



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:12 AM UTC

PDB ID : 1HHG / pdb_00001hhg
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 : 2.60 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) : **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

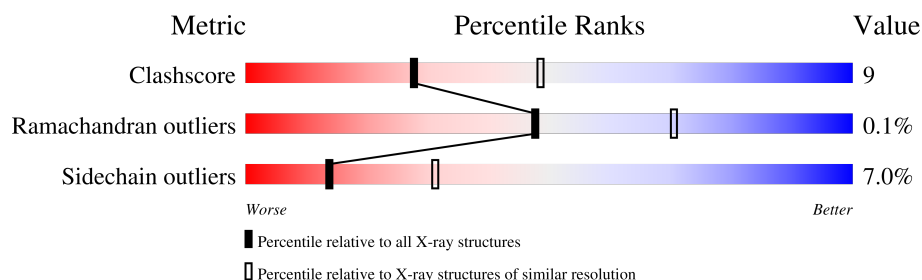
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)

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	61% 34% 5%
1	D	275	62% 33% 5%
2	B	100	61% 33% 6%
2	E	100	61% 34% 5%
3	C	9	67% 22% 11%
3	F	9	67% 22% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6294 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	15	0	0
			2247	1403	409	426	9			
1	D	275	Total	C	N	O	S	24	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	5	0	0
			837	533	141	159	4			

- Molecule 3 is a protein called HIV-1 GP120 ENVELOPE PROTEIN (RESIDUES 195-207).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			63	36	10	16	1			
3	F	9	Total	C	N	O	S	0	0	0
			63	36	10	16	1			

3 Residue-property plots [i](#)

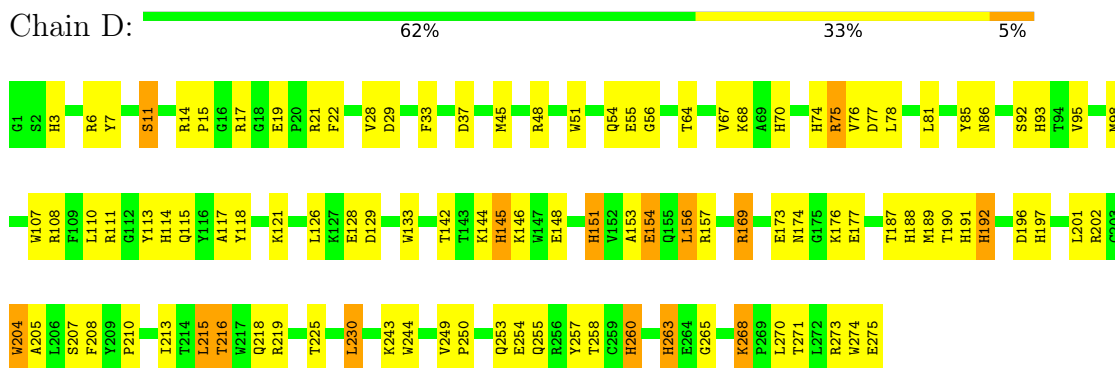
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

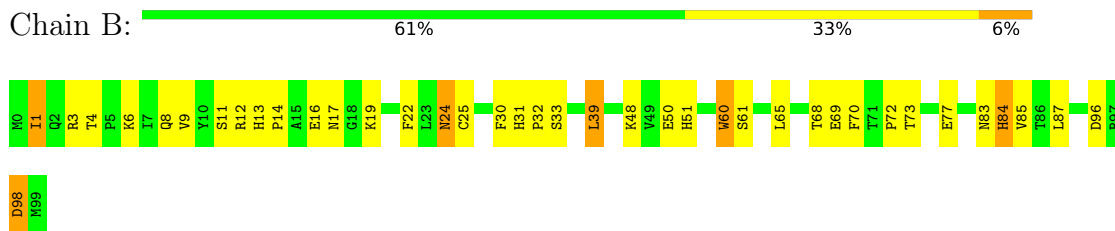
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN)



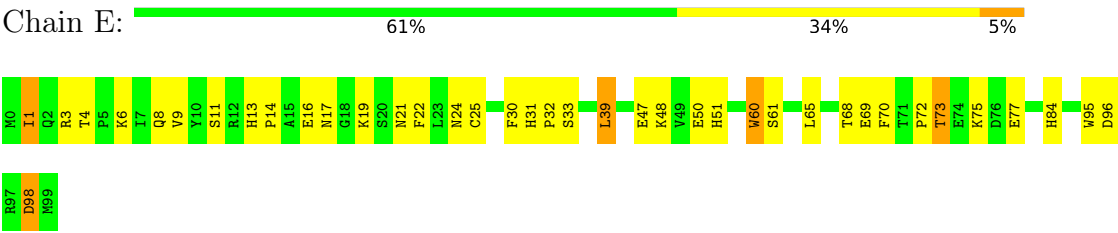
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN)



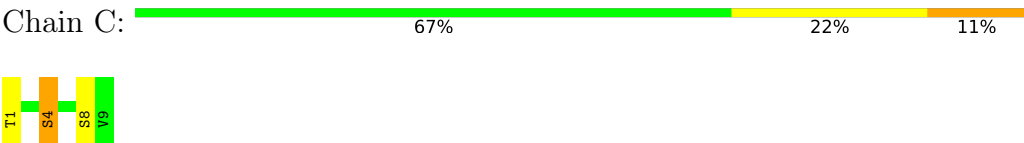
- Molecule 2: BETA 2-MICROGLOBULIN



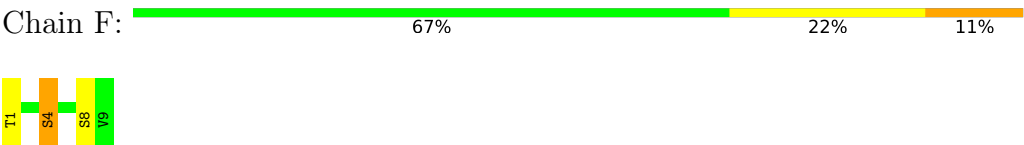
- Molecule 2: BETA 2-MICROGLOBULIN



● Molecule 3: HIV-1 GP120 ENVELOPE PROTEIN (RESIDUES 195-207)



● Molecule 3: HIV-1 GP120 ENVELOPE PROTEIN (RESIDUES 195-207)



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	62.70Å 87.00Å 79.40Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.277 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6294	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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	1.17	14/2312 (0.6%)	1.87	52/3137 (1.7%)
1	D	1.16	13/2312 (0.6%)	1.88	52/3137 (1.7%)
2	B	1.13	5/860 (0.6%)	1.80	24/1162 (2.1%)
2	E	1.13	5/860 (0.6%)	1.81	24/1162 (2.1%)
3	C	0.95	0/62	1.81	2/83 (2.4%)
3	F	0.95	0/62	1.81	2/83 (2.4%)
All	All	1.15	37/6468 (0.6%)	1.85	156/8764 (1.8%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	191	HIS	CD2-NE2	-7.96	1.29	1.37
2	B	84	HIS	CD2-NE2	-7.87	1.29	1.37
2	E	31	HIS	CD2-NE2	-7.66	1.29	1.37
2	B	31	HIS	CD2-NE2	-7.66	1.29	1.37
2	E	84	HIS	CD2-NE2	-7.47	1.29	1.37
1	D	263	HIS	CD2-NE2	-7.46	1.29	1.37
1	D	93	HIS	CD2-NE2	-7.42	1.29	1.37
1	A	263	HIS	CD2-NE2	-7.40	1.29	1.37
1	A	93	HIS	CD2-NE2	-7.38	1.29	1.37
2	B	51	HIS	CD2-NE2	-7.30	1.29	1.37
2	E	51	HIS	CD2-NE2	-7.22	1.29	1.37
1	D	114	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	114	HIS	CD2-NE2	-6.87	1.30	1.37
2	E	13	HIS	CD2-NE2	-6.86	1.30	1.37
1	D	145	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	151	HIS	CD2-NE2	-6.76	1.30	1.37
2	B	13	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	145	HIS	CD2-NE2	-6.71	1.30	1.37
1	D	151	HIS	CD2-NE2	-6.65	1.30	1.37
1	D	197	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	197	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	74	HIS	CD2-NE2	-6.49	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	HIS	CD2-NE2	-6.41	1.30	1.37
1	D	74	HIS	CD2-NE2	-6.38	1.30	1.37
1	D	260	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	188	HIS	CD2-NE2	-6.23	1.30	1.37
1	D	188	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	192	HIS	CD2-NE2	-6.10	1.31	1.37
1	D	192	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	70	HIS	CD2-NE2	-5.85	1.31	1.37
1	D	3	HIS	CG-ND1	-5.79	1.31	1.38
1	A	182	THR	CA-CB	5.71	1.61	1.52
1	A	3	HIS	CG-ND1	-5.68	1.31	1.38
1	D	70	HIS	CD2-NE2	-5.58	1.31	1.37
2	E	68	THR	CA-CB	5.09	1.62	1.53
2	B	68	THR	CA-CB	5.09	1.62	1.53
1	A	114	HIS	CG-ND1	-5.04	1.32	1.38

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	207	SER	CA-CB-OG	8.03	127.17	111.10
1	A	77	ASP	CA-CB-CG	8.01	120.61	112.60
1	D	77	ASP	CA-CB-CG	8.00	120.60	112.60
1	A	207	SER	CA-CB-OG	8.00	127.09	111.10
1	D	76	VAL	N-CA-C	-7.95	103.15	111.58
1	A	76	VAL	N-CA-C	-7.94	103.16	111.58
1	A	28	VAL	N-CA-C	-7.84	97.13	108.11
1	D	28	VAL	N-CA-C	-7.81	97.17	108.11
1	A	208	PHE	CA-CB-CG	7.76	121.56	113.80
2	E	17	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	D	208	PHE	CA-CB-CG	7.73	121.53	113.80
2	B	17	ASN	OD1-CG-ND2	-7.67	114.93	122.60
2	E	84	HIS	CB-CG-CD2	-7.61	121.30	131.20
2	E	31	HIS	CB-CG-CD2	-7.44	121.53	131.20
2	B	31	HIS	CB-CG-CD2	-7.42	121.56	131.20
2	B	84	HIS	CB-CG-CD2	-7.26	121.77	131.20
1	D	197	HIS	CB-CG-CD2	-7.24	121.78	131.20
1	A	197	HIS	CB-CG-CD2	-7.24	121.79	131.20
1	D	45	MET	N-CA-C	-7.21	98.29	109.76
1	A	45	MET	N-CA-C	-7.18	98.34	109.76
1	D	33	PHE	CA-CB-CG	6.99	120.78	113.80
1	A	33	PHE	CA-CB-CG	6.95	120.75	113.80
1	D	174	ASN	OD1-CG-ND2	-6.93	115.67	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ARG	CA-CB-CG	-6.70	100.70	114.10
1	D	108	ARG	CA-CB-CG	-6.66	100.77	114.10
1	D	191	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	D	174	ASN	CB-CG-ND2	6.60	126.30	116.40
1	D	78	LEU	N-CA-C	6.51	119.21	111.33
1	A	78	LEU	N-CA-C	6.50	119.19	111.33
1	A	86	ASN	OD1-CG-ND2	-6.47	116.13	122.60
2	B	70	PHE	CA-CB-CG	6.46	120.26	113.80
2	E	13	HIS	CB-CG-CD2	-6.44	122.83	131.20
2	E	70	PHE	CA-CB-CG	6.42	120.22	113.80
2	B	13	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	D	190	THR	CA-CB-OG1	-6.37	100.05	109.60
1	D	268	LYS	CA-CB-CG	6.36	126.81	114.10
1	A	268	LYS	CA-CB-CG	6.35	126.80	114.10
2	B	73	THR	N-CA-CB	-6.33	101.30	110.87
2	E	73	THR	N-CA-CB	-6.33	101.31	110.87
1	D	275	GLU	CA-CB-CG	6.30	126.71	114.10
1	A	275	GLU	CA-CB-CG	6.29	126.68	114.10
1	A	87	GLN	OE1-CD-NE2	-6.28	116.33	122.60
1	D	255	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	A	93	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	D	93	HIS	CB-CG-CD2	-6.17	123.17	131.20
2	B	51	HIS	CB-CG-CD2	-6.17	123.18	131.20
2	E	51	HIS	CB-CG-CD2	-6.16	123.20	131.20
1	D	260	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	A	260	HIS	CB-CG-CD2	-6.14	123.21	131.20
2	E	8	GLN	OE1-CD-NE2	-6.09	116.51	122.60
2	B	8	GLN	OE1-CD-NE2	-6.03	116.57	122.60
2	E	84	HIS	CB-CG-ND1	6.02	131.73	122.70
2	E	30	PHE	N-CA-C	5.98	119.37	110.52
2	B	30	PHE	N-CA-C	5.96	119.35	110.52
2	E	96	ASP	N-CA-C	-5.92	98.75	108.41
1	A	216	THR	N-CA-CB	-5.92	100.57	110.80
2	B	96	ASP	N-CA-C	-5.91	98.78	108.41
2	E	13	HIS	CB-CG-ND1	5.89	131.54	122.70
3	F	4	SER	N-CA-C	-5.89	97.57	107.99
1	D	216	THR	N-CA-CB	-5.89	100.62	110.80
1	A	132	SER	CA-CB-OG	5.87	122.84	111.10
3	C	4	SER	N-CA-C	-5.87	97.61	107.99
2	B	13	HIS	CB-CG-ND1	5.86	131.49	122.70
1	D	154	GLU	CA-CB-CG	5.80	125.71	114.10
1	D	29	ASP	CA-C-O	-5.79	112.22	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	ARG	CB-CG-CD	-5.76	98.06	111.30
2	E	47	GLU	N-CA-C	5.76	120.46	112.45
1	A	54	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	151	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	169	ARG	CB-CG-CD	-5.73	98.12	111.30
1	A	174	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	D	151	HIS	CA-CB-CG	-5.70	108.10	113.80
1	A	29	ASP	CA-C-O	-5.70	112.36	120.51
3	C	8	SER	CA-CB-OG	5.70	122.49	111.10
1	D	54	GLN	OE1-CD-NE2	-5.69	116.91	122.60
3	F	8	SER	CA-CB-OG	5.69	122.48	111.10
1	D	86	ASN	OD1-CG-ND2	-5.68	116.92	122.60
2	B	84	HIS	CB-CG-ND1	5.67	131.21	122.70
1	D	263	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	204	TRP	CG-CD1-NE1	-5.63	102.88	110.20
1	A	263	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	D	204	TRP	CG-CD1-NE1	-5.60	102.92	110.20
1	A	74	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	D	188	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	D	74	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	188	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	D	107	TRP	CG-CD2-CE3	5.52	139.42	133.90
1	A	244	TRP	CE2-CD2-CG	-5.51	100.59	107.20
1	D	244	TRP	CE2-CD2-CG	-5.47	100.63	107.20
2	B	31	HIS	CA-CB-CG	-5.47	108.33	113.80
2	E	6	LYS	N-CA-C	-5.47	102.39	110.48
1	A	145	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	255	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	E	31	HIS	CA-CB-CG	-5.46	108.34	113.80
2	E	4	THR	N-CA-C	5.45	116.69	109.93
2	B	4	THR	N-CA-C	5.45	116.69	109.93
2	B	6	LYS	N-CA-C	-5.44	102.43	110.48
1	D	145	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	D	254	GLU	CA-C-O	-5.44	114.79	120.55
1	A	197	HIS	CA-CB-CG	5.42	119.22	113.80
1	A	86	ASN	CA-CB-CG	-5.40	107.20	112.60
2	E	16	GLU	N-CA-C	-5.39	99.63	108.41
2	B	16	GLU	N-CA-C	-5.38	99.64	108.41
1	D	197	HIS	CA-CB-CG	5.38	119.18	113.80
1	A	204	TRP	CE2-CD2-CG	-5.35	100.78	107.20
1	A	274	TRP	CE2-CD2-CG	-5.33	100.80	107.20
2	E	39	LEU	O-C-N	-5.30	117.28	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	TRP	CE2-CD2-CG	-5.30	100.84	107.20
2	B	39	LEU	O-C-N	-5.30	117.28	123.27
1	D	274	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	D	128	GLU	N-CA-C	5.28	117.78	111.71
1	D	55	GLU	CB-CG-CD	5.27	121.56	112.60
2	E	98	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	55	GLU	CB-CG-CD	5.26	121.55	112.60
1	A	107	TRP	CG-CD2-CE3	5.26	139.16	133.90
1	D	197	HIS	CB-CG-ND1	5.22	130.53	122.70
1	A	174	ASN	CB-CG-ND2	5.21	124.21	116.40
2	B	98	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	197	HIS	CB-CG-ND1	5.20	130.50	122.70
1	A	174	ASN	CA-CB-CG	5.19	117.79	112.60
1	D	51	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	D	146	LYS	CB-CG-CD	-5.17	99.41	111.30
1	A	211	ALA	N-CA-C	5.17	117.65	111.71
2	B	60	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	204	TRP	N-CA-C	5.16	118.22	109.76
1	A	204	TRP	CD1-CG-CD2	5.15	114.54	106.30
1	A	51	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	A	146	LYS	CB-CG-CD	-5.15	99.46	111.30
2	E	32	PRO	CA-C-N	5.14	127.48	120.54
2	E	32	PRO	C-N-CA	5.14	127.48	120.54
1	D	204	TRP	CD1-CG-CD2	5.13	114.51	106.30
1	D	204	TRP	N-CA-C	5.12	118.17	109.76
1	D	151	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	A	151	HIS	CB-CG-CD2	-5.12	124.55	131.20
2	E	60	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	A	56	GLY	CA-C-N	5.11	125.14	119.32
1	A	56	GLY	C-N-CA	5.11	125.14	119.32
1	D	56	GLY	CA-C-N	5.10	125.13	119.32
1	D	56	GLY	C-N-CA	5.10	125.13	119.32
2	B	32	PRO	CA-C-N	5.09	127.42	120.54
2	B	32	PRO	C-N-CA	5.09	127.42	120.54
1	D	15	PRO	CB-CA-C	5.07	117.60	111.46
1	A	133	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	A	19	GLU	CB-CG-CD	5.06	121.20	112.60
2	B	85	VAL	N-CA-C	5.06	119.86	109.34
1	A	253	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	D	177	GLU	CB-CG-CD	5.05	121.18	112.60
2	B	73	THR	CA-CB-OG1	-5.04	102.04	109.60
1	D	133	TRP	CE2-CD2-CG	-5.04	101.15	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	73	THR	CA-CB-OG1	-5.03	102.06	109.60
1	D	244	TRP	CG-CD2-CE3	5.02	138.92	133.90
1	A	244	TRP	CG-CD2-CE3	5.01	138.91	133.90
2	E	95	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	D	176	LYS	N-CA-C	5.00	119.62	111.37
1	A	7	TYR	O-C-N	5.00	129.37	123.27
2	B	24	ASN	OD1-CG-ND2	-5.00	117.60	122.60

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	51	0
1	D	2247	0	2096	42	0
2	B	837	0	803	12	0
2	E	837	0	803	11	0
3	C	63	0	64	0	0
3	F	63	0	64	0	0
All	All	6294	0	5926	109	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 (109) 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:190:THR:CG2	1:A:202:ARG:HB3	1.78	1.13
1:A:190:THR:HG22	1:A:202:ARG:HB3	1.43	0.97
1:D:75:ARG:HH11	1:D:75:ARG:HB2	1.42	0.82
1:A:75:ARG:HB2	1:A:75:ARG:HH11	1.42	0.82
1:A:190:THR:HG21	1:A:202:ARG:HB3	1.70	0.71
1:D:14:ARG:HB3	1:D:17:ARG:HB2	1.71	0.71
1:A:189:MET:SD	1:A:217:TRP:HH2	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:HH11	1:D:6:ARG:HG3	1.60	0.66
1:A:6:ARG:HH11	1:A:6:ARG:HG3	1.60	0.66
1:A:111:ARG:HD2	1:A:113:TYR:OH	2.00	0.61
1:D:111:ARG:HD2	1:D:113:TYR:OH	2.00	0.61
1:A:210:PRO:O	1:A:263:HIS:HE1	1.84	0.61
1:A:201:LEU:HD22	1:A:249:VAL:HG21	1.81	0.60
1:D:201:LEU:HD22	1:D:249:VAL:HG21	1.81	0.60
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.38	0.59
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.40	0.57
1:A:153:ALA:HA	1:A:156:LEU:HB2	1.86	0.57
1:D:210:PRO:O	1:D:263:HIS:HE1	1.88	0.56
1:A:190:THR:HG22	1:A:202:ARG:CB	2.28	0.56
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.88	0.56
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.88	0.56
2:B:3:ARG:NH1	2:B:61:SER:HB3	2.22	0.54
2:E:3:ARG:NH1	2:E:61:SER:HB3	2.22	0.54
1:A:189:MET:SD	1:A:217:TRP:CH2	3.00	0.54
1:D:153:ALA:HA	1:D:156:LEU:HB2	1.89	0.54
1:A:11:SER:HA	1:A:21:ARG:O	2.08	0.54
1:D:11:SER:HA	1:D:21:ARG:O	2.08	0.54
1:D:81:LEU:HD13	1:D:118:TYR:CD1	2.42	0.54
1:D:121:LYS:HG3	2:E:1:ILE:HD12	1.90	0.54
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.42	0.53
1:A:144:LYS:O	1:A:148:GLU:HG3	2.09	0.53
1:D:144:LYS:O	1:D:148:GLU:HG3	2.09	0.53
1:D:19:GLU:H	1:D:19:GLU:CD	2.17	0.52
1:D:169:ARG:O	1:D:173:GLU:HG3	2.10	0.52
2:B:83:ASN:HA	2:B:87:LEU:HD12	1.92	0.51
1:A:230:LEU:HD22	1:A:243:LYS:HE3	1.94	0.50
1:A:189:MET:HA	1:A:202:ARG:O	2.12	0.50
1:D:230:LEU:HD22	1:D:243:LYS:HE3	1.94	0.49
1:D:189:MET:HA	1:D:202:ARG:O	2.12	0.49
1:A:187:THR:HA	1:A:204:TRP:O	2.12	0.49
1:D:187:THR:HA	1:D:204:TRP:O	2.12	0.49
1:A:129:ASP:O	1:A:157:ARG:NH1	2.46	0.48
1:A:213:ILE:HD12	1:A:263:HIS:HB2	1.94	0.48
2:B:19:LYS:O	2:B:72:PRO:HD2	2.14	0.48
2:E:19:LYS:O	2:E:72:PRO:HD2	2.14	0.48
1:A:230:LEU:CD2	1:A:243:LYS:HE3	2.44	0.47
1:D:230:LEU:CD2	1:D:243:LYS:HE3	2.44	0.47
1:A:218:GLN:O	1:A:257:TYR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:GLN:O	1:D:257:TYR:HA	2.14	0.47
1:A:6:ARG:HD2	1:A:98:MET:CE	2.44	0.46
1:D:6:ARG:HD2	1:D:98:MET:CE	2.44	0.46
1:D:126:LEU:HD22	1:D:156:LEU:HD23	1.97	0.46
2:B:22:PHE:CZ	2:B:69:GLU:HG2	2.51	0.46
2:E:22:PHE:CZ	2:E:69:GLU:HG2	2.51	0.46
1:D:250:PRO:O	1:D:253:GLN:HB2	2.16	0.46
1:A:126:LEU:HD22	1:A:156:LEU:HD23	1.98	0.46
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.97	0.46
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.98	0.46
1:A:6:ARG:HD2	1:A:98:MET:HE2	1.98	0.46
1:D:6:ARG:HD2	1:D:98:MET:HE2	1.98	0.46
1:D:98:MET:C	1:D:98:MET:SD	2.99	0.46
2:B:84:HIS:H	2:B:87:LEU:HD12	1.81	0.46
1:D:263:HIS:HD2	1:D:265:GLY:H	1.64	0.45
1:A:98:MET:SD	1:A:98:MET:C	2.99	0.45
1:A:263:HIS:HD2	1:A:265:GLY:H	1.64	0.45
1:D:260:HIS:HA	1:D:270:LEU:O	2.17	0.45
1:A:260:HIS:HA	1:A:270:LEU:O	2.17	0.45
1:D:126:LEU:HD22	1:D:156:LEU:CD2	2.46	0.45
1:A:184:ALA:HB2	1:A:265:GLY:O	2.17	0.45
1:D:192:HIS:HE1	2:E:98:ASP:CG	2.25	0.45
1:A:121:LYS:HG3	2:B:1:ILE:HD12	1.99	0.44
1:A:236:ALA:O	2:B:12:ARG:HG3	2.16	0.44
1:D:258:THR:HG22	1:D:273:ARG:HE	1.82	0.44
1:A:258:THR:HG22	1:A:273:ARG:HE	1.83	0.44
1:A:5:MET:SD	1:A:171:TYR:HE2	2.40	0.44
1:A:219:ARG:HD3	1:A:257:TYR:CZ	2.53	0.44
2:B:11:SER:HA	2:B:22:PHE:O	2.17	0.44
2:E:11:SER:HA	2:E:22:PHE:O	2.17	0.44
1:D:21:ARG:HH21	1:D:37:ASP:CG	2.26	0.43
1:D:219:ARG:HD3	1:D:257:TYR:CZ	2.53	0.43
1:A:21:ARG:HH21	1:A:37:ASP:CG	2.26	0.43
1:A:168:LEU:O	1:A:171:TYR:HB2	2.19	0.43
1:D:129:ASP:O	1:D:157:ARG:NH1	2.52	0.42
1:A:75:ARG:HB2	1:A:75:ARG:NH1	2.22	0.42
1:A:126:LEU:HD21	1:A:130:LEU:HA	2.01	0.42
1:D:81:LEU:O	1:D:85:TYR:HD2	2.01	0.42
1:A:81:LEU:O	1:A:85:TYR:HD2	2.02	0.42
1:D:7:TYR:O	1:D:98:MET:HA	2.20	0.42
1:A:7:TYR:O	1:A:98:MET:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:O	1:A:181:ARG:HD3	2.20	0.42
1:D:151:HIS:O	1:D:154:GLU:HB3	2.20	0.42
1:A:192:HIS:HE1	2:B:98:ASP:CG	2.28	0.41
1:D:64:THR:O	1:D:68:LYS:HD3	2.20	0.41
1:D:75:ARG:HB2	1:D:75:ARG:NH1	2.22	0.41
1:A:64:THR:O	1:A:68:LYS:HD3	2.20	0.41
1:A:142:THR:O	1:A:145:HIS:HB2	2.20	0.41
1:D:48:ARG:HA	1:D:48:ARG:HD2	1.86	0.41
1:D:142:THR:O	1:D:145:HIS:HB2	2.20	0.41
1:A:130:LEU:HB3	1:A:157:ARG:HG2	2.03	0.41
1:A:126:LEU:HD22	1:A:156:LEU:CD2	2.50	0.41
1:A:131:ARG:HA	1:A:153:ALA:HB1	2.04	0.40
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.56	0.40
1:D:205:ALA:HB2	1:D:215:LEU:HD11	2.03	0.40
1:A:48:ARG:HA	1:A:48:ARG:HD2	1.86	0.40
1:D:260:HIS:CE1	1:D:271:THR:HG23	2.55	0.40
1:A:22:PHE:HE2	1:A:67:VAL:HG22	1.86	0.40
1:D:22:PHE:HE2	1:D:67:VAL:HG22	1.86	0.40
2:E:11:SER:HB2	2:E:21:ASN:ND2	2.37	0.40
2:E:73:THR:HG22	2:E:75:LYS:H	1.86	0.40

There are no symmetry-related clashes.

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	273/275 (99%)	262 (96%)	10 (4%)	1 (0%)	30	51
1	D	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	98/100 (98%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	756/768 (98%)	730 (97%)	25 (3%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASN

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	231/231 (100%)	216 (94%)	15 (6%)	15	35
1	D	231/231 (100%)	217 (94%)	14 (6%)	17	37
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	29
2	E	95/95 (100%)	88 (93%)	7 (7%)	13	29
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	2
3	F	9/9 (100%)	7 (78%)	2 (22%)	1	2
All	All	670/670 (100%)	623 (93%)	47 (7%)	14	31

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	75	ARG
1	A	86	ASN
1	A	92	SER
1	A	95	VAL
1	A	110	LEU
1	A	115	GLN
1	A	156	LEU
1	A	196	ASP

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Mol	Chain	Res	Type
1	A	213	ILE
1	A	215	LEU
1	A	216	THR
1	A	225	THR
1	A	230	LEU
1	A	268	LYS
2	B	1	ILE
2	B	9	VAL
2	B	14	PRO
2	B	33	SER
2	B	48	LYS
2	B	50	GLU
2	B	77	GLU
3	C	1	THR
3	C	4	SER
1	D	11	SER
1	D	75	ARG
1	D	92	SER
1	D	95	VAL
1	D	110	LEU
1	D	115	GLN
1	D	156	LEU
1	D	196	ASP
1	D	213	ILE
1	D	215	LEU
1	D	216	THR
1	D	225	THR
1	D	230	LEU
1	D	268	LYS
2	E	1	ILE
2	E	9	VAL
2	E	14	PRO
2	E	33	SER
2	E	48	LYS
2	E	50	GLU
2	E	77	GLU
3	F	1	THR
3	F	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	86	ASN
1	A	93	HIS
1	A	114	HIS
1	A	151	HIS
1	A	192	HIS
1	A	224	GLN
1	A	263	HIS
2	B	8	GLN
1	D	70	HIS
1	D	93	HIS
1	D	114	HIS
1	D	180	GLN
1	D	192	HIS
1	D	224	GLN
1	D	263	HIS
2	E	8	GLN

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 ⓘ

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.