Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:05 am BST

PDB ID	:	1HHI
Title	:	THE ANTIGENIC IDENTITY OF PEPTIDE(SLASH)MHC COMPLEXES: A COMPARISON OF THE CONFORMATION OF FIVE PEPTIDES PRESENTED 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 following versions of software and data (see references ⓘ) were used in the production of this report:

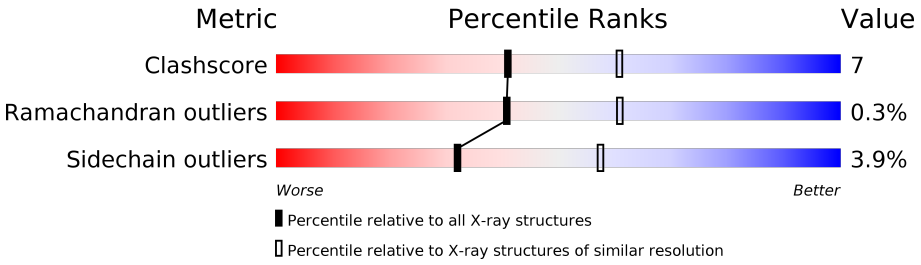
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	72% 25% •
1	D	275	73% 24% •
2	B	100	80% 18% •
2	E	100	79% 19% •
3	C	9	89% 11%
3	F	9	89% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6306 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	27	0	0
			2247	1403	409	426	9			
1	D	275	Total	C	N	O	S	27	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	20	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	20	0	0
			837	533	141	159	4			

- Molecule 3 is a protein called INFLUENZA A MATRIX PROTEIN M1 (RESIDUES 58-66).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			69	49	9	11			
3	F	9	Total	C	N	O	0	0	0
			69	49	9	11			

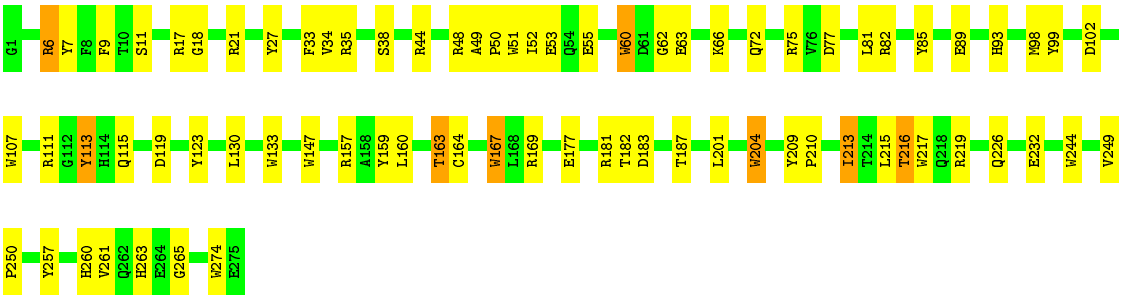
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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)

Chain A:

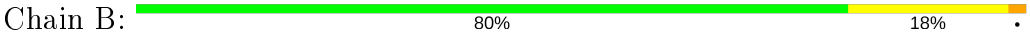


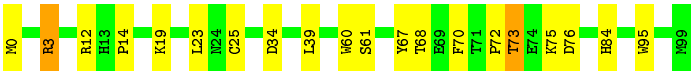
• Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN)

Chain D:

• Molecule 2: BETA 2-MICROGLOBULIN

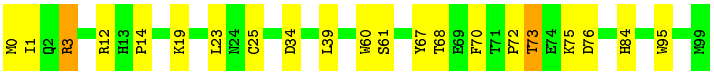
Chain B:





• Molecule 2: BETA 2-MICROGLOBULIN

Chain E:



• Molecule 3: INFLUENZA A MATRIX PROTEIN M1 (RESIDUES 58-66)

Chain C:

• Molecule 3: INFLUENZA A MATRIX PROTEIN M1 (RESIDUES 58-66)

Chain F:

4 Data and refinement statistics (i)

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	63.35Å 87.71Å 79.22Å 90.00° 90.10° 90.00°	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}	0.273 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6306	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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	0.98	4/2312 (0.2%)	1.67	48/3137 (1.5%)
1	D	0.97	2/2312 (0.1%)	1.61	44/3137 (1.4%)
2	B	0.90	0/860	1.39	7/1162 (0.6%)
2	E	0.84	0/860	1.42	7/1162 (0.6%)
3	C	0.61	0/70	1.18	0/92
3	F	0.61	0/70	1.18	0/92
All	All	0.94	6/6484 (0.1%)	1.57	106/8782 (1.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	CYS	N-CA	6.80	1.59	1.46
1	A	63	GLU	CD-OE1	-6.78	1.18	1.25
1	D	63	GLU	CD-OE1	-5.82	1.19	1.25
1	A	63	GLU	CD-OE2	-5.74	1.19	1.25
1	A	107	TRP	CD1-NE1	-5.39	1.28	1.38
1	D	60	TRP	CD1-NE1	-5.22	1.29	1.38

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	A	204	TRP	CD1-CG-CD2	10.56	114.75	106.30
1	D	204	TRP	CD1-CG-CD2	10.56	114.75	106.30
1	A	17	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	17	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	181	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	A	167	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	D	167	TRP	CD1-CG-CD2	9.17	113.64	106.30
1	D	274	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	D	204	TRP	CE2-CD2-CG	-8.61	100.41	107.30
1	A	274	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	A	204	TRP	CE2-CD2-CG	-8.59	100.43	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	D	133	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	A	133	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	D	51	TRP	CD1-CG-CD2	8.43	113.05	106.30
1	A	51	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	167	TRP	CE2-CD2-CG	-8.24	100.71	107.30
2	B	95	TRP	CD1-CG-CD2	8.23	112.89	106.30
2	E	95	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	D	167	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	A	133	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	D	133	TRP	CE2-CD2-CG	-7.96	100.93	107.30
1	A	274	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	D	274	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	A	51	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	D	51	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	D	217	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	A	217	TRP	CD1-CG-CD2	7.55	112.34	106.30
2	E	95	TRP	CE2-CD2-CG	-7.51	101.29	107.30
2	B	95	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	A	226	GLN	CA-CB-CG	-7.37	97.20	113.40
1	D	226	GLN	CA-CB-CG	-7.34	97.25	113.40
1	D	107	TRP	CD1-CG-CD2	7.32	112.16	106.30
1	A	244	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	D	244	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	D	244	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	A	244	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	D	6	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	147	TRP	CD1-CG-CD2	7.18	112.05	106.30
1	A	6	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	D	107	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	107	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	D	147	TRP	CD1-CG-CD2	7.03	111.93	106.30
1	A	204	TRP	CG-CD1-NE1	-7.01	103.09	110.10
1	A	217	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	D	204	TRP	CG-CD1-NE1	-7.00	103.10	110.10
1	D	217	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	219	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	60	TRP	CE2-CD2-CG	-6.74	101.91	107.30
2	B	60	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	D	60	TRP	CD1-CG-CD2	6.65	111.62	106.30
2	E	60	TRP	CD1-CG-CD2	6.65	111.62	106.30
2	E	60	TRP	CE2-CD2-CG	-6.63	102.00	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	167	TRP	CG-CD2-CE3	6.59	139.83	133.90
2	B	60	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	D	167	TRP	CG-CD2-CE3	6.53	139.78	133.90
1	A	60	TRP	CD1-CG-CD2	6.50	111.50	106.30
1	D	55	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	D	133	TRP	CG-CD2-CE3	6.38	139.64	133.90
1	A	133	TRP	CG-CD2-CE3	6.34	139.61	133.90
1	A	107	TRP	CD1-CG-CD2	6.31	111.35	106.30
1	A	147	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	D	147	TRP	CE2-CD2-CG	-6.13	102.39	107.30
1	A	257	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	D	204	TRP	CG-CD2-CE3	6.07	139.36	133.90
2	E	12	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	204	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	D	167	TRP	CB-CG-CD1	-6.04	119.15	127.00
1	D	232	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	A	167	TRP	CB-CG-CD1	-6.01	119.19	127.00
2	E	0	MET	CA-CB-CG	5.96	123.43	113.30
2	B	0	MET	CA-CB-CG	5.92	123.36	113.30
1	A	232	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	18	GLY	CA-C-N	-5.83	104.38	117.20
1	A	169	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	274	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	D	169	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	274	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	D	274	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	D	133	TRP	CB-CG-CD1	-5.71	119.58	127.00
1	D	63	GLU	OE1-CD-OE2	-5.70	116.47	123.30
1	A	274	TRP	CG-CD2-CE3	5.68	139.01	133.90
1	A	27	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	133	TRP	CB-CG-CD1	-5.64	119.67	127.00
1	D	113	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	113	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	D	27	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	D	217	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	D	167	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	A	167	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	D	173	GLU	CA-CB-CG	5.50	125.51	113.40
1	A	133	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	D	133	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	D	204	TRP	CB-CG-CD1	-5.43	119.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	D	107	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	D	108	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	55	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	A	217	TRP	CB-CG-CD1	-5.26	120.16	127.00
2	B	3	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	E	3	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	B	12	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	51	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	A	51	TRP	CB-CG-CD1	-5.09	120.39	127.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	36	0
1	D	2247	0	2096	35	0
2	B	837	0	803	7	0
2	E	837	0	803	9	0
3	C	69	0	75	2	0
3	F	69	0	75	2	0
All	All	6306	0	5948	85	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 7.

All (85) 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)
2:E:73:THR:HG22	2:E:76:ASP:H	1.48	0.77
2:B:73:THR:HG22	2:B:76:ASP:H	1.48	0.77
1:D:77:ASP:HB3	3:F:9:LEU:HD12	1.70	0.74
1:A:77:ASP:HB3	3:C:9:LEU:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:ARG:HH11	2:E:61:SER:HB3	1.61	0.65
2:B:3:ARG:HH11	2:B:61:SER:HB3	1.61	0.65
1:A:159:TYR:HA	1:A:163:THR:HG23	1.81	0.63
2:B:19:LYS:O	2:B:72:PRO:HD2	1.99	0.63
1:D:159:TYR:CD1	1:D:163:THR:HG23	2.36	0.61
2:E:19:LYS:O	2:E:72:PRO:HD2	2.03	0.59
1:A:213:ILE:HD12	1:A:263:HIS:HB2	1.85	0.59
1:D:19:GLU:HG3	1:D:20:PRO:HD2	1.85	0.58
1:D:159:TYR:HA	1:D:163:THR:CG2	2.34	0.58
1:D:62:GLY:O	1:D:66:LYS:HG3	2.03	0.57
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.88	0.57
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.88	0.56
1:D:215:LEU:HD12	1:D:261:VAL:HG22	1.89	0.55
1:D:44:ARG:HA	1:D:64:THR:HG23	1.88	0.55
1:A:215:LEU:HD12	1:A:261:VAL:HG22	1.89	0.54
1:D:176:LYS:HG3	1:D:180:GLN:OE1	2.07	0.54
1:A:159:TYR:HA	1:A:163:THR:CG2	2.38	0.54
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.90	0.53
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.90	0.53
1:A:210:PRO:O	1:A:263:HIS:HE1	1.92	0.51
1:A:123:TYR:CE2	3:C:9:LEU:HD22	2.45	0.51
1:D:123:TYR:CE2	3:F:9:LEU:HD22	2.45	0.51
1:A:163:THR:O	1:A:167:TRP:CD1	2.64	0.51
1:A:72:GLN:HE22	1:A:75:ARG:HD3	1.77	0.50
1:A:44:ARG:HH21	1:A:60:TRP:HB3	1.76	0.50
1:D:72:GLN:HE22	1:D:75:ARG:HD3	1.77	0.50
1:D:187:THR:HA	1:D:204:TRP:O	2.13	0.49
1:A:187:THR:HA	1:A:204:TRP:O	2.13	0.49
1:A:49:ALA:O	1:A:52:ILE:HG22	2.13	0.49
1:A:50:PRO:HA	1:A:53:GLU:OE1	2.13	0.49
1:D:49:ALA:O	1:D:52:ILE:HG22	2.13	0.49
1:A:21:ARG:HD2	1:A:38:SER:OG	2.13	0.48
1:D:21:ARG:HD2	1:D:38:SER:OG	2.13	0.48
1:D:44:ARG:HH21	1:D:60:TRP:HB3	1.78	0.48
1:D:121:LYS:HG2	2:E:1:ILE:HD11	1.94	0.48
1:A:82:ARG:HE	1:A:89:GLU:HA	1.79	0.48
2:B:34:ASP:O	2:B:84:HIS:HD2	1.97	0.48
1:D:82:ARG:HE	1:D:89:GLU:HA	1.80	0.47
1:D:45:MET:HG2	1:D:63:GLU:HB3	1.97	0.47
1:A:81:LEU:O	1:A:85:TYR:HD2	1.99	0.46
1:D:216:THR:HG22	1:D:260:HIS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:HG22	1:A:260:HIS:HB2	1.98	0.45
1:A:9:PHE:HE2	1:A:99:TYR:CE2	2.34	0.45
1:D:81:LEU:O	1:D:85:TYR:HD2	1.99	0.45
2:B:23:LEU:O	2:B:67:TYR:HA	2.17	0.45
1:D:9:PHE:HE2	1:D:99:TYR:CE2	2.34	0.45
1:A:111:ARG:HD2	1:A:113:TYR:OH	2.17	0.45
1:A:263:HIS:HD2	1:A:265:GLY:H	1.64	0.45
2:E:34:ASP:O	2:E:84:HIS:HD2	1.99	0.44
1:A:249:VAL:HA	1:A:250:PRO:HD3	1.89	0.44
1:A:183:ASP:HB2	1:A:209:TYR:N	2.33	0.44
1:A:201:LEU:HD22	1:A:249:VAL:HG21	1.99	0.44
2:E:23:LEU:O	2:E:67:TYR:HA	2.18	0.44
2:B:34:ASP:O	2:B:84:HIS:CD2	2.71	0.43
1:A:62:GLY:O	1:A:66:LYS:HG3	2.18	0.43
1:D:48:ARG:HA	1:D:48:ARG:HD2	1.82	0.43
1:D:201:LEU:HD22	1:D:249:VAL:HG21	1.99	0.43
1:D:159:TYR:HA	1:D:163:THR:HG22	1.99	0.43
1:D:249:VAL:HA	1:D:250:PRO:HD3	1.90	0.43
1:A:48:ARG:HA	1:A:48:ARG:HD2	1.82	0.43
1:A:7:TYR:O	1:A:98:MET:HA	2.19	0.43
1:D:7:TYR:O	1:D:98:MET:HA	2.19	0.43
1:D:120:GLY:O	2:E:3:ARG:NH2	2.52	0.42
2:E:34:ASP:O	2:E:84:HIS:CD2	2.73	0.42
1:A:263:HIS:CD2	1:A:265:GLY:H	2.37	0.42
1:A:82:ARG:HH21	1:A:89:GLU:HB2	1.84	0.42
1:A:72:GLN:NE2	1:A:75:ARG:HD3	2.34	0.42
1:D:72:GLN:NE2	1:D:75:ARG:HD3	2.34	0.42
1:A:130:LEU:HD22	1:A:160:LEU:HD12	2.01	0.41
1:D:159:TYR:HD1	1:D:163:THR:HG23	1.82	0.41
1:D:219:ARG:HD3	1:D:257:TYR:OH	2.19	0.41
1:A:163:THR:O	1:A:167:TRP:HD1	2.04	0.41
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.54	0.41
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.54	0.41
1:D:110:LEU:HA	1:D:110:LEU:HD12	1.86	0.41
1:A:9:PHE:CE2	1:A:99:TYR:CE2	3.09	0.41
1:D:111:ARG:HD2	1:D:113:TYR:OH	2.21	0.41
1:A:182:THR:HG21	1:A:265:GLY:CA	2.50	0.40
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.57	0.40
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.57	0.40
1:D:9:PHE:CE2	1:D:99:TYR:CE2	3.09	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%)	11 (4%)	0	100	100
1	D	273/275 (99%)	261 (96%)	12 (4%)	0	100	100
2	B	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	15	28
2	E	98/100 (98%)	92 (94%)	5 (5%)	1 (1%)	15	28
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	756/768 (98%)	720 (95%)	34 (4%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	14	PRO
2	E	14	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	A	231/231 (100%)	223 (96%)	8 (4%)	36	62
1	D	231/231 (100%)	221 (96%)	10 (4%)	29	53
2	B	95/95 (100%)	91 (96%)	4 (4%)	30	54
2	E	95/95 (100%)	91 (96%)	4 (4%)	30	54
3	C	7/7 (100%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	7/7 (100%)	7 (100%)	0	100 100
All	All	666/666 (100%)	640 (96%)	26 (4%)	32 57

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	35	ARG
1	A	115	GLN
1	A	157	ARG
1	A	163	THR
1	A	177	GLU
1	A	213	ILE
1	A	216	THR
2	B	68	THR
2	B	70	PHE
2	B	73	THR
2	B	75	LYS
1	D	11	SER
1	D	17	ARG
1	D	19	GLU
1	D	35	ARG
1	D	115	GLN
1	D	157	ARG
1	D	163	THR
1	D	177	GLU
1	D	213	ILE
1	D	216	THR
2	E	68	THR
2	E	70	PHE
2	E	73	THR
2	E	75	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	93	HIS
1	A	114	HIS
1	A	253	GLN
1	A	263	HIS

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Mol	Chain	Res	Type
1	D	72	GLN
1	D	114	HIS
1	D	253	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.