



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:42 am GMT

PDB ID : 1HSB
Title : DIFFERENT LENGTH PEPTIDES BIND TO HLA-AW68 SIMILARLY AT THEIR ENDS BUT BULGE OUT IN THE MIDDLE
Authors : Guo, H.-C.; Strominger, J.L.; Wiley, D.C.
Deposited on : 1993-03-30
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

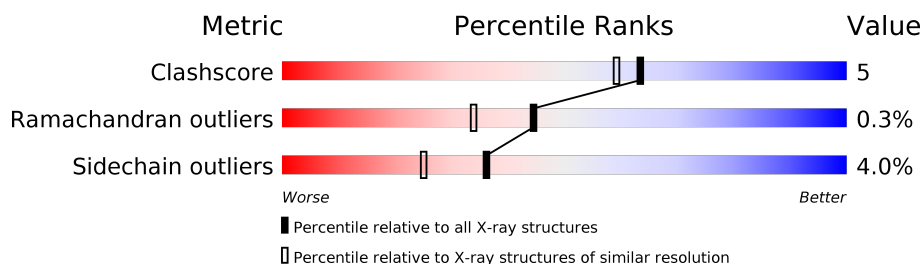
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	270	
2	B	99	
3	C	3	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3327 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-AW68.1).

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

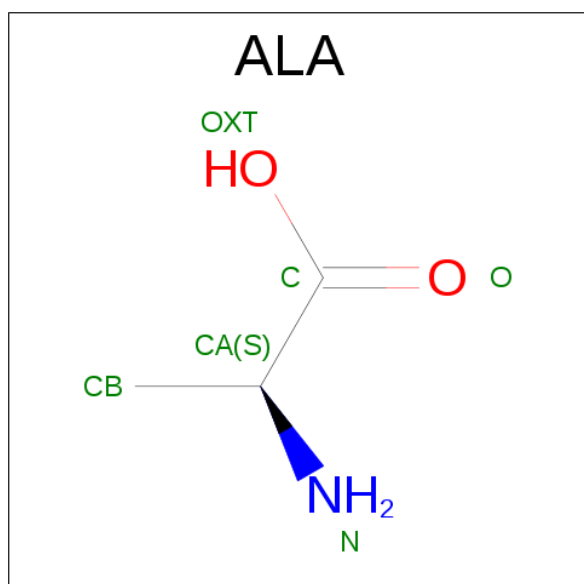
- Molecule 2 is a protein called BETA 2-MICROGLOBULIN.

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

- Molecule 3 is a protein called BOUND PEPTIDE FRAGMENT.

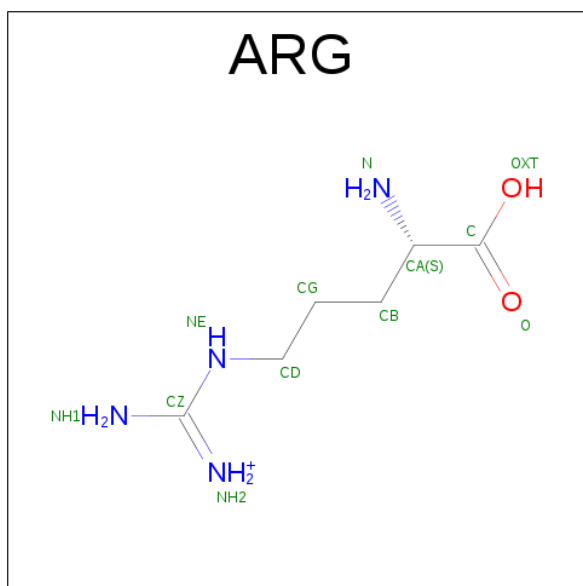
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			17	11	3	3			

- Molecule 4 is ALANINE (three-letter code: ALA) (formula: C₃H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 5 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 6 is water.

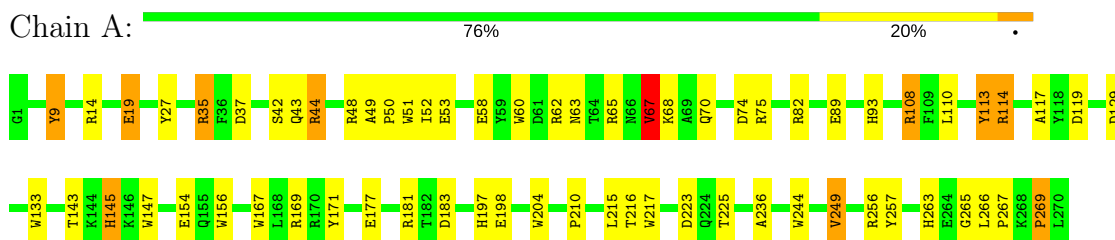
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	204	Total	O	0	0
			204	204		
6	B	66	Total	O	0	0
			66	66		

3 Residue-property plots

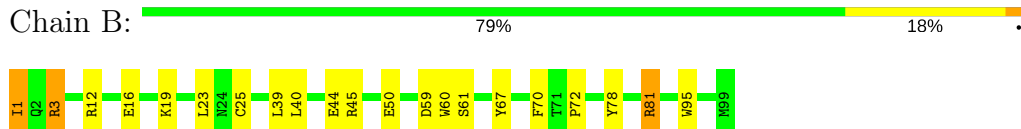
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

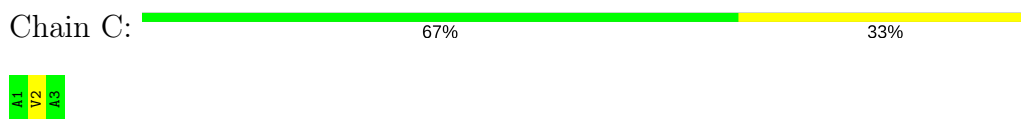
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-AW68.1)



- Molecule 2: BETA 2-MICROGLOBULIN



- Molecule 3: BOUND PEPTIDE FRAGMENT



4 Data and refinement statistics

Xtriage (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	59.43Å 78.47Å 111.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3327	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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	1.06	5/2253 (0.2%)	1.81	64/3056 (2.1%)
2	B	0.94	0/852	1.55	10/1152 (0.9%)
3	C	0.43	0/16	1.30	0/21
All	All	1.03	5/3121 (0.2%)	1.74	74/4229 (1.7%)

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	4
2	B	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	GLU	CG-CD	10.25	1.67	1.51
1	A	58	GLU	CB-CG	6.26	1.64	1.52
1	A	58	GLU	CG-CD	5.90	1.60	1.51
1	A	154	GLU	CD-OE2	-5.54	1.19	1.25
1	A	19	GLU	CB-CG	-5.21	1.42	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	GLU	OE1-CD-OE2	-16.41	103.60	123.30
1	A	58	GLU	OE1-CD-OE2	-15.71	104.45	123.30
1	A	82	ARG	NE-CZ-NH1	13.73	127.16	120.30
1	A	14	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	A	256	ARG	NE-CZ-NH2	-11.69	114.45	120.30
1	A	256	ARG	NE-CZ-NH1	10.08	125.34	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	TRP	CD1-CG-CD2	9.35	113.78	106.30
1	A	108	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	156	TRP	CD1-CG-CD2	9.18	113.64	106.30
1	A	114	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	27	TYR	CB-CG-CD1	-9.09	115.55	121.00
1	A	269	PRO	O-C-N	-8.86	108.53	122.70
1	A	19	GLU	CG-CD-OE1	8.67	135.65	118.30
1	A	217	TRP	CD1-CG-CD2	8.48	113.08	106.30
2	B	95	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	A	204	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	51	TRP	CE2-CD2-CG	-8.16	100.77	107.30
1	A	217	TRP	CE2-CD2-CG	-8.09	100.83	107.30
2	B	45	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	82	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	204	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	A	35	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	156	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	133	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	A	113	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	A	51	TRP	CG-CD2-CE3	7.25	140.43	133.90
1	A	244	TRP	CE2-CD2-CG	-7.12	101.60	107.30
2	B	95	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A	169	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	48	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	244	TRP	CD1-CG-CD2	6.83	111.77	106.30
1	A	60	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	A	181	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	147	TRP	CE2-CD2-CG	-6.73	101.91	107.30
1	A	48	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	133	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	60	TRP	CE2-CD2-CG	-6.64	101.98	107.30
1	A	114	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	51	TRP	CB-CG-CD1	-6.59	118.44	127.00
1	A	223	ASP	CB-CG-OD1	6.56	124.20	118.30
2	B	95	TRP	CG-CD2-CE3	6.47	139.72	133.90
1	A	167	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	A	167	TRP	CD1-CG-CD2	6.38	111.40	106.30
2	B	1	ILE	CB-CA-C	-6.28	99.03	111.60
2	B	16	GLU	OE1-CD-OE2	-6.17	115.89	123.30
1	A	156	TRP	CG-CD1-NE1	-6.16	103.94	110.10
2	B	3	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	74	ASP	CB-CG-OD1	5.96	123.67	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	216	THR	CA-CB-CG2	5.88	120.63	112.40
1	A	129	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	204	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	A	37	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	44	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	9	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	19	GLU	CB-CA-C	5.67	121.73	110.40
2	B	95	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	58	GLU	CG-CD-OE1	5.60	129.51	118.30
1	A	147	TRP	CG-CD2-CE3	5.60	138.94	133.90
1	A	19	GLU	CB-CG-CD	-5.57	99.17	114.20
1	A	249	VAL	N-CA-CB	-5.51	99.38	111.50
1	A	145	HIS	CA-CB-CG	-5.45	104.34	113.60
1	A	147	TRP	CD1-CG-CD2	5.38	110.61	106.30
1	A	14	ARG	CA-CB-CG	-5.37	101.59	113.40
1	A	225	THR	OG1-CB-CG2	-5.35	97.70	110.00
1	A	171	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	67	VAL	O-C-N	-5.27	114.27	122.70
1	A	223	ASP	CB-CG-OD2	-5.25	113.58	118.30
2	B	81	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	156	TRP	CB-CG-CD1	-5.22	120.22	127.00
1	A	44	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	B	45	ARG	CG-CD-NE	-5.19	100.90	111.80
1	A	108	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	65	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	GLU	Mainchain
1	A	266	LEU	Peptide
1	A	269	PRO	Mainchain
1	A	67	VAL	Mainchain
2	B	61	SER	Mainchain

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	2194	0	2045	21	0
2	B	829	0	794	9	0
3	C	17	0	21	1	0
4	A	5	0	4	0	0
5	A	12	0	13	1	0
6	A	204	0	0	4	0
6	B	66	0	0	2	0
All	All	3327	0	2877	28	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 5.

All (28) 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:B:3:ARG:NH1	6:B:752:HOH:O	2.31	0.62
1:A:9:TYR:CE2	1:A:70:GLN:HG2	2.35	0.62
2:B:81:ARG:HD2	6:B:550:HOH:O	1.98	0.62
1:A:210:PRO:O	1:A:263:HIS:HE1	1.89	0.55
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.89	0.54
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.88	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
1:A:75:ARG:NH1	6:A:720:HOH:O	2.38	0.53
1:A:145:HIS:CE1	6:A:729:HOH:O	2.62	0.52
1:A:42:SER:O	1:A:44:ARG:HG2	2.10	0.51
1:A:9:TYR:CD2	1:A:70:GLN:HG2	2.46	0.51
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.46	0.50
1:A:63:ASN:OD1	3:C:2:VAL:HG22	2.12	0.50
2:B:19:LYS:O	2:B:72:PRO:HD2	2.13	0.48
1:A:263:HIS:CD2	1:A:265:GLY:H	2.33	0.46
2:B:23:LEU:O	2:B:67:TYR:HA	2.15	0.46
1:A:143:THR:HG23	5:A:1002:ARG:HA	2.00	0.43
1:A:263:HIS:HD2	1:A:265:GLY:H	1.66	0.43
1:A:197:HIS:CE1	6:A:761:HOH:O	2.72	0.42
2:B:3:ARG:NH1	2:B:59:ASP:O	2.52	0.42
1:A:50:PRO:O	1:A:53:GLU:HB2	2.20	0.41
1:A:236:ALA:O	2:B:12:ARG:HG3	2.20	0.41
1:A:63:ASN:O	1:A:67:VAL:HG22	2.21	0.41
1:A:43:GLN:O	1:A:68:LYS:HE3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.41
1:A:62:ARG:HH11	1:A:62:ARG:HD3	1.72	0.41
1:A:75:ARG:HD3	6:A:665:HOH:O	2.20	0.41
2:B:40:LEU:O	2:B:78:TYR:HA	2.21	0.41

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%)	259 (97%)	8 (3%)	1 (0%)	38	26
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	1/3 (33%)	1 (100%)	0	0	100	100
All	All	366/372 (98%)	355 (97%)	10 (3%)	1 (0%)	44	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	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	227/227 (100%)	218 (96%)	9 (4%)	36	25
2	B	94/94 (100%)	90 (96%)	4 (4%)	33	22
3	C	1/1 (100%)	1 (100%)	0	100	100
All	All	322/322 (100%)	309 (96%)	13 (4%)	36	25

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	89	GLU
1	A	108	ARG
1	A	110	LEU
1	A	113	TYR
1	A	114	ARG
1	A	177	GLU
1	A	198	GLU
1	A	215	LEU
2	B	1	ILE
2	B	44	GLU
2	B	50	GLU
2	B	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	174	ASN
1	A	263	HIS

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ALA	A	1001	5	4,4,5	1.36	1 (25%)	1,4,6	0.23	0
5	ARG	A	1002	4	6,11,11	1.01	0	5,13,13	1.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ALA	A	1001	5	-	0/0/2/4	0/0/0/0
5	ARG	A	1002	4	-	0/7/11/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	ALA	CA-C	2.40	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	ARG	1	0

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.