wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 03:23 pm BST

PDB ID	:	3HAE
Title	:	Rational development of high-affinity T-cell receptor-like antibodies
Authors	:	Stewart-Jones, G.; Wadle, A.; Hombach, A.; Shenderov, E.; Held, G.; Fischer, E.
Deposited on	:	2009-05-01
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

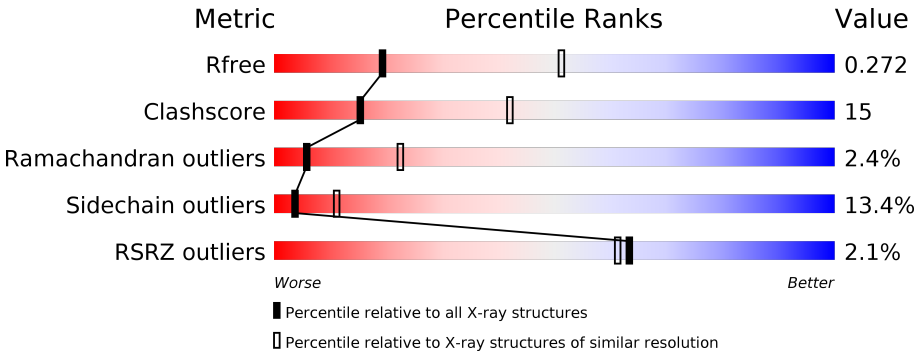
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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 <=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	276	2% 70% 25% 6%
1	D	276	% 68% 26% 5%
1	J	276	2% 72% 24% .
1	P	276	2% 66% 30% 5%
2	B	100	% 59% 36% 5%
2	E	100	% 65% 28% 6% .

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Mol	Chain	Length	Quality of chain
2	K	100	2% 60% 36%
2	Q	100	3% 62% 32% 6%
3	C	9	33% 44% 33% 22%
3	F	9	33% 33% 56% 11%
3	M	9	78% 11% 11%
3	R	9	44% 44% 11%
4	G	212	60% 32% 7%
4	L	212	67% 27% 5%
4	N	212	3% 59% 31% 9%
4	S	212	% 61% 34%
5	H	220	2% 67% 25% 5%
5	I	220	3% 65% 30% 5%
5	O	220	5% 64% 30% 6%
5	T	220	5% 62% 29% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25472 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, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	D	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	J	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	P	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	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	0	0	0
			836	533	141	158	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	K	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	Q	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769
E	0	MET	-	EXPRESSION TAG	UNP P61769
K	0	MET	-	EXPRESSION TAG	UNP P61769
Q	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called NYESO-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	M	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	R	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			

- Molecule 4 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	G	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	N	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	S	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			

- Molecule 5 is a protein called Antibody heavy chain.

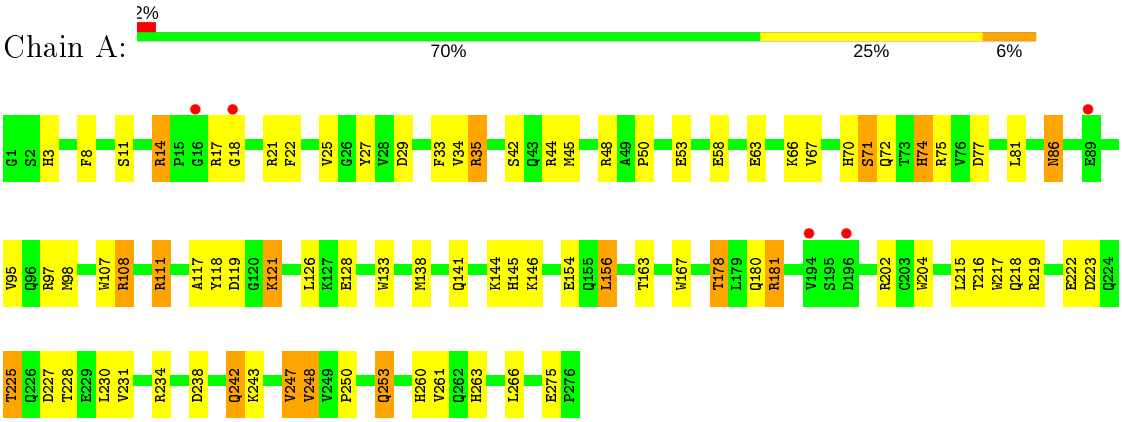
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	I	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	O	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	T	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			

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.

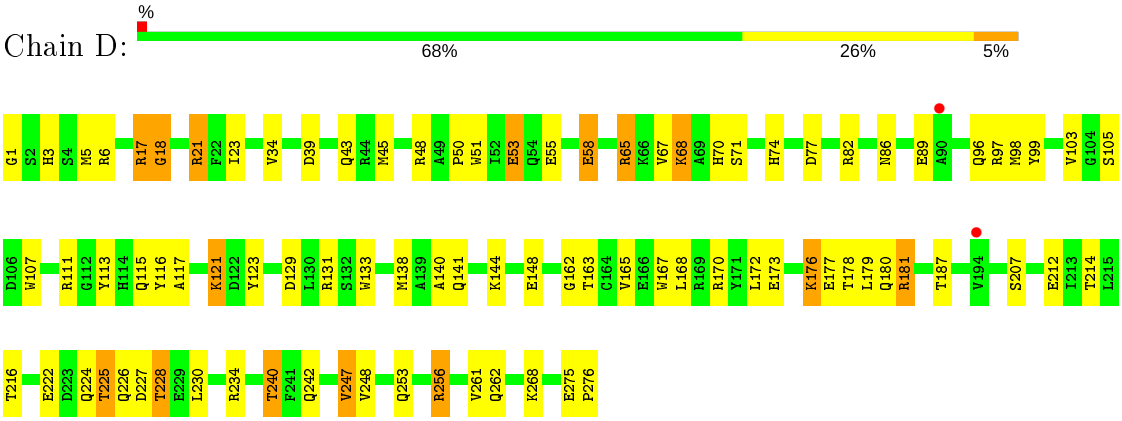
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



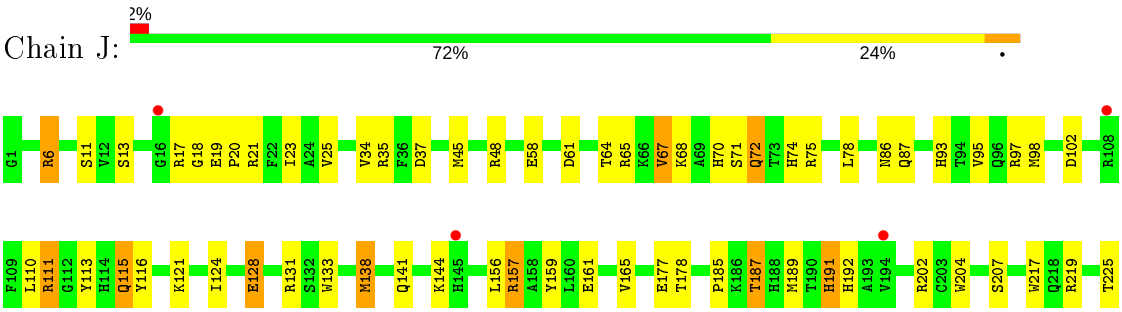
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

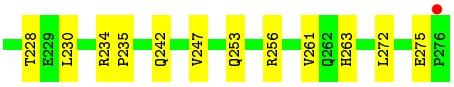
Chain D:



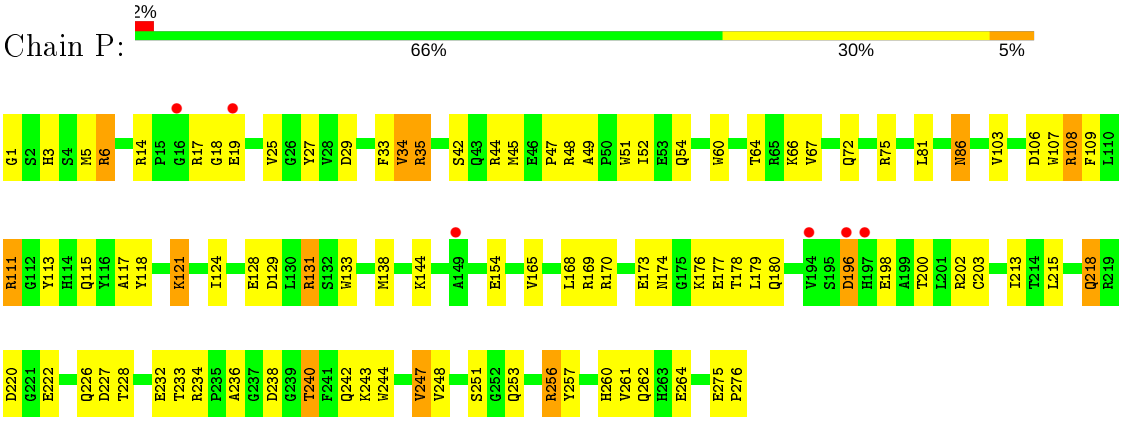
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain J:

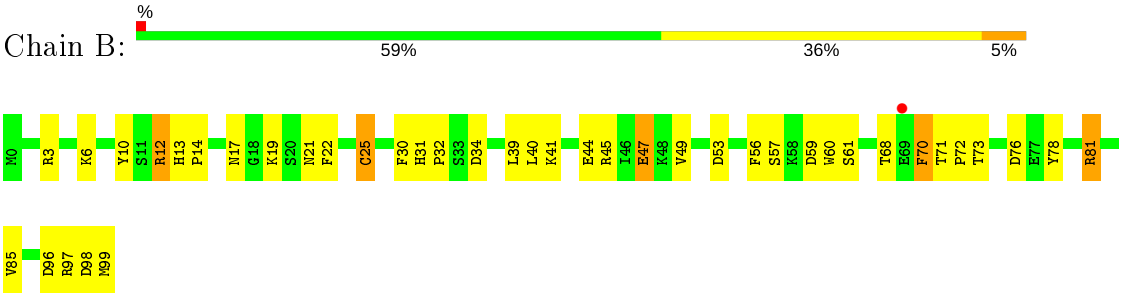




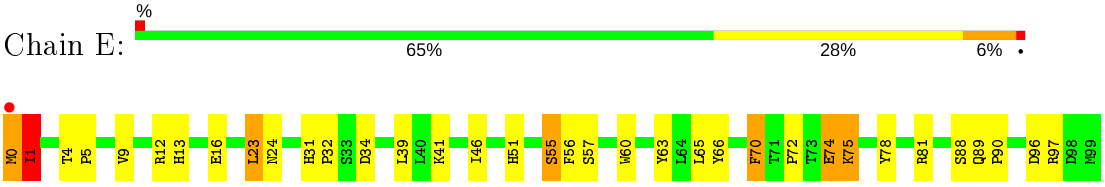
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



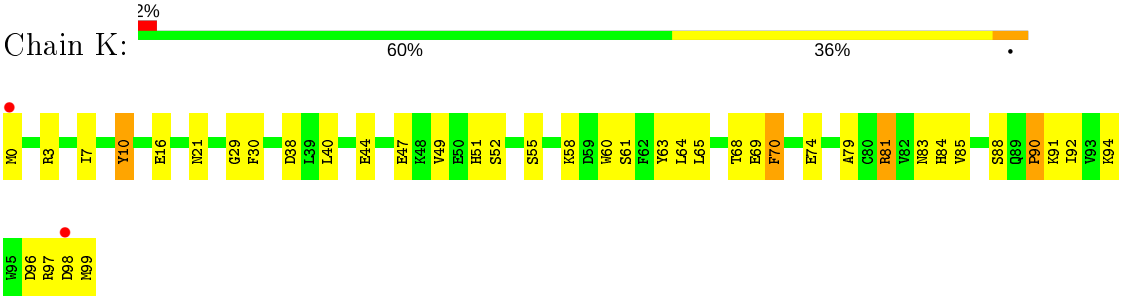
• Molecule 2: Beta-2-microglobulin



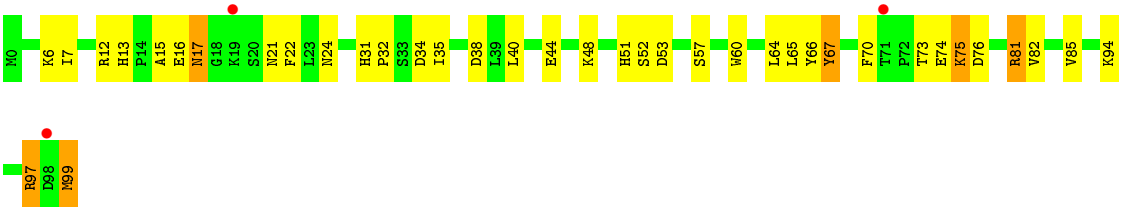
• Molecule 2: Beta-2-microglobulin



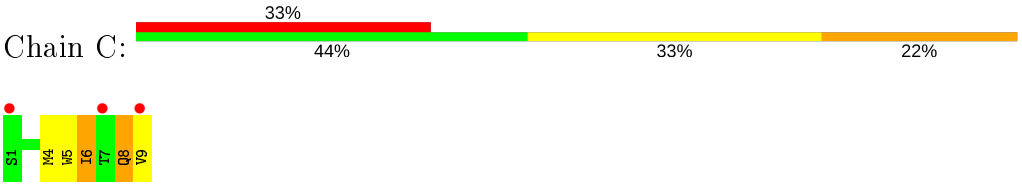
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 3: NYESO-1 peptide



• Molecule 3: NYESO-1 peptide

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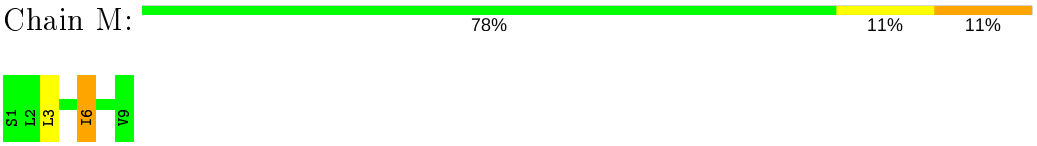
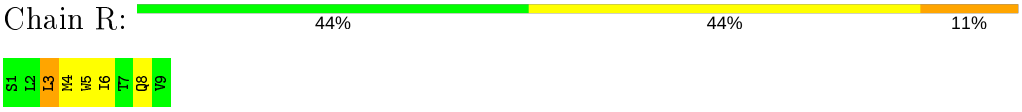
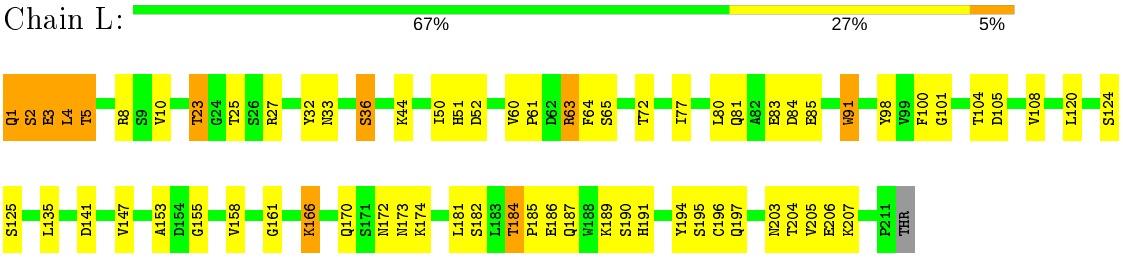


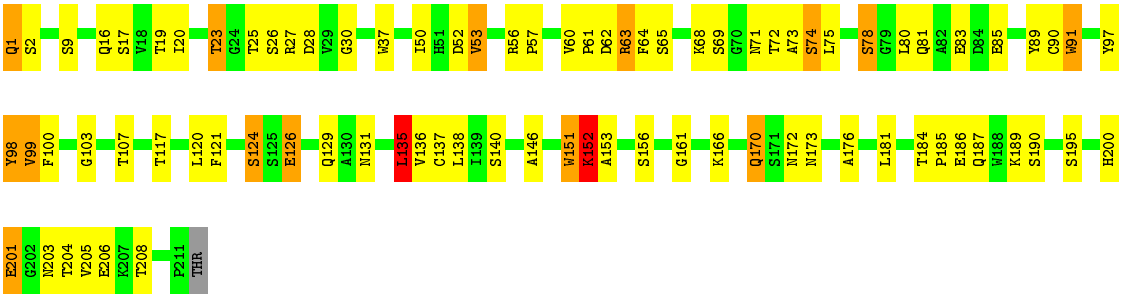
• Molecule 3: NYESO-1 peptide



• Molecule 4: Antibody light chain



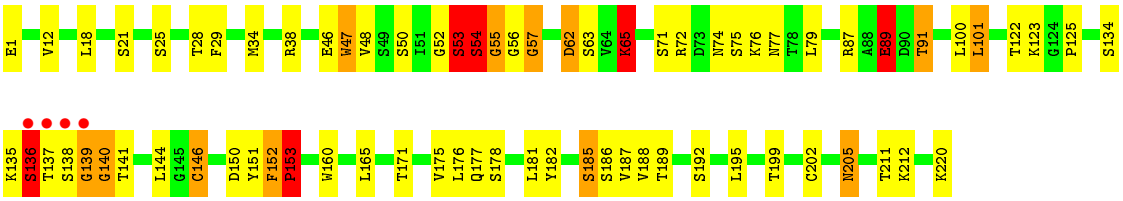
• Molecule 4: Antibody light chain



• Molecule 4: Antibody light chain

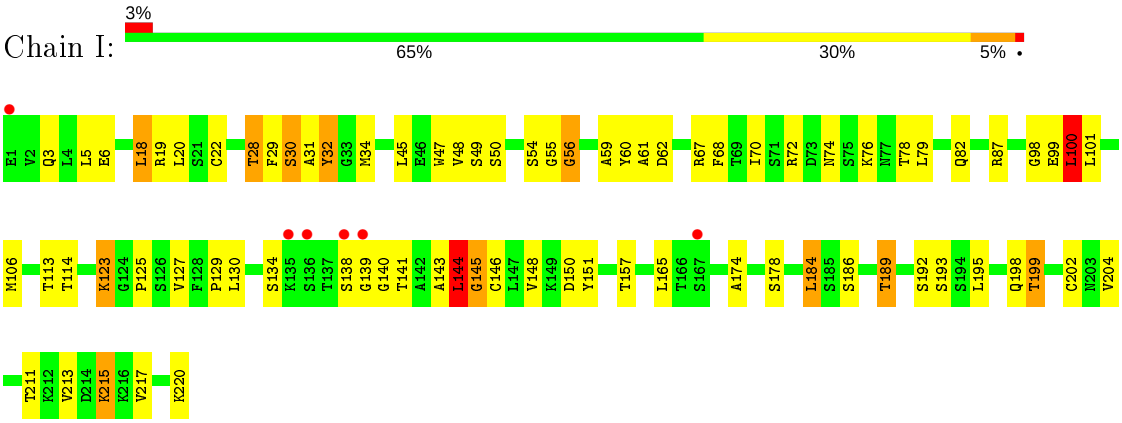
• Molecule 4: Antibody light chain

• Molecule 5: Antibody heavy chain



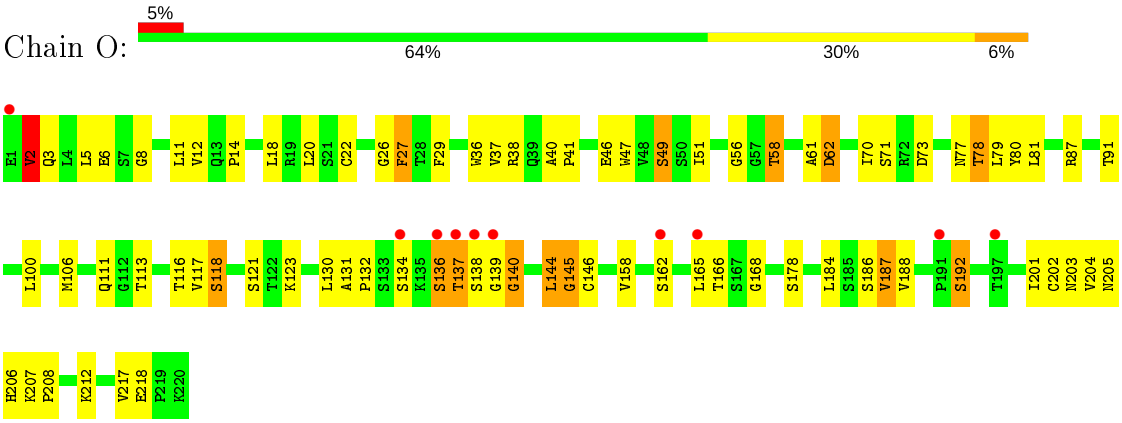
• Molecule 5: Antibody heavy chain

Chain I:



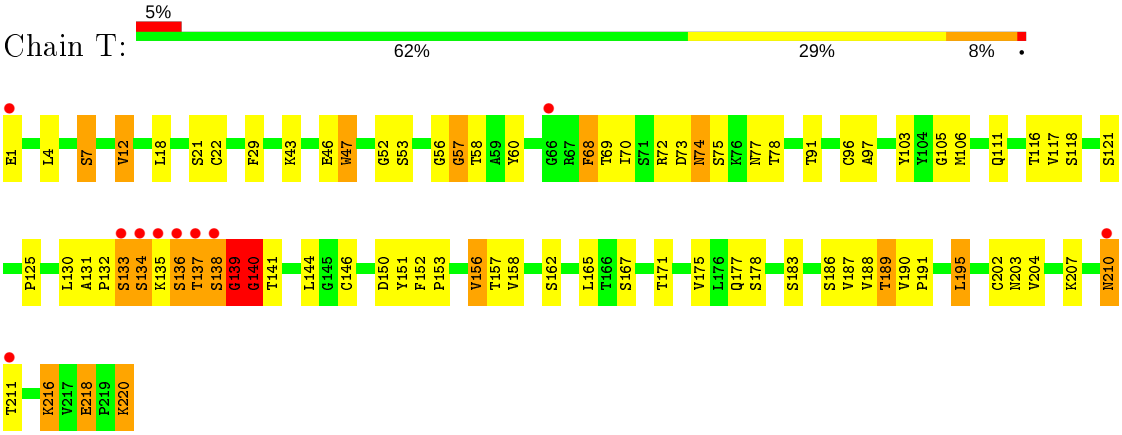
- Molecule 5: Antibody heavy chain

Chain O:



- Molecule 5: Antibody heavy chain

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.79Å 105.60Å 256.45Å 90.00° 92.26° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 29.74 – 2.86	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-2.90) 96.6 (29.74-2.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.283 0.194 , 0.272	Depositor DCC
R_{free} test set	4225 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 20.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25472	wwPDB-VP
Average B, all atoms (Å^2)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.91	1/2319 (0.0%)	0.92	2/3149 (0.1%)
1	D	0.92	1/2319 (0.0%)	0.91	2/3149 (0.1%)
1	J	0.79	2/2319 (0.1%)	0.84	1/3149 (0.0%)
1	P	0.94	5/2319 (0.2%)	0.89	2/3149 (0.1%)
2	B	0.85	0/859	0.93	2/1162 (0.2%)
2	E	0.87	0/859	0.91	0/1162
2	K	0.89	0/859	0.90	1/1162 (0.1%)
2	Q	0.94	0/859	0.85	0/1162
3	C	0.80	0/76	1.05	0/103
3	F	0.83	0/76	1.14	0/103
3	M	0.68	0/76	1.11	0/103
3	R	0.79	0/76	1.03	1/103 (1.0%)
4	G	0.83	1/1638 (0.1%)	0.91	3/2237 (0.1%)
4	L	0.86	0/1638	0.90	0/2237
4	N	0.77	0/1638	0.84	1/2237 (0.0%)
4	S	0.85	0/1638	0.84	2/2237 (0.1%)
5	H	0.85	1/1646 (0.1%)	0.96	6/2239 (0.3%)
5	I	0.92	0/1646	1.01	4/2239 (0.2%)
5	O	0.73	0/1646	0.83	1/2239 (0.0%)
5	T	0.86	1/1646 (0.1%)	0.90	4/2239 (0.2%)
All	All	0.86	12/26152 (0.0%)	0.90	32/35560 (0.1%)

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	1
4	G	0	1
4	L	0	2
4	N	0	2
5	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	T	0	1
All	All	0	10

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	19	GLU	CG-CD	7.12	1.62	1.51
1	P	198	GLU	CG-CD	7.08	1.62	1.51
1	A	154	GLU	CG-CD	6.59	1.61	1.51
5	T	96	CYS	CB-SG	-6.22	1.71	1.82
1	J	177	GLU	CG-CD	5.94	1.60	1.51

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	53	SER	N-CA-C	6.88	129.57	111.00
1	A	202	ARG	NE-CZ-NH2	-6.72	116.94	120.30
4	G	91	TRP	CA-CB-CG	6.51	126.08	113.70
4	G	135	LEU	CA-CB-CG	6.38	129.99	115.30
5	H	53	SER	C-N-CA	6.19	137.18	121.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Peptide
4	G	9	SER	Peptide
4	L	1	GLN	Peptide
4	L	2	SER	Peptide
4	N	2	SER	Peptide

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	2253	0	2103	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2253	0	2103	71	0
1	J	2253	0	2103	56	0
1	P	2253	0	2103	66	0
2	B	836	0	803	28	0
2	E	836	0	803	28	0
2	K	836	0	803	27	0
2	Q	836	0	803	26	0
3	C	75	0	83	15	0
3	F	75	0	83	12	0
3	M	75	0	83	3	0
3	R	75	0	83	3	0
4	G	1595	0	1537	61	0
4	L	1595	0	1537	56	0
4	N	1595	0	1537	54	0
4	S	1595	0	1537	54	0
5	H	1609	0	1577	58	0
5	I	1609	0	1577	51	0
5	O	1609	0	1577	51	0
5	T	1609	0	1577	55	0
All	All	25472	0	24412	744	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 15.

The worst 5 of 744 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:N:11:SER:HB3	4:N:107:THR:HG22	1.31	1.11
1:P:256:ARG:HH11	1:P:256:ARG:HG3	1.17	1.06
1:J:138:MET:HE2	1:J:138:MET:HA	1.39	1.03
1:J:6:ARG:HH22	1:J:113:TYR:HE1	1.08	1.00
1:P:111:ARG:HH12	1:P:128:GLU:HB3	1.26	0.99

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	274/276 (99%)	261 (95%)	10 (4%)	3 (1%)	14 42
1	D	274/276 (99%)	258 (94%)	15 (6%)	1 (0%)	34 66
1	J	274/276 (99%)	260 (95%)	12 (4%)	2 (1%)	22 54
1	P	274/276 (99%)	260 (95%)	11 (4%)	3 (1%)	14 42
2	B	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15 45
2	E	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	7 27
2	K	98/100 (98%)	90 (92%)	8 (8%)	0	100 100
2	Q	98/100 (98%)	86 (88%)	9 (9%)	3 (3%)	4 16
3	C	7/9 (78%)	7 (100%)	0	0	100 100
3	F	7/9 (78%)	7 (100%)	0	0	100 100
3	M	7/9 (78%)	7 (100%)	0	0	100 100
3	R	7/9 (78%)	7 (100%)	0	0	100 100
4	G	209/212 (99%)	182 (87%)	23 (11%)	4 (2%)	8 28
4	L	209/212 (99%)	186 (89%)	17 (8%)	6 (3%)	4 18
4	N	209/212 (99%)	183 (88%)	19 (9%)	7 (3%)	4 15
4	S	209/212 (99%)	186 (89%)	20 (10%)	3 (1%)	11 36
5	H	218/220 (99%)	197 (90%)	10 (5%)	11 (5%)	2 7
5	I	218/220 (99%)	189 (87%)	21 (10%)	8 (4%)	3 13
5	O	218/220 (99%)	189 (87%)	19 (9%)	10 (5%)	2 9
5	T	218/220 (99%)	188 (86%)	18 (8%)	12 (6%)	2 5
All	All	3224/3268 (99%)	2917 (90%)	231 (7%)	76 (2%)	6 22

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY

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Mol	Chain	Res	Type
1	D	18	GLY
1	J	18	GLY
1	P	18	GLY
4	L	2	SER

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	232/232 (100%)	202 (87%)	30 (13%)	4 13
1	D	232/232 (100%)	207 (89%)	25 (11%)	6 20
1	J	232/232 (100%)	205 (88%)	27 (12%)	5 16
1	P	232/232 (100%)	205 (88%)	27 (12%)	5 16
2	B	95/95 (100%)	83 (87%)	12 (13%)	4 13
2	E	95/95 (100%)	84 (88%)	11 (12%)	5 16
2	K	95/95 (100%)	83 (87%)	12 (13%)	4 13
2	Q	95/95 (100%)	82 (86%)	13 (14%)	3 11
3	C	9/9 (100%)	7 (78%)	2 (22%)	1 3
3	F	9/9 (100%)	8 (89%)	1 (11%)	6 19
3	M	9/9 (100%)	8 (89%)	1 (11%)	6 19
3	R	9/9 (100%)	7 (78%)	2 (22%)	1 3
4	G	178/179 (99%)	148 (83%)	30 (17%)	2 6
4	L	178/179 (99%)	159 (89%)	19 (11%)	6 20
4	N	178/179 (99%)	150 (84%)	28 (16%)	2 8
4	S	178/179 (99%)	155 (87%)	23 (13%)	4 13
5	H	178/178 (100%)	152 (85%)	26 (15%)	3 9
5	I	178/178 (100%)	151 (85%)	27 (15%)	3 8
5	O	178/178 (100%)	154 (86%)	24 (14%)	4 11
5	T	178/178 (100%)	148 (83%)	30 (17%)	2 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2768/2772 (100%)	2398 (87%)	370 (13%)	4 11

5 of 370 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	44	LYS
4	G	203	ASN
5	T	7	SER
4	L	158	VAL
4	G	53	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	174	ASN
2	Q	51	HIS
5	O	77	ASN
1	P	180	GLN
1	P	253	GLN

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

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

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, 95^{th} 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	276/276 (100%)	0.11	5 (1%)	68	67	2, 2, 2, 2	0
1	D	276/276 (100%)	0.12	2 (0%)	87	87	2, 2, 2, 2	0
1	J	276/276 (100%)	0.20	5 (1%)	68	67	2, 2, 2, 2	0
1	P	276/276 (100%)	0.06	6 (2%)	62	59	2, 2, 2, 2	0
2	B	100/100 (100%)	0.19	1 (1%)	82	82	2, 2, 2, 2	0
2	E	100/100 (100%)	0.17	1 (1%)	82	82	2, 2, 2, 2	0
2	K	100/100 (100%)	0.06	2 (2%)	65	63	2, 2, 2, 2	0
2	Q	100/100 (100%)	-0.01	3 (3%)	50	45	2, 2, 2, 2	0
3	C	9/9 (100%)	2.03	3 (33%)	0	0	2, 2, 2, 2	0
3	F	9/9 (100%)	1.62	3 (33%)	0	0	2, 2, 2, 2	0
3	M	9/9 (100%)	1.00	0	100	100	2, 2, 2, 2	0
3	R	9/9 (100%)	-0.54	0	100	100	2, 2, 2, 2	0
4	G	211/212 (99%)	0.15	0	100	100	2, 2, 2, 2	0
4	L	211/212 (99%)	0.00	0	100	100	2, 2, 2, 2	0
4	N	211/212 (99%)	0.33	7 (3%)	46	41	2, 2, 2, 2	0
4	S	211/212 (99%)	-0.20	2 (0%)	84	84	2, 2, 2, 2	0
5	H	220/220 (100%)	0.11	4 (1%)	68	67	2, 2, 2, 2	0
5	I	220/220 (100%)	0.23	6 (2%)	54	50	2, 2, 2, 2	0
5	O	220/220 (100%)	0.36	10 (4%)	33	29	2, 2, 2, 2	0
5	T	220/220 (100%)	-0.11	10 (4%)	33	29	2, 2, 2, 2	0
All	All	3264/3268 (99%)	0.12	70 (2%)	63	61	2, 2, 2, 2	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	136	SER	5.8
5	O	136	SER	4.2
5	O	165	LEU	3.8
5	O	137	THR	3.8
4	N	153	ALA	3.6

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.