



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2016 – 08:20 PM EDT

PDB ID : 1AO7
Title : COMPLEX BETWEEN HUMAN T-CELL RECEPTOR, VIRAL PEPTIDE (TAX), AND HLA-A 0201
Authors : Garboczi, D.N.; Ghosh, P.; Utz, U.; Fan, Q.R.; Biddison, W.E.; Wiley, D.C.
Deposited on : 1997-07-21
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

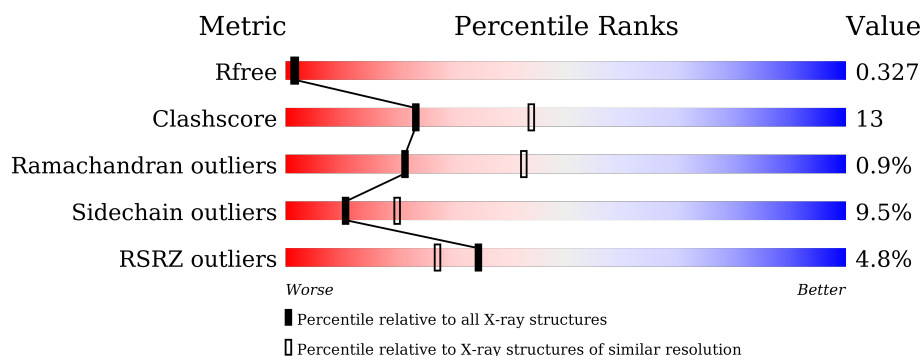
1 Overall quality at a glance ⓘ

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))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. 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.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
2	B	100	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
3	C	9	<div> <div></div> <div> <div>56%</div> <div>44%</div> </div> </div>
4	D	204	<div> <div>%</div> <div> <div></div> <div>38%</div> <div>16%</div> <div>.</div> <div>44%</div> </div> </div>
5	E	245	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>.</div> <div>15%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EMC	B	100	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5711 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 HLA-A 0201.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	122	0	0
			2237	1398	408	422	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
			828	524	140	158	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	CYS	TYR	CONFLICT	UNP P61769
B	91	CYS	LYS	CONFLICT	UNP P61769

- Molecule 3 is a protein called TAX PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			77	56	9	12			

- Molecule 4 is a protein called T CELL RECEPTOR ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	115	Total	C	N	O	S	25	0	0
			886	553	148	182	3			

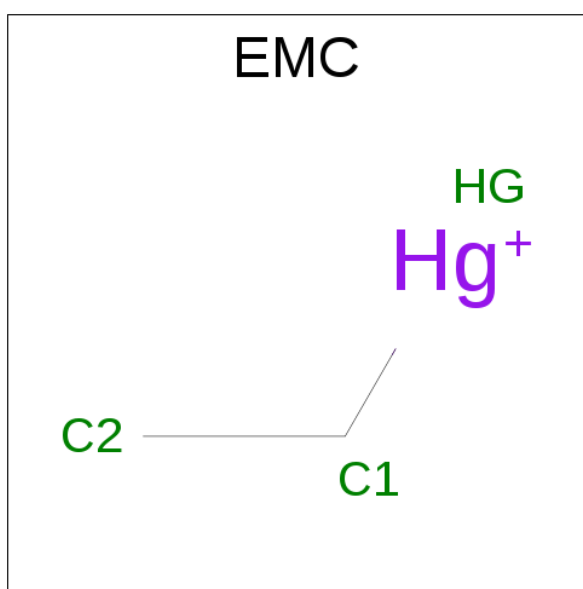
- Molecule 5 is a protein called T CELL RECEPTOR BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	209	Total	C	N	O	S	40	0	0
			1640	1041	286	305	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	ARG	SER	CONFLICT	UNP 3002925
E	96	PRO	PHE	CONFLICT	UNP 3002925
E	97	GLY	PRO	CONFLICT	UNP 3002925
E	98	LEU	ARG	CONFLICT	UNP 3002925
E	99	ALA	GLN	CONFLICT	UNP 3002925
E	100	GLY	PRO	CONFLICT	UNP 3002925
E	101	GLY	SER	CONFLICT	UNP 3002925
E	102	ARG	TYR	CONFLICT	UNP 3002925
E	103	PRO	ASN	CONFLICT	UNP 3002925
E	107	TYR	PHE	CONFLICT	UNP 3002925
E	116A	THR	LEU	CONFLICT	UNP 3002925
E	191	ALA	CYS	CONFLICT	UNP 3002925

- Molecule 6 is ETHYL MERCURY ION (three-letter code: EMC) (formula: C₂H₅Hg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	Hg	0	0
			3	2	1		
6	B	1	Total	C	Hg	0	0
			3	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total	O	0	0
			13	13		

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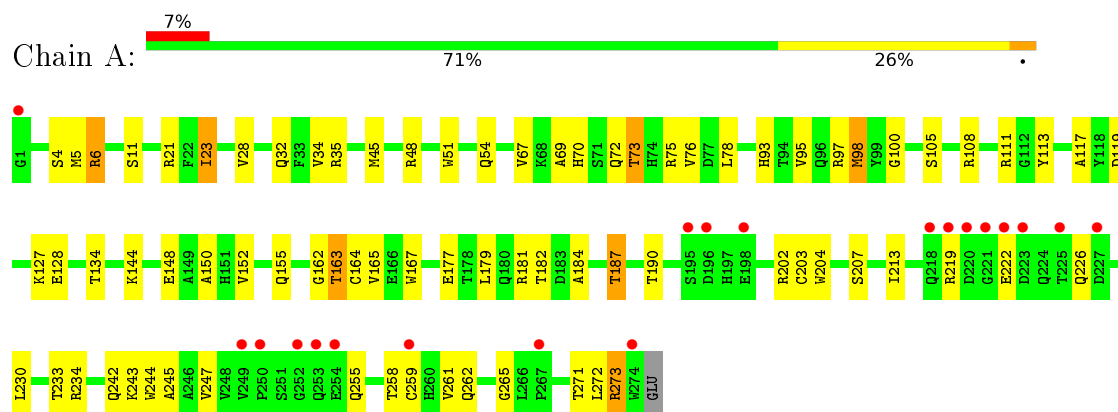
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	13	Total 13	O 13	0	0
7	C	1	Total 1	O 1	0	0
7	D	2	Total 2	O 2	0	0
7	E	8	Total 8	O 8	0	0

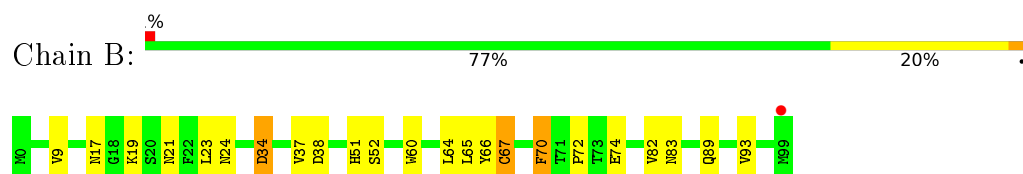
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

• Molecule 1: HLA-A 0201



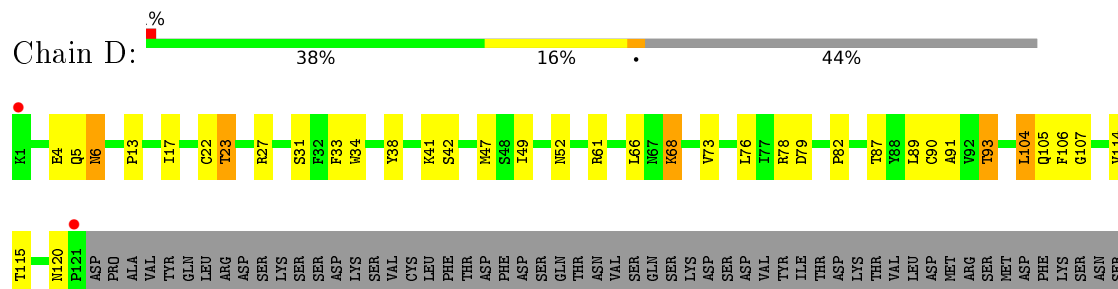
• Molecule 2: BETA-2 MICROGLOBULIN



• Molecule 3: TAX PEPTIDE

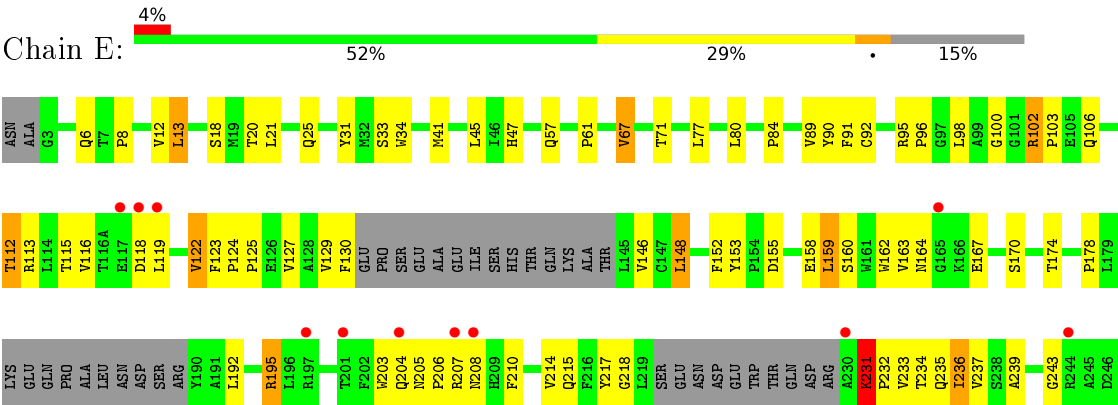


• Molecule 4: T CELL RECEPTOR ALPHA



ALA	ALA
VAL	VAL
ALA	ALA
TRP	TRP
SER	SER
ASN	ASN
LYS	LYS
SER	SER
ASP	ASP
PHE	PHE
ALA	ALA
CYS	CYS
ALA	ALA
ASN	ASN
ALA	ALA
PHE	PHE
ASN	ASN
SER	SER
ILE	ILE
PRO	PRO
GLU	GLU
ASP	ASP
THR	THR
PHE	PHE
PHE	PHE
PRO	PRO
SER	SER
PRO	PRO
GLU	GLU
SER	SER

• Molecule 5: T CELL RECEPTOR BETA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.30Å 49.50Å 96.00Å 90.00° 89.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60 11.95 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.9 (6.00-2.60) 85.9 (11.95-2.34)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.35Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.245 , 0.320 0.254 , 0.327	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5711	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EMC

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	0.38	0/2302	0.66	0/3125
2	B	0.40	0/850	0.75	1/1149 (0.1%)
3	C	0.51	0/80	0.82	0/108
4	D	0.41	0/905	0.74	1/1229 (0.1%)
5	E	0.39	0/1685	0.76	2/2292 (0.1%)
All	All	0.39	0/5822	0.72	4/7903 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	64	LEU	CA-CB-CG	6.51	130.26	115.30
5	E	231	LYS	N-CA-C	6.18	127.69	111.00
5	E	13	LEU	CA-CB-CG	5.61	128.20	115.30
4	D	120	ASN	N-CA-C	5.51	125.87	111.00

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	2237	0	2090	45	0
2	B	828	0	789	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	77	0	79	4	0
4	D	886	0	845	27	0
5	E	1640	0	1570	59	0
6	B	6	0	0	2	0
7	A	13	0	0	0	0
7	B	13	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
7	E	8	0	0	0	0
All	All	5711	0	5373	142	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 13.

The worst 5 of 142 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:21:ARG:NE	1:A:23:ILE:HD11	1.91	0.86
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.57	0.84
4:D:93:THR:HG21	4:D:104:LEU:HD22	1.60	0.83
1:A:32:GLN:HE21	1:A:48:ARG:HG3	1.44	0.81
5:E:21:LEU:HD12	5:E:77:LEU:HD23	1.62	0.80

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	272/275 (99%)	260 (96%)	12 (4%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	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
4	D	113/204 (55%)	105 (93%)	7 (6%)	1 (1%)	21	42
5	E	201/245 (82%)	182 (90%)	14 (7%)	5 (2%)	7	12
All	All	691/833 (83%)	649 (94%)	36 (5%)	6 (1%)	21	42

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	6	ASN
5	E	119	LEU
5	E	231	LYS
5	E	164	ASN
5	E	155	ASP

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	230/231 (100%)	208 (90%)	22 (10%)	10	20
2	B	95/95 (100%)	89 (94%)	6 (6%)	22	44
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	99/182 (54%)	90 (91%)	9 (9%)	12	22
5	E	177/209 (85%)	156 (88%)	21 (12%)	6	11
All	All	609/725 (84%)	551 (90%)	58 (10%)	11	20

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	83	ASN
4	D	68	LYS
5	E	174	THR
2	B	89	GLN
4	D	23	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	83	ASN
4	D	5	GLN
5	E	11	GLN
2	B	31	HIS
5	E	37	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
6	EMC	B	100	2	1,2,2	1.26	0	0,1,1	0.00	-
6	EMC	B	101	2	1,2,2	0.75	0	0,1,1	0.00	-

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
6	EMC	B	100	2	-	0/0/0/0	0/0/0/0
6	EMC	B	101	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	100	EMC	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/275 (99%)	-0.13	20 (7%) 18 12	6, 32, 119, 136	30 (10%)
2	B	100/100 (100%)	-0.67	1 (1%) 84 81	6, 25, 57, 81	2 (2%)
3	C	9/9 (100%)	-1.25	0 100 100	13, 19, 23, 24	0
4	D	115/204 (56%)	-0.43	2 (1%) 73 68	11, 33, 65, 76	7 (6%)
5	E	209/245 (85%)	-0.01	11 (5%) 30 23	16, 48, 90, 101	10 (4%)
All	All	707/833 (84%)	-0.23	34 (4%) 34 27	6, 35, 98, 136	49 (6%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	118	ASP	8.5
1	A	196	ASP	7.5
1	A	1	GLY	6.5
1	A	221	GLY	5.6
1	A	249	VAL	5.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	EMC	B	100	3/3	0.99	0.07	-1.76	44,44,57,69	0
6	EMC	B	101	3/3	0.99	0.06	-	50,50,51,53	3

6.5 Other polymers [i](#)

There are no such residues in this entry.