THR:HG23	1:E:89:GLY:N	2.33	0.44
1:I:293:VAL:HG22	1:I:296:ARG:NH1	2.33	0.44
1:K:256:GLN:NE2	2:K:568:HOH:O	2.26	0.44
1:A:57:VAL:O	1:A:57:VAL:HG12	2.18	0.44
1:C:294:GLU:OE1	1:C:303:ARG:NH2	2.49	0.44
1:G:159:ALA:HA	1:G:182:LYS:O	2.17	0.44
1:A:269:ASP:HB3	1:D:272:LEU:HD12	1.98	0.44
1:I:195:TYR:O	1:I:199:TYR:HB3	2.18	0.44
1:K:81:ASP:N	1:K:81:ASP:OD1	2.46	0.44
1:L:256:GLN:O	1:L:260:MET:HG2	2.17	0.44
1:C:202:ARG:HH11	1:C:269:ASP:CG	2.20	0.44
1:J:79:SER:HA	1:J:80:PRO:HD3	1.83	0.44
1:B:314:PHE:CE1	1:D:78:MET:HG2	2.52	0.44
1:H:306:ASP:OD2	1:H:308:SER:OG	2.34	0.43
1:K:79:SER:HA	1:K:80:PRO:HD3	1.88	0.43
1:D:183:GLN:HG2	1:D:213:PHE:CZ	2.53	0.43
1:D:310:PHE:HA	1:D:311:PRO:HD3	1.78	0.43
1:G:310:PHE:HA	1:G:311:PRO:HD3	1.67	0.43
2:G:454:HOH:O	1:K:313:TYR:HE2	2.01	0.43
1:J:189:GLY:HA2	1:K:254:SER:CB	2.48	0.43
1:K:57:VAL:CG1	1:K:57:VAL:O	2.65	0.43
1:B:287:TYR:CE2	1:B:296:ARG:NH1	2.86	0.43
1:F:177:GLU:O	1:H:180:ARG:NH1	2.51	0.43
1:J:195:TYR:O	1:J:199:TYR:HB3	2.18	0.43
1:K:183:GLN:HG2	1:K:213:PHE:CZ	2.54	0.43
1:G:183:GLN:HG2	1:G:213:PHE:CZ	2.53	0.43
1:G:25:TRP:HB3	1:G:40:HIS:HB3	2.00	0.43
1:F:57:VAL:HG13	1:F:57:VAL:O	2.19	0.43
1:I:147:PRO:HG3	1:L:314:PHE:HA	2.01	0.43
1:J:296:ARG:HD2	2:J:518:HOH:O	2.19	0.43
1:J:56:GLU:HB3	1:J:95:LYS:HD2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:HIS:HD2	2:G:362:HOH:O	2.02	0.42
1:E:195:TYR:O	1:E:199:TYR:HB3	2.19	0.42
1:I:58:ARG:NH1	2:I:431:HOH:O	2.52	0.42
1:L:301:GLN:H	1:L:301:GLN:HG3	1.62	0.42
1:B:185:ASP:HA	2:B:540:HOH:O	2.19	0.42
1:G:67:ASP:OD1	1:G:135:HIS:CD2	2.73	0.42
1:K:39:TYR:CG	1:K:72:VAL:HG13	2.54	0.42
1:A:310:PHE:HA	1:A:311:PRO:HD3	1.83	0.42
1:E:202:ARG:NE	2:E:417:HOH:O	2.45	0.42
1:F:294:GLU:OE1	1:F:294:GLU:HA	2.19	0.42
1:G:51:ALA:HA	1:G:88:THR:O	2.19	0.42
1:J:79:SER:O	1:J:148:LYS:NZ	2.53	0.42
1:A:293:VAL:HG22	1:A:296:ARG:NH2	2.35	0.42
1:B:80:PRO:O	1:D:312:ARG:HB2	2.19	0.42
1:L:45:ASP:HB3	2:L:336:HOH:O	2.19	0.42
1:B:134:LEU:HG	1:F:284:ARG:HH22	1.84	0.42
1:A:253:LYS:HD2	1:C:186:ALA:HB3	2.00	0.42
1:C:32:ASP:HB3	2:C:447:HOH:O	2.19	0.42
1:D:183:GLN:HG2	1:D:213:PHE:CE2	2.55	0.42
1:L:267:LEU:HD23	1:L:267:LEU:C	2.40	0.42
1:L:201:ALA:HA	1:L:209:ALA:HB2	2.00	0.42
1:H:67:ASP:OD1	1:H:135:HIS:CD2	2.72	0.42
1:A:288:MET:HE2	2:E:378:HOH:O	2.19	0.42
1:B:36:ASP:HB3	1:B:65:THR:HG23	2.01	0.42
1:C:306:ASP:CG	1:C:308:SER:HG	2.21	0.42
1:A:56:GLU:HB3	1:A:95:LYS:HE3	2.01	0.41
1:J:81:ASP:OD1	1:J:81:ASP:N	2.48	0.41
1:C:135:HIS:CA	2:C:543:HOH:O	2.68	0.41
1:E:303:ARG:HB3	2:E:542:HOH:O	2.20	0.41
1:F:195:TYR:O	1:F:199:TYR:HB3	2.20	0.41
1:K:39:TYR:CD2	1:K:72:VAL:HG13	2.55	0.41
1:L:183:GLN:HG2	1:L:213:PHE:CZ	2.55	0.41
1:B:267:LEU:HD23	1:B:267:LEU:C	2.40	0.41
1:B:304:PRO:HA	1:B:305:PRO:HD2	1.86	0.41
1:B:284:ARG:CZ	1:D:313:TYR:HB3	2.51	0.41
1:E:267:LEU:HD23	1:E:267:LEU:C	2.40	0.41
1:L:311:PRO:HG2	1:L:313:TYR:CZ	2.56	0.41
1:A:37:ILE:HA	1:A:51:ALA:O	2.21	0.41
1:B:256:GLN:O	1:B:260:MET:HG2	2.21	0.41
1:H:176:ARG:HB2	1:H:233:VAL:HG12	2.03	0.41
1:H:57:VAL:CG1	1:H:57:VAL:O	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:300:LEU:C	1:J:302:LYS:H	2.23	0.41
1:B:129:ALA:HB2	1:C:311:PRO:CB	2.50	0.41
1:C:307:TRP:HB2	2:C:552:HOH:O	2.20	0.41
1:C:37:ILE:HA	1:C:51:ALA:O	2.21	0.41
1:E:23:LYS:HE2	2:E:574:HOH:O	2.20	0.41
1:H:18:ASN:HA	1:H:19:PRO:HD3	1.92	0.41
1:I:56:GLU:CD	1:I:56:GLU:H	2.24	0.41
1:B:183:GLN:HG2	1:B:213:PHE:CE2	2.56	0.41
1:F:256:GLN:O	1:F:260:MET:HG2	2.20	0.41
1:J:183:GLN:HG2	1:J:213:PHE:CZ	2.56	0.41
1:L:260:MET:SD	1:L:281:GLU:HB3	2.61	0.41
1:F:183:GLN:HG2	1:F:213:PHE:CE2	2.56	0.41
1:I:57:VAL:O	1:I:57:VAL:CG1	2.69	0.41
1:L:51:ALA:HA	1:L:88:THR:O	2.20	0.41
1:G:303:ARG:HD2	2:G:557:HOH:O	2.21	0.41
1:K:307:TRP:C	1:K:309:PRO:HD2	2.41	0.41
1:C:79:SER:HA	1:C:80:PRO:HD3	1.82	0.40
1:D:244:LEU:HD23	1:D:244:LEU:HA	1.97	0.40
1:D:18:ASN:HA	1:D:19:PRO:HD3	1.95	0.40
1:E:51:ALA:HA	1:E:88:THR:O	2.21	0.40
1:K:183:GLN:HG2	1:K:213:PHE:CE2	2.57	0.40
1:I:254:SER:OG	1:L:291:GLU:OE1	2.30	0.40
1:C:195:TYR:O	1:C:199:TYR:HB3	2.20	0.40
1:D:36:ASP:HB3	1:D:65:THR:HG23	2.02	0.40
1:E:135:HIS:CD2	2:E:375:HOH:O	2.71	0.40
1:G:291:GLU:OE1	1:K:255:PRO:HD2	2.20	0.40
1:A:215:LEU:HD12	1:A:215:LEU:N	2.37	0.40
1:C:147:PRO:HG3	1:F:314:PHE:HA	2.04	0.40
1:G:195:TYR:O	1:G:199:TYR:HB3	2.21	0.40
1:H:255:PRO:HD2	1:J:291:GLU:OE1	2.21	0.40
1:L:284:ARG:HD3	2:L:440:HOH:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:532:HOH:O	2:L:398:HOH:O[1_556]	2.17	0.03
2:A:542:HOH:O	2:L:474:HOH:O[1_556]	2.18	0.02

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	265/314 (84%)	256 (97%)	9 (3%)	0	100	100
1	B	275/314 (88%)	264 (96%)	9 (3%)	2 (1%)	22	10
1	C	265/314 (84%)	260 (98%)	4 (2%)	1 (0%)	34	21
1	D	265/314 (84%)	258 (97%)	7 (3%)	0	100	100
1	E	265/314 (84%)	256 (97%)	9 (3%)	0	100	100
1	F	265/314 (84%)	249 (94%)	14 (5%)	2 (1%)	19	7
1	G	265/314 (84%)	254 (96%)	10 (4%)	1 (0%)	34	21
1	H	265/314 (84%)	259 (98%)	6 (2%)	0	100	100
1	I	265/314 (84%)	255 (96%)	10 (4%)	0	100	100
1	J	265/314 (84%)	255 (96%)	8 (3%)	2 (1%)	19	7
1	K	267/314 (85%)	259 (97%)	7 (3%)	1 (0%)	34	21
1	L	265/314 (84%)	258 (97%)	6 (2%)	1 (0%)	34	21
All	All	3192/3768 (85%)	3083 (97%)	99 (3%)	10 (0%)	41	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	302	LYS
1	F	301	GLN
1	G	302	LYS
1	J	302	LYS
1	B	302	LYS
1	F	298	ALA
1	C	267	LEU
1	J	301	GLN
1	K	267	LEU
1	B	132	GLY

5.3.2 Protein sidechains [i](#)

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	215/247 (87%)	204 (95%)	11 (5%)	24	10
1	B	222/247 (90%)	213 (96%)	9 (4%)	30	16
1	C	215/247 (87%)	205 (95%)	10 (5%)	26	12
1	D	215/247 (87%)	207 (96%)	8 (4%)	34	19
1	E	215/247 (87%)	207 (96%)	8 (4%)	34	19
1	F	215/247 (87%)	206 (96%)	9 (4%)	30	15
1	G	215/247 (87%)	206 (96%)	9 (4%)	30	15
1	H	215/247 (87%)	208 (97%)	7 (3%)	38	23
1	I	215/247 (87%)	207 (96%)	8 (4%)	34	19
1	J	215/247 (87%)	205 (95%)	10 (5%)	26	12
1	K	217/247 (88%)	211 (97%)	6 (3%)	43	30
1	L	215/247 (87%)	205 (95%)	10 (5%)	26	12
All	All	2589/2964 (87%)	2484 (96%)	105 (4%)	30	16

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	56	GLU
1	A	95	LYS
1	A	106	ASP
1	A	135	HIS
1	A	148	LYS
1	A	166	HIS
1	A	202	ARG
1	A	296	ARG
1	A	300	LEU
1	A	308	SER
1	B	29	ASP
1	B	32	ASP
1	B	95	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	125	THR
1	B	127	ASP
1	B	166	HIS
1	B	303	ARG
1	B	308	SER
1	B	312	ARG
1	C	29	ASP
1	C	32	ASP
1	C	41	ARG
1	C	56	GLU
1	C	57	VAL
1	C	71	ARG
1	C	135	HIS
1	C	166	HIS
1	C	224	MET
1	C	303	ARG
1	D	26	ARG
1	D	29	ASP
1	D	56	GLU
1	D	135	HIS
1	D	166	HIS
1	D	184	THR
1	D	202	ARG
1	D	302	LYS
1	E	29	ASP
1	E	57	VAL
1	E	135	HIS
1	E	166	HIS
1	E	184	THR
1	E	301	GLN
1	E	303	ARG
1	E	308	SER
1	F	29	ASP
1	F	32	ASP
1	F	56	GLU
1	F	57	VAL
1	F	135	HIS
1	F	166	HIS
1	F	284	ARG
1	F	303	ARG
1	F	308	SER
1	G	32	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	95	LYS
1	G	135	HIS
1	G	148	LYS
1	G	166	HIS
1	G	184	THR
1	G	302	LYS
1	G	303	ARG
1	G	308	SER
1	H	32	ASP
1	H	135	HIS
1	H	166	HIS
1	H	184	THR
1	H	303	ARG
1	H	306	ASP
1	H	308	SER
1	I	29	ASP
1	I	32	ASP
1	I	95	LYS
1	I	106	ASP
1	I	135	HIS
1	I	166	HIS
1	I	184	THR
1	I	308	SER
1	J	56	GLU
1	J	71	ARG
1	J	95	LYS
1	J	135	HIS
1	J	148	LYS
1	J	166	HIS
1	J	224	MET
1	J	300	LEU
1	J	303	ARG
1	J	312	ARG
1	K	29	ASP
1	K	56	GLU
1	K	135	HIS
1	K	166	HIS
1	K	184	THR
1	K	308	SER
1	L	23	LYS
1	L	95	LYS
1	L	135	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	148	LYS
1	L	166	HIS
1	L	301	GLN
1	L	302	LYS
1	L	303	ARG
1	L	306	ASP
1	L	308	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	256	GLN
1	B	256	GLN
1	C	135	HIS
1	C	256	GLN
1	D	256	GLN
1	E	256	GLN
1	F	256	GLN
1	G	135	HIS
1	H	135	HIS
1	H	256	GLN
1	I	135	HIS
1	I	256	GLN
1	J	256	GLN
1	K	256	GLN
1	L	135	HIS
1	L	256	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.