



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 AM UTC

PDB ID : 1HSL / pdb_00001hsl
Title : REFINED 1.89 ANGSTROMS STRUCTURE OF THE HISTIDINE-BINDING PROTEIN COMPLEXED WITH HISTIDINE AND ITS RELATIONSHIP WITH MANY OTHER ACTIVE TRANSPORT(SLASH)CHEM OSENSORY RECEPTORS
Authors : Yao, N.; Trakhanov, S.; Quiocho, F.A.
Deposited on : 1994-01-03
Resolution : 1.89 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

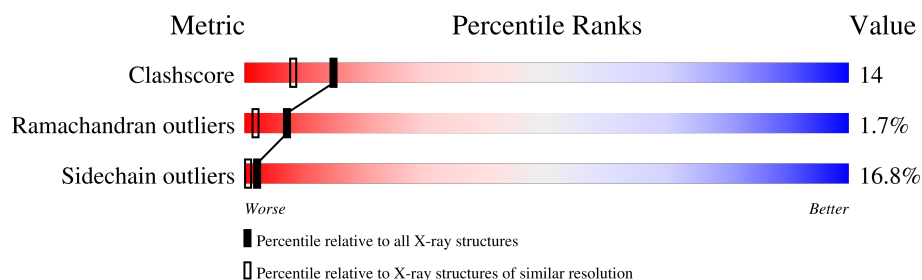
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	44% 41% 13% .
1	B	238	48% 36% 13% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4001 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.

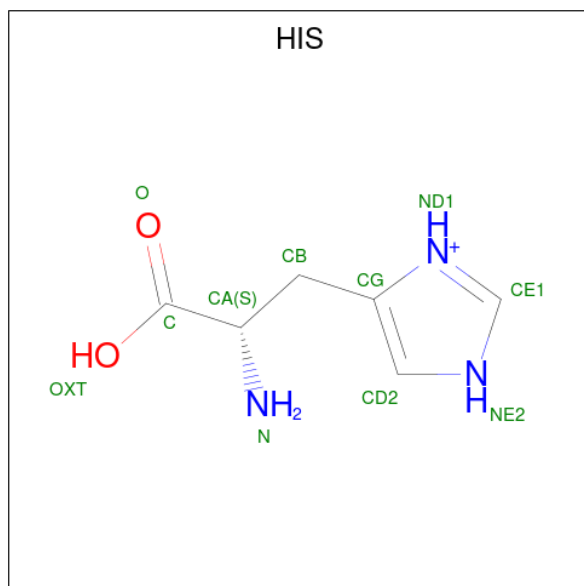
- Molecule 1 is a protein called HISTIDINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1843	1166	311	361	5			
1	B	238	Total	C	N	O	S	0	0	0
			1843	1166	311	361	5			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cd	0	0
			5	5		
2	B	2	Total	Cd	0	0
			2	2		

- Molecule 3 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	3	2		
3	B	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 4 is water.

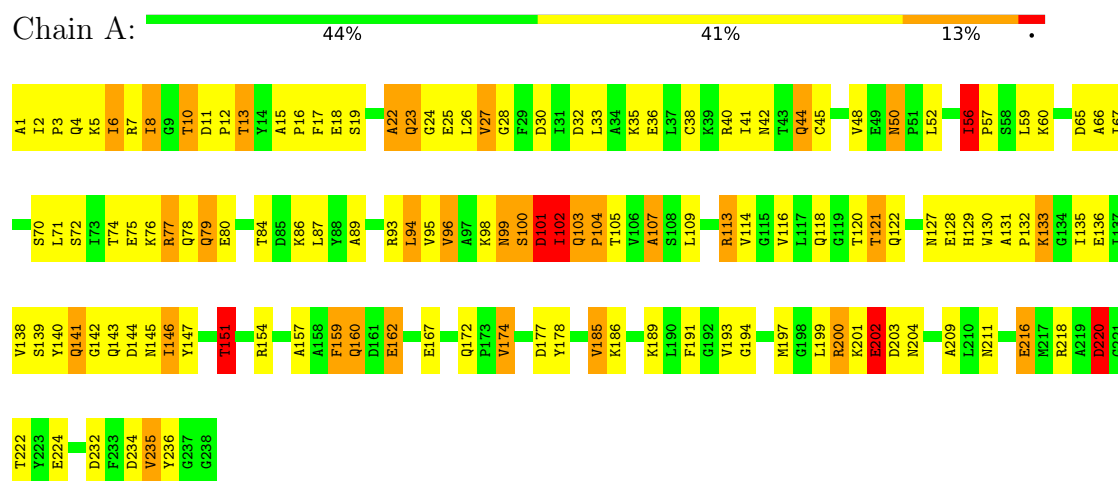
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	125	Total	O	0	0
			125	125		

3 Residue-property plots

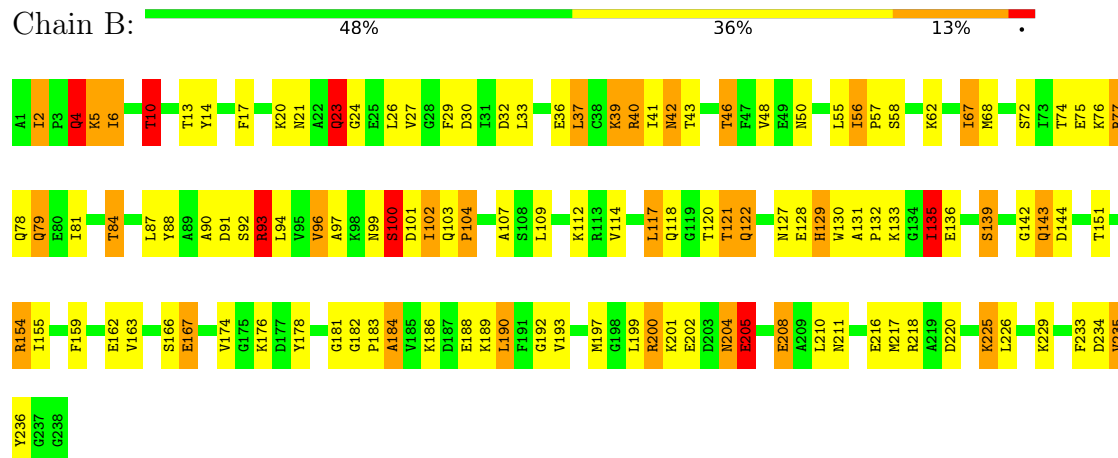
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: HISTIDINE-BINDING PROTEIN



• Molecule 1: HISTIDINE-BINDING PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.16Å 102.52Å 64.98Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	8.00 – 1.89	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.89)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4001	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CD

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	1.26	6/1874 (0.3%)	2.40	123/2522 (4.9%)
1	B	1.28	6/1874 (0.3%)	2.32	104/2522 (4.1%)
All	All	1.27	12/3748 (0.3%)	2.36	227/5044 (4.5%)

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	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	ILE	CA-CB	9.12	1.65	1.54
1	B	135	ILE	CA-CB	6.07	1.61	1.54
1	A	13	THR	CA-CB	5.95	1.61	1.53
1	B	129	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	129	HIS	CD2-NE2	-5.37	1.31	1.37
1	B	217	MET	CA-CB	-5.33	1.44	1.53
1	A	100	SER	CA-CB	-5.31	1.44	1.53
1	B	129	HIS	CB-CG	5.31	1.57	1.50
1	A	102	ILE	CA-CB	5.27	1.61	1.54
1	A	56	ILE	CA-CB	5.20	1.57	1.53
1	A	38	CYS	CA-CB	-5.20	1.45	1.53
1	B	48	VAL	CA-CB	-5.12	1.48	1.54

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ASP	CA-CB-CG	17.79	130.39	112.60
1	B	235	VAL	CB-CA-C	-12.95	95.08	112.04
1	B	23	GLN	OE1-CD-NE2	-12.68	109.92	122.60
1	B	78	GLN	OE1-CD-NE2	-12.03	110.57	122.60
1	A	103	GLN	N-CA-C	11.58	127.13	109.41
1	B	101	ASP	N-CA-C	11.38	127.13	112.34
1	A	204	ASN	OD1-CG-ND2	-11.06	111.54	122.60
1	A	100	SER	O-C-N	10.96	137.17	122.59
1	A	42	ASN	OD1-CG-ND2	-10.62	111.98	122.60
1	B	208	GLU	CA-CB-CG	10.48	135.07	114.10
1	B	42	ASN	OD1-CG-ND2	-10.40	112.20	122.60
1	B	186	LYS	N-CA-C	10.30	125.94	108.23
1	B	143	GLN	OE1-CD-NE2	-10.19	112.41	122.60
1	A	154	ARG	NE-CZ-NH2	10.02	128.22	119.20
1	A	99	ASN	CA-CB-CG	9.93	122.53	112.60
1	B	79	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	A	77	ARG	NE-CZ-NH2	9.62	127.85	119.20
1	B	77	ARG	NE-CZ-NH2	9.43	127.69	119.20
1	A	141	GLN	CA-CB-CG	-9.13	95.83	114.10
1	A	44	GLN	OE1-CD-NE2	-9.02	113.58	122.60
1	B	181	GLY	O-C-N	8.98	134.37	122.70
1	B	127	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	B	216	GLU	CA-CB-CG	-8.88	96.34	114.10
1	B	235	VAL	N-CA-CB	8.85	121.53	110.47
1	B	122	GLN	OE1-CD-NE2	-8.75	113.85	122.60
1	B	23	GLN	CA-CB-CG	8.75	131.59	114.10
1	A	186	LYS	N-CA-C	8.74	123.64	109.40
1	A	185	VAL	CA-C-O	8.48	129.42	120.51
1	A	193	VAL	N-CA-C	-8.40	100.51	112.35
1	A	160	GLN	OE1-CD-NE2	-8.39	114.21	122.60
1	A	220	ASP	CA-CB-CG	8.36	120.96	112.60
1	B	234	ASP	CA-CB-CG	8.16	120.77	112.60
1	A	211	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	A	127	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	B	10	THR	CB-CA-C	-7.86	92.11	109.56
1	A	185	VAL	N-CA-C	7.77	120.44	106.61
1	A	100	SER	CA-CB-OG	-7.74	95.62	111.10
1	A	1	ALA	CA-C-N	7.70	136.37	122.13
1	A	1	ALA	C-N-CA	7.70	136.37	122.13
1	A	204	ASN	CB-CG-ND2	7.69	127.94	116.40
1	B	120	THR	N-CA-C	7.65	120.87	110.55
1	A	4	GLN	OE1-CD-NE2	-7.61	114.99	122.60
1	A	79	GLN	OE1-CD-NE2	-7.61	115.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LYS	CA-CB-CG	7.60	129.30	114.10
1	B	21	ASN	OD1-CG-ND2	-7.58	115.02	122.60
1	A	144	ASP	CA-CB-CG	7.58	120.18	112.60
1	A	177	ASP	CB-CA-C	-7.58	99.58	111.17
1	A	204	ASN	N-CA-C	7.54	120.39	111.71
1	B	216	GLU	CB-CG-CD	7.47	125.31	112.60
1	A	218	ARG	N-CA-C	7.45	119.19	111.14
1	B	50	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	10	THR	CB-CA-C	-7.45	94.27	109.38
1	B	17	PHE	CA-CB-CG	-7.37	106.43	113.80
1	A	172	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	B	55	LEU	N-CA-C	7.31	119.04	111.14
1	A	23	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	145	ASN	OD1-CG-ND2	-7.25	115.36	122.60
1	A	162	GLU	N-CA-CB	-7.23	99.35	109.91
1	B	128	GLU	O-C-N	-7.17	114.57	122.03
1	A	78	GLN	CA-CB-CG	-7.11	99.88	114.10
1	A	101	ASP	N-CA-C	7.11	125.94	110.80
1	A	114	VAL	CA-C-N	7.07	127.92	120.43
1	A	114	VAL	C-N-CA	7.07	127.92	120.43
1	A	135	ILE	O-C-N	-7.05	114.92	122.95
1	A	35	LYS	CB-CG-CD	-7.02	95.16	111.30
1	A	93	ARG	CB-CG-CD	6.91	127.19	111.30
1	A	96	VAL	N-CA-CB	-6.90	99.02	111.92
1	A	11	ASP	O-C-N	-6.85	115.68	121.23
1	B	101	ASP	CA-C-O	6.84	127.68	119.61
1	A	103	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	A	1	ALA	N-CA-C	6.83	130.12	111.00
1	A	10	THR	N-CA-CB	6.82	123.34	111.13
1	B	42	ASN	CB-CG-ND2	6.81	126.62	116.40
1	A	167	GLU	O-C-N	-6.78	114.42	122.15
1	B	122	GLN	CA-CB-CG	6.76	127.62	114.10
1	A	103	GLN	CA-CB-CG	6.75	127.60	114.10
1	B	144	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	29	PHE	O-C-N	-6.75	114.33	122.22
1	A	101	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	145	ASN	CB-CG-ND2	6.61	126.32	116.40
1	B	167	GLU	CA-CB-CG	-6.60	100.89	114.10
1	A	32	ASP	N-CA-C	6.59	119.01	111.11
1	B	39	LYS	CA-C-O	6.57	127.94	120.90
1	A	189	LYS	N-CA-C	6.52	118.39	111.28
1	B	48	VAL	O-C-N	-6.51	115.80	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	THR	N-CA-CB	6.51	123.64	111.53
1	A	121	THR	CA-CB-OG1	-6.44	99.94	109.60
1	A	50	ASN	OD1-CG-ND2	-6.39	116.20	122.60
1	B	211	ASN	N-CA-C	6.38	119.05	111.33
1	A	6	ILE	N-CA-C	6.37	117.75	108.58
1	B	88	TYR	O-C-N	-6.36	116.62	123.42
1	A	191	PHE	O-C-N	-6.32	115.98	123.06
1	B	136	GLU	N-CA-C	6.27	119.73	109.76
1	B	204	ASN	N-CA-C	6.27	120.19	112.54
1	B	163	VAL	CA-C-O	-6.24	113.89	120.57
1	B	67	ILE	CA-C-O	-6.17	113.97	120.39
1	A	147	TYR	O-C-N	-6.17	115.58	122.12
1	A	204	ASN	CA-CB-CG	6.16	118.75	112.60
1	A	121	THR	O-C-N	-6.14	115.61	122.12
1	A	154	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	B	6	ILE	O-C-N	-6.11	116.25	123.03
1	B	127	ASN	CA-CB-CG	-6.11	106.49	112.60
1	A	120	THR	N-CA-C	6.02	119.43	110.52
1	A	218	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	99	ASN	OD1-CG-ND2	-6.00	116.59	122.60
1	A	185	VAL	O-C-N	5.99	128.52	122.71
1	A	3	PRO	N-CA-C	5.98	119.83	110.80
1	B	6	ILE	CA-C-O	5.96	126.95	120.57
1	A	27	VAL	N-CA-CB	-5.96	100.91	111.93
1	A	118	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	B	30	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	224	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	56	ILE	CB-CA-C	-5.90	108.09	114.35
1	A	93	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	B	162	GLU	N-CA-C	5.90	121.05	111.37
1	B	50	ASN	CB-CG-ND2	5.88	125.22	116.40
1	B	193	VAL	N-CA-C	5.88	117.81	112.29
1	B	135	ILE	O-C-N	-5.83	116.55	123.03
1	B	100	SER	CB-CA-C	-5.81	101.39	110.74
1	A	121	THR	N-CA-CB	-5.78	101.62	110.12
1	A	89	ALA	N-CA-C	5.77	118.20	110.35
1	A	94	LEU	N-CA-CB	5.77	119.81	110.41
1	A	218	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	A	151	THR	CA-CB-OG1	-5.76	100.97	109.60
1	B	77	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	B	20	LYS	N-CA-C	5.73	117.45	110.41
1	B	58	SER	CA-CB-OG	5.72	122.55	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ILE	O-C-N	-5.69	116.08	121.94
1	B	143	GLN	CG-CD-NE2	5.68	124.93	116.40
1	B	208	GLU	CB-CA-C	-5.66	101.40	110.79
1	A	100	SER	CA-C-O	5.65	128.59	120.51
1	B	154	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	A	172	GLN	CG-CD-NE2	5.62	124.83	116.40
1	A	159	PHE	O-C-N	-5.61	115.71	123.12
1	A	44	GLN	CG-CD-NE2	5.59	124.78	116.40
1	A	50	ASN	CA-C-N	5.59	125.52	119.76
1	A	50	ASN	C-N-CA	5.59	125.52	119.76
1	B	79	GLN	CB-CG-CD	5.57	122.07	112.60
1	A	15	ALA	CA-C-O	-5.56	114.63	120.02
1	B	14	TYR	N-CA-C	5.55	116.37	108.54
1	B	184	ALA	O-C-N	-5.55	116.19	123.02
1	A	136	GLU	N-CA-C	5.52	117.30	108.41
1	B	99	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	127	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	107	ALA	CA-C-O	-5.50	113.88	120.10
1	B	143	GLN	O-C-N	-5.50	116.29	122.12
1	A	102	ILE	N-CA-CB	-5.50	102.16	111.23
1	A	186	LYS	CA-C-O	5.49	126.63	120.70
1	B	200	ARG	CG-CD-NE	-5.49	99.92	112.00
1	A	22	ALA	N-CA-C	5.49	119.46	112.87
1	A	42	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	103	GLN	N-CA-CB	-5.49	102.95	109.59
1	A	203	ASP	N-CA-C	5.49	117.85	109.62
1	A	185	VAL	CB-CA-C	-5.48	105.01	111.09
1	B	4	GLN	N-CA-CB	-5.46	101.50	110.40
1	B	40	ARG	CG-CD-NE	-5.45	100.01	112.00
1	B	74	THR	CA-CB-OG1	-5.43	101.45	109.60
1	B	200	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	B	151	THR	O-C-N	-5.43	115.87	122.22
1	A	129	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	98	LYS	N-CA-C	5.42	117.89	110.24
1	A	232	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	114	VAL	O-C-N	-5.40	115.84	122.97
1	B	192	GLY	CA-C-O	-5.40	117.37	122.39
1	A	74	THR	O-C-N	-5.40	115.88	123.11
1	A	128	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	4	GLN	CG-CD-NE2	5.38	124.47	116.40
1	B	97	ALA	O-C-N	-5.38	116.51	122.86
1	A	8	ILE	CB-CG1-CD1	5.37	125.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASP	N-CA-C	5.37	117.23	108.63
1	A	121	THR	CA-CB-CG2	5.37	119.63	110.50
1	B	40	ARG	N-CA-C	5.37	117.88	111.71
1	B	93	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	128	GLU	N-CA-C	5.36	116.81	110.97
1	B	136	GLU	CB-CG-CD	5.35	121.70	112.60
1	B	174	VAL	CB-CA-C	-5.35	101.58	111.79
1	B	200	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	220	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	103	GLN	CB-CG-CD	-5.32	103.55	112.60
1	B	155	ILE	CA-CB-CG2	-5.32	101.46	110.50
1	A	95	VAL	N-CA-C	-5.30	100.84	108.53
1	A	13	THR	CA-CB-CG2	5.26	119.44	110.50
1	B	96	VAL	N-CA-CB	-5.26	102.64	112.36
1	B	4	GLN	CA-C-O	5.25	125.82	119.31
1	A	45	CYS	CA-CB-SG	-5.25	102.33	114.40
1	B	166	SER	CA-CB-OG	-5.24	100.61	111.10
1	B	102	ILE	CA-C-O	5.24	127.33	120.78
1	A	234	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	42	ASN	CB-CG-ND2	5.24	124.26	116.40
1	B	6	ILE	CB-CA-C	5.22	117.94	110.84
1	B	78	GLN	CG-CD-NE2	5.22	124.23	116.40
1	B	139	SER	CB-CA-C	-5.22	100.71	109.53
1	A	235	VAL	CB-CA-C	-5.22	99.93	111.77
1	B	121	THR	O-C-N	-5.21	116.60	122.12
1	A	75	GLU	CB-CG-CD	5.18	121.40	112.60
1	B	48	VAL	CA-C-N	-5.18	115.89	122.77
1	B	48	VAL	C-N-CA	-5.18	115.89	122.77
1	B	233	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	199	LEU	O-C-N	-5.17	117.49	123.33
1	A	33	LEU	O-C-N	-5.16	116.26	122.15
1	B	93	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	A	135	ILE	N-CA-CB	-5.16	105.10	110.72
1	A	80	GLU	N-CA-C	5.15	121.76	110.80
1	B	199	LEU	CA-C-O	-5.14	115.23	120.99
1	B	205	GLU	CB-CG-CD	5.14	121.33	112.60
1	A	118	GLN	N-CA-C	5.14	117.48	110.24
1	B	127	ASN	CB-CG-ND2	5.13	124.09	116.40
1	A	194	GLY	N-CA-C	5.11	118.60	111.19
1	B	84	THR	O-C-N	-5.11	115.80	122.59
1	A	185	VAL	CA-CB-CG1	-5.08	101.76	110.40
1	B	78	GLN	N-CA-C	5.08	118.97	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	LYS	CA-C-N	-5.08	116.53	122.93
1	B	5	LYS	C-N-CA	-5.08	116.53	122.93
1	A	28	GLY	O-C-N	-5.07	119.12	123.43
1	B	102	ILE	N-CA-C	5.07	119.89	109.34
1	B	120	THR	CA-C-N	5.06	127.06	120.28
1	B	120	THR	C-N-CA	5.06	127.06	120.28
1	A	104	PRO	O-C-N	-5.05	115.82	122.64
1	B	79	GLN	CG-CD-NE2	5.04	123.97	116.40
1	A	24	GLY	O-C-N	-5.04	116.11	122.41
1	B	90	ALA	O-C-N	-5.03	116.65	123.19
1	A	102	ILE	CB-CA-C	5.03	119.54	111.29
1	A	200	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	B	57	PRO	O-C-N	-5.02	116.50	122.17
1	B	236	TYR	O-C-N	-5.01	116.10	122.27
1	A	56	ILE	CA-C-O	-5.01	114.59	118.85
1	A	202	GLU	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	TYR	Sidechain
1	B	178	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	A	1843	0	1840	49	0
1	B	1843	0	1840	50	0
2	A	5	0	0	0	2
2	B	2	0	0	0	0
3	A	11	0	6	1	0
3	B	11	0	6	2	0
4	A	161	0	0	5	0
4	B	125	0	0	6	2
All	All	4001	0	3692	95	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (95) 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:A:113:ARG:NH2	1:A:138:VAL:HG21	1.91	0.85
1:B:121:THR:HG21	4:B:249:HOH:O	1.78	0.84
1:B:94:LEU:HD11	1:B:130:TRP:HH2	1.52	0.74
1:B:118:GLN:HG2	1:B:139:SER:HB3	1.70	0.74
1:B:109:LEU:HD13	1:B:135:ILE:HD13	1.70	0.71
1:A:56:ILE:HG13	1:A:57:PRO:HD3	1.74	0.69
1:B:62:LYS:HA	1:B:200:ARG:HH11	1.57	0.68
1:B:72:SER:HG	3:B:239:HIS:N	1.94	0.66
1:A:6:ILE:HG23	1:A:65:ASP:HB2	1.78	0.66
1:B:5:LYS:HE3	1:B:46:THR:HB	1.77	0.65
1:B:104:PRO:HG3	1:B:183:PRO:HD2	1.78	0.64
1:B:92:SER:O	1:B:184:ALA:HA	1.97	0.64
1:A:113:ARG:HH22	1:A:138:VAL:HG21	1.63	0.63
1:B:93:ARG:HG2	1:B:184:ALA:HA	1.82	0.62
1:A:7:ARG:HH11	1:A:48:VAL:HG21	1.65	0.61
1:A:41:ILE:HD12	1:A:209:ALA:HB1	1.81	0.61
1:A:113:ARG:HH21	1:A:113:ARG:HB3	1.67	0.60
1:A:94:LEU:HD23	1:A:159:PHE:HB2	1.83	0.59
1:A:84:THR:HG22	1:A:197:MET:H	1.66	0.58
1:B:76:LYS:HZ2	1:B:190:LEU:HA	1.67	0.58
1:A:102:ILE:HG13	1:A:109:LEU:HD23	1.85	0.57
1:B:56:ILE:HD12	1:B:56:ILE:H	1.70	0.57
1:B:104:PRO:HD3	1:B:182:GLY:HA3	1.87	0.57
1:A:122:GLN:HB3	1:A:159:PHE:CD2	2.40	0.56
1:A:121:THR:HG21	4:A:244:HOH:O	2.06	0.56
1:B:62:LYS:HA	1:B:200:ARG:NH1	2.21	0.56
1:B:122:GLN:HE22	3:B:239:HIS:HB2	1.70	0.55
1:B:13:THR:HG21	1:B:142:GLY:HA2	1.89	0.55
1:A:44:GLN:OE1	1:B:225:LYS:HB2	2.07	0.55
1:B:122:GLN:HB2	1:B:159:PHE:CD2	2.43	0.54
1:A:13:THR:O	1:A:143:GLN:HB3	2.08	0.53
1:A:200:ARG:HB3	1:A:202:GLU:HG2	1.89	0.53
1:A:5:LYS:HA	1:A:44:GLN:O	2.08	0.53
1:A:113:ARG:HH21	1:A:138:VAL:HG21	1.70	0.53
1:A:130:TRP:CZ2	1:A:185:VAL:HG11	2.43	0.53
1:A:67:ILE:HG21	1:A:71:LEU:HD22	1.92	0.52
1:B:130:TRP:HB3	1:B:135:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:H	1:B:205:GLU:CD	2.18	0.52
1:B:2:ILE:HD11	1:B:41:ILE:HD12	1.90	0.52
1:A:56:ILE:HG12	4:A:439:HOH:O	2.10	0.51
1:B:76:LYS:NZ	1:B:190:LEU:HA	2.25	0.51
1:A:8:ILE:HG12	1:A:66:ALA:HB3	1.92	0.51
1:B:117:LEU:HD21	4:B:356:HOH:O	2.10	0.51
1:B:218:ARG:HD2	4:B:387:HOH:O	2.10	0.50
1:B:104:PRO:CD	1:B:182:GLY:HA3	2.40	0.50
1:A:72:SER:HG	3:A:239:HIS:N	2.10	0.49
1:A:103:GLN:HB2	1:A:104:PRO:HD3	1.93	0.49
1:B:10:THR:HG23	1:B:68:MET:O	2.12	0.49
1:A:84:THR:CG2	1:A:197:MET:H	2.25	0.49
1:B:135:ILE:O	1:B:135:ILE:HG13	2.12	0.49
1:A:40:ARG:HH22	1:A:222:THR:HG21	1.77	0.49
1:A:22:ALA:HB3	1:B:42:ASN:HD21	1.79	0.48
1:A:142:GLY:N	4:A:816:HOH:O	2.47	0.48
1:B:13:THR:O	1:B:143:GLN:HB3	2.13	0.48
1:A:105:THR:HG22	1:A:107:ALA:H	1.77	0.48
1:A:216:GLU:O	1:A:220:ASP:HB3	2.13	0.48
1:B:109:LEU:HA	1:B:112:LYS:HG3	1.96	0.47
1:B:36:GLU:O	1:B:40:ARG:HG3	2.14	0.47
1:B:102:ILE:HG12	1:B:112:LYS:HD3	1.97	0.47
1:A:140:TYR:CD2	1:A:146:ILE:HG12	2.49	0.47
1:A:84:THR:HG22	1:A:197:MET:N	2.30	0.46
1:A:151:THR:HG22	4:A:833:HOH:O	2.15	0.46
1:B:32:ASP:HB3	1:B:226:LEU:HD22	1.98	0.46
1:A:57:PRO:O	1:A:60:LYS:HG2	2.15	0.46
1:B:37:LEU:HD23	1:B:197:MET:HE1	1.98	0.45
1:A:23:GLN:HG2	1:B:42:ASN:HD22	1.82	0.44
1:A:17:PHE:O	1:A:30:ASP:HB2	2.17	0.44
1:B:76:LYS:NZ	1:B:189:LYS:O	2.50	0.44
1:B:204:ASN:O	1:B:208:GLU:HG3	2.18	0.44
1:A:105:THR:HG22	1:A:107:ALA:N	2.32	0.44
1:B:4:GLN:H	1:B:4:GLN:HG3	1.34	0.44
1:A:130:TRP:HZ2	1:A:185:VAL:HG11	1.82	0.43
1:B:229:LYS:HD3	4:B:864:HOH:O	2.17	0.43
1:B:100:SER:HB3	1:B:102:ILE:HD12	2.00	0.43
1:B:131:ALA:N	1:B:132:PRO:HD2	2.34	0.43
1:A:12:PRO:O	1:A:19:SER:HA	2.18	0.43
1:A:56:ILE:HG12	1:A:56:ILE:H	1.65	0.42
1:B:76:LYS:HE2	1:B:76:LYS:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:HA	1:B:210:LEU:HD23	1.87	0.42
1:B:67:ILE:HG21	1:B:67:ILE:HD13	1.83	0.42
1:B:81:ILE:HA	4:B:801:HOH:O	2.18	0.42
1:B:94:LEU:HD11	1:B:130:TRP:CH2	2.42	0.42
1:A:41:ILE:HA	1:A:41:ILE:HD13	1.69	0.42
1:A:86:LYS:O	1:A:236:TYR:HE2	2.03	0.42
1:A:41:ILE:HD11	1:A:209:ALA:C	2.45	0.41
1:A:116:VAL:O	1:A:139:SER:HA	2.21	0.41
1:A:41:ILE:HD12	1:A:41:ILE:HG23	1.82	0.41
1:B:23:GLN:NE2	4:B:386:HOH:O	2.52	0.41
1:B:37:LEU:HD23	1:B:197:MET:CE	2.51	0.41
1:B:76:LYS:HD3	1:B:76:LYS:H	1.86	0.40
1:A:131:ALA:N	1:A:132:PRO:HD2	2.36	0.40
1:A:101:ASP:O	1:A:103:GLN:N	2.54	0.40
1:A:25:GLU:HB2	1:B:39:LYS:HB3	2.04	0.40
1:A:102:ILE:HD11	1:A:157:ALA:HB2	2.02	0.40
1:A:174:VAL:HG22	4:A:330:HOH:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:752:CD:CD	4:B:962:HOH:O[2_445]	1.59	0.61
2:A:756:CD:CD	4:B:956:HOH:O[2_445]	1.64	0.56

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	236/238 (99%)	215 (91%)	17 (7%)	4 (2%)	7	2
1	B	236/238 (99%)	214 (91%)	18 (8%)	4 (2%)	7	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	472/476 (99%)	429 (91%)	35 (7%)	8 (2%)	7	2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	101	ASP
1	A	100	SER
1	A	102	ILE
1	B	104	PRO
1	B	107	ALA
1	B	84	THR
1	B	24	GLY

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	193/193 (100%)	163 (84%)	30 (16%)	2	1
1	B	193/193 (100%)	158 (82%)	35 (18%)	2	0
All	All	386/386 (100%)	321 (83%)	65 (17%)	2	0

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	10	THR
1	A	16	PRO
1	A	18	GLU
1	A	26	LEU
1	A	27	VAL
1	A	36	GLU
1	A	50	ASN
1	A	52	LEU
1	A	56	ILE

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Mol	Chain	Res	Type
1	A	59	LEU
1	A	70	SER
1	A	76	LYS
1	A	77	ARG
1	A	79	GLN
1	A	87	LEU
1	A	96	VAL
1	A	113	ARG
1	A	133	LYS
1	A	141	GLN
1	A	151	THR
1	A	160	GLN
1	A	162	GLU
1	A	174	VAL
1	A	199	LEU
1	A	201	LYS
1	A	202	GLU
1	A	216	GLU
1	A	220	ASP
1	A	235	VAL
1	B	2	ILE
1	B	4	GLN
1	B	6	ILE
1	B	10	THR
1	B	23	GLN
1	B	26	LEU
1	B	27	VAL
1	B	33	LEU
1	B	37	LEU
1	B	43	THR
1	B	46	THR
1	B	56	ILE
1	B	75	GLU
1	B	77	ARG
1	B	79	GLN
1	B	87	LEU
1	B	91	ASP
1	B	93	ARG
1	B	96	VAL
1	B	100	SER
1	B	103	GLN
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	129	HIS
1	B	133	LYS
1	B	135	ILE
1	B	154	ARG
1	B	167	GLU
1	B	176	LYS
1	B	188	GLU
1	B	190	LEU
1	B	201	LYS
1	B	202	GLU
1	B	205	GLU
1	B	225	LYS
1	B	235	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	122	GLN
1	A	127	ASN
1	A	143	GLN
1	B	4	GLN
1	B	42	ASN
1	B	50	ASN
1	B	79	GLN
1	B	122	GLN
1	B	127	ASN
1	B	204	ASN

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

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	HIS	B	239	-	10,11,11	1.16	0	10,14,14	1.59	2 (20%)
3	HIS	A	239	-	10,11,11	1.37	2 (20%)	10,14,14	2.03	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HIS	B	239	-	-	2/8/8/8	0/1/1/1
3	HIS	A	239	-	-	2/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	239	HIS	CD2-NE2	-2.22	1.30	1.36
3	A	239	HIS	OXT-C	-2.10	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	239	HIS	CA-CB-CG	4.94	125.95	113.77
3	B	239	HIS	CA-CB-CG	3.05	121.30	113.77
3	A	239	HIS	CD2-NE2-CE1	2.89	112.52	107.36
3	B	239	HIS	CD2-NE2-CE1	2.73	112.23	107.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	239	HIS	CA-CB-CG-CD2
3	B	239	HIS	CA-CB-CG-ND1
3	B	239	HIS	CA-CB-CG-CD2
3	A	239	HIS	CA-CB-CG-ND1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	239	HIS	2	0
3	A	239	HIS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.