



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:02 AM UTC

PDB ID : 6CHB / pdb_00006chb
Title : Crystal structure of a natively-glycosylated BG505 SOSIP.664 HIV-1 Envelope Trimer in complex with the broadly-neutralizing antibodies BG18 and IOMA
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2018-02-22
Resolution : 6.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

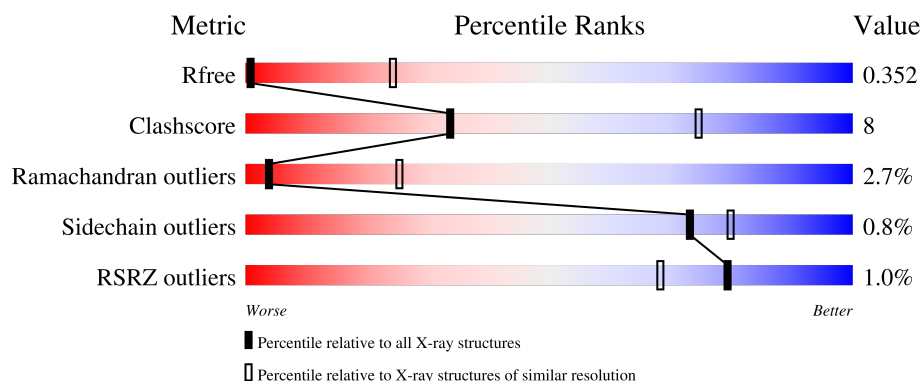
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.80 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}	180053	1165 (9.50-4.00)
Clashscore	190562	1006 (9.50-4.04)
Ramachandran outliers	187476	1052 (9.50-4.00)
Sidechain outliers	187428	1015 (9.50-4.00)
RSRZ outliers	180081	1158 (9.50-4.00)

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 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	153	
1	B	153	
1	C	153	
2	F	479	
2	G	479	

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Mol	Chain	Length	Quality of chain
2	H	479	 75% 17% 6%
3	I	241	 68% 26% 6%
3	J	241	 74% 20% 6%
3	Q	241	 75% 20% 6%
4	K	215	 80% 16% 5%
4	L	215	 74% 21% 5%
4	R	215	 80% 15% 5%
5	D	232	 42% 11% 46%
5	M	232	 41% 12% 46%
5	O	232	 43% 11% 46%
6	E	214	 44% 5% 50%
6	N	214	 43% 7% 49%
6	P	214	 37% 12% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28753 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			
1	A	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			
1	C	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	engineered mutation	UNP Q2N0S7
A	605	CYS	THR	engineered mutation	UNP Q2N0S7
C	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			
2	F	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			
2	H	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	engineered mutation	UNP Q2N0S6
H	332	ASN	THR	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	227	Total	C	N	O	S	0	0	0
			1723	1086	297	332	8			
3	I	227	Total	C	N	O	S	0	0	0
			1723	1086	297	332	8			
3	Q	227	Total	C	N	O	S	0	0	0
			1723	1086	297	332	8			

- Molecule 4 is a protein called BG18 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			
4	L	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			
4	R	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			

- Molecule 5 is a protein called IOMA Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	125	Total	C	N	O	S	0	0	0
			992	629	173	181	9			
5	M	125	Total	C	N	O	S	0	0	0
			992	629	173	181	9			
5	O	125	Total	C	N	O	S	0	0	0
			992	629	173	181	9			

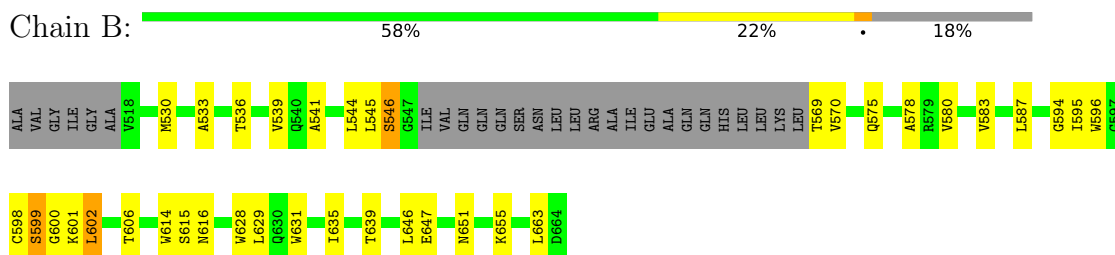
- Molecule 6 is a protein called IOMA Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	107	Total	C	N	O	S	0	0	0
			786	491	133	160	2			
6	N	109	Total	C	N	O	S	0	0	0
			799	498	136	163	2			
6	P	107	Total	C	N	O	S	0	0	0
			786	491	133	160	2			

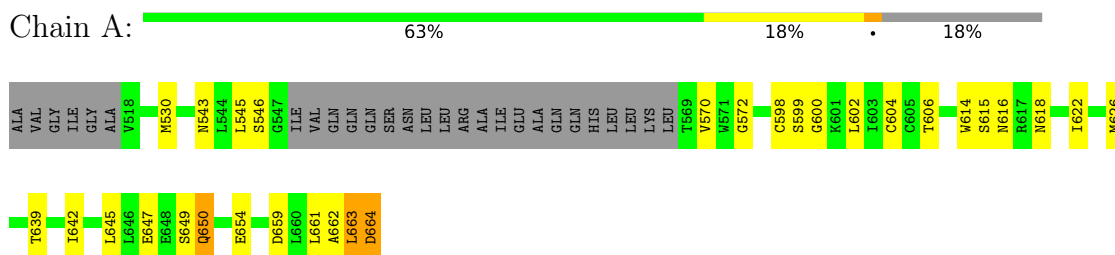
3 Residue-property plots [i](#)

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.

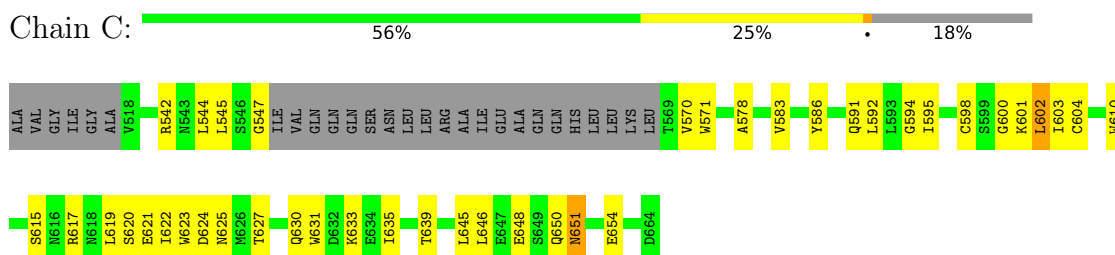
- Molecule 1: Envelope glycoprotein gp41



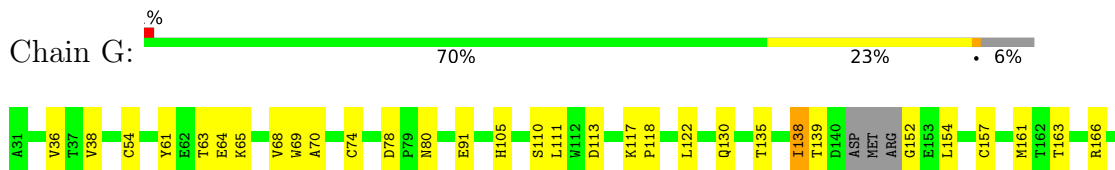
- Molecule 1: Envelope glycoprotein gp41

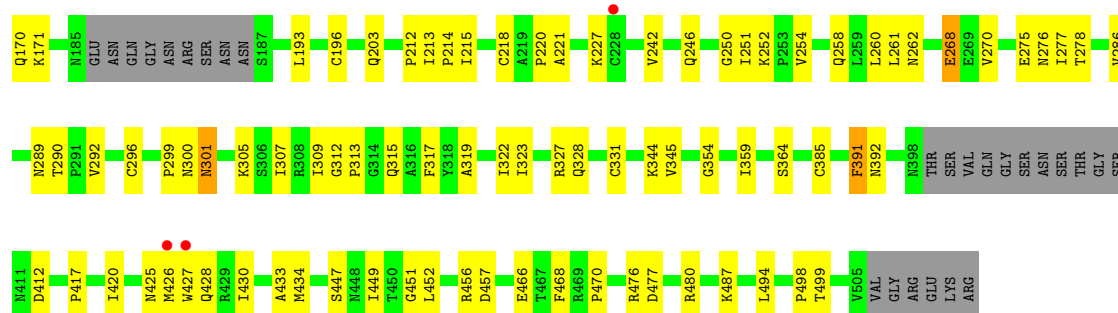


- Molecule 1: Envelope glycoprotein gp41

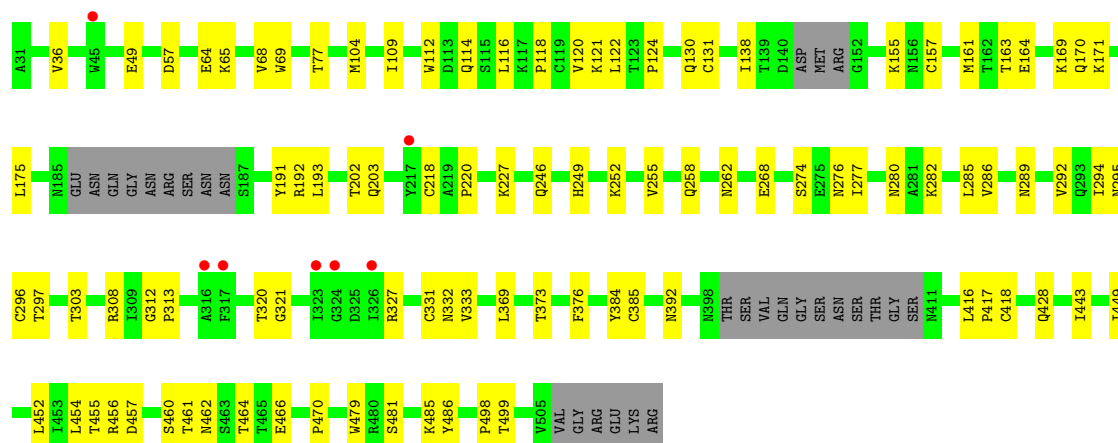
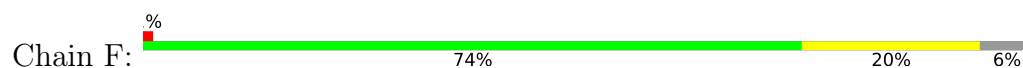


- Molecule 2: Envelope glycoprotein gp120

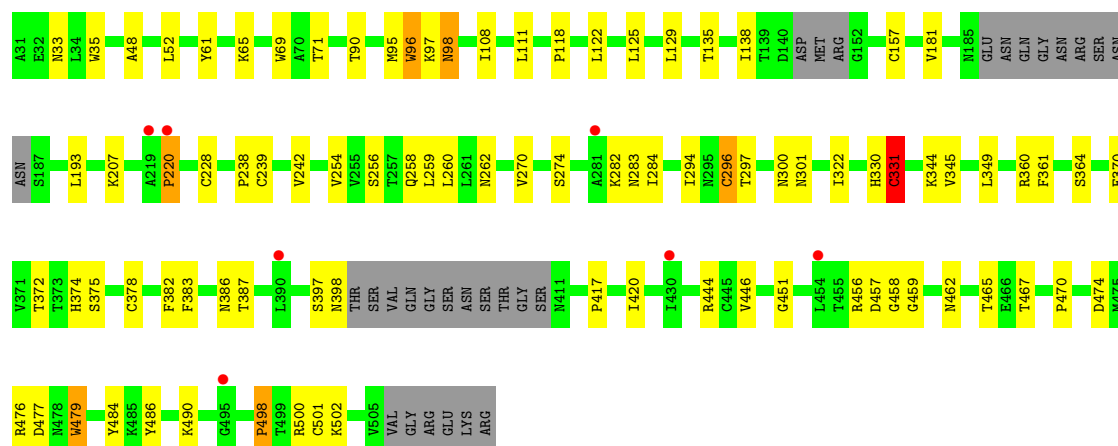
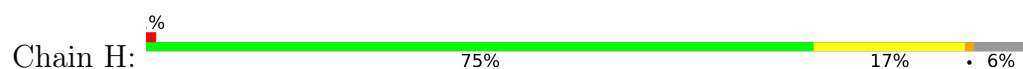




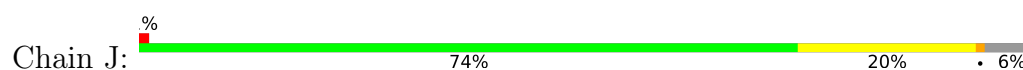
• Molecule 2: Envelope glycoprotein gp120

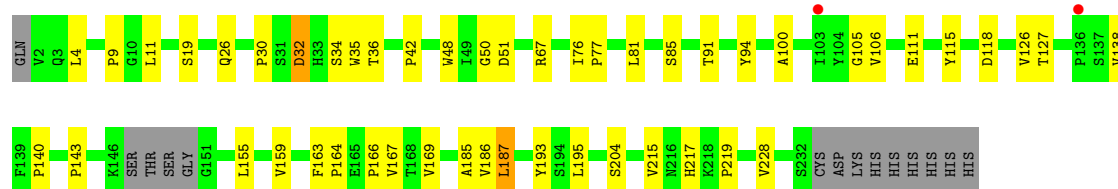


• Molecule 2: Envelope glycoprotein gp120

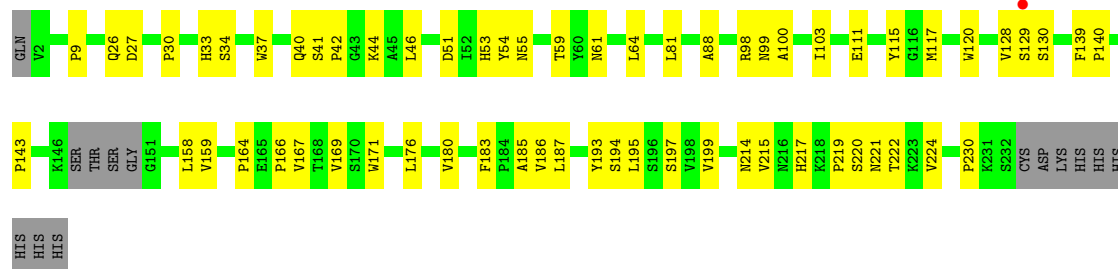


• Molecule 3: BG18 Heavy Chain

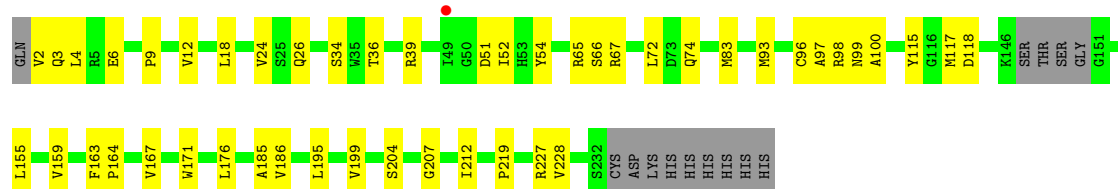




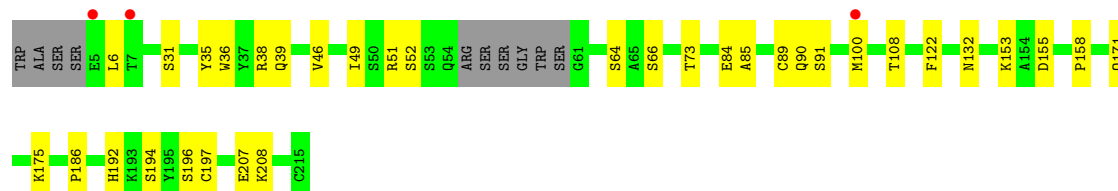
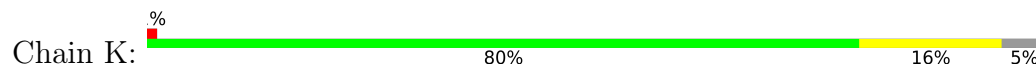
• Molecule 3: BG18 Heavy Chain



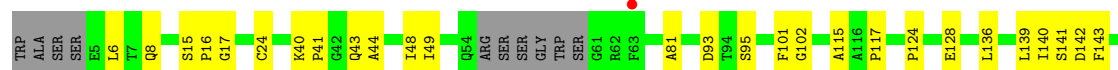
• Molecule 3: BG18 Heavy Chain

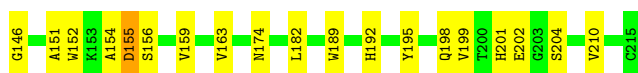


• Molecule 4: BG18 Light Chain

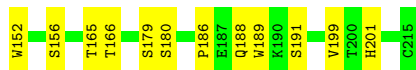
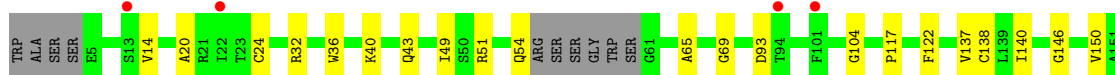
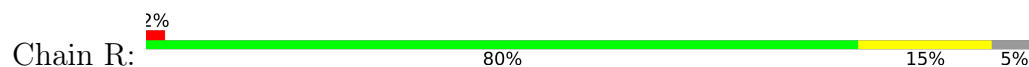


• Molecule 4: BG18 Light Chain

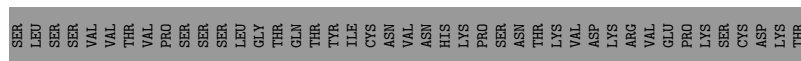
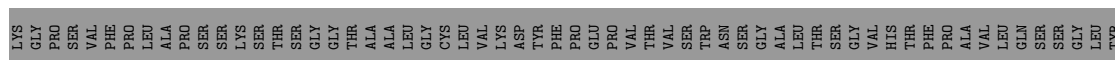
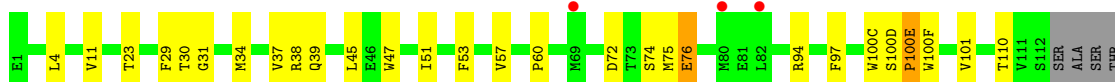




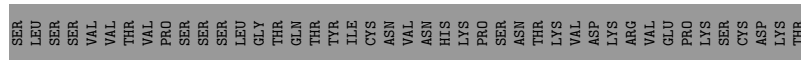
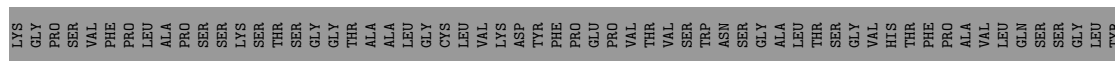
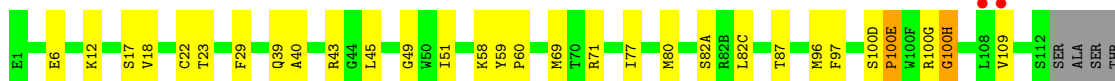
- Molecule 4: BG18 Light Chain



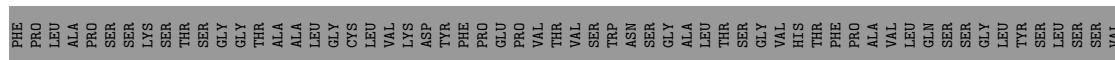
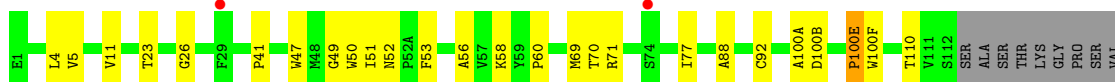
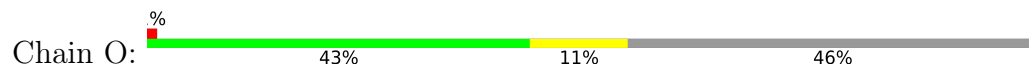
- Molecule 5: IOMA Heavy Chain



- Molecule 5: IOMA Heavy Chain

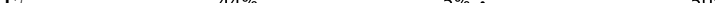


- Molecule 5: IOMA Heavy Chain



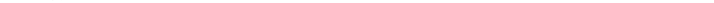
VAL	THR	VAL	PRO	SER	SER	SER	LEU	GLY	THR	GLN	THR	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	SER	ASN	THR	LYS	VAL	ASP	LYS	ARG	VAL	GLU	PRO	LYS	SER	SER	CYS	ASP	LYS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 6: IOMA Light Chain

Chain E:  44% 5% • 50%

[illegible]

- Molecule 6: IOMA Light Chain

Chain N:  %

HIS	SER	GLN
GLU	ASP	S2
GLY	PHE	A3
SER	THR	L4
THR	PRO	
VAL	GLY	D31
GLU	ALA	
LYS	VAL	Q38
THR	THR	H39
VAL	VAL	P40
ALA	ALA	
PRO	THR	L46
THR	LYS	I47
GLU	ALA	I48
CYS	ASP	Y49
SER	SER	P55
	PRO	
	VAL	I58
	LYS	
	ALA	A64
	GLY	
	VAL	A84
	GLU	
	THR	D93
	THR	G94
	THR	V96
	PRO	
	SER	G99
	LYS	
	GLN	Q108
	SER	
	ASN	
	LYS	
	THR	ALA
	ALA	ALA
	ALA	PRO
	SER	SER
	SER	VAL
	THR	THR
	THR	LEU
	LEU	PHE
	SER	PRO
	THR	PRO
	THR	SER
	PRO	SER
	GLU	GLU
	GLN	GLU
	THR	LEU
	LYS	GLN
	SER	ALA
	SER	ALA
	HIS	ASN
	ARG	LYS
	SER	ALA
	THR	THR
	SER	LEU
	CYS	VAL
	GLN	CYS
	VAL	LEU

- Molecule 6: IOMA Light Chain

Chain P: 37% 12% 50%

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.75Å 176.75Å 458.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.63 – 6.80 39.63 – 6.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.63-6.80) 99.1 (39.63-6.80)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 6.65Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.318 , 0.417 0.333 , 0.352	Depositor DCC
R_{free} test set	670 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	369.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 680.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	28753	wwPDB-VP
Average B, all atoms (Å ²)	411.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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

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	0.14	0/1019	0.43	0/1382
1	B	0.13	0/1019	0.42	1/1382 (0.1%)
1	C	0.15	0/1019	0.49	1/1382 (0.1%)
2	F	0.15	0/3611	0.43	0/4903
2	G	0.16	0/3611	0.44	0/4903
2	H	0.15	0/3611	0.44	0/4903
3	I	0.16	0/1767	0.43	0/2410
3	J	0.14	0/1767	0.43	0/2410
3	Q	0.15	0/1767	0.41	0/2410
4	K	0.13	0/1577	0.39	0/2153
4	L	0.14	0/1577	0.40	0/2153
4	R	0.14	0/1577	0.35	0/2153
5	D	0.17	0/1021	0.46	0/1384
5	M	0.13	0/1021	0.43	0/1384
5	O	0.17	0/1021	0.47	0/1384
6	E	0.15	0/803	0.39	0/1088
6	N	0.14	0/816	0.41	0/1105
6	P	0.13	0/803	0.43	0/1088
All	All	0.15	0/29407	0.43	2/39977 (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	A	0	1
5	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	544	LEU	N-CA-C	-5.37	108.50	114.62
1	B	602	LEU	CB-CA-C	-5.18	110.58	116.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	659	ASP	Peptide
5	D	100(C)	TRP	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	1001	0	978	17	1
1	B	1001	0	979	28	0
1	C	1001	0	979	25	0
2	F	3538	0	3488	54	0
2	G	3538	0	3493	68	0
2	H	3538	0	3491	47	0
3	I	1723	0	1696	36	0
3	J	1723	0	1694	27	0
3	Q	1723	0	1694	30	0
4	K	1540	0	1492	19	0
4	L	1540	0	1492	27	0
4	R	1540	0	1492	16	0
5	D	992	0	949	20	0
5	M	992	0	947	15	0
5	O	992	0	947	17	0
6	E	786	0	758	7	0
6	N	799	0	769	9	0
6	P	786	0	758	16	0
All	All	28753	0	28096	439	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 8.

The worst 5 of 439 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:Q:159:VAL:HG11	3:Q:167:VAL:HG11	1.67	0.77
6:P:83:GLU:HG3	6:P:105:THR:HA	1.66	0.77
3:J:140:PRO:HB3	3:J:228:VAL:HG13	1.73	0.71
2:F:295:ASN:HB2	2:F:332:ASN:HB2	1.72	0.70
2:G:212:PRO:HB2	2:G:252:LYS:HB3	1.74	0.69

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)
1:A:661:LEU:O	1:A:663:LEU:N[8_554]	2.16	0.04

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	122/153 (80%)	93 (76%)	24 (20%)	5 (4%)	2	18
1	B	122/153 (80%)	104 (85%)	15 (12%)	3 (2%)	4	26
1	C	122/153 (80%)	97 (80%)	20 (16%)	5 (4%)	2	18
2	F	442/479 (92%)	363 (82%)	71 (16%)	8 (2%)	6	34
2	G	442/479 (92%)	377 (85%)	51 (12%)	14 (3%)	3	21
2	H	442/479 (92%)	370 (84%)	57 (13%)	15 (3%)	3	21
3	I	223/241 (92%)	195 (87%)	21 (9%)	7 (3%)	3	22
3	J	223/241 (92%)	188 (84%)	27 (12%)	8 (4%)	2	20
3	Q	223/241 (92%)	195 (87%)	24 (11%)	4 (2%)	6	34
4	K	201/215 (94%)	175 (87%)	24 (12%)	2 (1%)	12	48
4	L	201/215 (94%)	174 (87%)	24 (12%)	3 (2%)	8	40
4	R	201/215 (94%)	175 (87%)	22 (11%)	4 (2%)	6	31
5	D	123/232 (53%)	103 (84%)	16 (13%)	4 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	123/232 (53%)	106 (86%)	12 (10%)	5 (4%)	2	18
5	O	123/232 (53%)	98 (80%)	22 (18%)	3 (2%)	4	27
6	E	105/214 (49%)	88 (84%)	16 (15%)	1 (1%)	12	48
6	N	107/214 (50%)	91 (85%)	13 (12%)	3 (3%)	4	24
6	P	105/214 (49%)	81 (77%)	20 (19%)	4 (4%)	2	19
All	All	3650/4602 (79%)	3073 (84%)	479 (13%)	98 (3%)	4	25

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	74	SER
5	D	100(E)	PRO
5	M	100(E)	PRO
3	I	30	PRO
3	I	166	PRO

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	108/129 (84%)	106 (98%)	2 (2%)	50	67
1	B	108/129 (84%)	106 (98%)	2 (2%)	50	67
1	C	108/129 (84%)	105 (97%)	3 (3%)	38	60
2	F	401/426 (94%)	398 (99%)	3 (1%)	76	81
2	G	401/426 (94%)	400 (100%)	1 (0%)	87	87
2	H	401/426 (94%)	395 (98%)	6 (2%)	57	72
3	I	195/208 (94%)	194 (100%)	1 (0%)	81	83
3	J	195/208 (94%)	193 (99%)	2 (1%)	68	78
3	Q	195/208 (94%)	195 (100%)	0	100	100
4	K	174/182 (96%)	173 (99%)	1 (1%)	78	83
4	L	174/182 (96%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	174/182 (96%)	173 (99%)	1 (1%)	78	83
5	D	104/197 (53%)	102 (98%)	2 (2%)	50	67
5	M	104/197 (53%)	103 (99%)	1 (1%)	68	78
5	O	104/197 (53%)	104 (100%)	0	100	100
6	E	85/177 (48%)	84 (99%)	1 (1%)	63	75
6	N	86/177 (49%)	85 (99%)	1 (1%)	63	75
6	P	85/177 (48%)	85 (100%)	0	100	100
All	All	3202/3957 (81%)	3175 (99%)	27 (1%)	73	80

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	M	59	TYR
1	C	603	ILE
2	H	331	CYS
3	I	26	GLN
1	C	604	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	422	GLN
4	R	188	GLN
3	I	172	ASN
3	Q	181	HIS
6	N	85	HIS

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 oligosaccharides 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 ⓘ

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	126/153 (82%)	-0.22	0 100 100	365, 471, 570, 691	0
1	B	126/153 (82%)	-0.13	0 100 100	309, 438, 494, 548	0
1	C	126/153 (82%)	-0.07	0 100 100	329, 445, 536, 592	0
2	F	450/479 (93%)	-0.13	7 (1%) 70 59	209, 400, 510, 597	0
2	G	450/479 (93%)	-0.10	3 (0%) 84 74	212, 372, 474, 595	0
2	H	450/479 (93%)	-0.10	7 (1%) 70 59	241, 392, 532, 589	0
3	I	227/241 (94%)	-0.21	1 (0%) 88 79	277, 411, 505, 576	0
3	J	227/241 (94%)	-0.20	2 (0%) 81 70	270, 380, 474, 594	0
3	Q	227/241 (94%)	-0.17	1 (0%) 88 79	341, 442, 578, 700	0
4	K	205/215 (95%)	-0.13	3 (1%) 72 60	297, 386, 473, 543	0
4	L	205/215 (95%)	-0.20	1 (0%) 87 77	324, 407, 503, 613	0
4	R	205/215 (95%)	-0.03	4 (1%) 65 56	354, 521, 620, 698	0
5	D	125/232 (53%)	-0.11	3 (2%) 59 52	237, 362, 466, 541	0
5	M	125/232 (53%)	-0.23	2 (1%) 70 59	303, 386, 510, 581	0
5	O	125/232 (53%)	-0.02	2 (1%) 70 59	223, 325, 420, 472	0
6	E	107/214 (50%)	-0.16	1 (0%) 81 70	319, 436, 537, 605	0
6	N	109/214 (50%)	-0.08	2 (1%) 67 58	351, 457, 555, 582	0
6	P	107/214 (50%)	-0.24	0 100 100	290, 406, 493, 559	0
All	All	3722/4602 (80%)	-0.14	39 (1%) 79 68	209, 409, 546, 700	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	22	ILE	5.7
2	G	427	TRP	5.2
3	Q	49	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	H	281	ALA	4.6
6	N	3	ALA	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.