



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:55 PM UTC

PDB ID : 1HSA / pdb_00001hsa
Title : THE THREE-DIMENSIONAL STRUCTURE OF HLA-B27 AT 2.1
ANGSTROMS RESOLUTION SUGGESTS A GENERAL MECHANISM
FOR TIGHT PEPTIDE BINDING TO MHC
Authors : Madden, D.R.; Gorga, J.C.; Strominger, J.L.; Wiley, D.C.
Deposited on : 1992-08-11
Resolution : 2.10 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

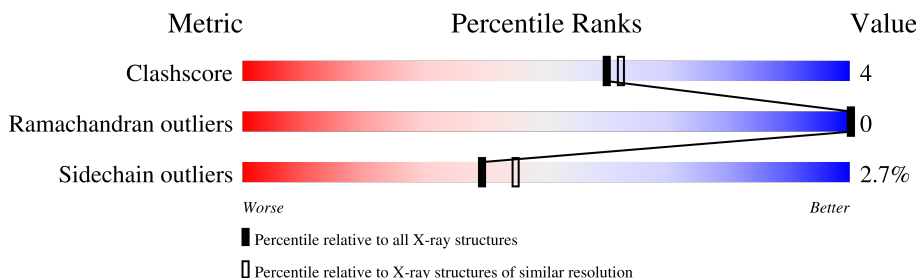
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	276	77% 21% .
1	D	276	76% 22% .
2	B	99	80% 17% .
2	E	99	82% 14% .
3	C	9	100%
3	F	9	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6706 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-B*2705).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	12	0	0
			2252	1401	408	436	7			
1	D	276	Total	C	N	O	S	12	0	0
			2252	1401	408	436	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	5	0	0
			829	528	140	158	3			
2	E	99	Total	C	N	O	S	5	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called MODEL PEPTIDE SEQUENCE - ARAAAAAAA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			52	30	12	10			
3	F	9	Total	C	N	O	0	0	0
			52	30	12	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	60	Total	O	0	0
			60	60		
4	C	4	Total	O	0	0
			4	4		
4	D	147	Total	O	0	0
			147	147		

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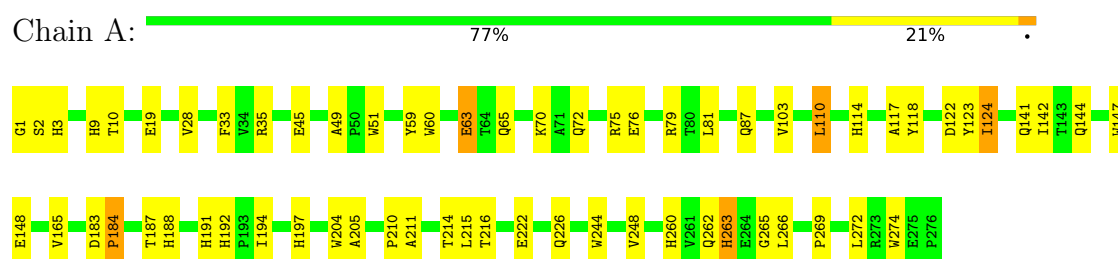
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	75	Total	O	0	0
			75	75		
4	F	5	Total	O	0	0
			5	5		

3 Residue-property plots

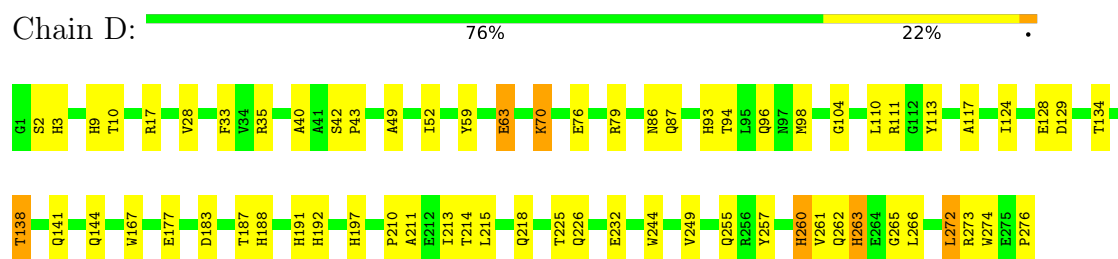
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

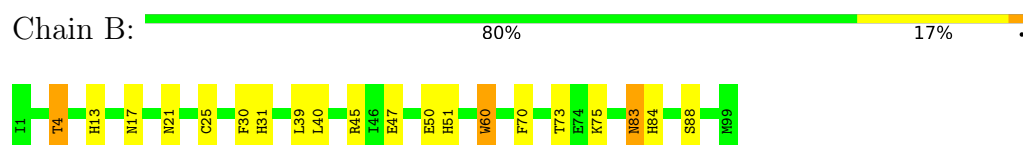
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-B*2705)



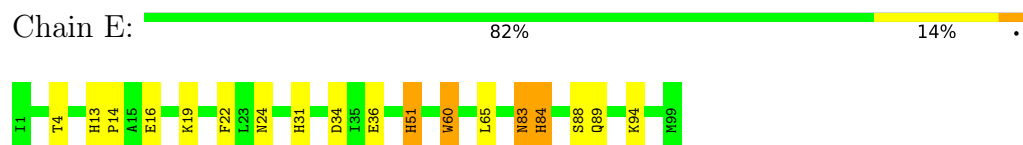
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-B*2705)



- Molecule 2: BETA 2-MICROGLOBULIN



- Molecule 2: BETA 2-MICROGLOBULIN



- Molecule 3: MODEL PEPTIDE SEQUENCE - ARAAAAAAA



There are no outlier residues recorded for this chain.

- Molecule 3: MODEL PEPTIDE SEQUENCE - ARAAAAAAA

Chain F:  100%

There are no outlier residues recorded for this chain.

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	45.10Å 69.80Å 81.10Å 80.30° 88.60° 89.90°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6706	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	1.14	17/2314 (0.7%)	1.64	25/3147 (0.8%)
1	D	1.16	16/2314 (0.7%)	1.67	26/3147 (0.8%)
2	B	1.14	5/852 (0.6%)	1.66	11/1152 (1.0%)
2	E	1.15	5/852 (0.6%)	1.66	9/1152 (0.8%)
3	C	0.86	0/51	1.20	0/67
3	F	1.00	0/51	1.27	0/67
All	All	1.15	43/6434 (0.7%)	1.65	71/8732 (0.8%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	31	HIS	CD2-NE2	-7.74	1.29	1.37
1	D	197	HIS	CD2-NE2	-6.89	1.30	1.37
2	B	31	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	3	HIS	CD2-NE2	-6.67	1.30	1.37
1	D	263	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	9	HIS	CD2-NE2	-6.61	1.30	1.37
1	D	188	HIS	CD2-NE2	-6.51	1.30	1.37
2	B	84	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	10	THR	CA-CB	6.45	1.64	1.53
1	A	197	HIS	CD2-NE2	-6.42	1.30	1.37
1	D	3	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	184	PRO	CA-CB	-6.21	1.48	1.54
1	D	93	HIS	CD2-NE2	-6.18	1.31	1.37
2	E	13	HIS	CD2-NE2	-6.14	1.31	1.37
2	E	84	HIS	CD2-NE2	-6.11	1.31	1.37
2	E	51	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	188	HIS	CG-ND1	-6.05	1.31	1.38
1	D	10	THR	CA-CB	5.98	1.63	1.53
1	A	260	HIS	CD2-NE2	-5.93	1.31	1.37
1	D	9	HIS	CD2-NE2	-5.89	1.31	1.37
1	D	188	HIS	CG-ND1	-5.88	1.31	1.38
2	B	13	HIS	CD2-NE2	-5.79	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	HIS	CD2-NE2	-5.79	1.31	1.37
1	D	191	HIS	CD2-NE2	-5.78	1.31	1.37
2	B	31	HIS	CG-ND1	-5.73	1.31	1.38
1	A	142	ILE	CA-CB	5.68	1.60	1.54
1	A	188	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	3	HIS	CG-ND1	-5.63	1.32	1.38
1	A	114	HIS	CA-CB	5.62	1.60	1.52
1	D	191	HIS	CG-ND1	-5.61	1.32	1.38
1	A	263	HIS	CD2-NE2	-5.49	1.31	1.37
1	D	28	VAL	CA-CB	5.48	1.60	1.54
1	D	260	HIS	CD2-NE2	-5.43	1.31	1.37
2	E	13	HIS	CG-ND1	-5.43	1.32	1.38
2	B	51	HIS	CD2-NE2	-5.42	1.31	1.37
1	D	192	HIS	CA-CB	5.32	1.60	1.52
1	D	192	HIS	CD2-NE2	-5.32	1.31	1.37
1	A	124	ILE	CA-CB	5.30	1.62	1.54
1	A	191	HIS	CD2-NE2	-5.23	1.32	1.37
1	D	3	HIS	CG-ND1	-5.11	1.32	1.38
1	D	249	VAL	CA-CB	5.06	1.60	1.54
1	A	192	HIS	CA-CB	5.04	1.59	1.52
1	A	192	HIS	CG-ND1	-5.02	1.32	1.38

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	83	ASN	OD1-CG-ND2	-10.48	112.12	122.60
1	A	65	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	D	2	SER	N-CA-C	-8.75	99.44	112.04
2	E	83	ASN	CB-CG-ND2	8.38	128.97	116.40
1	D	33	PHE	CA-CB-CG	8.21	122.01	113.80
2	B	83	ASN	CB-CG-ND2	8.11	128.57	116.40
2	B	83	ASN	OD1-CG-ND2	-8.06	114.54	122.60
2	B	21	ASN	CA-CB-CG	7.88	120.48	112.60
1	A	183	ASP	CA-C-N	7.71	125.21	119.66
1	A	183	ASP	C-N-CA	7.71	125.21	119.66
2	B	50	GLU	CA-CB-CG	-6.94	100.22	114.10
1	D	86	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	D	87	GLN	OE1-CD-NE2	-6.92	115.68	122.60
2	B	30	PHE	CA-CB-CG	6.81	120.61	113.80
2	B	51	HIS	CA-CB-CG	6.72	120.52	113.80
1	A	28	VAL	N-CA-C	-6.57	98.91	108.11
2	B	70	PHE	CA-CB-CG	6.54	120.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	ALA	N-CA-C	6.45	119.12	111.71
2	E	83	ASN	CA-CB-CG	-6.38	106.22	112.60
1	D	244	TRP	CG-CD2-CE3	6.31	140.21	133.90
1	D	129	ASP	CA-CB-CG	6.29	118.89	112.60
2	E	89	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	D	183	ASP	CA-C-N	6.24	124.21	119.66
1	D	183	ASP	C-N-CA	6.24	124.21	119.66
1	A	33	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	65	GLN	CG-CD-NE2	6.10	125.55	116.40
1	A	65	GLN	CA-CB-CG	6.04	126.19	114.10
1	A	226	GLN	OE1-CD-NE2	-6.01	116.59	122.60
2	B	4	THR	CB-CA-C	6.00	117.33	108.87
1	A	19	GLU	CB-CG-CD	5.92	122.67	112.60
2	B	17	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	49	ALA	CA-C-N	5.83	125.04	118.97
1	A	49	ALA	C-N-CA	5.83	125.04	118.97
1	D	138	THR	CA-CB-OG1	-5.83	100.85	109.60
1	A	274	TRP	CG-CD2-CE3	5.81	139.71	133.90
1	A	211	ALA	N-CA-C	5.78	117.58	111.28
1	A	266	LEU	CA-C-N	5.77	125.45	119.05
1	A	266	LEU	C-N-CA	5.77	125.45	119.05
1	A	141	GLN	OE1-CD-NE2	-5.73	116.87	122.60
2	B	47	GLU	N-CA-C	5.63	117.50	111.36
1	A	147	TRP	CG-CD2-CE3	5.59	139.49	133.90
1	D	104	GLY	CA-C-N	5.48	125.00	119.19
1	D	104	GLY	C-N-CA	5.48	125.00	119.19
2	E	22	PHE	CA-CB-CG	-5.47	108.33	113.80
2	E	34	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	183	ASP	CB-CA-C	5.40	115.52	110.17
1	D	87	GLN	CG-CD-NE2	5.38	124.48	116.40
1	D	266	LEU	CA-C-N	5.35	124.80	119.24
1	D	266	LEU	C-N-CA	5.35	124.80	119.24
1	A	51	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	D	134	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	87	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	D	144	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	D	167	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	D	96	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	45	GLU	CA-CB-CG	-5.20	103.69	114.10
1	D	28	VAL	N-CA-C	-5.20	100.27	107.80
1	D	94	THR	CA-CB-OG1	-5.18	101.83	109.60
1	D	177	GLU	CB-CG-CD	5.17	121.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	TRP	CG-CD2-CE3	5.16	139.06	133.90
2	E	4	THR	CB-CA-C	5.14	116.82	109.11
1	A	63	GLU	CB-CG-CD	5.13	121.33	112.60
1	D	63	GLU	CB-CG-CD	5.13	121.32	112.60
1	A	122	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	244	TRP	CE2-CD2-CG	-5.11	101.06	107.20
2	E	24	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	D	244	TRP	CB-CG-CD1	-5.07	119.30	126.90
1	A	244	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	60	TRP	CE2-CD2-CG	-5.05	101.14	107.20
2	B	60	TRP	CE2-CD2-CG	-5.03	101.17	107.20
2	E	60	TRP	CG-CD1-NE1	-5.03	103.67	110.20

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	2252	0	2109	19	0
1	D	2252	0	2109	24	0
2	B	829	0	794	5	0
2	E	829	0	794	6	0
3	C	52	0	55	0	0
3	F	52	0	55	0	0
4	A	149	0	0	1	0
4	B	60	0	0	1	0
4	C	4	0	0	0	0
4	D	147	0	0	3	0
4	E	75	0	0	2	0
4	F	5	0	0	0	0
All	All	6706	0	5916	52	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 4.

All (52) 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:D:76:GLU:HG2	1:D:79:ARG:HH21	1.53	0.73
1:D:111:ARG:HD2	4:D:787:HOH:O	1.97	0.65
1:A:144:GLN:O	1:A:148:GLU:HG3	2.00	0.61
1:D:111:ARG:NE	1:D:128:GLU:HG2	2.21	0.56
1:D:274:TRP:O	1:D:276:PRO:HD3	2.06	0.55
1:A:262:GLN:HG2	1:A:269:PRO:HB3	1.87	0.55
1:D:263:HIS:CD2	1:D:265:GLY:H	2.25	0.54
1:A:1:GLY:HA3	1:A:110:LEU:CD1	2.38	0.54
1:A:70:LYS:HE2	4:A:509:HOH:O	2.08	0.53
1:D:76:GLU:HG2	1:D:79:ARG:NH2	2.23	0.53
2:B:4:THR:HG22	4:B:606:HOH:O	2.09	0.52
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.43	0.52
2:E:16:GLU:CD	2:E:19:LYS:HG3	2.35	0.52
1:A:210:PRO:O	1:A:263:HIS:HE1	1.93	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.50
1:A:1:GLY:HA3	1:A:110:LEU:HD12	1.94	0.49
1:D:49:ALA:O	1:D:52:ILE:HG22	2.11	0.49
1:D:111:ARG:CD	1:D:128:GLU:HG2	2.42	0.49
1:A:205:ALA:HB2	1:A:215:LEU:HD21	1.95	0.49
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.94	0.48
1:A:76:GLU:HG2	1:A:79:ARG:HH21	1.79	0.47
2:E:83:ASN:HD22	2:E:84:HIS:H	1.61	0.47
1:D:40:ALA:O	1:D:43:PRO:HD3	2.15	0.47
1:D:255:GLN:O	1:D:273:ARG:NH1	2.47	0.46
1:D:187:THR:HB	1:D:272:LEU:HD21	1.98	0.46
1:A:214:THR:HB	1:A:262:GLN:HB2	1.99	0.45
1:D:218:GLN:O	1:D:257:TYR:HA	2.16	0.45
1:A:103:VAL:HG11	1:A:165:VAL:HG13	1.99	0.45
1:D:138:THR:O	1:D:141:GLN:HB2	2.16	0.45
2:E:94:LYS:HB3	4:E:825:HOH:O	2.17	0.45
2:E:36:GLU:HA	4:E:779:HOH:O	2.17	0.44
1:D:59:TYR:O	1:D:63:GLU:HG2	2.18	0.44
1:D:98:MET:HE1	1:D:113:TYR:HB3	1.99	0.44
1:D:213:ILE:HG13	1:D:263:HIS:HB2	1.99	0.44
1:D:210:PRO:O	1:D:263:HIS:HE1	2.00	0.44
1:D:214:THR:HB	1:D:262:GLN:HB2	1.99	0.44
1:A:187:THR:HA	1:A:204:TRP:O	2.18	0.43
1:A:184:PRO:HB3	1:A:265:GLY:O	2.19	0.43
1:D:17:ARG:HH11	1:D:17:ARG:HD2	1.69	0.43
1:D:70:LYS:HE2	4:D:524:HOH:O	2.19	0.43
1:A:59:TYR:O	1:A:63:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.54	0.42
1:D:218:GLN:OE1	1:D:260:HIS:NE2	2.52	0.42
2:E:51:HIS:HA	2:E:65:LEU:O	2.19	0.42
2:B:73:THR:OG1	2:B:75:LYS:HG3	2.20	0.42
1:A:194:ILE:HD12	1:A:248:VAL:HG13	2.03	0.41
2:B:40:LEU:HD23	2:B:45:ARG:HA	2.01	0.41
1:D:111:ARG:HA	4:D:787:HOH:O	2.20	0.41
1:A:187:THR:HB	1:A:272:LEU:HD21	2.02	0.41
1:A:72:GLN:OE1	1:A:75:ARG:NH1	2.54	0.40
1:D:215:LEU:HD22	1:D:261:VAL:HG22	2.03	0.40
1:A:123:TYR:HD2	1:A:124:ILE:HG22	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	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	D	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	E	97/99 (98%)	97 (100%)	0	0	100	100
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%)	734 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	235/235 (100%)	230 (98%)	5 (2%)	47	54
1	D	235/235 (100%)	226 (96%)	9 (4%)	29	32
2	B	94/94 (100%)	92 (98%)	2 (2%)	47	54
2	E	94/94 (100%)	92 (98%)	2 (2%)	47	54
3	C	1/1 (100%)	1 (100%)	0	100	100
3	F	1/1 (100%)	1 (100%)	0	100	100
All	All	660/660 (100%)	642 (97%)	18 (3%)	39	45

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	35	ARG
1	A	110	LEU
1	A	216	THR
1	A	222	GLU
2	B	83	ASN
2	B	88	SER
1	D	35	ARG
1	D	42	SER
1	D	70	LYS
1	D	110	LEU
1	D	124	ILE
1	D	225	THR
1	D	226	GLN
1	D	232	GLU
1	D	272	LEU
2	E	14	PRO
2	E	88	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	263	HIS
2	B	2	GLN
2	B	83	ASN
1	D	141	GLN
1	D	155	GLN
1	D	174	ASN
1	D	188	HIS
1	D	197	HIS
1	D	263	HIS
2	E	13	HIS
2	E	83	ASN

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.