



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 03:07 AM BST

PDB ID : 6VQO
Title : T cell receptor-p53-HLA-A2 complex
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Deposited on : 2020-02-05
Resolution : 3.00 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

<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	:	2.13.1
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)	:	2.13.1

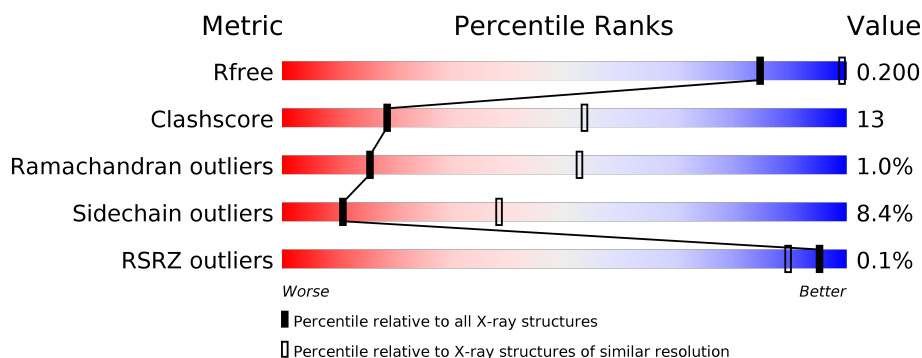
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	293	
1	F	293	
2	B	100	
2	G	100	
3	D	208	
3	H	208	

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Mol	Chain	Length	Quality of chain
4	E	244	 72% 23% . .
4	J	244	 63% 33% . .
5	P	9	 67% 33%
5	Q	9	 89% 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12740 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2198	1378	395	416	9			
1	F	254	Total	C	N	O	S	0	0	0
			1988	1250	355	375	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP F6IQS2
A	276	GLY	-	expression tag	UNP F6IQS2
A	277	GLY	-	expression tag	UNP F6IQS2
A	278	GLY	-	expression tag	UNP F6IQS2
A	279	LEU	-	expression tag	UNP F6IQS2
A	280	ASN	-	expression tag	UNP F6IQS2
A	281	ASP	-	expression tag	UNP F6IQS2
A	282	ILE	-	expression tag	UNP F6IQS2
A	283	PHE	-	expression tag	UNP F6IQS2
A	284	GLU	-	expression tag	UNP F6IQS2
A	285	ALA	-	expression tag	UNP F6IQS2
A	286	GLN	-	expression tag	UNP F6IQS2
A	287	LYS	-	expression tag	UNP F6IQS2
A	288	ILE	-	expression tag	UNP F6IQS2
A	289	GLU	-	expression tag	UNP F6IQS2
A	290	TRP	-	expression tag	UNP F6IQS2
A	291	HIS	-	expression tag	UNP F6IQS2
A	292	GLU	-	expression tag	UNP F6IQS2
F	0	MET	-	expression tag	UNP F6IQS2
F	276	GLY	-	expression tag	UNP F6IQS2
F	277	GLY	-	expression tag	UNP F6IQS2
F	278	GLY	-	expression tag	UNP F6IQS2
F	279	LEU	-	expression tag	UNP F6IQS2
F	280	ASN	-	expression tag	UNP F6IQS2
F	281	ASP	-	expression tag	UNP F6IQS2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	282	ILE	-	expression tag	UNP F6IQS2
F	283	PHE	-	expression tag	UNP F6IQS2
F	284	GLU	-	expression tag	UNP F6IQS2
F	285	ALA	-	expression tag	UNP F6IQS2
F	286	GLN	-	expression tag	UNP F6IQS2
F	287	LYS	-	expression tag	UNP F6IQS2
F	288	ILE	-	expression tag	UNP F6IQS2
F	289	GLU	-	expression tag	UNP F6IQS2
F	290	TRP	-	expression tag	UNP F6IQS2
F	291	HIS	-	expression tag	UNP F6IQS2
F	292	GLU	-	expression tag	UNP F6IQS2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			812	520	137	151	4			
2	G	99	Total	C	N	O	S	0	0	0
			785	504	132	146	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
G	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called T-cell receptor 1a2, alfa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	193	Total	C	N	O	S	0	0	0
			1493	941	237	305	10			
3	H	196	Total	C	N	O	S	0	0	0
			1514	948	244	312	10			

- Molecule 4 is a protein called TCR receptor 1a2, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	240	Total	C	N	O	S	0	0	0
			1882	1190	325	359	8			
4	J	241	Total	C	N	O	S	0	0	0
			1916	1212	333	363	8			

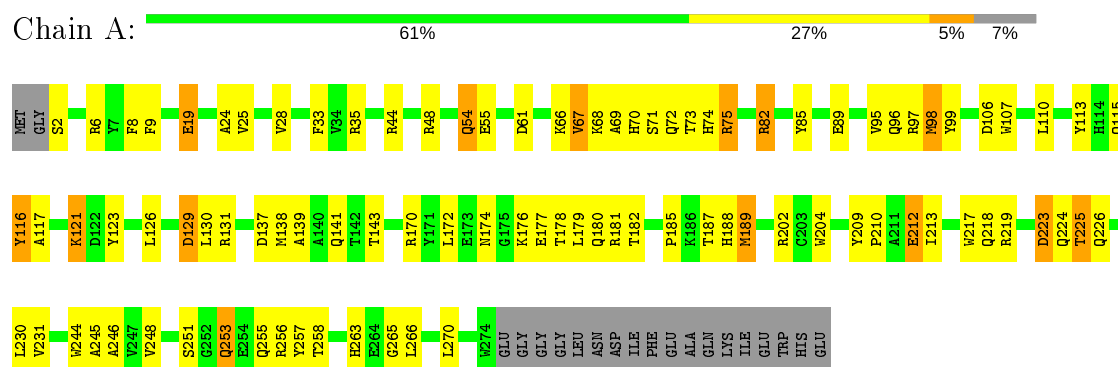
- Molecule 5 is a protein called peptide from p53 tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total	C	N	O	S	0	0	0
			76	45	16	13	2			
5	Q	9	Total	C	N	O	S	0	0	0
			76	45	16	13	2			

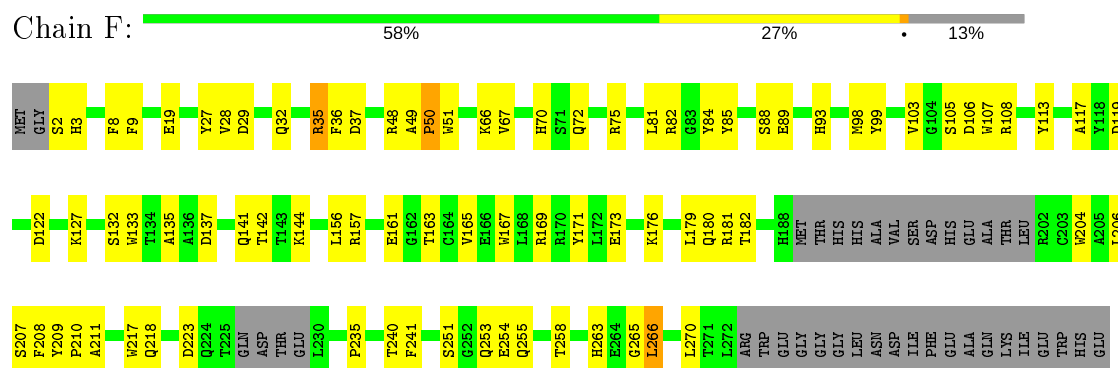
3 Residue-property plots [i](#)

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 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.

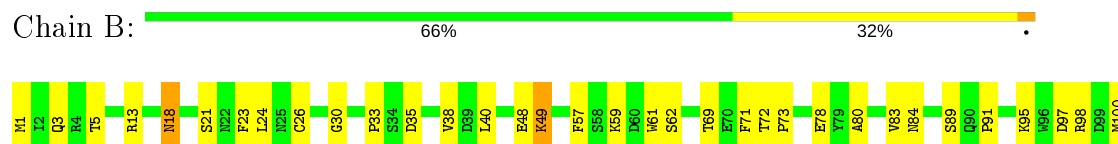
• Molecule 1: MHC class I antigen



• Molecule 1: MHC class I antigen

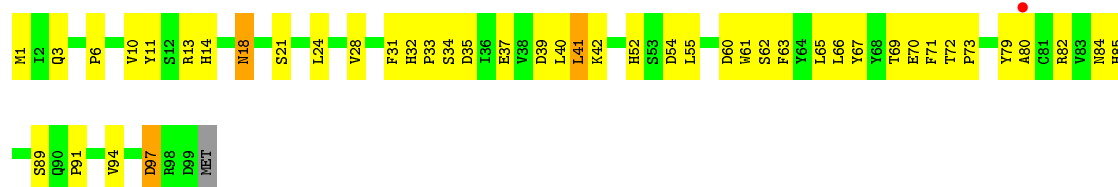


• Molecule 2: Beta-2-microglobulin

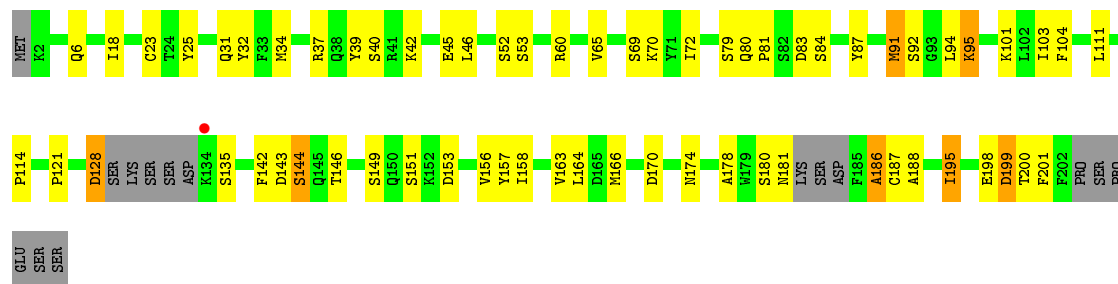


• Molecule 2: Beta-2-microglobulin

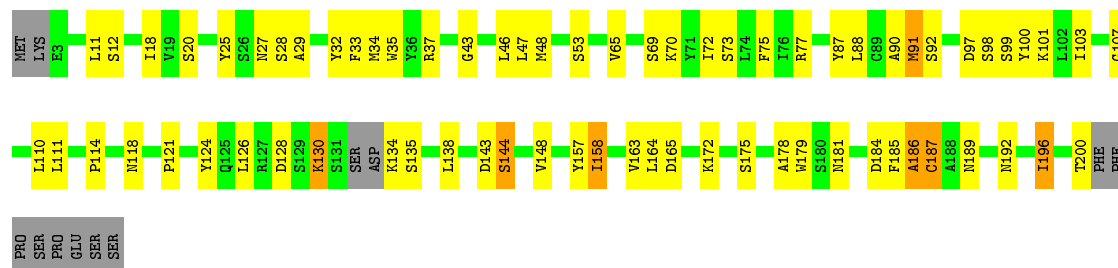




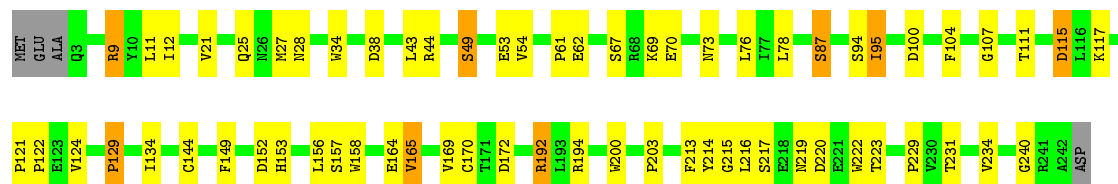
• Molecule 3: T-cell receptor 1a2, alfa chain



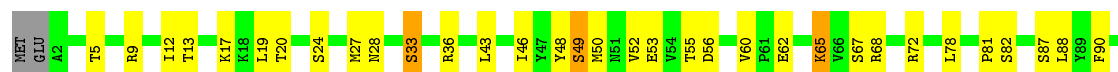
• Molecule 3: T-cell receptor 1a2, alfa chain

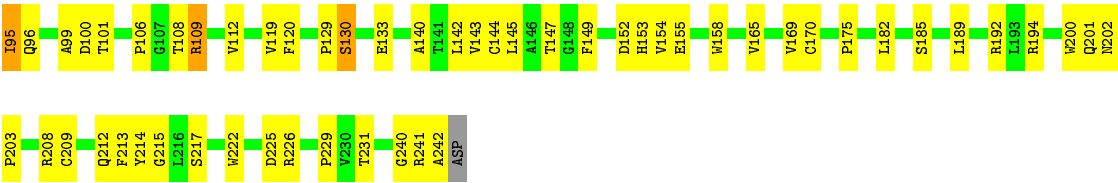


• Molecule 4: TCR receptor 1a2, beta chain



• Molecule 4: TCR receptor 1a2, beta chain

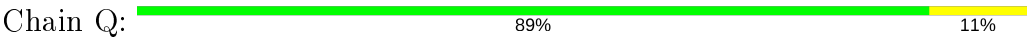




- Molecule 5: peptide from p53 tumor suppressor



- Molecule 5: peptide from p53 tumor suppressor



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	118.13Å 118.13Å 153.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 3.00 48.52 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.52-3.00) 97.2 (48.52-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.162 , 0.211 0.153 , 0.200	Depositor DCC
R_{free} test set	2271 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 15.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.098 for -h,-k,l 0.378 for h,-h-k,-l 0.098 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12740	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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	0.45	0/2262	0.89	1/3076 (0.0%)
1	F	0.37	0/2044	0.76	0/2781
2	B	0.45	0/835	0.90	0/1134
2	G	0.33	0/808	0.76	0/1102
3	D	0.41	0/1526	0.80	0/2071
3	H	0.42	0/1546	0.81	0/2096
4	E	0.40	0/1934	0.85	1/2643 (0.0%)
4	J	0.40	0/1968	0.79	1/2683 (0.0%)
5	P	0.52	0/77	0.97	0/101
5	Q	0.37	0/77	0.77	0/101
All	All	0.41	0/13077	0.82	3/17788 (0.0%)

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
3	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	208	ARG	NE-CZ-NH1	-5.84	117.38	120.30
4	E	44	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	82	ARG	NE-CZ-NH2	-5.42	117.59	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	199	ASP	Peptide

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	2198	0	2032	68	0
1	F	1988	0	1799	53	0
2	B	812	0	760	21	0
2	G	785	0	719	33	0
3	D	1493	0	1370	36	0
3	H	1514	0	1409	44	0
4	E	1882	0	1763	37	0
4	J	1916	0	1835	62	0
5	P	76	0	74	4	0
5	Q	76	0	74	1	0
All	All	12740	0	11835	324	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 324 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)
3:D:121:PRO:HB2	3:D:200:THR:CG2	1.84	1.07
2:G:21:SER:HA	2:G:72:THR:HG22	1.48	0.96
1:A:188:HIS:HB3	1:A:204:TRP:HB2	1.47	0.94
3:H:135:SER:HG	3:H:185:PHE:HD1	0.95	0.93
2:B:21:SER:HA	2:B:72:THR:HG22	1.58	0.85

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	271/293 (92%)	241 (89%)	29 (11%)	1 (0%)	34	72
1	F	248/293 (85%)	220 (89%)	23 (9%)	5 (2%)	7	34
2	B	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	15	53
2	G	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
3	D	187/208 (90%)	168 (90%)	16 (9%)	3 (2%)	9	40
3	H	192/208 (92%)	175 (91%)	15 (8%)	2 (1%)	15	53
4	E	238/244 (98%)	217 (91%)	18 (8%)	3 (1%)	12	45
4	J	239/244 (98%)	225 (94%)	13 (5%)	1 (0%)	34	72
5	P	7/9 (78%)	7 (100%)	0	0	100	100
5	Q	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1584/1708 (93%)	1438 (91%)	130 (8%)	16 (1%)	15	53

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	49	LYS
3	D	199	ASP
3	H	186	ALA
3	D	186	ALA
1	F	254	GLU

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	223/245 (91%)	203 (91%)	20 (9%)	9	35
1	F	194/245 (79%)	184 (95%)	10 (5%)	23	59
2	B	88/95 (93%)	80 (91%)	8 (9%)	9	34
2	G	83/95 (87%)	78 (94%)	5 (6%)	19	53
3	D	166/189 (88%)	148 (89%)	18 (11%)	6	26
3	H	171/189 (90%)	155 (91%)	16 (9%)	8	32
4	E	202/217 (93%)	184 (91%)	18 (9%)	9	35
4	J	210/217 (97%)	191 (91%)	19 (9%)	9	35
5	P	9/9 (100%)	9 (100%)	0	100	100
5	Q	9/9 (100%)	9 (100%)	0	100	100
All	All	1355/1510 (90%)	1241 (92%)	114 (8%)	11	38

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	67	SER
4	E	223	THR
4	J	72	ARG
4	E	87	SER
4	E	115	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	141	GLN
1	F	145	HIS
3	H	125	GLN
1	F	86	ASN
3	H	27	ASN

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 [i](#)

There are no monosaccharides 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 [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(Å²)	Q<0.9	
1	A	273/293 (93%)	-0.45	0	100	100	15, 43, 85, 132	0
1	F	254/293 (86%)	-0.35	0	100	100	28, 62, 110, 147	0
2	B	100/100 (100%)	-0.52	0	100	100	18, 35, 57, 72	0
2	G	99/100 (99%)	-0.28	1 (1%)	82	59	41, 69, 103, 119	0
3	D	193/208 (92%)	-0.22	1 (0%)	91	75	26, 55, 101, 115	0
3	H	196/208 (94%)	-0.34	0	100	100	35, 57, 81, 115	0
4	E	240/244 (98%)	-0.37	0	100	100	23, 55, 94, 107	0
4	J	241/244 (98%)	-0.40	0	100	100	31, 48, 79, 98	0
5	P	9/9 (100%)	-0.27	0	100	100	27, 32, 35, 42	0
5	Q	9/9 (100%)	-0.12	0	100	100	43, 50, 54, 64	0
All	All	1614/1708 (94%)	-0.37	2 (0%)	95	89	15, 52, 96, 147	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	80	ALA	2.6
3	D	134	LYS	2.5

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.