



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 09:23 am BST

PDB ID : 2HLA
Title : SPECIFICITY POCKETS FOR THE SIDE CHAINS OF PEPTIDE ANTIGENS IN HLA-AW68
Authors : Garrett, T.P.J.; Saper, M.A.; Wiley, D.C.
Deposited on : 1989-10-05
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (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

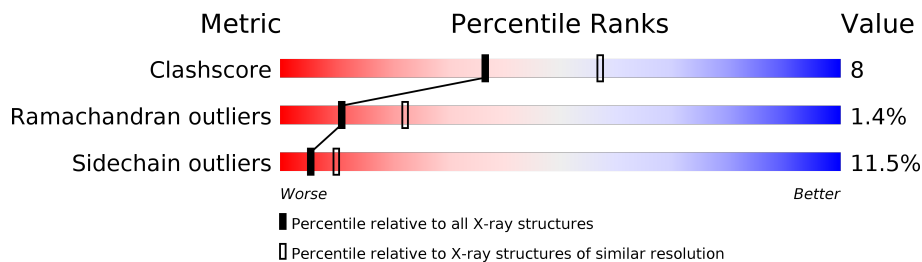
1 Overall quality at a glance

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	270	
2	B	99	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3033 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-Aw68).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2194	1362	399	423	10	0	0	0

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

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

- Molecule 3 is water.

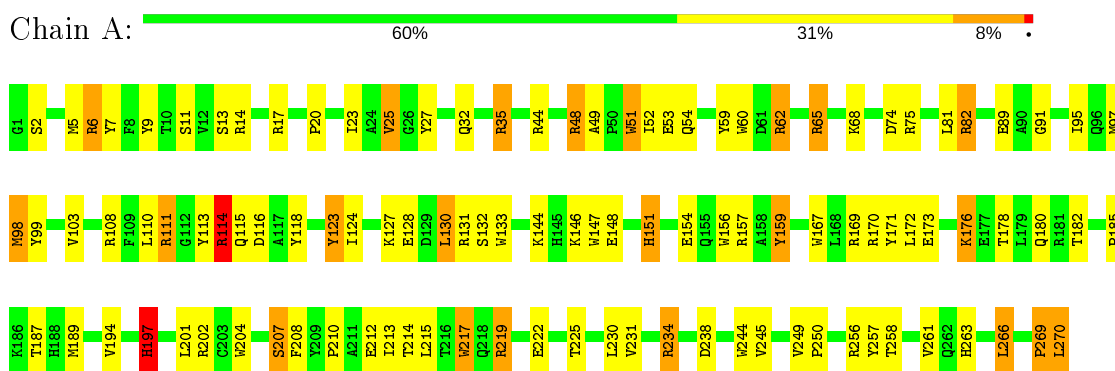
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

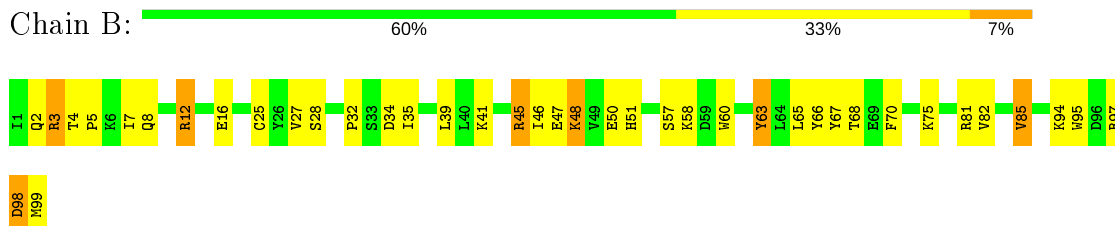
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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-Aw68)



- Molecule 2: BETA 2-MICROGLOBULIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.00Å 80.66Å 113.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3033	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.09	0/2253	2.03	94/3056 (3.1%)
2	B	1.07	0/852	1.95	24/1152 (2.1%)
All	All	1.08	0/3105	2.01	118/4208 (2.8%)

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

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	114	ARG	NE-CZ-NH1	-17.79	111.41	120.30
2	B	45	ARG	NE-CZ-NH1	-15.72	112.44	120.30
1	A	62	ARG	NE-CZ-NH1	-15.69	112.45	120.30
1	A	114	ARG	NE-CZ-NH2	15.32	127.96	120.30
2	B	66	TYR	CB-CG-CD1	-13.60	112.84	121.00
1	A	62	ARG	NE-CZ-NH2	13.20	126.90	120.30
1	A	170	ARG	NE-CZ-NH1	-13.12	113.74	120.30
2	B	45	ARG	NE-CZ-NH2	13.00	126.80	120.30
1	A	9	TYR	CB-CG-CD1	-12.01	113.80	121.00
1	A	131	ARG	NE-CZ-NH1	-11.76	114.42	120.30
1	A	256	ARG	NE-CZ-NH1	-11.47	114.57	120.30
1	A	219	ARG	NE-CZ-NH1	-11.31	114.65	120.30
1	A	48	ARG	NE-CZ-NH1	-11.01	114.80	120.30
2	B	95	TRP	CD1-CG-CD2	9.98	114.29	106.30
1	A	167	TRP	CD1-CG-CD2	9.71	114.06	106.30
1	A	202	ARG	NE-CZ-NH1	-9.54	115.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	A	6	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	A	35	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	A	65	ARG	NE-CZ-NH2	8.98	124.79	120.30
1	A	44	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	A	75	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	A	74	ASP	CA-CB-CG	8.52	132.14	113.40
2	B	60	TRP	CE2-CD2-CG	-8.49	100.51	107.30
1	A	51	TRP	CD1-CG-CD2	8.42	113.03	106.30
2	B	60	TRP	CD1-CG-CD2	8.40	113.02	106.30
2	B	95	TRP	CE2-CD2-CG	-8.37	100.61	107.30
1	A	159	TYR	CB-CG-CD2	-8.36	115.98	121.00
1	A	202	ARG	NE-CZ-NH2	8.05	124.32	120.30
1	A	60	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	A	167	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	197	HIS	CA-CB-CG	7.75	126.77	113.60
1	A	156	TRP	CD1-CG-CD2	7.67	112.43	106.30
2	B	3	ARG	NE-CZ-NH1	-7.53	116.53	120.30
1	A	171	TYR	CB-CG-CD1	-7.52	116.49	121.00
1	A	169	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	A	244	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	51	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	60	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	133	TRP	CD1-CG-CD2	7.23	112.09	106.30
1	A	123	TYR	CG-CD1-CE1	-7.22	115.52	121.30
1	A	217	TRP	CD1-CG-CD2	7.22	112.08	106.30
2	B	67	TYR	CB-CG-CD1	-7.18	116.69	121.00
1	A	167	TRP	CG-CD2-CE3	7.13	140.32	133.90
1	A	170	ARG	CG-CD-NE	-7.11	96.86	111.80
1	A	25	VAL	CG1-CB-CG2	-7.08	99.57	110.90
1	A	172	LEU	CB-CG-CD1	-7.06	99.00	111.00
1	A	234	ARG	NE-CZ-NH1	-7.05	116.77	120.30
2	B	60	TRP	CG-CD2-CE3	6.93	140.13	133.90
1	A	111	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	A	133	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	217	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	A	108	ARG	NE-CZ-NH1	-6.73	116.93	120.30
1	A	167	TRP	CG-CD1-NE1	-6.68	103.42	110.10
1	A	17	ARG	NE-CZ-NH2	6.66	123.63	120.30
2	B	81	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	156	TRP	CE2-CD2-CG	-6.55	102.06	107.30
2	B	99	MET	CG-SD-CE	-6.54	89.73	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	TRP	CB-CG-CD1	-6.46	118.60	127.00
1	A	95	ILE	CG1-CB-CG2	-6.40	97.32	111.40
1	A	82	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	219	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	5	MET	CA-CB-CG	-6.30	102.60	113.30
1	A	9	TYR	CB-CG-CD2	6.28	124.77	121.00
1	A	51	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	A	111	ARG	CA-CB-CG	6.16	126.94	113.40
1	A	244	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	A	244	TRP	CD1-CG-CD2	6.12	111.19	106.30
2	B	12	ARG	CB-CG-CD	-6.11	95.70	111.60
1	A	189	MET	CA-CB-CG	6.09	123.66	113.30
2	B	97	ARG	CB-CG-CD	-6.05	95.87	111.60
1	A	270	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	65	ARG	CB-CA-C	-5.98	98.44	110.40
1	A	60	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	A	147	TRP	CE2-CD2-CG	-5.94	102.55	107.30
1	A	99	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	A	9	TYR	CA-CB-CG	5.92	124.64	113.40
1	A	204	TRP	CD1-CG-CD2	5.85	110.98	106.30
1	A	147	TRP	CD1-CG-CD2	5.84	110.97	106.30
2	B	66	TYR	CB-CG-CD2	5.83	124.50	121.00
1	A	68	LYS	CA-CB-CG	-5.82	100.60	113.40
1	A	169	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	249	VAL	CG1-CB-CG2	-5.75	101.70	110.90
1	A	217	TRP	CG-CD2-CE3	5.75	139.07	133.90
1	A	231	VAL	CG1-CB-CG2	5.73	120.07	110.90
1	A	59	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	A	204	TRP	CE2-CD2-CG	-5.70	102.74	107.30
1	A	167	TRP	CB-CG-CD1	-5.70	119.59	127.00
1	A	266	LEU	CA-CB-CG	5.68	128.38	115.30
1	A	14	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	204	TRP	CE2-CD2-CE3	5.59	125.41	118.70
2	B	41	LYS	CB-CG-CD	-5.59	97.07	111.60
1	A	23	ILE	CB-CA-C	-5.58	100.43	111.60
2	B	98	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	B	63	TYR	CG-CD2-CE2	-5.56	116.85	121.30
1	A	207	SER	O-C-N	-5.50	113.89	122.70
1	A	151	HIS	CA-CB-CG	-5.49	104.26	113.60
1	A	159	TYR	CB-CG-CD1	5.49	124.29	121.00
1	A	133	TRP	CG-CD2-CE3	5.47	138.83	133.90
1	A	123	TYR	CD1-CG-CD2	5.46	123.91	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LYS	CB-CG-CD	-5.45	97.43	111.60
1	A	170	ARG	NH1-CZ-NH2	5.36	125.29	119.40
1	A	98	MET	CG-SD-CE	-5.31	91.70	100.20
2	B	85	VAL	CA-CB-CG2	-5.30	102.95	110.90
1	A	97	MET	CG-SD-CE	5.29	108.66	100.20
1	A	123	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	35	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	A	60	TRP	CG-CD1-NE1	-5.14	104.95	110.10
2	B	97	ARG	NE-CZ-NH1	-5.14	117.73	120.30
2	B	48	LYS	CA-CB-CG	5.13	124.69	113.40
2	B	60	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	156	TRP	CG-CD2-CE3	5.11	138.50	133.90
2	B	95	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	A	217	TRP	CB-CG-CD1	-5.09	120.39	127.00
1	A	156	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	7	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	60	TRP	CB-CG-CD1	-5.01	120.49	127.00
2	B	60	TRP	CB-CG-CD1	-5.00	120.49	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	TYR	Sidechain

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	2194	0	2045	33	0
2	B	829	0	794	16	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
All	All	3033	0	2839	46	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 8.

All (46) 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:62:ARG:HD2	1:A:65:ARG:NH1	2.07	0.69
1:A:13:SER:HA	1:A:20:PRO:HB3	1.76	0.66
2:B:2:GLN:HG2	2:B:32:PRO:HD3	1.78	0.66
1:A:62:ARG:HD2	1:A:65:ARG:HH11	1.60	0.65
2:B:7:ILE:HG12	2:B:82:VAL:HG21	1.82	0.61
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.83	0.59
1:A:173:GLU:O	1:A:176:LYS:HD3	2.03	0.59
1:A:238:ASP:HB3	2:B:12:ARG:HH11	1.67	0.58
2:B:46:ILE:HD13	2:B:68:THR:HG21	1.86	0.57
2:B:47:GLU:O	2:B:48:LYS:HB3	2.06	0.54
1:A:2:SER:HB2	1:A:103:VAL:O	2.07	0.54
1:A:130:LEU:HB3	1:A:157:ARG:HG3	1.90	0.54
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.90	0.54
1:A:25:VAL:HG12	1:A:27:TYR:CE2	2.43	0.54
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.90	0.53
1:A:238:ASP:HB3	2:B:12:ARG:HE	1.74	0.51
1:A:62:ARG:HA	1:A:65:ARG:NH1	2.26	0.51
1:A:25:VAL:HG12	1:A:27:TYR:HE2	1.76	0.50
1:A:49:ALA:O	1:A:52:ILE:HG22	2.12	0.50
1:A:32:GLN:NE2	1:A:48:ARG:HG3	2.27	0.49
1:A:82:ARG:NH1	1:A:91:GLY:O	2.46	0.49
1:A:176:LYS:HA	1:A:180:GLN:HG3	1.95	0.49
2:B:27:VAL:HG11	2:B:35:ILE:HD13	1.94	0.48
2:B:45:ARG:HH12	2:B:47:GLU:CD	2.17	0.48
1:A:213:ILE:HD12	1:A:263:HIS:HB2	1.97	0.47
1:A:230:LEU:HD12	1:A:245:VAL:HB	1.97	0.46
1:A:219:ARG:HG3	1:A:257:TYR:CZ	2.51	0.46
1:A:116:ASP:OD2	1:A:123:TYR:HB3	2.15	0.46
1:A:144:LYS:O	1:A:148:GLU:HG3	2.16	0.46
1:A:51:TRP:O	1:A:54:GLN:HG2	2.15	0.45
1:A:114:ARG:NH1	1:A:124:ILE:HG23	2.31	0.45
1:A:123:TYR:HD1	1:A:124:ILE:HG22	1.82	0.45
2:B:25:CYS:HB2	2:B:39:LEU:CD2	2.47	0.45
2:B:51:HIS:HA	2:B:65:LEU:O	2.17	0.45
1:A:215:LEU:CD1	1:A:261:VAL:HG22	2.48	0.44
1:A:210:PRO:O	1:A:263:HIS:HE1	2.00	0.44
1:A:234:ARG:HD3	2:B:8:GLN:OE1	2.19	0.43
1:A:201:LEU:HB3	1:A:217:TRP:CH2	2.53	0.43
2:B:48:LYS:HE3	2:B:48:LYS:HB3	1.79	0.42
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NE	1:A:89:GLU:HA	2.34	0.42
1:A:215:LEU:HD12	1:A:261:VAL:HG22	2.00	0.42
2:B:28:SER:HA	2:B:63:TYR:HA	2.01	0.42
1:A:197:HIS:O	1:A:250:PRO:HA	2.21	0.41
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.51	0.40
2:B:4:THR:HA	2:B:5:PRO:HD2	1.97	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	268/270 (99%)	245 (91%)	18 (7%)	5 (2%)	8	15
2	B	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
All	All	365/369 (99%)	335 (92%)	25 (7%)	5 (1%)	11	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	A	194	VAL
1	A	197	HIS
1	A	176	LYS
1	A	151	HIS

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	227/227 (100%)	201 (88%)	26 (12%)	5	10
2	B	94/94 (100%)	83 (88%)	11 (12%)	5	10
All	All	321/321 (100%)	284 (88%)	37 (12%)	5	10

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	11	SER
1	A	35	ARG
1	A	53	GLU
1	A	98	MET
1	A	110	LEU
1	A	111	ARG
1	A	113	TYR
1	A	114	ARG
1	A	115	GLN
1	A	128	GLU
1	A	130	LEU
1	A	132	SER
1	A	146	LYS
1	A	154	GLU
1	A	178	THR
1	A	182	THR
1	A	207	SER
1	A	212	GLU
1	A	214	THR
1	A	222	GLU
1	A	225	THR
1	A	258	THR
1	A	266	LEU
1	A	269	PRO
1	A	270	LEU
2	B	3	ARG
2	B	16	GLU
2	B	34	ASP
2	B	50	GLU
2	B	57	SER
2	B	58	LYS
2	B	70	PHE

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Mol	Chain	Res	Type
2	B	75	LYS
2	B	85	VAL
2	B	94	LYS
2	B	98	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	66	ASN
1	A	255	GLN
1	A	263	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 carbohydrates 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.