



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 PM UTC

PDB ID : 1LTB / pdb_00001ltb
Title : 2.6 ANGSTROMS CRYSTAL STRUCTURE OF PARTIALLY-ACTIVATED
E. COLI HEAT-LABILE ENTEROTOXIN (LT)
Authors : Merritt, E.A.; Sixma, T.K.; Hol, W.G.J.
Deposited on : 1993-09-15
Resolution : 2.60 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

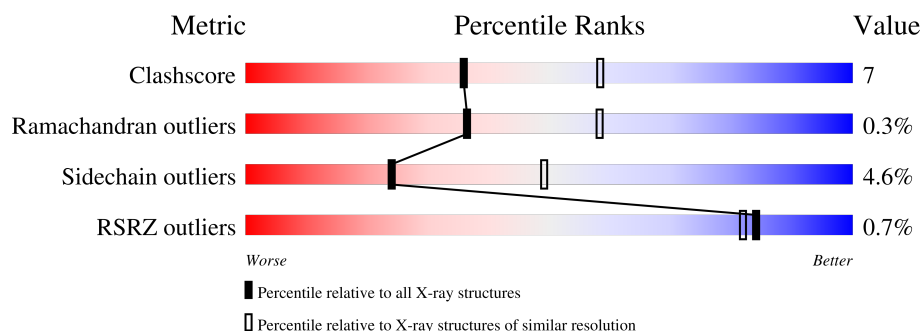
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	D	103	
1	E	103	
1	F	103	
1	G	103	
1	H	103	
2	A	185	

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Mol	Chain	Length	Quality of chain
3	C	45	2% 44% 44% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6175 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 HEAT-LABILE ENTEROTOXIN, SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	E	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	F	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	G	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	H	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			

- Molecule 2 is a protein called HEAT-LABILE ENTEROTOXIN, SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	185	Total	C	N	O	S	0	0	0
			1511	953	276	278	4			

- Molecule 3 is a protein called HEAT-LABILE ENTEROTOXIN, SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	41	Total	C	N	O	S	0	0	0
			347	214	59	73	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	32	Total	O	0	0
			32	32		
4	E	24	Total	O	0	0
			24	24		
4	F	21	Total	O	0	0
			21	21		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	27	Total 27	O 27	0	0
4	H	30	Total 30	O 30	0	0
4	A	41	Total 41	O 41	0	0
4	C	22	Total 22	O 22	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain D: 



- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain E: 



- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain F: 



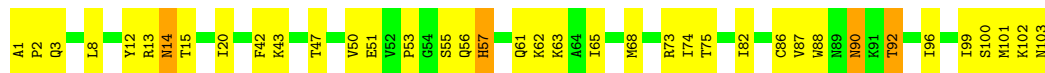
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain G: 



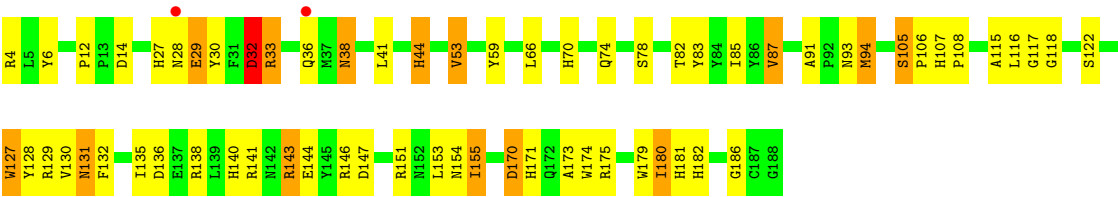
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain H: 

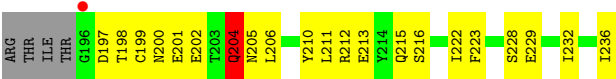


- Molecule 2: HEAT-LABILE ENTEROTOXIN, SUBUNIT A

Chain A: 



● Molecule 3: HEAT-LABILE ENTEROTOXIN, SUBUNIT A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.20Å 98.20Å 64.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60 75.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60) 89.8 (75.79-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6175	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% 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	D	1.09	1/835 (0.1%)	1.87	19/1124 (1.7%)
1	E	1.12	3/835 (0.4%)	1.84	13/1124 (1.2%)
1	F	1.00	3/835 (0.4%)	1.86	24/1124 (2.1%)
1	G	1.07	3/835 (0.4%)	1.84	15/1124 (1.3%)
1	H	1.09	1/835 (0.1%)	1.90	15/1124 (1.3%)
2	A	1.18	11/1559 (0.7%)	1.91	44/2120 (2.1%)
3	C	1.03	0/351	2.10	15/472 (3.2%)
All	All	1.10	22/6085 (0.4%)	1.89	145/8212 (1.8%)

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
2	A	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	12	PRO	CA-CB	-7.63	1.47	1.54
1	D	57	HIS	CD2-NE2	-7.13	1.30	1.37
2	A	70	HIS	CD2-NE2	-6.87	1.30	1.37
1	E	57	HIS	CD2-NE2	-6.78	1.30	1.37
1	H	57	HIS	CD2-NE2	-6.68	1.30	1.37
2	A	181	HIS	CD2-NE2	-6.60	1.30	1.37
1	F	57	HIS	CD2-NE2	-6.46	1.30	1.37
2	A	27	HIS	CD2-NE2	-6.22	1.31	1.37
2	A	182	HIS	CD2-NE2	-6.14	1.31	1.37
1	G	5	ILE	CA-CB	5.99	1.61	1.54
1	G	57	HIS	CD2-NE2	-5.93	1.31	1.37
2	A	107	HIS	CD2-NE2	-5.91	1.31	1.37
1	E	58	ILE	CA-CB	5.73	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	74	ILE	CA-CB	5.71	1.62	1.54
2	A	140	HIS	CD2-NE2	-5.45	1.31	1.37
1	F	57	HIS	CG-ND1	-5.43	1.32	1.38
1	G	24	ILE	CA-CB	5.34	1.60	1.54
2	A	171	HIS	CD2-NE2	-5.32	1.32	1.37
2	A	107	HIS	CG-ND1	-5.23	1.32	1.38
1	E	57	HIS	CG-ND1	-5.19	1.32	1.38
2	A	131	ASN	CA-CB	-5.09	1.45	1.53
2	A	171	HIS	CG-ND1	-5.08	1.32	1.38

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	32	ASP	CA-CB-CG	12.65	125.25	112.60
3	C	204	GLN	CG-CD-NE2	9.69	130.94	116.40
2	A	180	ILE	CB-CA-C	-9.62	99.43	112.04
1	E	50	VAL	N-CA-C	-9.61	94.72	108.17
2	A	118	GLY	CA-C-O	-9.10	115.89	122.45
2	A	179	TRP	CG-CD2-CE3	8.88	142.78	133.90
2	A	136	ASP	CA-CB-CG	8.79	121.39	112.60
1	D	50	VAL	N-CA-C	-8.74	95.13	107.80
1	D	70	ASP	CA-CB-CG	8.41	121.01	112.60
1	G	50	VAL	N-CA-C	-8.36	96.41	108.36
1	D	94	ASN	OD1-CG-ND2	-8.20	114.40	122.60
1	G	90	ASN	CA-CB-CG	8.16	120.77	112.60
1	E	70	ASP	CA-CB-CG	8.12	120.72	112.60
1	D	102	LYS	O-C-N	8.03	132.58	123.27
2	A	28	ASN	N-CA-C	7.75	119.72	111.28
1	H	86	CYS	N-CA-C	-7.51	96.98	109.07
3	C	215	GLN	OE1-CD-NE2	-7.42	115.17	122.60
2	A	170	ASP	CA-CB-CG	7.40	120.00	112.60
3	C	204	GLN	OE1-CD-NE2	-7.33	115.27	122.60
3	C	204	GLN	CA-CB-CG	-7.30	99.51	114.10
1	F	86	CYS	N-CA-C	-7.22	97.44	109.07
1	F	65	ILE	N-CA-C	-7.17	103.48	110.72
1	F	10	SER	CA-CB-OG	7.12	125.33	111.10
2	A	180	ILE	N-CA-CB	6.95	119.16	110.47
3	C	197	ASP	CA-CB-CG	6.91	119.50	112.60
1	H	50	VAL	N-CA-C	-6.90	97.67	107.75
2	A	132	PHE	CA-CB-CG	-6.84	106.96	113.80
1	E	21	ASN	OD1-CG-ND2	-6.80	115.80	122.60
2	A	87	VAL	N-CA-C	-6.77	98.68	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	205	ASN	CA-CB-CG	6.73	119.33	112.60
1	H	103	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	H	51	GLU	N-CA-C	6.57	118.77	110.24
2	A	179	TRP	CB-CG-CD1	-6.56	117.06	126.90
2	A	181	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	G	102	LYS	O-C-N	6.50	131.19	123.33
2	A	38	ASN	OD1-CG-ND2	-6.45	116.16	122.60
2	A	173	ALA	N-CA-C	6.42	119.10	111.33
1	H	90	ASN	OD1-CG-ND2	-6.37	116.23	122.60
2	A	135	ILE	CB-CA-C	-6.36	104.37	111.23
1	G	70	ASP	CA-CB-CG	6.30	118.90	112.60
1	G	31	MET	N-CA-C	-6.24	104.94	113.30
3	C	216	SER	N-CA-C	-6.20	103.83	111.40
1	E	57	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	F	71	THR	CA-CB-OG1	-6.17	100.34	109.60
3	C	216	SER	O-C-N	-6.14	114.73	122.17
2	A	36	GLN	N-CA-C	-6.12	97.71	108.23
1	E	19	THR	N-CA-C	-6.09	97.78	108.20
1	F	88	TRP	CB-CG-CD1	-6.08	117.78	126.90
2	A	174	TRP	CG-CD2-CE3	6.07	139.97	133.90
1	D	94	ASN	CB-CG-ND2	6.05	125.48	116.40
1	D	57	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	D	16	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	F	70	ASP	CA-CB-CG	6.00	118.60	112.60
1	D	102	LYS	CA-CB-CG	6.00	126.09	114.10
1	F	88	TRP	CG-CD2-CE3	5.99	139.89	133.90
1	F	50	VAL	N-CA-C	-5.99	97.76	107.28
2	A	27	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	F	58	ILE	O-C-N	-5.97	116.18	122.57
2	A	83	TYR	CA-CB-CG	5.95	124.60	113.90
2	A	30	TYR	N-CA-C	5.94	118.52	111.33
1	H	65	ILE	N-CA-C	-5.93	104.96	110.53
1	G	3	GLN	N-CA-C	-5.89	105.74	113.17
2	A	144	GLU	CA-CB-CG	-5.88	102.34	114.10
1	D	86	CYS	N-CA-C	-5.88	98.94	108.52
1	D	49	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	H	14	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	F	11	GLU	N-CA-CB	-5.84	101.51	110.44
1	F	22	ASP	CA-CB-CG	5.83	118.44	112.60
2	A	41	LEU	CA-C-O	-5.83	114.70	120.82
1	H	63	LYS	N-CA-CB	5.80	118.74	110.16
1	E	76	TYR	O-C-N	-5.77	115.86	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5	ILE	CA-C-O	-5.76	114.96	120.95
1	D	14	ASN	N-CA-C	5.76	119.61	112.24
1	D	95	SER	N-CA-CB	-5.74	101.28	110.63
2	A	107	HIS	CB-CG-CD2	-5.71	123.77	131.20
3	C	210	TYR	O-C-N	-5.70	116.07	122.12
1	G	21	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	H	56	GLN	N-CA-C	-5.65	98.76	110.80
1	E	96	ILE	N-CA-C	5.62	116.31	108.89
1	F	95	SER	N-CA-CB	-5.62	101.75	110.57
2	A	154	ASN	CA-CB-CG	-5.60	107.00	112.60
2	A	105	SER	CA-C-N	5.59	125.26	119.05
2	A	105	SER	C-N-CA	5.59	125.26	119.05
1	F	95	SER	CA-CB-OG	5.59	122.28	111.10
2	A	153	LEU	O-C-N	5.59	129.45	122.86
1	E	99	ILE	N-CA-C	-5.58	99.77	108.81
3	C	201	GLU	N-CA-C	-5.53	104.66	111.40
1	H	63	LYS	CB-CA-C	-5.51	101.48	110.85
1	H	61	GLN	N-CA-C	-5.49	105.45	111.82
1	H	56	GLN	CA-CB-CG	5.46	125.03	114.10
1	F	55	SER	N-CA-C	5.45	117.64	111.11
1	E	95	SER	N-CA-CB	-5.44	101.54	110.52
2	A	44	HIS	CB-CG-CD2	-5.44	124.13	131.20
2	A	94	MET	CA-CB-CG	5.43	124.96	114.10
2	A	179	TRP	CE2-CD2-CG	-5.42	100.70	107.20
2	A	141	ARG	CA-CB-CG	-5.42	103.27	114.10
1	E	86	CYS	N-CA-C	-5.41	99.91	108.73
1	G	57	HIS	CB-CG-CD2	-5.41	124.16	131.20
3	C	198	THR	CA-CB-OG1	-5.39	101.51	109.60
1	H	92	THR	CA-CB-OG1	-5.38	101.52	109.60
2	A	174	TRP	CE2-CD2-CG	-5.37	100.75	107.20
1	F	92	THR	O-C-N	-5.35	116.63	121.39
3	C	200	ASN	OD1-CG-ND2	-5.34	117.25	122.60
2	A	182	HIS	CB-CG-ND1	5.31	130.67	122.70
1	G	69	LYS	CA-CB-CG	-5.30	103.50	114.10
3	C	205	ASN	N-CA-CB	-5.30	102.31	110.16
3	C	215	GLN	CG-CD-NE2	5.29	124.34	116.40
1	F	9	CYS	CA-C-N	5.28	128.09	120.38
1	F	9	CYS	C-N-CA	5.28	128.09	120.38
1	E	4	THR	CA-CB-OG1	-5.28	101.69	109.60
2	A	33	ARG	CA-CB-CG	5.27	124.65	114.10
1	E	31	MET	N-CA-C	-5.26	106.09	112.88
1	F	88	TRP	CE2-CD2-CG	-5.25	100.89	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	76	TYR	N-CA-C	-5.25	105.25	110.97
2	A	182	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	D	82	ILE	CA-CB-CG1	-5.23	101.50	110.40
1	F	5	ILE	CA-C-O	-5.23	115.31	120.85
1	G	77	LEU	CA-C-O	-5.23	115.01	120.55
2	A	38	ASN	CA-CB-CG	-5.22	107.38	112.60
2	A	155	ILE	CB-CA-C	5.19	117.27	111.45
1	F	60	SER	N-CA-C	-5.19	105.80	111.82
1	G	46	GLU	CA-CB-CG	-5.18	103.73	114.10
3	C	229	GLU	CB-CG-CD	5.18	121.40	112.60
1	E	72	LEU	CA-C-O	-5.17	115.07	120.55
2	A	174	TRP	CG-CD1-NE1	-5.15	103.50	110.20
2	A	36	GLN	CA-C-O	5.14	126.54	120.98
1	F	21	ASN	CA-CB-CG	-5.14	107.46	112.60
1	G	61	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	H	73	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	G	103	ASN	CA-CB-CG	-5.10	107.50	112.60
2	A	127	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	H	51	GLU	CA-CB-CG	5.07	124.24	114.10
1	D	20	ILE	N-CA-CB	-5.06	106.56	111.57
2	A	93	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	F	75	THR	CA-CB-OG1	-5.05	102.02	109.60
1	D	3	GLN	CG-CD-NE2	5.05	123.97	116.40
1	F	20	ILE	N-CA-CB	-5.04	103.57	110.68
1	D	16	GLN	CA-CB-CG	5.04	124.19	114.10
1	D	102	LYS	CA-C-N	5.04	130.76	121.70
1	D	102	LYS	C-N-CA	5.04	130.76	121.70
2	A	91	ALA	O-C-N	-5.03	117.98	121.65
1	F	61	GLN	CA-CB-CG	-5.02	104.06	114.10
2	A	53	VAL	N-CA-C	-5.02	103.11	109.58
2	A	146	ARG	CB-CG-CD	-5.01	99.79	111.30
1	D	56	GLN	OE1-CD-NE2	-5.00	117.59	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	128	TYR	Sidechain

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	D	824	0	841	15	1
1	E	824	0	841	13	0
1	F	824	0	841	8	0
1	G	824	0	841	16	0
1	H	824	0	841	22	0
2	A	1511	0	1407	21	0
3	C	347	0	327	9	0
4	A	41	0	0	1	0
4	C	22	0	0	1	0
4	D	32	0	0	1	0
4	E	24	0	0	0	0
4	F	21	0	0	1	0
4	G	27	0	0	4	0
4	H	30	0	0	4	1
All	All	6175	0	5939	87	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 7.

All (87) 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:G:10:SER:HB2	4:G:127:HOH:O	1.59	1.00
1:H:13:ARG:HA	4:H:127:HOH:O	1.78	0.81
1:D:3:GLN:HG2	1:E:93:PRO:HG3	1.69	0.74
1:G:101:MET:HE3	4:H:129:HOH:O	1.91	0.70
2:A:38:ASN:HA	3:C:204:GLN:OE1	1.91	0.70
2:A:170:ASP:HA	2:A:175:ARG:NH2	2.07	0.68
1:H:87:VAL:HG12	1:H:96:ILE:HA	1.78	0.65
2:A:129:ARG:NH1	2:A:131:ASN:HD21	1.96	0.64
1:G:101:MET:CE	4:H:129:HOH:O	2.45	0.63
1:G:6:THR:HG21	4:G:125:HOH:O	2.00	0.60
1:F:9:CYS:SG	1:F:15:THR:HB	2.41	0.60
1:E:59:ASP:HA	1:E:62:LYS:HD2	1.83	0.59
2:A:94:MET:HB2	2:A:155:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:94:MET:SD	2:A:115:ALA:HB2	2.43	0.58
1:D:93:PRO:HG3	1:H:3:GLN:HG2	1.87	0.57
1:E:58:ILE:HG13	1:E:61:GLN:HG3	1.86	0.57
1:H:57:HIS:HB2	1:H:62:LYS:HE2	1.87	0.56
1:E:15:THR:HA	1:E:87:VAL:O	2.06	0.55
1:H:68:MET:HE1	1:H:99:ILE:HG22	1.88	0.55
1:F:65:ILE:HG22	1:F:69:LYS:HE2	1.89	0.54
1:G:1:ALA:HA	1:H:92:THR:O	2.08	0.54
1:G:3:GLN:HE22	1:H:92:THR:HG22	1.72	0.53
1:F:24:ILE:HD11	1:F:82:ILE:HD11	1.90	0.53
1:D:41:THR:HG22	1:D:47:THR:OG1	2.10	0.52
3:C:212:ARG:NH1	4:C:187:HOH:O	2.43	0.52
1:G:3:GLN:HB3	1:H:47:THR:HG21	1.92	0.51
1:G:54:GLY:H	1:G:57:HIS:HD2	1.57	0.51
3:C:232:ILE:O	3:C:236:ILE:HG12	2.13	0.49
1:F:14:ASN:O	1:F:88:TRP:HA	2.13	0.49
1:F:15:THR:HA	1:F:87:VAL:O	2.12	0.49
3:C:202:GLU:O	3:C:206:LEU:HG	2.12	0.49
2:A:105:SER:O	2:A:108:PRO:HD3	2.12	0.49
1:D:25:LEU:HD22	1:D:43:LYS:HA	1.95	0.49
1:H:74:ILE:HD11	3:C:228:SER:HB2	1.95	0.49
1:E:65:ILE:HG22	1:E:69:LYS:HE2	1.94	0.49
1:G:6:THR:HG22	1:G:17:ILE:HG13	1.95	0.49
1:H:55:SER:HA	4:H:130:HOH:O	2.14	0.48
2:A:53:VAL:HG23	4:A:190:HOH:O	2.12	0.48
2:A:74:GLN:O	2:A:78:SER:HB2	2.13	0.48
1:G:49:GLN:HB3	1:G:93:PRO:HG2	1.97	0.47
2:A:129:ARG:HH11	2:A:131:ASN:HD21	1.63	0.47
2:A:127:TRP:HH2	2:A:143:ARG:HH22	1.62	0.47
2:A:105:SER:HA	2:A:106:PRO:HD3	1.75	0.46
1:H:75:THR:HG21	1:H:101:MET:CE	2.46	0.46
1:D:30:SER:HB2	1:H:8:LEU:HD11	1.97	0.46
2:A:170:ASP:HA	2:A:175:ARG:HH22	1.80	0.45
1:E:44:SER:OG	1:E:46:GLU:HG2	2.16	0.45
2:A:29:GLU:HG3	2:A:32:ASP:HB3	1.98	0.45
2:A:82:THR:HA	2:A:130:VAL:O	2.16	0.45
2:A:186:GLY:O	3:C:199:CYS:HB2	2.17	0.45
1:H:15:THR:HA	1:H:87:VAL:O	2.17	0.45
2:A:6:TYR:CE2	2:A:87:VAL:HG22	2.52	0.45
2:A:147:ASP:O	2:A:151:ARG:HB2	2.17	0.45
1:D:36:GLU:O	1:D:52:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:MET:HE3	1:F:27:TYR:HD1	1.82	0.44
1:H:1:ALA:HB1	1:H:2:PRO:HD2	2.00	0.44
1:H:43:LYS:HA	1:H:43:LYS:HD2	1.82	0.43
1:E:57:HIS:HB2	1:E:62:LYS:HE2	2.00	0.43
1:D:65:ILE:HG12	1:E:31:MET:HE1	1.99	0.43
1:H:53:PRO:HA	1:H:57:HIS:ND1	2.34	0.43
1:H:102:LYS:HE2	1:H:102:LYS:HB3	1.63	0.43
1:E:63:LYS:HB3	3:C:236:ILE:HD13	2.01	0.43
2:A:4:ARG:HD2	2:A:87:VAL:CG1	2.49	0.43
1:D:32:ALA:HB1	1:H:12:TYR:CZ	2.54	0.42
1:H:14:ASN:O	1:H:88:TRP:HA	2.19	0.42
1:D:103:ASN:HB2	1:E:76:TYR:CE1	2.55	0.42
1:F:49:GLN:HG2	1:F:93:PRO:HG2	2.02	0.42
1:F:57:HIS:O	1:F:62:LYS:NZ	2.48	0.42
2:A:117:GLY:HA3	3:C:211:LEU:HD13	2.02	0.42
1:G:35:ARG:HG3	1:G:37:MET:SD	2.59	0.42
1:H:82:ILE:HD13	1:H:99:ILE:HD11	2.01	0.42
1:D:65:ILE:HG12	1:E:31:MET:CE	2.50	0.42
1:G:13:ARG:O	1:G:14:ASN:HB2	2.20	0.42
1:D:9:CYS:SG	1:D:15:THR:HB	2.60	0.41
1:D:12:TYR:CZ	1:E:32:ALA:HB1	2.55	0.41
1:D:61:GLN:O	1:D:65:ILE:HG13	2.20	0.41
2:A:44:HIS:CG	2:A:59:TYR:HB2	2.56	0.41
2:A:66:LEU:CD1	2:A:85:ILE:HG21	2.51	0.41
1:G:9:CYS:HB3	4:G:111:HOH:O	2.21	0.41
1:G:6:THR:CG2	4:G:125:HOH:O	2.63	0.41
1:H:20:ILE:HG21	1:H:42:PHE:CE1	2.56	0.41
4:F:107:HOH:O	1:G:31:MET:HE1	2.20	0.41
1:D:21:ASN:HB3	4:D:127:HOH:O	2.20	0.40
1:D:99:ILE:HG21	1:D:99:ILE:HD13	1.85	0.40
1:G:58:ILE:H	1:G:58:ILE:HG13	1.68	0.40
1:H:99:ILE:HG12	1:H:100:SER:N	2.35	0.40
3:C:222:ILE:HG13	3:C:223:PHE:CD1	2.57	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:D:6:THR:OG1	4:H:131:HOH:O[3_555]	2.17	0.03

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	D	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	28
1	E	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
1	F	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	12	28
1	G	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
1	H	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
2	A	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
3	C	39/45 (87%)	39 (100%)	0	0	100	100
All	All	727/745 (98%)	687 (94%)	38 (5%)	2 (0%)	36	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	56	GLN
1	F	53	PRO

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	D	95/95 (100%)	92 (97%)	3 (3%)	34	62
1	E	95/95 (100%)	92 (97%)	3 (3%)	34	62
1	F	95/95 (100%)	89 (94%)	6 (6%)	16	36
1	G	95/95 (100%)	88 (93%)	7 (7%)	13	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	95/95 (100%)	94 (99%)	1 (1%)	65	84
2	A	155/155 (100%)	146 (94%)	9 (6%)	18	39
3	C	40/44 (91%)	38 (95%)	2 (5%)	22	46
All	All	670/674 (99%)	639 (95%)	31 (5%)	24	49

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	6	THR
1	D	10	SER
1	D	103	ASN
1	E	55	SER
1	E	56	GLN
1	E	82	ILE
1	F	6	THR
1	F	8	LEU
1	F	15	THR
1	F	44	SER
1	F	56	GLN
1	F	59	ASP
1	G	3	GLN
1	G	13	ARG
1	G	35	ARG
1	G	58	ILE
1	G	62	LYS
1	G	91	LYS
1	G	103	ASN
1	H	90	ASN
2	A	14	ASP
2	A	29	GLU
2	A	32	ASP
2	A	33	ARG
2	A	116	LEU
2	A	122	SER
2	A	138	ARG
2	A	143	ARG
2	A	180	ILE
3	C	204	GLN
3	C	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	E	21	ASN
1	E	49	GLN
1	E	94	ASN
1	F	56	GLN
1	F	61	GLN
1	G	3	GLN
1	H	3	GLN
1	H	21	ASN
1	H	90	ASN
2	A	27	HIS
2	A	38	ASN
2	A	74	GLN
2	A	111	GLN
2	A	131	ASN
3	C	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	103/103 (100%)	-0.83	0 100 100	2, 11, 40, 53	0
1	E	103/103 (100%)	-0.84	0 100 100	2, 10, 40, 56	0
1	F	103/103 (100%)	-0.62	2 (1%) 66 61	2, 15, 51, 84	0
1	G	103/103 (100%)	-0.72	0 100 100	2, 17, 41, 60	0
1	H	103/103 (100%)	-0.71	0 100 100	2, 11, 48, 64	0
2	A	185/185 (100%)	-0.49	2 (1%) 78 74	3, 19, 51, 67	0
3	C	41/45 (91%)	-0.48	1 (2%) 59 54	3, 12, 51, 65	0
All	All	741/745 (99%)	-0.66	5 (0%) 84 82	2, 15, 49, 84	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	196	GLY	3.0
1	F	58	ILE	2.7
2	A	36	GLN	2.3
1	F	56	GLN	2.2
2	A	28	ASN	2.1

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.