



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:24 am BST

PDB ID : 4LCY
Title : Crystal structure of HLA-b46 at 1.6 angstrom resolution
Authors : Liu, J.X.
Deposited on : 2013-06-24
Resolution : 1.60 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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

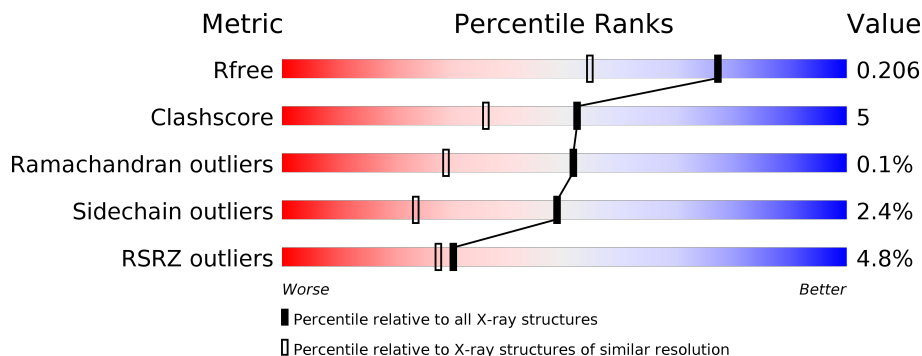
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 $\leq 5\%$. 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	274	<p>3% 92% 6% .</p>
1	F	274	<p>9% 90% 7% .</p>
2	B	100	<p>2% 92% 8%</p>
2	H	100	<p>2% 95% . .</p>
3	C	9	<p>100%</p>
3	J	9	<p>100%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7457 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 class I histocompatibility antigen, B-46 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	Total	C	N	O	S	0	0	0
			2242	1395	413	426	8			
1	F	274	Total	C	N	O	S	0	0	0
			2241	1395	413	425	8			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769
H	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called dengue1 poly peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	9	Total	C	N	O	S	0	0	0
			74	49	12	12	1			
3	J	9	Total	C	N	O	S	0	0	0
			74	49	12	12	1			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total	Na	0
			1	1	

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	2	Total Na 2 2	0	0
4	F	2	Total Na 2 2	0	0

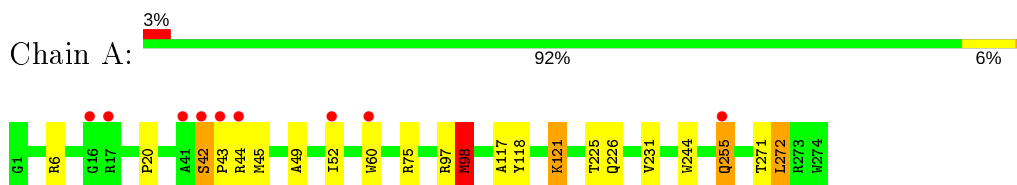
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	404	Total O 404 404	0	0
5	B	167	Total O 167 167	0	0
5	C	18	Total O 18 18	0	0
5	F	349	Total O 349 349	0	0
5	H	188	Total O 188 188	0	0
5	J	20	Total O 20 20	0	0

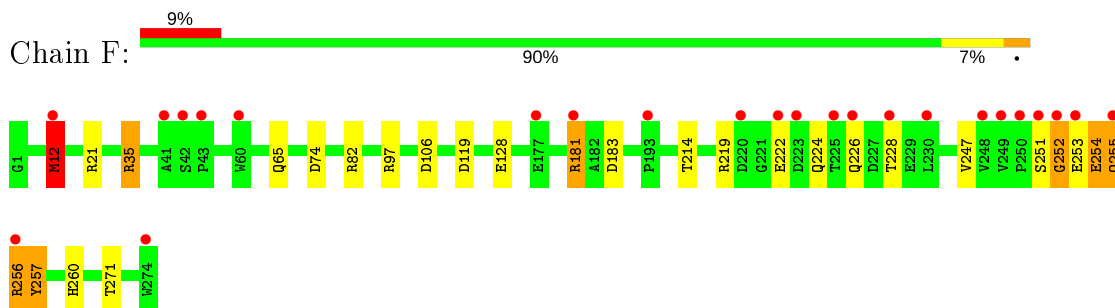
3 Residue-property plots [i](#)

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 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.

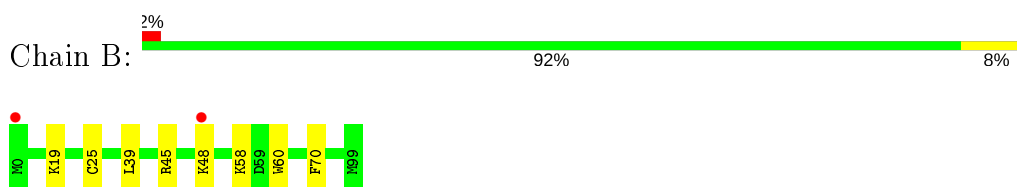
- Molecule 1: HLA class I histocompatibility antigen, B-46 alpha chain



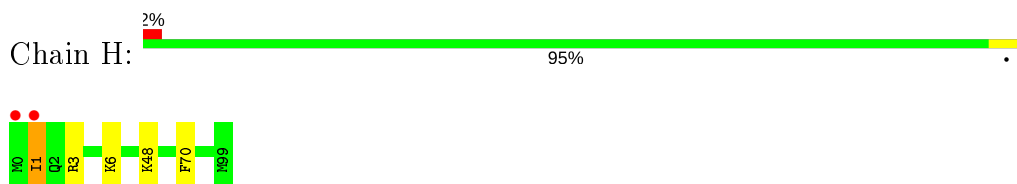
- Molecule 1: HLA class I histocompatibility antigen, B-46 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: dengue1 poly peptide



There are no outlier residues recorded for this chain.

- Molecule 3: dengue1 poly peptide

Chain J:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.95Å 89.73Å 94.62Å 90.00° 98.45° 90.00°	Depositor
Resolution (Å)	25.20 – 1.60 25.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.20-1.60) 98.9 (25.20-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.87 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.201 0.179 , 0.206	Depositor DCC
R_{free} test set	5346 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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, 0.333 respectively for untwinned datasets, and 0.375, 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:
NA

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	0.64	0/2305	0.84	4/3130 (0.1%)
1	F	0.68	1/2304 (0.0%)	0.86	5/3130 (0.2%)
2	B	0.59	0/860	0.74	0/1162
2	H	0.61	0/860	0.78	0/1162
3	C	0.60	0/75	0.77	0/99
3	J	0.69	0/75	0.77	0/99
All	All	0.65	1/6479 (0.0%)	0.82	9/8782 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	257	TYR	CE1-CZ	-5.63	1.31	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	6	ARG	CG-CD-NE	-5.93	99.34	111.80
1	F	106	ASP	CB-CG-OD1	5.88	123.59	118.30
1	F	256	ARG	CB-CA-C	5.62	121.63	110.40
1	A	44	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	98	MET	N-CA-CB	5.47	120.44	110.60
1	F	82	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	F	74	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	6	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	F	12	MET	CB-CG-SD	5.06	127.57	112.40

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	2242	0	2103	22	0
1	F	2241	0	2103	39	0
2	B	837	0	803	5	0
2	H	837	0	803	4	0
3	C	74	0	83	0	0
3	J	74	0	83	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
5	A	404	0	0	2	0
5	B	167	0	0	2	0
5	C	18	0	0	0	0
5	F	349	0	0	9	0
5	H	188	0	0	4	0
5	J	20	0	0	0	0
All	All	7457	0	5978	67	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 (67) 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:45:MET:HE1	1:A:60:TRP:CE3	1.56	1.40
1:F:219:ARG:O	1:F:222:GLU:HG2	1.38	1.20
1:A:45:MET:CE	1:A:60:TRP:CE3	2.26	1.18
1:F:253:GLU:O	1:F:255:GLN:HB2	1.43	1.16
1:A:45:MET:HE2	1:A:60:TRP:CZ3	1.91	1.04
1:A:45:MET:CE	1:A:60:TRP:HE3	1.68	1.02
1:A:45:MET:HE1	1:A:60:TRP:HE3	0.81	0.95
1:A:45:MET:CE	1:A:60:TRP:CZ3	2.49	0.93
1:A:118:TYR:O	1:A:121:LYS:HD3	1.73	0.89
1:A:45:MET:HE2	1:A:60:TRP:HZ3	1.30	0.89
1:F:254:GLU:HA	1:F:255:GLN:CB	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:GLU:N	1:F:254:GLU:OE2	2.17	0.78
1:F:255:GLN:HE21	1:F:255:GLN:CA	2.01	0.71
1:F:12:MET:SD	5:F:482:HOH:O	2.49	0.69
1:F:222:GLU:HG3	1:F:224:GLN:NE2	2.07	0.69
1:F:255:GLN:HE21	1:F:255:GLN:HA	1.63	0.62
1:A:255:GLN:NE2	5:A:771:HOH:O	2.33	0.61
1:F:214:THR:HG23	5:F:690:HOH:O	2.01	0.60
1:F:222:GLU:HG3	1:F:224:GLN:HE21	1.66	0.59
1:A:271:THR:C	1:A:272:LEU:HD12	2.23	0.58
1:F:224:GLN:O	1:F:228:THR:HG23	2.04	0.57
1:F:254:GLU:HA	1:F:255:GLN:HB2	1.85	0.57
1:F:260:HIS:CE1	1:F:271:THR:HG22	2.41	0.54
1:F:253:GLU:C	1:F:255:GLN:HB2	2.25	0.54
1:F:119:ASP:O	2:H:1:ILE:HG23	2.09	0.53
1:F:254:GLU:CA	1:F:255:GLN:CB	2.84	0.53
1:F:260:HIS:ND1	1:F:271:THR:HG22	2.23	0.52
1:F:181:ARG:O	1:F:181:ARG:NE	2.43	0.51
1:F:255:GLN:NE2	1:F:255:GLN:HA	2.25	0.51
1:F:12:MET:HG3	5:H:206:HOH:O	2.10	0.51
1:F:35:ARG:NH1	5:F:620:HOH:O	2.43	0.51
1:A:20:PRO:HD2	1:A:75:ARG:HG2	1.93	0.51
1:F:254:GLU:CA	1:F:255:GLN:HB2	2.40	0.51
2:H:1:ILE:HD11	2:H:3:ARG:NE	2.26	0.51
1:F:252:GLY:O	1:F:253:GLU:HB3	2.11	0.50
1:F:255:GLN:NE2	1:F:255:GLN:CA	2.73	0.50
1:A:98:MET:HE1	2:B:58:LYS:HD2	1.94	0.49
1:A:121:LYS:HD2	5:B:297:HOH:O	2.13	0.49
1:F:21:ARG:NH1	5:F:699:HOH:O	2.46	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.48
1:F:255:GLN:HE21	1:F:255:GLN:N	2.10	0.48
1:A:225:THR:OG1	1:A:226:GLN:N	2.48	0.47
1:F:251:SER:C	1:F:253:GLU:H	2.18	0.47
1:A:272:LEU:N	1:A:272:LEU:HD12	2.29	0.47
1:F:228:THR:HG22	1:F:247:VAL:CG1	2.45	0.46
1:F:254:GLU:HA	1:F:255:GLN:HB3	1.93	0.46
2:H:6:LYS:HD2	5:H:291:HOH:O	2.16	0.46
2:B:45:ARG:NH1	5:B:266:HOH:O	2.49	0.45
2:H:48:LYS:NZ	5:H:346:HOH:O	2.50	0.45
2:B:19:LYS:HE2	5:H:327:HOH:O	2.16	0.45
1:F:228:THR:HG21	5:F:733:HOH:O	2.17	0.45
1:F:255:GLN:O	1:F:256:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.00	0.43
1:F:252:GLY:O	1:F:253:GLU:CB	2.66	0.43
1:F:181:ARG:NH1	1:F:183:ASP:OD1	2.52	0.43
1:A:97:ARG:NH2	5:A:775:HOH:O	2.45	0.43
1:F:271:THR:HG23	5:F:651:HOH:O	2.19	0.43
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.54	0.42
1:A:49:ALA:O	1:A:52:ILE:HG22	2.18	0.42
1:F:97:ARG:NH2	5:F:729:HOH:O	2.37	0.42
1:F:181:ARG:NE	5:F:695:HOH:O	2.53	0.42
1:A:255:GLN:C	1:A:255:GLN:HE21	2.23	0.42
1:A:272:LEU:N	1:A:272:LEU:CD1	2.83	0.42
1:F:254:GLU:HB2	1:F:257:TYR:HD1	1.85	0.41
1:A:42:SER:HA	1:A:43:PRO:HA	1.76	0.41
1:F:65:GLN:NE2	5:F:734:HOH:O	2.53	0.41
1:F:251:SER:O	1:F:253:GLU:N	2.54	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	272/274 (99%)	265 (97%)	7 (3%)	0	100	100
1	F	272/274 (99%)	267 (98%)	4 (2%)	1 (0%)	34	15
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	H	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100
All	All	754/766 (98%)	740 (98%)	13 (2%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	252	GLY

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	230/230 (100%)	225 (98%)	5 (2%)	52	27
1	F	230/230 (100%)	223 (97%)	7 (3%)	41	16
2	B	95/95 (100%)	93 (98%)	2 (2%)	53	29
2	H	95/95 (100%)	93 (98%)	2 (2%)	53	29
3	C	9/9 (100%)	9 (100%)	0	100	100
3	J	9/9 (100%)	9 (100%)	0	100	100
All	All	668/668 (100%)	652 (98%)	16 (2%)	49	24

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	98	MET
1	A	121	LYS
1	A	255	GLN
1	A	272	LEU
2	B	48	LYS
2	B	70	PHE
1	F	12	MET
1	F	35	ARG
1	F	128	GLU
1	F	181	ARG
1	F	226	GLN
1	F	254	GLU
1	F	255	GLN
2	H	1	ILE
2	H	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	F	224	GLN
1	F	255	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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	274/274 (100%)	0.17	9 (3%) 46 43	6, 13, 31, 64	2 (0%)
1	F	274/274 (100%)	0.37	24 (8%) 10 9	6, 16, 41, 77	0
2	B	100/100 (100%)	0.03	2 (2%) 65 64	8, 15, 31, 42	0
2	H	100/100 (100%)	0.05	2 (2%) 65 64	8, 16, 31, 36	0
3	C	9/9 (100%)	-0.15	0 100 100	9, 9, 13, 14	0
3	J	9/9 (100%)	-0.06	0 100 100	11, 12, 16, 21	0
All	All	766/766 (100%)	0.20	37 (4%) 30 28	6, 14, 35, 77	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	253	GLU	8.6
1	A	41	ALA	8.2
1	F	255	GLN	8.0
1	A	42	SER	7.9
1	A	43	PRO	7.6
1	F	274	TRP	5.6
1	F	256	ARG	4.8
1	F	252	GLY	4.7
2	H	1	ILE	4.6
1	F	42	SER	4.2
1	F	60	TRP	3.8
1	F	249	VAL	3.5
1	F	41	ALA	3.3
1	F	220	ASP	3.2
1	A	16	GLY	3.1
1	A	17	ARG	3.0
1	A	44	ARG	2.9
1	A	60	TRP	2.8
1	F	223	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	226	GLN	2.7
2	B	0	MET	2.7
1	F	181	ARG	2.7
1	F	12	MET	2.6
2	B	48	LYS	2.5
2	H	0	MET	2.4
1	A	52	ILE	2.4
1	F	43	PRO	2.3
1	F	193	PRO	2.3
1	F	251	SER	2.2
1	F	230	LEU	2.2
1	A	255	GLN	2.2
1	F	228	THR	2.2
1	F	248	VAL	2.1
1	F	177	GLU	2.1
1	F	225	THR	2.1
1	F	222	GLU	2.1
1	F	250	PRO	2.0

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. 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	B-factors(Å ²)	Q<0.9
4	NA	B	101	1/1	0.93	0.17	31,31,31,31	0
4	NA	H	101	1/1	0.94	0.13	30,30,30,30	0
4	NA	A	302	1/1	0.97	0.12	26,26,26,26	0
4	NA	F	301	1/1	0.97	0.07	20,20,20,20	0
4	NA	A	301	1/1	0.97	0.11	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	F	302	1/1	0.99	0.05	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.