



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 07:49 am BST

PDB ID : 4NHH  
Title : 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 : 6.50 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

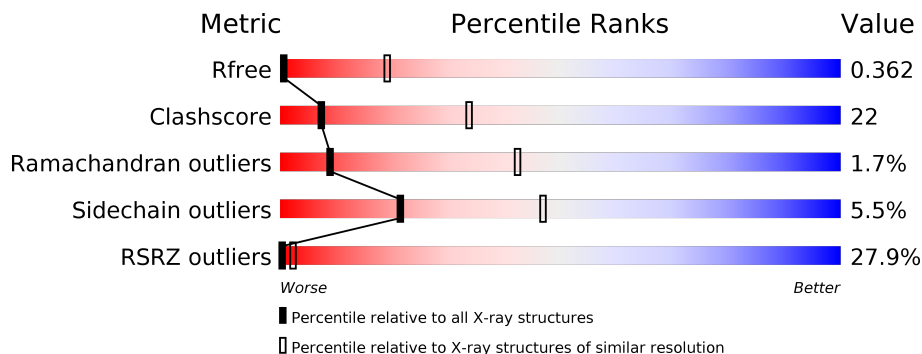
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.50 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	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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  $\geq 3$ , 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	F	213	
1	G	213	
1	K	213	
1	L	213	
1	P	213	
1	Q	213	

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Mol	Chain	Length	Quality of chain
2	E	229	
2	H	229	
2	I	229	
2	M	229	
2	O	229	
2	R	229	
3	A	211	
3	B	211	
3	C	211	
3	D	211	
3	J	211	
3	N	211	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 28972 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 light chain.

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

- Molecule 2 is a protein called Hepatitis B virus receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	209	Total 1565	C 988	N 268	O 303	S 6	0	0	0
2	M	206	Total 1542	C 974	N 263	O 299	S 6	0	0	0
2	E	210	Total 1574	C 994	N 270	O 304	S 6	0	0	0
2	I	206	Total 1544	C 976	N 265	O 297	S 6	0	0	0
2	O	208	Total 1555	C 982	N 265	O 302	S 6	0	0	0
2	R	206	Total 1542	C 974	N 263	O 299	S 6	0	0	0

There are 1158 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLU	SER	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	PHE	CONFLICT	UNP Q6PYX1
H	5	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	6	GLU	-	EXPRESSION TAG	UNP Q6PYX1
H	7	SER	-	EXPRESSION TAG	UNP Q6PYX1
H	8	GLY	-	EXPRESSION TAG	UNP Q6PYX1
H	9	GLY	-	EXPRESSION TAG	UNP Q6PYX1
H	10	GLY	PHE	CONFLICT	UNP Q6PYX1
H	11	LEU	PRO	CONFLICT	UNP Q6PYX1
H	12	VAL	PRO	CONFLICT	UNP Q6PYX1
H	14	ALA	PRO	CONFLICT	UNP Q6PYX1
H	15	GLY	LYS	CONFLICT	UNP Q6PYX1
H	16	GLY	ASP	CONFLICT	UNP Q6PYX1
H	17	SER	THR	CONFLICT	UNP Q6PYX1
H	19	ILE	MET	CONFLICT	UNP Q6PYX1
H	20	LEU	ILE	CONFLICT	UNP Q6PYX1
H	?	-	ARG	DELETION	UNP Q6PYX1
H	?	-	THR	DELETION	UNP Q6PYX1
H	?	-	PRO	DELETION	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	?	-	VAL	DELETION	UNP Q6PYX1
H	?	-	THR	DELETION	UNP Q6PYX1
H	23	GLY	VAL	CONFLICT	UNP Q6PYX1
H	25	SER	-	EXPRESSION TAG	UNP Q6PYX1
H	26	ASN	-	EXPRESSION TAG	UNP Q6PYX1
H	27	PHE	VAL	CONFLICT	UNP Q6PYX1
H	28	ARG	ASP	CONFLICT	UNP Q6PYX1
H	29	ILE	VAL	CONFLICT	UNP Q6PYX1
H	31	ALA	-	EXPRESSION TAG	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	?	-	ASP	DELETION	UNP Q6PYX1
H	?	-	PRO	DELETION	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	?	-	VAL	DELETION	UNP Q6PYX1
H	33	THR	LYS	CONFLICT	UNP Q6PYX1
H	34	MET	PHE	CONFLICT	UNP Q6PYX1
H	37	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	38	ARG	-	EXPRESSION TAG	UNP Q6PYX1
H	39	ARG	TYR	CONFLICT	UNP Q6PYX1
H	41	PRO	-	EXPRESSION TAG	UNP Q6PYX1
H	42	GLY	-	EXPRESSION TAG	UNP Q6PYX1
H	43	GLY	ASP	CONFLICT	UNP Q6PYX1
H	45	LEU	VAL	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	47	TRP	-	EXPRESSION TAG	UNP Q6PYX1
H	?	-	HIS	DELETION	UNP Q6PYX1
H	?	-	ASN	DELETION	UNP Q6PYX1
H	?	-	LYS	DELETION	UNP Q6PYX1
H	?	-	THR	DELETION	UNP Q6PYX1
H	?	-	LYS	DELETION	UNP Q6PYX1
H	?	-	PRO	DELETION	UNP Q6PYX1
H	?	-	ARG	DELETION	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	50	SER	GLU	CONFLICT	UNP Q6PYX1
H	51	ILE	GLN	CONFLICT	UNP Q6PYX1
H	52	SER	TYR	CONFLICT	UNP Q6PYX1
H	53	SER	ASN	CONFLICT	UNP Q6PYX1
H	58	ASP	-	EXPRESSION TAG	UNP Q6PYX1
H	59	TYR	-	EXPRESSION TAG	UNP Q6PYX1
H	60	ALA	-	EXPRESSION TAG	UNP Q6PYX1
H	61	ASP	-	EXPRESSION TAG	UNP Q6PYX1
H	62	ALA	-	EXPRESSION TAG	UNP Q6PYX1
H	64	LYS	VAL	CONFLICT	UNP Q6PYX1
H	65	GLY	SER	CONFLICT	UNP Q6PYX1
H	66	ARG	VAL	CONFLICT	UNP Q6PYX1
H	67	PHE	LEU	CONFLICT	UNP Q6PYX1
H	70	SER	-	EXPRESSION TAG	UNP Q6PYX1
H	71	ARG	-	EXPRESSION TAG	UNP Q6PYX1
H	72	ASP	-	EXPRESSION TAG	UNP Q6PYX1
H	73	ASP	-	EXPRESSION TAG	UNP Q6PYX1
H	?	-	HIS	DELETION	UNP Q6PYX1
H	75	GLU	GLN	CONFLICT	UNP Q6PYX1
H	77	PHE	-	EXPRESSION TAG	UNP Q6PYX1
H	78	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	79	TYR	TRP	CONFLICT	UNP Q6PYX1
H	81	GLN	-	EXPRESSION TAG	UNP Q6PYX1
H	82	MET	ASN	CONFLICT	UNP Q6PYX1
H	83	HIS	GLY	CONFLICT	UNP Q6PYX1
H	85	ARG	-	EXPRESSION TAG	UNP Q6PYX1
H	86	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	88	ASP	-	EXPRESSION TAG	UNP Q6PYX1
H	89	THR	-	EXPRESSION TAG	UNP Q6PYX1
H	90	ALA	-	EXPRESSION TAG	UNP Q6PYX1
H	91	ILE	-	EXPRESSION TAG	UNP Q6PYX1
H	93	TYR	LYS	CONFLICT	UNP Q6PYX1
H	95	ALA	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	96	ARG	-	EXPRESSION TAG	UNP Q6PYX1
H	98	GLY	VAL	CONFLICT	UNP Q6PYX1
H	?	-	ASN	DELETION	UNP Q6PYX1
H	100	ASP	LYS	CONFLICT	UNP Q6PYX1
H	101	ARG	ALA	CONFLICT	UNP Q6PYX1
H	103	ASP	PRO	CONFLICT	UNP Q6PYX1
H	105	TRP	-	EXPRESSION TAG	UNP Q6PYX1
H	106	GLY	-	EXPRESSION TAG	UNP Q6PYX1
H	108	GLY	-	EXPRESSION TAG	UNP Q6PYX1
H	109	THR	ILE	CONFLICT	UNP Q6PYX1
H	110	VAL	GLU	CONFLICT	UNP Q6PYX1
H	111	VAL	LYS	CONFLICT	UNP Q6PYX1
H	113	VAL	ILE	CONFLICT	UNP Q6PYX1
H	115	PRO	LYS	CONFLICT	UNP Q6PYX1
H	117	SER	-	EXPRESSION TAG	UNP Q6PYX1
H	118	THR	-	EXPRESSION TAG	UNP Q6PYX1
H	?	-	GLN	DELETION	UNP Q6PYX1
H	?	-	PRO	DELETION	UNP Q6PYX1
H	?	-	ARG	DELETION	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	122	SER	GLN	CONFLICT	UNP Q6PYX1
H	124	PHE	TYR	CONFLICT	UNP Q6PYX1
H	125	PRO	THR	CONFLICT	UNP Q6PYX1
H	127	ALA	PRO	CONFLICT	UNP Q6PYX1
H	?	-	ARG	DELETION	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	130	GLY	MET	CONFLICT	UNP Q6PYX1
H	?	-	LYS	DELETION	UNP Q6PYX1
H	?	-	ASN	DELETION	UNP Q6PYX1
H	?	-	GLN	DELETION	UNP Q6PYX1
H	132	ALA	VAL	CONFLICT	UNP Q6PYX1
H	133	ALA	SER	CONFLICT	UNP Q6PYX1
H	135	GLY	THR	CONFLICT	UNP Q6PYX1
H	140	ASP	GLY	CONFLICT	UNP Q6PYX1
H	141	TYR	PHE	CONFLICT	UNP Q6PYX1
H	142	PHE	TYR	CONFLICT	UNP Q6PYX1
H	144	GLU	SER	CONFLICT	UNP Q6PYX1
H	145	PRO	ASP	CONFLICT	UNP Q6PYX1
H	146	VAL	ILE	CONFLICT	UNP Q6PYX1
H	147	THR	ALA	CONFLICT	UNP Q6PYX1
H	149	SER	GLU	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	151	ASN	GLU	CONFLICT	UNP Q6PYX1
H	?	-	ASN	DELETION	UNP Q6PYX1
H	154	ALA	GLN	CONFLICT	UNP Q6PYX1
H	155	LEU	PRO	CONFLICT	UNP Q6PYX1
H	156	THR	GLU	CONFLICT	UNP Q6PYX1
H	157	SER	ASN	CONFLICT	UNP Q6PYX1
H	158	GLY	ASN	CONFLICT	UNP Q6PYX1
H	159	VAL	TYR	CONFLICT	UNP Q6PYX1
H	160	HIS	LYS	CONFLICT	UNP Q6PYX1
H	162	PHE	THR	CONFLICT	UNP Q6PYX1
H	164	ALA	PRO	CONFLICT	UNP Q6PYX1
H	167	GLN	ASP	CONFLICT	UNP Q6PYX1
H	169	SER	ASP	CONFLICT	UNP Q6PYX1
H	?	-	SER	DELETION	UNP Q6PYX1
H	?	-	PHE	DELETION	UNP Q6PYX1
H	?	-	PHE	DELETION	UNP Q6PYX1
H	?	-	LYS	DELETION	UNP Q6PYX1
H	175	SER	-	EXPRESSION TAG	UNP Q6PYX1
H	176	SER	-	EXPRESSION TAG	UNP Q6PYX1
H	177	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	178	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	181	PRO	ASP	CONFLICT	UNP Q6PYX1
H	182	SER	LYS	CONFLICT	UNP Q6PYX1
H	?	-	ARG	DELETION	UNP Q6PYX1
H	?	-	TRP	DELETION	UNP Q6PYX1
H	184	SER	GLN	CONFLICT	UNP Q6PYX1
H	185	LEU	GLN	CONFLICT	UNP Q6PYX1
H	187	THR	-	EXPRESSION TAG	UNP Q6PYX1
H	188	GLN	ASN	CONFLICT	UNP Q6PYX1
H	189	THR	VAL	CONFLICT	UNP Q6PYX1
H	190	TYR	PHE	CONFLICT	UNP Q6PYX1
H	191	ILE	SER	CONFLICT	UNP Q6PYX1
H	193	ASN	SER	CONFLICT	UNP Q6PYX1
H	?	-	MET	DELETION	UNP Q6PYX1
H	?	-	HIS	DELETION	UNP Q6PYX1
H	?	-	GLU	DELETION	UNP Q6PYX1
H	?	-	ALA	DELETION	UNP Q6PYX1
H	?	-	LEU	DELETION	UNP Q6PYX1
H	?	-	HIS	DELETION	UNP Q6PYX1
H	197	LYS	-	EXPRESSION TAG	UNP Q6PYX1
H	198	PRO	-	EXPRESSION TAG	UNP Q6PYX1
H	199	SER	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	200	ASN	TYR	CONFLICT	UNP Q6PYX1
H	202	LYS	-	EXPRESSION TAG	UNP Q6PYX1
H	203	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	204	ASP	-	EXPRESSION TAG	UNP Q6PYX1
H	205	LYS	-	EXPRESSION TAG	UNP Q6PYX1
H	206	LYS	-	EXPRESSION TAG	UNP Q6PYX1
H	207	VAL	-	EXPRESSION TAG	UNP Q6PYX1
H	208	GLU	-	EXPRESSION TAG	UNP Q6PYX1
H	209	PRO	GLN	CONFLICT	UNP Q6PYX1
H	212	CYS	-	EXPRESSION TAG	UNP Q6PYX1
H	213	ASP	-	EXPRESSION TAG	UNP Q6PYX1
H	214	LYS	-	EXPRESSION TAG	UNP Q6PYX1
H	215	THR	LEU	CONFLICT	UNP Q6PYX1
H	217	THR	LEU	CONFLICT	UNP Q6PYX1
H	218	CYS	SER	CONFLICT	UNP Q6PYX1
H	220	PRO	-	EXPRESSION TAG	UNP Q6PYX1
H	221	CYS	-	EXPRESSION TAG	UNP Q6PYX1
H	222	PRO	-	EXPRESSION TAG	UNP Q6PYX1
H	223	ALA	-	EXPRESSION TAG	UNP Q6PYX1
H	224	PRO	-	EXPRESSION TAG	UNP Q6PYX1
H	225	GLU	-	EXPRESSION TAG	UNP Q6PYX1
H	226	LEU	-	EXPRESSION TAG	UNP Q6PYX1
H	227	LEU	-	EXPRESSION TAG	UNP Q6PYX1
H	229	GLY	LYS	CONFLICT	UNP Q6PYX1
M	1	GLU	SER	CONFLICT	UNP Q6PYX1
M	3	GLN	PHE	CONFLICT	UNP Q6PYX1
M	5	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	6	GLU	-	EXPRESSION TAG	UNP Q6PYX1
M	7	SER	-	EXPRESSION TAG	UNP Q6PYX1
M	8	GLY	-	EXPRESSION TAG	UNP Q6PYX1
M	9	GLY	-	EXPRESSION TAG	UNP Q6PYX1
M	10	GLY	PHE	CONFLICT	UNP Q6PYX1
M	11	LEU	PRO	CONFLICT	UNP Q6PYX1
M	12	VAL	PRO	CONFLICT	UNP Q6PYX1
M	14	ALA	PRO	CONFLICT	UNP Q6PYX1
M	15	GLY	LYS	CONFLICT	UNP Q6PYX1
M	16	GLY	ASP	CONFLICT	UNP Q6PYX1
M	17	SER	THR	CONFLICT	UNP Q6PYX1
M	19	ILE	MET	CONFLICT	UNP Q6PYX1
M	20	LEU	ILE	CONFLICT	UNP Q6PYX1
M	?	-	ARG	DELETION	UNP Q6PYX1
M	?	-	THR	DELETION	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	PRO	DELETION	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	?	-	VAL	DELETION	UNP Q6PYX1
M	?	-	THR	DELETION	UNP Q6PYX1
M	23	GLY	VAL	CONFLICT	UNP Q6PYX1
M	25	SER	-	EXPRESSION TAG	UNP Q6PYX1
M	26	ASN	-	EXPRESSION TAG	UNP Q6PYX1
M	27	PHE	VAL	CONFLICT	UNP Q6PYX1
M	28	ARG	ASP	CONFLICT	UNP Q6PYX1
M	29	ILE	VAL	CONFLICT	UNP Q6PYX1
M	31	ALA	-	EXPRESSION TAG	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	?	-	ASP	DELETION	UNP Q6PYX1
M	?	-	PRO	DELETION	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	?	-	VAL	DELETION	UNP Q6PYX1
M	33	THR	LYS	CONFLICT	UNP Q6PYX1
M	34	MET	PHE	CONFLICT	UNP Q6PYX1
M	37	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	38	ARG	-	EXPRESSION TAG	UNP Q6PYX1
M	39	ARG	TYR	CONFLICT	UNP Q6PYX1
M	41	PRO	-	EXPRESSION TAG	UNP Q6PYX1
M	42	GLY	-	EXPRESSION TAG	UNP Q6PYX1
M	43	GLY	ASP	CONFLICT	UNP Q6PYX1
M	45	LEU	VAL	CONFLICT	UNP Q6PYX1
M	47	TRP	-	EXPRESSION TAG	UNP Q6PYX1
M	?	-	HIS	DELETION	UNP Q6PYX1
M	?	-	ASN	DELETION	UNP Q6PYX1
M	?	-	LYS	DELETION	UNP Q6PYX1
M	?	-	THR	DELETION	UNP Q6PYX1
M	?	-	LYS	DELETION	UNP Q6PYX1
M	?	-	PRO	DELETION	UNP Q6PYX1
M	?	-	ARG	DELETION	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	50	SER	GLU	CONFLICT	UNP Q6PYX1
M	51	ILE	GLN	CONFLICT	UNP Q6PYX1
M	52	SER	TYR	CONFLICT	UNP Q6PYX1
M	53	SER	ASN	CONFLICT	UNP Q6PYX1
M	58	ASP	-	EXPRESSION TAG	UNP Q6PYX1
M	59	TYR	-	EXPRESSION TAG	UNP Q6PYX1
M	60	ALA	-	EXPRESSION TAG	UNP Q6PYX1
M	61	ASP	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	62	ALA	-	EXPRESSION TAG	UNP Q6PYX1
M	64	LYS	VAL	CONFLICT	UNP Q6PYX1
M	65	GLY	SER	CONFLICT	UNP Q6PYX1
M	66	ARG	VAL	CONFLICT	UNP Q6PYX1
M	67	PHE	LEU	CONFLICT	UNP Q6PYX1
M	70	SER	-	EXPRESSION TAG	UNP Q6PYX1
M	71	ARG	-	EXPRESSION TAG	UNP Q6PYX1
M	72	ASP	-	EXPRESSION TAG	UNP Q6PYX1
M	73	ASP	-	EXPRESSION TAG	UNP Q6PYX1
M	?	-	HIS	DELETION	UNP Q6PYX1
M	75	GLU	GLN	CONFLICT	UNP Q6PYX1
M	77	PHE	-	EXPRESSION TAG	UNP Q6PYX1
M	78	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	79	TYR	TRP	CONFLICT	UNP Q6PYX1
M	81	GLN	-	EXPRESSION TAG	UNP Q6PYX1
M	82	MET	ASN	CONFLICT	UNP Q6PYX1
M	82A	HIS	GLY	CONFLICT	UNP Q6PYX1
M	83	ARG	-	EXPRESSION TAG	UNP Q6PYX1
M	84	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	86	ASP	-	EXPRESSION TAG	UNP Q6PYX1
M	87	THR	-	EXPRESSION TAG	UNP Q6PYX1
M	88	ALA	-	EXPRESSION TAG	UNP Q6PYX1
M	89	ILE	-	EXPRESSION TAG	UNP Q6PYX1
M	91	TYR	LYS	CONFLICT	UNP Q6PYX1
M	93	ALA	-	EXPRESSION TAG	UNP Q6PYX1
M	94	ARG	-	EXPRESSION TAG	UNP Q6PYX1
M	96	GLY	VAL	CONFLICT	UNP Q6PYX1
M	?	-	ASN	DELETION	UNP Q6PYX1
M	98	ASP	LYS	CONFLICT	UNP Q6PYX1
M	99	ARG	ALA	CONFLICT	UNP Q6PYX1
M	101	ASP	PRO	CONFLICT	UNP Q6PYX1
M	103	TRP	-	EXPRESSION TAG	UNP Q6PYX1
M	104	GLY	-	EXPRESSION TAG	UNP Q6PYX1
M	106	GLY	-	EXPRESSION TAG	UNP Q6PYX1
M	107	THR	ILE	CONFLICT	UNP Q6PYX1
M	108	VAL	GLU	CONFLICT	UNP Q6PYX1
M	109	VAL	LYS	CONFLICT	UNP Q6PYX1
M	111	VAL	ILE	CONFLICT	UNP Q6PYX1
M	113	PRO	LYS	CONFLICT	UNP Q6PYX1
M	115	SER	-	EXPRESSION TAG	UNP Q6PYX1
M	116	THR	-	EXPRESSION TAG	UNP Q6PYX1
M	?	-	GLN	DELETION	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	PRO	DELETION	UNP Q6PYX1
M	?	-	ARG	DELETION	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	120	SER	GLN	CONFLICT	UNP Q6PYX1
M	122	PHE	TYR	CONFLICT	UNP Q6PYX1
M	123	PRO	THR	CONFLICT	UNP Q6PYX1
M	125	ALA	PRO	CONFLICT	UNP Q6PYX1
M	?	-	ARG	DELETION	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	136	GLY	MET	CONFLICT	UNP Q6PYX1
M	?	-	LYS	DELETION	UNP Q6PYX1
M	?	-	ASN	DELETION	UNP Q6PYX1
M	?	-	GLN	DELETION	UNP Q6PYX1
M	138	ALA	VAL	CONFLICT	UNP Q6PYX1
M	139	ALA	SER	CONFLICT	UNP Q6PYX1
M	141	GLY	THR	CONFLICT	UNP Q6PYX1
M	146	ASP	GLY	CONFLICT	UNP Q6PYX1
M	147	TYR	PHE	CONFLICT	UNP Q6PYX1
M	148	PHE	TYR	CONFLICT	UNP Q6PYX1
M	150	GLU	SER	CONFLICT	UNP Q6PYX1
M	151	PRO	ASP	CONFLICT	UNP Q6PYX1
M	152	VAL	ILE	CONFLICT	UNP Q6PYX1
M	153	THR	ALA	CONFLICT	UNP Q6PYX1
M	156	SER	GLU	CONFLICT	UNP Q6PYX1
M	162	ASN	GLU	CONFLICT	UNP Q6PYX1
M	?	-	ASN	DELETION	UNP Q6PYX1
M	165	ALA	GLN	CONFLICT	UNP Q6PYX1
M	166	LEU	PRO	CONFLICT	UNP Q6PYX1
M	167	THR	GLU	CONFLICT	UNP Q6PYX1
M	168	SER	ASN	CONFLICT	UNP Q6PYX1
M	169	GLY	ASN	CONFLICT	UNP Q6PYX1
M	171	VAL	TYR	CONFLICT	UNP Q6PYX1
M	172	HIS	LYS	CONFLICT	UNP Q6PYX1
M	174	PHE	THR	CONFLICT	UNP Q6PYX1
M	176	ALA	PRO	CONFLICT	UNP Q6PYX1
M	179	GLN	ASP	CONFLICT	UNP Q6PYX1
M	182	SER	ASP	CONFLICT	UNP Q6PYX1
M	?	-	SER	DELETION	UNP Q6PYX1
M	?	-	PHE	DELETION	UNP Q6PYX1
M	?	-	PHE	DELETION	UNP Q6PYX1
M	?	-	LYS	DELETION	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	188	SER	-	EXPRESSION TAG	UNP Q6PYX1
M	189	SER	-	EXPRESSION TAG	UNP Q6PYX1
M	190	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	191	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	194	PRO	ASP	CONFLICT	UNP Q6PYX1
M	195	SER	LYS	CONFLICT	UNP Q6PYX1
M	?	-	ARG	DELETION	UNP Q6PYX1
M	?	-	TRP	DELETION	UNP Q6PYX1
M	197	SER	GLN	CONFLICT	UNP Q6PYX1
M	198	LEU	GLN	CONFLICT	UNP Q6PYX1
M	200	THR	-	EXPRESSION TAG	UNP Q6PYX1
M	203	GLN	ASN	CONFLICT	UNP Q6PYX1
M	205	THR	VAL	CONFLICT	UNP Q6PYX1
M	206	TYR	PHE	CONFLICT	UNP Q6PYX1
M	207	ILE	SER	CONFLICT	UNP Q6PYX1
M	209	ASN	SER	CONFLICT	UNP Q6PYX1
M	?	-	MET	DELETION	UNP Q6PYX1
M	?	-	HIS	DELETION	UNP Q6PYX1
M	?	-	GLU	DELETION	UNP Q6PYX1
M	?	-	ALA	DELETION	UNP Q6PYX1
M	?	-	LEU	DELETION	UNP Q6PYX1
M	?	-	HIS	DELETION	UNP Q6PYX1
M	213	LYS	-	EXPRESSION TAG	UNP Q6PYX1
M	214	PRO	-	EXPRESSION TAG	UNP Q6PYX1
M	215	SER	-	EXPRESSION TAG	UNP Q6PYX1
M	216	ASN	TYR	CONFLICT	UNP Q6PYX1
M	218	LYS	-	EXPRESSION TAG	UNP Q6PYX1
M	219	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	220	ASP	-	EXPRESSION TAG	UNP Q6PYX1
M	221	LYS	-	EXPRESSION TAG	UNP Q6PYX1
M	222	LYS	-	EXPRESSION TAG	UNP Q6PYX1
M	225	VAL	-	EXPRESSION TAG	UNP Q6PYX1
M	226	GLU	-	EXPRESSION TAG	UNP Q6PYX1
M	227	PRO	GLN	CONFLICT	UNP Q6PYX1
M	230	CYS	-	EXPRESSION TAG	UNP Q6PYX1
M	231	ASP	-	EXPRESSION TAG	UNP Q6PYX1
M	232	LYS	-	EXPRESSION TAG	UNP Q6PYX1
M	233	THR	LEU	CONFLICT	UNP Q6PYX1
M	235	THR	LEU	CONFLICT	UNP Q6PYX1
M	236	CYS	SER	CONFLICT	UNP Q6PYX1
M	238	PRO	-	EXPRESSION TAG	UNP Q6PYX1
M	239	CYS	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	240	PRO	-	EXPRESSION TAG	UNP Q6PYX1
M	241	ALA	-	EXPRESSION TAG	UNP Q6PYX1
M	242	PRO	-	EXPRESSION TAG	UNP Q6PYX1
M	243	GLU	-	EXPRESSION TAG	UNP Q6PYX1
M	244	LEU	-	EXPRESSION TAG	UNP Q6PYX1
M	245	LEU	-	EXPRESSION TAG	UNP Q6PYX1
M	247	GLY	LYS	CONFLICT	UNP Q6PYX1
E	1	GLU	SER	CONFLICT	UNP Q6PYX1
E	3	GLN	PHE	CONFLICT	UNP Q6PYX1
E	5	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	6	GLU	-	EXPRESSION TAG	UNP Q6PYX1
E	7	SER	-	EXPRESSION TAG	UNP Q6PYX1
E	8	GLY	-	EXPRESSION TAG	UNP Q6PYX1
E	9	GLY	-	EXPRESSION TAG	UNP Q6PYX1
E	10	GLY	PHE	CONFLICT	UNP Q6PYX1
E	11	LEU	PRO	CONFLICT	UNP Q6PYX1
E	12	VAL	PRO	CONFLICT	UNP Q6PYX1
E	14	ALA	PRO	CONFLICT	UNP Q6PYX1
E	15	GLY	LYS	CONFLICT	UNP Q6PYX1
E	16	GLY	ASP	CONFLICT	UNP Q6PYX1
E	17	SER	THR	CONFLICT	UNP Q6PYX1
E	19	ILE	MET	CONFLICT	UNP Q6PYX1
E	20	LEU	ILE	CONFLICT	UNP Q6PYX1
E	?	-	ARG	DELETION	UNP Q6PYX1
E	?	-	THR	DELETION	UNP Q6PYX1
E	?	-	PRO	DELETION	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	?	-	VAL	DELETION	UNP Q6PYX1
E	?	-	THR	DELETION	UNP Q6PYX1
E	23	GLY	VAL	CONFLICT	UNP Q6PYX1
E	25	SER	-	EXPRESSION TAG	UNP Q6PYX1
E	26	ASN	-	EXPRESSION TAG	UNP Q6PYX1
E	27	PHE	VAL	CONFLICT	UNP Q6PYX1
E	28	ARG	ASP	CONFLICT	UNP Q6PYX1
E	29	ILE	VAL	CONFLICT	UNP Q6PYX1
E	31	ALA	-	EXPRESSION TAG	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	?	-	ASP	DELETION	UNP Q6PYX1
E	?	-	PRO	DELETION	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	?	-	VAL	DELETION	UNP Q6PYX1
E	33	THR	LYS	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	34	MET	PHE	CONFLICT	UNP Q6PYX1
E	37	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	38	ARG	-	EXPRESSION TAG	UNP Q6PYX1
E	39	ARG	TYR	CONFLICT	UNP Q6PYX1
E	41	PRO	-	EXPRESSION TAG	UNP Q6PYX1
E	42	GLY	-	EXPRESSION TAG	UNP Q6PYX1
E	43	GLY	ASP	CONFLICT	UNP Q6PYX1
E	45	LEU	VAL	CONFLICT	UNP Q6PYX1
E	47	TRP	-	EXPRESSION TAG	UNP Q6PYX1
E	?	-	HIS	DELETION	UNP Q6PYX1
E	?	-	ASN	DELETION	UNP Q6PYX1
E	?	-	LYS	DELETION	UNP Q6PYX1
E	?	-	THR	DELETION	UNP Q6PYX1
E	?	-	LYS	DELETION	UNP Q6PYX1
E	?	-	PRO	DELETION	UNP Q6PYX1
E	?	-	ARG	DELETION	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	50	SER	GLU	CONFLICT	UNP Q6PYX1
E	51	ILE	GLN	CONFLICT	UNP Q6PYX1
E	52	SER	TYR	CONFLICT	UNP Q6PYX1
E	53	SER	ASN	CONFLICT	UNP Q6PYX1
E	58	ASP	-	EXPRESSION TAG	UNP Q6PYX1
E	59	TYR	-	EXPRESSION TAG	UNP Q6PYX1
E	60	ALA	-	EXPRESSION TAG	UNP Q6PYX1
E	61	ASP	-	EXPRESSION TAG	UNP Q6PYX1
E	62	ALA	-	EXPRESSION TAG	UNP Q6PYX1
E	64	LYS	VAL	CONFLICT	UNP Q6PYX1
E	65	GLY	SER	CONFLICT	UNP Q6PYX1
E	66	ARG	VAL	CONFLICT	UNP Q6PYX1
E	67	PHE	LEU	CONFLICT	UNP Q6PYX1
E	70	SER	-	EXPRESSION TAG	UNP Q6PYX1
E	71	ARG	-	EXPRESSION TAG	UNP Q6PYX1
E	72	ASP	-	EXPRESSION TAG	UNP Q6PYX1
E	73	ASP	-	EXPRESSION TAG	UNP Q6PYX1
E	?	-	HIS	DELETION	UNP Q6PYX1
E	75	GLU	GLN	CONFLICT	UNP Q6PYX1
E	77	PHE	-	EXPRESSION TAG	UNP Q6PYX1
E	78	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	79	TYR	TRP	CONFLICT	UNP Q6PYX1
E	81	GLN	-	EXPRESSION TAG	UNP Q6PYX1
E	82	MET	ASN	CONFLICT	UNP Q6PYX1
E	83	HIS	GLY	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	85	ARG	-	EXPRESSION TAG	UNP Q6PYX1
E	86	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	88	ASP	-	EXPRESSION TAG	UNP Q6PYX1
E	89	THR	-	EXPRESSION TAG	UNP Q6PYX1
E	90	ALA	-	EXPRESSION TAG	UNP Q6PYX1
E	91	ILE	-	EXPRESSION TAG	UNP Q6PYX1
E	93	TYR	LYS	CONFLICT	UNP Q6PYX1
E	95	ALA	-	EXPRESSION TAG	UNP Q6PYX1
E	96	ARG	-	EXPRESSION TAG	UNP Q6PYX1
E	98	GLY	VAL	CONFLICT	UNP Q6PYX1
E	?	-	ASN	DELETION	UNP Q6PYX1
E	100	ASP	LYS	CONFLICT	UNP Q6PYX1
E	101	ARG	ALA	CONFLICT	UNP Q6PYX1
E	103	ASP	PRO	CONFLICT	UNP Q6PYX1
E	105	TRP	-	EXPRESSION TAG	UNP Q6PYX1
E	106	GLY	-	EXPRESSION TAG	UNP Q6PYX1
E	108	GLY	-	EXPRESSION TAG	UNP Q6PYX1
E	109	THR	ILE	CONFLICT	UNP Q6PYX1
E	110	VAL	GLU	CONFLICT	UNP Q6PYX1
E	111	VAL	LYS	CONFLICT	UNP Q6PYX1
E	113	VAL	ILE	CONFLICT	UNP Q6PYX1
E	115	PRO	LYS	CONFLICT	UNP Q6PYX1
E	117	SER	-	EXPRESSION TAG	UNP Q6PYX1
E	118	THR	-	EXPRESSION TAG	UNP Q6PYX1
E	?	-	GLN	DELETION	UNP Q6PYX1
E	?	-	PRO	DELETION	UNP Q6PYX1
E	?	-	ARG	DELETION	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	122	SER	GLN	CONFLICT	UNP Q6PYX1
E	124	PHE	TYR	CONFLICT	UNP Q6PYX1
E	125	PRO	THR	CONFLICT	UNP Q6PYX1
E	127	ALA	PRO	CONFLICT	UNP Q6PYX1
E	?	-	ARG	DELETION	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	130	GLY	MET	CONFLICT	UNP Q6PYX1
E	?	-	LYS	DELETION	UNP Q6PYX1
E	?	-	ASN	DELETION	UNP Q6PYX1
E	?	-	GLN	DELETION	UNP Q6PYX1
E	132	ALA	VAL	CONFLICT	UNP Q6PYX1
E	133	ALA	SER	CONFLICT	UNP Q6PYX1
E	135	GLY	THR	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	140	ASP	GLY	CONFLICT	UNP Q6PYX1
E	141	TYR	PHE	CONFLICT	UNP Q6PYX1
E	142	PHE	TYR	CONFLICT	UNP Q6PYX1
E	144	GLU	SER	CONFLICT	UNP Q6PYX1
E	145	PRO	ASP	CONFLICT	UNP Q6PYX1
E	146	VAL	ILE	CONFLICT	UNP Q6PYX1
E	147	THR	ALA	CONFLICT	UNP Q6PYX1
E	149	SER	GLU	CONFLICT	UNP Q6PYX1
E	151	ASN	GLU	CONFLICT	UNP Q6PYX1
E	?	-	ASN	DELETION	UNP Q6PYX1
E	154	ALA	GLN	CONFLICT	UNP Q6PYX1
E	155	LEU	PRO	CONFLICT	UNP Q6PYX1
E	156	THR	GLU	CONFLICT	UNP Q6PYX1
E	157	SER	ASN	CONFLICT	UNP Q6PYX1
E	158	GLY	ASN	CONFLICT	UNP Q6PYX1
E	159	VAL	TYR	CONFLICT	UNP Q6PYX1
E	160	HIS	LYS	CONFLICT	UNP Q6PYX1
E	162	PHE	THR	CONFLICT	UNP Q6PYX1
E	164	ALA	PRO	CONFLICT	UNP Q6PYX1
E	167	GLN	ASP	CONFLICT	UNP Q6PYX1
E	169	SER	ASP	CONFLICT	UNP Q6PYX1
E	?	-	SER	DELETION	UNP Q6PYX1
E	?	-	PHE	DELETION	UNP Q6PYX1
E	?	-	PHE	DELETION	UNP Q6PYX1
E	?	-	LYS	DELETION	UNP Q6PYX1
E	175	SER	-	EXPRESSION TAG	UNP Q6PYX1
E	176	SER	-	EXPRESSION TAG	UNP Q6PYX1
E	177	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	178	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	181	PRO	ASP	CONFLICT	UNP Q6PYX1
E	182	SER	LYS	CONFLICT	UNP Q6PYX1
E	?	-	ARG	DELETION	UNP Q6PYX1
E	?	-	TRP	DELETION	UNP Q6PYX1
E	184	SER	GLN	CONFLICT	UNP Q6PYX1
E	185	LEU	GLN	CONFLICT	UNP Q6PYX1
E	187	THR	-	EXPRESSION TAG	UNP Q6PYX1
E	188	GLN	ASN	CONFLICT	UNP Q6PYX1
E	189	THR	VAL	CONFLICT	UNP Q6PYX1
E	190	TYR	PHE	CONFLICT	UNP Q6PYX1
E	191	ILE	SER	CONFLICT	UNP Q6PYX1
E	193	ASN	SER	CONFLICT	UNP Q6PYX1
E	?	-	MET	DELETION	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	HIS	DELETION	UNP Q6PYX1
E	?	-	GLU	DELETION	UNP Q6PYX1
E	?	-	ALA	DELETION	UNP Q6PYX1
E	?	-	LEU	DELETION	UNP Q6PYX1
E	?	-	HIS	DELETION	UNP Q6PYX1
E	197	LYS	-	EXPRESSION TAG	UNP Q6PYX1
E	198	PRO	-	EXPRESSION TAG	UNP Q6PYX1
E	199	SER	-	EXPRESSION TAG	UNP Q6PYX1
E	200	ASN	TYR	CONFLICT	UNP Q6PYX1
E	202	LYS	-	EXPRESSION TAG	UNP Q6PYX1
E	203	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	204	ASP	-	EXPRESSION TAG	UNP Q6PYX1
E	205	LYS	-	EXPRESSION TAG	UNP Q6PYX1
E	206	LYS	-	EXPRESSION TAG	UNP Q6PYX1
E	207	VAL	-	EXPRESSION TAG	UNP Q6PYX1
E	208	GLU	-	EXPRESSION TAG	UNP Q6PYX1
E	209	PRO	GLN	CONFLICT	UNP Q6PYX1
E	212	CYS	-	EXPRESSION TAG	UNP Q6PYX1
E	213	ASP	-	EXPRESSION TAG	UNP Q6PYX1
E	214	LYS	-	EXPRESSION TAG	UNP Q6PYX1
E	215	THR	LEU	CONFLICT	UNP Q6PYX1
E	217	THR	LEU	CONFLICT	UNP Q6PYX1
E	218	CYS	SER	CONFLICT	UNP Q6PYX1
E	220	PRO	-	EXPRESSION TAG	UNP Q6PYX1
E	221	CYS	-	EXPRESSION TAG	UNP Q6PYX1
E	222	PRO	-	EXPRESSION TAG	UNP Q6PYX1
E	223	ALA	-	EXPRESSION TAG	UNP Q6PYX1
E	224	PRO	-	EXPRESSION TAG	UNP Q6PYX1
E	225	GLU	-	EXPRESSION TAG	UNP Q6PYX1
E	226	LEU	-	EXPRESSION TAG	UNP Q6PYX1
E	227	LEU	-	EXPRESSION TAG	UNP Q6PYX1
E	229	GLY	LYS	CONFLICT	UNP Q6PYX1
I	1	GLU	SER	CONFLICT	UNP Q6PYX1
I	3	GLN	PHE	CONFLICT	UNP Q6PYX1
I	5	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	6	GLU	-	EXPRESSION TAG	UNP Q6PYX1
I	7	SER	-	EXPRESSION TAG	UNP Q6PYX1
I	8	GLY	-	EXPRESSION TAG	UNP Q6PYX1
I	9	GLY	-	EXPRESSION TAG	UNP Q6PYX1
I	10	GLY	PHE	CONFLICT	UNP Q6PYX1
I	11	LEU	PRO	CONFLICT	UNP Q6PYX1
I	12	VAL	PRO	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	14	ALA	PRO	CONFLICT	UNP Q6PYX1
I	15	GLY	LYS	CONFLICT	UNP Q6PYX1
I	16	GLY	ASP	CONFLICT	UNP Q6PYX1
I	17	SER	THR	CONFLICT	UNP Q6PYX1
I	19	ILE	MET	CONFLICT	UNP Q6PYX1
I	20	LEU	ILE	CONFLICT	UNP Q6PYX1
I	?	-	ARG	DELETION	UNP Q6PYX1
I	?	-	THR	DELETION	UNP Q6PYX1
I	?	-	PRO	DELETION	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1
I	?	-	VAL	DELETION	UNP Q6PYX1
I	?	-	THR	DELETION	UNP Q6PYX1
I	23	GLY	VAL	CONFLICT	UNP Q6PYX1
I	25	SER	-	EXPRESSION TAG	UNP Q6PYX1
I	26	ASN	-	EXPRESSION TAG	UNP Q6PYX1
I	27	PHE	VAL	CONFLICT	UNP Q6PYX1
I	28	ARG	ASP	CONFLICT	UNP Q6PYX1
I	29	ILE	VAL	CONFLICT	UNP Q6PYX1
I	31	ALA	-	EXPRESSION TAG	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1
I	?	-	ASP	DELETION	UNP Q6PYX1
I	?	-	PRO	DELETION	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1
I	?	-	VAL	DELETION	UNP Q6PYX1
I	33	THR	LYS	CONFLICT	UNP Q6PYX1
I	34	MET	PHE	CONFLICT	UNP Q6PYX1
I	37	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	38	ARG	-	EXPRESSION TAG	UNP Q6PYX1
I	39	ARG	TYR	CONFLICT	UNP Q6PYX1
I	41	PRO	-	EXPRESSION TAG	UNP Q6PYX1
I	42	GLY	-	EXPRESSION TAG	UNP Q6PYX1
I	43	GLY	ASP	CONFLICT	UNP Q6PYX1
I	45	LEU	VAL	CONFLICT	UNP Q6PYX1
I	47	TRP	-	EXPRESSION TAG	UNP Q6PYX1
I	?	-	HIS	DELETION	UNP Q6PYX1
I	?	-	ASN	DELETION	UNP Q6PYX1
I	?	-	LYS	DELETION	UNP Q6PYX1
I	?	-	THR	DELETION	UNP Q6PYX1
I	?	-	LYS	DELETION	UNP Q6PYX1
I	?	-	PRO	DELETION	UNP Q6PYX1
I	?	-	ARG	DELETION	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	50	SER	GLU	CONFLICT	UNP Q6PYX1
I	51	ILE	GLN	CONFLICT	UNP Q6PYX1
I	52	SER	TYR	CONFLICT	UNP Q6PYX1
I	53	SER	ASN	CONFLICT	UNP Q6PYX1
I	58	ASP	-	EXPRESSION TAG	UNP Q6PYX1
I	59	TYR	-	EXPRESSION TAG	UNP Q6PYX1
I	60	ALA	-	EXPRESSION TAG	UNP Q6PYX1
I	61	ASP	-	EXPRESSION TAG	UNP Q6PYX1
I	62	ALA	-	EXPRESSION TAG	UNP Q6PYX1
I	64	LYS	VAL	CONFLICT	UNP Q6PYX1
I	65	GLY	SER	CONFLICT	UNP Q6PYX1
I	66	ARG	VAL	CONFLICT	UNP Q6PYX1
I	67	PHE	LEU	CONFLICT	UNP Q6PYX1
I	70	SER	-	EXPRESSION TAG	UNP Q6PYX1
I	71	ARG	-	EXPRESSION TAG	UNP Q6PYX1
I	72	ASP	-	EXPRESSION TAG	UNP Q6PYX1
I	73	ASP	-	EXPRESSION TAG	UNP Q6PYX1
I	?	-	HIS	DELETION	UNP Q6PYX1
I	75	GLU	GLN	CONFLICT	UNP Q6PYX1
I	77	PHE	-	EXPRESSION TAG	UNP Q6PYX1
I	78	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	79	TYR	TRP	CONFLICT	UNP Q6PYX1
I	81	GLN	-	EXPRESSION TAG	UNP Q6PYX1
I	82	MET	ASN	CONFLICT	UNP Q6PYX1
I	83	HIS	GLY	CONFLICT	UNP Q6PYX1
I	85	ARG	-	EXPRESSION TAG	UNP Q6PYX1
I	86	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	88	ASP	-	EXPRESSION TAG	UNP Q6PYX1
I	89	THR	-	EXPRESSION TAG	UNP Q6PYX1
I	90	ALA	-	EXPRESSION TAG	UNP Q6PYX1
I	91	ILE	-	EXPRESSION TAG	UNP Q6PYX1
I	93	TYR	LYS	CONFLICT	UNP Q6PYX1
I	95	ALA	-	EXPRESSION TAG	UNP Q6PYX1
I	96	ARG	-	EXPRESSION TAG	UNP Q6PYX1
I	98	GLY	VAL	CONFLICT	UNP Q6PYX1
I	?	-	ASN	DELETION	UNP Q6PYX1
I	100	ASP	LYS	CONFLICT	UNP Q6PYX1
I	101	ARG	ALA	CONFLICT	UNP Q6PYX1
I	103	ASP	PRO	CONFLICT	UNP Q6PYX1
I	105	TRP	-	EXPRESSION TAG	UNP Q6PYX1
I	106	GLY	-	EXPRESSION TAG	UNP Q6PYX1
I	108	GLY	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	109	THR	ILE	CONFLICT	UNP Q6PYX1
I	110	VAL	GLU	CONFLICT	UNP Q6PYX1
I	111	VAL	LYS	CONFLICT	UNP Q6PYX1
I	113	VAL	ILE	CONFLICT	UNP Q6PYX1
I	115	PRO	LYS	CONFLICT	UNP Q6PYX1
I	117	SER	-	EXPRESSION TAG	UNP Q6PYX1
I	118	THR	-	EXPRESSION TAG	UNP Q6PYX1
I	?	-	GLN	DELETION	UNP Q6PYX1
I	?	-	PRO	DELETION	UNP Q6PYX1
I	?	-	ARG	DELETION	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1
I	122	SER	GLN	CONFLICT	UNP Q6PYX1
I	124	PHE	TYR	CONFLICT	UNP Q6PYX1
I	125	PRO	THR	CONFLICT	UNP Q6PYX1
I	127	ALA	PRO	CONFLICT	UNP Q6PYX1
I	?	-	ARG	DELETION	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1
I	130	GLY	MET	CONFLICT	UNP Q6PYX1
I	?	-	LYS	DELETION	UNP Q6PYX1
I	?	-	ASN	DELETION	UNP Q6PYX1
I	?	-	GLN	DELETION	UNP Q6PYX1
I	132	ALA	VAL	CONFLICT	UNP Q6PYX1
I	133	ALA	SER	CONFLICT	UNP Q6PYX1
I	135	GLY	THR	CONFLICT	UNP Q6PYX1
I	140	ASP	GLY	CONFLICT	UNP Q6PYX1
I	141	TYR	PHE	CONFLICT	UNP Q6PYX1
I	142	PHE	TYR	CONFLICT	UNP Q6PYX1
I	144	GLU	SER	CONFLICT	UNP Q6PYX1
I	145	PRO	ASP	CONFLICT	UNP Q6PYX1
I	146	VAL	ILE	CONFLICT	UNP Q6PYX1
I	147	THR	ALA	CONFLICT	UNP Q6PYX1
I	149	SER	GLU	CONFLICT	UNP Q6PYX1
I	151	ASN	GLU	CONFLICT	UNP Q6PYX1
I	?	-	ASN	DELETION	UNP Q6PYX1
I	154	ALA	GLN	CONFLICT	UNP Q6PYX1
I	155	LEU	PRO	CONFLICT	UNP Q6PYX1
I	156	THR	GLU	CONFLICT	UNP Q6PYX1
I	157	SER	ASN	CONFLICT	UNP Q6PYX1
I	158	GLY	ASN	CONFLICT	UNP Q6PYX1
I	159	VAL	TYR	CONFLICT	UNP Q6PYX1
I	160	HIS	LYS	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	162	PHE	THR	CONFLICT	UNP Q6PYX1
I	164	ALA	PRO	CONFLICT	UNP Q6PYX1
I	167	GLN	ASP	CONFLICT	UNP Q6PYX1
I	169	SER	ASP	CONFLICT	UNP Q6PYX1
I	?	-	SER	DELETION	UNP Q6PYX1
I	?	-	PHE	DELETION	UNP Q6PYX1
I	?	-	PHE	DELETION	UNP Q6PYX1
I	?	-	LYS	DELETION	UNP Q6PYX1
I	175	SER	-	EXPRESSION TAG	UNP Q6PYX1
I	176	SER	-	EXPRESSION TAG	UNP Q6PYX1
I	177	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	178	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	181	PRO	ASP	CONFLICT	UNP Q6PYX1
I	182	SER	LYS	CONFLICT	UNP Q6PYX1
I	?	-	ARG	DELETION	UNP Q6PYX1
I	?	-	TRP	DELETION	UNP Q6PYX1
I	184	SER	GLN	CONFLICT	UNP Q6PYX1
I	185	LEU	GLN	CONFLICT	UNP Q6PYX1
I	187	THR	-	EXPRESSION TAG	UNP Q6PYX1
I	188	GLN	ASN	CONFLICT	UNP Q6PYX1
I	189	THR	VAL	CONFLICT	UNP Q6PYX1
I	190	TYR	PHE	CONFLICT	UNP Q6PYX1
I	191	ILE	SER	CONFLICT	UNP Q6PYX1
I	193	ASN	SER	CONFLICT	UNP Q6PYX1
I	?	-	MET	DELETION	UNP Q6PYX1
I	?	-	HIS	DELETION	UNP Q6PYX1
I	?	-	GLU	DELETION	UNP Q6PYX1
I	?	-	ALA	DELETION	UNP Q6PYX1
I	?	-	LEU	DELETION	UNP Q6PYX1
I	?	-	HIS	DELETION	UNP Q6PYX1
I	197	LYS	-	EXPRESSION TAG	UNP Q6PYX1
I	198	PRO	-	EXPRESSION TAG	UNP Q6PYX1
I	199	SER	-	EXPRESSION TAG	UNP Q6PYX1
I	200	ASN	TYR	CONFLICT	UNP Q6PYX1
I	202	LYS	-	EXPRESSION TAG	UNP Q6PYX1
I	203	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	204	ASP	-	EXPRESSION TAG	UNP Q6PYX1
I	205	LYS	-	EXPRESSION TAG	UNP Q6PYX1
I	206	LYS	-	EXPRESSION TAG	UNP Q6PYX1
I	207	VAL	-	EXPRESSION TAG	UNP Q6PYX1
I	208	GLU	-	EXPRESSION TAG	UNP Q6PYX1
I	209	PRO	GLN	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	212	CYS	-	EXPRESSION TAG	UNP Q6PYX1
I	213	ASP	-	EXPRESSION TAG	UNP Q6PYX1
I	214	LYS	-	EXPRESSION TAG	UNP Q6PYX1
I	215	THR	LEU	CONFLICT	UNP Q6PYX1
I	217	THR	LEU	CONFLICT	UNP Q6PYX1
I	218	CYS	SER	CONFLICT	UNP Q6PYX1
I	220	PRO	-	EXPRESSION TAG	UNP Q6PYX1
I	221	CYS	-	EXPRESSION TAG	UNP Q6PYX1
I	222	PRO	-	EXPRESSION TAG	UNP Q6PYX1
I	223	ALA	-	EXPRESSION TAG	UNP Q6PYX1
I	224	PRO	-	EXPRESSION TAG	UNP Q6PYX1
I	225	GLU	-	EXPRESSION TAG	UNP Q6PYX1
I	226	LEU	-	EXPRESSION TAG	UNP Q6PYX1
I	227	LEU	-	EXPRESSION TAG	UNP Q6PYX1
I	229	GLY	LYS	CONFLICT	UNP Q6PYX1
O	1	GLU	SER	CONFLICT	UNP Q6PYX1
O	3	GLN	PHE	CONFLICT	UNP Q6PYX1
O	5	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	6	GLU	-	EXPRESSION TAG	UNP Q6PYX1
O	7	SER	-	EXPRESSION TAG	UNP Q6PYX1
O	8	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	9	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	10	GLY	PHE	CONFLICT	UNP Q6PYX1
O	11	LEU	PRO	CONFLICT	UNP Q6PYX1
O	12	VAL	PRO	CONFLICT	UNP Q6PYX1
O	14	ALA	PRO	CONFLICT	UNP Q6PYX1
O	15	GLY	LYS	CONFLICT	UNP Q6PYX1
O	16	GLY	ASP	CONFLICT	UNP Q6PYX1
O	17	SER	THR	CONFLICT	UNP Q6PYX1
O	19	ILE	MET	CONFLICT	UNP Q6PYX1
O	20	LEU	ILE	CONFLICT	UNP Q6PYX1
O	?	-	ARG	DELETION	UNP Q6PYX1
O	?	-	THR	DELETION	UNP Q6PYX1
O	?	-	PRO	DELETION	UNP Q6PYX1
O	?	-	GLU	DELETION	UNP Q6PYX1
O	?	-	VAL	DELETION	UNP Q6PYX1
O	?	-	THR	DELETION	UNP Q6PYX1
O	23	GLY	VAL	CONFLICT	UNP Q6PYX1
O	25	SER	-	EXPRESSION TAG	UNP Q6PYX1
O	26	ASN	-	EXPRESSION TAG	UNP Q6PYX1
O	27	PHE	VAL	CONFLICT	UNP Q6PYX1
O	28	ARG	ASP	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	29	ILE	VAL	CONFLICT	UNP Q6PYX1
O	31	ALA	-	EXPRESSION TAG	UNP Q6PYX1
O	?	-	GLU	DELETION	UNP Q6PYX1
O	?	-	ASP	DELETION	UNP Q6PYX1
O	?	-	PRO	DELETION	UNP Q6PYX1
O	?	-	GLU	DELETION	UNP Q6PYX1
O	?	-	VAL	DELETION	UNP Q6PYX1
O	33	THR	LYS	CONFLICT	UNP Q6PYX1
O	34	MET	PHE	CONFLICT	UNP Q6PYX1
O	37	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	38	ARG	-	EXPRESSION TAG	UNP Q6PYX1
O	39	ARG	TYR	CONFLICT	UNP Q6PYX1
O	41	PRO	-	EXPRESSION TAG	UNP Q6PYX1
O	42	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	43	GLY	ASP	CONFLICT	UNP Q6PYX1
O	45	LEU	VAL	CONFLICT	UNP Q6PYX1
O	47	TRP	-	EXPRESSION TAG	UNP Q6PYX1
O	?	-	HIS	DELETION	UNP Q6PYX1
O	?	-	ASN	DELETION	UNP Q6PYX1
O	?	-	LYS	DELETION	UNP Q6PYX1
O	?	-	THR	DELETION	UNP Q6PYX1
O	?	-	LYS	DELETION	UNP Q6PYX1
O	?	-	PRO	DELETION	UNP Q6PYX1
O	?	-	ARG	DELETION	UNP Q6PYX1
O	?	-	GLU	DELETION	UNP Q6PYX1
O	50	SER	GLU	CONFLICT	UNP Q6PYX1
O	51	ILE	GLN	CONFLICT	UNP Q6PYX1
O	52	SER	TYR	CONFLICT	UNP Q6PYX1
O	53	SER	ASN	CONFLICT	UNP Q6PYX1
O	58	ASP	-	EXPRESSION TAG	UNP Q6PYX1
O	59	TYR	-	EXPRESSION TAG	UNP Q6PYX1
O	60	ALA	-	EXPRESSION TAG	UNP Q6PYX1
O	61	ASP	-	EXPRESSION TAG	UNP Q6PYX1
O	62	ALA	-	EXPRESSION TAG	UNP Q6PYX1
O	64	LYS	VAL	CONFLICT	UNP Q6PYX1
O	65	GLY	SER	CONFLICT	UNP Q6PYX1
O	66	ARG	VAL	CONFLICT	UNP Q6PYX1
O	67	PHE	LEU	CONFLICT	UNP Q6PYX1
O	70	SER	-	EXPRESSION TAG	UNP Q6PYX1
O	71	ARG	-	EXPRESSION TAG	UNP Q6PYX1
O	72	ASP	-	EXPRESSION TAG	UNP Q6PYX1
O	73	ASP	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	HIS	DELETION	UNP Q6PYX1
O	75	GLU	GLN	CONFLICT	UNP Q6PYX1
O	77	PHE	-	EXPRESSION TAG	UNP Q6PYX1
O	78	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	79	TYR	TRP	CONFLICT	UNP Q6PYX1
O	81	GLN	-	EXPRESSION TAG	UNP Q6PYX1
O	82	MET	ASN	CONFLICT	UNP Q6PYX1
O	82A	HIS	GLY	CONFLICT	UNP Q6PYX1
O	83	ARG	-	EXPRESSION TAG	UNP Q6PYX1
O	84	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	86	ASP	-	EXPRESSION TAG	UNP Q6PYX1
O	87	THR	-	EXPRESSION TAG	UNP Q6PYX1
O	88	ALA	-	EXPRESSION TAG	UNP Q6PYX1
O	89	ILE	-	EXPRESSION TAG	UNP Q6PYX1
O	91	TYR	LYS	CONFLICT	UNP Q6PYX1
O	93	ALA	-	EXPRESSION TAG	UNP Q6PYX1
O	94	ARG	-	EXPRESSION TAG	UNP Q6PYX1
O	96	GLY	VAL	CONFLICT	UNP Q6PYX1
O	?	-	ASN	DELETION	UNP Q6PYX1
O	98	ASP	LYS	CONFLICT	UNP Q6PYX1
O	99	ARG	ALA	CONFLICT	UNP Q6PYX1
O	101	ASP	PRO	CONFLICT	UNP Q6PYX1
O	103	TRP	-	EXPRESSION TAG	UNP Q6PYX1
O	104	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	106	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	107	THR	ILE	CONFLICT	UNP Q6PYX1
O	108	VAL	GLU	CONFLICT	UNP Q6PYX1
O	109	VAL	LYS	CONFLICT	UNP Q6PYX1
O	111	VAL	ILE	CONFLICT	UNP Q6PYX1
O	113	PRO	LYS	CONFLICT	UNP Q6PYX1
O	115	SER	-	EXPRESSION TAG	UNP Q6PYX1
O	116	THR	-	EXPRESSION TAG	UNP Q6PYX1
O	?	-	GLN	DELETION	UNP Q6PYX1
O	?	-	PRO	DELETION	UNP Q6PYX1
O	?	-	ARG	DELETION	UNP Q6PYX1
O	?	-	GLU	DELETION	UNP Q6PYX1
O	120	SER	GLN	CONFLICT	UNP Q6PYX1
O	122	PHE	TYR	CONFLICT	UNP Q6PYX1
O	123	PRO	THR	CONFLICT	UNP Q6PYX1
O	125	ALA	PRO	CONFLICT	UNP Q6PYX1
O	?	-	ARG	DELETION	UNP Q6PYX1
O	?	-	GLU	DELETION	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	GLU	DELETION	UNP Q6PYX1
O	136	GLY	MET	CONFLICT	UNP Q6PYX1
O	?	-	LYS	DELETION	UNP Q6PYX1
O	?	-	ASN	DELETION	UNP Q6PYX1
O	?	-	GLN	DELETION	UNP Q6PYX1
O	138	ALA	VAL	CONFLICT	UNP Q6PYX1
O	139	ALA	SER	CONFLICT	UNP Q6PYX1
O	141	GLY	THR	CONFLICT	UNP Q6PYX1
O	146	ASP	GLY	CONFLICT	UNP Q6PYX1
O	147	TYR	PHE	CONFLICT	UNP Q6PYX1
O	148	PHE	TYR	CONFLICT	UNP Q6PYX1
O	150	GLU	SER	CONFLICT	UNP Q6PYX1
O	151	PRO	ASP	CONFLICT	UNP Q6PYX1
O	152	VAL	ILE	CONFLICT	UNP Q6PYX1
O	153	THR	ALA	CONFLICT	UNP Q6PYX1
O	156	SER	GLU	CONFLICT	UNP Q6PYX1
O	162	ASN	GLU	CONFLICT	UNP Q6PYX1
O	?	-	ASN	DELETION	UNP Q6PYX1
O	165	ALA	GLN	CONFLICT	UNP Q6PYX1
O	166	LEU	PRO	CONFLICT	UNP Q6PYX1
O	167	THR	GLU	CONFLICT	UNP Q6PYX1
O	168	SER	ASN	CONFLICT	UNP Q6PYX1
O	169	GLY	ASN	CONFLICT	UNP Q6PYX1
O	171	VAL	TYR	CONFLICT	UNP Q6PYX1
O	172	HIS	LYS	CONFLICT	UNP Q6PYX1
O	174	PHE	THR	CONFLICT	UNP Q6PYX1
O	176	ALA	PRO	CONFLICT	UNP Q6PYX1
O	179	GLN	ASP	CONFLICT	UNP Q6PYX1
O	182	SER	ASP	CONFLICT	UNP Q6PYX1
O	?	-	SER	DELETION	UNP Q6PYX1
O	?	-	PHE	DELETION	UNP Q6PYX1
O	?	-	PHE	DELETION	UNP Q6PYX1
O	?	-	LYS	DELETION	UNP Q6PYX1
O	188	SER	-	EXPRESSION TAG	UNP Q6PYX1
O	189	SER	-	EXPRESSION TAG	UNP Q6PYX1
O	190	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	191	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	194	PRO	ASP	CONFLICT	UNP Q6PYX1
O	195	SER	LYS	CONFLICT	UNP Q6PYX1
O	?	-	ARG	DELETION	UNP Q6PYX1
O	?	-	TRP	DELETION	UNP Q6PYX1
O	197	SER	GLN	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	198	LEU	GLN	CONFLICT	UNP Q6PYX1
O	200	THR	-	EXPRESSION TAG	UNP Q6PYX1
O	203	GLN	ASN	CONFLICT	UNP Q6PYX1
O	205	THR	VAL	CONFLICT	UNP Q6PYX1
O	206	TYR	PHE	CONFLICT	UNP Q6PYX1
O	207	ILE	SER	CONFLICT	UNP Q6PYX1
O	209	ASN	SER	CONFLICT	UNP Q6PYX1
O	?	-	MET	DELETION	UNP Q6PYX1
O	?	-	HIS	DELETION	UNP Q6PYX1
O	?	-	GLU	DELETION	UNP Q6PYX1
O	?	-	ALA	DELETION	UNP Q6PYX1
O	?	-	LEU	DELETION	UNP Q6PYX1
O	?	-	HIS	DELETION	UNP Q6PYX1
O	213	LYS	-	EXPRESSION TAG	UNP Q6PYX1
O	214	PRO	-	EXPRESSION TAG	UNP Q6PYX1
O	215	SER	-	EXPRESSION TAG	UNP Q6PYX1
O	216	ASN	TYR	CONFLICT	UNP Q6PYX1
O	218	LYS	-	EXPRESSION TAG	UNP Q6PYX1
O	219	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	220	ASP	-	EXPRESSION TAG	UNP Q6PYX1
O	221	LYS	-	EXPRESSION TAG	UNP Q6PYX1
O	222	LYS	-	EXPRESSION TAG	UNP Q6PYX1
O	225	VAL	-	EXPRESSION TAG	UNP Q6PYX1
O	226	GLU	-	EXPRESSION TAG	UNP Q6PYX1
O	227	PRO	GLN	CONFLICT	UNP Q6PYX1
O	230	CYS	-	EXPRESSION TAG	UNP Q6PYX1
O	231	ASP	-	EXPRESSION TAG	UNP Q6PYX1
O	232	LYS	-	EXPRESSION TAG	UNP Q6PYX1
O	233	THR	LEU	CONFLICT	UNP Q6PYX1
O	235	THR	LEU	CONFLICT	UNP Q6PYX1
O	236	CYS	SER	CONFLICT	UNP Q6PYX1
O	238	PRO	-	EXPRESSION TAG	UNP Q6PYX1
O	239	CYS	-	EXPRESSION TAG	UNP Q6PYX1
O	240	PRO	-	EXPRESSION TAG	UNP Q6PYX1
O	241	ALA	-	EXPRESSION TAG	UNP Q6PYX1
O	242	PRO	-	EXPRESSION TAG	UNP Q6PYX1
O	243	GLU	-	EXPRESSION TAG	UNP Q6PYX1
O	244	LEU	-	EXPRESSION TAG	UNP Q6PYX1
O	245	LEU	-	EXPRESSION TAG	UNP Q6PYX1
O	247	GLY	LYS	CONFLICT	UNP Q6PYX1
R	1	GLU	SER	CONFLICT	UNP Q6PYX1
R	3	GLN	PHE	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	5	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	6	GLU	-	EXPRESSION TAG	UNP Q6PYX1
R	7	SER	-	EXPRESSION TAG	UNP Q6PYX1
R	8	GLY	-	EXPRESSION TAG	UNP Q6PYX1
R	9	GLY	-	EXPRESSION TAG	UNP Q6PYX1
R	10	GLY	PHE	CONFLICT	UNP Q6PYX1
R	11	LEU	PRO	CONFLICT	UNP Q6PYX1
R	12	VAL	PRO	CONFLICT	UNP Q6PYX1
R	14	ALA	PRO	CONFLICT	UNP Q6PYX1
R	15	GLY	LYS	CONFLICT	UNP Q6PYX1
R	16	GLY	ASP	CONFLICT	UNP Q6PYX1
R	17	SER	THR	CONFLICT	UNP Q6PYX1
R	19	ILE	MET	CONFLICT	UNP Q6PYX1
R	20	LEU	ILE	CONFLICT	UNP Q6PYX1
R	?	-	ARG	DELETION	UNP Q6PYX1
R	?	-	THR	DELETION	UNP Q6PYX1
R	?	-	PRO	DELETION	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	?	-	VAL	DELETION	UNP Q6PYX1
R	?	-	THR	DELETION	UNP Q6PYX1
R	23	GLY	VAL	CONFLICT	UNP Q6PYX1
R	25	SER	-	EXPRESSION TAG	UNP Q6PYX1
R	26	ASN	-	EXPRESSION TAG	UNP Q6PYX1
R	27	PHE	VAL	CONFLICT	UNP Q6PYX1
R	28	ARG	ASP	CONFLICT	UNP Q6PYX1
R	29	ILE	VAL	CONFLICT	UNP Q6PYX1
R	31	ALA	-	EXPRESSION TAG	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	?	-	ASP	DELETION	UNP Q6PYX1
R	?	-	PRO	DELETION	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	?	-	VAL	DELETION	UNP Q6PYX1
R	33	THR	LYS	CONFLICT	UNP Q6PYX1
R	34	MET	PHE	CONFLICT	UNP Q6PYX1
R	37	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	38	ARG	-	EXPRESSION TAG	UNP Q6PYX1
R	39	ARG	TYR	CONFLICT	UNP Q6PYX1
R	41	PRO	-	EXPRESSION TAG	UNP Q6PYX1
R	42	GLY	-	EXPRESSION TAG	UNP Q6PYX1
R	43	GLY	ASP	CONFLICT	UNP Q6PYX1
R	45	LEU	VAL	CONFLICT	UNP Q6PYX1
R	47	TRP	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	HIS	DELETION	UNP Q6PYX1
R	?	-	ASN	DELETION	UNP Q6PYX1
R	?	-	LYS	DELETION	UNP Q6PYX1
R	?	-	THR	DELETION	UNP Q6PYX1
R	?	-	LYS	DELETION	UNP Q6PYX1
R	?	-	PRO	DELETION	UNP Q6PYX1
R	?	-	ARG	DELETION	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	50	SER	GLU	CONFLICT	UNP Q6PYX1
R	51	ILE	GLN	CONFLICT	UNP Q6PYX1
R	52	SER	TYR	CONFLICT	UNP Q6PYX1
R	53	SER	ASN	CONFLICT	UNP Q6PYX1
R	58	ASP	-	EXPRESSION TAG	UNP Q6PYX1
R	59	TYR	-	EXPRESSION TAG	UNP Q6PYX1
R	60	ALA	-	EXPRESSION TAG	UNP Q6PYX1
R	61	ASP	-	EXPRESSION TAG	UNP Q6PYX1
R	62	ALA	-	EXPRESSION TAG	UNP Q6PYX1
R	64	LYS	VAL	CONFLICT	UNP Q6PYX1
R	65	GLY	SER	CONFLICT	UNP Q6PYX1
R	66	ARG	VAL	CONFLICT	UNP Q6PYX1
R	67	PHE	LEU	CONFLICT	UNP Q6PYX1
R	70	SER	-	EXPRESSION TAG	UNP Q6PYX1
R	71	ARG	-	EXPRESSION TAG	UNP Q6PYX1
R	72	ASP	-	EXPRESSION TAG	UNP Q6PYX1
R	73	ASP	-	EXPRESSION TAG	UNP Q6PYX1
R	?	-	HIS	DELETION	UNP Q6PYX1
R	75	GLU	GLN	CONFLICT	UNP Q6PYX1
R	77	PHE	-	EXPRESSION TAG	UNP Q6PYX1
R	78	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	79	TYR	TRP	CONFLICT	UNP Q6PYX1
R	81	GLN	-	EXPRESSION TAG	UNP Q6PYX1
R	82	MET	ASN	CONFLICT	UNP Q6PYX1
R	82A	HIS	GLY	CONFLICT	UNP Q6PYX1
R	83	ARG	-	EXPRESSION TAG	UNP Q6PYX1
R	84	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	86	ASP	-	EXPRESSION TAG	UNP Q6PYX1
R	87	THR	-	EXPRESSION TAG	UNP Q6PYX1
R	88	ALA	-	EXPRESSION TAG	UNP Q6PYX1
R	89	ILE	-	EXPRESSION TAG	UNP Q6PYX1
R	91	TYR	LYS	CONFLICT	UNP Q6PYX1
R	93	ALA	-	EXPRESSION TAG	UNP Q6PYX1
R	94	ARG	-	EXPRESSION TAG	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	96	GLY	VAL	CONFLICT	UNP Q6PYX1
R	?	-	ASN	DELETION	UNP Q6PYX1
R	98	ASP	LYS	CONFLICT	UNP Q6PYX1
R	99	ARG	ALA	CONFLICT	UNP Q6PYX1
R	101	ASP	PRO	CONFLICT	UNP Q6PYX1
R	103	TRP	-	EXPRESSION TAG	UNP Q6PYX1
R	104	GLY	-	EXPRESSION TAG	UNP Q6PYX1
R	106	GLY	-	EXPRESSION TAG	UNP Q6PYX1
R	107	THR	ILE	CONFLICT	UNP Q6PYX1
R	108	VAL	GLU	CONFLICT	UNP Q6PYX1
R	109	VAL	LYS	CONFLICT	UNP Q6PYX1
R	111	VAL	ILE	CONFLICT	UNP Q6PYX1
R	113	PRO	LYS	CONFLICT	UNP Q6PYX1
R	115	SER	-	EXPRESSION TAG	UNP Q6PYX1
R	116	THR	-	EXPRESSION TAG	UNP Q6PYX1
R	?	-	GLN	DELETION	UNP Q6PYX1
R	?	-	PRO	DELETION	UNP Q6PYX1
R	?	-	ARG	DELETION	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	120	SER	GLN	CONFLICT	UNP Q6PYX1
R	122	PHE	TYR	CONFLICT	UNP Q6PYX1
R	123	PRO	THR	CONFLICT	UNP Q6PYX1
R	125	ALA	PRO	CONFLICT	UNP Q6PYX1
R	?	-	ARG	DELETION	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	136	GLY	MET	CONFLICT	UNP Q6PYX1
R	?	-	LYS	DELETION	UNP Q6PYX1
R	?	-	ASN	DELETION	UNP Q6PYX1
R	?	-	GLN	DELETION	UNP Q6PYX1
R	138	ALA	VAL	CONFLICT	UNP Q6PYX1
R	139	ALA	SER	CONFLICT	UNP Q6PYX1
R	141	GLY	THR	CONFLICT	UNP Q6PYX1
R	146	ASP	GLY	CONFLICT	UNP Q6PYX1
R	147	TYR	PHE	CONFLICT	UNP Q6PYX1
R	148	PHE	TYR	CONFLICT	UNP Q6PYX1
R	150	GLU	SER	CONFLICT	UNP Q6PYX1
R	151	PRO	ASP	CONFLICT	UNP Q6PYX1
R	152	VAL	ILE	CONFLICT	UNP Q6PYX1
R	153	THR	ALA	CONFLICT	UNP Q6PYX1
R	156	SER	GLU	CONFLICT	UNP Q6PYX1
R	162	ASN	GLU	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	ASN	DELETION	UNP Q6PYX1
R	165	ALA	GLN	CONFLICT	UNP Q6PYX1
R	166	LEU	PRO	CONFLICT	UNP Q6PYX1
R	167	THR	GLU	CONFLICT	UNP Q6PYX1
R	168	SER	ASN	CONFLICT	UNP Q6PYX1
R	169	GLY	ASN	CONFLICT	UNP Q6PYX1
R	171	VAL	TYR	CONFLICT	UNP Q6PYX1
R	172	HIS	LYS	CONFLICT	UNP Q6PYX1
R	174	PHE	THR	CONFLICT	UNP Q6PYX1
R	176	ALA	PRO	CONFLICT	UNP Q6PYX1
R	179	GLN	ASP	CONFLICT	UNP Q6PYX1
R	182	SER	ASP	CONFLICT	UNP Q6PYX1
R	?	-	SER	DELETION	UNP Q6PYX1
R	?	-	PHE	DELETION	UNP Q6PYX1
R	?	-	PHE	DELETION	UNP Q6PYX1
R	?	-	LYS	DELETION	UNP Q6PYX1
R	188	SER	-	EXPRESSION TAG	UNP Q6PYX1
R	189	SER	-	EXPRESSION TAG	UNP Q6PYX1
R	190	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	191	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	194	PRO	ASP	CONFLICT	UNP Q6PYX1
R	195	SER	LYS	CONFLICT	UNP Q6PYX1
R	?	-	ARG	DELETION	UNP Q6PYX1
R	?	-	TRP	DELETION	UNP Q6PYX1
R	197	SER	GLN	CONFLICT	UNP Q6PYX1
R	198	LEU	GLN	CONFLICT	UNP Q6PYX1
R	200	THR	-	EXPRESSION TAG	UNP Q6PYX1
R	203	GLN	ASN	CONFLICT	UNP Q6PYX1
R	205	THR	VAL	CONFLICT	UNP Q6PYX1
R	206	TYR	PHE	CONFLICT	UNP Q6PYX1
R	207	ILE	SER	CONFLICT	UNP Q6PYX1
R	209	ASN	SER	CONFLICT	UNP Q6PYX1
R	?	-	MET	DELETION	UNP Q6PYX1
R	?	-	HIS	DELETION	UNP Q6PYX1
R	?	-	GLU	DELETION	UNP Q6PYX1
R	?	-	ALA	DELETION	UNP Q6PYX1
R	?	-	LEU	DELETION	UNP Q6PYX1
R	?	-	HIS	DELETION	UNP Q6PYX1
R	213	LYS	-	EXPRESSION TAG	UNP Q6PYX1
R	214	PRO	-	EXPRESSION TAG	UNP Q6PYX1
R	215	SER	-	EXPRESSION TAG	UNP Q6PYX1
R	216	ASN	TYR	CONFLICT	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	218	LYS	-	EXPRESSION TAG	UNP Q6PYX1
R	219	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	220	ASP	-	EXPRESSION TAG	UNP Q6PYX1
R	221	LYS	-	EXPRESSION TAG	UNP Q6PYX1
R	222	LYS	-	EXPRESSION TAG	UNP Q6PYX1
R	225	VAL	-	EXPRESSION TAG	UNP Q6PYX1
R	226	GLU	-	EXPRESSION TAG	UNP Q6PYX1
R	227	PRO	GLN	CONFLICT	UNP Q6PYX1
R	230	CYS	-	EXPRESSION TAG	UNP Q6PYX1
R	231	ASP	-	EXPRESSION TAG	UNP Q6PYX1
R	232	LYS	-	EXPRESSION TAG	UNP Q6PYX1
R	233	THR	LEU	CONFLICT	UNP Q6PYX1
R	235	THR	LEU	CONFLICT	UNP Q6PYX1
R	236	CYS	SER	CONFLICT	UNP Q6PYX1
R	238	PRO	-	EXPRESSION TAG	UNP Q6PYX1
R	239	CYS	-	EXPRESSION TAG	UNP Q6PYX1
R	240	PRO	-	EXPRESSION TAG	UNP Q6PYX1
R	241	ALA	-	EXPRESSION TAG	UNP Q6PYX1
R	242	PRO	-	EXPRESSION TAG	UNP Q6PYX1
R	243	GLU	-	EXPRESSION TAG	UNP Q6PYX1
R	244	LEU	-	EXPRESSION TAG	UNP Q6PYX1
R	245	LEU	-	EXPRESSION TAG	UNP Q6PYX1
R	247	GLY	LYS	CONFLICT	UNP Q6PYX1

- Molecule 3 is a protein called 2G12 IgG dimer heavy chain.

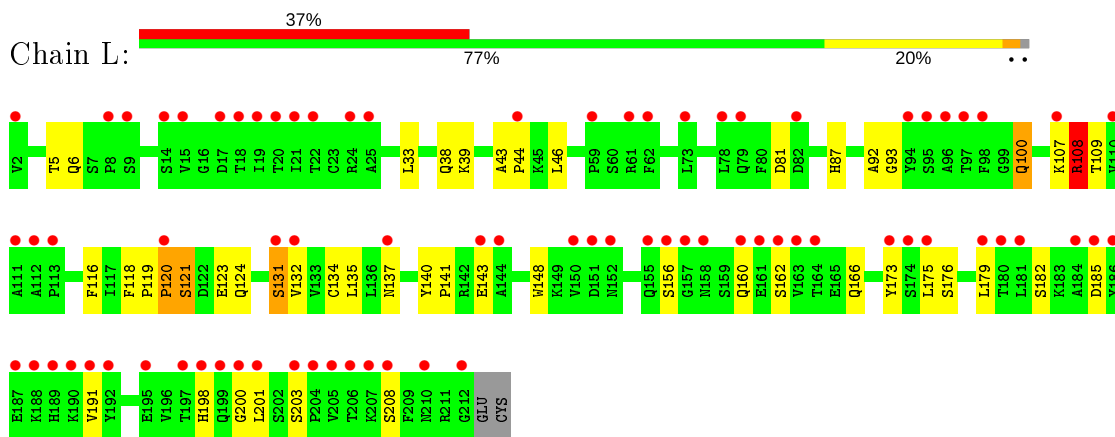
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	B	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	C	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	D	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	J	207	Total	C	N	O	S	0	0	0
			1660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



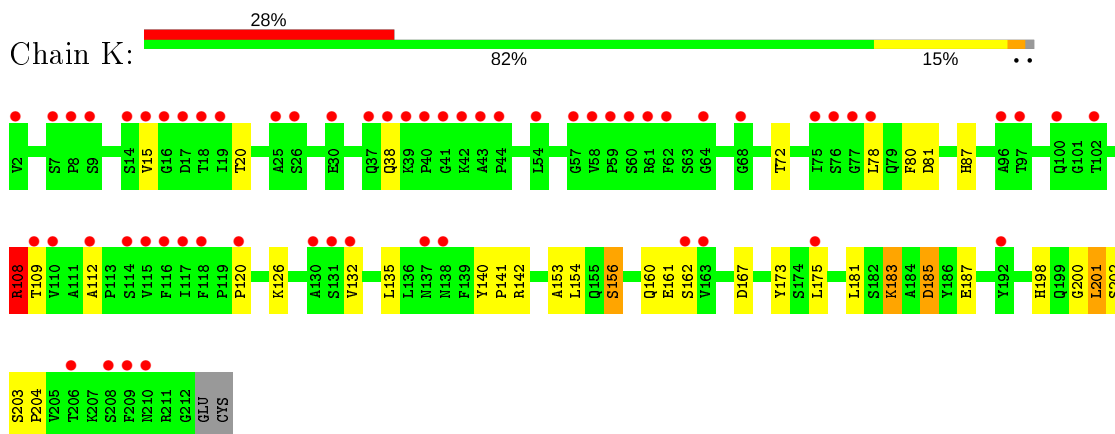
### 3 Residue-property plots [i](#)

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.

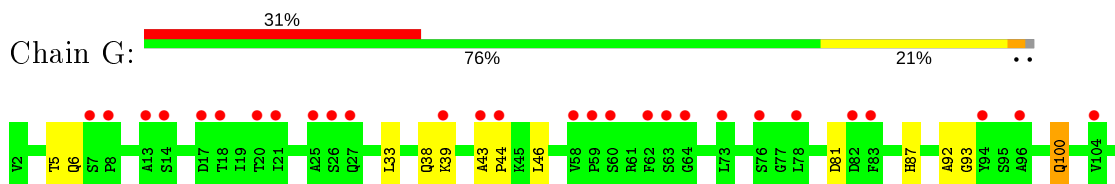
- Molecule 1: 2G12 IgG dimer light chain

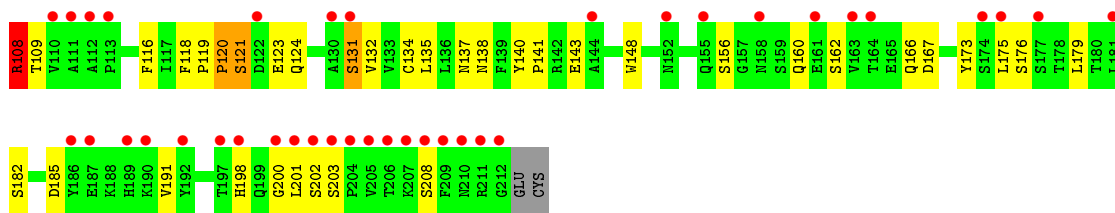


- Molecule 1: 2G12 IgG dimer light chain

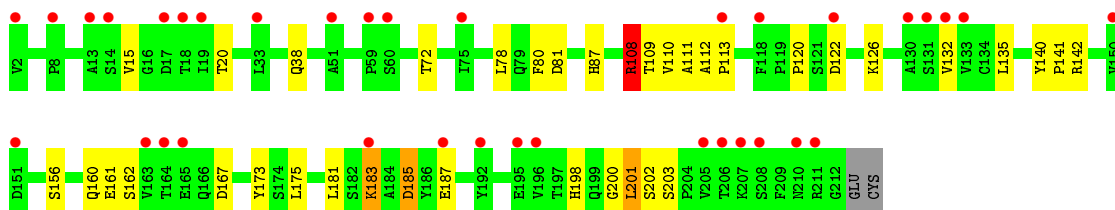
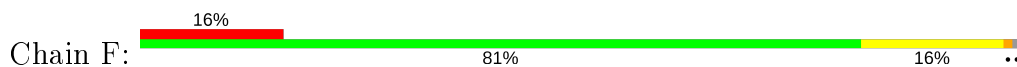


- Molecule 1: 2G12 IgG dimer light chain

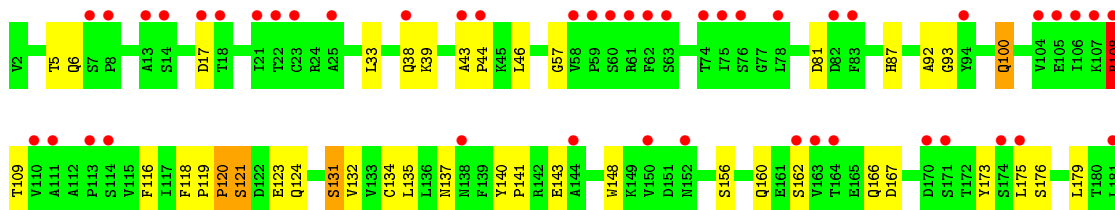
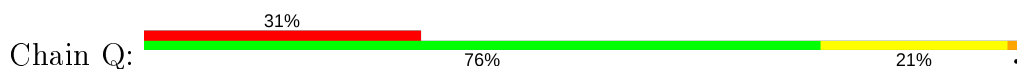




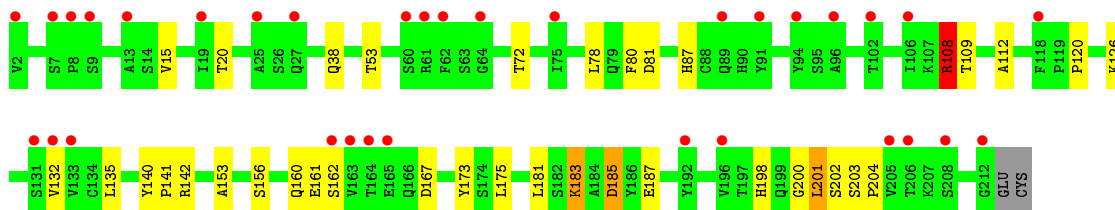
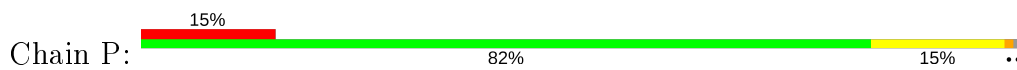
- Molecule 1: 2G12 IgG dimer light chain



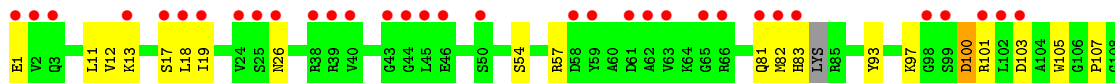
- Molecule 1: 2G12 IgG dimer light chain



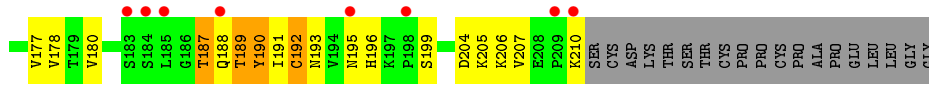
- Molecule 1: 2G12 IgG dimer light chain



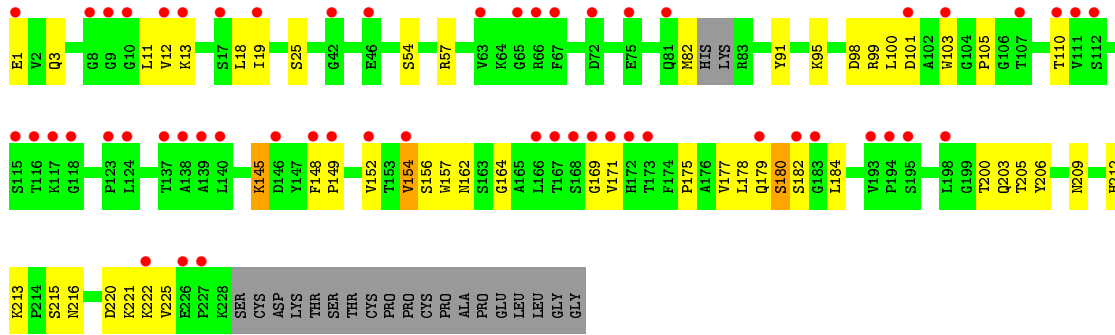
- Molecule 2: Hepatitis B virus receptor binding protein



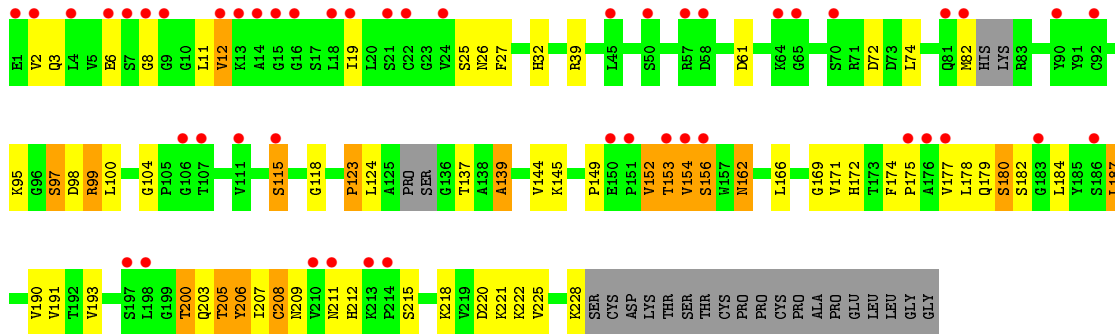




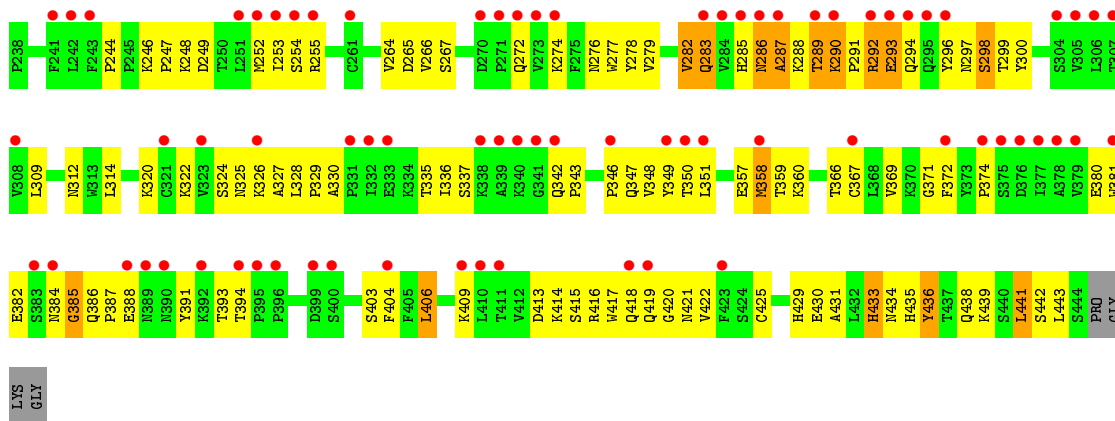
• Molecule 2: Hepatitis B virus receptor binding protein



• Molecule 2: Hepatitis B virus receptor binding protein



• Molecule 3: 2G12 IgG dimer heavy chain



• Molecule 3: 2G12 IgG dimer heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	374.73Å 374.73Å 64.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.91 – 6.50 64.91 – 5.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (64.91-6.50) 99.9 (64.91-5.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 6.17Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.381 , 0.366 0.380 , 0.362	Depositor DCC
$R_{free}$ test set	675 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	243.9	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.14 , 259.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	28972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	481.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4512e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	F	0.53	1/1654 (0.1%)	0.85	6/2246 (0.3%)
1	G	0.97	6/1654 (0.4%)	0.81	5/2246 (0.2%)
1	K	0.53	1/1654 (0.1%)	0.84	5/2246 (0.2%)
1	L	0.97	6/1654 (0.4%)	0.81	4/2246 (0.2%)
1	P	0.53	1/1654 (0.1%)	0.85	5/2246 (0.2%)
1	Q	0.97	6/1654 (0.4%)	0.81	6/2246 (0.3%)
2	E	0.89	2/1600 (0.1%)	0.78	3/2162 (0.1%)
2	H	0.89	2/1591 (0.1%)	0.78	3/2151 (0.1%)
2	I	1.18	9/1569 (0.6%)	0.83	5/2120 (0.2%)
2	M	1.18	9/1568 (0.6%)	0.84	5/2122 (0.2%)
2	O	0.89	2/1582 (0.1%)	0.79	3/2142 (0.1%)
2	R	1.18	9/1568 (0.6%)	0.84	5/2122 (0.2%)
3	A	0.42	0/1706	0.68	0/2323
3	B	0.37	0/1699	0.64	0/2312
3	C	0.43	0/1706	0.68	0/2323
3	D	0.37	0/1699	0.64	0/2312
3	J	0.42	0/1706	0.68	0/2323
3	N	0.37	0/1699	0.64	0/2312
All	All	0.78	54/29617 (0.2%)	0.77	55/40200 (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
3	B	0	1
3	D	0	1
3	N	0	1
All	All	0	3

The worst 5 of 54 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	180	SER	C-N	27.91	1.98	1.34
2	I	168	SER	C-N	27.90	1.98	1.34
2	R	180	SER	C-N	27.85	1.98	1.34
1	G	121	SER	CB-OG	24.55	1.74	1.42
1	Q	121	SER	CB-OG	24.55	1.74	1.42

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	108	ARG	NE-CZ-NH2	-13.67	113.46	120.30
1	P	108	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	K	108	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	L	108	ARG	NE-CZ-NH2	-12.31	114.15	120.30
1	L	108	ARG	NE-CZ-NH1	12.09	126.34	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	373	TYR	Sidechain
3	D	373	TYR	Sidechain
3	N	373	TYR	Sidechain

## 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	F	1618	0	1580	69	0
1	G	1618	0	1580	60	1
1	K	1618	0	1579	47	2
1	L	1618	0	1580	59	1
1	P	1618	0	1580	39	3
1	Q	1618	0	1580	63	0
2	E	1574	0	1546	53	41
2	H	1565	0	1533	51	38
2	I	1544	0	1517	89	3
2	M	1542	0	1516	103	0
2	O	1555	0	1525	82	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1542	0	1516	87	1
3	A	1660	0	1632	102	79
3	B	1654	0	1627	151	43
3	C	1660	0	1626	182	1
3	D	1654	0	1627	122	34
3	J	1660	0	1632	101	60
3	N	1654	0	1627	190	2
All	All	28972	0	28403	1283	155

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 22.

The worst 5 of 1283 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:C:253:ILE:HG21	3:N:310:HIS:CE1	1.27	1.67
1:F:201:LEU:CD1	2:O:99:ARG:CG	1.80	1.57
1:F:112:ALA:HB3	2:O:99:ARG:CB	1.23	1.56
1:F:112:ALA:CB	2:O:99:ARG:CB	1.81	1.55
1:F:201:LEU:HD11	2:O:99:ARG:CD	1.45	1.46

The worst 5 of 155 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:1:GLU:N	3:J:294:GLN:CB[3_565]	0.39	1.81
3:A:253:ILE:N	3:B:253:ILE:CB[6_555]	0.53	1.67
2:H:1:GLU:N	3:A:294:GLN:CB[5_555]	0.53	1.67
3:A:382:GLU:OE1	3:B:433:HIS:CD2[6_555]	0.60	1.60
3:D:253:ILE:CG2	3:J:253:ILE:CA[3_565]	0.68	1.52

## 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	F	209/213 (98%)	202 (97%)	7 (3%)	0	100	100
1	G	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
1	K	209/213 (98%)	202 (97%)	7 (3%)	0	100	100
1	L	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
1	P	209/213 (98%)	202 (97%)	7 (3%)	0	100	100
1	Q	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
2	E	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
2	H	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
2	I	185/229 (81%)	177 (96%)	8 (4%)	0	100	100
2	M	187/229 (82%)	179 (96%)	8 (4%)	0	100	100
2	O	189/229 (82%)	186 (98%)	3 (2%)	0	100	100
2	R	187/229 (82%)	179 (96%)	8 (4%)	0	100	100
3	A	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	19
3	B	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	20
3	C	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	19
3	D	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	20
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	19
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	20
All	All	3605/3918 (92%)	3348 (93%)	194 (5%)	63 (2%)	9	42

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	283	GLN
3	A	287	ALA
3	A	289	THR
3	A	433	HIS
3	B	298	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	F	182/184 (99%)	174 (96%)	8 (4%)	28	53
1	G	182/184 (99%)	172 (94%)	10 (6%)	21	47
1	K	182/184 (99%)	174 (96%)	8 (4%)	28	53
1	L	182/184 (99%)	172 (94%)	10 (6%)	21	47
1	P	182/184 (99%)	174 (96%)	8 (4%)	28	53
1	Q	182/184 (99%)	172 (94%)	10 (6%)	21	47
2	E	176/192 (92%)	167 (95%)	9 (5%)	24	49
2	H	175/192 (91%)	166 (95%)	9 (5%)	24	49
2	I	172/192 (90%)	157 (91%)	15 (9%)	10	31
2	M	172/192 (90%)	157 (91%)	15 (9%)	10	31
2	O	174/192 (91%)	165 (95%)	9 (5%)	23	48
2	R	172/192 (90%)	156 (91%)	16 (9%)	9	29
3	A	193/196 (98%)	187 (97%)	6 (3%)	40	62
3	B	192/196 (98%)	180 (94%)	12 (6%)	18	43
3	C	193/196 (98%)	187 (97%)	6 (3%)	40	62
3	D	192/196 (98%)	180 (94%)	12 (6%)	18	43
3	J	193/196 (98%)	187 (97%)	6 (3%)	40	62
3	N	192/196 (98%)	180 (94%)	12 (6%)	18	43
All	All	3288/3432 (96%)	3107 (94%)	181 (6%)	21	47

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	126	LYS
2	I	210	LYS
3	J	436	TYR
1	F	181	LEU
2	I	117	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	32	HIS

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Mol	Chain	Res	Type
3	C	421	ASN
3	N	312	ASN
2	I	83	HIS
3	C	325	ASN

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	13
2	H	12
2	O	11
2	I	10
2	R	10
2	M	10

The worst 5 of 66 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	102:LEU	C	103:ASP	N	11.62
1	E	102:LEU	C	103:ASP	N	11.62
1	O	100:LEU	C	101:ASP	N	11.62
1	H	129:SER	C	130:GLY	N	11.41
1	E	129:SER	C	130:GLY	N	11.41

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	F	211/213 (99%)	0.88	35 (16%) 1 4	467, 467, 467, 467	0
1	G	211/213 (99%)	1.54	66 (31%) 0 2	526, 526, 526, 526	0
1	K	211/213 (99%)	1.43	60 (28%) 0 2	487, 487, 487, 487	0
1	L	211/213 (99%)	1.73	78 (36%) 0 1	547, 547, 547, 547	0
1	P	211/213 (99%)	0.87	33 (15%) 2 5	467, 467, 467, 467	0
1	Q	211/213 (99%)	1.50	66 (31%) 0 2	527, 527, 527, 527	0
2	E	210/229 (91%)	1.28	56 (26%) 0 2	407, 407, 407, 407	0
2	H	209/229 (91%)	1.61	63 (30%) 0 2	427, 427, 427, 427	0
2	I	206/229 (89%)	1.18	48 (23%) 0 2	456, 456, 456, 456	0
2	M	206/229 (89%)	1.89	80 (38%) 0 1	477, 477, 477, 477	0
2	O	208/229 (90%)	1.29	55 (26%) 0 2	407, 407, 407, 407	0
2	R	206/229 (89%)	1.29	48 (23%) 0 2	457, 457, 457, 457	0
3	A	207/211 (98%)	1.80	74 (35%) 0 1	516, 516, 516, 516	0
3	B	206/211 (97%)	2.00	78 (37%) 0 1	520, 520, 520, 520	0
3	C	207/211 (98%)	1.67	63 (30%) 0 2	485, 485, 485, 485	0
3	D	206/211 (97%)	1.15	37 (17%) 1 4	489, 489, 489, 489	0
3	J	207/211 (98%)	1.72	65 (31%) 0 2	490, 490, 490, 490	0
3	N	206/211 (97%)	1.26	43 (20%) 1 3	494, 494, 494, 494	0
All	All	3750/3918 (95%)	1.45	1048 (27%) 0 2	407, 487, 547, 547	0

The worst 5 of 1048 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	254	SER	11.7
3	C	348	VAL	11.5
1	G	208	SER	11.3

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Mol	Chain	Res	Type	RSRZ
1	K	38	GLN	10.7
1	Q	208	SER	9.6

## 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.