



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:28 PM UTC

PDB ID : 5EXV / pdb_00005exv
Title : Crystal structure of heme binding protein HutX from *Vibrio cholerae*
Authors : Sekine, Y.; Tanaka, Y.; Uchida, T.
Deposited on : 2015-11-24
Resolution : 2.90 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

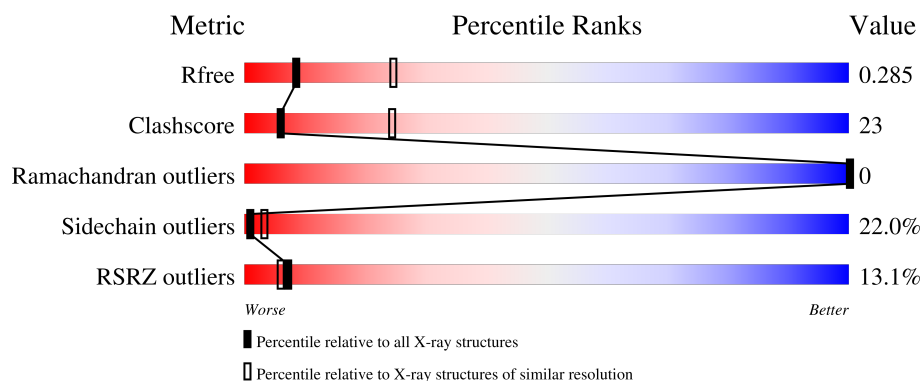
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	189	8% 35% 36% 15% 14%
1	B	189	55% 28% 6% 12%
1	C	189	6% 49% 27% 12% 13%
1	D	189	% 55% 25% 6% 13%
1	E	189	31% 40% 38% 11% 12%

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Mol	Chain	Length	Quality of chain
1	F	189	23% 38% 38% 13% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7856 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 Hemin-degrading HemS.ChuX domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1286	823	221	236	6			
1	B	167	Total	C	N	O	S	0	0	0
			1321	844	227	243	7			
1	C	165	Total	C	N	O	S	0	0	0
			1303	833	223	240	7			
1	D	165	Total	C	N	O	S	0	0	0
			1304	834	224	240	6			
1	E	167	Total	C	N	O	S	0	0	0
			1321	844	227	243	7			
1	F	167	Total	C	N	O	S	0	0	0
			1321	844	227	243	7			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A0A085SE34
A	-20	GLY	-	expression tag	UNP A0A085SE34
A	-19	SER	-	expression tag	UNP A0A085SE34
A	-18	SER	-	expression tag	UNP A0A085SE34
A	-17	HIS	-	expression tag	UNP A0A085SE34
A	-16	HIS	-	expression tag	UNP A0A085SE34
A	-15	HIS	-	expression tag	UNP A0A085SE34
A	-14	HIS	-	expression tag	UNP A0A085SE34
A	-13	HIS	-	expression tag	UNP A0A085SE34
A	-12	HIS	-	expression tag	UNP A0A085SE34
A	-11	SER	-	expression tag	UNP A0A085SE34
A	-10	SER	-	expression tag	UNP A0A085SE34
A	-9	GLY	-	expression tag	UNP A0A085SE34
A	-8	LEU	-	expression tag	UNP A0A085SE34
A	-7	GLU	-	expression tag	UNP A0A085SE34
A	-6	VAL	-	expression tag	UNP A0A085SE34
A	-5	LEU	-	expression tag	UNP A0A085SE34

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PHE	-	expression tag	UNP A0A085SE34
A	-3	GLN	-	expression tag	UNP A0A085SE34
A	-2	GLY	-	expression tag	UNP A0A085SE34
A	-1	PRO	-	expression tag	UNP A0A085SE34
A	0	HIS	-	expression tag	UNP A0A085SE34
B	-21	MET	-	expression tag	UNP A0A085SE34
B	-20	GLY	-	expression tag	UNP A0A085SE34
B	-19	SER	-	expression tag	UNP A0A085SE34
B	-18	SER	-	expression tag	UNP A0A085SE34
B	-17	HIS	-	expression tag	UNP A0A085SE34
B	-16	HIS	-	expression tag	UNP A0A085SE34
B	-15	HIS	-	expression tag	UNP A0A085SE34
B	-14	HIS	-	expression tag	UNP A0A085SE34
B	-13	HIS	-	expression tag	UNP A0A085SE34
B	-12	HIS	-	expression tag	UNP A0A085SE34
B	-11	SER	-	expression tag	UNP A0A085SE34
B	-10	SER	-	expression tag	UNP A0A085SE34
B	-9	GLY	-	expression tag	UNP A0A085SE34
B	-8	LEU	-	expression tag	UNP A0A085SE34
B	-7	GLU	-	expression tag	UNP A0A085SE34
B	-6	VAL	-	expression tag	UNP A0A085SE34
B	-5	LEU	-	expression tag	UNP A0A085SE34
B	-4	PHE	-	expression tag	UNP A0A085SE34
B	-3	GLN	-	expression tag	UNP A0A085SE34
B	-2	GLY	-	expression tag	UNP A0A085SE34
B	-1	PRO	-	expression tag	UNP A0A085SE34
B	0	HIS	-	expression tag	UNP A0A085SE34
C	-21	MET	-	expression tag	UNP A0A085SE34
C	-20	GLY	-	expression tag	UNP A0A085SE34
C	-19	SER	-	expression tag	UNP A0A085SE34
C	-18	SER	-	expression tag	UNP A0A085SE34
C	-17	HIS	-	expression tag	UNP A0A085SE34
C	-16	HIS	-	expression tag	UNP A0A085SE34
C	-15	HIS	-	expression tag	UNP A0A085SE34
C	-14	HIS	-	expression tag	UNP A0A085SE34
C	-13	HIS	-	expression tag	UNP A0A085SE34
C	-12	HIS	-	expression tag	UNP A0A085SE34
C	-11	SER	-	expression tag	UNP A0A085SE34
C	-10	SER	-	expression tag	UNP A0A085SE34
C	-9	GLY	-	expression tag	UNP A0A085SE34
C	-8	LEU	-	expression tag	UNP A0A085SE34
C	-7	GLU	-	expression tag	UNP A0A085SE34

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	VAL	-	expression tag	UNP A0A085SE34
C	-5	LEU	-	expression tag	UNP A0A085SE34
C	-4	PHE	-	expression tag	UNP A0A085SE34
C	-3	GLN	-	expression tag	UNP A0A085SE34
C	-2	GLY	-	expression tag	UNP A0A085SE34
C	-1	PRO	-	expression tag	UNP A0A085SE34
C	0	HIS	-	expression tag	UNP A0A085SE34
D	-21	MET	-	expression tag	UNP A0A085SE34
D	-20	GLY	-	expression tag	UNP A0A085SE34
D	-19	SER	-	expression tag	UNP A0A085SE34
D	-18	SER	-	expression tag	UNP A0A085SE34
D	-17	HIS	-	expression tag	UNP A0A085SE34
D	-16	HIS	-	expression tag	UNP A0A085SE34
D	-15	HIS	-	expression tag	UNP A0A085SE34
D	-14	HIS	-	expression tag	UNP A0A085SE34
D	-13	HIS	-	expression tag	UNP A0A085SE34
D	-12	HIS	-	expression tag	UNP A0A085SE34
D	-11	SER	-	expression tag	UNP A0A085SE34
D	-10	SER	-	expression tag	UNP A0A085SE34
D	-9	GLY	-	expression tag	UNP A0A085SE34
D	-8	LEU	-	expression tag	UNP A0A085SE34
D	-7	GLU	-	expression tag	UNP A0A085SE34
D	-6	VAL	-	expression tag	UNP A0A085SE34
D	-5	LEU	-	expression tag	UNP A0A085SE34
D	-4	PHE	-	expression tag	UNP A0A085SE34
D	-3	GLN	-	expression tag	UNP A0A085SE34
D	-2	GLY	-	expression tag	UNP A0A085SE34
D	-1	PRO	-	expression tag	UNP A0A085SE34
D	0	HIS	-	expression tag	UNP A0A085SE34
E	-21	MET	-	expression tag	UNP A0A085SE34
E	-20	GLY	-	expression tag	UNP A0A085SE34
E	-19	SER	-	expression tag	UNP A0A085SE34
E	-18	SER	-	expression tag	UNP A0A085SE34
E	-17	HIS	-	expression tag	UNP A0A085SE34
E	-16	HIS	-	expression tag	UNP A0A085SE34
E	-15	HIS	-	expression tag	UNP A0A085SE34
E	-14	HIS	-	expression tag	UNP A0A085SE34
E	-13	HIS	-	expression tag	UNP A0A085SE34
E	-12	HIS	-	expression tag	UNP A0A085SE34
E	-11	SER	-	expression tag	UNP A0A085SE34
E	-10	SER	-	expression tag	UNP A0A085SE34
E	-9	GLY	-	expression tag	UNP A0A085SE34

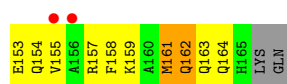
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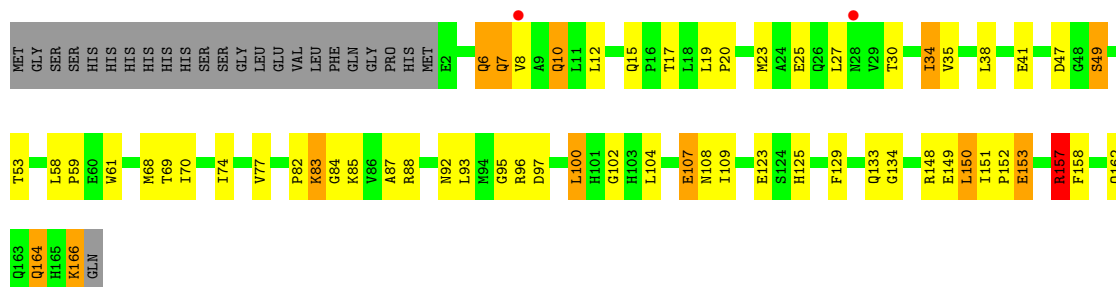
Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	LEU	-	expression tag	UNP A0A085SE34
E	-7	GLU	-	expression tag	UNP A0A085SE34
E	-6	VAL	-	expression tag	UNP A0A085SE34
E	-5	LEU	-	expression tag	UNP A0A085SE34
E	-4	PHE	-	expression tag	UNP A0A085SE34
E	-3	GLN	-	expression tag	UNP A0A085SE34
E	-2	GLY	-	expression tag	UNP A0A085SE34
E	-1	PRO	-	expression tag	UNP A0A085SE34
E	0	HIS	-	expression tag	UNP A0A085SE34
F	-21	MET	-	expression tag	UNP A0A085SE34
F	-20	GLY	-	expression tag	UNP A0A085SE34
F	-19	SER	-	expression tag	UNP A0A085SE34
F	-18	SER	-	expression tag	UNP A0A085SE34
F	-17	HIS	-	expression tag	UNP A0A085SE34
F	-16	HIS	-	expression tag	UNP A0A085SE34
F	-15	HIS	-	expression tag	UNP A0A085SE34
F	-14	HIS	-	expression tag	UNP A0A085SE34
F	-13	HIS	-	expression tag	UNP A0A085SE34
F	-12	HIS	-	expression tag	UNP A0A085SE34
F	-11	SER	-	expression tag	UNP A0A085SE34
F	-10	SER	-	expression tag	UNP A0A085SE34
F	-9	GLY	-	expression tag	UNP A0A085SE34
F	-8	LEU	-	expression tag	UNP A0A085SE34
F	-7	GLU	-	expression tag	UNP A0A085SE34
F	-6	VAL	-	expression tag	UNP A0A085SE34
F	-5	LEU	-	expression tag	UNP A0A085SE34
F	-4	PHE	-	expression tag	UNP A0A085SE34
F	-3	GLN	-	expression tag	UNP A0A085SE34
F	-2	GLY	-	expression tag	UNP A0A085SE34
F	-1	PRO	-	expression tag	UNP A0A085SE34
F	0	HIS	-	expression tag	UNP A0A085SE34

- Molecule 1: Hemin-degrading HemS.ChuX domain protein

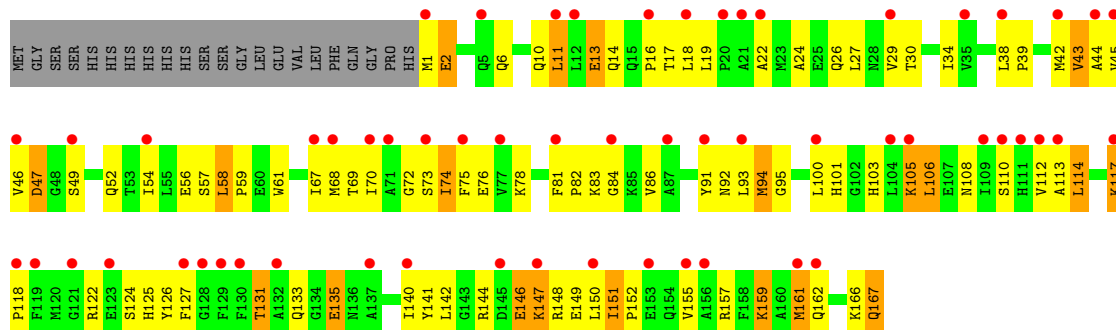




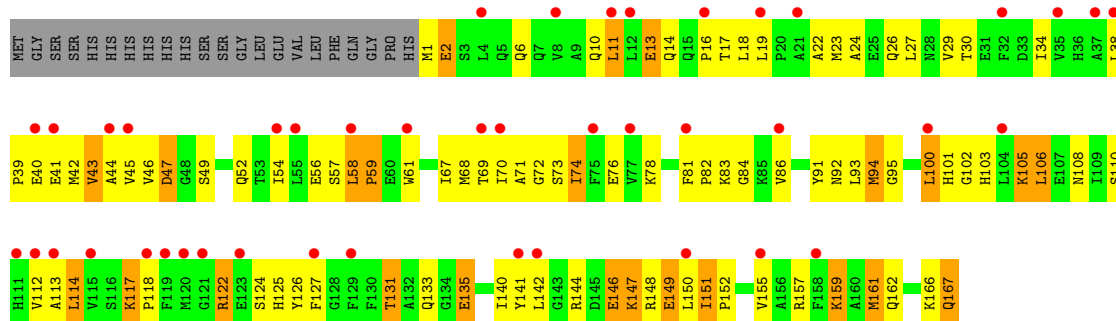
- Molecule 1: Hemin-degrading HemS.ChuX domain protein



- Molecule 1: Hemin-degrading HemS.ChuX domain protein



- Molecule 1: Hemin-degrading HemS.ChuX domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.20Å 80.88Å 111.09Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	48.66 – 2.90 48.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.66-2.90) 98.3 (48.66-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.246 , 0.278 0.258 , 0.285	Depositor DCC
R_{free} test set	1186 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7856	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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	0.51	1/1316 (0.1%)	0.98	2/1780 (0.1%)
1	B	0.37	0/1351	0.84	2/1825 (0.1%)
1	C	0.47	0/1333	0.93	3/1802 (0.2%)
1	D	0.50	2/1334 (0.1%)	0.89	1/1803 (0.1%)
1	E	0.89	7/1351 (0.5%)	1.03	11/1825 (0.6%)
1	F	0.88	9/1351 (0.7%)	1.03	11/1825 (0.6%)
All	All	0.64	19/8036 (0.2%)	0.95	30/10860 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	157	ARG	CA-C	-5.99	1.45	1.52
1	E	117	LYS	C-N	5.69	1.41	1.33
1	F	117	LYS	C-N	5.58	1.40	1.33
1	E	38	LEU	C-N	5.48	1.41	1.33
1	E	39	PRO	N-CD	5.41	1.55	1.47
1	F	38	LEU	C-N	5.40	1.40	1.33
1	F	39	PRO	N-CD	5.35	1.55	1.47
1	E	16	PRO	N-CD	5.30	1.55	1.47
1	F	19	LEU	C-N	5.29	1.40	1.33
1	E	19	LEU	C-N	5.28	1.40	1.33
1	E	152	PRO	N-CD	5.25	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	152	PRO	N-CD	5.23	1.55	1.47
1	F	16	PRO	N-CD	5.20	1.55	1.47
1	A	149	GLU	CA-C	-5.19	1.45	1.53
1	F	118	PRO	N-CD	5.16	1.54	1.47
1	D	157	ARG	CD-NE	-5.15	1.39	1.46
1	E	118	PRO	N-CD	5.12	1.54	1.47
1	F	58	LEU	C-N	5.06	1.40	1.34
1	F	59	PRO	N-CD	5.00	1.54	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLU	N-CA-C	8.12	122.31	109.65
1	C	8	VAL	N-CA-C	-6.97	105.82	111.81
1	D	157	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	F	38	LEU	CA-C-N	-6.35	113.42	119.89
1	F	38	LEU	C-N-CA	-6.35	113.42	119.89
1	E	38	LEU	CA-C-N	-6.33	113.43	119.89
1	E	38	LEU	C-N-CA	-6.33	113.43	119.89
1	E	117	LYS	CA-C-N	-6.13	113.45	119.76
1	E	117	LYS	C-N-CA	-6.13	113.45	119.76
1	F	117	LYS	CA-C-N	-6.13	113.45	119.76
1	F	117	LYS	C-N-CA	-6.13	113.45	119.76
1	F	43	VAL	N-CA-C	5.91	116.87	108.42
1	E	43	VAL	N-CA-C	5.88	116.83	108.42
1	A	84	GLY	N-CA-C	5.71	118.83	110.38
1	B	90	TYR	N-CA-C	5.58	117.10	109.18
1	C	150	LEU	CA-C-N	-5.57	118.58	122.59
1	C	150	LEU	C-N-CA	-5.57	118.58	122.59
1	F	19	LEU	CA-C-N	-5.39	113.35	119.28
1	F	19	LEU	C-N-CA	-5.39	113.35	119.28
1	E	19	LEU	CA-C-N	-5.37	113.38	119.28
1	E	19	LEU	C-N-CA	-5.37	113.38	119.28
1	B	97	ASP	CB-CA-C	-5.21	110.14	117.23
1	E	58	LEU	CA-C-N	-5.20	113.27	119.05
1	E	58	LEU	C-N-CA	-5.20	113.27	119.05
1	F	58	LEU	CA-C-N	-5.17	113.31	119.05
1	F	58	LEU	C-N-CA	-5.17	113.31	119.05
1	E	151	ILE	CA-C-N	-5.07	113.42	119.05
1	E	151	ILE	C-N-CA	-5.07	113.42	119.05
1	F	151	ILE	CA-C-N	-5.07	113.43	119.05
1	F	151	ILE	C-N-CA	-5.07	113.43	119.05

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	GLU	Peptide
1	C	4	LEU	Peptide
1	D	8	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1286	0	1275	84	0
1	B	1321	0	1314	34	1
1	C	1303	0	1293	51	1
1	D	1304	0	1294	37	0
1	E	1321	0	1313	92	0
1	F	1321	0	1313	104	0
All	All	7856	0	7802	357	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 23.

All (357) 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:159:LYS:NZ	1:E:162:GLN:OE1	1.88	1.05
1:F:159:LYS:NZ	1:F:162:GLN:OE1	1.87	1.05
1:C:13:GLU:CD	1:F:122:ARG:HH21	1.69	1.00
1:E:131:THR:HG21	1:E:135:GLU:HG2	1.44	1.00
1:F:131:THR:HG21	1:F:135:GLU:HG2	1.44	0.99
1:E:72:GLY:C	1:F:105:LYS:HG2	1.88	0.98
1:F:105:LYS:CD	1:F:108:ASN:HB3	1.94	0.98
1:E:105:LYS:CD	1:E:108:ASN:HB3	1.93	0.98
1:F:105:LYS:HD2	1:F:108:ASN:HB3	1.47	0.97
1:E:105:LYS:HD2	1:E:108:ASN:HB3	1.47	0.94
1:E:76:GLU:N	1:F:101:HIS:O	2.00	0.94
1:E:74:ILE:HG23	1:F:103:HIS:H	1.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:LEU:O	1:F:117:LYS:NZ	2.08	0.87
1:E:18:LEU:O	1:E:117:LYS:NZ	2.08	0.86
1:E:74:ILE:CG2	1:F:103:HIS:HB2	2.06	0.86
1:E:105:LYS:HE3	1:F:71:ALA:O	1.76	0.84
1:E:67:ILE:HD12	1:E:141:TYR:CD2	2.15	0.82
1:F:124:SER:C	1:F:125:HIS:HD1	1.88	0.81
1:E:124:SER:C	1:E:125:HIS:HD1	1.88	0.81
1:F:67:ILE:HD12	1:F:141:TYR:CD2	2.15	0.81
1:E:105:LYS:HG2	1:F:72:GLY:C	2.07	0.80
1:E:131:THR:CG2	1:E:135:GLU:HG2	2.13	0.79
1:E:74:ILE:HG22	1:F:103:HIS:O	1.83	0.78
1:B:18:LEU:O	1:B:117:LYS:NZ	2.17	0.78
1:E:72:GLY:C	1:F:105:LYS:CG	2.56	0.78
1:F:131:THR:CG2	1:F:135:GLU:HG2	2.13	0.78
1:D:30:THR:HB	1:D:134:GLY:HA3	1.66	0.77
1:E:105:LYS:HG2	1:F:72:GLY:O	1.86	0.76
1:C:123:GLU:HB3	1:C:125:HIS:HE1	1.50	0.76
1:E:124:SER:O	1:E:125:HIS:ND1	2.16	0.76
1:E:74:ILE:HG23	1:F:103:HIS:N	2.01	0.75
1:A:11:LEU:O	1:A:15:GLN:N	2.20	0.74
1:E:10:GLN:O	1:E:14:GLN:HG3	1.88	0.74
1:E:72:GLY:CA	1:F:105:LYS:HG2	2.18	0.74
1:E:146:GLU:H	1:E:146:GLU:CD	1.95	0.74
1:C:125:HIS:HB2	1:C:142:LEU:HD22	1.70	0.73
1:E:105:LYS:CE	1:F:71:ALA:O	2.36	0.73
1:F:10:GLN:O	1:F:14:GLN:HG3	1.88	0.73
1:A:144:ARG:HD2	1:A:148:ARG:O	1.87	0.73
1:F:146:GLU:CD	1:F:146:GLU:H	1.95	0.73
1:B:159:LYS:NZ	1:B:162:GLN:OE1	2.21	0.73
1:F:124:SER:O	1:F:125:HIS:ND1	2.16	0.73
1:E:108:ASN:ND2	1:F:71:ALA:O	2.21	0.72
1:C:123:GLU:HB3	1:C:125:HIS:CE1	2.25	0.72
1:A:7:GLN:HG3	1:A:8:VAL:HG22	1.72	0.71
1:A:6:GLN:NE2	1:F:1:MET:O	2.24	0.71
1:E:105:LYS:HD3	1:E:108:ASN:HB3	1.72	0.71
1:E:92:ASN:OD1	1:E:103:HIS:ND1	2.24	0.71
1:E:72:GLY:O	1:F:105:LYS:HG2	1.89	0.71
1:F:105:LYS:HD3	1:F:108:ASN:HB3	1.72	0.70
1:E:73:SER:OG	1:F:105:LYS:NZ	2.25	0.70
1:F:92:ASN:OD1	1:F:103:HIS:ND1	2.24	0.70
1:A:61:TRP:CD1	1:A:154:GLN:HG2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLU:OE2	1:F:122:ARG:NH2	2.26	0.69
1:B:105:LYS:HD2	1:B:108:ASN:HB3	1.74	0.68
1:F:52:GLN:HB2	1:F:106:LEU:HD23	1.75	0.68
1:E:52:GLN:HB2	1:E:106:LEU:HD23	1.76	0.68
1:F:124:SER:C	1:F:125:HIS:ND1	2.51	0.68
1:E:124:SER:C	1:E:125:HIS:ND1	2.51	0.68
1:F:83:LYS:HB2	1:F:94:MET:HE2	1.75	0.68
1:A:61:TRP:HD1	1:A:154:GLN:HG2	1.57	0.68
1:E:72:GLY:HA3	1:F:105:LYS:HG2	1.75	0.68
1:F:105:LYS:HD2	1:F:105:LYS:O	1.94	0.68
1:A:125:HIS:HB2	1:A:142:LEU:HD22	1.76	0.67
1:E:105:LYS:HG3	1:F:73:SER:OG	1.93	0.67
1:F:114:LEU:N	1:F:114:LEU:HD23	2.09	0.67
1:F:1:MET:O	1:F:1:MET:HG3	1.95	0.67
1:E:83:LYS:HB2	1:E:94:MET:HE2	1.75	0.67
1:E:105:LYS:HD2	1:E:105:LYS:O	1.94	0.67
1:E:114:LEU:HD23	1:E:114:LEU:N	2.09	0.66
1:C:151:ILE:HB	1:F:41:GLU:HB2	1.77	0.66
1:E:166:LYS:C	1:E:167:GLN:HG3	2.20	0.66
1:F:24:ALA:HA	1:F:34:ILE:HD11	1.78	0.66
1:A:93:LEU:HB3	1:A:102:GLY:HA2	1.78	0.66
1:B:83:LYS:HB2	1:B:94:MET:HE2	1.78	0.65
1:E:1:MET:HG3	1:E:1:MET:O	1.95	0.65
1:D:133:GLN:OE1	1:D:133:GLN:N	2.30	0.65
1:A:107:GLU:N	1:A:107:GLU:OE1	2.29	0.65
1:C:116:SER:OG	1:C:162:GLN:OE1	2.15	0.65
1:F:166:LYS:C	1:F:167:GLN:HG3	2.20	0.65
1:A:118:PRO:HA	1:A:123:GLU:HA	1.78	0.65
1:E:24:ALA:HA	1:E:34:ILE:HD11	1.78	0.65
1:C:13:GLU:CD	1:F:122:ARG:NH2	2.51	0.64
1:C:52:GLN:NE2	1:C:56:GLU:OE2	2.30	0.64
1:E:67:ILE:HD12	1:E:141:TYR:HD2	1.63	0.64
1:E:151:ILE:O	1:E:155:VAL:HG23	1.98	0.63
1:A:123:GLU:OE1	1:A:123:GLU:N	2.28	0.63
1:D:7:GLN:HG2	1:D:27:LEU:HD22	1.80	0.63
1:F:151:ILE:O	1:F:155:VAL:HG23	1.98	0.62
1:F:67:ILE:HD12	1:F:141:TYR:HD2	1.63	0.62
1:F:125:HIS:HB2	1:F:142:LEU:HD13	1.81	0.62
1:E:125:HIS:HB2	1:E:142:LEU:HD13	1.81	0.61
1:F:162:GLN:O	1:F:166:LYS:HG3	2.01	0.61
1:E:162:GLN:O	1:E:166:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:PRO:HB3	1:D:95:GLY:HA2	1.83	0.60
1:B:146:GLU:H	1:B:146:GLU:CD	2.10	0.60
1:D:6:GLN:O	1:D:10:GLN:HB2	2.01	0.60
1:D:151:ILE:HG22	1:D:153:GLU:HG2	1.84	0.60
1:C:151:ILE:HB	1:F:41:GLU:CB	2.31	0.59
1:F:54:ILE:O	1:F:57:SER:OG	2.20	0.59
1:B:24:ALA:HA	1:B:34:ILE:HD11	1.83	0.59
1:C:145:ASP:N	1:C:146:GLU:HA	2.17	0.59
1:A:66:THR:HG23	1:A:140:ILE:HD13	1.85	0.59
1:A:47:ASP:OD1	1:A:47:ASP:N	2.36	0.59
1:F:67:ILE:CD1	1:F:141:TYR:CD2	2.86	0.59
1:C:153:GLU:HG3	1:C:154:GLN:HG2	1.85	0.59
1:B:92:ASN:OD1	1:B:103:HIS:ND1	2.32	0.59
1:E:54:ILE:O	1:E:57:SER:OG	2.20	0.58
1:C:40:GLU:HB2	1:F:149:GLU:OE2	2.03	0.58
1:A:145:ASP:HB3	1:A:147:LYS:HG3	1.85	0.58
1:A:20:PRO:HA	1:A:23:MET:HG3	1.86	0.58
1:A:93:LEU:N	1:A:102:GLY:O	2.37	0.58
1:D:157:ARG:HG2	1:D:157:ARG:HH21	1.69	0.58
1:C:119:PHE:CZ	1:C:120:MET:HG2	2.39	0.58
1:A:3:SER:O	1:A:7:GLN:HB3	2.04	0.58
1:E:105:LYS:HD3	1:F:71:ALA:O	2.04	0.58
1:A:89:GLY:O	1:A:105:LYS:NZ	2.36	0.58
1:E:67:ILE:CD1	1:E:141:TYR:CD2	2.86	0.58
1:A:11:LEU:HD13	1:A:11:LEU:H	1.68	0.57
1:A:117:LYS:O	1:A:124:SER:OG	2.21	0.57
1:D:157:ARG:HD3	1:D:157:ARG:H	1.69	0.57
1:A:17:THR:HG1	1:A:119:PHE:HE1	1.52	0.57
1:A:119:PHE:N	1:A:122:ARG:O	2.34	0.57
1:F:29:VAL:HG23	1:F:34:ILE:HD11	1.87	0.57
1:A:116:SER:HB2	1:A:125:HIS:ND1	2.20	0.57
1:D:30:THR:CB	1:D:134:GLY:HA3	2.34	0.57
1:E:29:VAL:HG23	1:E:34:ILE:HD11	1.87	0.57
1:C:41:GLU:N	1:F:149:GLU:OE1	2.38	0.56
1:E:74:ILE:HG22	1:F:103:HIS:HB2	1.85	0.56
1:F:144:ARG:HG2	1:F:144:ARG:HH11	1.71	0.56
1:A:93:LEU:HD23	1:A:101:HIS:HB3	1.88	0.56
1:F:131:THR:HG22	1:F:135:GLU:O	2.06	0.56
1:F:146:GLU:OE1	1:F:146:GLU:N	2.37	0.56
1:B:84:GLY:HA3	1:B:91:TYR:CZ	2.41	0.56
1:C:149:GLU:HG2	1:F:40:GLU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLU:HB3	1:D:85:LYS:HB3	1.89	0.55
1:A:105:LYS:HD2	1:A:107:GLU:HB2	1.87	0.55
1:B:105:LYS:CD	1:B:108:ASN:HB3	2.36	0.55
1:E:144:ARG:HH11	1:E:144:ARG:HG2	1.71	0.55
1:C:3:SER:OG	1:C:5:GLN:O	2.11	0.55
1:C:2:GLU:HB3	1:C:6:GLN:OE1	2.07	0.55
1:E:131:THR:HG22	1:E:135:GLU:O	2.06	0.55
1:D:34:ILE:HG13	1:D:35:VAL:N	2.21	0.54
1:F:95:GLY:HA3	1:F:101:HIS:CD2	2.42	0.54
1:D:157:ARG:HG2	1:D:157:ARG:NH2	2.21	0.54
1:D:157:ARG:HD3	1:D:157:ARG:N	2.22	0.54
1:E:95:GLY:HA3	1:E:101:HIS:CD2	2.42	0.54
1:D:87:ALA:O	1:D:92:ASN:ND2	2.37	0.54
1:C:154:GLN:HB3	1:C:157:ARG:HG3	1.88	0.54
1:F:131:THR:CG2	1:F:135:GLU:CG	2.86	0.54
1:B:123:GLU:HG2	1:B:150:LEU:HD23	1.89	0.54
1:E:131:THR:CG2	1:E:135:GLU:CG	2.85	0.54
1:E:146:GLU:OE1	1:E:146:GLU:N	2.38	0.53
1:D:157:ARG:HH21	1:D:157:ARG:CG	2.21	0.53
1:A:4:LEU:HD11	1:A:29:VAL:HG21	1.90	0.53
1:D:123:GLU:OE1	1:D:150:LEU:HD23	2.08	0.53
1:F:67:ILE:HG21	1:F:74:ILE:HD11	1.91	0.53
1:A:14:GLN:O	1:A:16:PRO:HD3	2.09	0.53
1:A:162:GLN:CD	1:A:163:GLN:HA	2.33	0.53
1:D:58:LEU:O	1:D:61:TRP:HB2	2.08	0.53
1:A:44:ALA:HB3	1:A:114:LEU:HB2	1.91	0.52
1:A:30:THR:N	1:A:33:ASP:OD2	2.40	0.52
1:E:54:ILE:HG23	1:E:161:MET:HE1	1.91	0.52
1:E:74:ILE:CG2	1:F:103:HIS:CB	2.83	0.52
1:A:84:GLY:HA3	1:A:91:TYR:CE2	2.45	0.52
1:B:54:ILE:HG23	1:B:161:MET:HE1	1.90	0.52
1:D:23:MET:HB2	1:D:34:ILE:HD13	1.91	0.52
1:E:147:LYS:O	1:E:148:ARG:HB2	2.09	0.52
1:E:67:ILE:HG21	1:E:74:ILE:HD11	1.91	0.52
1:E:72:GLY:O	1:F:105:LYS:CG	2.54	0.52
1:E:74:ILE:O	1:F:102:GLY:HA3	2.09	0.52
1:F:147:LYS:O	1:F:148:ARG:HB2	2.09	0.52
1:F:54:ILE:HG23	1:F:161:MET:HE1	1.91	0.52
1:E:105:LYS:CD	1:F:71:ALA:O	2.58	0.52
1:C:15:GLN:HE22	1:C:18:LEU:HD22	1.74	0.51
1:D:107:GLU:N	1:D:107:GLU:OE1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:GLU:CD	1:D:153:GLU:H	2.17	0.51
1:C:2:GLU:OE2	1:C:2:GLU:N	2.43	0.51
1:A:66:THR:O	1:A:76:GLU:HA	2.10	0.51
1:E:74:ILE:CG2	1:F:103:HIS:O	2.58	0.51
1:C:102:GLY:HA3	1:D:74:ILE:O	2.11	0.51
1:B:125:HIS:HB2	1:B:142:LEU:HD13	1.92	0.51
1:C:1:MET:N	1:C:2:GLU:OE2	2.38	0.51
1:C:74:ILE:O	1:D:102:GLY:HA3	2.11	0.51
1:A:83:LYS:HD3	1:A:94:MET:HE2	1.93	0.51
1:A:61:TRP:C	1:A:154:GLN:HE21	2.20	0.50
1:B:77:VAL:HG11	1:B:100:LEU:HB2	1.93	0.50
1:C:14:GLN:O	1:C:15:GLN:HG3	2.12	0.50
1:F:131:THR:HG23	1:F:135:GLU:H	1.77	0.50
1:A:30:THR:HG1	1:A:33:ASP:CG	2.18	0.50
1:C:1:MET:HE3	1:C:1:MET:O	2.11	0.50
1:A:8:VAL:HG11	1:A:27:LEU:HD21	1.93	0.50
1:E:30:THR:O	1:E:34:ILE:HD12	2.12	0.50
1:E:131:THR:HG23	1:E:135:GLU:H	1.77	0.49
1:A:64:VAL:HG12	1:A:141:TYR:O	2.12	0.49
1:F:30:THR:O	1:F:34:ILE:HD12	2.12	0.49
1:A:55:LEU:HD21	1:A:129:PHE:CE2	2.46	0.49
1:E:56:GLU:O	1:E:59:PRO:HD2	2.12	0.49
1:E:22:ALA:O	1:E:26:GLN:HG2	2.13	0.49
1:F:56:GLU:O	1:F:59:PRO:HD2	2.12	0.49
1:C:38:LEU:HD21	1:C:43:VAL:CG2	2.42	0.49
1:C:145:ASP:N	1:C:145:ASP:OD1	2.44	0.49
1:E:46:VAL:HG13	1:E:112:VAL:HB	1.95	0.49
1:F:13:GLU:HG3	1:F:14:GLN:HG2	1.94	0.49
1:A:24:ALA:O	1:A:28:ASN:N	2.46	0.49
1:A:84:GLY:HA3	1:A:91:TYR:HE2	1.78	0.48
1:A:5:GLN:HB3	1:A:37:ALA:O	2.13	0.48
1:C:150:LEU:O	1:C:152:PRO:HD3	2.13	0.48
1:A:114:LEU:HD22	1:A:127:PHE:CD1	2.49	0.48
1:A:70:ILE:HB	1:B:70:ILE:CD1	2.44	0.48
1:E:13:GLU:HG3	1:E:14:GLN:HG2	1.94	0.48
1:F:22:ALA:O	1:F:26:GLN:HG2	2.13	0.48
1:A:53:THR:HA	1:A:56:GLU:OE2	2.14	0.48
1:A:133:GLN:OE1	1:A:133:GLN:N	2.25	0.48
1:F:46:VAL:HG13	1:F:112:VAL:HB	1.95	0.48
1:A:48:GLY:HA3	1:A:110:SER:O	2.14	0.48
1:A:55:LEU:HD21	1:A:129:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:GLN:HB3	1:C:37:ALA:O	2.13	0.48
1:D:162:GLN:O	1:D:166:LYS:HB2	2.14	0.48
1:A:105:LYS:HA	1:A:105:LYS:HD3	1.64	0.47
1:B:10:GLN:O	1:B:14:GLN:HG3	2.14	0.47
1:C:125:HIS:HB3	1:C:158:PHE:CE2	2.50	0.47
1:A:29:VAL:HB	1:A:33:ASP:CB	2.44	0.47
1:A:150:LEU:H	1:A:150:LEU:HD22	1.78	0.47
1:A:127:PHE:HB3	1:A:129:PHE:HE1	1.80	0.47
1:A:12:LEU:HA	1:A:13:GLU:HA	1.41	0.47
1:C:144:ARG:HA	1:C:145:ASP:HA	1.71	0.47
1:A:29:VAL:HB	1:A:33:ASP:HB2	1.96	0.47
1:B:2:GLU:H	1:B:2:GLU:HG2	1.65	0.46
1:F:127:PHE:HB2	1:F:140:ILE:HB	1.97	0.46
1:A:91:TYR:CD1	1:A:106:LEU:HD11	2.49	0.46
1:B:46:VAL:HG13	1:B:112:VAL:HB	1.98	0.46
1:B:105:LYS:HD2	1:B:105:LYS:O	2.15	0.46
1:E:166:LYS:C	1:E:167:GLN:CG	2.86	0.46
1:D:19:LEU:O	1:D:23:MET:HG3	2.15	0.46
1:D:109:ILE:HD12	1:D:129:PHE:HB3	1.97	0.46
1:A:129:PHE:N	1:A:129:PHE:HD1	2.13	0.46
1:B:32:PHE:CD2	1:D:164:GLN:HG2	2.49	0.46
1:E:84:GLY:HA3	1:E:91:TYR:CZ	2.51	0.46
1:A:81:PHE:CG	1:A:82:PRO:HD2	2.50	0.46
1:B:108:ASN:OD1	1:D:53:THR:HG21	2.15	0.46
1:E:27:LEU:N	1:E:27:LEU:HD23	2.31	0.46
1:A:131:THR:HB	1:A:133:GLN:OE1	2.16	0.46
1:E:43:VAL:HG22	1:E:44:ALA:N	2.31	0.46
1:B:22:ALA:O	1:B:26:GLN:HG2	2.16	0.46
1:E:29:VAL:HG23	1:E:34:ILE:CD1	2.46	0.46
1:E:127:PHE:HB2	1:E:140:ILE:HB	1.97	0.46
1:F:166:LYS:C	1:F:167:GLN:CG	2.86	0.46
1:A:133:GLN:H	1:A:133:GLN:CD	2.16	0.46
1:D:59:PRO:HG2	1:D:83:LYS:HG2	1.98	0.45
1:D:157:ARG:N	1:D:157:ARG:CD	2.79	0.45
1:A:65:THR:HG23	1:A:78:LYS:HG3	1.99	0.45
1:E:131:THR:CG2	1:E:135:GLU:H	2.29	0.45
1:A:129:PHE:N	1:A:129:PHE:CD1	2.84	0.45
1:F:84:GLY:HA3	1:F:91:TYR:CZ	2.51	0.45
1:A:116:SER:HB2	1:A:125:HIS:CE1	2.51	0.45
1:B:34:ILE:HD12	1:B:34:ILE:H	1.81	0.45
1:F:27:LEU:N	1:F:27:LEU:HD23	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:HA	1:A:164:GLN:OE1	2.16	0.45
1:C:114:LEU:CD2	1:C:161:MET:HB3	2.47	0.45
1:E:126:TYR:CD1	1:E:126:TYR:C	2.94	0.45
1:F:81:PHE:CG	1:F:82:PRO:HD2	2.52	0.45
1:E:2:GLU:HB2	1:E:6:GLN:HB2	1.99	0.45
1:E:58:LEU:O	1:E:61:TRP:HB2	2.17	0.45
1:E:81:PHE:CG	1:E:82:PRO:HD2	2.52	0.45
1:F:126:TYR:CD1	1:F:126:TYR:C	2.94	0.45
1:F:131:THR:CG2	1:F:135:GLU:H	2.30	0.45
1:A:3:SER:O	1:A:6:GLN:HG2	2.17	0.45
1:A:17:THR:OG1	1:A:119:PHE:HE1	1.98	0.45
1:F:29:VAL:HG23	1:F:34:ILE:CD1	2.46	0.45
1:C:96:ARG:H	1:C:96:ARG:HG2	1.43	0.45
1:E:75:PHE:HB3	1:F:100:LEU:HD11	1.98	0.45
1:F:13:GLU:HG3	1:F:14:GLN:N	2.32	0.45
1:A:24:ALA:HB1	1:A:29:VAL:O	2.16	0.44
1:A:5:GLN:HA	1:A:37:ALA:HB1	1.98	0.44
1:A:9:ALA:HA	1:A:12:LEU:HD23	1.99	0.44
1:B:21:ALA:O	1:B:24:ALA:HB3	2.17	0.44
1:B:151:ILE:O	1:B:155:VAL:HG23	2.17	0.44
1:F:2:GLU:HB2	1:F:6:GLN:HB2	1.99	0.44
1:F:114:LEU:N	1:F:114:LEU:CD2	2.78	0.44
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.77	0.44
1:C:4:LEU:HB3	1:C:37:ALA:HB1	1.99	0.44
1:F:157:ARG:HA	1:F:157:ARG:HD2	1.76	0.44
1:C:38:LEU:HD21	1:C:43:VAL:HG23	1.97	0.44
1:E:74:ILE:HG21	1:F:103:HIS:HB2	1.91	0.44
1:F:58:LEU:O	1:F:61:TRP:HB2	2.17	0.44
1:C:85:LYS:HB2	1:C:94:MET:CE	2.47	0.44
1:E:142:LEU:HD12	1:E:142:LEU:N	2.33	0.44
1:F:43:VAL:HG22	1:F:44:ALA:N	2.31	0.44
1:C:67:ILE:HA	1:C:75:PHE:O	2.18	0.43
1:D:125:HIS:HB3	1:D:158:PHE:CE2	2.52	0.43
1:F:142:LEU:N	1:F:142:LEU:HD12	2.32	0.43
1:D:96:ARG:HA	1:D:96:ARG:HD3	1.56	0.43
1:E:2:GLU:HB3	1:E:6:GLN:OE1	2.18	0.43
1:C:100:LEU:H	1:C:100:LEU:HD23	1.83	0.43
1:E:11:LEU:HD23	1:E:11:LEU:HA	1.80	0.43
1:E:13:GLU:HG3	1:E:14:GLN:N	2.32	0.43
1:E:101:HIS:O	1:F:76:GLU:O	2.36	0.43
1:E:74:ILE:O	1:F:103:HIS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LEU:N	1:E:114:LEU:CD2	2.78	0.43
1:F:2:GLU:HB3	1:F:6:GLN:OE1	2.18	0.43
1:B:114:LEU:HD22	1:B:127:PHE:CD1	2.54	0.43
1:A:41:GLU:HG3	1:A:42:MET:N	2.34	0.43
1:F:113:ALA:C	1:F:114:LEU:HD23	2.43	0.43
1:C:131:THR:HG23	1:C:133:GLN:OE1	2.19	0.43
1:A:10:GLN:HG3	1:F:14:GLN:HE22	1.83	0.43
1:C:18:LEU:HD12	1:C:18:LEU:HA	1.84	0.43
1:F:147:LYS:HD2	1:F:147:LYS:HA	1.85	0.43
1:A:21:ALA:O	1:A:24:ALA:HB3	2.19	0.42
1:A:89:GLY:C	1:A:90:TYR:HD1	2.27	0.42
1:B:157:ARG:HA	1:B:157:ARG:HD2	1.82	0.42
1:F:82:PRO:HG2	1:F:93:LEU:HD22	2.01	0.42
1:A:161:MET:HA	1:A:165:HIS:CE1	2.53	0.42
1:B:54:ILE:O	1:B:57:SER:OG	2.36	0.42
1:D:47:ASP:OD2	1:D:49:SER:OG	2.30	0.42
1:E:113:ALA:C	1:E:114:LEU:HD23	2.43	0.42
1:F:67:ILE:CG2	1:F:74:ILE:HD11	2.49	0.42
1:A:68:MET:HE3	1:A:68:MET:HB3	1.86	0.42
1:C:24:ALA:HB1	1:C:29:VAL:O	2.20	0.42
1:B:52:GLN:HB2	1:B:106:LEU:HD23	2.00	0.42
1:C:131:THR:OG1	1:C:132:ALA:N	2.53	0.42
1:A:18:LEU:O	1:A:117:LYS:NZ	2.31	0.42
1:B:131:THR:OG1	1:B:132:ALA:N	2.53	0.42
1:E:157:ARG:HA	1:E:157:ARG:HD2	1.76	0.42
1:C:142:LEU:HD23	1:C:155:VAL:HG22	2.00	0.42
1:E:67:ILE:CG2	1:E:74:ILE:HD11	2.49	0.42
1:E:82:PRO:HG2	1:E:93:LEU:HD22	2.01	0.42
1:A:161:MET:O	1:A:164:GLN:HA	2.20	0.41
1:B:82:PRO:HG2	1:B:93:LEU:HD22	2.03	0.41
1:C:23:MET:HE3	1:C:34:ILE:HG21	2.03	0.41
1:F:105:LYS:HD3	1:F:108:ASN:HD22	1.86	0.41
1:A:90:TYR:N	1:A:90:TYR:CD1	2.89	0.41
1:C:120:MET:O	1:C:120:MET:HG3	2.19	0.41
1:A:8:VAL:HG21	1:A:27:LEU:HD13	2.02	0.41
1:A:35:VAL:HG21	1:A:130:PHE:CZ	2.55	0.41
1:A:35:VAL:HG21	1:A:130:PHE:HZ	1.86	0.41
1:A:122:ARG:HD2	1:A:149:GLU:OE1	2.21	0.41
1:D:95:GLY:HA3	1:D:100:LEU:O	2.20	0.41
1:A:72:GLY:C	1:B:105:LYS:HG2	2.45	0.41
1:B:95:GLY:HA3	1:B:101:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLU:HB2	1:B:6:GLN:HB2	2.03	0.41
1:C:3:SER:O	1:C:7:GLN:HB2	2.21	0.41
1:C:60:GLU:HG2	1:C:157:ARG:HH12	1.85	0.41
1:C:147:LYS:HD3	1:C:149:GLU:HB3	2.03	0.41
1:D:20:PRO:HA	1:D:34:ILE:HD11	2.01	0.41
1:F:46:VAL:HG22	1:F:47:ASP:N	2.36	0.40
1:E:46:VAL:HG22	1:E:47:ASP:N	2.36	0.40
1:E:105:LYS:HD3	1:E:108:ASN:HD22	1.86	0.40
1:A:11:LEU:O	1:A:14:GLN:N	2.54	0.40
1:D:58:LEU:HA	1:D:61:TRP:CD1	2.57	0.40
1:D:84:GLY:O	1:D:85:LYS:HD2	2.21	0.40
1:F:105:LYS:HZ2	1:F:105:LYS:HG3	1.73	0.40
1:F:11:LEU:HD13	1:F:23:MET:HG2	2.03	0.40
1:A:101:HIS:HA	1:A:102:GLY:HA2	1.94	0.40
1:C:81:PHE:HA	1:C:82:PRO:HD3	1.87	0.40
1:C:159:LYS:NZ	1:C:162:GLN:HE22	2.19	0.40
1:D:151:ILE:HA	1:D:152:PRO:HD3	1.92	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:B:157:ARG:NH2	1:C:133:GLN:O[2_557]	2.12	0.08

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	161/189 (85%)	147 (91%)	14 (9%)	0	100	100
1	B	165/189 (87%)	159 (96%)	6 (4%)	0	100	100
1	C	163/189 (86%)	153 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	163/189 (86%)	157 (96%)	6 (4%)	0	100	100
1	E	165/189 (87%)	159 (96%)	6 (4%)	0	100	100
1	F	165/189 (87%)	159 (96%)	6 (4%)	0	100	100
All	All	982/1134 (87%)	934 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	136/159 (86%)	101 (74%)	35 (26%)	0	2
1	B	140/159 (88%)	117 (84%)	23 (16%)	2	8
1	C	138/159 (87%)	105 (76%)	33 (24%)	1	3
1	D	138/159 (87%)	108 (78%)	30 (22%)	1	3
1	E	140/159 (88%)	109 (78%)	31 (22%)	1	3
1	F	140/159 (88%)	109 (78%)	31 (22%)	1	3
All	All	832/954 (87%)	649 (78%)	183 (22%)	1	3

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	GLN
1	A	8	VAL
1	A	11	LEU
1	A	12	LEU
1	A	17	THR
1	A	18	LEU
1	A	23	MET
1	A	25	GLU
1	A	26	GLN

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Mol	Chain	Res	Type
1	A	29	VAL
1	A	30	THR
1	A	36	HIS
1	A	38	LEU
1	A	40	GLU
1	A	47	ASP
1	A	54	ILE
1	A	58	LEU
1	A	64	VAL
1	A	68	MET
1	A	70	ILE
1	A	74	ILE
1	A	90	TYR
1	A	93	LEU
1	A	106	LEU
1	A	114	LEU
1	A	129	PHE
1	A	131	THR
1	A	139	LYS
1	A	140	ILE
1	A	147	LYS
1	A	150	LEU
1	A	162	GLN
1	A	163	GLN
1	A	164	GLN
1	B	2	GLU
1	B	11	LEU
1	B	13	GLU
1	B	17	THR
1	B	42	MET
1	B	47	ASP
1	B	49	SER
1	B	68	MET
1	B	69	THR
1	B	70	ILE
1	B	78	LYS
1	B	86	VAL
1	B	94	MET
1	B	100	LEU
1	B	105	LYS
1	B	106	LEU
1	B	114	LEU

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Mol	Chain	Res	Type
1	B	122	ARG
1	B	135	GLU
1	B	150	LEU
1	B	159	LYS
1	B	161	MET
1	B	167	GLN
1	C	1	MET
1	C	2	GLU
1	C	5	GLN
1	C	12	LEU
1	C	13	GLU
1	C	18	LEU
1	C	38	LEU
1	C	46	VAL
1	C	52	GLN
1	C	55	LEU
1	C	58	LEU
1	C	68	MET
1	C	70	ILE
1	C	85	LYS
1	C	94	MET
1	C	96	ARG
1	C	99	GLU
1	C	100	LEU
1	C	101	HIS
1	C	105	LYS
1	C	116	SER
1	C	119	PHE
1	C	127	PHE
1	C	131	THR
1	C	133	GLN
1	C	135	GLU
1	C	145	ASP
1	C	147	LYS
1	C	149	GLU
1	C	161	MET
1	C	162	GLN
1	C	163	GLN
1	C	164	GLN
1	D	6	GLN
1	D	7	GLN
1	D	10	GLN

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Mol	Chain	Res	Type
1	D	12	LEU
1	D	15	GLN
1	D	17	THR
1	D	25	GLU
1	D	34	ILE
1	D	38	LEU
1	D	41	GLU
1	D	49	SER
1	D	68	MET
1	D	69	THR
1	D	70	ILE
1	D	77	VAL
1	D	83	LYS
1	D	88	ARG
1	D	93	LEU
1	D	97	ASP
1	D	100	LEU
1	D	104	LEU
1	D	107	GLU
1	D	108	ASN
1	D	148	ARG
1	D	149	GLU
1	D	150	LEU
1	D	153	GLU
1	D	157	ARG
1	D	164	GLN
1	D	166	LYS
1	E	2	GLU
1	E	11	LEU
1	E	13	GLU
1	E	17	THR
1	E	42	MET
1	E	45	VAL
1	E	47	ASP
1	E	49	SER
1	E	68	MET
1	E	69	THR
1	E	70	ILE
1	E	74	ILE
1	E	78	LYS
1	E	86	VAL
1	E	94	MET

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Mol	Chain	Res	Type
1	E	100	LEU
1	E	105	LYS
1	E	106	LEU
1	E	110	SER
1	E	114	LEU
1	E	122	ARG
1	E	131	THR
1	E	133	GLN
1	E	135	GLU
1	E	146	GLU
1	E	147	LYS
1	E	149	GLU
1	E	150	LEU
1	E	159	LYS
1	E	161	MET
1	E	167	GLN
1	F	2	GLU
1	F	11	LEU
1	F	13	GLU
1	F	17	THR
1	F	42	MET
1	F	45	VAL
1	F	47	ASP
1	F	49	SER
1	F	68	MET
1	F	69	THR
1	F	70	ILE
1	F	74	ILE
1	F	78	LYS
1	F	86	VAL
1	F	94	MET
1	F	100	LEU
1	F	105	LYS
1	F	106	LEU
1	F	110	SER
1	F	114	LEU
1	F	122	ARG
1	F	131	THR
1	F	133	GLN
1	F	135	GLU
1	F	146	GLU
1	F	147	LYS

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Mol	Chain	Res	Type
1	F	149	GLU
1	F	150	LEU
1	F	159	LYS
1	F	161	MET
1	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	165	HIS
1	B	7	GLN
1	B	101	HIS
1	B	111	HIS
1	B	165	HIS
1	C	5	GLN
1	C	10	GLN
1	C	15	GLN
1	C	162	GLN
1	D	10	GLN
1	D	108	ASN
1	D	164	GLN
1	E	7	GLN
1	F	7	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

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	163/189 (86%)	0.93	15 (9%) 14 12	42, 98, 138, 155	0
1	B	167/189 (88%)	-0.05	0 100 100	23, 41, 66, 90	0
1	C	165/189 (87%)	0.51	12 (7%) 21 17	27, 62, 116, 148	0
1	D	165/189 (87%)	-0.00	2 (1%) 76 69	28, 47, 87, 127	0
1	E	167/189 (88%)	1.81	58 (34%) 1 1	122, 152, 168, 184	0
1	F	167/189 (88%)	1.52	43 (25%) 1 1	117, 157, 172, 185	0
All	All	994/1134 (87%)	0.79	130 (13%) 7 6	23, 89, 166, 185	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	112	VAL	7.8
1	F	104	LEU	5.2
1	F	121	GLY	4.6
1	F	58	LEU	4.6
1	F	38	LEU	4.5
1	E	45	VAL	4.4
1	A	37	ALA	4.2
1	E	113	ALA	4.2
1	E	44	ALA	4.1
1	E	128	GLY	3.9
1	E	42	MET	3.8
1	C	151	ILE	3.8
1	E	70	ILE	3.8
1	E	118	PRO	3.7
1	C	150	LEU	3.7
1	F	70	ILE	3.7
1	F	37	ALA	3.7
1	F	77	VAL	3.7
1	F	21	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	41	GLU	3.5
1	E	119	PHE	3.4
1	E	104	LEU	3.3
1	E	38	LEU	3.3
1	E	21	ALA	3.3
1	E	161	MET	3.3
1	E	123	GLU	3.3
1	F	8	VAL	3.3
1	E	73	SER	3.3
1	C	145	ASP	3.2
1	E	12	LEU	3.2
1	A	38	LEU	3.1
1	F	35	VAL	3.1
1	C	121	GLY	3.1
1	E	67	ILE	3.1
1	F	112	VAL	3.1
1	A	17	THR	3.0
1	E	77	VAL	3.0
1	E	109	ILE	3.0
1	E	137	ALA	2.9
1	E	1	MET	2.9
1	E	84	GLY	2.9
1	F	141	TYR	2.8
1	F	54	ILE	2.8
1	E	71	ALA	2.8
1	E	11	LEU	2.8
1	E	87	ALA	2.8
1	E	35	VAL	2.8
1	F	120	MET	2.8
1	A	43	VAL	2.7
1	E	150	LEU	2.7
1	F	11	LEU	2.7
1	E	155	VAL	2.7
1	E	93	LEU	2.7
1	F	100	LEU	2.7
1	A	94	MET	2.7
1	E	111	HIS	2.7
1	F	118	PRO	2.7
1	E	81	PHE	2.6
1	F	61	TRP	2.6
1	E	121	GLY	2.6
1	A	9	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	158	PHE	2.6
1	E	105	LYS	2.6
1	C	155	VAL	2.6
1	E	20	PRO	2.6
1	E	127	PHE	2.6
1	E	156	ALA	2.6
1	F	44	ALA	2.6
1	E	68	MET	2.5
1	F	4	LEU	2.5
1	C	156	ALA	2.5
1	D	8	VAL	2.5
1	E	100	LEU	2.5
1	A	8	VAL	2.5
1	F	113	ALA	2.5
1	C	1	MET	2.4
1	F	12	LEU	2.4
1	E	54	ILE	2.4
1	E	129	PHE	2.4
1	F	32	PHE	2.4
1	E	18	LEU	2.4
1	F	45	VAL	2.4
1	E	75	PHE	2.4
1	F	55	LEU	2.4
1	E	145	ASP	2.4
1	F	129	PHE	2.4
1	D	28	ASN	2.4
1	F	123	GLU	2.3
1	C	37	ALA	2.3
1	E	49	SER	2.3
1	A	58	LEU	2.3
1	F	40	GLU	2.3
1	C	100	LEU	2.3
1	F	142	LEU	2.3
1	C	17	THR	2.3
1	E	46	VAL	2.3
1	F	75	PHE	2.2
1	F	119	PHE	2.2
1	C	149	GLU	2.2
1	E	91	TYR	2.2
1	E	130	PHE	2.2
1	E	140	ILE	2.2
1	A	164	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	16	PRO	2.2
1	E	29	VAL	2.2
1	E	147	LYS	2.2
1	E	132	ALA	2.2
1	F	86	VAL	2.1
1	F	115	VAL	2.1
1	F	81	PHE	2.1
1	A	13	GLU	2.1
1	F	111	HIS	2.1
1	F	16	PRO	2.1
1	F	69	THR	2.1
1	A	4	LEU	2.1
1	A	12	LEU	2.1
1	F	127	PHE	2.1
1	E	162	GLN	2.1
1	E	22	ALA	2.1
1	E	110	SER	2.1
1	F	155	VAL	2.1
1	A	93	LEU	2.1
1	F	150	LEU	2.1
1	E	117	LYS	2.0
1	A	152	PRO	2.0
1	F	19	LEU	2.0
1	E	153	GLU	2.0
1	A	6	GLN	2.0
1	E	5	GLN	2.0
1	C	16	PRO	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.