



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:02 PM GMT

PDB ID : 4NHG
Title : Crystal Structure of 2G12 IgG Dimer
Authors : Wu, Y.; West Jr., A.P.; Kim, H.J.; Thornton, M.E.; Ward, A.B.; Bjorkman, P.J.
Deposited on : 2013-11-05
Resolution : 8.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

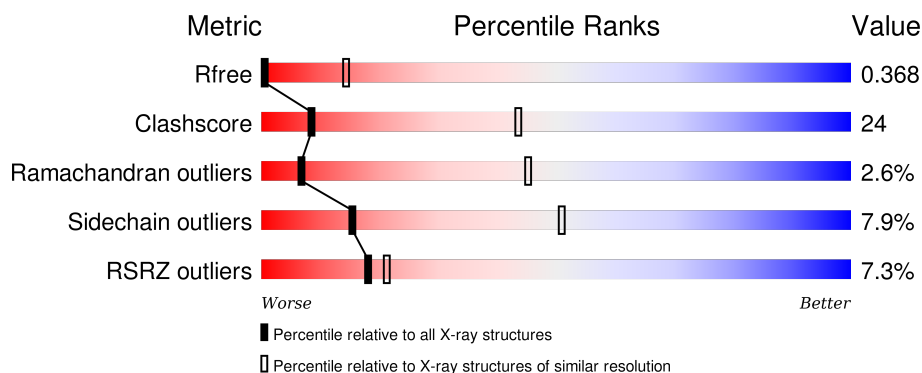
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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. 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	243	<div> <div>4%</div> <div>53%</div> <div>33%</div> <div>•</div> <div>12%</div> </div>
1	D	243	<div> <div>2%</div> <div>50%</div> <div>33%</div> <div>5%</div> <div>12%</div> </div>
1	E	243	<div> <div>10%</div> <div>50%</div> <div>33%</div> <div>5%</div> <div>12%</div> </div>
1	H	243	<div> <div>2%</div> <div>50%</div> <div>35%</div> <div>•</div> <div>12%</div> </div>
1	I	243	<div> <div>9%</div> <div>50%</div> <div>36%</div> <div>•</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	243	
2	B	213	
2	C	213	
2	F	213	
2	G	213	
2	K	213	
2	L	213	
3	J	211	
3	N	211	
3	O	211	
3	P	211	
3	X	211	
3	Y	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29250 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 2G12 IgG dimer heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	D	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			
1	E	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	I	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			
1	H	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	M	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			

- Molecule 2 is a protein called 2G12 IgG dimer light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	C	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	F	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	G	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	K	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	L	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			

- Molecule 3 is a protein called Hepatitis B virus receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	N	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	X	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	Y	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	O	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	P	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	272	GLN	GLU	CONFLICT	UNP Q6PYX1
X	283	GLN	GLU	CONFLICT	UNP Q6PYX1
X	294	GLN	GLU	CONFLICT	UNP Q6PYX1
X	312	ASN	ASP	CONFLICT	UNP Q6PYX1
X	315	ASP	ASN	CONFLICT	UNP Q6PYX1
X	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
Y	272	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	283	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	294	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	312	ASN	ASP	CONFLICT	UNP Q6PYX1
Y	315	ASP	ASN	CONFLICT	UNP Q6PYX1
Y	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
J	272	GLN	GLU	CONFLICT	UNP Q6PYX1
J	283	GLN	GLU	CONFLICT	UNP Q6PYX1
J	294	GLN	GLU	CONFLICT	UNP Q6PYX1
J	312	ASN	ASP	CONFLICT	UNP Q6PYX1
J	315	ASP	ASN	CONFLICT	UNP Q6PYX1
J	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
N	272	GLN	GLU	CONFLICT	UNP Q6PYX1
N	283	GLN	GLU	CONFLICT	UNP Q6PYX1
N	294	GLN	GLU	CONFLICT	UNP Q6PYX1
N	312	ASN	ASP	CONFLICT	UNP Q6PYX1
N	315	ASP	ASN	CONFLICT	UNP Q6PYX1
N	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	272	GLN	GLU	CONFLICT	UNP Q6PYX1
O	283	GLN	GLU	CONFLICT	UNP Q6PYX1
O	294	GLN	GLU	CONFLICT	UNP Q6PYX1
O	312	ASN	ASP	CONFLICT	UNP Q6PYX1

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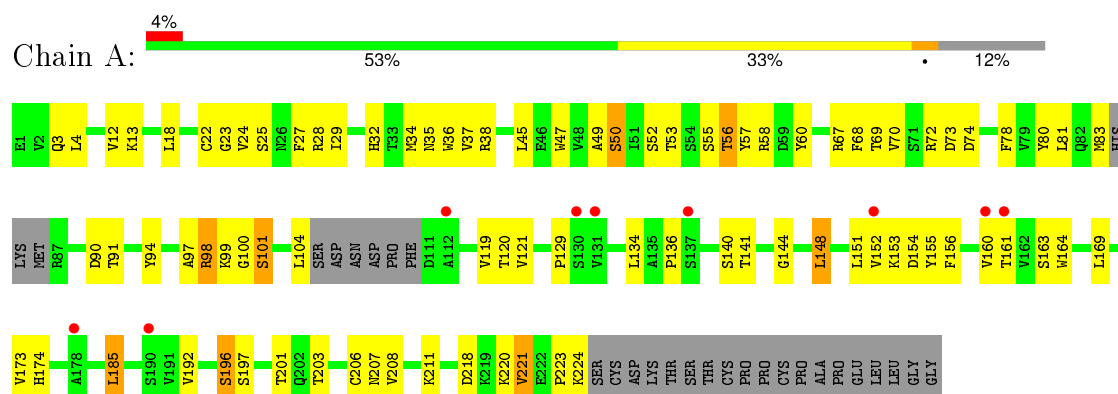
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Chain	Residue	Modelled	Actual	Comment	Reference
O	315	ASP	ASN	CONFLICT	UNP Q6PYX1
O	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
P	272	GLN	GLU	CONFLICT	UNP Q6PYX1
P	283	GLN	GLU	CONFLICT	UNP Q6PYX1
P	294	GLN	GLU	CONFLICT	UNP Q6PYX1
P	312	ASN	ASP	CONFLICT	UNP Q6PYX1
P	315	ASP	ASN	CONFLICT	UNP Q6PYX1
P	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1

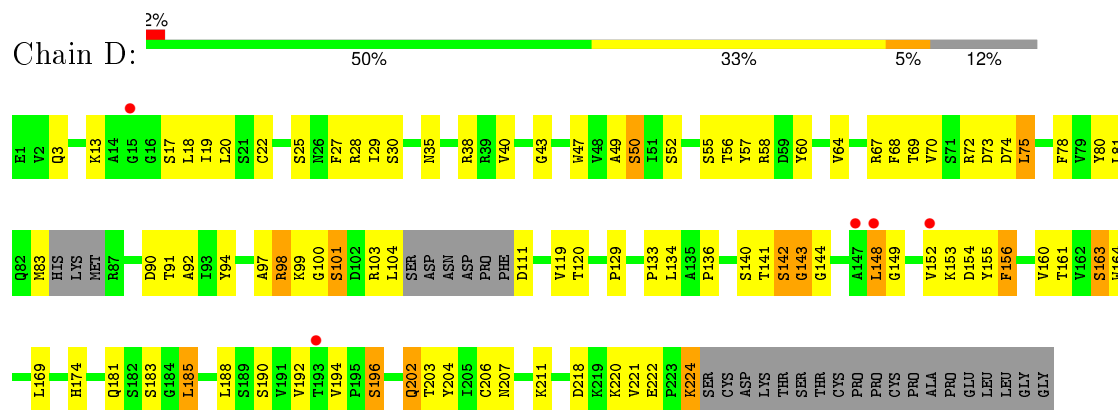
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

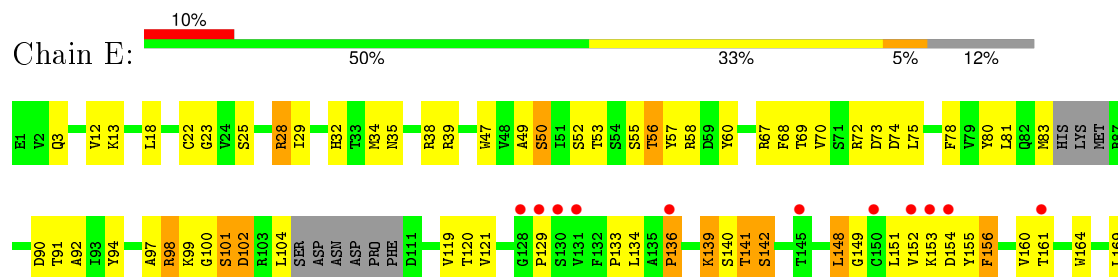
• Molecule 1: 2G12 IgG dimer heavy chain

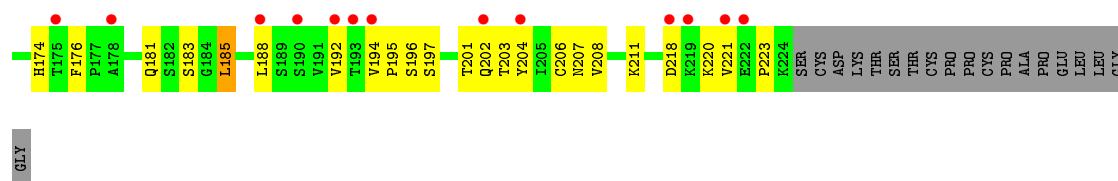


• Molecule 1: 2G12 IgG dimer heavy chain

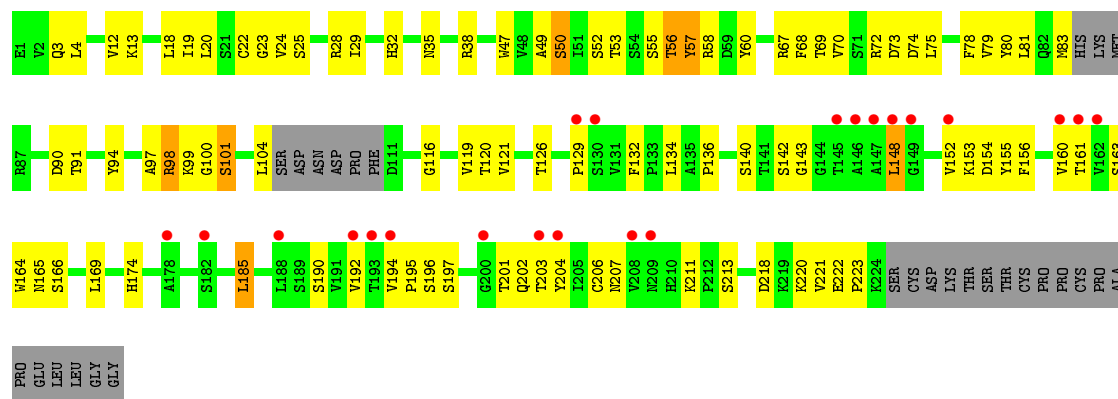


• Molecule 1: 2G12 IgG dimer heavy chain

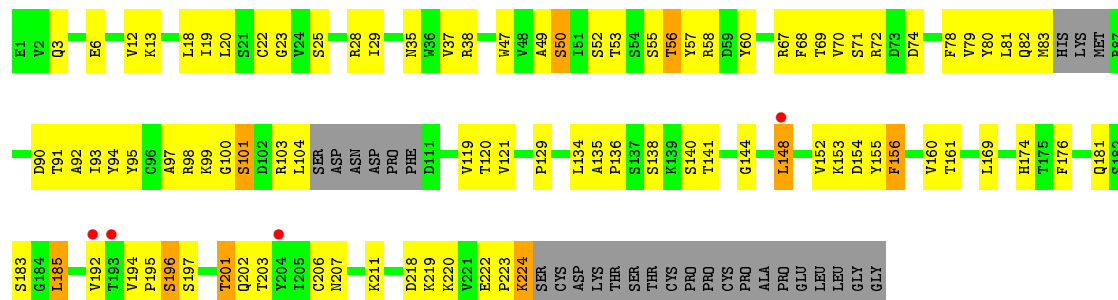




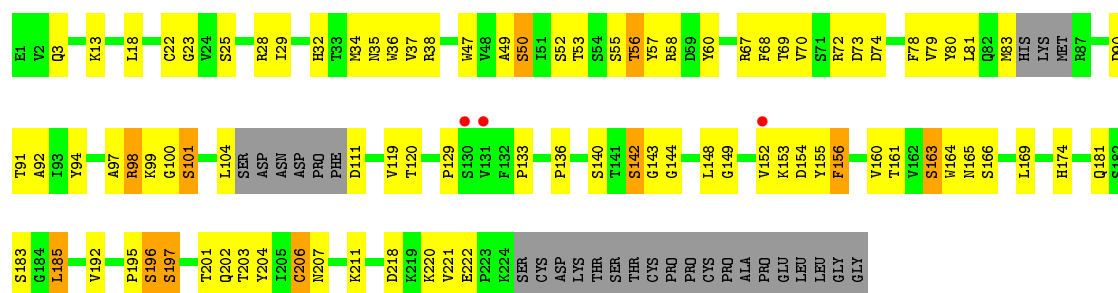
• Molecule 1: 2G12 IgG dimer heavy chain



• Molecule 1: 2G12 IgG dimer heavy chain



• Molecule 1: 2G12 IgG dimer heavy chain



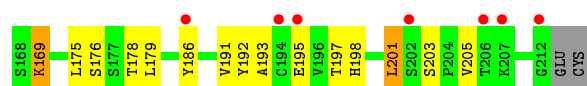
• Molecule 2: 2G12 IgG dimer light chain

H198	V110	V2
L201	A111	T5
S202	A112	D6
S203	P113	S7
P204	F118	
V205	P119	D17
S208	P120	T18
	S121	T19
	D122	T20
	E123	
	G124	T29
	L125	E30
	A130	T31
	S131	X32
	V132	L33
	V133	
	C134	T36
	L135	Q37
	L136	Q38
	H137	X39
	M138	
	F139	K45
	P140	L46
	P141	L47
	R142	X50
	E143	
		T56
	W148	R61
	K149	
	V150	E70
	D151	F71
	M152	
		T72
	E161	L73
	S162	T74
	V163	T75
	T164	S76
	E165	G77
	Q166	L78
	D167	
	S168	D81
	K169	
	D170	A84
	S171	
	T172	
		D89
	L175	R90
	S176	T91
		A92
		X93
	L179	
		Q100
	V191	G101
	V192	T102
	A193	
	C194	T106
	E195	K107
	V196	R108
	T197	T109
G10		
CYS		

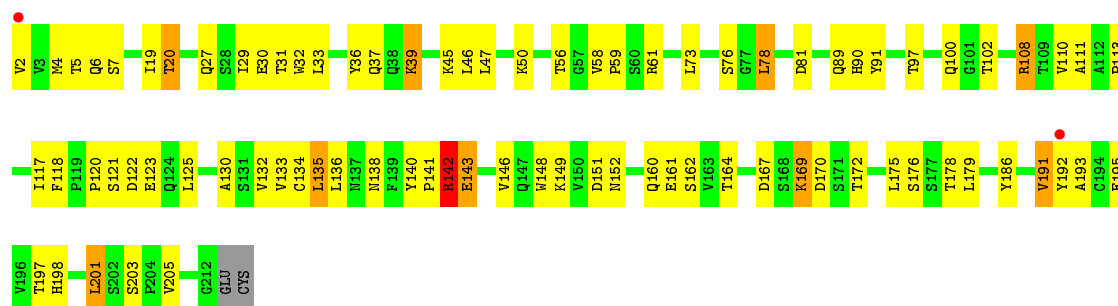
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|------|------|------|
| Y192 | R108 | V2 |
| A193 | T109 | V3 |
| C194 | G110 | V4 |
| E195 | A111 | T5 |
| Y196 | A112 | Q6 |
| T197 | P113 | S7 |
| H198 | F118 | I19 |
| Q199 | P119 | T20 |
| L201 | S121 | I21 |
| S202 | D122 | I29 |
| S203 | E123 | E30 |
| P204 | Q124 | T31 |
| V205 | G125 | W32 |
| G212 | K126 | L33 |
| GLU | A130 | Y36 |
| CYS | S131 | Q37 |
| | V132 | Q38 |
| | G133 | R39 |
| | G134 | P44 |
| | L135 | K45 |
| | L136 | L46 |
| | N137 | L47 |
| | N138 | K50 |
| | F139 | T56 |
| | P141 | R61 |
| | Y140 | E70 |
| | R142 | F71 |
| | E143 | T72 |
| | K145 | L73 |
| | V146 | T74 |
| | Q147 | L75 |
| | W148 | S76 |
| | K149 | G77 |
| | D151 | L78 |
| | N152 | D81 |
| | A153 | D82 |
| | Q160 | F83 |
| | S162 | H87 |
| | K169 | R90 |
| | L175 | Y91 |
| | S176 | T97 |
| | S177 | Q100 |
| | T178 | T102 |
| | L179 | I106 |
| | K183 | Y108 |
| | Y186 | T109 |
| | E187 | L113 |
| | W191 | |

- | Protein | Position | Residue | Frequency | Conservation | Pathway |
|---------|----------|---------|-----------|--------------|---------|
| V2 | L175 | Q100 | 0.00 | 0.00 | 0.00 |
| | S176 | G101 | 0.00 | 0.00 | 0.00 |
| | T177 | T102 | 0.00 | 0.00 | 0.00 |
| | T178 | T106 | 0.00 | 0.00 | 0.00 |
| | L179 | K107 | 0.00 | 0.00 | 0.00 |
| | V191 | R108 | 0.00 | 0.00 | 0.00 |
| | Y192 | T109 | 0.00 | 0.00 | 0.00 |
| | A193 | V110 | 0.00 | 0.00 | 0.00 |
| | C194 | A111 | 0.00 | 0.00 | 0.00 |
| | E195 | A112 | 0.00 | 0.00 | 0.00 |
| V2 | V196 | P113 | 0.00 | 0.00 | 0.00 |
| | T197 | S114 | 0.00 | 0.00 | 0.00 |
| | H198 | V115 | 0.00 | 0.00 | 0.00 |
| | Q199 | F116 | 0.00 | 0.00 | 0.00 |
| | G200 | I117 | 0.00 | 0.00 | 0.00 |
| | L201 | F118 | 0.00 | 0.00 | 0.00 |
| | S202 | P119 | 0.00 | 0.00 | 0.00 |
| | S203 | P120 | 0.00 | 0.00 | 0.00 |
| | P204 | S121 | 0.00 | 0.00 | 0.00 |
| | V205 | D122 | 0.00 | 0.00 | 0.00 |
| V2 | T206 | E123 | 0.00 | 0.00 | 0.00 |
| | K207 | A130 | 0.00 | 0.00 | 0.00 |
| | S208 | S131 | 0.00 | 0.00 | 0.00 |
| | G212 | V132 | 0.00 | 0.00 | 0.00 |
| | GLU | V133 | 0.00 | 0.00 | 0.00 |
| | CYS | C134 | 0.00 | 0.00 | 0.00 |
| | | L135 | 0.00 | 0.00 | 0.00 |
| | | L136 | 0.00 | 0.00 | 0.00 |
| | | N137 | 0.00 | 0.00 | 0.00 |
| | | N138 | 0.00 | 0.00 | 0.00 |
| V2 | | F139 | 0.00 | 0.00 | 0.00 |
| | | Y140 | 0.00 | 0.00 | 0.00 |
| | | P141 | 0.00 | 0.00 | 0.00 |
| | | R142 | 0.00 | 0.00 | 0.00 |
| | | E143 | 0.00 | 0.00 | 0.00 |
| | | A144 | 0.00 | 0.00 | 0.00 |
| | | K145 | 0.00 | 0.00 | 0.00 |
| | | V146 | 0.00 | 0.00 | 0.00 |
| | | Q147 | 0.00 | 0.00 | 0.00 |
| | | V148 | 0.00 | 0.00 | 0.00 |
| V2 | | K149 | 0.00 | 0.00 | 0.00 |
| | | V150 | 0.00 | 0.00 | 0.00 |
| | | D151 | 0.00 | 0.00 | 0.00 |
| | | N152 | 0.00 | 0.00 | 0.00 |
| | | Q155 | 0.00 | 0.00 | 0.00 |
| | | S156 | 0.00 | 0.00 | 0.00 |
| | | Q160 | 0.00 | 0.00 | 0.00 |
| | | E161 | 0.00 | 0.00 | 0.00 |
| | | S162 | 0.00 | 0.00 | 0.00 |
| | | V163 | 0.00 | 0.00 | 0.00 |
| V2 | | T164 | 0.00 | 0.00 | 0.00 |
| | | D167 | 0.00 | 0.00 | 0.00 |
| | | S168 | 0.00 | 0.00 | 0.00 |
| | | V169 | 0.00 | 0.00 | 0.00 |
| | | V170 | 0.00 | 0.00 | 0.00 |
| | | V171 | 0.00 | 0.00 | 0.00 |
| | | V172 | 0.00 | 0.00 | 0.00 |
| | | V173 | 0.00 | 0.00 | 0.00 |
| | | V174 | 0.00 | 0.00 | 0.00 |
| | | V175 | 0.00 | 0.00 | 0.00 |
| V2 | | V176 | 0.00 | 0.00 | 0.00 |
| | | V177 | 0.00 | 0.00 | 0.00 |
| | | V178 | 0.00 | 0.00 | 0.00 |
| | | V179 | 0.00 | 0.00 | 0.00 |
| | | V180 | 0.00 | 0.00 | 0.00 |
| | | V181 | 0.00 | 0.00 | 0.00 |
| | | V182 | 0.00 | 0.00 | 0.00 |
| | | V183 | 0.00 | 0.00 | 0.00 |
| | | V184 | 0.00 | 0.00 | 0.00 |
| | | V185 | 0.00 | 0.00 | 0.00 |
| V2 | | V186 | 0.00 | 0.00 | 0.00 |
| | | V187 | 0.00 | 0.00 | 0.00 |
| | | V188 | 0.00 | 0.00 | 0.00 |
| | | V189 | 0.00 | 0.00 | 0.00 |
| | | V190 | 0.00 | 0.00 | 0.00 |

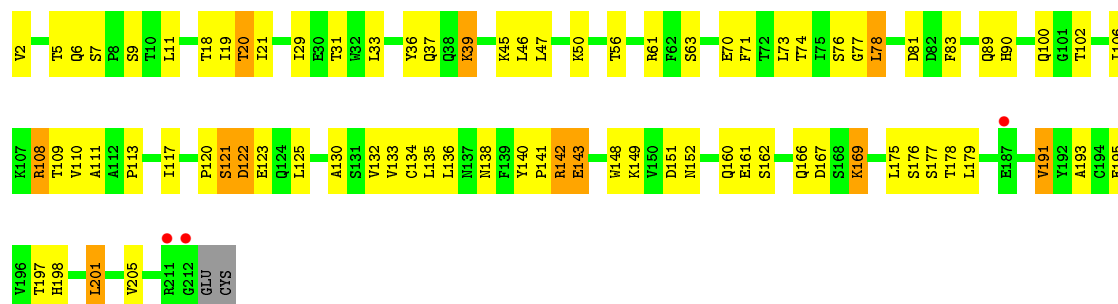
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|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| H90 | Q100 | G101 | Ti02 | K107 | R108 | Ti09 | V110 | A111 | A112 | P113 | S114 | V115 | I117 | F118 | P119 | F119 | P120 | S121 | D122 | E123 | I125 | G128 | Ti29 | A130 | S131 | V132 | V133 | C134 | L135 | L136 | M137 | M138 | F139 | P140 | P141 | R142 | E143 | A144 | R145 | V146 | Q147 | K148 | M149 | M152 | A153 | L154 | Q155 | Q160 | E161 | S162 | T167 |
| V2 | T5 | D6 | S7 | S12 | A13 | S14 | V15 | T19 | T20 | T21 | T29 | F30 | T31 | W32 | L33 | V36 | Q37 | Q38 | R39 | P44 | K45 | L46 | L47 | L48 | V49 | K50 | T53 | T56 | S57 | V58 | P59 | S60 | R61 | F62 | S63 | L73 | T74 | T75 | S76 | G77 | L78 | D79 | F80 | D81 | D82 | F83 | H87 | R88 | T89 | | |



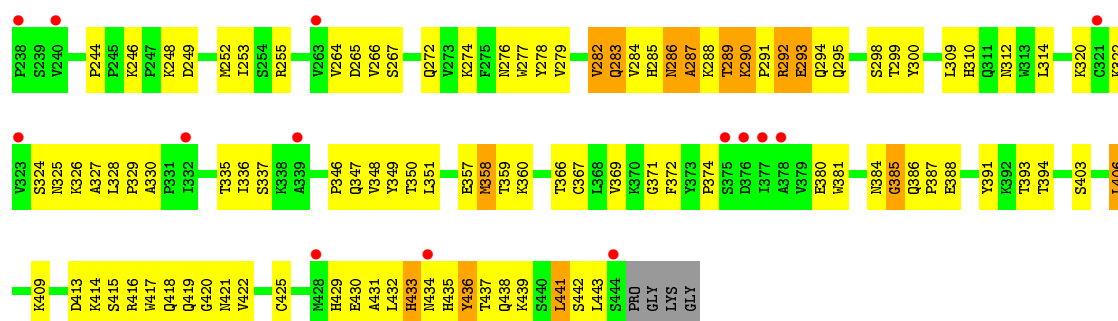
- Molecule 2: 2G12 IgG dimer light chain



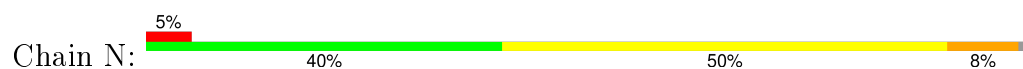
- Molecule 2: 2G12 IgG dimer light chain

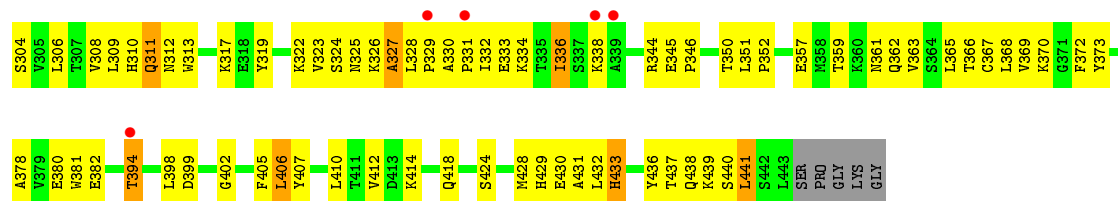


- Molecule 3: Hepatitis B virus receptor binding protein

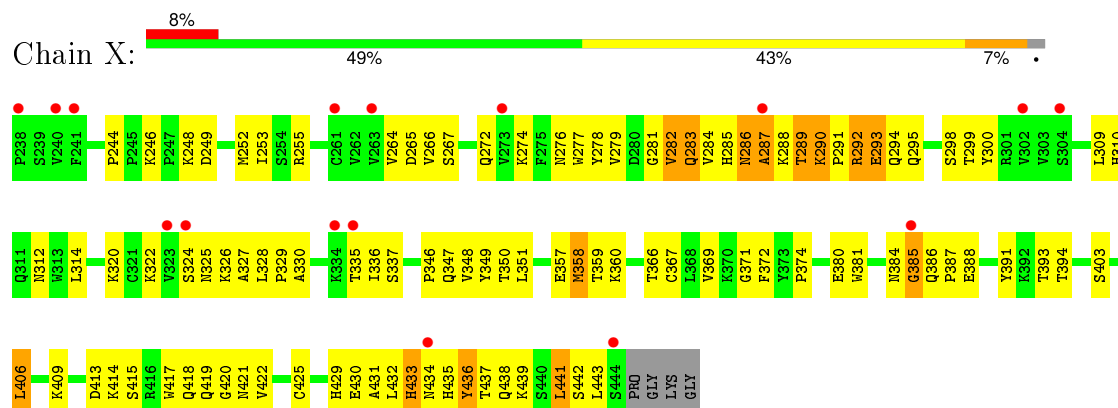


- Molecule 3: Hepatitis B virus receptor binding protein

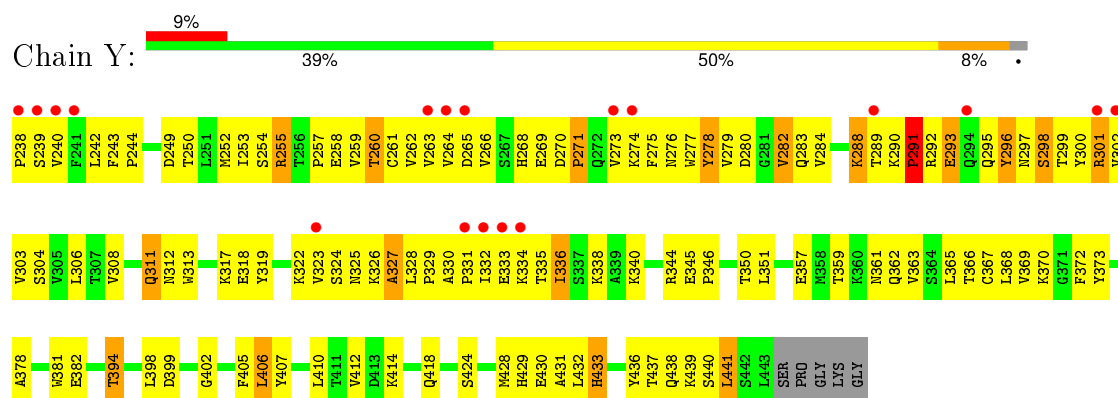




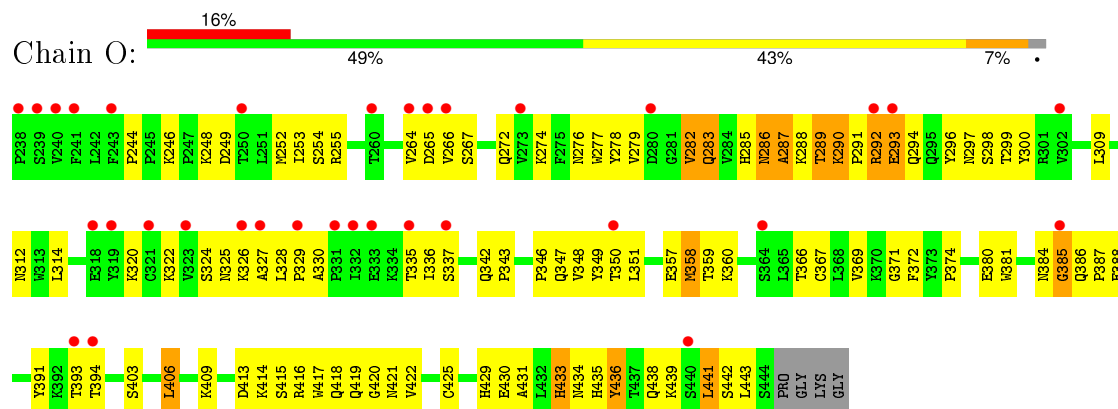
• Molecule 3: Hepatitis B virus receptor binding protein



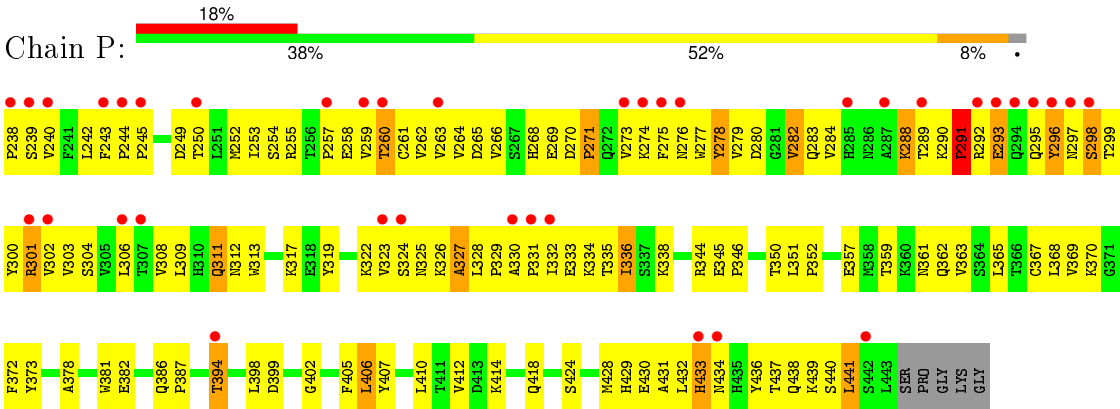
• Molecule 3: Hepatitis B virus receptor binding protein



• Molecule 3: Hepatitis B virus receptor binding protein



• Molecule 3: Hepatitis B virus receptor binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	246.25Å 246.25Å 657.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.75 – 8.00 39.75 – 7.43	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.75-8.00) 82.2 (39.75-7.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 7.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.359 , 0.369 0.352 , 0.368	Depositor DCC
R_{free} test set	1263 reflections (9.99%)	DCC
Wilson B-factor (Å ²)	296.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 280.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 13337 reflections	Xtriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	29250	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.69	1/1633 (0.1%)	0.95	4/2220 (0.2%)
1	D	0.63	0/1631	0.85	3/2214 (0.1%)
1	E	0.67	0/1633	0.93	4/2220 (0.2%)
1	H	0.63	0/1633	0.92	3/2220 (0.1%)
1	I	0.68	0/1631	0.83	3/2214 (0.1%)
1	M	0.68	2/1631 (0.1%)	0.85	3/2214 (0.1%)
2	B	0.63	0/1654	0.75	1/2246 (0.0%)
2	C	0.70	1/1654 (0.1%)	0.78	2/2246 (0.1%)
2	F	0.69	0/1654	0.77	2/2246 (0.1%)
2	G	0.69	1/1654 (0.1%)	0.77	1/2246 (0.0%)
2	K	0.63	0/1654	0.77	3/2246 (0.1%)
2	L	0.67	1/1654 (0.1%)	0.78	1/2246 (0.0%)
3	J	0.43	0/1706	0.68	0/2323
3	N	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	O	0.43	0/1706	0.68	0/2323
3	P	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	X	0.43	0/1706	0.68	0/2323
3	Y	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
All	All	0.60	9/29931 (0.0%)	0.78	36/40683 (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	E	0	3
3	N	0	1
3	P	0	1
3	Y	0	1
All	All	0	6

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	433	HIS	CA-C	11.57	1.83	1.52
3	N	433	HIS	CA-C	11.50	1.82	1.52
3	P	433	HIS	CA-C	11.50	1.82	1.52
1	M	36	TRP	CB-CG	6.40	1.61	1.50
2	C	143	GLU	CB-CG	6.03	1.63	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH1	-17.15	111.73	120.30
1	H	28	ARG	NE-CZ-NH1	-16.64	111.98	120.30
1	E	28	ARG	NE-CZ-NH1	-15.56	112.52	120.30
1	A	28	ARG	NE-CZ-NH2	14.53	127.56	120.30
1	E	28	ARG	NE-CZ-NH2	13.74	127.17	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	139	LYS	Peptide
1	E	140	SER	Peptide
1	E	142	SER	Peptide
3	N	373	TYR	Sidechain
3	Y	373	TYR	Sidechain

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	1600	0	1581	73	0
1	D	1600	0	1579	96	11
1	E	1600	0	1581	72	0
1	H	1600	0	1580	78	2
1	I	1600	0	1578	78	0
1	M	1600	0	1579	85	0
2	B	1618	0	1580	49	23
2	C	1618	0	1580	54	0
2	F	1618	0	1580	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1618	0	1580	58	2
2	K	1618	0	1580	54	0
2	L	1618	0	1580	57	19
3	J	1660	0	1632	99	60
3	N	1654	0	1627	114	37
3	O	1660	0	1630	93	19
3	P	1654	0	1624	123	37
3	X	1660	0	1632	98	56
3	Y	1654	0	1627	118	37
All	All	29250	0	28730	1381	174

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 24.

The worst 5 of 1381 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:D:103:ARG:C	2:F:50:LYS:HZ2	1.05	1.59
3:P:433:HIS:C	3:P:433:HIS:CA	1.82	1.45
3:N:433:HIS:C	3:N:433:HIS:CA	1.82	1.45
3:Y:433:HIS:C	3:Y:433:HIS:CA	1.83	1.45
1:D:103:ARG:CA	2:F:50:LYS:NZ	1.90	1.34

The worst 5 of 174 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)
3:Y:252:MET:O	3:Y:253:ILE:CG1[12_555]	0.41	1.79
3:J:252:MET:O	3:X:253:ILE:CD1[12_545]	0.48	1.72
3:O:253:ILE:CA	3:O:253:ILE:CB[10_444]	0.59	1.61
3:J:253:ILE:CD1	3:X:252:MET:O[12_545]	0.66	1.54
3:Y:253:ILE:CA	3:Y:253:ILE:CA[12_555]	0.70	1.50

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	207/243 (85%)	184 (89%)	19 (9%)	4 (2%)	10	52
1	D	204/243 (84%)	185 (91%)	15 (7%)	4 (2%)	9	51
1	E	207/243 (85%)	186 (90%)	18 (9%)	3 (1%)	14	58
1	H	207/243 (85%)	187 (90%)	16 (8%)	4 (2%)	10	52
1	I	204/243 (84%)	182 (89%)	17 (8%)	5 (2%)	7	46
1	M	204/243 (84%)	186 (91%)	13 (6%)	5 (2%)	7	46
2	B	209/213 (98%)	187 (90%)	21 (10%)	1 (0%)	34	77
2	C	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	34	77
2	F	209/213 (98%)	184 (88%)	24 (12%)	1 (0%)	34	77
2	G	209/213 (98%)	186 (89%)	22 (10%)	1 (0%)	34	77
2	K	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	34	77
2	L	209/213 (98%)	186 (89%)	21 (10%)	2 (1%)	19	65
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	29
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
3	O	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	29
3	P	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
3	X	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	29
3	Y	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
All	All	3714/4002 (93%)	3276 (88%)	343 (9%)	95 (3%)	7	45

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	SER
1	A	141	THR
1	A	223	PRO
1	D	136	PRO
1	D	140	SER

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	180/205 (88%)	163 (91%)	17 (9%)	11	42
1	D	180/205 (88%)	162 (90%)	18 (10%)	9	38
1	E	180/205 (88%)	162 (90%)	18 (10%)	9	38
1	H	180/205 (88%)	165 (92%)	15 (8%)	14	49
1	I	180/205 (88%)	165 (92%)	15 (8%)	14	49
1	M	180/205 (88%)	163 (91%)	17 (9%)	11	42
2	B	182/184 (99%)	164 (90%)	18 (10%)	10	39
2	C	182/184 (99%)	165 (91%)	17 (9%)	11	42
2	F	182/184 (99%)	164 (90%)	18 (10%)	10	39
2	G	182/184 (99%)	164 (90%)	18 (10%)	10	39
2	K	182/184 (99%)	163 (90%)	19 (10%)	9	36
2	L	182/184 (99%)	164 (90%)	18 (10%)	10	39
3	J	193/196 (98%)	187 (97%)	6 (3%)	47	77
3	N	192/196 (98%)	180 (94%)	12 (6%)	22	59
3	O	193/196 (98%)	187 (97%)	6 (3%)	47	77
3	P	192/196 (98%)	180 (94%)	12 (6%)	22	59
3	X	193/196 (98%)	187 (97%)	6 (3%)	47	77
3	Y	192/196 (98%)	180 (94%)	12 (6%)	22	59
All	All	3327/3510 (95%)	3065 (92%)	262 (8%)	15	51

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	142	ARG
3	N	260	THR
1	M	211	LYS
2	G	197	THR
1	I	156	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
3	X	390	ASN
3	Y	312	ASN
3	P	361	ASN
3	X	418	GLN
3	Y	272	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 carbohydrates 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	209/243 (86%)	0.33	9 (4%) 39 37	114, 118, 126, 134	0
1	D	207/243 (85%)	0.29	5 (2%) 62 58	113, 118, 125, 139	0
1	E	209/243 (86%)	0.81	24 (11%) 6 12	178, 182, 190, 198	0
1	H	209/243 (86%)	0.26	4 (1%) 70 65	96, 100, 107, 115	0
1	I	207/243 (85%)	0.67	22 (10%) 8 13	177, 182, 189, 203	0
1	M	207/243 (85%)	0.17	3 (1%) 78 72	94, 100, 107, 121	0
2	B	211/213 (99%)	0.12	3 (1%) 78 72	113, 118, 124, 139	0
2	C	211/213 (99%)	0.29	9 (4%) 39 37	113, 118, 123, 143	0
2	F	211/213 (99%)	0.94	32 (15%) 3 9	177, 182, 188, 203	0
2	G	211/213 (99%)	0.90	29 (13%) 4 10	177, 182, 187, 207	0
2	K	211/213 (99%)	0.29	2 (0%) 85 81	94, 100, 105, 120	0
2	L	211/213 (99%)	0.25	3 (1%) 78 72	94, 100, 105, 124	0
3	J	207/211 (98%)	0.61	14 (6%) 20 23	176, 176, 176, 176	0
3	N	206/211 (97%)	0.63	11 (5%) 30 31	179, 179, 179, 179	0
3	O	207/211 (98%)	1.00	33 (15%) 3 8	274, 274, 274, 274	0
3	P	206/211 (97%)	1.02	38 (18%) 2 7	277, 277, 277, 277	0
3	X	207/211 (98%)	0.54	16 (7%) 16 20	167, 167, 167, 167	0
3	Y	206/211 (97%)	0.59	18 (8%) 13 17	171, 171, 171, 171	0
All	All	3753/4002 (93%)	0.54	275 (7%) 18 21	94, 167, 277, 277	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	134	CYS	6.7
3	O	238	PRO	6.0
1	E	193	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	190	SER	5.4
1	I	152	VAL	5.2

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.