



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:10 PM UTC

PDB ID : 1HHJ / pdb_00001hhj
Title : THE ANTIGENIC IDENTITY OF PEPTIDE(SLASH)MHC COMPLEXES:
A COMPARISON OF THE CONFORMATION OF FIVE PEPTIDES PRE-
SENTED BY HLA-A2
Authors : Madden, D.R.; Garboczi, D.N.; Wiley, D.C.
Deposited on : 1993-06-30
Resolution : 2.50 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)	:	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

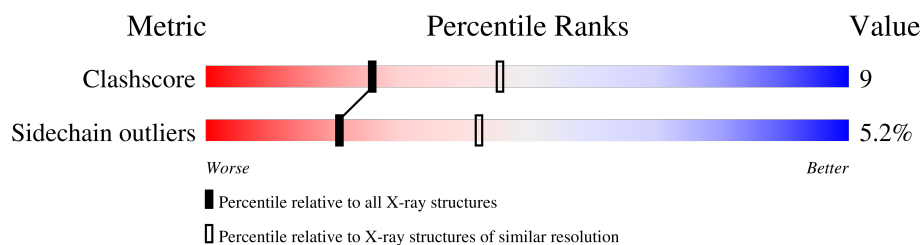
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	275	66% 28% 6% .
1	D	275	63% 30% 6% .
2	B	100	64% 28% 8%
2	E	100	64% 30% 6%
3	C	9	56% 44%
3	F	9	44% 56%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6308 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 CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
1	D	275	Total	C	N	O	S	17	0	0
			2247	1403	409	426	9			

- Molecule 2 is a protein called BETA 2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	10	0	0
			837	533	141	159	4			

- Molecule 3 is a protein called HIV-1 REVERSE TRANSCRIPTASE (RESIDUES 309-317).

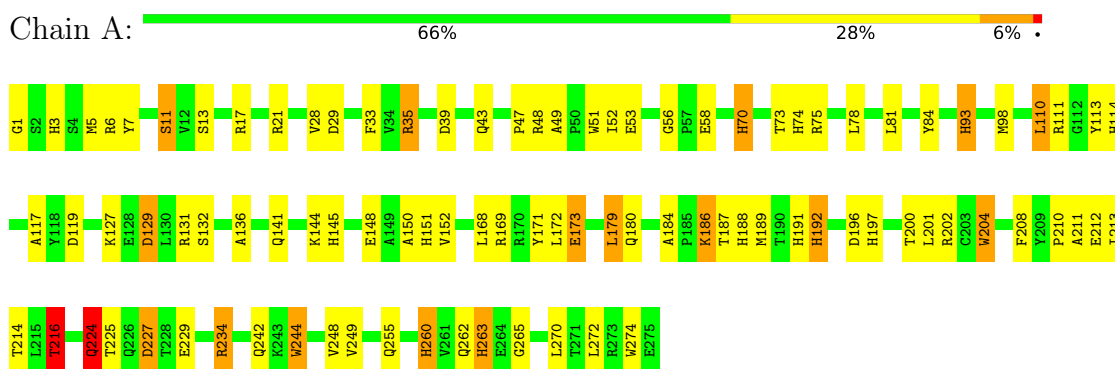
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			70	46	12	12			
3	F	9	Total	C	N	O	0	0	0
			70	46	12	12			

3 Residue-property plots

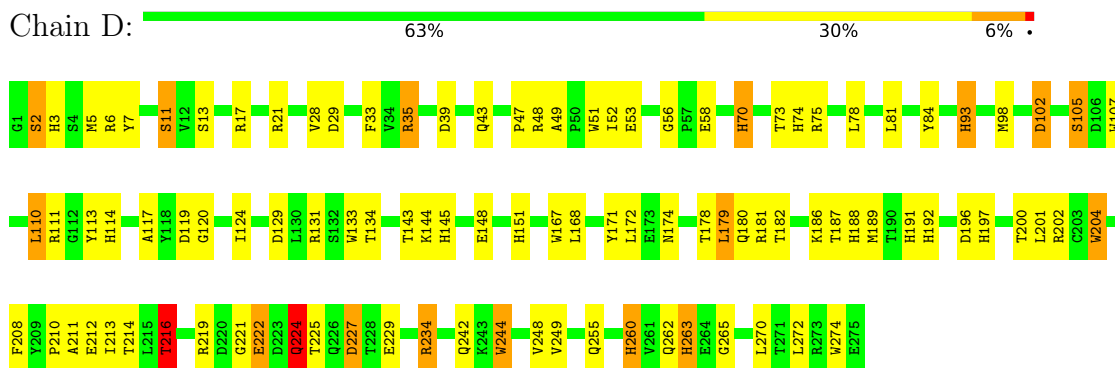
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

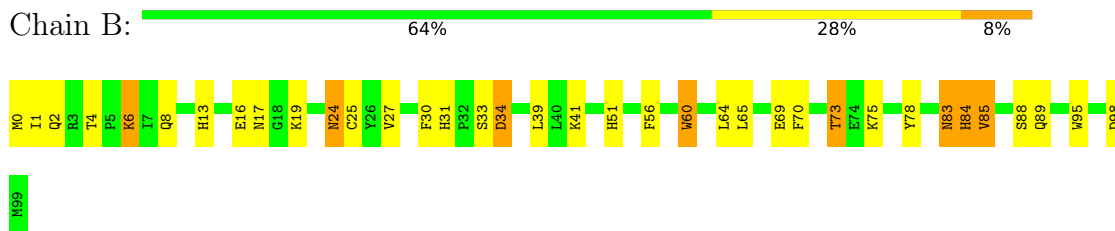
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN)



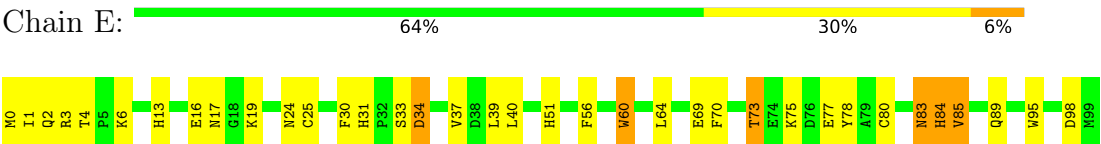
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN)



- Molecule 2: BETA 2-MICROGLOBULIN



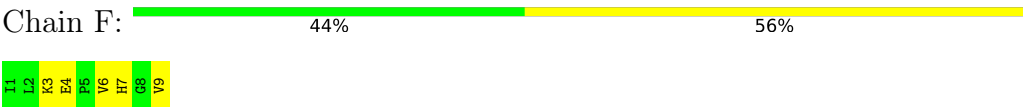
- Molecule 2: BETA 2-MICROGLOBULIN



● Molecule 3: HIV-1 REVERSE TRANSCRIPTASE (RESIDUES 309-317)



● Molecule 3: HIV-1 REVERSE TRANSCRIPTASE (RESIDUES 309-317)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.37Å 63.60Å 74.75Å 81.53° 75.72° 77.48°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.278 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6308	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.12	14/2312 (0.6%)	1.79	42/3137 (1.3%)
1	D	1.13	16/2312 (0.7%)	1.80	48/3137 (1.5%)
2	B	1.07	5/860 (0.6%)	1.77	24/1162 (2.1%)
2	E	1.09	5/860 (0.6%)	1.78	25/1162 (2.2%)
3	C	1.29	1/71 (1.4%)	1.67	0/94
3	F	1.29	1/71 (1.4%)	1.67	0/94
All	All	1.11	42/6486 (0.6%)	1.79	139/8786 (1.6%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	84	HIS	CD2-NE2	-7.91	1.29	1.37
2	B	84	HIS	CD2-NE2	-7.84	1.29	1.37
1	D	191	HIS	CD2-NE2	-7.25	1.29	1.37
1	A	191	HIS	CD2-NE2	-7.20	1.29	1.37
1	A	74	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	93	HIS	CD2-NE2	-7.07	1.30	1.37
1	D	93	HIS	CD2-NE2	-7.00	1.30	1.37
1	D	74	HIS	CD2-NE2	-6.97	1.30	1.37
2	E	13	HIS	CD2-NE2	-6.93	1.30	1.37
2	B	13	HIS	CD2-NE2	-6.90	1.30	1.37
1	D	260	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	114	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	260	HIS	CD2-NE2	-6.80	1.30	1.37
2	B	51	HIS	CD2-NE2	-6.68	1.30	1.37
1	D	114	HIS	CD2-NE2	-6.67	1.30	1.37
2	E	51	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	263	HIS	CD2-NE2	-6.61	1.30	1.37
1	D	263	HIS	CD2-NE2	-6.58	1.30	1.37
2	E	31	HIS	CD2-NE2	-6.55	1.30	1.37
2	B	31	HIS	CD2-NE2	-6.50	1.30	1.37
1	D	145	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	70	HIS	CD2-NE2	-6.42	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	192	HIS	CD2-NE2	-6.25	1.30	1.37
1	D	188	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	188	HIS	CD2-NE2	-6.17	1.31	1.37
3	C	7	HIS	CD2-NE2	-6.00	1.31	1.37
3	F	7	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	197	HIS	CD2-NE2	-5.76	1.31	1.37
1	D	212	GLU	CA-CB	-5.74	1.44	1.53
1	D	197	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	212	GLU	CA-CB	-5.69	1.44	1.53
1	D	192	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	145	HIS	CD2-NE2	-5.61	1.31	1.37
1	D	3	HIS	CG-ND1	-5.57	1.32	1.38
1	D	3	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	74	HIS	CG-ND1	-5.47	1.32	1.38
1	D	74	HIS	CG-ND1	-5.45	1.32	1.38
1	A	191	HIS	CG-ND1	-5.26	1.32	1.38
1	D	151	HIS	CD2-NE2	-5.12	1.32	1.37
2	E	51	HIS	CG-ND1	-5.01	1.32	1.38
2	B	51	HIS	CG-ND1	-5.01	1.32	1.38

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	ASP	N-CA-C	8.43	121.53	111.33
1	A	33	PHE	CA-CB-CG	8.19	121.99	113.80
1	D	33	PHE	CA-CB-CG	8.18	121.98	113.80
2	E	24	ASN	CA-CB-CG	8.03	120.63	112.60
2	B	24	ASN	CA-CB-CG	7.98	120.58	112.60
1	D	70	HIS	CB-CG-CD2	-7.65	121.25	131.20
1	A	208	PHE	CA-CB-CG	7.63	121.43	113.80
1	A	70	HIS	CB-CG-CD2	-7.61	121.31	131.20
1	D	208	PHE	CA-CB-CG	7.58	121.38	113.80
2	E	13	HIS	CB-CG-CD2	-7.19	121.85	131.20
2	B	84	HIS	CB-CG-CD2	-7.11	121.95	131.20
2	B	13	HIS	CB-CG-CD2	-7.11	121.95	131.20
2	E	84	HIS	CB-CG-CD2	-7.08	122.00	131.20
1	A	196	ASP	N-CA-C	7.08	121.01	112.38
1	D	174	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	D	180	GLN	OE1-CD-NE2	-7.03	115.57	122.60
2	E	98	ASP	CA-CB-CG	7.01	119.61	112.60
1	D	28	VAL	N-CA-C	-7.00	98.37	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	98	ASP	CA-CB-CG	6.97	119.57	112.60
1	D	224	GLN	OE1-CD-NE2	-6.93	115.67	122.60
2	E	2	GLN	OE1-CD-NE2	-6.79	115.81	122.60
2	B	2	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	D	196	ASP	CB-CA-C	-6.66	99.36	110.68
2	B	17	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	A	151	HIS	CA-C-N	6.62	129.03	120.56
1	A	151	HIS	C-N-CA	6.62	129.03	120.56
2	E	17	ASN	OD1-CG-ND2	-6.59	116.01	122.60
2	E	83	ASN	CA-CB-CG	-6.56	106.04	112.60
1	D	191	HIS	CB-CG-CD2	-6.54	122.69	131.20
2	B	83	ASN	CA-CB-CG	-6.53	106.07	112.60
1	D	29	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	28	VAL	N-CA-C	-6.49	98.39	107.80
1	A	29	ASP	CA-CB-CG	6.48	119.08	112.60
2	B	70	PHE	CA-CB-CG	6.47	120.27	113.80
2	E	70	PHE	CA-CB-CG	6.41	120.21	113.80
1	D	255	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	A	255	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	A	39	ASP	CA-CB-CG	6.28	118.88	112.60
1	D	39	ASP	CA-CB-CG	6.26	118.86	112.60
2	B	31	HIS	CB-CG-CD2	-6.21	123.13	131.20
2	E	31	HIS	CB-CG-CD2	-6.18	123.17	131.20
1	D	222	GLU	CB-CG-CD	6.13	123.02	112.60
2	E	56	PHE	CA-CB-CG	6.10	119.90	113.80
1	D	93	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	93	HIS	CB-CG-CD2	-6.07	123.30	131.20
2	B	56	PHE	CA-CB-CG	6.06	119.86	113.80
1	D	260	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	D	70	HIS	CB-CG-ND1	5.99	131.68	122.70
1	A	70	HIS	CB-CG-ND1	5.97	131.66	122.70
1	A	191	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	A	260	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	110	LEU	N-CA-C	-5.86	105.13	112.93
1	A	188	HIS	CB-CG-CD2	-5.84	123.60	131.20
1	D	188	HIS	CB-CG-CD2	-5.83	123.62	131.20
2	B	84	HIS	CB-CG-ND1	5.82	131.43	122.70
2	E	84	HIS	CB-CG-ND1	5.81	131.42	122.70
1	D	3	HIS	CA-CB-CG	-5.80	108.00	113.80
1	D	211	ALA	N-CA-C	5.76	119.78	112.87
1	A	274	TRP	CG-CD2-CE3	5.75	139.65	133.90
1	A	229	GLU	CA-CB-CG	-5.73	102.64	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	TRP	CG-CD2-CE3	5.73	139.63	133.90
1	D	229	GLU	CA-CB-CG	-5.72	102.66	114.10
1	A	197	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	244	TRP	CG-CD2-CE3	5.70	139.59	133.90
1	D	151	HIS	CA-CB-CG	-5.69	108.11	113.80
1	A	211	ALA	N-CA-C	5.65	119.65	112.87
1	D	244	TRP	CG-CD2-CE3	5.60	139.50	133.90
2	B	33	SER	N-CA-C	5.59	119.95	113.18
2	E	1	ILE	N-CA-C	5.59	116.62	109.30
2	B	1	ILE	N-CA-C	5.58	116.62	109.30
1	A	179	LEU	N-CA-C	5.58	119.78	112.92
2	E	33	SER	N-CA-C	5.57	119.92	113.18
1	A	263	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	A	204	TRP	CE2-CD2-CG	-5.50	100.60	107.20
2	B	6	LYS	N-CA-C	-5.49	101.59	110.32
1	D	263	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	D	204	TRP	CE2-CD2-CG	-5.48	100.62	107.20
1	D	43	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	D	221	GLY	CA-C-N	5.48	130.49	121.39
1	D	221	GLY	C-N-CA	5.48	130.49	121.39
1	A	43	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	A	179	LEU	CA-C-O	5.46	125.95	119.56
2	E	6	LYS	N-CA-C	-5.45	101.66	110.32
2	E	95	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	D	274	TRP	CE2-CD2-CG	-5.42	100.69	107.20
1	D	105	SER	O-C-N	5.42	128.56	122.22
1	A	188	HIS	CA-CB-CG	5.42	119.22	113.80
1	A	216	THR	N-CA-CB	-5.41	101.47	111.53
1	D	188	HIS	CA-CB-CG	5.41	119.21	113.80
1	D	56	GLY	CA-C-N	5.41	125.23	119.28
1	D	56	GLY	C-N-CA	5.41	125.23	119.28
1	D	216	THR	N-CA-CB	-5.41	101.47	111.53
1	A	56	GLY	CA-C-N	5.40	125.22	119.28
1	A	56	GLY	C-N-CA	5.40	125.22	119.28
1	A	274	TRP	CE2-CD2-CG	-5.40	100.72	107.20
2	B	95	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	A	224	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	180	GLN	N-CA-C	-5.37	105.42	112.41
2	E	89	GLN	CA-C-N	5.35	126.53	119.84
2	E	89	GLN	C-N-CA	5.35	126.53	119.84
1	A	186	LYS	N-CA-C	-5.32	99.85	108.41
1	A	244	TRP	CE2-CD2-CG	-5.32	100.82	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	186	LYS	N-CA-C	-5.30	99.88	108.41
1	D	244	TRP	CE2-CD2-CG	-5.30	100.84	107.20
1	D	110	LEU	N-CA-C	-5.28	106.16	113.18
2	B	85	VAL	CB-CA-C	-5.26	104.00	112.16
1	D	102	ASP	CA-CB-CG	5.26	117.86	112.60
2	E	85	VAL	CB-CA-C	-5.25	104.03	112.16
2	E	24	ASN	OD1-CG-ND2	-5.24	117.36	122.60
2	B	73	THR	CA-CB-OG1	-5.23	101.75	109.60
2	E	73	THR	CA-CB-OG1	-5.21	101.78	109.60
2	E	51	HIS	CB-CG-CD2	-5.21	124.42	131.20
2	B	51	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	D	180	GLN	CG-CD-NE2	5.20	124.19	116.40
2	B	60	TRP	CE2-CD2-CG	-5.19	100.97	107.20
2	B	24	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	D	131	ARG	CA-C-N	-5.17	114.70	122.81
1	D	131	ARG	C-N-CA	-5.17	114.70	122.81
1	D	227	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	141	GLN	OE1-CD-NE2	-5.13	117.47	122.60
2	E	60	TRP	CE2-CD2-CG	-5.13	101.05	107.20
2	B	60	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	A	227	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	244	TRP	CB-CG-CD1	-5.08	119.27	126.90
2	E	60	TRP	CG-CD2-CE3	5.08	138.98	133.90
2	E	95	TRP	CE2-CD2-CG	-5.07	101.11	107.20
1	D	58	GLU	N-CA-CB	-5.07	102.66	110.01
1	D	244	TRP	CB-CG-CD1	-5.04	119.33	126.90
2	B	95	TRP	CE2-CD2-CG	-5.04	101.15	107.20
2	E	77	GLU	CB-CG-CD	-5.04	104.04	112.60
2	B	89	GLN	CA-C-N	5.03	126.13	119.84
2	B	89	GLN	C-N-CA	5.03	126.13	119.84
1	A	129	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	167	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	D	51	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	A	58	GLU	N-CA-CB	-5.02	102.74	110.01
1	A	136	ALA	N-CA-C	5.02	116.75	111.28
1	A	51	TRP	CE2-CD2-CG	-5.00	101.19	107.20
1	D	129	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2247	0	2096	46	0
1	D	2247	0	2096	49	0
2	B	837	0	803	12	0
2	E	837	0	803	10	0
3	C	70	0	78	4	0
3	F	70	0	78	5	0
All	All	6308	0	5954	115	0

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 9.

All (115) 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:35:ARG:HG2	1:A:48:ARG:HD3	1.66	0.78
1:D:35:ARG:HG2	1:D:48:ARG:HD3	1.66	0.77
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.80	0.64
1:D:49:ALA:O	1:D:52:ILE:HG22	1.98	0.63
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.80	0.63
1:A:49:ALA:O	1:A:52:ILE:HG22	1.98	0.62
1:D:178:THR:O	1:D:181:ARG:HG2	1.99	0.61
1:A:1:GLY:O	1:A:3:HIS:CD2	2.54	0.59
2:B:73:THR:HG22	2:B:75:LYS:H	1.68	0.59
1:A:110:LEU:HG	1:A:111:ARG:NH1	2.19	0.57
1:A:17:ARG:HG2	1:A:17:ARG:HH11	1.70	0.57
1:D:17:ARG:HG2	1:D:17:ARG:HH11	1.70	0.57
1:A:11:SER:HA	1:A:21:ARG:O	2.05	0.57
1:A:150:ALA:HB3	1:A:152:VAL:HG23	1.87	0.56
1:D:11:SER:HA	1:D:21:ARG:O	2.05	0.56
1:A:70:HIS:CE1	3:C:6:VAL:HG21	2.41	0.56
1:D:35:ARG:NH1	1:D:48:ARG:NH1	2.54	0.56
1:A:35:ARG:NH1	1:A:48:ARG:NH1	2.54	0.55
1:D:70:HIS:CE1	3:F:6:VAL:HG21	2.41	0.55
1:A:189:MET:HE3	1:A:272:LEU:HB2	1.89	0.54
1:D:189:MET:HE3	1:D:272:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:HIS:HE1	3:C:3:LYS:O	1.92	0.53
2:E:73:THR:HG22	2:E:75:LYS:H	1.74	0.53
1:A:110:LEU:HG	1:A:111:ARG:HH12	1.73	0.53
1:A:224:GLN:HG3	1:A:227:ASP:HB2	1.91	0.52
1:D:70:HIS:HE1	3:F:3:LYS:O	1.92	0.52
1:D:81:LEU:HD23	1:D:84:TYR:HD2	1.75	0.52
1:A:214:THR:HB	1:A:262:GLN:HB2	1.91	0.52
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.43	0.51
1:D:214:THR:HB	1:D:262:GLN:HB2	1.91	0.51
1:D:224:GLN:HG3	1:D:227:ASP:HB2	1.93	0.51
1:D:47:PRO:HB2	1:D:53:GLU:HG2	1.92	0.51
1:A:47:PRO:HB2	1:A:53:GLU:HG2	1.93	0.50
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.45	0.50
1:D:5:MET:SD	1:D:171:TYR:HE2	2.34	0.50
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.45	0.50
2:B:41:LYS:HE3	2:B:78:TYR:OH	2.11	0.50
1:A:81:LEU:HD23	1:A:84:TYR:HD2	1.75	0.50
1:D:172:LEU:HA	1:D:179:LEU:CD1	2.41	0.50
2:B:30:PHE:HZ	2:B:64:LEU:HD12	1.77	0.50
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.94	0.49
1:D:172:LEU:HA	1:D:179:LEU:HD11	1.95	0.49
1:A:144:LYS:O	1:A:148:GLU:HG3	2.12	0.49
2:E:30:PHE:HZ	2:E:64:LEU:HD12	1.77	0.49
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.94	0.48
1:D:187:THR:HA	1:D:204:TRP:O	2.13	0.48
1:D:201:LEU:HD22	1:D:249:VAL:HG21	1.96	0.48
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.48	0.48
1:A:127:LYS:HD2	1:A:132:SER:OG	2.14	0.48
1:A:187:THR:HA	1:A:204:TRP:O	2.13	0.48
1:D:182:THR:CG2	1:D:265:GLY:CA	2.91	0.48
1:A:201:LEU:HD22	1:A:249:VAL:HG21	1.95	0.47
1:A:213:ILE:HG13	1:A:262:GLN:O	2.14	0.47
1:D:110:LEU:HG	1:D:111:ARG:HH12	1.78	0.47
1:A:73:THR:HG21	3:C:6:VAL:HG12	1.96	0.47
1:D:73:THR:HG21	3:F:6:VAL:HG12	1.96	0.47
2:E:34:ASP:O	2:E:84:HIS:HD2	1.97	0.47
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.83	0.47
2:B:34:ASP:O	2:B:84:HIS:HD2	1.97	0.47
1:D:260:HIS:HA	1:D:270:LEU:O	2.14	0.47
1:A:5:MET:SD	1:A:171:TYR:HE2	2.38	0.47
1:A:260:HIS:HA	1:A:270:LEU:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.83	0.46
1:D:213:ILE:HG13	1:D:262:GLN:O	2.14	0.46
1:A:172:LEU:HA	1:A:179:LEU:HD11	1.98	0.46
1:D:182:THR:HG21	1:D:265:GLY:CA	2.46	0.46
1:D:2:SER:H	1:D:105:SER:HA	1.81	0.45
1:D:7:TYR:O	1:D:98:MET:HA	2.17	0.45
3:F:3:LYS:HG2	3:F:4:GLU:N	2.31	0.45
2:E:40:LEU:O	2:E:78:TYR:HA	2.17	0.45
1:A:169:ARG:O	1:A:173:GLU:HG2	2.17	0.45
1:A:7:TYR:O	1:A:98:MET:HA	2.17	0.45
1:D:35:ARG:NH1	1:D:48:ARG:HH11	2.15	0.44
1:A:35:ARG:NH1	1:A:48:ARG:HH11	2.15	0.44
3:C:3:LYS:HG2	3:C:4:GLU:N	2.31	0.44
1:D:234:ARG:HD3	1:D:242:GLN:HB2	2.00	0.44
1:D:133:TRP:HB2	1:D:144:LYS:HG3	1.98	0.44
1:A:234:ARG:HD3	1:A:242:GLN:HB2	2.00	0.43
2:B:73:THR:HG22	2:B:75:LYS:HB3	1.99	0.43
1:A:172:LEU:HA	1:A:179:LEU:CD1	2.48	0.43
1:A:189:MET:HA	1:A:202:ARG:O	2.19	0.43
1:A:93:HIS:HD2	1:A:119:ASP:OD2	2.02	0.43
1:D:120:GLY:O	2:E:3:ARG:NH2	2.52	0.43
1:D:189:MET:HA	1:D:202:ARG:O	2.19	0.43
1:A:210:PRO:O	1:A:263:HIS:HE1	2.01	0.42
1:D:210:PRO:O	1:D:263:HIS:HE1	2.01	0.42
1:D:93:HIS:HD2	1:D:119:ASP:OD2	2.01	0.42
1:D:143:THR:HG23	3:F:9:VAL:HA	2.00	0.42
1:D:144:LYS:HE2	1:D:148:GLU:OE2	2.19	0.42
1:A:234:ARG:NH1	2:B:8:GLN:OE1	2.52	0.42
1:D:5:MET:SD	1:D:171:TYR:CE2	3.12	0.42
2:E:37:VAL:HG13	2:E:80:CYS:SG	2.60	0.42
1:A:216:THR:HG22	1:A:260:HIS:HB2	2.02	0.42
1:D:98:MET:C	1:D:98:MET:SD	3.03	0.42
1:D:182:THR:HG21	1:D:265:GLY:HA2	2.00	0.42
1:A:184:ALA:O	1:A:186:LYS:NZ	2.49	0.41
1:A:129:ASP:O	1:A:131:ARG:HG3	2.21	0.41
1:A:263:HIS:CD2	1:A:265:GLY:H	2.38	0.41
1:D:263:HIS:CD2	1:D:265:GLY:H	2.38	0.41
1:D:107:TRP:CE2	1:D:172:LEU:HD13	2.55	0.41
1:A:98:MET:SD	1:A:98:MET:C	3.03	0.41
2:E:34:ASP:O	2:E:84:HIS:CD2	2.73	0.41
1:D:124:ILE:HA	1:D:134:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:LYS:O	2:B:27:VAL:HA	2.22	0.40
2:B:16:GLU:HB2	2:B:19:LYS:HD2	2.03	0.40
1:D:13:SER:HB3	1:D:78:LEU:HD13	2.04	0.40
1:D:219:ARG:O	1:D:222:GLU:HG2	2.21	0.40
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.03	0.40
1:D:216:THR:HG22	1:D:260:HIS:HB2	2.02	0.40
2:B:34:ASP:O	2:B:84:HIS:CD2	2.73	0.40
2:E:16:GLU:HB2	2:E:19:LYS:HD2	2.03	0.40
1:A:13:SER:HB3	1:A:78:LEU:HD13	2.03	0.40
1:A:169:ARG:HH11	1:A:169:ARG:HD3	1.70	0.40
1:A:179:LEU:H	1:A:179:LEU:HG	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/231 (100%)	220 (95%)	11 (5%)	23	46
1	D	231/231 (100%)	220 (95%)	11 (5%)	23	46
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	27
2	E	95/95 (100%)	89 (94%)	6 (6%)	16	34
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	668/668 (100%)	633 (95%)	35 (5%)	21	42

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	35	ARG
1	A	75	ARG
1	A	173	GLU
1	A	192	HIS
1	A	200	THR
1	A	216	THR
1	A	224	GLN
1	A	225	THR
1	A	234	ARG
1	A	248	VAL
2	B	0	MET
2	B	4	THR
2	B	34	ASP
2	B	69	GLU
2	B	83	ASN
2	B	85	VAL
2	B	88	SER
1	D	2	SER
1	D	11	SER
1	D	35	ARG
1	D	75	ARG
1	D	179	LEU
1	D	200	THR
1	D	216	THR
1	D	224	GLN
1	D	225	THR
1	D	234	ARG
1	D	248	VAL
2	E	0	MET
2	E	4	THR
2	E	34	ASP
2	E	69	GLU
2	E	83	ASN
2	E	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	141	GLN

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	174	ASN
1	A	180	GLN
1	A	192	HIS
2	B	13	HIS
1	D	174	ASN
1	D	180	GLN
2	E	13	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.