



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:48 PM UTC

PDB ID : 8JFJ / pdb_00008j fj
Title : Crystal structure of enoyl-ACP reductase FabI from Helicobacter pylori
Authors : Song, W.Y.; Zhang, L.
Deposited on : 2023-05-18
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 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

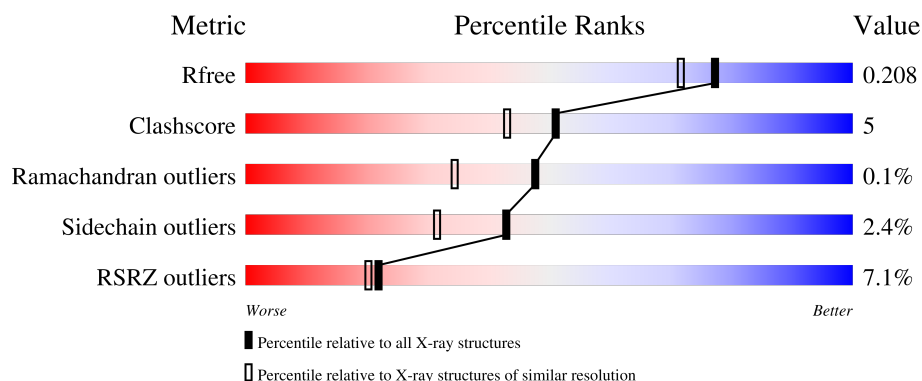
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	275	7% 74% 20% 5% ..
1	B	275	5% 77% 16% • 5%
1	C	275	8% 79% 14% 6% •
1	D	275	7% 77% 15% • 6%
1	E	275	8% 79% 15% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	275	7% 71% 19% 5% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13195 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2090	1336	350	395	9			
1	B	262	Total	C	N	O	S	0	1	0
			2018	1293	336	380	9			
1	C	272	Total	C	N	O	S	0	0	0
			2081	1330	348	394	9			
1	D	258	Total	C	N	O	S	0	0	0
			1983	1272	332	370	9			
1	E	263	Total	C	N	O	S	0	0	0
			2018	1294	336	380	8			
1	F	265	Total	C	N	O	S	0	0	0
			2036	1304	340	383	9			

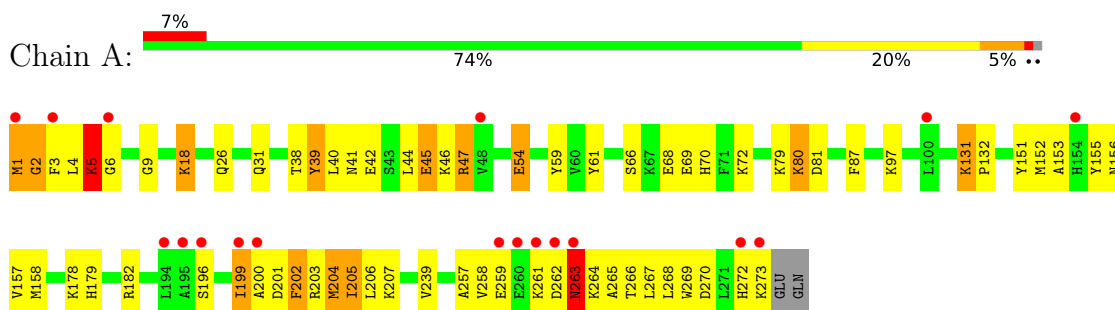
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	169	Total	O	0	0
			169	169		
2	B	172	Total	O	0	0
			172	172		
2	C	153	Total	O	0	0
			153	153		
2	D	172	Total	O	0	0
			172	172		
2	E	165	Total	O	0	0
			165	165		
2	F	138	Total	O	0	0
			138	138		

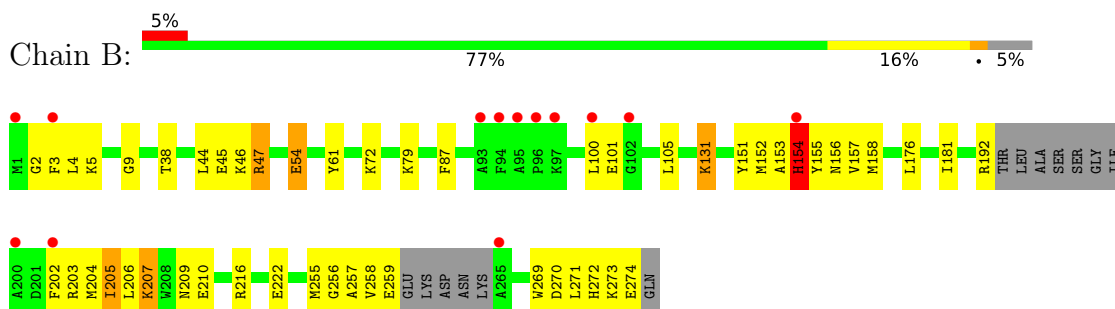
3 Residue-property plots

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.

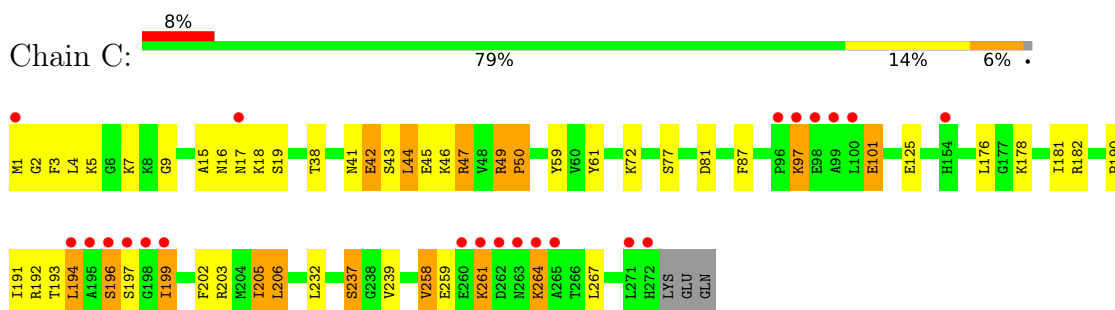
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



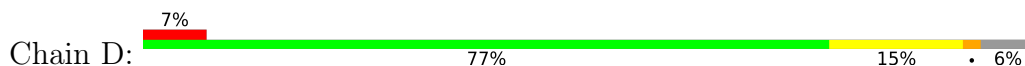
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

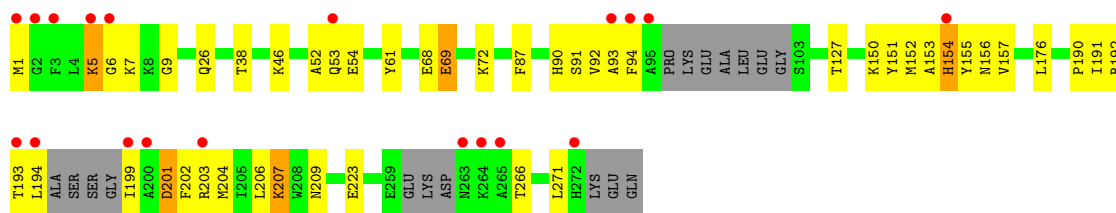


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

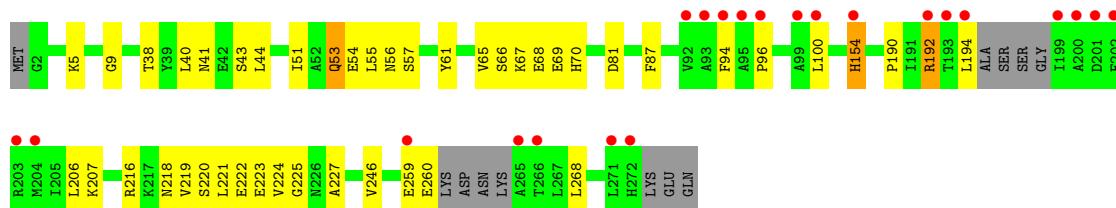
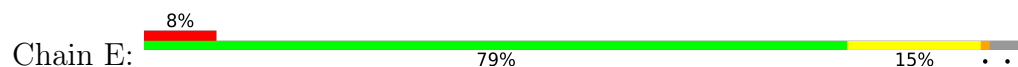


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

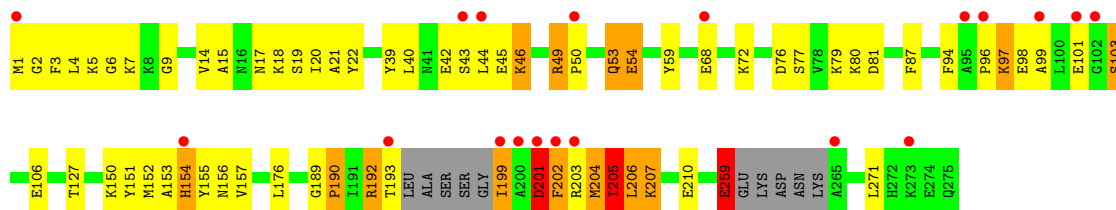




- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	265.76Å 68.34Å 88.16Å 90.00° 108.59° 90.00°	Depositor
Resolution (Å)	41.43 – 1.80 41.43 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (41.43-1.80) 97.4 (41.43-1.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.192 , 0.206 0.194 , 0.208	Depositor DCC
R_{free} test set	6731 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13195	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.94% 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	1.29	49/2128 (2.3%)	1.17	27/2876 (0.9%)
1	B	1.10	35/2057 (1.7%)	0.99	20/2778 (0.7%)
1	C	1.01	29/2119 (1.4%)	0.94	14/2865 (0.5%)
1	D	1.09	29/2017 (1.4%)	1.11	20/2724 (0.7%)
1	E	1.05	27/2054 (1.3%)	0.86	10/2777 (0.4%)
1	F	1.24	43/2072 (2.1%)	1.28	28/2799 (1.0%)
All	All	1.14	212/12447 (1.7%)	1.07	119/16819 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	F	0	3
All	All	0	5

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	57	SER	C-N	16.41	1.46	1.33
1	F	190	PRO	N-CA	15.73	1.66	1.47
1	A	131	LYS	C-N	11.69	1.47	1.33
1	D	190	PRO	C-O	-11.62	1.10	1.23
1	B	131	LYS	C-N	11.52	1.48	1.34
1	F	156	ASN	C-O	-11.17	1.13	1.24
1	A	72	LYS	C-N	10.94	1.47	1.34
1	C	72	LYS	C-N	9.94	1.47	1.34
1	B	256	GLY	C-O	-9.87	1.13	1.23
1	B	72	LYS	C-N	9.86	1.47	1.34
1	E	222	GLU	C-O	-9.73	1.12	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	54	GLU	C-O	-9.65	1.12	1.24
1	A	158	MET	C-O	-9.50	1.12	1.24
1	C	2	GLY	C-O	-9.43	1.14	1.23
1	A	257	ALA	C-O	-9.39	1.11	1.23
1	F	22	TYR	C-O	-9.37	1.13	1.24
1	A	39	TYR	C-O	-9.33	1.13	1.24
1	D	151	TYR	C-O	-9.21	1.12	1.23
1	A	44	LEU	C-O	-9.18	1.12	1.24
1	C	72	LYS	C-O	-8.95	1.15	1.24
1	B	158	MET	C-O	-8.89	1.13	1.24
1	E	220	SER	C-O	-8.79	1.12	1.23
1	E	221	LEU	C-O	-8.79	1.13	1.24
1	A	72	LYS	C-O	-8.78	1.16	1.24
1	A	269	TRP	C-O	-8.60	1.14	1.24
1	E	68	GLU	C-O	-8.60	1.14	1.24
1	D	69	GLU	CD-OE1	-8.47	1.09	1.25
1	E	65	VAL	C-O	-8.36	1.12	1.24
1	B	5	LYS	C-O	-8.34	1.13	1.24
1	C	203	ARG	C-O	-8.30	1.14	1.24
1	F	19	SER	C-O	-8.29	1.13	1.23
1	F	14	VAL	C-O	-8.29	1.14	1.24
1	C	205	ILE	C-O	-8.25	1.14	1.24
1	A	26	GLN	C-O	-8.19	1.14	1.24
1	A	152	MET	C-O	-8.10	1.14	1.23
1	A	203	ARG	C-O	-8.05	1.14	1.24
1	E	55	LEU	C-O	-8.04	1.13	1.24
1	D	153	ALA	C-O	-8.00	1.13	1.23
1	F	21	ALA	C-O	-7.99	1.14	1.24
1	A	97	LYS	C-O	-7.99	1.14	1.24
1	B	2	GLY	C-O	-7.97	1.13	1.23
1	D	156	ASN	C-O	-7.96	1.14	1.24
1	D	207	LYS	C-O	-7.95	1.14	1.24
1	B	209	ASN	C-O	-7.94	1.14	1.24
1	B	157	VAL	C-O	-7.91	1.14	1.24
1	F	3	PHE	C-O	-7.90	1.14	1.24
1	B	151	TYR	C-O	-7.86	1.14	1.23
1	F	7	LYS	C-O	-7.85	1.14	1.23
1	B	72	LYS	C-O	-7.82	1.17	1.24
1	D	152	MET	C-O	-7.80	1.14	1.23
1	D	5	LYS	CB-CG	-7.74	1.29	1.52
1	F	151	TYR	C-O	-7.73	1.14	1.23
1	E	223	GLU	C-O	-7.68	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	17	ASN	C-O	-7.67	1.13	1.24
1	C	206	LEU	C-O	-7.67	1.15	1.24
1	C	16	ASN	C-O	-7.65	1.16	1.24
1	D	155	TYR	C-O	-7.65	1.14	1.24
1	B	203	ARG	C-O	-7.63	1.15	1.24
1	A	206	LEU	C-O	-7.60	1.15	1.24
1	D	69	GLU	C-O	-7.59	1.14	1.24
1	B	270	ASP	CG-OD2	-7.57	1.10	1.25
1	F	202	PHE	C-O	-7.57	1.15	1.24
1	E	5	LYS	C-O	-7.56	1.14	1.23
1	A	266	THR	C-O	-7.52	1.14	1.23
1	A	46	LYS	C-O	-7.49	1.14	1.24
1	A	40	LEU	C-O	-7.48	1.15	1.24
1	A	157	VAL	C-O	-7.46	1.15	1.24
1	A	268	LEU	C-O	-7.44	1.15	1.24
1	B	269	TRP	C-O	-7.43	1.15	1.24
1	F	68	GLU	CB-CG	-7.42	1.30	1.52
1	F	68	GLU	CG-CD	-7.42	1.33	1.52
1	D	90	HIS	C-O	-7.36	1.15	1.23
1	E	69	GLU	C-O	-7.34	1.14	1.24
1	C	19	SER	C-O	-7.33	1.15	1.23
1	B	153	ALA	C-O	-7.33	1.15	1.23
1	A	179	HIS	C-O	-7.24	1.14	1.24
1	A	3	PHE	C-O	-7.20	1.14	1.24
1	C	43	SER	C-O	-7.19	1.15	1.24
1	C	17	ASN	C-O	-7.16	1.14	1.24
1	A	205	ILE	C-O	-7.15	1.15	1.24
1	B	255	MET	C-O	-7.14	1.16	1.23
1	B	272	HIS	C-O	-7.10	1.15	1.24
1	B	257	ALA	C-O	-7.10	1.14	1.23
1	E	224	VAL	C-O	-7.05	1.15	1.24
1	A	79	LYS	C-O	-7.04	1.15	1.24
1	F	153	ALA	C-O	-7.04	1.15	1.23
1	F	94	PHE	C-O	-7.03	1.14	1.23
1	F	155	TYR	C-O	-6.94	1.15	1.24
1	A	155	TYR	C-O	-6.93	1.15	1.24
1	D	202	PHE	C-O	-6.88	1.16	1.24
1	F	203	ARG	C-O	-6.86	1.16	1.24
1	D	94	PHE	C-O	-6.84	1.15	1.24
1	F	207	LYS	C-O	-6.83	1.16	1.24
1	C	49	ARG	C-O	-6.81	1.18	1.24
1	D	93	ALA	C-O	-6.79	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	ASN	C-O	-6.76	1.16	1.24
1	F	6	GLY	C-O	-6.74	1.15	1.24
1	E	223	GLU	CD-OE1	-6.73	1.12	1.25
1	A	156	ASN	C-O	-6.69	1.15	1.24
1	D	157	VAL	C-O	-6.67	1.16	1.24
1	F	210	GLU	CD-OE2	-6.61	1.12	1.25
1	E	56	ASN	C-O	-6.59	1.14	1.23
1	F	157	VAL	C-O	-6.57	1.16	1.24
1	A	267	LEU	C-O	-6.56	1.15	1.23
1	D	204	MET	C-O	-6.54	1.16	1.24
1	A	270	ASP	C-O	-6.53	1.16	1.24
1	B	207	LYS	C-O	-6.53	1.15	1.24
1	A	41	ASN	C-O	-6.50	1.16	1.23
1	E	53	GLN	C-O	-6.50	1.16	1.24
1	C	5	LYS	C-O	-6.43	1.16	1.23
1	F	54	GLU	C-N	-6.42	1.25	1.33
1	B	270	ASP	CG-OD1	-6.39	1.13	1.25
1	A	68	GLU	C-O	-6.39	1.16	1.24
1	A	151	TYR	C-O	-6.38	1.16	1.23
1	C	47	ARG	C-O	-6.34	1.15	1.23
1	A	45	GLU	C-O	-6.31	1.16	1.24
1	C	18	LYS	C-O	-6.30	1.15	1.23
1	B	156	ASN	C-O	-6.29	1.16	1.24
1	A	204	MET	C-O	-6.28	1.16	1.24
1	B	4	LEU	C-O	-6.27	1.14	1.23
1	C	50	PRO	C-O	-6.25	1.16	1.24
1	C	4	LEU	C-O	-6.25	1.14	1.23
1	C	202	PHE	C-O	-6.24	1.16	1.24
1	F	205	ILE	C-O	-6.24	1.16	1.24
1	B	205	ILE	C-O	-6.21	1.16	1.24
1	E	70	HIS	C-O	-6.17	1.16	1.24
1	F	50	PRO	CB-CG	-6.15	1.19	1.49
1	A	70	HIS	CG-ND1	-6.14	1.31	1.38
1	E	51	ILE	C-O	-6.14	1.17	1.24
1	C	42	GLU	C-O	-6.12	1.17	1.24
1	B	45	GLU	CD-OE1	-6.11	1.13	1.25
1	B	152	MET	C-O	-6.10	1.16	1.23
1	D	203	ARG	C-O	-6.08	1.17	1.24
1	B	44	LEU	C-O	-6.06	1.16	1.24
1	F	189	GLY	C-N	6.04	1.40	1.33
1	A	42	GLU	C-O	-6.02	1.17	1.24
1	A	265	ALA	C-O	-6.01	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	15	ALA	C-O	-6.01	1.15	1.23
1	A	202	PHE	C-O	-6.00	1.17	1.24
1	F	206	LEU	C-O	-5.99	1.17	1.24
1	A	178	LYS	C-O	-5.98	1.16	1.24
1	D	53	GLN	CB-CG	-5.97	1.34	1.52
1	A	69	GLU	C-O	-5.96	1.16	1.24
1	E	223	GLU	CD-OE2	-5.96	1.14	1.25
1	A	258	VAL	C-O	-5.93	1.17	1.23
1	C	7	LYS	C-O	-5.93	1.16	1.23
1	D	68	GLU	C-O	-5.91	1.16	1.24
1	F	4	LEU	C-O	-5.90	1.15	1.24
1	F	20	ILE	C-O	-5.89	1.17	1.24
1	F	204	MET	C-O	-5.88	1.17	1.24
1	D	46	LYS	C-O	-5.85	1.16	1.24
1	B	270	ASP	C-O	-5.83	1.17	1.24
1	F	190	PRO	C-O	-5.83	1.16	1.23
1	D	53	GLN	CD-OE1	5.82	1.34	1.23
1	E	225	GLY	C-O	-5.82	1.16	1.23
1	C	50	PRO	N-CD	-5.81	1.39	1.47
1	F	18	LYS	C-O	-5.80	1.16	1.23
1	A	70	HIS	CE1-NE2	-5.79	1.26	1.32
1	C	41	ASN	C-O	-5.78	1.18	1.24
1	C	197	SER	C-O	-5.75	1.16	1.24
1	F	152	MET	C-O	-5.75	1.17	1.23
1	A	45	GLU	CD-OE2	-5.74	1.14	1.25
1	C	191	ILE	C-O	-5.73	1.17	1.24
1	C	46	LYS	C-O	-5.73	1.17	1.24
1	B	47	ARG	C-O	-5.72	1.16	1.24
1	C	44	LEU	C-O	-5.67	1.16	1.24
1	B	271	LEU	C-O	-5.67	1.17	1.24
1	E	70	HIS	CG-ND1	-5.66	1.32	1.38
1	F	103	SER	C-O	-5.66	1.16	1.23
1	D	92	VAL	C-O	-5.65	1.18	1.24
1	E	192	ARG	CG-CD	-5.65	1.35	1.52
1	A	54	GLU	C-O	-5.64	1.17	1.24
1	E	67	LYS	C-O	-5.63	1.17	1.24
1	E	66	SER	C-O	-5.60	1.16	1.24
1	A	66	SER	C-O	-5.57	1.16	1.24
1	A	18	LYS	C-O	-5.54	1.16	1.24
1	F	2	GLY	C-O	-5.52	1.16	1.23
1	B	258	VAL	C-O	-5.49	1.17	1.23
1	E	219	VAL	C-O	-5.49	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	96	PRO	C-O	-5.48	1.17	1.23
1	A	201	ASP	C-O	-5.47	1.17	1.24
1	F	19	SER	CA-CB	-5.46	1.44	1.53
1	B	3	PHE	C-O	-5.43	1.17	1.24
1	F	99	ALA	C-O	-5.42	1.17	1.24
1	B	46	LYS	C-O	-5.42	1.17	1.24
1	F	192	ARG	C-O	-5.39	1.17	1.24
1	E	54	GLU	C-O	-5.38	1.17	1.24
1	A	153	ALA	C-O	-5.38	1.17	1.23
1	C	45	GLU	C-O	-5.37	1.17	1.24
1	C	194	LEU	C-O	-5.35	1.17	1.24
1	C	15	ALA	C-O	-5.35	1.16	1.23
1	A	200	ALA	C-O	-5.33	1.18	1.24
1	F	49	ARG	CB-CG	-5.33	1.36	1.52
1	C	3	PHE	C-O	-5.29	1.17	1.24
1	E	207	LYS	CG-CD	-5.28	1.36	1.52
1	D	192	ARG	C-O	-5.28	1.17	1.23
1	F	150	LYS	C-O	-5.27	1.17	1.23
1	B	131	LYS	C-O	-5.26	1.19	1.24
1	D	91	SER	C-O	-5.26	1.15	1.23
1	D	150	LYS	C-O	-5.23	1.17	1.23
1	D	207	LYS	C-N	-5.23	1.27	1.33
1	E	70	HIS	CE1-NE2	-5.19	1.27	1.32
1	A	2	GLY	C-O	-5.17	1.17	1.23
1	B	204	MET	C-O	-5.14	1.18	1.24
1	B	155	TYR	C-O	-5.13	1.15	1.23
1	A	270	ASP	CG-OD1	-5.13	1.15	1.25
1	D	191	ILE	C-O	-5.08	1.18	1.24
1	A	199	ILE	C-O	-5.06	1.18	1.24
1	D	90	HIS	CE1-NE2	-5.04	1.27	1.32
1	B	45	GLU	C-O	-5.03	1.17	1.24
1	F	210	GLU	C-O	-5.03	1.18	1.24
1	E	218	ASN	C-O	-5.00	1.17	1.23

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	LYS	CB-CG-CD	-14.65	77.61	111.30
1	F	259	GLU	CG-CD-OE1	14.02	150.65	118.40
1	F	189	GLY	CA-C-N	13.67	134.59	119.83
1	F	189	GLY	C-N-CA	13.67	134.59	119.83
1	F	259	GLU	CG-CD-OE2	-13.59	87.15	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	259	GLU	OE1-CD-OE2	-12.81	92.16	122.90
1	D	53	GLN	N-CA-C	-12.66	97.47	113.16
1	F	201	ASP	CB-CA-C	12.16	130.98	110.79
1	D	52	ALA	CA-C-N	-11.25	102.01	122.38
1	D	52	ALA	C-N-CA	-11.25	102.01	122.38
1	A	47	ARG	CA-C-O	-11.22	106.47	119.60
1	F	80	LYS	CA-C-O	-10.97	108.79	120.42
1	D	6	GLY	N-CA-C	-10.96	100.79	115.36
1	F	190	PRO	CB-CA-C	10.81	125.27	111.64
1	D	192	ARG	CG-CD-NE	-10.74	88.38	112.00
1	D	93	ALA	CA-C-O	-10.59	108.67	120.32
1	A	47	ARG	CG-CD-NE	-10.44	89.03	112.00
1	C	72	LYS	O-C-N	-10.09	111.50	120.48
1	A	72	LYS	CA-C-N	10.06	129.81	118.85
1	A	72	LYS	C-N-CA	10.06	129.81	118.85
1	F	42	GLU	CA-CB-CG	10.02	134.14	114.10
1	B	72	LYS	O-C-N	-9.91	111.66	120.48
1	C	42	GLU	CB-CG-CD	9.69	129.06	112.60
1	C	42	GLU	CB-CA-C	9.59	126.71	110.79
1	A	47	ARG	CA-C-N	-9.58	103.81	120.29
1	A	47	ARG	C-N-CA	-9.58	103.81	120.29
1	B	131	LYS	O-C-N	-9.49	111.30	120.70
1	E	192	ARG	CA-CB-CG	-9.28	95.53	114.10
1	E	192	ARG	CB-CG-CD	9.18	132.41	111.30
1	C	101	GLU	CB-CA-C	-8.95	92.30	109.66
1	D	201	ASP	CA-CB-CG	8.81	121.41	112.60
1	A	72	LYS	O-C-N	-8.73	112.51	120.71
1	F	201	ASP	CA-CB-CG	8.54	121.14	112.60
1	A	131	LYS	O-C-N	-8.31	112.78	120.51
1	F	53	GLN	O-C-N	-8.18	113.64	122.07
1	F	202	PHE	CB-CA-C	-8.15	96.99	110.85
1	A	262	ASP	CA-C-N	7.91	133.59	122.36
1	A	262	ASP	C-N-CA	7.91	133.59	122.36
1	E	57	SER	O-C-N	-7.84	114.41	121.39
1	B	155	TYR	CB-CA-C	7.76	121.38	109.34
1	B	54	GLU	CB-CA-C	-7.72	97.97	110.79
1	A	131	LYS	CA-C-N	7.70	127.41	119.56
1	A	131	LYS	C-N-CA	7.70	127.41	119.56
1	A	5	LYS	CA-C-N	-7.65	108.21	122.05
1	A	5	LYS	C-N-CA	-7.65	108.21	122.05
1	B	3	PHE	CA-CB-CG	7.56	121.36	113.80
1	B	72	LYS	CA-C-N	7.53	127.41	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	LYS	C-N-CA	7.53	127.41	119.05
1	B	273	LYS	CA-C-N	7.52	135.24	121.70
1	B	273	LYS	C-N-CA	7.52	135.24	121.70
1	B	222[A]	GLU	CA-C-O	7.52	128.59	120.10
1	B	222[B]	GLU	CA-C-O	7.52	128.59	120.10
1	F	190	PRO	N-CA-C	-7.48	99.51	111.03
1	D	206	LEU	CA-C-O	-7.41	113.04	120.82
1	F	80	LYS	CA-C-N	-7.23	106.23	121.64
1	F	80	LYS	C-N-CA	-7.23	106.23	121.64
1	B	54	GLU	OE1-CD-OE2	-7.22	105.58	122.90
1	B	274	GLU	CB-CG-CD	7.16	124.77	112.60
1	F	155	TYR	CB-CA-C	7.14	122.99	110.85
1	D	54	GLU	N-CA-CB	7.12	121.31	110.28
1	B	154	HIS	CA-C-O	-7.08	112.07	120.57
1	C	178	LYS	CA-CB-CG	7.04	128.19	114.10
1	D	68	GLU	CA-C-O	-7.02	110.99	119.49
1	E	192	ARG	NE-CZ-NH2	-6.97	112.93	119.20
1	F	49	ARG	CG-CD-NE	-6.96	96.70	112.00
1	E	192	ARG	N-CA-C	6.95	119.80	109.59
1	A	264	LYS	N-CA-C	6.91	124.10	113.19
1	A	263	ASN	CA-C-O	-6.84	113.90	121.84
1	A	202	PHE	CA-CB-CG	-6.82	106.98	113.80
1	D	5	LYS	CB-CA-C	-6.77	99.68	109.84
1	C	72	LYS	CA-C-N	6.67	126.46	119.05
1	C	72	LYS	C-N-CA	6.67	126.46	119.05
1	A	80	LYS	CB-CG-CD	6.54	126.35	111.30
1	C	178	LYS	CB-CA-C	6.38	124.46	110.18
1	D	53	GLN	CG-CD-NE2	-6.35	106.88	116.40
1	A	178	LYS	CB-CA-C	-6.34	98.89	110.63
1	D	154	HIS	CA-CB-CG	6.26	120.06	113.80
1	E	57	SER	CA-C-N	6.23	128.22	121.00
1	E	57	SER	C-N-CA	6.23	128.22	121.00
1	A	262	ASP	CB-CA-C	6.15	120.77	111.80
1	D	93	ALA	N-CA-CB	-6.12	100.95	110.55
1	A	97	LYS	CA-C-O	-6.09	114.09	120.55
1	E	154	HIS	CA-CB-CG	6.06	119.86	113.80
1	A	46	LYS	N-CA-C	-5.98	104.83	111.71
1	A	3	PHE	CA-CB-CG	-5.90	107.90	113.80
1	F	49	ARG	CB-CA-C	-5.90	98.54	110.17
1	D	94	PHE	N-CA-C	5.87	123.31	110.80
1	C	47	ARG	CB-CG-CD	-5.87	97.80	111.30
1	A	259	GLU	CA-C-N	-5.81	112.87	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	GLU	C-N-CA	-5.81	112.87	121.24
1	B	54	GLU	CG-CD-OE1	5.80	131.74	118.40
1	D	201	ASP	CB-CA-C	5.77	120.65	110.85
1	C	97	LYS	CB-CG-CD	-5.76	98.05	111.30
1	F	203	ARG	CB-CG-CD	5.75	124.54	111.30
1	E	54	GLU	CB-CG-CD	5.73	122.34	112.60
1	F	42	GLU	N-CA-C	5.71	119.05	111.75
1	D	5	LYS	CG-CD-CE	-5.66	98.28	111.30
1	E	192	ARG	CD-NE-CZ	5.63	132.29	124.40
1	C	264	LYS	CB-CG-CD	5.62	124.23	111.30
1	B	54	GLU	CG-CD-OE2	-5.57	105.58	118.40
1	F	46	LYS	CB-CA-C	5.51	121.51	109.99
1	F	189	GLY	O-C-N	-5.49	115.78	122.03
1	D	193	THR	CA-CB-OG1	-5.46	101.42	109.60
1	B	72	LYS	N-CA-CB	5.38	118.31	110.30
1	F	206	LEU	N-CA-CB	-5.35	102.26	110.01
1	C	258	VAL	CA-C-N	-5.28	113.62	122.92
1	C	258	VAL	C-N-CA	-5.28	113.62	122.92
1	B	131	LYS	CA-C-N	5.25	124.86	119.56
1	B	131	LYS	C-N-CA	5.25	124.86	119.56
1	A	259	GLU	CB-CA-C	-5.24	98.98	109.35
1	A	262	ASP	CA-CB-CG	5.23	117.83	112.60
1	F	50	PRO	N-CA-C	-5.22	105.32	113.78
1	F	42	GLU	CB-CG-CD	-5.16	103.84	112.60
1	D	5	LYS	N-CA-C	5.15	117.81	110.24
1	B	72	LYS	CB-CA-C	-5.11	103.26	112.76
1	F	49	ARG	N-CA-C	5.07	121.02	109.81
1	F	201	ASP	CA-C-N	5.07	127.48	120.29
1	F	201	ASP	C-N-CA	5.07	127.48	120.29
1	C	72	LYS	N-CA-C	-5.02	105.92	112.75

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	54	GLU	Sidechain
1	C	259	GLU	Sidechain
1	F	259	GLU	Sidechain
1	F	53	GLN	Mainchain
1	F	79	LYS	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	2090	0	2122	18	0
1	B	2018	0	2043	12	0
1	C	2081	0	2109	30	0
1	D	1983	0	2014	20	0
1	E	2018	0	2041	27	0
1	F	2036	0	2063	34	0
2	A	169	0	0	3	1
2	B	172	0	0	3	1
2	C	153	0	0	2	0
2	D	172	0	0	2	1
2	E	165	0	0	2	1
2	F	138	0	0	4	1
All	All	13195	0	12392	129	3

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 5.

All (129) 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:F:154:HIS:CD2	1:F:201:ASP:OD2	1.66	1.44
1:F:154:HIS:HD2	1:F:201:ASP:CG	1.56	1.12
1:F:154:HIS:HD2	1:F:201:ASP:OD2	1.06	1.12
1:F:97:LYS:H	1:F:97:LYS:HD2	1.15	1.08
1:C:192:ARG:HD2	1:E:53:GLN:HG2	1.46	0.97
1:C:261:LYS:O	1:C:264:LYS:HG2	1.65	0.95
1:F:154:HIS:CD2	1:F:201:ASP:CG	2.36	0.95
1:E:259:GLU:OE1	2:E:301:HOH:O	1.83	0.94
1:C:192:ARG:CD	1:E:53:GLN:HG2	2.04	0.87
1:A:1:MET:HA	1:A:5:LYS:HG2	1.54	0.87
1:D:154:HIS:CG	1:D:201:ASP:OD2	2.30	0.84
1:F:76:ASP:OD2	2:F:301:HOH:O	1.94	0.83
1:F:98:GLU:OE1	1:F:98:GLU:N	2.12	0.82
1:F:97:LYS:HD2	1:F:97:LYS:N	1.95	0.81
1:C:97:LYS:N	1:C:97:LYS:HD3	1.97	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:LYS:H	1:F:97:LYS:CD	1.95	0.79
1:F:154:HIS:NE2	1:F:201:ASP:OD2	2.15	0.79
1:E:94:PHE:CZ	1:E:96:PRO:HG3	2.18	0.78
1:F:259:GLU:HG2	1:F:271:LEU:HD11	1.66	0.78
1:F:45:GLU:OE2	2:F:302:HOH:O	2.03	0.76
1:F:199:ILE:HG22	1:F:202:PHE:H	1.52	0.74
1:A:80:LYS:HE3	2:A:376:HOH:O	1.88	0.73
1:D:154:HIS:CD2	1:D:201:ASP:OD2	2.40	0.73
1:D:5:LYS:NZ	1:E:192:ARG:HD2	2.04	0.73
1:D:5:LYS:HZ2	1:E:192:ARG:HD2	1.55	0.71
1:A:263:ASN:O	1:A:263:ASN:ND2	2.17	0.71
1:E:100:LEU:CD2	1:E:154:HIS:CD2	2.75	0.70
1:A:80:LYS:CE	2:A:376:HOH:O	2.40	0.69
1:B:79:LYS:NZ	2:B:303:HOH:O	2.25	0.69
1:C:49:ARG:HB3	1:C:50:PRO:HD3	1.74	0.69
1:F:49:ARG:NH2	2:F:302:HOH:O	2.15	0.68
1:C:192:ARG:HA	1:C:206:LEU:HD21	1.74	0.68
1:F:49:ARG:NE	2:F:302:HOH:O	2.19	0.67
1:F:40:LEU:HB3	1:F:44:LEU:HD12	1.77	0.65
1:C:199:ILE:N	1:C:199:ILE:HD13	2.13	0.64
1:F:77:SER:O	1:F:81:ASP:N	2.31	0.64
1:E:41:ASN:OD1	1:E:43:SER:HB3	1.98	0.63
1:F:154:HIS:CD2	1:F:201:ASP:OD1	2.52	0.61
1:E:100:LEU:HD21	1:E:154:HIS:CD2	2.37	0.59
1:A:196:SER:HB3	1:A:202:PHE:CD2	2.38	0.59
1:C:261:LYS:O	1:C:264:LYS:CG	2.45	0.58
1:D:69:GLU:HG3	2:D:313:HOH:O	2.02	0.58
1:C:237:SER:OG	1:D:223:GLU:OE2	2.10	0.58
1:D:5:LYS:C	1:D:7:LYS:H	2.13	0.57
1:D:5:LYS:C	1:D:7:LYS:N	2.63	0.56
1:A:263:ASN:HD22	1:A:263:ASN:C	2.12	0.56
2:C:431:HOH:O	1:E:194:LEU:HD23	2.06	0.54
1:D:5:LYS:NZ	1:E:192:ARG:CD	2.71	0.53
1:F:59:TYR:CE1	1:F:81:ASP:HB3	2.44	0.53
1:C:192:ARG:HD3	1:E:53:GLN:HG2	1.88	0.52
1:F:154:HIS:ND1	1:F:154:HIS:C	2.68	0.52
1:E:81:ASP:OD2	2:E:302:HOH:O	2.19	0.52
1:C:61:TYR:CE1	1:C:77:SER:HB3	2.45	0.52
1:F:39:TYR:CD1	1:F:45:GLU:HB2	2.45	0.52
1:D:69:GLU:H	1:D:69:GLU:CD	2.19	0.50
1:B:38:THR:HA	1:B:61:TYR:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLU:OE2	2:C:301:HOH:O	2.19	0.49
1:B:100:LEU:O	1:B:154:HIS:CD2	2.66	0.49
1:D:38:THR:HA	1:D:61:TYR:O	2.13	0.49
1:E:94:PHE:O	1:E:96:PRO:HD3	2.13	0.49
1:F:54:GLU:O	1:F:54:GLU:HG2	2.13	0.48
1:F:72:LYS:HE2	1:F:76:ASP:OD1	2.14	0.48
1:F:103:SER:OG	1:F:106:GLU:HG3	2.13	0.48
1:F:204:MET:HB3	1:F:204:MET:HE3	1.38	0.48
1:D:266:THR:HG21	1:D:271:LEU:HD21	1.96	0.47
1:D:5:LYS:HE3	1:D:5:LYS:HB2	1.43	0.47
1:B:9:GLY:HA3	1:B:87:PHE:CZ	2.49	0.47
1:C:97:LYS:N	1:C:97:LYS:CD	2.74	0.47
1:A:263:ASN:ND2	1:A:263:ASN:C	2.73	0.47
1:C:237:SER:HB3	1:D:223:GLU:HG2	1.95	0.46
1:C:192:ARG:HD3	1:E:53:GLN:CG	2.46	0.46
1:A:2:GLY:HA3	1:A:31:GLN:OE1	2.14	0.46
1:F:98:GLU:HA	1:F:101:GLU:HG3	1.98	0.46
1:D:127:THR:HG21	1:D:176:LEU:HD11	1.97	0.46
1:A:38:THR:HA	1:A:61:TYR:O	2.15	0.45
1:C:176:LEU:HB3	1:C:181:ILE:HB	1.97	0.45
1:E:216:ARG:NH2	1:E:268:LEU:HD11	2.30	0.45
1:E:38:THR:HA	1:E:61:TYR:O	2.16	0.45
1:E:190:PRO:HB2	1:E:206:LEU:HD23	1.97	0.45
1:D:9:GLY:HA3	1:D:87:PHE:CZ	2.51	0.45
1:F:192:ARG:HA	1:F:206:LEU:HD21	1.98	0.45
1:C:193:THR:HG1	1:C:196:SER:HG	1.56	0.45
1:E:94:PHE:CE2	1:E:96:PRO:HG3	2.52	0.45
1:F:207:LYS:HD2	1:F:207:LYS:HA	1.77	0.45
1:B:176:LEU:HB3	1:B:181:ILE:HB	1.98	0.45
1:C:38:THR:HA	1:C:61:TYR:O	2.16	0.45
1:F:43:SER:O	1:F:46:LYS:HG2	2.17	0.45
1:E:259:GLU:O	1:E:260:GLU:HB2	2.17	0.44
1:C:1:MET:HE3	1:C:1:MET:HB2	1.75	0.44
1:A:131:LYS:HB3	1:A:132:PRO:HD3	2.00	0.44
1:A:59:TYR:CE1	1:A:81:ASP:HB3	2.53	0.44
1:C:47:ARG:HD3	1:C:47:ARG:HA	1.62	0.44
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.81	0.43
1:C:59:TYR:CE1	1:C:81:ASP:HB3	2.52	0.43
1:E:40:LEU:HB3	1:E:44:LEU:HD22	1.99	0.43
1:C:97:LYS:HB2	1:C:97:LYS:HE2	1.78	0.43
1:C:190:PRO:HB2	1:C:206:LEU:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLY:HA3	1:A:87:PHE:CZ	2.53	0.43
1:B:216:ARG:NE	2:B:302:HOH:O	2.22	0.43
1:C:9:GLY:HA3	1:C:87:PHE:CZ	2.53	0.43
1:C:182:ARG:HD2	1:C:239:VAL:O	2.18	0.43
1:D:5:LYS:HZ3	1:E:192:ARG:HD2	1.84	0.43
1:E:100:LEU:HD21	1:E:154:HIS:HD2	1.84	0.43
1:A:6:GLY:HA2	2:A:322:HOH:O	2.19	0.43
1:B:101:GLU:HB2	2:B:398:HOH:O	2.19	0.43
1:C:258:VAL:HG12	1:C:267:LEU:HD23	2.00	0.43
1:A:272:HIS:O	1:A:273:LYS:HB2	2.19	0.42
1:B:202:PHE:HA	1:B:205:ILE:HG22	2.01	0.42
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.83	0.42
1:C:261:LYS:HE3	1:C:261:LYS:HB2	1.63	0.42
1:F:9:GLY:HA3	1:F:87:PHE:CZ	2.53	0.42
1:D:26:GLN:HG2	2:D:302:HOH:O	2.19	0.42
1:A:182:ARG:HD2	1:A:239:VAL:O	2.19	0.42
1:E:9:GLY:HA3	1:E:87:PHE:CZ	2.54	0.42
1:F:190:PRO:HB2	1:F:206:LEU:HD13	2.02	0.42
1:F:205:ILE:HD12	1:F:205:ILE:O	2.19	0.41
1:C:9:GLY:HA3	1:C:87:PHE:CE2	2.55	0.41
1:A:39:TYR:CD1	1:A:45:GLU:HB2	2.55	0.41
1:C:87:PHE:HB2	1:C:232:LEU:HD22	2.03	0.41
1:F:127:THR:HG21	1:F:176:LEU:HD11	2.02	0.41
1:C:192:ARG:CD	1:E:53:GLN:CG	2.87	0.41
1:D:5:LYS:HZ3	1:E:192:ARG:CD	2.33	0.41
1:B:47:ARG:HH11	1:B:47:ARG:HD2	1.74	0.40
1:B:192:ARG:HA	1:B:206:LEU:HD11	2.02	0.40
1:E:227:ALA:CB	1:E:246:VAL:HG21	2.51	0.40
1:D:154:HIS:CB	1:D:201:ASP:OD2	2.70	0.40
1:F:1:MET:O	1:F:1:MET:HG3	2.20	0.40
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.90	0.40
1:B:207:LYS:NZ	1:B:210:GLU:OE2	2.44	0.40

All (3) 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:E:409:HOH:O	2:F:435:HOH:O[2_555]	1.87	0.33
2:D:450:HOH:O	2:D:450:HOH:O[2_554]	1.97	0.23
2:A:408:HOH:O	2:B:443:HOH:O[4_554]	2.03	0.17

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	271/275 (98%)	262 (97%)	9 (3%)	0	100	100
1	B	257/275 (94%)	253 (98%)	4 (2%)	0	100	100
1	C	270/275 (98%)	264 (98%)	5 (2%)	1 (0%)	30	19
1	D	250/275 (91%)	240 (96%)	10 (4%)	0	100	100
1	E	257/275 (94%)	251 (98%)	6 (2%)	0	100	100
1	F	259/275 (94%)	256 (99%)	3 (1%)	0	100	100
All	All	1564/1650 (95%)	1526 (98%)	37 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	237	SER

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	225/227 (99%)	215 (96%)	10 (4%)	25	13
1	B	217/227 (96%)	214 (99%)	3 (1%)	59	52
1	C	224/227 (99%)	216 (96%)	8 (4%)	31	18
1	D	214/227 (94%)	210 (98%)	4 (2%)	50	41
1	E	217/227 (96%)	217 (100%)	0	100	100
1	F	219/227 (96%)	212 (97%)	7 (3%)	34	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1316/1362 (97%)	1284 (98%)	32 (2%)	43 31

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	18	LYS
1	A	47	ARG
1	A	54	GLU
1	A	199	ILE
1	A	204	MET
1	A	205	ILE
1	A	261	LYS
1	A	263	ASN
1	B	131	LYS
1	B	154	HIS
1	B	259	GLU
1	C	42	GLU
1	C	44	LEU
1	C	101	GLU
1	C	194	LEU
1	C	196	SER
1	C	199	ILE
1	C	205	ILE
1	C	261	LYS
1	D	1	MET
1	D	194	LEU
1	D	199	ILE
1	D	207	LYS
1	F	5	LYS
1	F	97	LYS
1	F	154	HIS
1	F	193	THR
1	F	199	ILE
1	F	201	ASP
1	F	205	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	136	ASN
1	A	154	HIS
1	B	154	HIS
1	B	251	HIS
1	B	272	HIS
1	C	26	GLN
1	C	128	ASN
1	C	154	HIS
1	C	272	HIS
1	D	154	HIS
1	E	154	HIS
1	F	154	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	273/275 (99%)	0.16	18 (6%)	24 23	11, 18, 43, 57	0
1	B	262/275 (95%)	0.21	13 (4%)	34 33	12, 20, 44, 60	1 (0%)
1	C	272/275 (98%)	0.33	22 (8%)	18 16	11, 21, 49, 64	0
1	D	258/275 (93%)	0.13	19 (7%)	20 19	10, 17, 41, 67	0
1	E	263/275 (95%)	0.21	22 (8%)	17 15	11, 20, 45, 64	0
1	F	265/275 (96%)	0.27	19 (7%)	21 20	11, 20, 48, 61	0
All	All	1593/1650 (96%)	0.22	113 (7%)	22 20	10, 20, 47, 67	1 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	94	PHE	5.9
1	E	99	ALA	5.7
1	B	154	HIS	5.4
1	E	199	ILE	5.3
1	D	199	ILE	5.1
1	F	154	HIS	5.0
1	B	100	LEU	4.9
1	D	5	LYS	4.7
1	D	93	ALA	4.6
1	F	199	ILE	4.6
1	A	261	LYS	4.4
1	D	194	LEU	4.4
1	B	96	PRO	4.3
1	E	95	ALA	4.3
1	C	196	SER	4.2
1	D	95	ALA	4.2
1	F	265	ALA	4.2
1	D	272	HIS	4.1
1	E	265	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	ASN	4.0
1	C	194	LEU	3.9
1	D	265	ALA	3.7
1	E	96	PRO	3.6
1	C	262	ASP	3.6
1	B	200	ALA	3.5
1	E	93	ALA	3.5
1	B	1	MET	3.5
1	D	154	HIS	3.5
1	A	273	LYS	3.5
1	D	263	ASN	3.4
1	A	1	MET	3.4
1	B	95	ALA	3.4
1	B	265	ALA	3.3
1	D	200	ALA	3.3
1	A	260	GLU	3.3
1	A	196	SER	3.3
1	C	261	LYS	3.3
1	C	264	LYS	3.2
1	C	195	ALA	3.2
1	E	194	LEU	3.2
1	A	154	HIS	3.2
1	F	1	MET	3.1
1	E	202	PHE	3.1
1	A	200	ALA	3.1
1	D	2	GLY	3.0
1	F	273	LYS	3.0
1	D	6	GLY	3.0
1	C	265	ALA	3.0
1	C	154	HIS	2.9
1	B	93	ALA	2.9
1	C	272	HIS	2.9
1	A	48	VAL	2.8
1	B	97	LYS	2.8
1	F	95	ALA	2.8
1	E	92	VAL	2.8
1	E	192	ARG	2.8
1	F	201	ASP	2.8
1	D	1	MET	2.8
1	E	100	LEU	2.8
1	C	260	GLU	2.8
1	C	198	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	262	ASP	2.7
1	C	96	PRO	2.7
1	E	154	HIS	2.6
1	C	1	MET	2.6
1	C	263	ASN	2.6
1	A	195	ALA	2.6
1	A	199	ILE	2.6
1	B	3	PHE	2.5
1	E	271	LEU	2.5
1	D	193	THR	2.5
1	F	200	ALA	2.5
1	D	94	PHE	2.4
1	E	200	ALA	2.4
1	C	100	LEU	2.4
1	E	266	THR	2.4
1	C	99	ALA	2.4
1	A	194	LEU	2.4
1	F	96	PRO	2.4
1	E	272	HIS	2.4
1	F	193	THR	2.3
1	F	203	ARG	2.3
1	E	201	ASP	2.3
1	A	100	LEU	2.3
1	A	3	PHE	2.3
1	F	102	GLY	2.3
1	E	259	GLU	2.2
1	C	197	SER	2.2
1	D	53	GLN	2.2
1	F	99	ALA	2.2
1	B	202	PHE	2.2
1	A	6	GLY	2.2
1	B	102	GLY	2.2
1	F	50	PRO	2.2
1	F	101	GLU	2.2
1	D	203	ARG	2.2
1	B	94	PHE	2.1
1	C	17	ASN	2.1
1	C	271	LEU	2.1
1	F	44	LEU	2.1
1	A	272	HIS	2.1
1	D	3	PHE	2.1
1	C	199	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	193	THR	2.1
1	E	204	MET	2.1
1	F	43	SER	2.1
1	D	264	LYS	2.1
1	F	68	GLU	2.1
1	A	259	GLU	2.0
1	C	97	LYS	2.0
1	C	98	GLU	2.0
1	F	202	PHE	2.0
1	E	203	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.