wwPDB X-ray Structure Validation Summary Report (i)

Aug 17, 2023 – 04:09 PM JST

PDB ID	:	8IVW
Title	:	Crystal structure of NRP2 in complex with aNRP2-10 Fab fragment
Authors	:	Geng, Y.; Zhai, L.
Deposited on	:	2023-03-29
Resolution	:	3.21 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

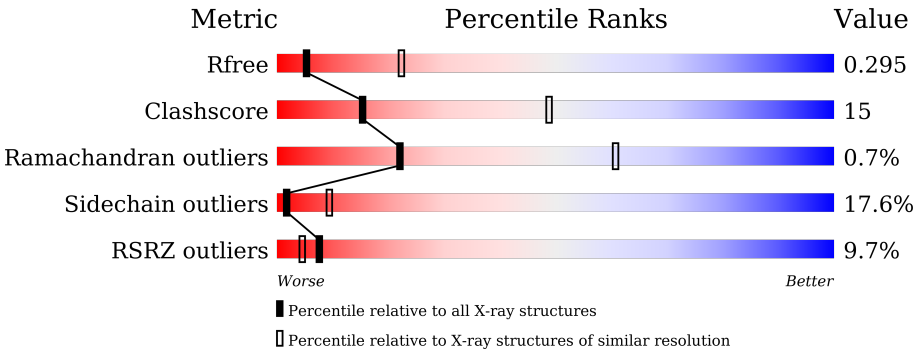
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	583	6% 51% 19% · 27%
1	D	583	9% 51% 17% · 28%
1	G	583	14% 46% 20% · 31%
1	J	583	12% 51% 17% 5% 27%
2	B	228	4% 63% 26% 7% ·
2	E	228	2% 63% 25% 8% ·

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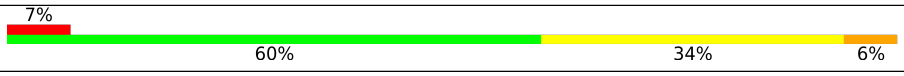
Mol	Chain	Length	Quality of chain
2	H	228	
2	K	228	
3	C	215	
3	F	215	
3	I	215	
3	L	215	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26621 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 Neuropilin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3412	2169	594	632	17			
1	D	420	Total	C	N	O	S	0	0	0
			3337	2122	575	623	17			
1	G	402	Total	C	N	O	S	0	0	0
			3202	2030	557	599	16			
1	J	427	Total	C	N	O	S	0	0	0
			3410	2166	591	636	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	-	expression tag	UNP O60462
A	14	HIS	-	expression tag	UNP O60462
A	15	HIS	-	expression tag	UNP O60462
A	16	HIS	-	expression tag	UNP O60462
A	17	HIS	-	expression tag	UNP O60462
A	18	HIS	-	expression tag	UNP O60462
A	19	GLU	-	expression tag	UNP O60462
A	20	ASN	-	expression tag	UNP O60462
A	21	LEU	-	expression tag	UNP O60462
A	22	TYR	-	expression tag	UNP O60462
A	23	PHE	-	expression tag	UNP O60462
A	24	GLN	-	expression tag	UNP O60462
D	13	HIS	-	expression tag	UNP O60462
D	14	HIS	-	expression tag	UNP O60462
D	15	HIS	-	expression tag	UNP O60462
D	16	HIS	-	expression tag	UNP O60462
D	17	HIS	-	expression tag	UNP O60462
D	18	HIS	-	expression tag	UNP O60462
D	19	GLU	-	expression tag	UNP O60462
D	20	ASN	-	expression tag	UNP O60462
D	21	LEU	-	expression tag	UNP O60462

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	TYR	-	expression tag	UNP O60462
D	23	PHE	-	expression tag	UNP O60462
D	24	GLN	-	expression tag	UNP O60462
G	13	HIS	-	expression tag	UNP O60462
G	14	HIS	-	expression tag	UNP O60462
G	15	HIS	-	expression tag	UNP O60462
G	16	HIS	-	expression tag	UNP O60462
G	17	HIS	-	expression tag	UNP O60462
G	18	HIS	-	expression tag	UNP O60462
G	19	GLU	-	expression tag	UNP O60462
G	20	ASN	-	expression tag	UNP O60462
G	21	LEU	-	expression tag	UNP O60462
G	22	TYR	-	expression tag	UNP O60462
G	23	PHE	-	expression tag	UNP O60462
G	24	GLN	-	expression tag	UNP O60462
J	13	HIS	-	expression tag	UNP O60462
J	14	HIS	-	expression tag	UNP O60462
J	15	HIS	-	expression tag	UNP O60462
J	16	HIS	-	expression tag	UNP O60462
J	17	HIS	-	expression tag	UNP O60462
J	18	HIS	-	expression tag	UNP O60462
J	19	GLU	-	expression tag	UNP O60462
J	20	ASN	-	expression tag	UNP O60462
J	21	LEU	-	expression tag	UNP O60462
J	22	TYR	-	expression tag	UNP O60462
J	23	PHE	-	expression tag	UNP O60462
J	24	GLN	-	expression tag	UNP O60462

- Molecule 2 is a protein called Heavy chian of antibody 10V8 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1664	1053	273	331	7			
2	E	220	Total	C	N	O	S	0	0	0
			1668	1055	274	332	7			
2	H	220	Total	C	N	O	S	0	0	0
			1668	1055	274	332	7			
2	K	220	Total	C	N	O	S	0	0	0
			1668	1055	274	332	7			

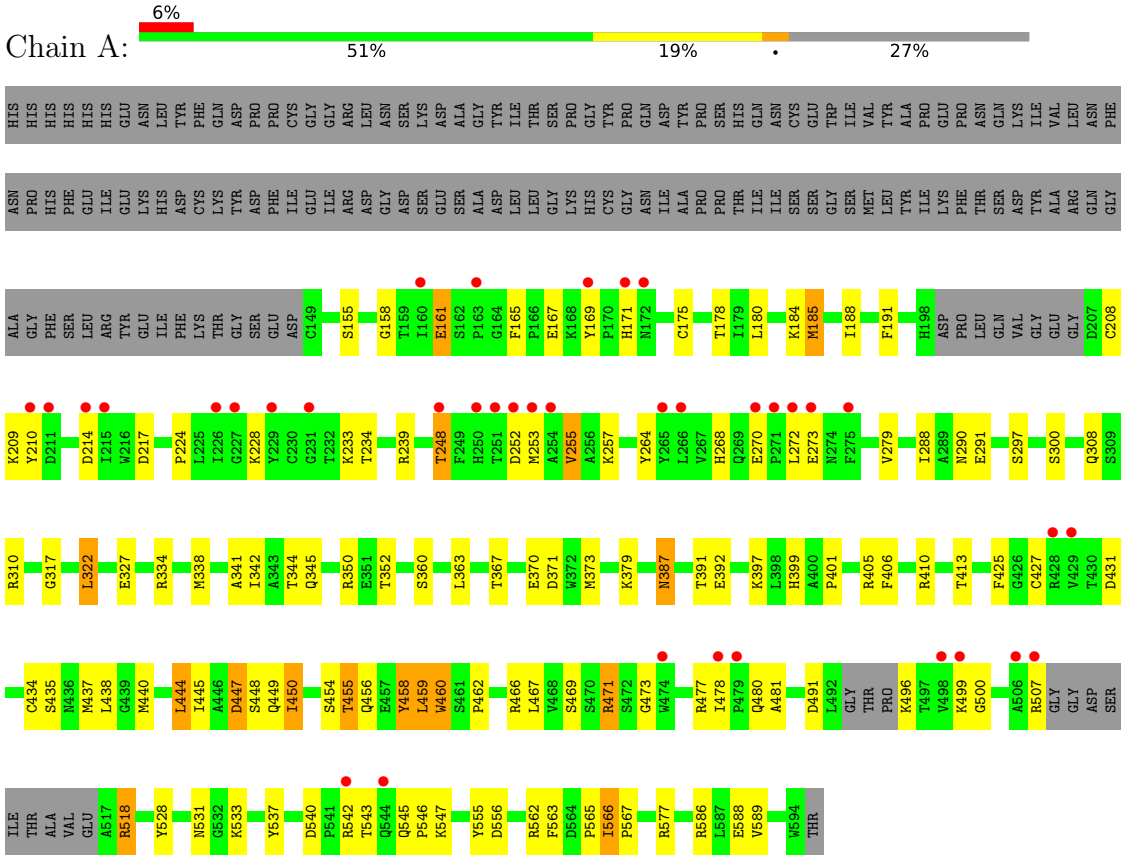
- Molecule 3 is a protein called Light chain of antibody 10V8 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1648	1029	277	336	6			
3	F	215	Total	C	N	O	S	0	0	0
			1648	1029	277	336	6			
3	I	215	Total	C	N	O	S	0	0	0
			1648	1029	277	336	6			
3	L	215	Total	C	N	O	S	0	0	0
			1648	1029	277	336	6			

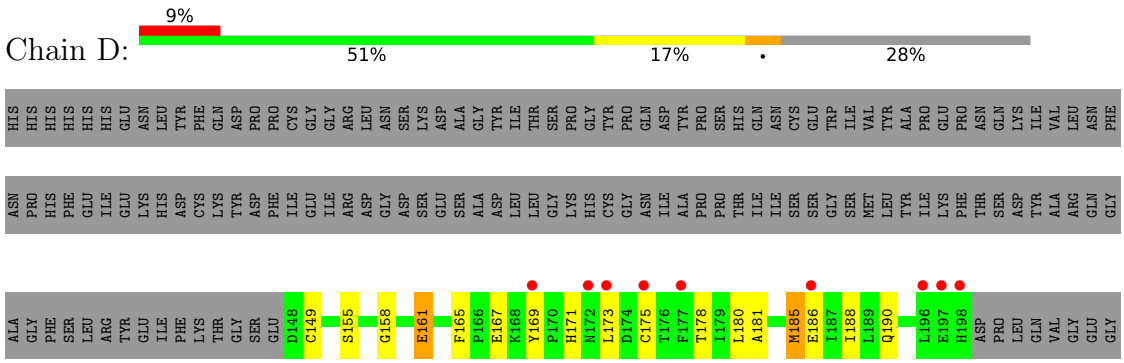
3 Residue-property plots (i)

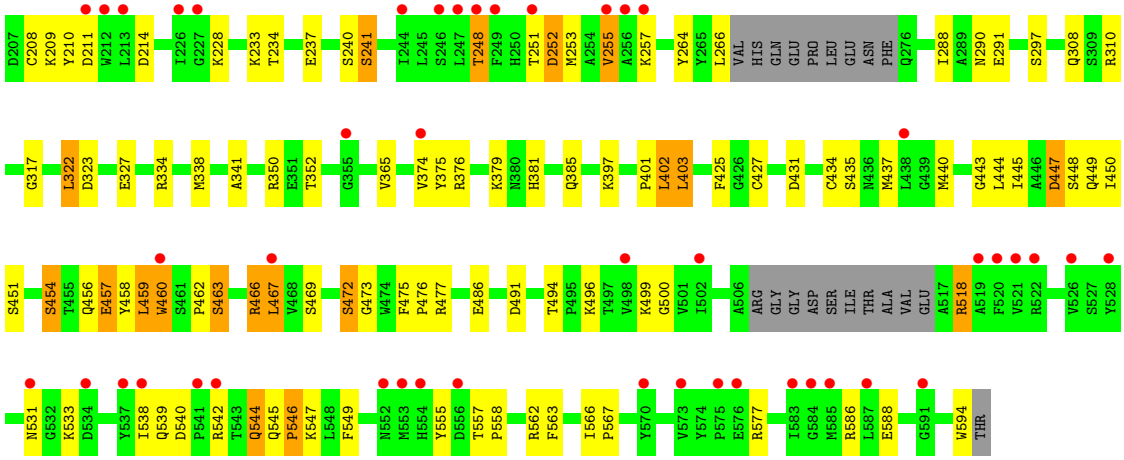
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neuropilin-2



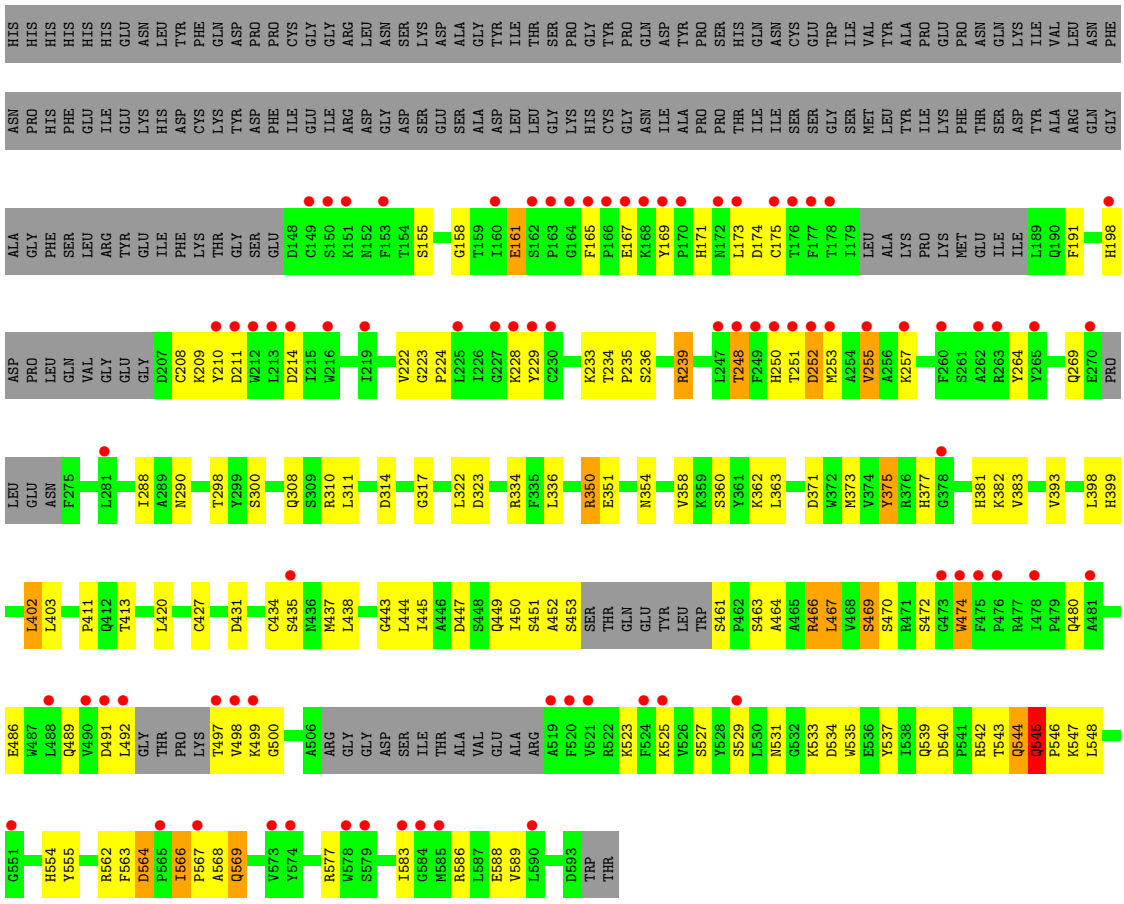
• Molecule 1: Neuropilin-2





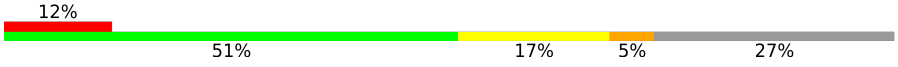
• Molecule 1: Neuropilin-2

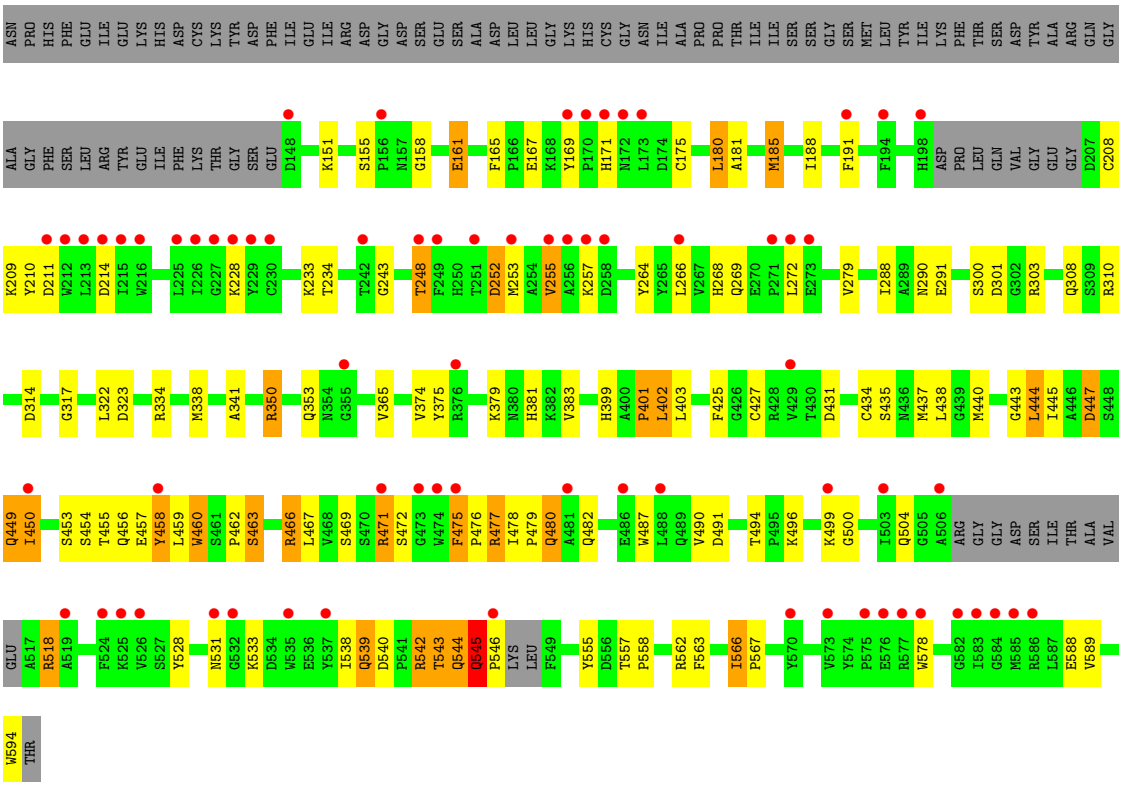
Chain G:



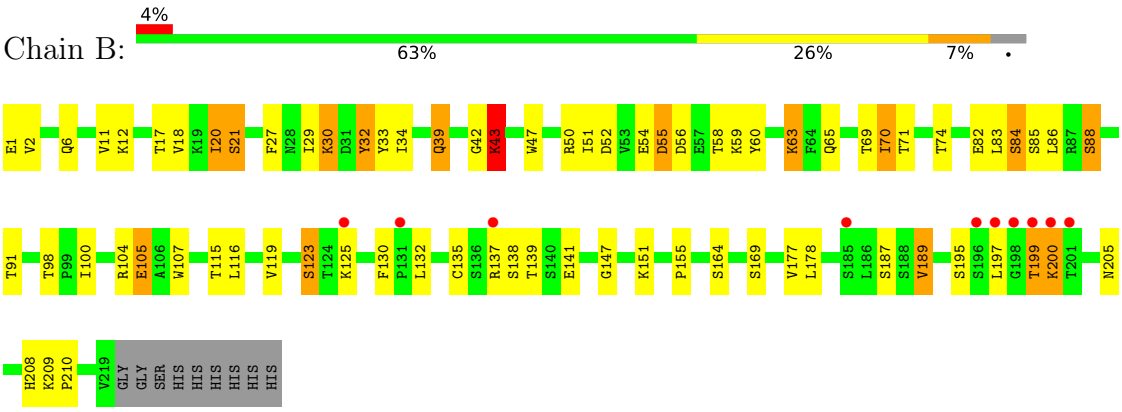
• Molecule 1: Neuropilin-2

Chain J:

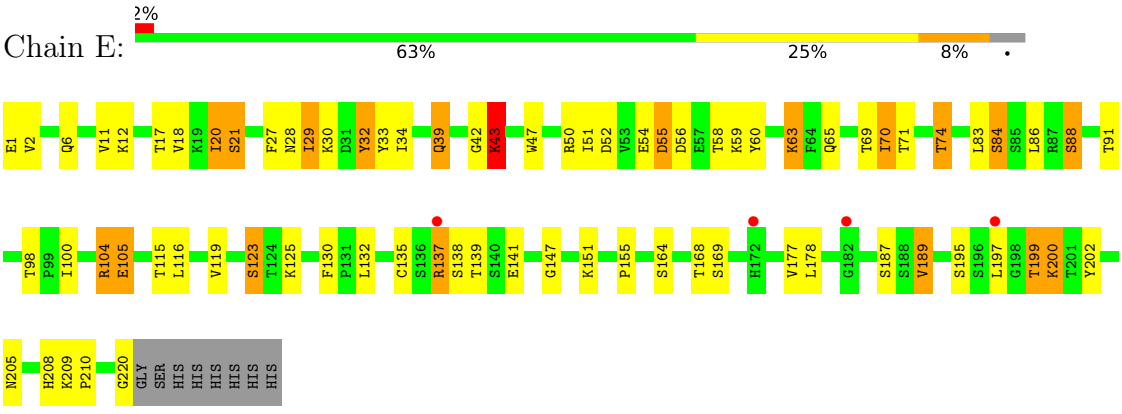




• Molecule 2: Heavy chian of antibody 10V8 Fab fragment

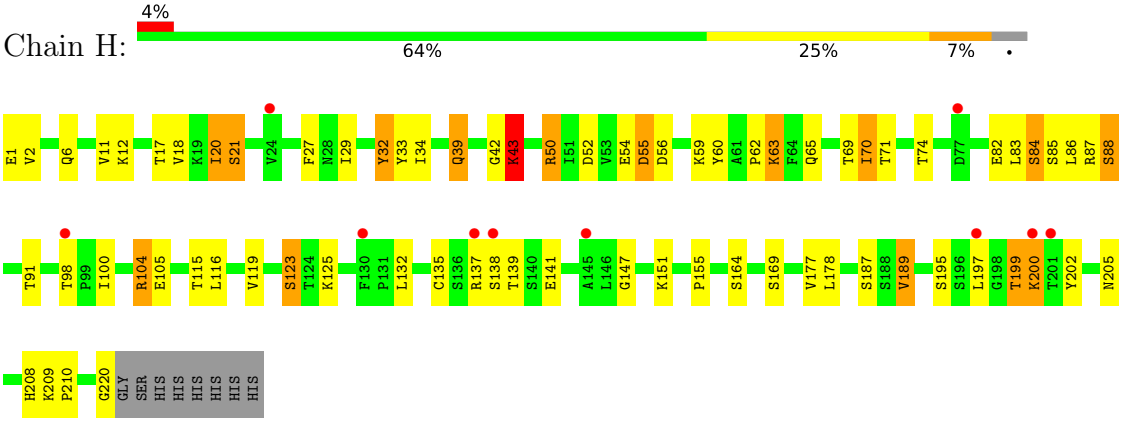


• Molecule 2: Heavy chian of antibody 10V8 Fab fragment



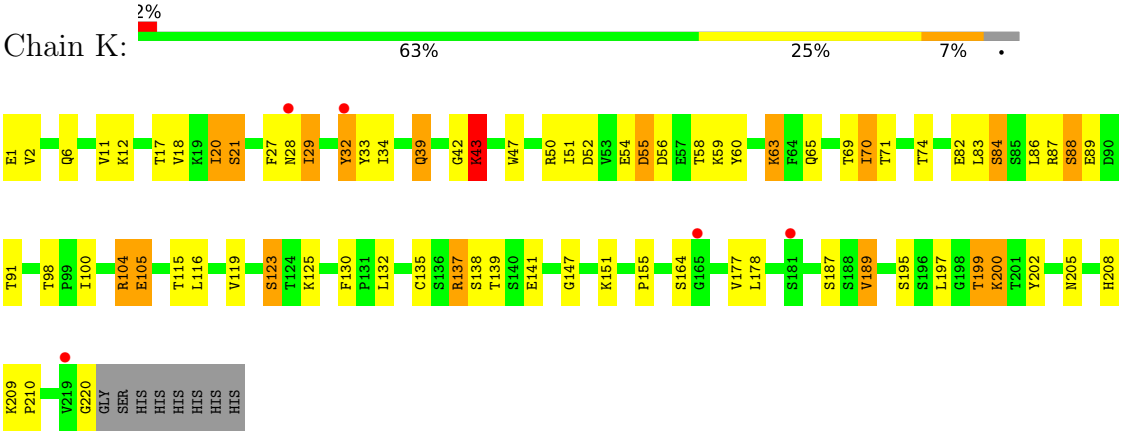
• Molecule 2: Heavy chian of antibody 10V8 Fab fragment

Chain H:



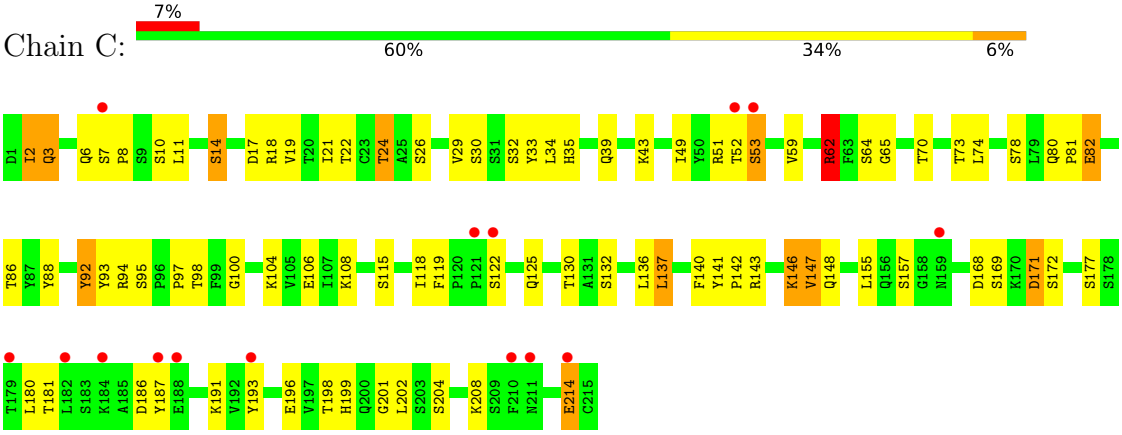
• Molecule 2: Heavy chian of antibody 10V8 Fab fragment

Chain K:



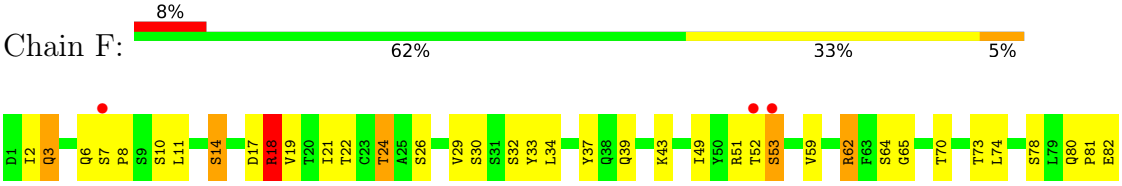
• Molecule 3: Light chain of antibody 10V8 Fab fragment

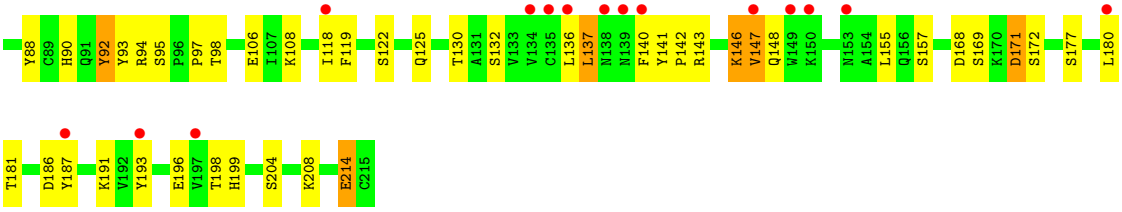
Chain C:



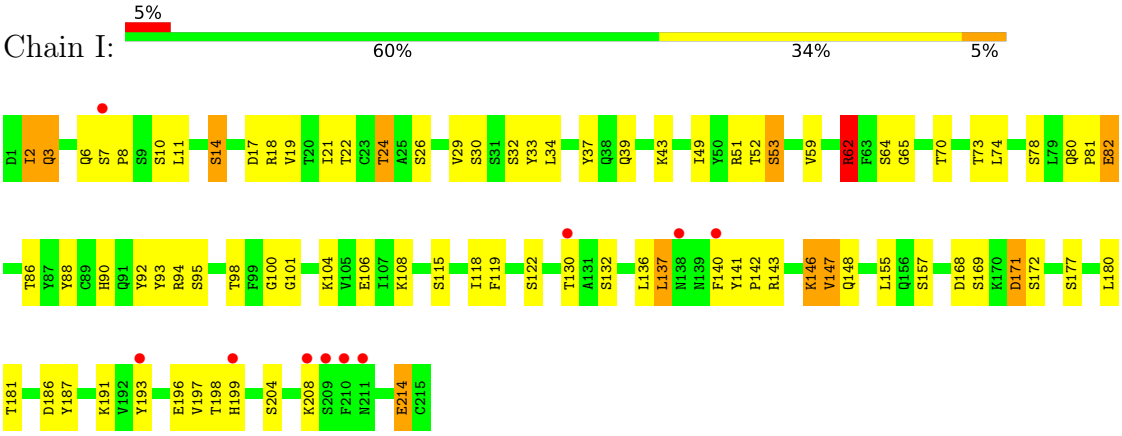
• Molecule 3: Light chain of antibody 10V8 Fab fragment

Chain F:

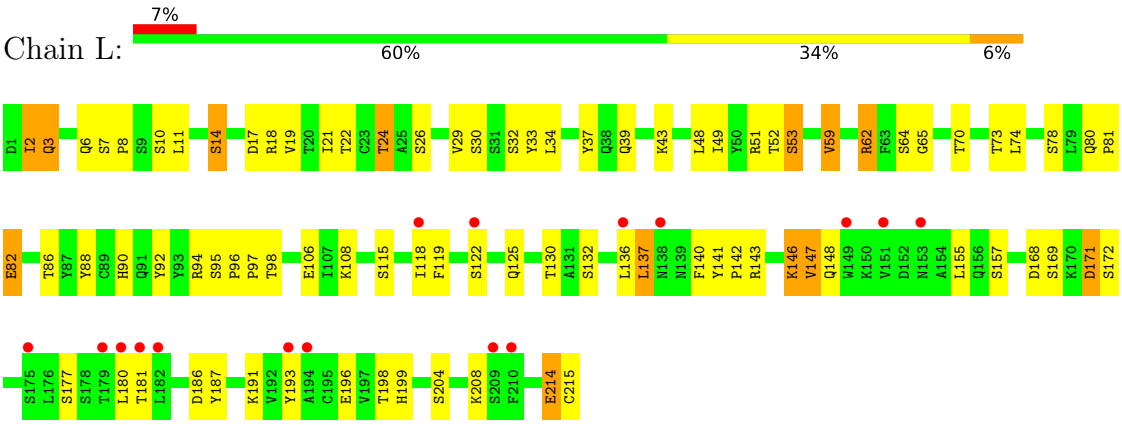




• Molecule 3: Light chain of antibody 10V8 Fab fragment



• Molecule 3: Light chain of antibody 10V8 Fab fragment



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.42Å 225.16Å 143.00Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	49.65 – 3.21 49.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.6 (49.65-3.21) 84.7 (49.60-3.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.248 , 0.294 0.249 , 0.295	Depositor DCC
R_{free} test set	3309 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	26621	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.36	0/3503	0.69	0/4755
1	D	0.35	0/3426	0.67	0/4654
1	G	0.36	0/3283	0.69	1/4452 (0.0%)
1	J	0.35	0/3502	0.67	0/4757
2	B	0.33	0/1705	0.72	0/2326
2	E	0.34	0/1709	0.72	0/2331
2	H	0.34	0/1709	0.74	0/2331
2	K	0.34	0/1709	0.73	0/2331
3	C	0.37	0/1686	0.74	1/2289 (0.0%)
3	F	0.36	0/1686	0.74	0/2289
3	I	0.37	0/1686	0.74	1/2289 (0.0%)
3	L	0.37	0/1686	0.73	0/2289
All	All	0.35	0/27290	0.71	3/37093 (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
1	D	0	1
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
3	F	0	1
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	62	ARG	NE-CZ-NH1	-5.71	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	545	GLN	CB-CA-C	5.25	120.90	110.40
3	I	62	ARG	NE-CZ-NH1	-5.15	117.73	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	123	SER	Peptide
1	D	542	ARG	Sidechain
2	E	123	SER	Peptide
3	F	18	ARG	Sidechain
2	H	123	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	3412	0	3313	93	0
1	D	3337	0	3230	88	0
1	G	3202	0	3088	97	1
1	J	3410	0	3297	140	0
2	B	1664	0	1627	54	0
2	E	1668	0	1630	52	1
2	H	1668	0	1630	54	0
2	K	1668	0	1630	60	0
3	C	1648	0	1595	53	0
3	F	1648	0	1595	51	0
3	I	1648	0	1595	57	0
3	L	1648	0	1595	57	0
All	All	26621	0	25825	780	1

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 780 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:G:443:GLY:HA2	1:G:466:ARG:NH1	1.44	1.31
1:J:449:GLN:NE2	1:J:491:ASP:O	1.71	1.24
1:J:272:LEU:CD1	1:J:279:VAL:HG21	1.69	1.20
1:A:272:LEU:CD1	1:A:279:VAL:HG21	1.71	1.17
1:J:447:ASP:HB3	1:J:462:PRO:CG	1.74	1.17

All (1) 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)
2:E:27:PHE:O	1:G:531:ASN:OD1[2_546]	1.96	0.24

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	418/583 (72%)	393 (94%)	23 (6%)	2 (0%)	29	67
1	D	412/583 (71%)	390 (95%)	20 (5%)	2 (0%)	29	67
1	G	388/583 (67%)	365 (94%)	18 (5%)	5 (1%)	12	47
1	J	419/583 (72%)	391 (93%)	23 (6%)	5 (1%)	13	49
2	B	217/228 (95%)	199 (92%)	16 (7%)	2 (1%)	17	56
2	E	218/228 (96%)	200 (92%)	16 (7%)	2 (1%)	17	56
2	H	218/228 (96%)	200 (92%)	16 (7%)	2 (1%)	17	56
2	K	218/228 (96%)	201 (92%)	15 (7%)	2 (1%)	17	56
3	C	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
3	F	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
3	I	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
3	L	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
All	All	3360/4104 (82%)	3155 (94%)	183 (5%)	22 (1%)	22	61

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	ILE
2	B	43	LYS
2	E	29	ILE
1	G	545	GLN
2	H	29	ILE

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	372/506 (74%)	331 (89%)	41 (11%)	6 26
1	D	363/506 (72%)	323 (89%)	40 (11%)	6 26
1	G	350/506 (69%)	313 (89%)	37 (11%)	6 27
1	J	372/506 (74%)	324 (87%)	48 (13%)	4 19
2	B	187/194 (96%)	145 (78%)	42 (22%)	1 4
2	E	187/194 (96%)	144 (77%)	43 (23%)	1 3
2	H	187/194 (96%)	146 (78%)	41 (22%)	1 5
2	K	187/194 (96%)	146 (78%)	41 (22%)	1 5
3	C	190/190 (100%)	142 (75%)	48 (25%)	0 2
3	F	190/190 (100%)	145 (76%)	45 (24%)	1 3
3	I	190/190 (100%)	142 (75%)	48 (25%)	0 2
3	L	190/190 (100%)	143 (75%)	47 (25%)	0 2
All	All	2965/3560 (83%)	2444 (82%)	521 (18%)	2 9

5 of 521 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	139	THR
3	L	10	SER
2	K	138	SER
3	L	214	GLU

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Mol	Chain	Res	Type
2	E	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	3	GLN
1	J	380	ASN
2	H	39	GLN
3	I	159	ASN
1	J	539	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	426/583 (73%)	0.49	37 (8%) 10 5	37, 79, 167, 239	0
1	D	420/583 (72%)	0.59	55 (13%) 3 2	39, 110, 168, 220	0
1	G	402/583 (68%)	1.05	80 (19%) 1 1	42, 114, 196, 269	0
1	J	427/583 (73%)	0.77	70 (16%) 1 1	38, 111, 174, 256	0
2	B	219/228 (96%)	0.20	10 (4%) 32 20	35, 72, 122, 168	0
2	E	220/228 (96%)	0.19	4 (1%) 68 55	36, 74, 131, 198	0
2	H	220/228 (96%)	0.26	10 (4%) 33 21	34, 67, 124, 166	0
2	K	220/228 (96%)	0.21	5 (2%) 60 47	34, 70, 124, 161	0
3	C	215/215 (100%)	0.42	15 (6%) 16 9	28, 61, 135, 169	0
3	F	215/215 (100%)	0.43	18 (8%) 11 6	29, 62, 140, 159	0
3	I	215/215 (100%)	0.27	10 (4%) 31 19	29, 57, 122, 158	0
3	L	215/215 (100%)	0.37	16 (7%) 14 8	28, 65, 132, 152	0
All	All	3414/4104 (83%)	0.50	330 (9%) 7 4	28, 82, 160, 269	0

The worst 5 of 330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	170	PRO	19.8
1	A	272	LEU	14.9
1	G	172	ASN	13.4
1	J	169	TYR	11.0
1	G	169	TYR	10.1

6.2 Non-standard residues in protein, DNA, RNA chains

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.