



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2021 – 12:46 PM EST

PDB ID : 6W51
Title : Structure of the antibody fragment H2 in complex with HLA-A*02:01/p53R175H
Authors : Wright, K.M.; Gabelli, S.B.
Deposited on : 2020-03-12
Resolution : 3.53 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
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)	:	2.17.1

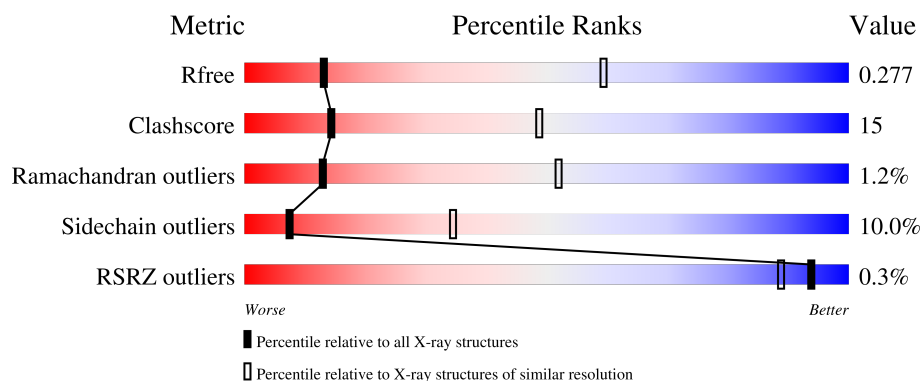
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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 of 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	296	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 67% 21% • 9% </div> </div>
1	D	296	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 68% 21% • 7% </div>
1	G	296	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 60% 27% 5% 8% </div>
1	J	296	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 71% 19% • 7% </div> </div>
2	B	119	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 66% 15% • 17% </div>

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Mol	Chain	Length	Quality of chain
2	E	119	
2	H	119	
2	K	119	
3	C	9	
3	F	9	
3	I	9	
3	L	9	
4	M	223	
4	O	223	
4	Q	223	
4	S	223	
5	N	215	
5	P	215	
5	R	215	
5	T	215	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25900 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	268	Total	C	N	O	S	0	3	0
			2201	1373	401	418	9			
1	D	274	Total	C	N	O	S	0	3	0
			2258	1409	412	428	9			
1	G	272	Total	C	N	O	S	0	3	0
			2241	1401	405	426	9			
1	J	275	Total	C	N	O	S	0	3	0
			2265	1414	412	430	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP U5YKE0
A	277	GLY	-	expression tag	UNP U5YKE0
A	278	SER	-	expression tag	UNP U5YKE0
A	279	GLY	-	expression tag	UNP U5YKE0
A	280	SER	-	expression tag	UNP U5YKE0
A	281	GLY	-	expression tag	UNP U5YKE0
A	282	LEU	-	expression tag	UNP U5YKE0
A	283	ASN	-	expression tag	UNP U5YKE0
A	284	ASP	-	expression tag	UNP U5YKE0
A	285	ILE	-	expression tag	UNP U5YKE0
A	286	PHE	-	expression tag	UNP U5YKE0
A	287	GLU	-	expression tag	UNP U5YKE0
A	288	ALA	-	expression tag	UNP U5YKE0
A	289	GLN	-	expression tag	UNP U5YKE0
A	290	LYS	-	expression tag	UNP U5YKE0
A	291	ILE	-	expression tag	UNP U5YKE0
A	292	GLU	-	expression tag	UNP U5YKE0
A	293	TRP	-	expression tag	UNP U5YKE0
A	294	HIS	-	expression tag	UNP U5YKE0
A	295	GLU	-	expression tag	UNP U5YKE0
D	0	MET	-	initiating methionine	UNP U5YKE0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	277	GLY	-	expression tag	UNP U5YKE0
D	278	SER	-	expression tag	UNP U5YKE0
D	279	GLY	-	expression tag	UNP U5YKE0
D	280	SER	-	expression tag	UNP U5YKE0
D	281	GLY	-	expression tag	UNP U5YKE0
D	282	LEU	-	expression tag	UNP U5YKE0
D	283	ASN	-	expression tag	UNP U5YKE0
D	284	ASP	-	expression tag	UNP U5YKE0
D	285	ILE	-	expression tag	UNP U5YKE0
D	286	PHE	-	expression tag	UNP U5YKE0
D	287	GLU	-	expression tag	UNP U5YKE0
D	288	ALA	-	expression tag	UNP U5YKE0
D	289	GLN	-	expression tag	UNP U5YKE0
D	290	LYS	-	expression tag	UNP U5YKE0
D	291	ILE	-	expression tag	UNP U5YKE0
D	292	GLU	-	expression tag	UNP U5YKE0
D	293	TRP	-	expression tag	UNP U5YKE0
D	294	HIS	-	expression tag	UNP U5YKE0
D	295	GLU	-	expression tag	UNP U5YKE0
G	0	MET	-	initiating methionine	UNP U5YKE0
G	277	GLY	-	expression tag	UNP U5YKE0
G	278	SER	-	expression tag	UNP U5YKE0
G	279	GLY	-	expression tag	UNP U5YKE0
G	280	SER	-	expression tag	UNP U5YKE0
G	281	GLY	-	expression tag	UNP U5YKE0
G	282	LEU	-	expression tag	UNP U5YKE0
G	283	ASN	-	expression tag	UNP U5YKE0
G	284	ASP	-	expression tag	UNP U5YKE0
G	285	ILE	-	expression tag	UNP U5YKE0
G	286	PHE	-	expression tag	UNP U5YKE0
G	287	GLU	-	expression tag	UNP U5YKE0
G	288	ALA	-	expression tag	UNP U5YKE0
G	289	GLN	-	expression tag	UNP U5YKE0
G	290	LYS	-	expression tag	UNP U5YKE0
G	291	ILE	-	expression tag	UNP U5YKE0
G	292	GLU	-	expression tag	UNP U5YKE0
G	293	TRP	-	expression tag	UNP U5YKE0
G	294	HIS	-	expression tag	UNP U5YKE0
G	295	GLU	-	expression tag	UNP U5YKE0
J	0	MET	-	initiating methionine	UNP U5YKE0
J	277	GLY	-	expression tag	UNP U5YKE0
J	278	SER	-	expression tag	UNP U5YKE0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	279	GLY	-	expression tag	UNP U5YKE0
J	280	SER	-	expression tag	UNP U5YKE0
J	281	GLY	-	expression tag	UNP U5YKE0
J	282	LEU	-	expression tag	UNP U5YKE0
J	283	ASN	-	expression tag	UNP U5YKE0
J	284	ASP	-	expression tag	UNP U5YKE0
J	285	ILE	-	expression tag	UNP U5YKE0
J	286	PHE	-	expression tag	UNP U5YKE0
J	287	GLU	-	expression tag	UNP U5YKE0
J	288	ALA	-	expression tag	UNP U5YKE0
J	289	GLN	-	expression tag	UNP U5YKE0
J	290	LYS	-	expression tag	UNP U5YKE0
J	291	ILE	-	expression tag	UNP U5YKE0
J	292	GLU	-	expression tag	UNP U5YKE0
J	293	TRP	-	expression tag	UNP U5YKE0
J	294	HIS	-	expression tag	UNP U5YKE0
J	295	GLU	-	expression tag	UNP U5YKE0

- 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	1	0
			836	532	142	159	3			
2	E	100	Total	C	N	O	S	0	1	0
			837	535	141	158	3			
2	H	100	Total	C	N	O	S	0	1	0
			841	535	143	160	3			
2	K	99	Total	C	N	O	S	0	1	0
			836	532	142	159	3			

- Molecule 3 is a protein called Cellular tumor antigen p53 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			75	45	16	12	2			
3	F	9	Total	C	N	O	S	0	0	0
			75	45	16	12	2			
3	I	9	Total	C	N	O	S	0	0	0
			75	45	16	12	2			
3	L	9	Total	C	N	O	S	0	0	0
			75	45	16	12	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	HIS	ARG	engineered mutation	UNP P04637
F	8	HIS	ARG	engineered mutation	UNP P04637
I	8	HIS	ARG	engineered mutation	UNP P04637
L	8	HIS	ARG	engineered mutation	UNP P04637

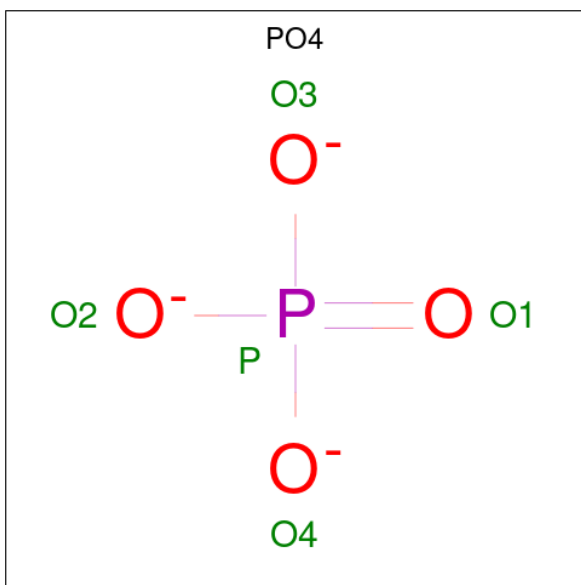
- Molecule 4 is a protein called Immunoglobulin heavy chain H2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	223	Total	C	N	O	S	0	0	0
			1673	1059	274	333	7			
4	O	223	Total	C	N	O	S	0	0	0
			1673	1059	274	333	7			
4	Q	221	Total	C	N	O	S	0	0	0
			1660	1052	272	329	7			
4	S	222	Total	C	N	O	S	0	0	0
			1664	1054	273	330	7			

- Molecule 5 is a protein called Immunoglobulin light chain H2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	214	Total	C	N	O	S	0	0	0
			1660	1042	278	335	5			
5	P	214	Total	C	N	O	S	0	0	0
			1660	1042	278	335	5			
5	R	214	Total	C	N	O	S	0	0	0
			1660	1042	278	335	5			
5	T	210	Total	C	N	O	S	0	0	0
			1629	1023	274	327	5			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	S	1	Total	O	P	0	0
			5	4	1		

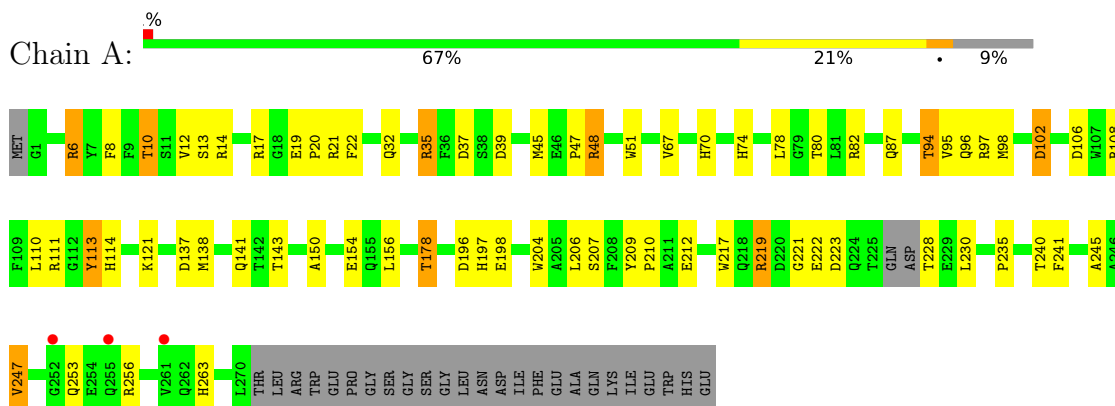
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	N	1	Total	O	0	0
			1	1		

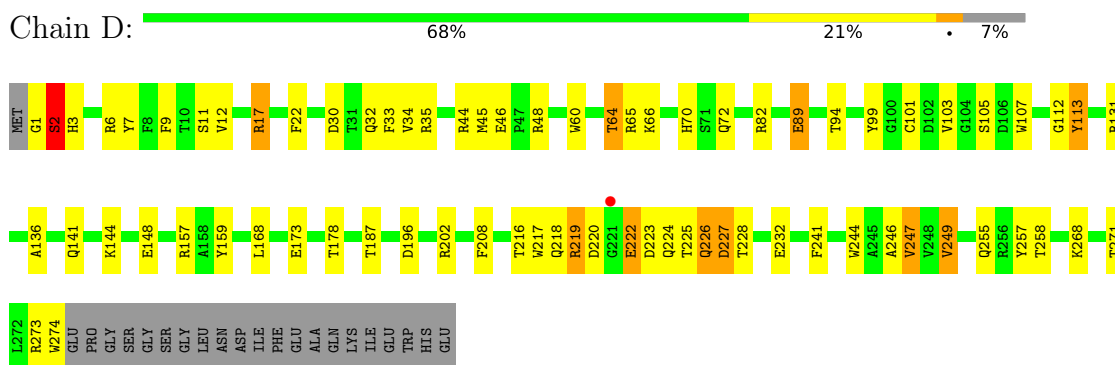
3 Residue-property plots [i](#)

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.

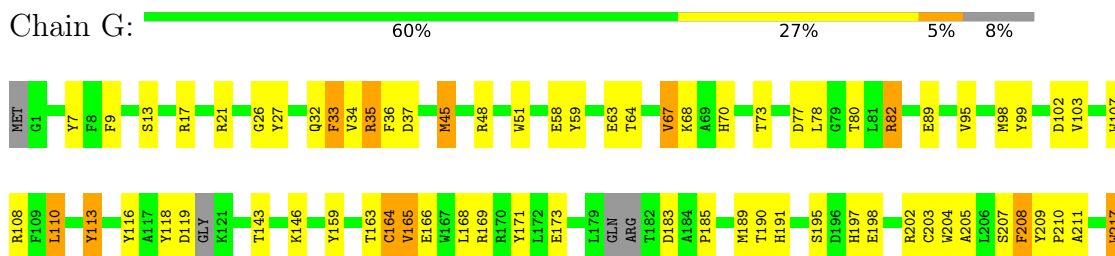
• Molecule 1: MHC class I antigen

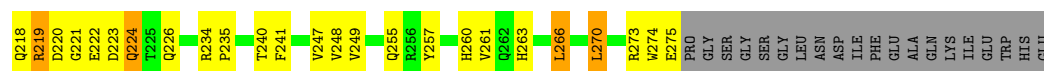


• Molecule 1: MHC class I antigen

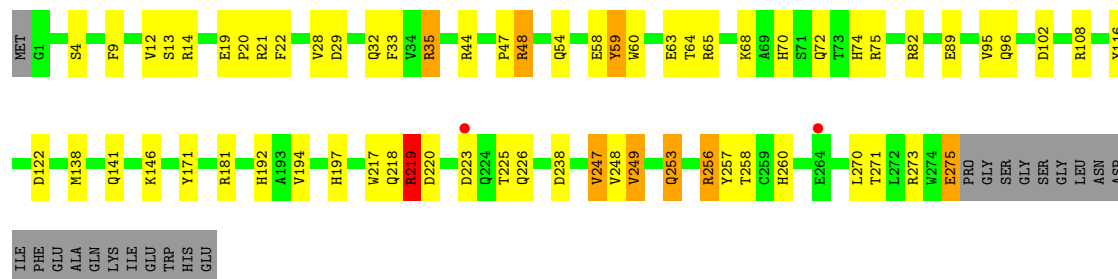


• Molecule 1: MHC class I antigen





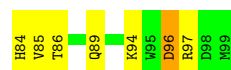
- Molecule 1: MHC class I antigen



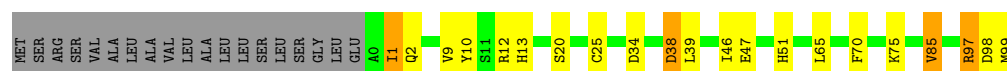
- Molecule 2: Beta-2-microglobulin



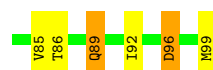
- Molecule 2: Beta-2-microglobulin



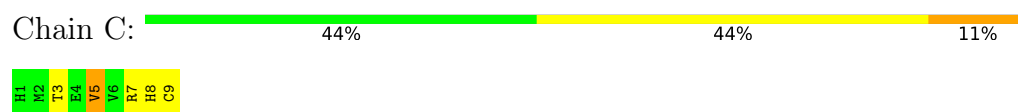
- Molecule 2: Beta-2-microglobulin



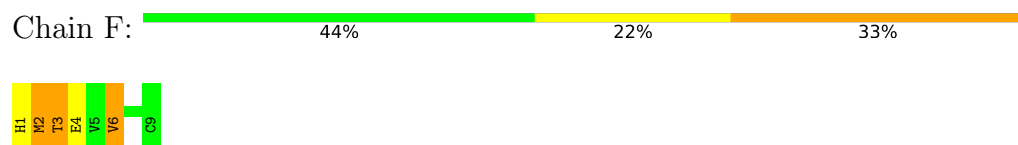
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Cellular tumor antigen p53 peptide



- Molecule 3: Cellular tumor antigen p53 peptide



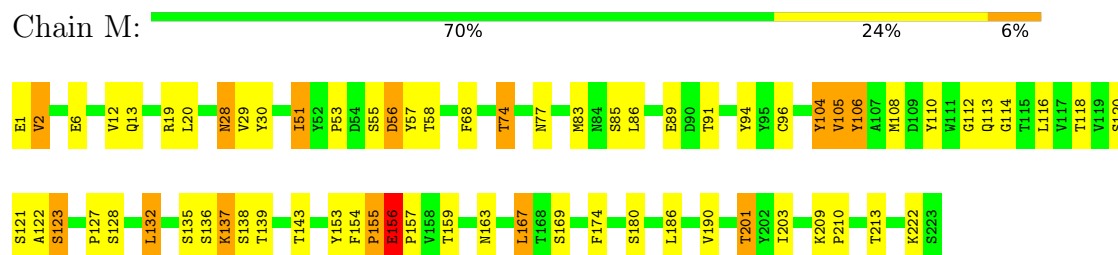
- Molecule 3: Cellular tumor antigen p53 peptide



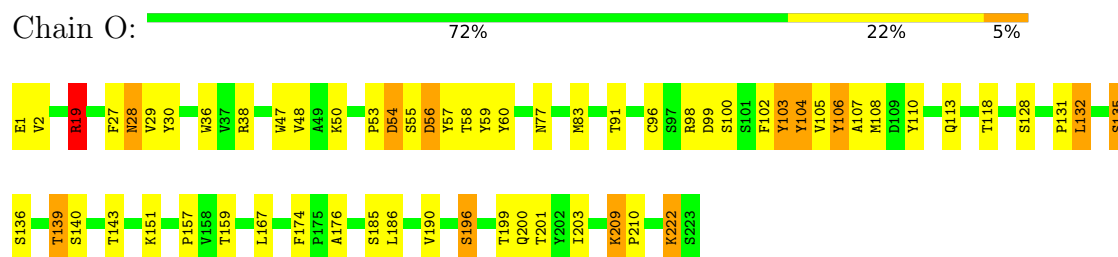
- Molecule 3: Cellular tumor antigen p53 peptide



- Molecule 4: Immunoglobulin heavy chain H2

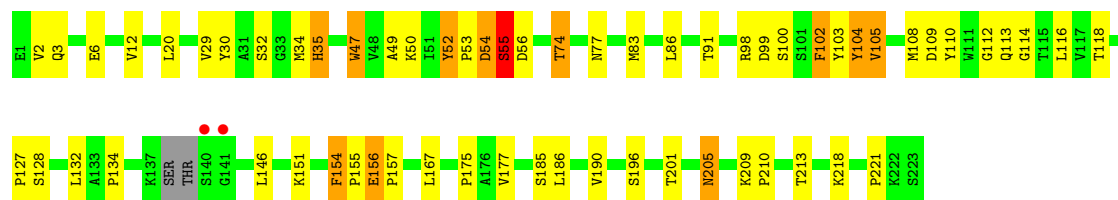


- Molecule 4: Immunoglobulin heavy chain H2



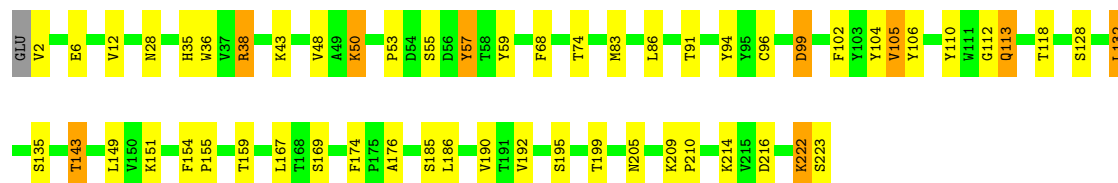
- Molecule 4: Immunoglobulin heavy chain H2





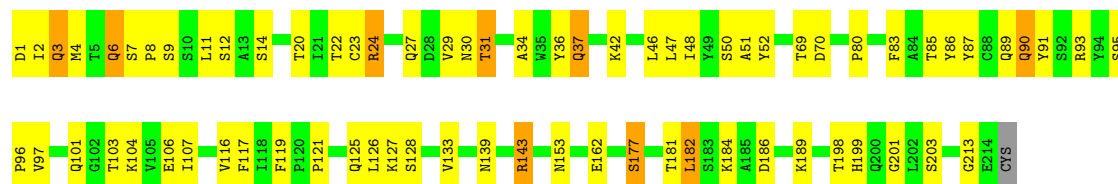
• Molecule 4: Immunoglobulin heavy chain H2

Chain S: 74% 21% .



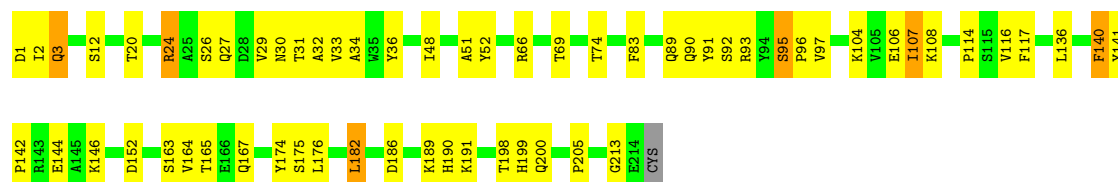
• Molecule 5: Immunoglobulin light chain H2

Chain N: 66% 29% .



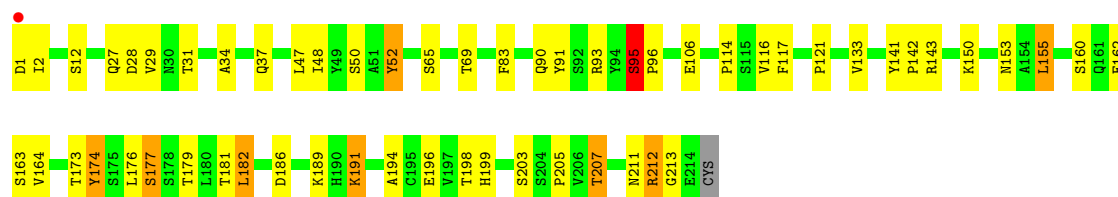
• Molecule 5: Immunoglobulin light chain H2

Chain P: 71% 26% .



• Molecule 5: Immunoglobulin light chain H2

Chain R: 73% 22% .



• Molecule 5: Immunoglobulin light chain H2

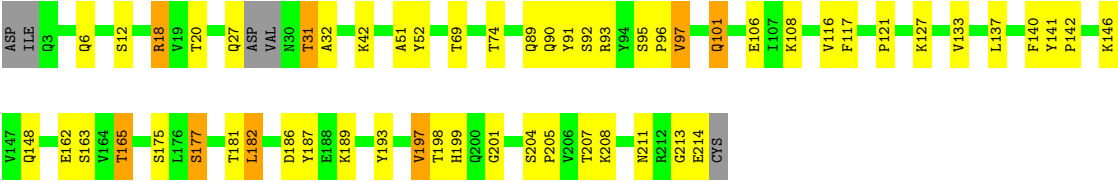
Chain T:

72%

22%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.21Å 123.69Å 136.91Å 90.00° 100.36° 90.00°	Depositor
Resolution (Å)	30.37 – 3.53 30.37 – 3.53	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.37-3.53) 95.3 (30.37-3.53)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.56Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.200 , 0.283 0.201 , 0.277	Depositor DCC
R_{free} test set	2193 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25900	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: PO4

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	0.65	0/2263	0.86	0/3069
1	D	0.68	0/2323	0.90	0/3153
1	G	0.69	0/2304	0.90	1/3126 (0.0%)
1	J	0.66	0/2330	0.85	1/3163 (0.0%)
2	B	0.67	0/859	0.89	0/1163
2	E	0.68	0/863	0.93	0/1169
2	H	0.67	0/864	0.90	0/1170
2	K	0.66	0/859	0.87	0/1163
3	C	0.90	0/76	1.21	0/101
3	F	0.63	0/76	0.98	0/101
3	I	0.89	1/76 (1.3%)	1.15	0/101
3	L	0.71	0/76	0.89	0/101
4	M	0.71	0/1716	0.99	0/2340
4	O	0.75	0/1716	0.98	2/2340 (0.1%)
4	Q	0.72	0/1702	0.97	2/2319 (0.1%)
4	S	0.73	0/1707	0.94	1/2328 (0.0%)
5	N	0.75	1/1697 (0.1%)	0.93	0/2305
5	P	0.69	0/1697	0.96	2/2305 (0.1%)
5	R	0.72	0/1697	0.93	1/2305 (0.0%)
5	T	0.68	0/1665	0.83	0/2259
All	All	0.70	2/26566 (0.0%)	0.92	10/36081 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	14	SER	CA-CB	-5.26	1.45	1.52
3	I	4	GLU	CD-OE2	5.08	1.31	1.25

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	24	ARG	CG-CD-NE	-11.48	87.68	111.80
4	O	19	ARG	CG-CD-NE	7.44	127.43	111.80
1	J	219	ARG	CB-CA-C	6.58	123.55	110.40
4	Q	102	PHE	CB-CA-C	5.97	122.35	110.40
4	O	38	ARG	NE-CZ-NH2	-5.93	117.34	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2201	0	2051	75	1
1	D	2258	0	2105	95	0
1	G	2241	0	2086	112	0
1	J	2265	0	2112	53	1
2	B	836	0	799	11	0
2	E	837	0	808	44	1
2	H	841	0	804	14	0
2	K	836	0	799	29	0
3	C	75	0	74	11	0
3	F	75	0	74	10	0
3	I	75	0	74	9	1
3	L	75	0	74	2	0
4	M	1673	0	1620	60	1
4	O	1673	0	1620	55	1
4	Q	1660	0	1607	57	1
4	S	1664	0	1611	43	0
5	N	1660	0	1612	51	0
5	P	1660	0	1612	55	0
5	R	1660	0	1612	40	0
5	T	1629	0	1580	49	1
6	S	5	0	0	0	0
7	N	1	0	0	0	0
All	All	25900	0	24734	783	4

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 15.

The worst 5 of 783 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)
4:O:100:SER:OG	4:O:105:VAL:HG13	1.18	1.34
4:Q:100:SER:HB2	4:Q:109:ASP:OD2	1.35	1.21
2:E:35:ILE:HG22	2:E:84:HIS:HD2	1.08	1.13
1:D:228:THR:HG22	1:D:247:VAL:CG1	1.80	1.10
2:E:35:ILE:HG22	2:E:84:HIS:CD2	1.88	1.09

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:OG1	4:M:57:TYR:OH[1_655]	2.07	0.13
3:I:8:HIS:CE1	4:Q:54:ASP:OD2[2_546]	2.09	0.11
1:J:72:GLN:NE2	5:T:92:SER:OG[1_455]	2.09	0.11
2:E:96:ASP:OD2	4:O:140:SER:O[1_655]	2.18	0.02

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	267/296 (90%)	257 (96%)	9 (3%)	1 (0%)	34	71
1	D	275/296 (93%)	264 (96%)	8 (3%)	3 (1%)	14	54
1	G	269/296 (91%)	245 (91%)	20 (7%)	4 (2%)	10	47
1	J	276/296 (93%)	268 (97%)	7 (2%)	1 (0%)	34	71
2	B	98/119 (82%)	95 (97%)	2 (2%)	1 (1%)	15	55
2	E	99/119 (83%)	92 (93%)	5 (5%)	2 (2%)	7	42
2	H	99/119 (83%)	95 (96%)	2 (2%)	2 (2%)	7	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	98/119 (82%)	92 (94%)	3 (3%)	3 (3%)	4	32
3	C	7/9 (78%)	4 (57%)	2 (29%)	1 (14%)	0	3
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	M	221/223 (99%)	207 (94%)	9 (4%)	5 (2%)	6	38
4	O	221/223 (99%)	206 (93%)	10 (4%)	5 (2%)	6	38
4	Q	217/223 (97%)	210 (97%)	4 (2%)	3 (1%)	11	48
4	S	220/223 (99%)	211 (96%)	8 (4%)	1 (0%)	29	68
5	N	212/215 (99%)	199 (94%)	10 (5%)	3 (1%)	11	48
5	P	212/215 (99%)	200 (94%)	10 (5%)	2 (1%)	17	58
5	R	212/215 (99%)	200 (94%)	10 (5%)	2 (1%)	17	58
5	T	206/215 (96%)	196 (95%)	10 (5%)	0	100	100
All	All	3230/3448 (94%)	3058 (95%)	133 (4%)	39 (1%)	13	52

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	SER
1	D	227	ASP
2	H	1	ILE
2	K	47	GLU
2	K	48	LYS

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	227/248 (92%)	210 (92%)	17 (8%)	13	45
1	D	233/248 (94%)	213 (91%)	20 (9%)	10	40
1	G	232/248 (94%)	212 (91%)	20 (9%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	234/248 (94%)	211 (90%)	23 (10%)	8	35
2	B	95/109 (87%)	86 (90%)	9 (10%)	8	36
2	E	95/109 (87%)	84 (88%)	11 (12%)	5	29
2	H	95/109 (87%)	86 (90%)	9 (10%)	8	36
2	K	95/109 (87%)	80 (84%)	15 (16%)	2	16
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	30
3	F	9/9 (100%)	6 (67%)	3 (33%)	0	2
3	I	9/9 (100%)	7 (78%)	2 (22%)	1	5
3	L	9/9 (100%)	6 (67%)	3 (33%)	0	2
4	M	186/186 (100%)	161 (87%)	25 (13%)	4	23
4	O	186/186 (100%)	169 (91%)	17 (9%)	9	38
4	Q	184/186 (99%)	164 (89%)	20 (11%)	6	31
4	S	185/186 (100%)	166 (90%)	19 (10%)	7	33
5	N	189/190 (100%)	166 (88%)	23 (12%)	5	26
5	P	189/190 (100%)	177 (94%)	12 (6%)	18	52
5	R	189/190 (100%)	172 (91%)	17 (9%)	9	38
5	T	185/190 (97%)	167 (90%)	18 (10%)	8	35
All	All	2835/2968 (96%)	2551 (90%)	284 (10%)	7	34

5 of 284 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	28	ASP
5	R	95	SER
4	S	143	THR
1	J	54	GLN
1	J	29	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
5	P	3	GLN
5	R	3	GLN
5	P	30	ASN
4	Q	3	GLN

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Mol	Chain	Res	Type
4	S	113	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PO4	S	301	-	4,4,4	0.74	0	6,6,6	0.43	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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	268/296 (90%)	-0.31	3 (1%) 80 69	30, 69, 132, 186	0
1	D	274/296 (92%)	-0.44	1 (0%) 92 87	34, 65, 121, 160	0
1	G	272/296 (91%)	-0.47	0 100 100	28, 65, 110, 149	0
1	J	275/296 (92%)	-0.22	2 (0%) 87 79	34, 88, 134, 180	0
2	B	99/119 (83%)	-0.45	0 100 100	37, 68, 114, 132	0
2	E	100/119 (84%)	-0.54	0 100 100	34, 62, 93, 109	0
2	H	100/119 (84%)	-0.49	0 100 100	33, 61, 94, 104	0
2	K	99/119 (83%)	-0.34	0 100 100	46, 84, 131, 144	0
3	C	9/9 (100%)	-0.54	0 100 100	43, 57, 72, 78	0
3	F	9/9 (100%)	-0.77	0 100 100	37, 48, 56, 69	0
3	I	9/9 (100%)	-0.69	0 100 100	34, 46, 68, 77	0
3	L	9/9 (100%)	-0.59	0 100 100	55, 59, 74, 76	0
4	M	223/223 (100%)	-0.67	0 100 100	26, 50, 88, 191	0
4	O	223/223 (100%)	-0.63	0 100 100	29, 53, 83, 200	0
4	Q	221/223 (99%)	-0.60	2 (0%) 84 73	35, 56, 91, 141	0
4	S	222/223 (99%)	-0.49	0 100 100	38, 64, 96, 161	0
5	N	214/215 (99%)	-0.60	0 100 100	30, 55, 88, 111	0
5	P	214/215 (99%)	-0.68	0 100 100	29, 57, 88, 113	0
5	R	214/215 (99%)	-0.58	1 (0%) 91 84	33, 57, 88, 128	0
5	T	210/215 (97%)	-0.42	0 100 100	39, 74, 102, 148	0
All	All	3264/3448 (94%)	-0.49	9 (0%) 94 89	26, 63, 112, 200	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	223	ASP	3.1
1	A	255	GLN	3.0
1	J	264	GLU	2.8
4	Q	140	SER	2.6
1	D	221	GLY	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 [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(\AA^2)	Q<0.9
6	PO4	S	301	5/5	0.60	0.34	155,157,164,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.