Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

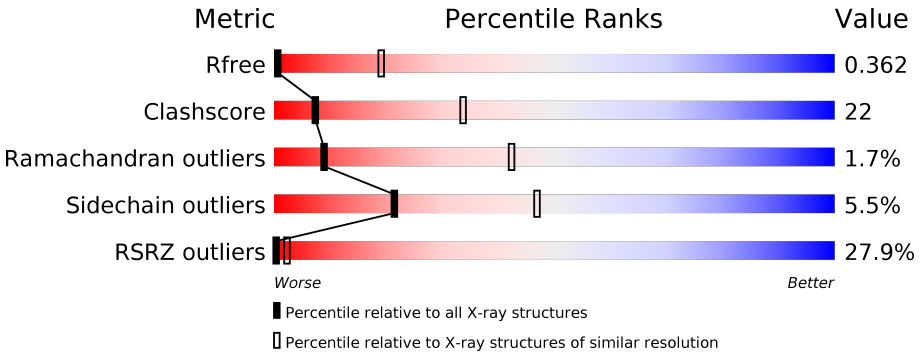
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	213	16% 81% 16%
1	G	213	31% 76% 21%
1	K	213	28% 82% 15%
1	L	213	37% 77% 20%
1	P	213	15% 82% 15%
1	Q	213	31% 76% 21%

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Mol	Chain	Length	Quality of chain
2	E	229	24% 68% 22% • 8%
2	H	229	28% 69% 21% • 9%
2	I	229	21% 60% 23% 7% 10%
2	M	229	35% 60% 22% 7% 10%
2	O	229	24% 69% 21% • 9%
2	R	229	21% 60% 22% 7% 10%
3	A	211	35% 47% 44% 7% •
3	B	211	37% 39% 51% 8% •
3	C	211	30% 45% 45% 7% •
3	D	211	18% 39% 51% 7% •
3	J	211	31% 49% 42% 7% •
3	N	211	20% 39% 51% 8% •

2 Entry composition

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
1	L	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	K	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	G	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	F	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	Q	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	P	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			

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

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

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.

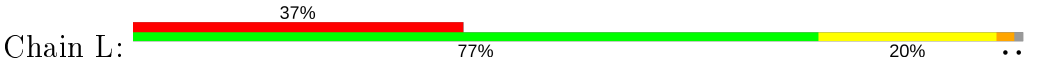
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	B	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	C	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	D	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	J	207	Total	C	N	O	S	0	0	0
			1660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

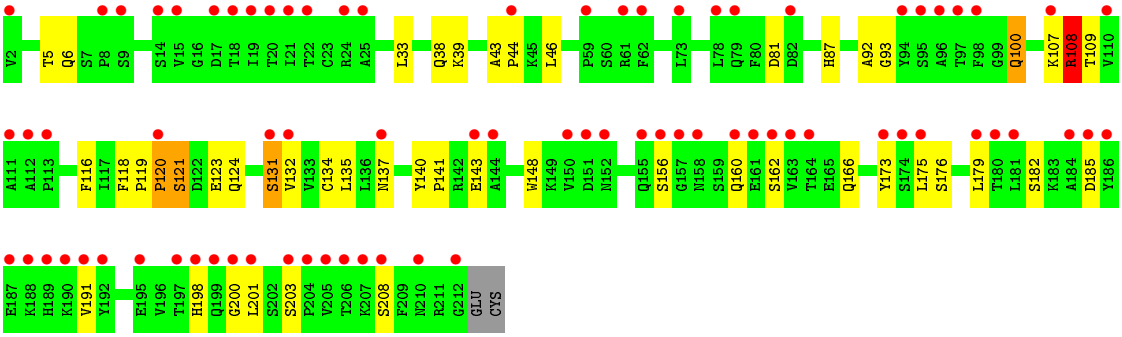
3 Residue-property plots (i)

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

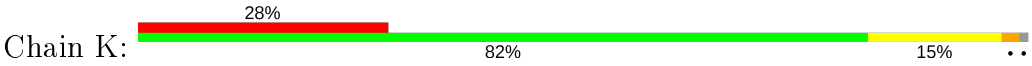
Chain L:

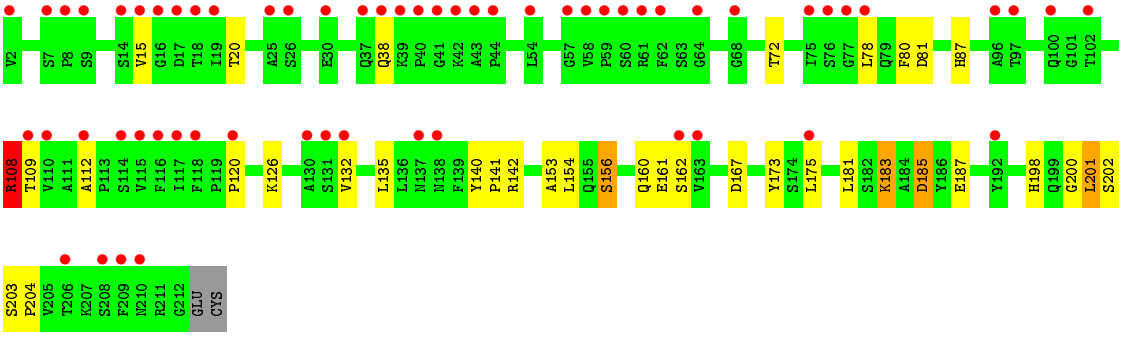




- Molecule 1: 2G12 IgG dimer light chain

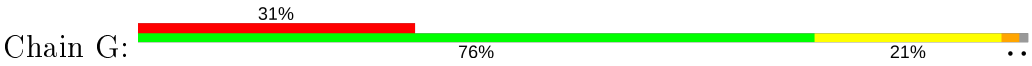
Chain K:

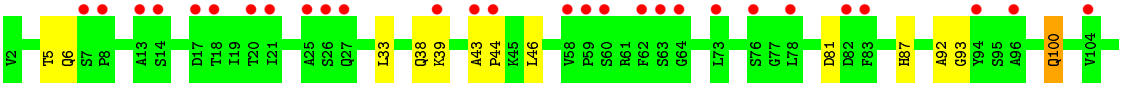


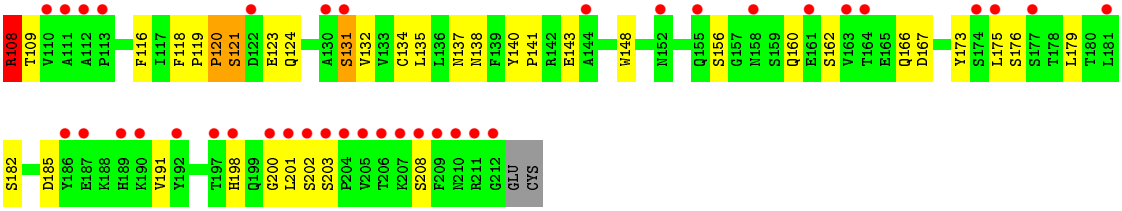


- Molecule 1: 2G12 IgG dimer light chain

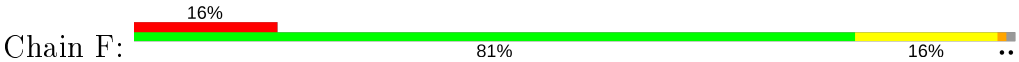
Chain G:

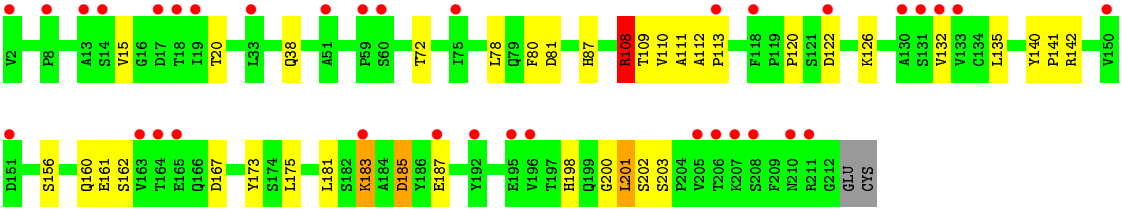




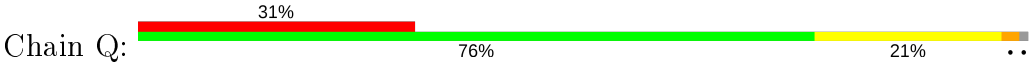


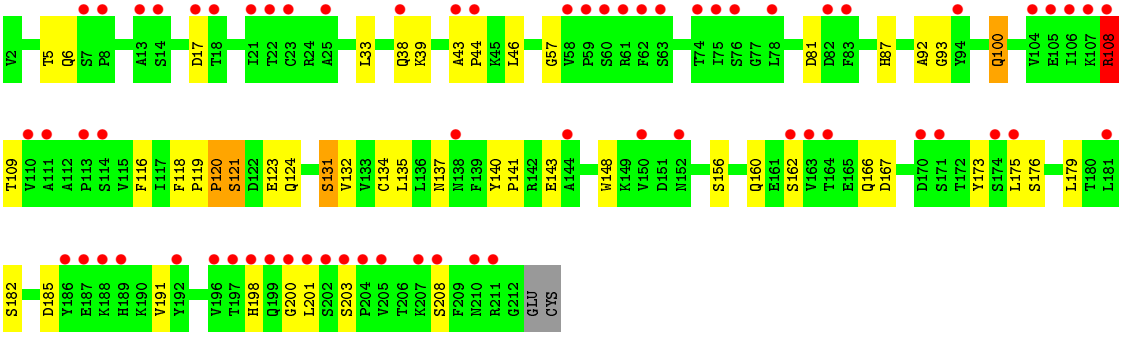
• Molecule 1: 2G12 IgG dimer light chain



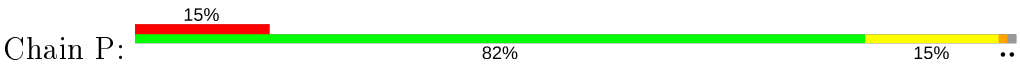


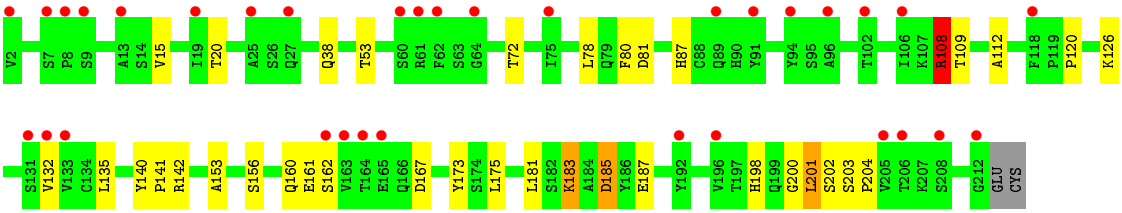
• Molecule 1: 2G12 IgG dimer light chain



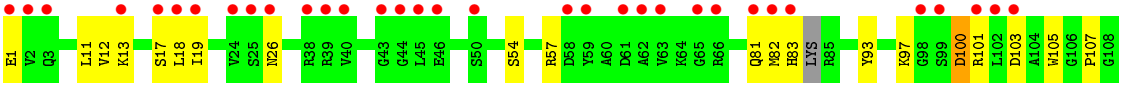


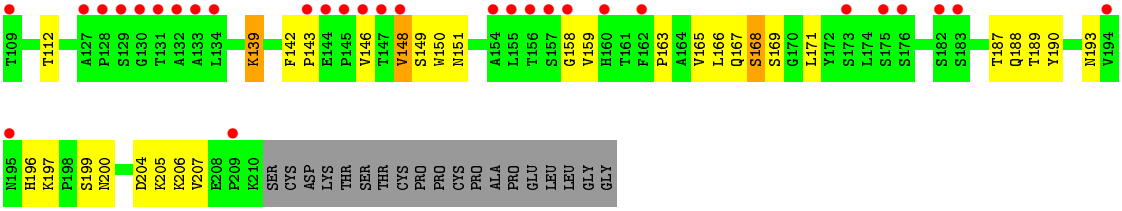
• Molecule 1: 2G12 IgG dimer light chain



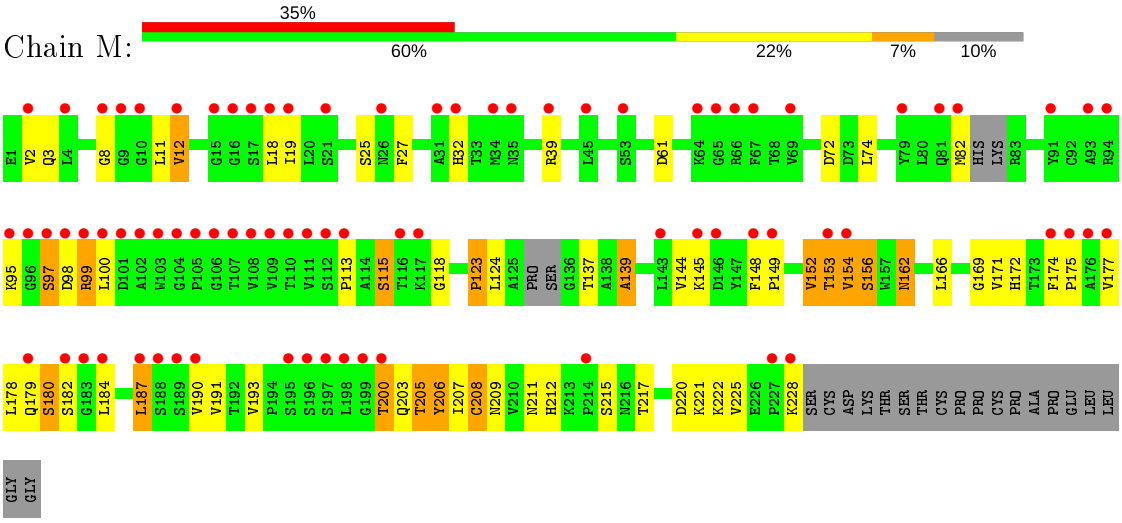


• Molecule 2: Hepatitis B virus receptor binding protein

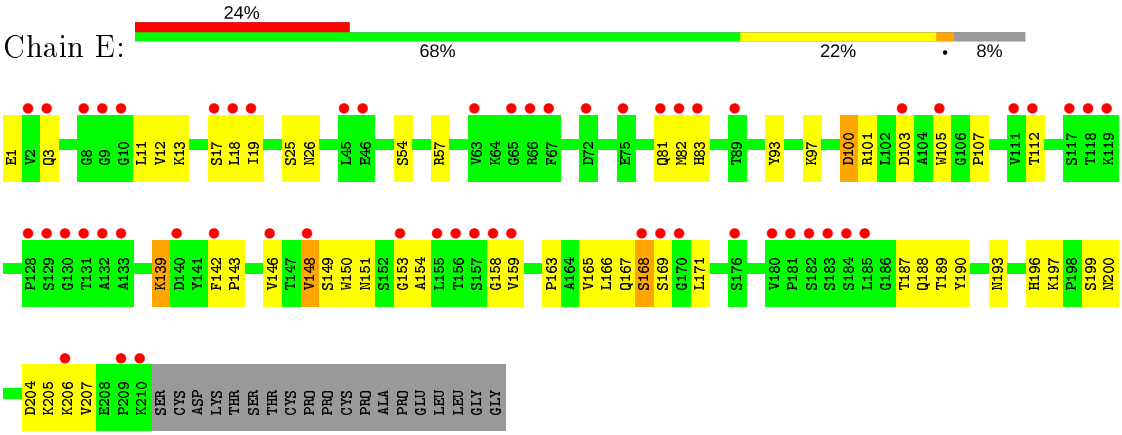




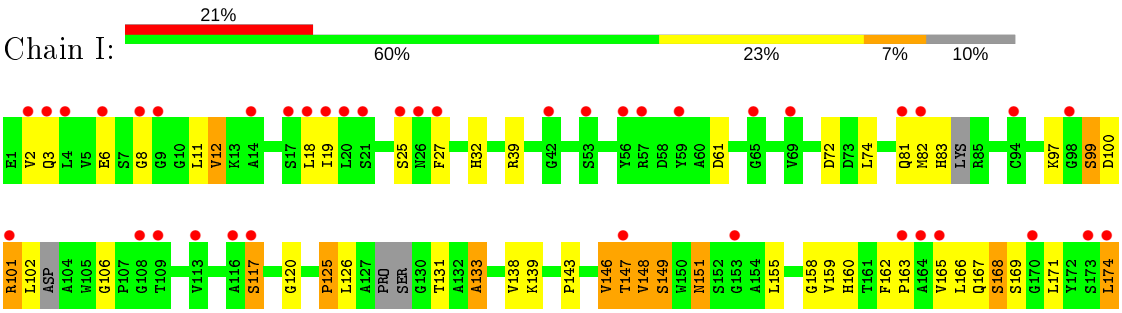
• Molecule 2: Hepatitis B virus receptor binding protein

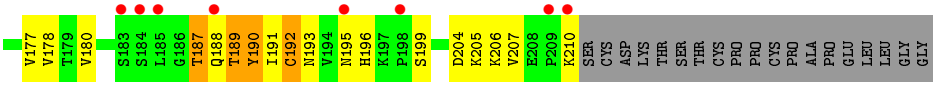


• Molecule 2: Hepatitis B virus receptor binding protein



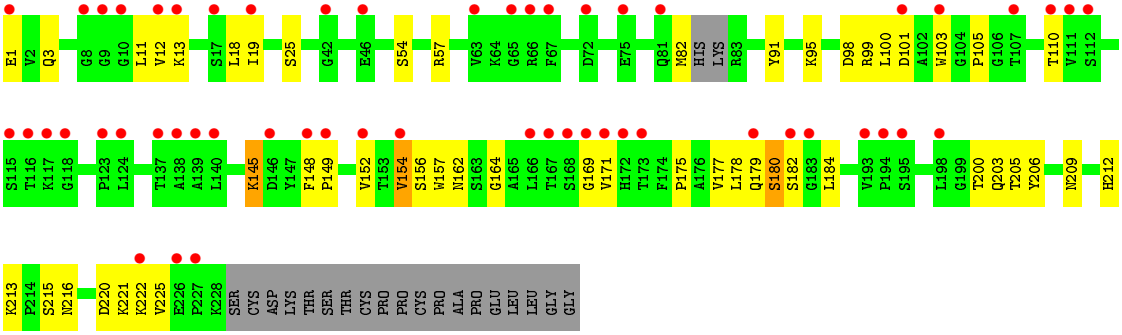
• Molecule 2: Hepatitis B virus receptor binding protein





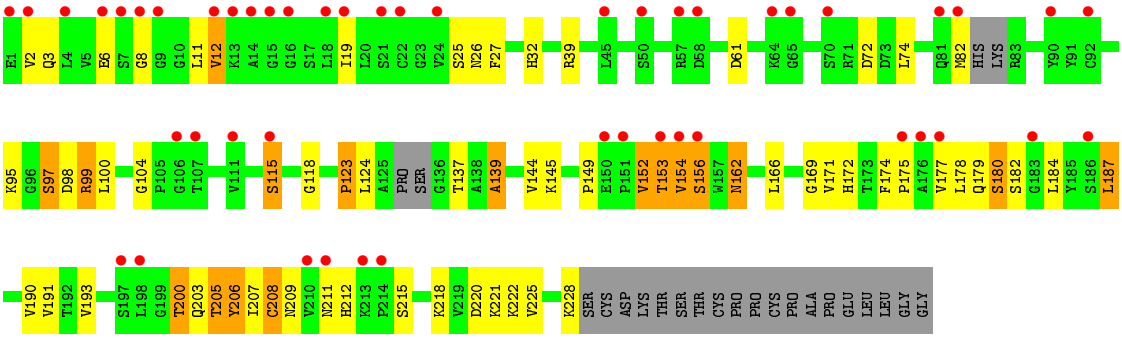
- Molecule 2: Hepatitis B virus receptor binding protein

Chain O:



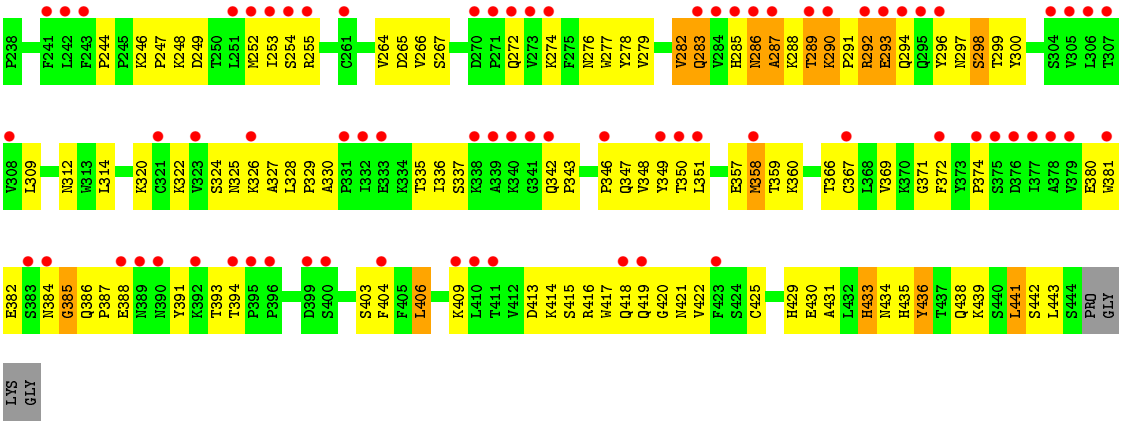
- Molecule 2: Hepatitis B virus receptor binding protein

Chain R:

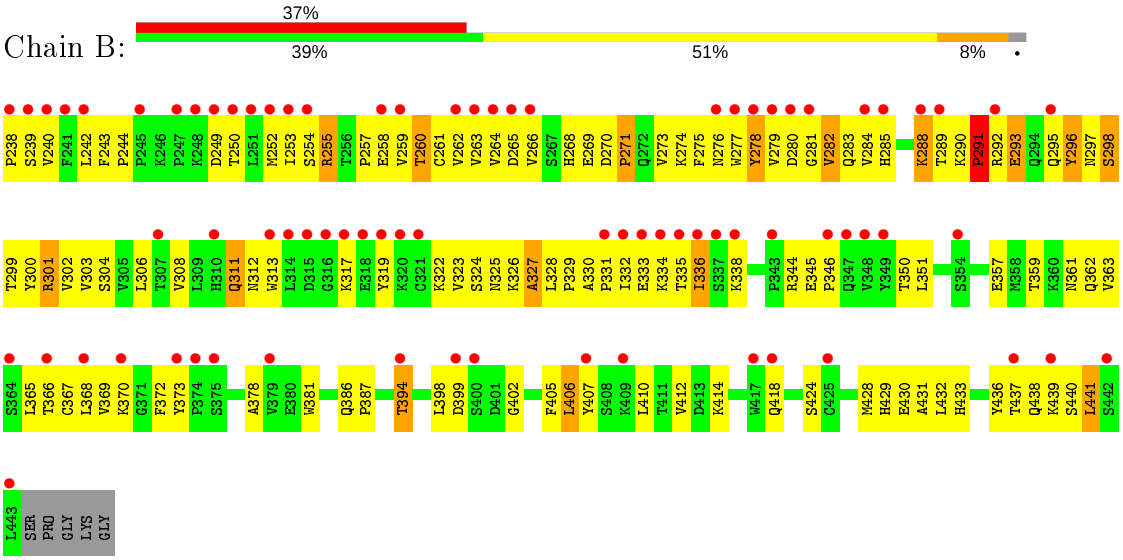


- Molecule 3: 2G12 IgG dimer heavy chain

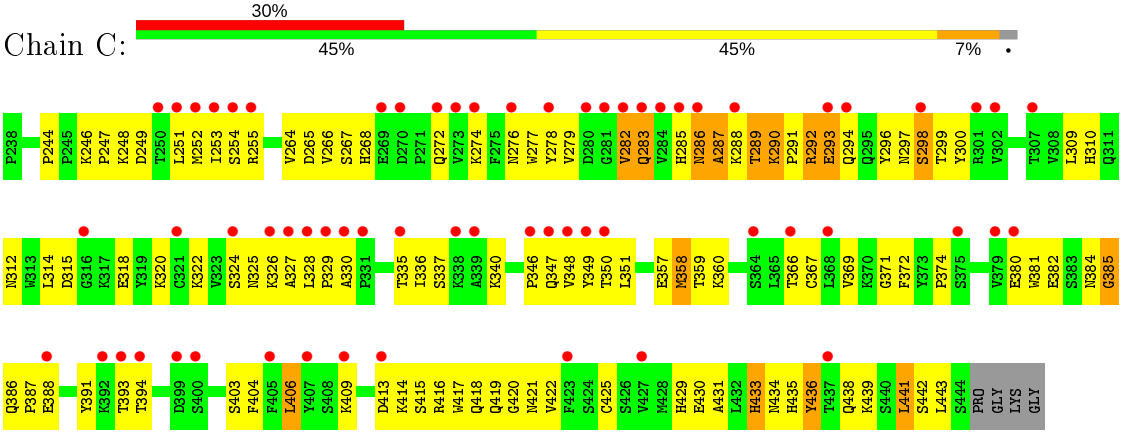
Chain A:



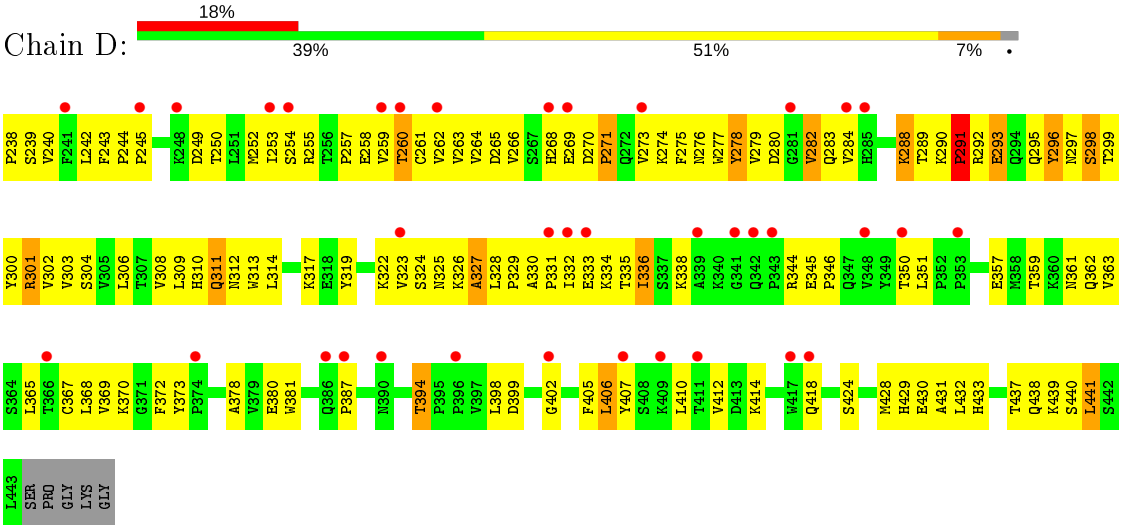
- Molecule 3: 2G12 IgG dimer heavy chain



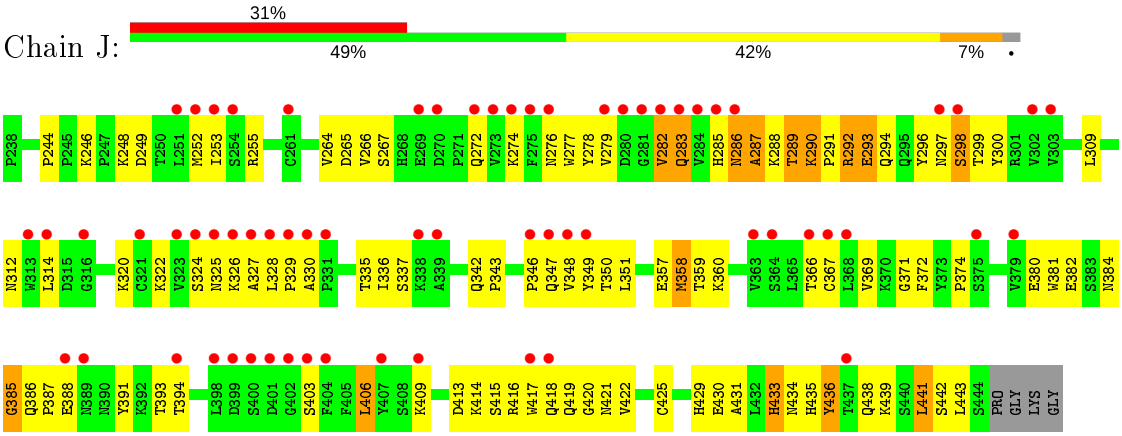
- Molecule 3: 2G12 IgG dimer heavy chain



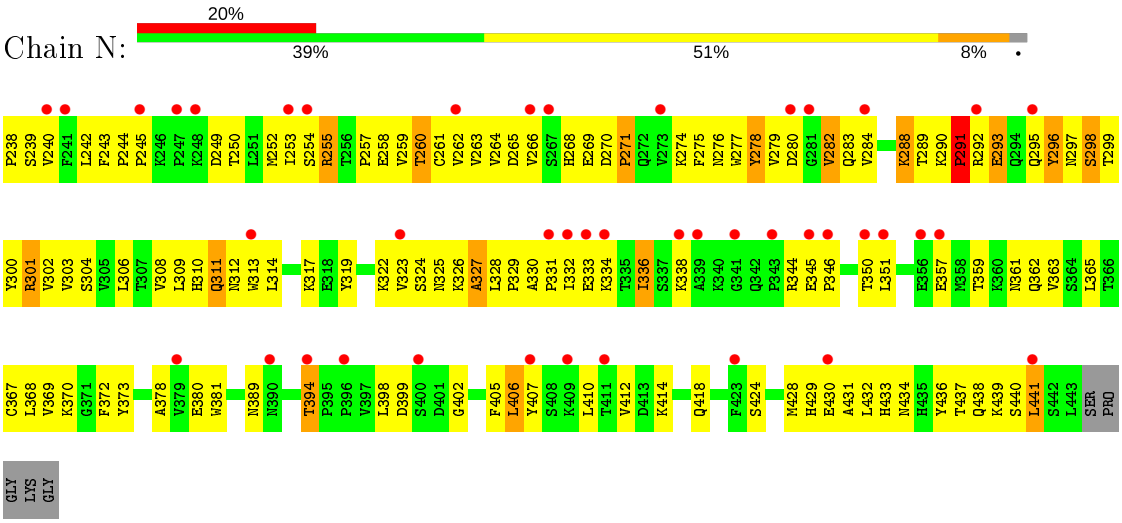
- Molecule 3: 2G12 IgG dimer heavy chain



- Molecule 3: 2G12 IgG dimer heavy chain



- Molecule 3: 2G12 IgG dimer heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.77 (at 6.17Å)	Xtriage
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^2)	243.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.14 , 259.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	28972	wwPDB-VP
Average B, all atoms (Å^2)	481.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	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

All (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
1	L	121	SER	CB-OG	24.52	1.74	1.42
2	E	168	SER	C-N	23.32	1.87	1.34
2	O	180	SER	C-N	23.31	1.87	1.34
2	H	168	SER	C-N	23.29	1.87	1.34
2	I	148	VAL	C-N	22.64	1.86	1.34
2	R	154	VAL	C-N	22.64	1.86	1.34
2	M	154	VAL	C-N	22.59	1.86	1.34
2	E	148	VAL	C-N	16.81	1.72	1.34
2	O	154	VAL	C-N	16.81	1.72	1.34
2	H	148	VAL	C-N	16.78	1.72	1.34
1	L	119	PRO	C-O	12.54	1.48	1.23
1	Q	119	PRO	C-O	12.46	1.48	1.23
1	G	119	PRO	C-O	12.46	1.48	1.23
1	L	131	SER	CB-OG	12.04	1.57	1.42
1	Q	131	SER	CB-OG	11.99	1.57	1.42
1	G	131	SER	CB-OG	11.98	1.57	1.42
1	L	182	SER	CB-OG	8.19	1.52	1.42
1	Q	182	SER	CB-OG	8.19	1.52	1.42
1	G	182	SER	CB-OG	8.14	1.52	1.42
2	I	131	THR	C-O	6.95	1.36	1.23
2	M	137	THR	C-O	6.90	1.36	1.23
2	R	137	THR	C-O	6.90	1.36	1.23
2	I	133	ALA	C-O	6.80	1.36	1.23
2	R	139	ALA	C-O	6.75	1.36	1.23
2	M	139	ALA	C-O	6.75	1.36	1.23
1	Q	119	PRO	C-N	6.27	1.46	1.34
1	P	183	LYS	C-O	6.20	1.35	1.23
1	K	183	LYS	C-O	6.16	1.35	1.23
1	G	119	PRO	C-N	6.16	1.46	1.34
1	F	183	LYS	C-O	6.15	1.35	1.23
1	L	119	PRO	C-N	6.15	1.46	1.34
1	Q	120	PRO	N-CD	5.95	1.56	1.47
2	R	208	CYS	CB-SG	5.92	1.92	1.82
1	L	120	PRO	N-CD	5.90	1.56	1.47
1	G	120	PRO	N-CD	5.89	1.56	1.47
2	M	208	CYS	CB-SG	5.88	1.92	1.82
2	I	192	CYS	CB-SG	5.88	1.92	1.82
2	M	206	TYR	CE1-CZ	5.57	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	206	TYR	CG-CD2	5.57	1.46	1.39
2	M	206	TYR	CG-CD2	5.53	1.46	1.39
2	I	190	TYR	CG-CD2	5.51	1.46	1.39
2	I	190	TYR	CE1-CZ	5.51	1.45	1.38
2	R	206	TYR	CE1-CZ	5.50	1.45	1.38
2	I	125	PRO	C-O	5.48	1.34	1.23
2	R	123	PRO	C-O	5.46	1.34	1.23
2	M	123	PRO	C-O	5.44	1.34	1.23
2	M	137	THR	C-N	5.26	1.46	1.34
2	I	131	THR	C-N	5.25	1.46	1.34
2	R	137	THR	C-N	5.22	1.46	1.34

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	Q	108	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	Q	108	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	G	108	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	G	108	ARG	NE-CZ-NH1	12.02	126.31	120.30
1	F	108	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	P	108	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	K	108	ARG	NE-CZ-NH1	10.28	125.44	120.30
2	E	168	SER	O-C-N	-8.46	109.17	122.70
2	H	168	SER	O-C-N	-8.43	109.21	122.70
2	O	180	SER	O-C-N	-8.43	109.22	122.70
2	R	154	VAL	C-N-CA	-6.45	105.57	121.70
2	I	148	VAL	C-N-CA	-6.42	105.64	121.70
2	M	154	VAL	C-N-CA	-6.42	105.66	121.70
2	I	168	SER	O-C-N	-6.36	112.53	122.70
2	M	180	SER	O-C-N	-6.35	112.54	122.70
2	R	180	SER	O-C-N	-6.34	112.55	122.70
1	K	81	ASP	CB-CG-OD2	6.26	123.93	118.30
1	P	81	ASP	CB-CG-OD2	6.24	123.92	118.30
1	F	81	ASP	CB-CG-OD2	6.19	123.87	118.30
1	Q	81	ASP	CB-CG-OD2	6.15	123.83	118.30
1	G	81	ASP	CB-CG-OD2	6.14	123.83	118.30
1	L	81	ASP	CB-CG-OD2	6.13	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	100	ASP	CB-CG-OD2	5.81	123.53	118.30
2	R	98	ASP	CB-CG-OD2	5.79	123.51	118.30
2	M	98	ASP	CB-CG-OD2	5.76	123.48	118.30
2	I	204	ASP	CB-CG-OD2	5.63	123.37	118.30
2	M	220	ASP	CB-CG-OD2	5.61	123.35	118.30
2	R	220	ASP	CB-CG-OD2	5.54	123.29	118.30
2	E	204	ASP	CB-CG-OD2	5.50	123.25	118.30
2	H	204	ASP	CB-CG-OD2	5.50	123.25	118.30
2	O	220	ASP	CB-CG-OD2	5.50	123.25	118.30
1	L	185	ASP	CB-CG-OD2	5.32	123.09	118.30
1	Q	185	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	185	ASP	CB-CG-OD2	5.18	122.97	118.30
2	E	100	ASP	CB-CG-OD2	5.17	122.95	118.30
2	R	61	ASP	CB-CG-OD2	5.17	122.95	118.30
1	P	185	ASP	CB-CG-OD2	5.16	122.94	118.30
2	M	61	ASP	CB-CG-OD2	5.15	122.93	118.30
2	I	61	ASP	CB-CG-OD2	5.12	122.91	118.30
2	H	100	ASP	CB-CG-OD2	5.11	122.90	118.30
1	G	167	ASP	CB-CG-OD2	5.09	122.89	118.30
1	F	167	ASP	CB-CG-OD2	5.09	122.89	118.30
1	F	185	ASP	CB-CG-OD2	5.08	122.88	118.30
1	P	167	ASP	CB-CG-OD2	5.05	122.85	118.30
1	Q	167	ASP	CB-CG-OD2	5.05	122.85	118.30
1	K	167	ASP	CB-CG-OD2	5.05	122.84	118.30
1	Q	17	ASP	CB-CG-OD2	5.04	122.84	118.30
1	K	185	ASP	CB-CG-OD2	5.04	122.84	118.30
2	O	98	ASP	CB-CG-OD2	5.03	122.82	118.30
1	F	122	ASP	CB-CG-OD2	5.02	122.82	118.30

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 (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	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
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.

All (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
1:F:112:ALA:CB	2:O:99:ARG:HB3	1.39	1.45
3:C:310:HIS:CD2	3:N:253:ILE:HD12	1.50	1.42
2:O:154:VAL:C	2:O:156:SER:N	1.72	1.42
2:E:148:VAL:C	2:E:149:SER:N	1.72	1.41
3:C:253:ILE:CG2	3:N:310:HIS:CE1	2.03	1.41
2:H:148:VAL:C	2:H:149:SER:N	1.72	1.39
3:C:253:ILE:HG21	3:N:310:HIS:NE2	1.40	1.36
1:Q:121:SER:CB	1:Q:121:SER:OG	1.74	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:SER:OG	1:G:121:SER:CB	1.74	1.35
1:L:121:SER:OG	1:L:121:SER:CB	1.74	1.35
1:F:112:ALA:HB1	2:O:99:ARG:CG	1.56	1.33
2:M:115:SER:N	3:B:282:VAL:HG12	1.36	1.33
2:R:154:VAL:C	2:R:156:SER:N	1.86	1.29
2:M:154:VAL:C	2:M:156:SER:N	1.86	1.28
2:O:180:SER:C	2:O:182:SER:N	1.87	1.28
2:I:148:VAL:C	2:I:149:SER:N	1.86	1.27
1:F:201:LEU:HD13	2:O:99:ARG:CG	1.48	1.27
2:H:168:SER:C	2:H:169:SER:N	1.87	1.27
2:E:168:SER:C	2:E:169:SER:N	1.87	1.25
3:C:252:MET:C	3:N:253:ILE:HD13	1.58	1.23
1:F:112:ALA:CB	2:O:99:ARG:CG	2.14	1.20
1:F:202:SER:O	3:C:297:ASN:CA	1.89	1.20
2:E:11:LEU:HD11	2:I:166:LEU:HD21	1.24	1.17
1:F:202:SER:O	3:C:297:ASN:HA	1.39	1.17
2:I:168:SER:C	2:I:169:SER:N	1.98	1.17
2:R:180:SER:C	2:R:182:SER:N	1.98	1.16
1:P:203:SER:CB	3:J:298:SER:HB3	1.76	1.16
2:M:180:SER:C	2:M:182:SER:N	1.98	1.16
1:P:203:SER:HB2	3:J:298:SER:HB3	1.20	1.15
1:K:156:SER:CB	3:B:333:GLU:OE2	1.95	1.15
2:O:11:LEU:HD11	2:R:178:LEU:HD21	1.24	1.14
1:F:112:ALA:CB	2:O:99:ARG:HG2	1.74	1.14
2:M:115:SER:HB2	3:B:282:VAL:CG1	1.77	1.14
1:F:201:LEU:CD1	2:O:99:ARG:CD	2.17	1.13
2:H:11:LEU:HD11	2:M:178:LEU:HD21	1.24	1.13
1:K:202:SER:HB2	3:A:296:TYR:O	1.47	1.12
1:F:112:ALA:HB2	2:O:99:ARG:HA	1.22	1.12
3:C:310:HIS:CD2	3:N:253:ILE:CD1	2.33	1.12
2:H:11:LEU:CD1	2:M:178:LEU:HD21	1.79	1.11
1:K:202:SER:CB	3:A:296:TYR:O	1.99	1.11
2:O:11:LEU:CD1	2:R:178:LEU:HD21	1.79	1.11
2:E:11:LEU:CD1	2:I:166:LEU:HD21	1.79	1.10
1:F:201:LEU:HD12	2:O:99:ARG:HG3	1.21	1.09
1:F:201:LEU:CD1	2:O:99:ARG:HG3	1.58	1.08
3:C:310:HIS:HD2	3:N:253:ILE:CD1	1.64	1.08
2:I:117:SER:HB2	3:D:282:VAL:HG12	1.30	1.07
1:P:203:SER:HB2	3:J:298:SER:CB	1.84	1.07
1:F:112:ALA:CB	2:O:99:ARG:CA	2.30	1.06
2:M:115:SER:CB	3:B:282:VAL:CG1	2.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ALA:HB2	2:O:99:ARG:CA	1.86	1.05
2:O:178:LEU:HD21	2:R:11:LEU:HD11	1.07	1.05
3:C:436:TYR:CE2	3:N:434:ASN:HB2	1.91	1.04
1:F:203:SER:CB	3:C:298:SER:HB3	1.87	1.04
1:F:110:VAL:HB	2:O:100:LEU:HD12	1.34	1.04
2:H:166:LEU:HD21	2:M:11:LEU:HD11	1.07	1.03
1:F:201:LEU:CD1	2:O:99:ARG:HG2	1.66	1.02
2:E:166:LEU:HD21	2:I:11:LEU:HD11	1.07	1.02
2:M:115:SER:CB	3:B:282:VAL:HG11	1.90	1.01
2:I:117:SER:HB2	3:D:282:VAL:CG1	1.90	1.01
2:E:166:LEU:HD21	2:I:11:LEU:CD1	1.91	1.01
1:F:203:SER:HB2	3:C:298:SER:CB	1.90	1.01
2:H:166:LEU:HD21	2:M:11:LEU:CD1	1.91	1.01
3:C:252:MET:C	3:N:253:ILE:CD1	2.29	1.01
2:O:178:LEU:HD21	2:R:11:LEU:CD1	1.91	0.99
3:C:294:GLN:HG2	2:O:1:GLU:O	1.21	0.99
3:B:266:VAL:HB	3:B:300:TYR:HB2	1.44	0.99
3:C:294:GLN:CG	2:O:1:GLU:O	2.08	0.99
3:D:266:VAL:HB	3:D:300:TYR:HB2	1.44	0.98
1:F:201:LEU:CD1	2:O:99:ARG:HD3	1.87	0.98
2:H:158:GLY:C	2:H:159:VAL:N	2.17	0.98
2:O:169:GLY:C	2:O:171:VAL:N	2.17	0.98
3:N:266:VAL:HB	3:N:300:TYR:HB2	1.45	0.98
1:F:203:SER:HB2	3:C:298:SER:HB3	0.99	0.97
3:C:254:SER:HA	3:N:311:GLN:OE1	1.65	0.97
2:M:113:PRO:HB2	3:B:281:GLY:HA3	1.47	0.96
1:K:156:SER:HB3	3:B:333:GLU:OE2	1.63	0.96
2:E:158:GLY:C	2:E:159:VAL:N	2.17	0.96
1:K:156:SER:CB	3:B:333:GLU:CD	2.34	0.96
3:C:252:MET:O	3:N:253:ILE:HD13	1.66	0.96
1:K:156:SER:HB2	3:B:333:GLU:OE2	1.64	0.95
3:C:436:TYR:CE2	3:N:434:ASN:CB	2.50	0.94
1:K:156:SER:OG	3:B:333:GLU:OE1	1.86	0.94
3:C:253:ILE:HD13	3:N:310:HIS:HE2	1.29	0.94
3:C:382:GLU:OE1	3:N:433:HIS:CD2	2.20	0.94
1:F:20:THR:HG23	1:F:72:THR:HG23	1.48	0.94
2:O:11:LEU:HD11	2:R:178:LEU:CD2	1.97	0.93
1:P:20:THR:HG23	1:P:72:THR:HG23	1.48	0.93
2:H:11:LEU:HD11	2:M:178:LEU:CD2	1.97	0.93
1:Q:120:PRO:HD3	1:Q:132:VAL:HG12	1.50	0.93
2:E:11:LEU:HD11	2:I:166:LEU:CD2	1.97	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:115:SER:HB2	3:B:282:VAL:CB	1.99	0.92
1:L:120:PRO:HD3	1:L:132:VAL:HG12	1.50	0.92
1:K:20:THR:HG23	1:K:72:THR:HG23	1.48	0.92
1:F:112:ALA:HB1	2:O:99:ARG:HG2	0.92	0.91
2:M:115:SER:OG	3:B:282:VAL:HG11	1.69	0.91
2:M:115:SER:H	3:B:282:VAL:CG1	1.82	0.91
1:F:201:LEU:HD11	2:O:99:ARG:HD3	0.92	0.91
2:M:115:SER:H	3:B:282:VAL:HG12	1.00	0.91
1:G:120:PRO:HD3	1:G:132:VAL:HG12	1.50	0.91
3:C:434:ASN:ND2	3:N:428:MET:HE1	1.85	0.90
3:A:272:GLN:HE22	3:A:326:LYS:HD2	1.35	0.90
1:K:202:SER:HB2	3:A:296:TYR:C	1.90	0.90
1:F:201:LEU:HD13	2:O:99:ARG:HG2	0.90	0.90
3:J:272:GLN:HE22	3:J:326:LYS:HD2	1.35	0.90
3:C:282:VAL:O	3:C:283:GLN:HB2	1.72	0.89
2:M:115:SER:N	3:B:282:VAL:CG1	2.33	0.89
1:Q:118:PHE:CE1	2:R:139:ALA:O	2.25	0.89
1:G:118:PHE:CE1	2:I:133:ALA:O	2.25	0.89
3:C:436:TYR:HE2	3:N:434:ASN:OD1	1.56	0.89
2:H:166:LEU:CD2	2:M:11:LEU:HD11	2.01	0.89
1:P:203:SER:CB	3:J:298:SER:CB	2.44	0.89
1:L:118:PHE:CE1	2:M:139:ALA:O	2.25	0.89
3:J:282:VAL:O	3:J:283:GLN:HB2	1.72	0.88
1:K:108:ARG:HD3	1:K:109:THR:O	1.74	0.88
2:M:115:SER:CA	3:B:282:VAL:HG12	2.04	0.88
3:C:272:GLN:HE22	3:C:326:LYS:HD2	1.35	0.88
1:F:108:ARG:HD3	1:F:109:THR:O	1.74	0.88
2:O:178:LEU:CD2	2:R:11:LEU:HD11	2.01	0.88
1:K:20:THR:HG23	1:K:72:THR:CG2	2.04	0.87
1:P:20:THR:HG23	1:P:72:THR:CG2	2.04	0.87
3:B:311:GLN:H	3:B:311:GLN:NE2	1.71	0.87
3:A:282:VAL:O	3:A:283:GLN:HB2	1.72	0.87
1:F:20:THR:HG23	1:F:72:THR:CG2	2.04	0.87
2:M:115:SER:HB2	3:B:282:VAL:HB	1.56	0.86
3:D:311:GLN:H	3:D:311:GLN:NE2	1.71	0.86
3:N:311:GLN:NE2	3:N:311:GLN:H	1.71	0.86
3:C:436:TYR:CD2	3:N:434:ASN:CB	2.59	0.86
1:F:110:VAL:O	2:O:100:LEU:HB2	1.75	0.86
2:E:81:GLN:HE21	2:E:83:HIS:HE1	1.23	0.85
1:P:108:ARG:HD3	1:P:109:THR:O	1.74	0.85
2:H:81:GLN:HE21	2:H:83:HIS:HE1	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:LEU:CD2	2:I:11:LEU:HD11	2.01	0.85
3:N:328:LEU:HD21	3:N:332:ILE:HG13	1.59	0.85
3:C:436:TYR:CE2	3:N:434:ASN:OD1	2.30	0.85
3:B:328:LEU:HD21	3:B:332:ILE:HG13	1.59	0.84
2:M:217:THR:OG1	3:B:285:HIS:CD2	2.31	0.84
3:C:253:ILE:HD13	3:N:310:HIS:NE2	1.93	0.84
3:D:328:LEU:HD21	3:D:332:ILE:HG13	1.59	0.83
3:C:253:ILE:HG22	3:N:310:HIS:CE1	2.13	0.83
3:C:346:PRO:HB3	3:C:372:PHE:HB3	1.60	0.83
2:R:115:SER:HB2	3:N:282:VAL:CG1	2.07	0.83
3:N:291:PRO:HB3	3:N:304:SER:HA	1.60	0.82
3:A:346:PRO:HB3	3:A:372:PHE:HB3	1.60	0.82
1:Q:6:GLN:H	1:Q:100:GLN:HE22	1.27	0.82
1:F:202:SER:O	3:C:297:ASN:C	2.17	0.82
3:D:291:PRO:HB3	3:D:304:SER:HA	1.60	0.82
3:A:314:LEU:HD22	3:A:430:GLU:HG3	1.62	0.82
3:B:243:PHE:HB2	3:B:260:THR:HG23	1.60	0.81
3:B:291:PRO:HB3	3:B:304:SER:HA	1.60	0.81
2:H:206:LYS:HA	2:H:207:VAL:N	1.95	0.81
3:N:243:PHE:HB2	3:N:260:THR:HG23	1.60	0.81
2:O:222:LYS:HA	2:O:225:VAL:N	1.94	0.81
3:C:314:LEU:HD22	3:C:430:GLU:HG3	1.62	0.81
3:J:346:PRO:HB3	3:J:372:PHE:HB3	1.60	0.81
3:J:314:LEU:HD22	3:J:430:GLU:HG3	1.62	0.81
3:D:243:PHE:HB2	3:D:260:THR:HG23	1.60	0.80
1:G:6:GLN:H	1:G:100:GLN:HE22	1.27	0.80
2:E:206:LYS:HA	2:E:207:VAL:N	1.95	0.80
3:C:252:MET:N	3:N:253:ILE:HD11	1.97	0.80
1:L:6:GLN:H	1:L:100:GLN:HE22	1.27	0.80
1:L:118:PHE:HE1	2:M:139:ALA:O	1.65	0.80
3:D:289:THR:HG22	3:D:290:LYS:H	1.48	0.79
3:D:346:PRO:HB3	3:D:372:PHE:HB3	1.63	0.79
2:R:115:SER:HB2	3:N:282:VAL:HG11	1.64	0.79
3:N:346:PRO:HB3	3:N:372:PHE:HB3	1.63	0.79
1:G:92:ALA:O	2:E:97:LYS:NZ	2.16	0.79
3:B:346:PRO:HB3	3:B:372:PHE:HB3	1.63	0.79
3:B:289:THR:HG22	3:B:290:LYS:H	1.48	0.79
3:A:291:PRO:C	3:A:292:ARG:HD2	2.03	0.79
1:G:118:PHE:HE1	2:I:133:ALA:O	1.65	0.79
1:G:108:ARG:HD3	1:G:109:THR:O	1.83	0.79
1:Q:108:ARG:HD3	1:Q:109:THR:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:291:PRO:C	3:J:292:ARG:HD2	2.03	0.78
3:N:289:THR:HG22	3:N:290:LYS:H	1.48	0.78
3:N:429:HIS:HD2	3:N:431:ALA:H	1.31	0.78
1:Q:92:ALA:O	2:O:95:LYS:NZ	2.16	0.78
1:L:108:ARG:HD3	1:L:109:THR:O	1.83	0.78
1:Q:118:PHE:HE1	2:R:139:ALA:O	1.65	0.78
3:B:263:VAL:O	3:B:301:ARG:HA	1.84	0.78
3:C:291:PRO:C	3:C:292:ARG:HD2	2.03	0.78
3:A:292:ARG:O	3:A:293:GLU:HB3	1.84	0.78
3:D:429:HIS:HD2	3:D:431:ALA:H	1.31	0.78
1:L:92:ALA:O	2:H:97:LYS:NZ	2.16	0.77
3:B:429:HIS:HD2	3:B:431:ALA:H	1.31	0.77
3:C:268:HIS:HB3	1:Q:57:GLY:HA2	1.66	0.77
1:G:160:GLN:NE2	2:I:165:VAL:CG1	2.48	0.77
3:C:436:TYR:CD2	3:N:434:ASN:HB3	2.20	0.77
3:N:263:VAL:O	3:N:301:ARG:HA	1.84	0.77
3:C:252:MET:C	3:N:253:ILE:CG1	2.46	0.77
3:D:263:VAL:O	3:D:301:ARG:HA	1.84	0.77
3:D:429:HIS:CD2	3:D:431:ALA:H	2.03	0.77
2:M:113:PRO:CB	3:B:281:GLY:HA3	2.15	0.76
3:B:429:HIS:CD2	3:B:431:ALA:H	2.03	0.76
3:C:253:ILE:CD1	3:N:310:HIS:HE2	1.98	0.76
1:Q:160:GLN:NE2	2:R:177:VAL:CG1	2.48	0.76
3:N:429:HIS:CD2	3:N:431:ALA:H	2.03	0.76
3:C:292:ARG:O	3:C:293:GLU:HB3	1.84	0.76
1:L:160:GLN:NE2	2:M:177:VAL:CG1	2.48	0.76
3:C:253:ILE:CG2	3:N:310:HIS:ND1	2.47	0.76
2:I:81:GLN:HE21	2:I:83:HIS:HE1	1.33	0.76
3:N:252:MET:SD	3:N:428:MET:HE1	2.26	0.76
1:L:198:HIS:CD2	1:L:200:GLY:H	2.04	0.75
3:B:266:VAL:HB	3:B:300:TYR:CB	2.15	0.75
3:C:272:GLN:NE2	3:C:326:LYS:HD2	2.01	0.75
1:Q:198:HIS:CD2	1:Q:200:GLY:H	2.04	0.75
3:B:328:LEU:HD12	3:B:329:PRO:HD2	1.69	0.75
3:C:253:ILE:CD1	3:N:310:HIS:NE2	2.49	0.75
3:C:252:MET:N	3:N:253:ILE:CD1	2.49	0.75
3:D:266:VAL:HB	3:D:300:TYR:CB	2.15	0.75
3:J:272:GLN:NE2	3:J:326:LYS:HD2	2.01	0.75
3:D:365:LEU:HD12	3:D:410:LEU:HD23	1.69	0.74
3:B:365:LEU:HD12	3:B:410:LEU:HD23	1.69	0.74
3:D:328:LEU:HD12	3:D:329:PRO:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:HIS:CD2	1:G:200:GLY:H	2.04	0.74
3:J:292:ARG:O	3:J:293:GLU:HB3	1.85	0.74
3:N:328:LEU:HD12	3:N:329:PRO:HD2	1.69	0.74
3:N:365:LEU:HD12	3:N:410:LEU:HD23	1.69	0.74
3:J:429:HIS:CD2	3:J:431:ALA:H	2.05	0.74
3:N:266:VAL:HB	3:N:300:TYR:CB	2.16	0.74
3:A:272:GLN:NE2	3:A:326:LYS:HD2	2.01	0.74
3:A:429:HIS:CD2	3:A:431:ALA:H	2.05	0.74
1:F:112:ALA:HB3	2:O:99:ARG:CA	2.03	0.74
3:C:429:HIS:CD2	3:C:431:ALA:H	2.05	0.74
3:C:434:ASN:ND2	3:N:428:MET:CE	2.51	0.74
3:C:310:HIS:HD2	3:N:253:ILE:HD12	0.93	0.72
3:N:288:LYS:H	3:N:288:LYS:HD3	1.54	0.72
2:E:81:GLN:HE21	2:E:83:HIS:CE1	2.07	0.72
3:B:288:LYS:HD3	3:B:288:LYS:H	1.54	0.72
2:M:113:PRO:HB2	3:B:281:GLY:CA	2.19	0.72
1:P:153:ALA:HA	3:N:330:ALA:CB	2.20	0.72
1:F:198:HIS:CD2	1:F:200:GLY:H	2.08	0.71
1:P:198:HIS:CD2	1:P:200:GLY:H	2.08	0.71
3:D:288:LYS:H	3:D:288:LYS:HD3	1.54	0.71
1:G:43:ALA:HB2	2:E:107:PRO:HA	1.72	0.71
1:K:198:HIS:HD2	1:K:200:GLY:H	1.39	0.71
1:L:43:ALA:HB2	2:H:107:PRO:HA	1.72	0.71
1:K:198:HIS:CD2	1:K:200:GLY:H	2.08	0.71
2:H:11:LEU:HD12	2:M:178:LEU:HD21	1.70	0.70
1:F:110:VAL:O	2:O:100:LEU:CB	2.39	0.70
2:H:81:GLN:HE21	2:H:83:HIS:CE1	2.07	0.70
3:C:253:ILE:HG21	3:N:310:HIS:CD2	2.26	0.70
1:L:160:GLN:HB3	2:M:177:VAL:HG11	1.74	0.70
3:C:251:LEU:C	3:N:253:ILE:HD11	2.11	0.70
1:Q:43:ALA:HB2	2:O:105:PRO:HA	1.72	0.70
1:P:112:ALA:HB1	1:P:201:LEU:HD13	1.73	0.69
3:A:422:VAL:HG22	3:A:442:SER:OG	1.92	0.69
3:C:253:ILE:HG22	3:N:310:HIS:ND1	2.06	0.69
2:M:215:SER:O	3:B:285:HIS:HB2	1.91	0.69
3:C:422:VAL:HG22	3:C:442:SER:OG	1.92	0.69
2:M:115:SER:CB	3:B:282:VAL:HG12	2.13	0.69
2:M:145:LYS:HE2	2:M:179:GLN:HE22	1.58	0.69
1:G:137:ASN:OD1	2:I:160:HIS:CD2	2.46	0.69
3:J:422:VAL:HG22	3:J:442:SER:OG	1.92	0.69
2:H:143:PRO:O	2:H:196:HIS:HE1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ALA:CB	2:O:99:ARG:HA	2.01	0.69
3:C:434:ASN:HA	3:N:252:MET:CE	2.23	0.69
2:O:149:PRO:O	2:O:212:HIS:HE1	1.75	0.69
3:A:252:MET:HB2	3:A:255:ARG:HG3	1.75	0.69
3:C:436:TYR:CD1	3:N:436:TYR:HD1	2.11	0.69
1:P:198:HIS:HD2	1:P:200:GLY:H	1.39	0.69
1:L:137:ASN:OD1	2:M:172:HIS:CD2	2.46	0.68
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.58	0.68
2:E:143:PRO:O	2:E:196:HIS:HE1	1.75	0.68
1:K:112:ALA:HB1	1:K:201:LEU:HD13	1.73	0.68
2:R:145:LYS:HE2	2:R:179:GLN:HE22	1.58	0.68
1:F:110:VAL:CB	2:O:100:LEU:HD12	2.19	0.68
1:F:198:HIS:HD2	1:F:200:GLY:H	1.39	0.68
1:G:160:GLN:HB3	2:I:165:VAL:HG11	1.74	0.68
3:C:253:ILE:CG2	3:N:310:HIS:NE2	2.32	0.68
1:K:202:SER:OG	3:A:296:TYR:O	2.12	0.68
3:J:325:ASN:HD21	3:J:327:ALA:HB3	1.58	0.68
1:Q:137:ASN:OD1	2:R:172:HIS:CD2	2.46	0.68
3:B:270:ASP:N	3:B:271:PRO:HD3	2.09	0.68
2:H:81:GLN:NE2	2:H:83:HIS:HE1	1.91	0.68
2:I:139:LYS:HE2	2:I:167:GLN:HE22	1.58	0.68
1:K:156:SER:OG	3:B:333:GLU:CD	2.31	0.68
1:F:111:ALA:HA	2:O:100:LEU:O	1.93	0.68
2:E:81:GLN:NE2	2:E:83:HIS:HE1	1.91	0.68
3:J:252:MET:HB2	3:J:255:ARG:HG3	1.75	0.68
3:C:436:TYR:CD1	3:N:436:TYR:CD1	2.82	0.68
3:N:270:ASP:N	3:N:271:PRO:HD3	2.09	0.67
3:C:252:MET:HB2	3:C:255:ARG:HG3	1.75	0.67
3:J:429:HIS:HD2	3:J:431:ALA:H	1.43	0.67
3:D:270:ASP:N	3:D:271:PRO:HD3	2.09	0.67
1:Q:160:GLN:HB3	2:R:177:VAL:HG11	1.74	0.67
3:C:429:HIS:HD2	3:C:431:ALA:H	1.42	0.67
2:E:11:LEU:HD12	2:I:166:LEU:HD21	1.70	0.67
1:F:112:ALA:HB1	1:F:201:LEU:HD13	1.73	0.67
1:F:20:THR:CG2	1:F:72:THR:HG23	2.24	0.67
2:O:11:LEU:HD12	2:R:178:LEU:HD21	1.70	0.67
3:J:418:GLN:HA	3:J:443:LEU:CD2	2.24	0.67
1:P:20:THR:CG2	1:P:72:THR:HG23	2.24	0.67
3:A:325:ASN:ND2	3:A:327:ALA:HB3	2.10	0.66
3:A:418:GLN:HA	3:A:443:LEU:CD2	2.24	0.66
3:C:418:GLN:HA	3:C:443:LEU:CD2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:THR:HB	3:C:441:LEU:HG	1.77	0.66
3:A:325:ASN:HD21	3:A:327:ALA:HB3	1.58	0.66
3:B:290:LYS:HE3	3:B:292:ARG:HH22	1.61	0.66
3:J:350:THR:HB	3:J:441:LEU:HG	1.77	0.66
3:A:350:THR:HB	3:A:441:LEU:HG	1.77	0.65
2:M:154:VAL:C	2:M:156:SER:CA	2.65	0.65
2:E:12:VAL:HG11	2:E:82:MET:CE	2.26	0.65
2:I:81:GLN:HE21	2:I:83:HIS:CE1	2.13	0.65
2:O:12:VAL:HG11	2:O:82:MET:CE	2.26	0.65
2:H:12:VAL:HG11	2:H:82:MET:CE	2.26	0.65
1:K:20:THR:CG2	1:K:72:THR:HG23	2.24	0.65
3:J:325:ASN:ND2	3:J:327:ALA:HB3	2.10	0.65
1:Q:160:GLN:CD	2:R:177:VAL:HG11	2.17	0.65
3:A:429:HIS:HD2	3:A:431:ALA:H	1.43	0.65
2:E:11:LEU:HD11	2:I:166:LEU:CG	2.27	0.65
1:L:160:GLN:CD	2:M:177:VAL:HG11	2.17	0.65
1:P:153:ALA:HA	3:N:330:ALA:HB2	1.77	0.65
2:O:11:LEU:HD11	2:R:178:LEU:CG	2.27	0.65
1:F:203:SER:HB3	3:C:298:SER:CA	2.26	0.65
3:A:279:VAL:O	3:A:282:VAL:HG13	1.97	0.64
3:A:328:LEU:HG	3:A:330:ALA:O	1.98	0.64
3:D:290:LYS:HE3	3:D:292:ARG:HH22	1.61	0.64
3:J:328:LEU:HG	3:J:330:ALA:O	1.98	0.64
3:C:325:ASN:ND2	3:C:327:ALA:HB3	2.10	0.64
3:C:328:LEU:HG	3:C:330:ALA:O	1.98	0.64
3:D:330:ALA:HB1	3:D:331:PRO:HD2	1.79	0.64
1:G:160:GLN:CD	2:I:165:VAL:HG11	2.17	0.64
3:N:290:LYS:HE3	3:N:292:ARG:HH22	1.61	0.64
3:C:433:HIS:NE2	3:N:380:GLU:OE1	2.29	0.64
2:I:148:VAL:C	2:I:149:SER:CA	2.65	0.64
3:J:279:VAL:O	3:J:282:VAL:HG13	1.97	0.64
2:R:169:GLY:C	2:R:171:VAL:N	2.51	0.64
3:B:330:ALA:HB1	3:B:331:PRO:HD2	1.79	0.64
2:O:12:VAL:HG11	2:O:82:MET:HE3	1.79	0.64
1:Q:132:VAL:HG22	1:Q:179:LEU:HB3	1.80	0.64
1:P:203:SER:OG	3:J:298:SER:HB3	1.96	0.64
1:L:137:ASN:OD1	2:M:172:HIS:HD2	1.81	0.64
1:G:132:VAL:HG22	1:G:179:LEU:HB3	1.79	0.63
2:R:154:VAL:C	2:R:156:SER:CA	2.64	0.63
2:H:11:LEU:HD11	2:M:178:LEU:CG	2.27	0.63
1:L:132:VAL:HG22	1:L:179:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:169:GLY:C	2:M:171:VAL:N	2.52	0.63
3:A:288:LYS:HD2	3:A:288:LYS:H	1.63	0.63
1:G:162:SER:OG	2:I:163:PRO:HD2	1.99	0.63
3:N:330:ALA:HB1	3:N:331:PRO:HD2	1.80	0.63
3:B:332:ILE:HG22	3:B:333:GLU:N	2.13	0.63
3:C:279:VAL:O	3:C:282:VAL:HG13	1.97	0.63
1:Q:162:SER:OG	2:R:175:PRO:HD2	1.99	0.63
1:F:202:SER:O	3:C:296:TYR:O	2.17	0.63
2:I:158:GLY:C	2:I:159:VAL:N	2.52	0.63
3:J:288:LYS:H	3:J:288:LYS:HD2	1.63	0.63
1:L:162:SER:OG	2:M:175:PRO:HD2	1.99	0.63
1:G:5:THR:HA	1:G:100:GLN:HE22	1.64	0.63
1:L:100:GLN:CD	1:L:100:GLN:H	2.02	0.63
1:Q:137:ASN:OD1	2:R:172:HIS:HD2	1.81	0.63
3:N:332:ILE:HG22	3:N:333:GLU:N	2.13	0.62
1:G:118:PHE:CZ	2:I:133:ALA:O	2.52	0.62
2:I:81:GLN:NE2	2:I:83:HIS:HE1	1.98	0.62
1:Q:100:GLN:H	1:Q:100:GLN:CD	2.02	0.62
3:C:288:LYS:HD2	3:C:288:LYS:H	1.63	0.62
3:D:332:ILE:HG22	3:D:333:GLU:N	2.13	0.62
1:G:137:ASN:OD1	2:I:160:HIS:HD2	1.82	0.62
2:M:12:VAL:HG11	2:M:82:MET:HE3	1.81	0.62
1:L:118:PHE:CZ	2:M:139:ALA:O	2.52	0.62
1:Q:118:PHE:CZ	2:R:139:ALA:O	2.52	0.62
2:I:12:VAL:HG11	2:I:82:MET:HE3	1.82	0.62
1:L:5:THR:HA	1:L:100:GLN:HE22	1.64	0.62
2:R:115:SER:HB2	3:N:282:VAL:HG12	1.81	0.62
2:I:12:VAL:HG11	2:I:82:MET:CE	2.30	0.62
2:R:12:VAL:HG11	2:R:82:MET:CE	2.30	0.61
1:Q:5:THR:HA	1:Q:100:GLN:HE22	1.64	0.61
1:G:100:GLN:H	1:G:100:GLN:CD	2.02	0.61
3:C:436:TYR:CE2	3:N:434:ASN:CG	2.74	0.61
1:F:202:SER:O	3:C:297:ASN:N	2.33	0.61
3:B:394:THR:HG23	3:B:407:TYR:O	2.01	0.61
3:C:434:ASN:HA	3:N:252:MET:HE1	1.82	0.61
2:M:113:PRO:O	3:B:282:VAL:N	2.33	0.61
1:G:118:PHE:HB2	2:I:126:LEU:HD22	1.83	0.61
2:M:12:VAL:HG11	2:M:82:MET:CE	2.30	0.61
1:Q:118:PHE:HB2	2:R:124:LEU:HD22	1.83	0.61
3:C:435:HIS:CE1	3:N:254:SER:OG	2.53	0.60
1:Q:121:SER:CB	2:R:123:PRO:HD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:MET:CA	3:N:253:ILE:CD1	2.79	0.60
3:C:434:ASN:CG	3:N:428:MET:CE	2.70	0.60
1:G:160:GLN:CD	2:I:165:VAL:CG1	2.70	0.60
3:B:406:LEU:HD12	3:B:406:LEU:C	2.22	0.60
3:N:274:LYS:HE2	3:N:276:ASN:HD21	1.67	0.60
3:N:406:LEU:HD12	3:N:406:LEU:C	2.22	0.60
2:H:150:TRP:C	2:H:151:ASN:N	2.55	0.60
3:J:384:ASN:O	3:J:386:GLN:N	2.31	0.60
3:D:394:THR:HG23	3:D:407:TYR:O	2.01	0.60
3:C:417:TRP:CH2	3:C:441:LEU:HD22	2.37	0.60
1:G:121:SER:CB	2:I:125:PRO:HD2	2.32	0.60
3:N:394:THR:HG23	3:N:407:TYR:O	2.01	0.60
1:L:121:SER:CB	2:M:123:PRO:HD2	2.31	0.60
2:O:157:TRP:C	2:O:162:ASN:N	2.55	0.60
3:D:274:LYS:HE2	3:D:276:ASN:HD21	1.67	0.59
3:D:406:LEU:C	3:D:406:LEU:HD12	2.22	0.59
3:C:382:GLU:OE1	3:N:433:HIS:CG	2.56	0.59
3:C:382:GLU:OE1	3:N:433:HIS:NE2	2.35	0.59
1:Q:160:GLN:CD	2:R:177:VAL:CG1	2.70	0.59
1:L:135:LEU:HD22	2:M:190:VAL:HG21	1.84	0.59
3:B:274:LYS:HE2	3:B:276:ASN:HD21	1.67	0.59
2:E:150:TRP:C	2:E:151:ASN:N	2.55	0.59
1:G:135:LEU:HD22	2:I:177:VAL:HG21	1.84	0.59
1:L:160:GLN:CD	2:M:177:VAL:CG1	2.70	0.59
2:M:203:GLN:OE1	2:M:205:THR:N	2.36	0.59
3:C:417:TRP:HH2	3:C:441:LEU:HD22	1.67	0.59
3:C:433:HIS:ND1	3:C:434:ASN:OD1	2.35	0.59
3:J:433:HIS:ND1	3:J:434:ASN:OD1	2.35	0.59
3:C:436:TYR:CE1	3:N:436:TYR:HD1	2.20	0.59
3:D:257:PRO:HB2	3:D:308:VAL:HB	1.85	0.59
1:L:46:LEU:HD22	2:H:103:ASP:HA	1.84	0.59
2:R:203:GLN:OE1	2:R:205:THR:N	2.36	0.59
3:A:417:TRP:CH2	3:A:441:LEU:HD22	2.37	0.59
3:A:417:TRP:HH2	3:A:441:LEU:HD22	1.68	0.59
3:B:257:PRO:HB2	3:B:308:VAL:HB	1.85	0.59
3:C:252:MET:CA	3:N:253:ILE:HG12	2.33	0.59
1:G:176:SER:HB3	2:I:162:PHE:CE1	2.37	0.59
2:I:188:GLN:OE1	2:I:189:THR:N	2.36	0.59
2:E:139:LYS:HE2	2:E:167:GLN:OE1	2.03	0.59
3:J:421:ASN:N	3:J:421:ASN:HD22	2.00	0.59
1:Q:176:SER:HB3	2:R:174:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:266:VAL:CB	3:B:300:TYR:HB2	2.28	0.59
1:G:46:LEU:HD22	2:E:103:ASP:HA	1.84	0.59
1:F:202:SER:O	3:C:297:ASN:O	2.17	0.59
1:L:118:PHE:HB2	2:M:124:LEU:HD22	1.83	0.59
1:L:176:SER:HB3	2:M:174:PHE:CE1	2.37	0.59
3:J:417:TRP:CH2	3:J:441:LEU:HD22	2.37	0.59
3:J:417:TRP:HH2	3:J:441:LEU:HD22	1.67	0.59
3:A:286:ASN:O	3:A:287:ALA:HB2	2.03	0.58
1:L:118:PHE:CD1	2:M:124:LEU:HB3	2.38	0.58
3:N:269:GLU:O	3:N:269:GLU:HG2	2.03	0.58
3:C:436:TYR:HD1	3:N:436:TYR:CD1	2.20	0.58
1:Q:132:VAL:CG2	1:Q:179:LEU:HB3	2.34	0.58
1:Q:135:LEU:HD22	2:R:190:VAL:HG21	1.84	0.58
3:C:421:ASN:HD22	3:C:421:ASN:N	2.00	0.58
3:N:279:VAL:HG23	3:N:279:VAL:O	2.03	0.58
1:Q:118:PHE:CD1	2:R:124:LEU:HB3	2.38	0.58
1:G:166:GLN:HG3	1:G:173:TYR:CZ	2.39	0.58
1:L:160:GLN:CB	2:M:177:VAL:HG11	2.33	0.58
3:D:296:TYR:CE1	3:D:301:ARG:HD3	2.38	0.58
3:N:296:TYR:CE1	3:N:301:ARG:HD3	2.38	0.58
1:L:132:VAL:CG2	1:L:179:LEU:HB3	2.33	0.58
3:N:424:SER:OG	3:N:438:GLN:HG2	2.04	0.58
1:Q:46:LEU:HD22	2:O:101:ASP:HA	1.84	0.58
3:A:384:ASN:O	3:A:386:GLN:N	2.31	0.58
3:A:433:HIS:ND1	3:A:434:ASN:OD1	2.36	0.58
2:O:145:LYS:HE2	2:O:179:GLN:OE1	2.03	0.58
1:P:183:LYS:O	1:P:187:GLU:HG3	2.04	0.58
3:B:279:VAL:O	3:B:279:VAL:HG23	2.04	0.58
3:D:288:LYS:HE2	3:D:306:LEU:HD11	1.86	0.58
1:K:154:LEU:N	3:B:330:ALA:HB3	2.19	0.58
3:B:296:TYR:CE1	3:B:301:ARG:HD3	2.38	0.57
3:D:279:VAL:HG23	3:D:279:VAL:O	2.04	0.57
3:J:415:SER:O	3:J:419:GLN:HG3	2.04	0.57
1:L:166:GLN:HG3	1:L:173:TYR:CZ	2.38	0.57
3:N:257:PRO:HB2	3:N:308:VAL:HB	1.85	0.57
1:G:132:VAL:CG2	1:G:179:LEU:HB3	2.33	0.57
1:G:118:PHE:CD1	2:I:126:LEU:HB3	2.38	0.57
1:G:160:GLN:CB	2:I:165:VAL:HG11	2.33	0.57
3:N:265:ASP:HA	3:N:299:THR:HB	1.86	0.57
3:B:325:ASN:HD22	3:B:326:LYS:H	1.51	0.57
1:K:183:LYS:O	1:K:187:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:5:THR:HA	1:Q:100:GLN:NE2	2.19	0.57
1:Q:166:GLN:HG3	1:Q:173:TYR:CZ	2.39	0.57
3:A:421:ASN:HD22	3:A:421:ASN:N	2.00	0.57
3:C:276:ASN:HB2	3:C:322:LYS:HB3	1.86	0.57
3:C:286:ASN:O	3:C:287:ALA:HB2	2.03	0.57
1:F:203:SER:CB	3:C:298:SER:CB	2.66	0.57
3:J:286:ASN:O	3:J:287:ALA:HB2	2.03	0.57
3:B:269:GLU:HG2	3:B:269:GLU:O	2.03	0.57
3:B:424:SER:OG	3:B:438:GLN:HG2	2.04	0.57
3:D:424:SER:OG	3:D:438:GLN:HG2	2.04	0.57
3:D:265:ASP:HA	3:D:299:THR:HB	1.85	0.57
2:H:12:VAL:HG11	2:H:82:MET:HE3	1.85	0.57
1:Q:160:GLN:CB	2:R:177:VAL:HG11	2.33	0.57
1:F:183:LYS:O	1:F:187:GLU:HG3	2.04	0.57
1:G:5:THR:HA	1:G:100:GLN:NE2	2.18	0.57
2:H:139:LYS:HE2	2:H:167:GLN:OE1	2.03	0.57
2:I:120:GLY:HA2	2:I:196:HIS:CD2	2.40	0.57
1:L:5:THR:HA	1:L:100:GLN:NE2	2.19	0.57
2:R:118:GLY:HA2	2:R:212:HIS:CD2	2.40	0.57
3:C:415:SER:O	3:C:419:GLN:HG3	2.04	0.57
1:K:156:SER:CB	3:B:333:GLU:OE1	2.46	0.56
3:D:325:ASN:HD22	3:D:326:LYS:H	1.50	0.56
2:M:162:ASN:N	2:M:162:ASN:OD1	2.38	0.56
3:N:288:LYS:HE2	3:N:306:LEU:HD11	1.86	0.56
3:A:276:ASN:HB2	3:A:322:LYS:HB3	1.86	0.56
3:B:328:LEU:HG	3:B:330:ALA:O	2.05	0.56
3:B:439:LYS:HE3	3:B:440:SER:O	2.05	0.56
3:C:384:ASN:O	3:C:386:GLN:N	2.31	0.56
1:K:38:GLN:NE2	2:M:39:ARG:HD2	2.20	0.56
3:A:415:SER:O	3:A:419:GLN:HG3	2.04	0.56
3:N:325:ASN:HD22	3:N:326:LYS:H	1.50	0.56
2:R:166:LEU:HD21	2:R:191:VAL:HG21	1.86	0.56
3:B:311:GLN:CD	3:B:311:GLN:H	2.08	0.56
3:D:269:GLU:HG2	3:D:269:GLU:O	2.03	0.56
3:D:328:LEU:HG	3:D:330:ALA:O	2.05	0.56
3:J:276:ASN:HB2	3:J:322:LYS:HB3	1.86	0.56
2:M:153:THR:HG22	2:M:211:ASN:HB3	1.87	0.56
2:M:118:GLY:HA2	2:M:212:HIS:CD2	2.40	0.56
3:N:311:GLN:CD	3:N:311:GLN:H	2.08	0.56
3:N:328:LEU:HG	3:N:330:ALA:O	2.06	0.56
3:B:265:ASP:HA	3:B:299:THR:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:439:LYS:HE3	3:D:440:SER:O	2.05	0.56
1:P:38:GLN:NE2	2:R:39:ARG:HD2	2.20	0.56
3:N:301:ARG:HE	3:N:303:VAL:CG2	2.18	0.56
1:Q:118:PHE:CB	2:R:124:LEU:HD22	2.36	0.56
3:D:311:GLN:CD	3:D:311:GLN:H	2.08	0.56
3:D:325:ASN:ND2	3:D:326:LYS:H	2.03	0.56
2:H:206:LYS:CA	2:H:207:VAL:N	2.67	0.56
3:A:328:LEU:HD12	3:A:329:PRO:HD2	1.88	0.56
3:B:288:LYS:HE2	3:B:306:LEU:HD11	1.86	0.56
3:C:320:LYS:HG3	3:C:335:THR:HG22	1.87	0.56
2:E:158:GLY:O	2:E:159:VAL:N	2.38	0.56
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
3:A:288:LYS:O	3:A:289:THR:O	2.24	0.56
3:A:320:LYS:HG3	3:A:335:THR:HG22	1.87	0.56
3:B:301:ARG:HE	3:B:303:VAL:CG2	2.18	0.56
3:D:301:ARG:HE	3:D:303:VAL:CG2	2.18	0.56
1:F:203:SER:CB	3:C:298:SER:CA	2.84	0.56
1:F:38:GLN:NE2	2:I:39:ARG:HD2	2.20	0.56
1:G:118:PHE:CB	2:I:126:LEU:HD22	2.36	0.56
2:I:155:LEU:HD21	2:I:178:VAL:HG21	1.87	0.56
2:M:166:LEU:HD21	2:M:191:VAL:HG21	1.87	0.56
3:N:325:ASN:ND2	3:N:326:LYS:H	2.04	0.56
1:Q:135:LEU:CD2	2:R:190:VAL:HG21	2.36	0.56
1:G:135:LEU:CD2	2:I:177:VAL:HG21	2.36	0.56
1:P:203:SER:HA	3:J:297:ASN:CB	2.33	0.56
2:R:12:VAL:HG11	2:R:82:MET:HE3	1.87	0.56
3:C:288:LYS:O	3:C:289:THR:O	2.24	0.56
3:D:270:ASP:OD2	3:D:327:ALA:HB2	2.06	0.56
2:E:12:VAL:HG11	2:E:82:MET:HE3	1.88	0.56
1:L:135:LEU:CD2	2:M:190:VAL:HG21	2.36	0.56
3:C:434:ASN:CG	3:N:428:MET:HE3	2.27	0.55
1:G:6:GLN:N	1:G:100:GLN:HE22	2.02	0.55
2:H:165:VAL:HG11	1:K:160:GLN:CD	2.27	0.55
2:R:162:ASN:OD1	2:R:162:ASN:N	2.38	0.55
2:E:188:GLN:HB2	2:E:190:TYR:CZ	2.42	0.55
2:I:147:THR:HG22	2:I:195:ASN:HB3	1.87	0.55
3:N:439:LYS:HE3	3:N:440:SER:O	2.05	0.55
2:O:203:GLN:HB2	2:O:206:TYR:CZ	2.42	0.55
2:O:177:VAL:HG11	1:P:160:GLN:CD	2.27	0.55
2:R:153:THR:HG22	2:R:211:ASN:HB3	1.87	0.55
2:E:12:VAL:HG11	2:E:82:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:GLN:HB2	2:H:190:TYR:CZ	2.42	0.55
1:L:118:PHE:CB	2:M:124:LEU:HD22	2.35	0.55
2:O:169:GLY:O	2:O:171:VAL:N	2.38	0.55
2:I:151:ASN:N	2:I:151:ASN:OD1	2.38	0.55
1:K:204:PRO:HD3	3:A:297:ASN:HB2	1.88	0.55
3:B:325:ASN:ND2	3:B:326:LYS:H	2.04	0.55
1:F:202:SER:O	3:C:296:TYR:C	2.45	0.55
3:J:320:LYS:HG3	3:J:335:THR:HG22	1.87	0.55
3:B:270:ASP:OD2	3:B:327:ALA:HB2	2.06	0.55
3:C:328:LEU:HD12	3:C:329:PRO:HD2	1.88	0.55
3:N:270:ASP:OD2	3:N:327:ALA:HB2	2.06	0.55
1:P:15:VAL:HG21	1:P:80:PHE:CZ	2.42	0.55
3:A:289:THR:O	3:A:290:LYS:HB2	2.07	0.54
2:E:165:VAL:HG11	1:F:160:GLN:CD	2.27	0.54
1:F:38:GLN:HE22	2:I:39:ARG:HD2	1.72	0.54
1:K:153:ALA:HB1	3:B:331:PRO:HD2	1.89	0.54
2:O:13:LYS:HD3	2:O:148:PHE:CE1	2.42	0.54
3:J:328:LEU:HD12	3:J:329:PRO:HD2	1.88	0.54
2:H:158:GLY:O	2:H:159:VAL:N	2.38	0.54
2:I:180:VAL:HG11	2:I:190:TYR:CE1	2.43	0.54
1:P:38:GLN:HE22	2:R:39:ARG:HD2	1.72	0.54
3:B:275:PHE:HE1	3:B:302:VAL:HG12	1.72	0.54
3:C:414:LYS:HE2	3:C:418:GLN:NE2	2.22	0.54
3:D:238:PRO:CG	3:D:328:LEU:HD13	2.37	0.54
3:D:262:VAL:HG13	3:D:303:VAL:HG22	1.90	0.54
3:J:289:THR:O	3:J:290:LYS:HB2	2.07	0.54
3:J:414:LYS:O	3:J:418:GLN:HG3	2.07	0.54
2:M:193:VAL:HG11	2:M:206:TYR:CE1	2.43	0.54
3:N:238:PRO:CG	3:N:328:LEU:HD13	2.37	0.54
3:A:414:LYS:HE2	3:A:418:GLN:NE2	2.22	0.54
3:A:414:LYS:O	3:A:418:GLN:HG3	2.08	0.54
1:F:15:VAL:HG21	1:F:80:PHE:CZ	2.42	0.54
2:H:13:LYS:HD3	2:H:142:PHE:CE1	2.42	0.54
3:C:253:ILE:CG2	3:N:310:HIS:CD2	2.88	0.54
1:Q:198:HIS:HD2	1:Q:200:GLY:H	1.53	0.54
3:B:238:PRO:CG	3:B:328:LEU:HD13	2.37	0.54
3:B:322:LYS:HE3	3:B:333:GLU:OE2	2.08	0.54
3:C:253:ILE:HD13	3:N:255:ARG:O	2.08	0.54
2:E:13:LYS:HD3	2:E:142:PHE:CE1	2.42	0.54
3:B:240:VAL:O	3:B:334:LYS:HE3	2.08	0.54
3:D:322:LYS:HE3	3:D:333:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:193:VAL:HG11	2:R:206:TYR:CE1	2.43	0.54
3:B:351:LEU:C	3:B:441:LEU:HD11	2.28	0.54
2:E:206:LYS:CA	2:E:207:VAL:N	2.67	0.54
2:E:190:TYR:O	2:E:207:VAL:N	2.41	0.54
3:N:322:LYS:HE3	3:N:333:GLU:OE2	2.08	0.54
3:N:240:VAL:O	3:N:334:LYS:HE3	2.08	0.54
3:B:262:VAL:HG13	3:B:303:VAL:HG22	1.90	0.54
1:P:203:SER:HA	3:J:297:ASN:HB2	1.90	0.54
3:J:414:LYS:HE2	3:J:418:GLN:NE2	2.22	0.54
3:N:351:LEU:C	3:N:441:LEU:HD11	2.28	0.54
2:O:222:LYS:CA	2:O:225:VAL:N	2.67	0.54
3:A:418:GLN:HA	3:A:443:LEU:HD22	1.90	0.54
2:I:117:SER:HB2	3:D:282:VAL:HG11	1.85	0.54
1:K:38:GLN:HE22	2:M:39:ARG:HD2	1.72	0.53
2:R:149:PRO:O	2:R:212:HIS:HE1	1.92	0.53
3:C:418:GLN:HA	3:C:443:LEU:HD22	1.90	0.53
1:G:6:GLN:H	1:G:100:GLN:NE2	2.03	0.53
3:J:418:GLN:HA	3:J:443:LEU:HD22	1.90	0.53
3:C:414:LYS:O	3:C:418:GLN:HG3	2.08	0.53
1:K:15:VAL:HG21	1:K:80:PHE:CZ	2.42	0.53
3:N:275:PHE:HE1	3:N:302:VAL:HG12	1.72	0.53
3:C:289:THR:O	3:C:290:LYS:HB2	2.07	0.53
3:D:351:LEU:C	3:D:441:LEU:HD11	2.28	0.53
2:H:190:TYR:O	2:H:207:VAL:N	2.41	0.53
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.91	0.53
2:O:212:HIS:HD2	2:O:215:SER:OG	1.92	0.53
3:C:285:HIS:O	3:C:286:ASN:HB2	2.08	0.53
3:D:275:PHE:HE1	3:D:302:VAL:HG12	1.72	0.53
3:D:291:PRO:HB3	3:D:304:SER:CA	2.37	0.53
1:L:93:GLY:O	2:H:97:LYS:HE2	2.09	0.53
2:H:57:ARG:NH1	2:M:72:ASP:OD2	2.37	0.53
3:D:240:VAL:O	3:D:334:LYS:HE3	2.08	0.53
2:E:196:HIS:HD2	2:E:199:SER:OG	1.92	0.53
1:G:93:GLY:O	2:E:97:LYS:HE2	2.09	0.53
2:O:206:TYR:O	2:O:225:VAL:N	2.41	0.53
1:K:202:SER:C	3:A:296:TYR:O	2.42	0.53
1:L:198:HIS:HD2	1:L:200:GLY:H	1.53	0.53
3:C:351:LEU:HB2	3:C:366:THR:HB	1.90	0.53
2:H:188:GLN:HA	2:H:189:THR:N	2.24	0.53
2:I:143:PRO:O	2:I:196:HIS:HE1	1.91	0.53
2:O:57:ARG:NH1	2:R:72:ASP:OD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:351:LEU:HB2	3:A:366:THR:HB	1.90	0.52
2:H:196:HIS:HD2	2:H:199:SER:OG	1.92	0.52
3:J:285:HIS:O	3:J:286:ASN:HB2	2.09	0.52
1:L:175:LEU:C	2:M:174:PHE:CE2	2.82	0.52
1:Q:116:PHE:CG	2:R:139:ALA:HB3	2.44	0.52
3:A:393:THR:HG22	3:A:394:THR:O	2.10	0.52
1:F:110:VAL:HB	2:O:100:LEU:CD1	2.23	0.52
3:D:312:ASN:ND2	3:D:317:LYS:HD2	2.24	0.52
1:G:116:PHE:CG	2:I:133:ALA:HB3	2.44	0.52
3:N:262:VAL:HG13	3:N:303:VAL:HG22	1.90	0.52
1:Q:175:LEU:C	2:R:174:PHE:CE2	2.82	0.52
1:F:203:SER:HB3	3:C:298:SER:HA	1.90	0.52
3:J:393:THR:HG22	3:J:394:THR:O	2.10	0.52
3:N:312:ASN:ND2	3:N:317:LYS:HD2	2.24	0.52
3:C:393:THR:HG22	3:C:394:THR:O	2.10	0.52
1:L:116:PHE:CG	2:M:139:ALA:HB3	2.44	0.52
3:N:291:PRO:HB3	3:N:304:SER:CA	2.37	0.52
2:O:203:GLN:HA	2:O:205:THR:N	2.24	0.52
3:J:351:LEU:HB2	3:J:366:THR:HB	1.90	0.52
1:L:175:LEU:CA	2:M:174:PHE:HE2	2.23	0.52
3:N:297:ASN:O	3:N:298:SER:HB3	2.09	0.52
3:B:297:ASN:O	3:B:298:SER:HB3	2.09	0.52
3:B:312:ASN:ND2	3:B:317:LYS:HD2	2.24	0.52
3:D:297:ASN:O	3:D:298:SER:HB3	2.09	0.52
2:M:149:PRO:O	2:M:212:HIS:HE1	1.91	0.52
1:Q:93:GLY:O	2:O:95:LYS:HE2	2.09	0.52
3:C:294:GLN:NE2	2:O:1:GLU:O	2.43	0.52
3:D:378:ALA:HB3	3:D:428:MET:HB2	1.92	0.52
1:L:44:PRO:HG2	2:H:105:TRP:CE3	2.45	0.52
1:P:120:PRO:HD3	1:P:132:VAL:HG22	1.91	0.52
1:Q:121:SER:HB2	2:R:123:PRO:HD2	1.92	0.52
3:A:285:HIS:O	3:A:286:ASN:HB2	2.08	0.52
3:A:436:TYR:C	3:A:436:TYR:CD1	2.84	0.52
3:D:249:ASP:O	3:D:257:PRO:HG3	2.10	0.52
1:L:121:SER:HB2	2:M:123:PRO:HD2	1.92	0.52
3:B:378:ALA:HB3	3:B:428:MET:HB2	1.92	0.51
3:J:436:TYR:CD1	3:J:436:TYR:C	2.84	0.51
3:N:296:TYR:HE1	3:N:301:ARG:HD3	1.74	0.51
1:G:44:PRO:HG2	2:E:105:TRP:CE3	2.45	0.51
1:G:175:LEU:C	2:I:162:PHE:CE2	2.82	0.51
1:Q:175:LEU:CA	2:R:174:PHE:HE2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:436:TYR:C	3:C:436:TYR:CD1	2.84	0.51
3:D:289:THR:HG22	3:D:290:LYS:N	2.21	0.51
3:D:325:ASN:ND2	3:D:326:LYS:N	2.58	0.51
2:I:196:HIS:CD2	2:I:199:SER:OG	2.64	0.51
3:N:325:ASN:ND2	3:N:326:LYS:N	2.59	0.51
2:M:212:HIS:CD2	2:M:215:SER:OG	2.64	0.51
3:N:378:ALA:HB3	3:N:428:MET:HB2	1.92	0.51
3:B:325:ASN:ND2	3:B:326:LYS:N	2.59	0.51
1:G:175:LEU:CA	2:I:162:PHE:HE2	2.23	0.51
3:J:350:THR:HB	3:J:441:LEU:CG	2.40	0.51
3:B:296:TYR:HE1	3:B:301:ARG:HD3	1.74	0.51
3:C:350:THR:HB	3:C:441:LEU:CG	2.40	0.51
1:Q:44:PRO:HG2	2:O:103:TRP:CE3	2.45	0.51
3:D:332:ILE:CG2	3:D:333:GLU:N	2.74	0.51
1:F:120:PRO:HD3	1:F:132:VAL:HG22	1.91	0.51
1:G:198:HIS:HD2	1:G:200:GLY:H	1.53	0.51
3:C:283:GLN:C	3:C:285:HIS:N	2.63	0.51
3:D:266:VAL:CB	3:D:300:TYR:HB2	2.28	0.51
1:G:162:SER:OG	2:I:163:PRO:CD	2.59	0.51
3:N:249:ASP:O	3:N:257:PRO:HG3	2.11	0.51
3:C:443:LEU:O	3:C:443:LEU:HG	2.11	0.51
3:D:278:TYR:CD1	3:D:278:TYR:N	2.79	0.51
3:D:296:TYR:HE1	3:D:301:ARG:HD3	1.74	0.51
3:A:418:GLN:C	3:A:420:GLY:H	2.15	0.51
3:C:429:HIS:O	3:C:435:HIS:HA	2.11	0.51
2:E:188:GLN:HA	2:E:189:THR:N	2.24	0.51
2:H:12:VAL:HG11	2:H:82:MET:HE1	1.91	0.51
3:J:418:GLN:C	3:J:420:GLY:H	2.15	0.51
3:J:443:LEU:HG	3:J:443:LEU:O	2.11	0.51
2:M:144:VAL:HG11	2:M:152:VAL:HG11	1.93	0.51
2:M:203:GLN:O	2:M:205:THR:HA	2.11	0.51
3:N:266:VAL:CB	3:N:300:TYR:HB2	2.28	0.50
3:B:291:PRO:CB	3:B:304:SER:HA	2.37	0.50
3:D:261:CYS:HB2	3:D:277:TRP:CZ2	2.47	0.50
1:L:162:SER:OG	2:M:175:PRO:CD	2.59	0.50
2:R:212:HIS:CD2	2:R:215:SER:OG	2.64	0.50
3:B:261:CYS:HB2	3:B:277:TRP:CZ2	2.47	0.50
3:C:357:GLU:C	3:C:359:THR:H	2.15	0.50
3:N:278:TYR:N	3:N:278:TYR:CD1	2.79	0.50
3:B:291:PRO:HB3	3:B:304:SER:CA	2.37	0.50
3:B:332:ILE:CG2	3:B:333:GLU:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:ILE:HD12	3:N:310:HIS:CD2	2.47	0.50
3:C:360:LYS:O	3:C:414:LYS:HD2	2.11	0.50
3:J:360:LYS:O	3:J:414:LYS:HD2	2.11	0.50
3:N:261:CYS:HB2	3:N:277:TRP:CZ2	2.47	0.50
3:A:429:HIS:O	3:A:435:HIS:HA	2.11	0.50
3:B:249:ASP:O	3:B:257:PRO:HG3	2.11	0.50
3:C:268:HIS:HB3	1:Q:57:GLY:CA	2.39	0.50
3:C:409:LYS:HB2	3:D:407:TYR:OH	2.12	0.50
2:I:138:VAL:HG11	2:I:146:VAL:HG11	1.93	0.50
3:J:357:GLU:C	3:J:359:THR:H	2.15	0.50
1:Q:162:SER:OG	2:R:175:PRO:CD	2.59	0.50
3:B:249:ASP:C	3:B:257:PRO:HG3	2.32	0.50
3:B:432:LEU:CD1	3:B:437:THR:HG22	2.42	0.50
3:D:406:LEU:O	3:D:406:LEU:HD12	2.12	0.50
1:K:154:LEU:N	3:B:330:ALA:CB	2.70	0.50
1:G:124:GLN:NE2	1:G:131:SER:OG	2.40	0.50
1:L:124:GLN:NE2	1:L:131:SER:OG	2.40	0.50
1:Q:6:GLN:N	1:Q:100:GLN:HE22	2.02	0.50
3:A:246:LYS:HB2	3:A:249:ASP:OD2	2.12	0.50
3:A:283:GLN:C	3:A:285:HIS:N	2.62	0.50
3:C:253:ILE:HD11	3:N:255:ARG:H	1.76	0.50
3:C:418:GLN:C	3:C:420:GLY:H	2.15	0.50
3:C:380:GLU:O	3:C:425:CYS:HA	2.12	0.50
3:A:294:GLN:O	3:A:300:TYR:CD1	2.65	0.50
3:A:409:LYS:HB2	3:B:407:TYR:OH	2.12	0.50
3:B:250:THR:HG22	3:B:257:PRO:HB3	1.94	0.50
3:C:294:GLN:O	3:C:300:TYR:CD1	2.65	0.50
3:D:250:THR:HG22	3:D:257:PRO:HB3	1.94	0.50
3:J:380:GLU:O	3:J:425:CYS:HA	2.12	0.50
3:J:429:HIS:O	3:J:435:HIS:HA	2.11	0.50
3:C:253:ILE:HB	3:N:310:HIS:CD2	2.47	0.50
1:G:121:SER:HB2	2:I:125:PRO:HD2	1.92	0.49
3:N:250:THR:HG22	3:N:257:PRO:HB3	1.94	0.49
3:N:406:LEU:HD12	3:N:406:LEU:O	2.12	0.49
2:R:203:GLN:O	2:R:205:THR:HA	2.11	0.49
3:D:292:ARG:O	3:D:293:GLU:HB3	2.12	0.49
3:D:432:LEU:CD1	3:D:437:THR:HG22	2.42	0.49
3:J:283:GLN:C	3:J:285:HIS:N	2.62	0.49
3:N:292:ARG:O	3:N:293:GLU:HB3	2.12	0.49
3:A:357:GLU:C	3:A:359:THR:H	2.15	0.49
3:A:380:GLU:O	3:A:425:CYS:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:278:TYR:N	3:B:278:TYR:CD1	2.79	0.49
3:B:289:THR:HG22	3:B:290:LYS:N	2.21	0.49
2:I:188:GLN:O	2:I:189:THR:HA	2.11	0.49
3:N:249:ASP:C	3:N:257:PRO:HG3	2.32	0.49
3:N:432:LEU:CD1	3:N:437:THR:HG22	2.42	0.49
2:R:144:VAL:HG11	2:R:152:VAL:HG11	1.93	0.49
3:A:350:THR:HB	3:A:441:LEU:CG	2.40	0.49
3:A:360:LYS:O	3:A:414:LYS:HD2	2.11	0.49
3:B:292:ARG:O	3:B:293:GLU:HB3	2.12	0.49
3:D:369:VAL:O	3:D:405:PHE:HA	2.12	0.49
3:J:246:LYS:HB2	3:J:249:ASP:OD2	2.12	0.49
3:J:294:GLN:O	3:J:300:TYR:CD1	2.65	0.49
3:N:332:ILE:CG2	3:N:333:GLU:N	2.74	0.49
2:O:203:GLN:O	2:O:205:THR:HA	2.13	0.49
3:A:277:TRP:O	3:A:283:GLN:HB3	2.13	0.49
3:A:443:LEU:HG	3:A:443:LEU:O	2.11	0.49
3:C:246:LYS:HB2	3:C:249:ASP:OD2	2.12	0.49
3:C:266:VAL:O	3:C:300:TYR:HB2	2.13	0.49
3:D:249:ASP:C	3:D:257:PRO:HG3	2.32	0.49
3:B:369:VAL:O	3:B:405:PHE:HA	2.12	0.49
3:J:409:LYS:HB2	3:N:407:TYR:OH	2.12	0.49
3:J:277:TRP:O	3:J:283:GLN:HB3	2.13	0.49
3:D:398:LEU:HD11	3:D:402:GLY:HA2	1.95	0.49
3:C:252:MET:HA	3:N:253:ILE:HG12	1.94	0.49
1:P:20:THR:CG2	1:P:72:THR:CG2	2.86	0.49
3:A:248:LYS:O	3:A:255:ARG:HD3	2.13	0.49
3:A:266:VAL:O	3:A:300:TYR:HB2	2.13	0.49
3:B:406:LEU:HD12	3:B:406:LEU:O	2.12	0.49
3:C:277:TRP:O	3:C:283:GLN:HB3	2.13	0.49
3:J:266:VAL:O	3:J:300:TYR:HB2	2.13	0.49
3:J:278:TYR:HB2	3:J:320:LYS:HB3	1.95	0.49
3:N:244:PRO:HB3	3:N:336:ILE:HD11	1.95	0.49
3:A:278:TYR:HB2	3:A:320:LYS:HB3	1.95	0.49
3:A:384:ASN:OD1	3:A:385:GLY:N	2.41	0.48
2:E:188:GLN:O	2:E:189:THR:HA	2.12	0.48
3:N:369:VAL:O	3:N:405:PHE:HA	2.12	0.48
1:Q:124:GLN:NE2	1:Q:131:SER:OG	2.40	0.48
3:C:278:TYR:HB2	3:C:320:LYS:HB3	1.94	0.48
3:C:283:GLN:CD	3:C:287:ALA:HB2	2.34	0.48
3:N:398:LEU:HD11	3:N:402:GLY:HA2	1.95	0.48
2:O:11:LEU:HD11	2:R:178:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:108:ARG:HD2	1:K:140:TYR:CB	2.43	0.48
3:N:259:VAL:HG23	3:N:308:VAL:CG2	2.43	0.48
1:P:108:ARG:HD2	1:P:140:TYR:CB	2.43	0.48
1:Q:176:SER:N	2:R:174:PHE:CE2	2.81	0.48
3:A:282:VAL:O	3:A:283:GLN:CB	2.52	0.48
3:A:283:GLN:CD	3:A:287:ALA:HB2	2.34	0.48
2:E:57:ARG:HH22	2:I:72:ASP:CG	2.16	0.48
3:A:358:MET:O	3:A:414:LYS:HE3	2.14	0.48
3:B:350:THR:HB	3:B:441:LEU:HG	1.95	0.48
3:C:248:LYS:O	3:C:255:ARG:HD3	2.13	0.48
3:C:346:PRO:CB	3:C:372:PHE:HB3	2.39	0.48
1:F:108:ARG:HD2	1:F:140:TYR:CB	2.43	0.48
3:J:248:LYS:O	3:J:255:ARG:HD3	2.13	0.48
3:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	0.48
3:J:346:PRO:CB	3:J:372:PHE:HB3	2.39	0.48
3:B:259:VAL:HG23	3:B:308:VAL:CG2	2.43	0.48
3:D:259:VAL:HG23	3:D:308:VAL:CG2	2.43	0.48
3:J:358:MET:O	3:J:414:LYS:HE3	2.14	0.48
3:D:350:THR:HB	3:D:441:LEU:HG	1.95	0.48
1:G:176:SER:N	2:I:162:PHE:CE2	2.81	0.48
2:E:57:ARG:NH1	2:I:72:ASP:OD2	2.37	0.48
1:K:156:SER:HB3	3:B:333:GLU:CD	2.22	0.48
2:R:118:GLY:HA2	2:R:212:HIS:HD2	1.77	0.48
3:D:291:PRO:CB	3:D:304:SER:HA	2.37	0.48
1:L:176:SER:N	2:M:174:PHE:CE2	2.81	0.48
2:O:57:ARG:HH22	2:R:72:ASP:CG	2.16	0.48
3:B:312:ASN:HB3	3:B:319:TYR:OH	2.14	0.48
3:D:244:PRO:HB3	3:D:336:ILE:HD11	1.95	0.48
2:H:57:ARG:HH22	2:M:72:ASP:CG	2.16	0.48
3:C:252:MET:CA	3:N:253:ILE:HD13	2.36	0.48
3:B:398:LEU:HD11	3:B:402:GLY:HA2	1.95	0.48
2:E:11:LEU:HD11	2:I:166:LEU:HD11	1.95	0.47
3:N:289:THR:HG22	3:N:290:LYS:N	2.21	0.47
1:Q:6:GLN:H	1:Q:100:GLN:NE2	2.03	0.47
3:B:368:LEU:HD12	3:B:369:VAL:H	1.79	0.47
3:C:253:ILE:CG2	3:N:310:HIS:CG	2.96	0.47
1:G:162:SER:OG	2:I:163:PRO:O	2.28	0.47
1:L:6:GLN:N	1:L:100:GLN:HE22	2.02	0.47
3:A:292:ARG:O	3:A:293:GLU:CB	2.58	0.47
3:A:388:GLU:OE2	3:A:416:ARG:NH2	2.42	0.47
3:D:368:LEU:HD12	3:D:369:VAL:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:GLN:O	2:H:189:THR:HA	2.13	0.47
3:J:414:LYS:HG2	3:J:418:GLN:NE2	2.29	0.47
2:M:2:VAL:HG13	2:M:27:PHE:CD2	2.49	0.47
3:N:350:THR:HB	3:N:441:LEU:HG	1.95	0.47
3:B:244:PRO:HB3	3:B:336:ILE:HD11	1.95	0.47
3:C:358:MET:O	3:C:414:LYS:HE3	2.14	0.47
2:I:120:GLY:HA2	2:I:196:HIS:HD2	1.77	0.47
3:D:432:LEU:HD22	3:D:437:THR:HB	1.97	0.47
2:H:11:LEU:HD11	2:M:178:LEU:HD11	1.95	0.47
3:J:384:ASN:OD1	3:J:385:GLY:N	2.41	0.47
2:M:212:HIS:HD2	2:M:215:SER:OG	1.97	0.47
3:A:414:LYS:HG2	3:A:418:GLN:NE2	2.29	0.47
3:C:289:THR:CG2	3:C:290:LYS:N	2.78	0.47
3:D:312:ASN:HB3	3:D:319:TYR:OH	2.14	0.47
1:G:176:SER:HB3	2:I:162:PHE:CD1	2.50	0.47
2:M:118:GLY:HA2	2:M:212:HIS:HD2	1.77	0.47
2:M:32:HIS:HD2	2:M:95:LYS:O	1.97	0.47
3:N:368:LEU:HD12	3:N:369:VAL:H	1.80	0.47
3:N:432:LEU:HD22	3:N:437:THR:HB	1.97	0.47
2:R:2:VAL:HG13	2:R:27:PHE:CD2	2.49	0.47
3:A:438:GLN:O	3:A:439:LYS:HD3	2.15	0.47
3:C:384:ASN:OD1	3:C:385:GLY:N	2.41	0.47
3:C:414:LYS:HG2	3:C:418:GLN:NE2	2.29	0.47
3:D:275:PHE:HZ	3:D:302:VAL:O	1.98	0.47
3:J:371:GLY:HA2	3:J:403:SER:OG	2.14	0.47
3:J:438:GLN:O	3:J:439:LYS:HD3	2.15	0.47
3:A:388:GLU:HA	3:A:388:GLU:OE1	2.14	0.47
3:B:432:LEU:HD22	3:B:437:THR:HB	1.97	0.47
2:I:196:HIS:HD2	2:I:199:SER:OG	1.97	0.47
3:J:388:GLU:OE1	3:J:388:GLU:HA	2.14	0.47
3:N:312:ASN:HB3	3:N:319:TYR:OH	2.14	0.47
2:R:208:CYS:SG	2:R:221:LYS:HB3	2.55	0.47
3:B:278:TYR:CE2	3:B:284:VAL:HG22	2.50	0.47
3:C:371:GLY:HA2	3:C:403:SER:OG	2.14	0.47
2:I:2:VAL:HG13	2:I:27:PHE:CD2	2.49	0.47
3:N:275:PHE:HZ	3:N:302:VAL:O	1.97	0.47
3:B:261:CYS:HB2	3:B:277:TRP:CH2	2.50	0.47
3:D:278:TYR:CE2	3:D:284:VAL:HG22	2.50	0.47
3:C:288:LYS:CD	3:C:288:LYS:H	2.27	0.46
3:C:388:GLU:OE1	3:C:388:GLU:HA	2.14	0.46
3:C:438:GLN:O	3:C:439:LYS:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:32:HIS:HD2	2:I:97:LYS:O	1.97	0.46
1:K:154:LEU:H	3:B:330:ALA:HB3	1.77	0.46
3:N:261:CYS:HB2	3:N:277:TRP:CH2	2.50	0.46
3:N:291:PRO:CB	3:N:304:SER:HA	2.37	0.46
2:R:212:HIS:HD2	2:R:215:SER:OG	1.97	0.46
3:C:286:ASN:O	3:C:287:ALA:CB	2.63	0.46
3:J:289:THR:CG2	3:J:290:LYS:N	2.78	0.46
1:L:6:GLN:H	1:L:100:GLN:NE2	2.03	0.46
1:P:153:ALA:CB	3:N:330:ALA:HB1	2.45	0.46
1:P:202:SER:HB2	3:J:296:TYR:O	2.14	0.46
3:A:371:GLY:HA2	3:A:403:SER:OG	2.15	0.46
3:B:300:TYR:O	3:B:301:ARG:HB2	2.16	0.46
2:E:17:SER:OG	2:E:83:HIS:HD2	1.99	0.46
3:B:308:VAL:HG11	3:B:313:TRP:HB2	1.97	0.46
3:B:432:LEU:HD11	3:B:437:THR:HG22	1.98	0.46
2:E:18:LEU:N	2:E:82:MET:HE2	2.30	0.46
3:N:322:LYS:HG3	3:N:333:GLU:HG2	1.97	0.46
3:A:288:LYS:CD	3:A:288:LYS:H	2.27	0.46
3:A:289:THR:CG2	3:A:290:LYS:N	2.78	0.46
3:D:361:ASN:ND2	3:D:362:GLN:HG3	2.31	0.46
3:J:286:ASN:O	3:J:287:ALA:CB	2.63	0.46
1:Q:176:SER:HB3	2:R:174:PHE:CD1	2.50	0.46
3:B:275:PHE:HZ	3:B:302:VAL:O	1.98	0.46
3:B:311:GLN:N	3:B:311:GLN:NE2	2.53	0.46
3:B:344:ARG:O	3:B:372:PHE:HA	2.16	0.46
3:D:311:GLN:NE2	3:D:311:GLN:N	2.53	0.46
2:M:208:CYS:SG	2:M:221:LYS:HB3	2.55	0.46
3:N:279:VAL:O	3:N:282:VAL:HG22	2.15	0.46
3:N:300:TYR:O	3:N:301:ARG:HB2	2.16	0.46
2:H:17:SER:OG	2:H:83:HIS:HD2	1.99	0.46
2:O:19:ILE:HD13	2:R:19:ILE:O	2.16	0.46
3:D:261:CYS:HB2	3:D:277:TRP:CH2	2.50	0.46
2:H:163:PRO:HD2	1:K:162:SER:OG	2.16	0.46
3:N:344:ARG:O	3:N:372:PHE:HA	2.16	0.46
2:R:32:HIS:HD2	2:R:95:LYS:O	1.97	0.46
2:R:97:SER:C	2:R:99:ARG:H	2.19	0.46
3:A:346:PRO:CB	3:A:372:PHE:HB3	2.39	0.46
3:D:242:LEU:HD13	3:D:336:ILE:HG22	1.98	0.46
3:D:279:VAL:O	3:D:282:VAL:HG22	2.15	0.46
2:I:99:SER:C	2:I:101:ARG:H	2.19	0.46
3:N:406:LEU:CD1	3:N:406:LEU:C	2.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:12:VAL:HG11	2:O:82:MET:HE1	1.98	0.46
3:A:265:ASP:HA	3:A:299:THR:HB	1.98	0.46
3:A:296:TYR:HB3	3:A:297:ASN:H	1.56	0.46
3:B:279:VAL:O	3:B:282:VAL:HG22	2.15	0.46
3:D:300:TYR:O	3:D:301:ARG:HB2	2.16	0.46
3:D:322:LYS:HG3	3:D:333:GLU:HG2	1.97	0.46
3:N:278:TYR:CE2	3:N:284:VAL:HG22	2.50	0.46
1:P:153:ALA:CB	3:N:330:ALA:CB	2.94	0.46
3:A:266:VAL:HB	3:A:300:TYR:HB2	1.98	0.45
3:B:242:LEU:HD13	3:B:336:ILE:HG22	1.98	0.45
3:B:279:VAL:O	3:B:280:ASP:HB2	2.17	0.45
3:B:322:LYS:HG3	3:B:333:GLU:HG2	1.97	0.45
1:L:121:SER:CB	1:L:121:SER:HG	2.17	0.45
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	0.45
3:N:279:VAL:O	3:N:280:ASP:HB2	2.16	0.45
3:N:361:ASN:ND2	3:N:362:GLN:HG3	2.31	0.45
3:N:439:LYS:HA	3:N:439:LYS:HD2	1.81	0.45
3:A:421:ASN:ND2	3:A:421:ASN:N	2.64	0.45
3:D:406:LEU:C	3:D:406:LEU:CD1	2.84	0.45
1:F:141:PRO:O	1:F:198:HIS:HE1	2.00	0.45
2:H:11:LEU:HD21	2:M:179:GLN:O	2.16	0.45
3:J:296:TYR:HB3	3:J:297:ASN:H	1.56	0.45
1:L:176:SER:HB3	2:M:174:PHE:CD1	2.50	0.45
2:M:97:SER:C	2:M:99:ARG:H	2.19	0.45
3:C:253:ILE:CB	3:N:310:HIS:CD2	3.00	0.45
3:N:345:GLU:HA	3:N:431:ALA:HB3	1.98	0.45
1:Q:92:ALA:O	2:O:95:LYS:CE	2.64	0.45
3:D:344:ARG:O	3:D:372:PHE:HA	2.16	0.45
1:G:160:GLN:NE2	2:I:165:VAL:HG12	2.31	0.45
1:Q:121:SER:HG	1:Q:121:SER:CB	2.17	0.45
3:A:286:ASN:O	3:A:287:ALA:CB	2.63	0.45
3:C:374:PRO:O	3:C:429:HIS:HE1	2.00	0.45
3:D:308:VAL:HG11	3:D:313:TRP:HB2	1.97	0.45
3:D:326:LYS:C	3:D:328:LEU:H	2.20	0.45
1:G:118:PHE:CG	2:I:126:LEU:HB3	2.52	0.45
2:I:192:CYS:SG	2:I:205:LYS:HB3	2.55	0.45
1:K:141:PRO:O	1:K:198:HIS:HE1	2.00	0.45
3:N:308:VAL:HG11	3:N:313:TRP:HB2	1.97	0.45
3:N:432:LEU:HD11	3:N:437:THR:HG22	1.98	0.45
3:C:265:ASP:HA	3:C:299:THR:HB	1.98	0.45
3:C:292:ARG:O	3:C:293:GLU:CB	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:175:PRO:HD2	1:P:162:SER:OG	2.16	0.45
3:B:361:ASN:ND2	3:B:362:GLN:HG3	2.31	0.45
3:C:278:TYR:CD1	3:C:278:TYR:N	2.85	0.45
3:D:269:GLU:C	3:D:271:PRO:HD3	2.36	0.45
3:D:345:GLU:HA	3:D:431:ALA:HB3	1.99	0.45
1:G:92:ALA:O	2:E:97:LYS:CE	2.64	0.45
3:J:374:PRO:O	3:J:429:HIS:HE1	2.00	0.45
2:M:18:LEU:HB2	2:M:82:MET:HE1	1.99	0.45
3:N:238:PRO:CB	3:N:328:LEU:HD13	2.47	0.45
3:B:323:VAL:HG12	3:B:324:SER:N	2.32	0.45
3:D:238:PRO:CB	3:D:328:LEU:HD13	2.47	0.45
3:J:278:TYR:N	3:J:278:TYR:CD1	2.85	0.45
3:B:300:TYR:O	3:B:301:ARG:CB	2.64	0.45
3:B:406:LEU:C	3:B:406:LEU:CD1	2.84	0.45
3:D:432:LEU:HD11	3:D:437:THR:HG22	1.98	0.45
2:M:200:THR:HB	2:M:203:GLN:N	2.32	0.45
1:Q:118:PHE:CG	2:R:124:LEU:HB3	2.52	0.45
3:A:244:PRO:HB3	3:A:336:ILE:HD13	1.99	0.45
3:B:238:PRO:CB	3:B:328:LEU:HD13	2.47	0.45
3:B:269:GLU:C	3:B:271:PRO:HD3	2.36	0.45
3:B:301:ARG:HG2	3:B:303:VAL:HG23	1.99	0.45
3:C:244:PRO:HB3	3:C:336:ILE:HD13	1.99	0.45
3:D:279:VAL:O	3:D:280:ASP:HB2	2.17	0.45
3:D:300:TYR:O	3:D:301:ARG:CB	2.65	0.45
3:D:323:VAL:HG12	3:D:324:SER:N	2.32	0.45
1:L:92:ALA:O	2:H:97:LYS:CE	2.64	0.45
2:H:165:VAL:CG1	1:K:160:GLN:CD	2.86	0.45
1:Q:116:PHE:CG	2:R:139:ALA:CB	3.00	0.45
3:B:265:ASP:HA	3:B:299:THR:CB	2.47	0.45
3:D:290:LYS:HE3	3:D:292:ARG:HH12	1.82	0.45
3:D:301:ARG:HG2	3:D:303:VAL:HG23	1.99	0.45
2:E:19:ILE:HD13	2:I:19:ILE:O	2.16	0.45
3:J:292:ARG:O	3:J:293:GLU:CB	2.58	0.45
3:J:388:GLU:OE2	3:J:416:ARG:NH2	2.42	0.45
3:J:421:ASN:N	3:J:421:ASN:ND2	2.64	0.45
1:P:204:PRO:HD3	3:J:297:ASN:HB2	1.99	0.45
3:C:347:GLN:NE2	3:C:349:TYR:OH	2.50	0.44
2:E:163:PRO:HD2	1:F:162:SER:OG	2.16	0.44
3:J:265:ASP:HA	3:J:299:THR:HB	1.98	0.44
3:J:266:VAL:HB	3:J:300:TYR:HB2	1.98	0.44
3:N:300:TYR:O	3:N:301:ARG:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:326:LYS:C	3:N:328:LEU:H	2.20	0.44
3:B:239:SER:HB3	3:B:264:VAL:CG2	2.48	0.44
3:D:296:TYR:HB3	3:D:297:ASN:H	1.34	0.44
1:F:112:ALA:HB3	2:O:99:ARG:HB3	0.48	0.44
1:P:153:ALA:CA	3:N:330:ALA:HB2	2.45	0.44
1:P:141:PRO:O	1:P:198:HIS:HE1	2.00	0.44
2:R:115:SER:H	3:N:282:VAL:HG12	1.82	0.44
2:O:11:LEU:HD21	2:R:179:GLN:O	2.17	0.44
3:A:291:PRO:O	3:A:292:ARG:HD2	2.17	0.44
3:B:326:LYS:C	3:B:328:LEU:H	2.20	0.44
3:C:296:TYR:HB3	3:C:297:ASN:H	1.56	0.44
1:G:116:PHE:CG	2:I:133:ALA:CB	3.00	0.44
2:H:19:ILE:HD13	2:M:19:ILE:O	2.16	0.44
3:N:265:ASP:HA	3:N:299:THR:CB	2.47	0.44
3:N:290:LYS:HE3	3:N:292:ARG:HH12	1.82	0.44
3:N:311:GLN:NE2	3:N:311:GLN:N	2.53	0.44
2:O:177:VAL:CG1	1:P:160:GLN:CD	2.86	0.44
3:B:258:GLU:HA	3:B:308:VAL:HG23	1.99	0.44
3:C:266:VAL:HB	3:C:300:TYR:HB2	1.98	0.44
2:E:11:LEU:HD21	2:I:167:GLN:O	2.16	0.44
2:H:18:LEU:N	2:H:82:MET:HE2	2.32	0.44
1:L:118:PHE:CG	2:M:124:LEU:HB3	2.52	0.44
3:N:242:LEU:HD13	3:N:336:ILE:HG22	1.97	0.44
2:R:200:THR:HB	2:R:203:GLN:N	2.32	0.44
3:A:278:TYR:N	3:A:278:TYR:CD1	2.85	0.44
3:B:296:TYR:HB3	3:B:297:ASN:H	1.34	0.44
3:C:309:LEU:O	3:C:312:ASN:N	2.51	0.44
3:C:318:GLU:OE1	3:C:340:LYS:NZ	2.45	0.44
3:D:239:SER:HB3	3:D:264:VAL:CG2	2.47	0.44
3:D:258:GLU:HA	3:D:308:VAL:HG23	1.99	0.44
3:J:288:LYS:H	3:J:288:LYS:CD	2.27	0.44
3:J:347:GLN:NE2	3:J:349:TYR:OH	2.50	0.44
3:N:239:SER:HB3	3:N:264:VAL:CG2	2.47	0.44
3:D:265:ASP:HA	3:D:299:THR:CB	2.47	0.44
3:B:345:GLU:HA	3:B:431:ALA:HB3	1.98	0.44
3:D:439:LYS:HD2	3:D:439:LYS:HA	1.82	0.44
2:I:18:LEU:HB2	2:I:82:MET:HE1	1.99	0.44
3:N:323:VAL:HG12	3:N:324:SER:N	2.32	0.44
1:Q:38:GLN:NE2	2:O:91:TYR:OH	2.48	0.44
2:R:206:TYR:O	2:R:225:VAL:N	2.51	0.44
1:K:153:ALA:HB2	3:B:329:PRO:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:VAL:CG1	1:F:160:GLN:CD	2.86	0.44
2:I:187:THR:HB	2:I:188:GLN:N	2.32	0.44
2:I:190:TYR:O	2:I:207:VAL:N	2.51	0.44
3:N:258:GLU:HA	3:N:308:VAL:HG23	1.99	0.44
3:C:436:TYR:CD2	3:N:434:ASN:OD1	2.71	0.44
3:C:291:PRO:O	3:C:292:ARG:HD2	2.17	0.44
3:C:421:ASN:ND2	3:C:421:ASN:N	2.64	0.44
3:A:278:TYR:HA	3:A:282:VAL:O	2.18	0.43
3:A:287:ALA:O	3:A:288:LYS:C	2.56	0.43
2:M:115:SER:HB2	3:B:282:VAL:HG11	1.58	0.43
3:D:363:VAL:HG22	3:D:412:VAL:O	2.18	0.43
3:J:244:PRO:HB3	3:J:336:ILE:HD13	1.99	0.43
3:A:374:PRO:O	3:A:429:HIS:HE1	2.00	0.43
1:L:38:GLN:NE2	2:H:93:TYR:OH	2.48	0.43
1:L:116:PHE:CG	2:M:139:ALA:CB	3.00	0.43
3:A:348:VAL:O	3:A:439:LYS:HG3	2.19	0.43
3:C:294:GLN:HG3	2:O:1:GLU:HB2	1.65	0.43
2:E:19:ILE:CD1	2:I:19:ILE:O	2.67	0.43
3:C:310:HIS:CG	3:N:253:ILE:HD12	2.33	0.43
3:C:436:TYR:CD2	3:N:434:ASN:CG	2.90	0.43
1:Q:160:GLN:NE2	2:R:177:VAL:HG12	2.31	0.43
3:A:347:GLN:NE2	3:A:349:TYR:OH	2.51	0.43
3:C:278:TYR:HA	3:C:282:VAL:O	2.18	0.43
3:C:388:GLU:OE2	3:C:416:ARG:NH2	2.42	0.43
3:J:278:TYR:HA	3:J:282:VAL:O	2.18	0.43
3:N:301:ARG:HG2	3:N:303:VAL:HG23	1.99	0.43
3:N:363:VAL:HG22	3:N:412:VAL:O	2.18	0.43
3:N:414:LYS:O	3:N:418:GLN:HG3	2.19	0.43
3:C:293:GLU:OE1	2:O:1:GLU:CG	2.66	0.43
1:P:142:ARG:HD3	1:P:173:TYR:CE2	2.54	0.43
3:B:266:VAL:HB	3:B:300:TYR:CD2	2.54	0.43
3:B:386:GLN:HA	3:B:387:PRO:HD3	1.76	0.43
1:F:113:PRO:O	2:O:99:ARG:HD2	2.17	0.43
3:N:296:TYR:HB3	3:N:297:ASN:H	1.34	0.43
3:A:264:VAL:O	3:A:265:ASP:HB2	2.18	0.43
3:B:363:VAL:HG22	3:B:412:VAL:O	2.18	0.43
3:C:282:VAL:O	3:C:283:GLN:CB	2.52	0.43
3:C:436:TYR:CE1	3:N:436:TYR:O	2.72	0.43
2:O:11:LEU:HD11	2:R:178:LEU:CD1	2.49	0.43
3:C:287:ALA:O	3:C:288:LYS:C	2.56	0.43
3:D:338:LYS:NZ	3:D:430:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:414:LYS:O	3:D:418:GLN:HG3	2.18	0.43
2:M:206:TYR:O	2:M:225:VAL:N	2.51	0.43
1:K:202:SER:CB	3:A:296:TYR:C	2.66	0.43
3:B:278:TYR:HE2	3:B:284:VAL:HG22	1.83	0.43
3:C:348:VAL:O	3:C:439:LYS:HG3	2.19	0.43
2:H:19:ILE:CD1	2:M:19:ILE:O	2.66	0.43
3:N:338:LYS:NZ	3:N:430:GLU:OE2	2.52	0.43
3:B:290:LYS:HE3	3:B:292:ARG:HH12	1.82	0.43
3:C:253:ILE:CD1	3:N:310:HIS:CD2	3.02	0.43
3:D:368:LEU:HD12	3:D:369:VAL:N	2.34	0.43
2:H:11:LEU:HD11	2:M:178:LEU:CD1	2.49	0.43
2:M:115:SER:H	3:B:282:VAL:CB	2.30	0.43
2:I:192:CYS:SG	2:I:192:CYS:O	2.77	0.43
3:J:291:PRO:O	3:J:292:ARG:HD2	2.17	0.43
3:N:278:TYR:HE2	3:N:284:VAL:HG22	1.83	0.43
3:N:238:PRO:HB2	3:N:328:LEU:HD13	2.01	0.43
2:O:19:ILE:CD1	2:R:19:ILE:O	2.67	0.43
2:R:222:LYS:HA	2:R:225:VAL:N	2.34	0.43
3:C:391:TYR:C	3:C:391:TYR:CD2	2.92	0.42
1:K:203:SER:HA	3:A:297:ASN:HB2	1.15	0.42
2:M:208:CYS:O	2:M:208:CYS:SG	2.77	0.42
1:P:161:GLU:HG2	1:P:175:LEU:HD21	2.01	0.42
3:B:368:LEU:HD12	3:B:369:VAL:N	2.34	0.42
3:C:328:LEU:HA	3:C:329:PRO:HD3	1.94	0.42
1:G:108:ARG:CD	1:G:109:THR:O	2.62	0.42
3:J:248:LYS:NZ	3:J:380:GLU:OE2	2.47	0.42
1:K:15:VAL:HG21	1:K:80:PHE:CE2	2.54	0.42
2:M:222:LYS:HA	2:M:225:VAL:N	2.34	0.42
3:D:278:TYR:HE2	3:D:284:VAL:HG22	1.83	0.42
3:J:287:ALA:O	3:J:288:LYS:C	2.56	0.42
3:N:368:LEU:HD12	3:N:369:VAL:N	2.34	0.42
1:Q:108:ARG:HD2	1:Q:140:TYR:CB	2.50	0.42
3:A:391:TYR:CD2	3:A:391:TYR:C	2.92	0.42
3:B:414:LYS:O	3:B:418:GLN:HG3	2.19	0.42
3:C:283:GLN:C	3:C:285:HIS:H	2.23	0.42
3:D:252:MET:SD	3:D:428:MET:HE3	2.59	0.42
3:D:357:GLU:C	3:D:359:THR:H	2.23	0.42
2:E:11:LEU:HD11	2:I:166:LEU:CD1	2.49	0.42
1:G:38:GLN:NE2	2:E:93:TYR:OH	2.48	0.42
1:K:156:SER:HB2	3:B:333:GLU:CD	2.18	0.42
1:K:38:GLN:OE1	1:K:87:HIS:HE1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:266:VAL:HB	3:N:300:TYR:CD2	2.54	0.42
3:N:357:GLU:C	3:N:359:THR:H	2.23	0.42
3:B:350:THR:HB	3:B:441:LEU:CD1	2.50	0.42
3:C:264:VAL:O	3:C:265:ASP:HB2	2.18	0.42
1:P:153:ALA:HB1	3:N:330:ALA:HB1	2.02	0.42
3:B:357:GLU:C	3:B:359:THR:H	2.23	0.42
3:D:266:VAL:HB	3:D:300:TYR:CD2	2.54	0.42
1:F:142:ARG:HD3	1:F:173:TYR:CE2	2.54	0.42
1:F:15:VAL:HG21	1:F:80:PHE:CE2	2.54	0.42
1:G:138:ASN:OD1	2:I:160:HIS:NE2	2.48	0.42
3:J:386:GLN:HG3	3:J:387:PRO:HD2	2.02	0.42
1:K:161:GLU:HG2	1:K:175:LEU:HD21	2.01	0.42
2:H:19:ILE:CD1	2:M:8:GLY:HA3	2.49	0.42
3:C:433:HIS:CE1	3:N:380:GLU:OE1	2.73	0.42
1:P:15:VAL:HG21	1:P:80:PHE:CE2	2.54	0.42
2:R:208:CYS:O	2:R:208:CYS:SG	2.77	0.42
2:O:19:ILE:CD1	2:R:8:GLY:HA3	2.49	0.42
3:D:291:PRO:O	3:D:292:ARG:HB3	2.19	0.42
2:I:206:LYS:HA	2:I:207:VAL:N	2.34	0.42
3:J:264:VAL:O	3:J:265:ASP:HB2	2.18	0.42
1:K:142:ARG:HD3	1:K:173:TYR:CE2	2.54	0.42
2:M:3:GLN:HB2	2:M:25:SER:HB2	2.02	0.42
3:N:291:PRO:O	3:N:292:ARG:HB3	2.19	0.42
2:R:12:VAL:HG11	2:R:82:MET:HE1	1.99	0.42
3:B:291:PRO:O	3:B:292:ARG:HB3	2.19	0.42
3:B:338:LYS:NZ	3:B:430:GLU:OE2	2.52	0.42
1:G:141:PRO:O	1:G:198:HIS:HE1	2.02	0.42
3:J:391:TYR:CD2	3:J:391:TYR:C	2.93	0.42
1:L:100:GLN:CD	1:L:100:GLN:N	2.71	0.42
2:M:162:ASN:N	2:M:207:ILE:O	2.53	0.42
1:P:38:GLN:OE1	1:P:87:HIS:HE1	2.03	0.42
3:A:328:LEU:HD12	3:A:329:PRO:CD	2.50	0.42
3:A:367:CYS:HB2	3:A:381:TRP:CH2	2.55	0.42
3:B:238:PRO:HB2	3:B:328:LEU:HD13	2.01	0.42
3:C:372:PHE:O	3:C:404:PHE:N	2.44	0.42
3:D:350:THR:HB	3:D:441:LEU:CD1	2.50	0.42
1:K:108:ARG:HD2	1:K:140:TYR:CG	2.55	0.42
1:Q:141:PRO:O	1:Q:198:HIS:HE1	2.02	0.42
3:A:283:GLN:C	3:A:285:HIS:H	2.23	0.41
1:F:20:THR:CG2	1:F:72:THR:CG2	2.86	0.41
3:A:372:PHE:O	3:A:404:PHE:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:268:HIS:O	3:B:271:PRO:CG	2.68	0.41
3:C:384:ASN:CG	3:C:385:GLY:H	2.22	0.41
2:E:54:SER:HB2	2:I:74:LEU:HD12	2.02	0.41
1:F:161:GLU:HG2	1:F:175:LEU:HD21	2.01	0.41
3:J:348:VAL:O	3:J:439:LYS:HG3	2.19	0.41
3:A:336:ILE:HG12	3:A:337:SER:N	2.35	0.41
3:A:369:VAL:HB	3:A:406:LEU:HD12	2.02	0.41
3:D:300:TYR:HB3	3:D:301:ARG:H	1.37	0.41
3:D:238:PRO:HB2	3:D:328:LEU:HD13	2.01	0.41
1:G:100:GLN:N	1:G:100:GLN:CD	2.71	0.41
1:Q:100:GLN:CD	1:Q:100:GLN:N	2.72	0.41
3:A:342:GLN:HA	3:A:343:PRO:HD3	1.83	0.41
2:M:217:THR:HG1	3:B:285:HIS:CD2	2.36	0.41
3:C:434:ASN:HA	3:N:252:MET:HE3	2.00	0.41
3:D:325:ASN:HD22	3:D:326:LYS:N	2.15	0.41
1:F:108:ARG:HD2	1:F:140:TYR:CG	2.55	0.41
2:I:151:ASN:N	2:I:191:ILE:O	2.53	0.41
1:L:141:PRO:O	1:L:198:HIS:HE1	2.02	0.41
1:L:160:GLN:NE2	2:M:177:VAL:HG12	2.31	0.41
3:N:325:ASN:HD22	3:N:326:LYS:N	2.15	0.41
1:P:108:ARG:HD2	1:P:140:TYR:CG	2.55	0.41
3:A:246:LYS:HA	3:A:247:PRO:HD3	1.94	0.41
3:B:325:ASN:HD22	3:B:326:LYS:N	2.15	0.41
3:C:328:LEU:HD12	3:C:329:PRO:CD	2.50	0.41
3:C:367:CYS:HB2	3:C:381:TRP:CH2	2.55	0.41
2:E:19:ILE:CD1	2:I:8:GLY:HA3	2.49	0.41
3:J:274:LYS:HE2	3:J:324:SER:HB2	2.02	0.41
3:J:309:LEU:O	3:J:312:ASN:N	2.51	0.41
3:J:328:LEU:HD12	3:J:329:PRO:CD	2.50	0.41
3:J:367:CYS:HB2	3:J:381:TRP:CH2	2.55	0.41
1:L:108:ARG:HD2	1:L:140:TYR:CB	2.50	0.41
1:L:38:GLN:OE1	1:L:87:HIS:HE1	2.04	0.41
1:Q:108:ARG:CD	1:Q:109:THR:O	2.62	0.41
3:A:274:LYS:HE2	3:A:324:SER:HB2	2.02	0.41
3:B:276:ASN:HB3	3:B:278:TYR:CE1	2.56	0.41
1:G:108:ARG:HD2	1:G:140:TYR:CB	2.49	0.41
1:G:38:GLN:OE1	1:G:87:HIS:HE1	2.04	0.41
2:O:54:SER:HB2	2:R:74:LEU:HD12	2.02	0.41
1:P:108:ARG:HD2	1:P:140:TYR:HB3	2.03	0.41
2:R:3:GLN:HB2	2:R:25:SER:HB2	2.02	0.41
3:B:273:VAL:HB	3:B:302:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:386:GLN:HG3	3:C:387:PRO:HD2	2.02	0.41
1:G:134:CYS:HB2	1:G:148:TRP:CH2	2.56	0.41
1:G:175:LEU:CA	2:I:162:PHE:CE2	3.03	0.41
3:J:283:GLN:C	3:J:285:HIS:H	2.23	0.41
3:J:369:VAL:HB	3:J:406:LEU:HD12	2.02	0.41
1:K:20:THR:CG2	1:K:72:THR:CG2	2.86	0.41
1:L:143:GLU:CD	1:L:143:GLU:H	2.24	0.41
1:Q:38:GLN:OE1	1:Q:87:HIS:HE1	2.04	0.41
3:B:252:MET:SD	3:B:428:MET:HE3	2.60	0.41
3:D:335:THR:O	3:D:336:ILE:HB	2.21	0.41
1:G:143:GLU:H	1:G:143:GLU:CD	2.24	0.41
2:I:3:GLN:HB2	2:I:25:SER:HB2	2.02	0.41
2:M:148:PHE:HA	2:M:149:PRO:HA	1.92	0.41
3:N:268:HIS:O	3:N:271:PRO:CG	2.68	0.41
3:A:328:LEU:HA	3:A:329:PRO:HD3	1.94	0.41
3:C:286:ASN:HB3	3:C:287:ALA:H	1.63	0.41
3:C:382:GLU:OE1	3:N:433:HIS:CE1	2.74	0.41
1:F:108:ARG:HD2	1:F:140:TYR:HB3	2.03	0.41
1:F:38:GLN:OE1	1:F:87:HIS:HE1	2.03	0.41
1:L:175:LEU:CA	2:M:174:PHE:CE2	3.03	0.41
3:N:350:THR:HB	3:N:441:LEU:CD1	2.50	0.41
1:Q:175:LEU:CA	2:R:174:PHE:CE2	3.03	0.41
2:R:162:ASN:N	2:R:207:ILE:O	2.53	0.41
3:B:367:CYS:HB2	3:B:381:TRP:CZ2	2.56	0.41
3:C:274:LYS:HE2	3:C:324:SER:HB2	2.02	0.41
3:D:268:HIS:O	3:D:271:PRO:CG	2.68	0.41
3:J:336:ILE:HG12	3:J:337:SER:N	2.35	0.41
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.41
1:K:204:PRO:HD2	3:A:298:SER:OG	2.21	0.41
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.56	0.41
2:M:154:VAL:CA	2:M:156:SER:N	2.79	0.41
1:Q:134:CYS:HB2	1:Q:148:TRP:CH2	2.56	0.41
1:Q:143:GLU:H	1:Q:143:GLU:CD	2.24	0.41
3:A:309:LEU:O	3:A:312:ASN:N	2.51	0.41
3:B:350:THR:HB	3:B:441:LEU:HD12	2.03	0.41
2:H:54:SER:HB2	2:M:74:LEU:HD12	2.02	0.41
2:I:205:LYS:HA	2:I:205:LYS:HD3	1.97	0.41
3:J:386:GLN:HA	3:J:387:PRO:HD3	1.88	0.41
3:N:367:CYS:HB2	3:N:381:TRP:CZ2	2.56	0.41
2:O:18:LEU:N	2:O:82:MET:HE2	2.36	0.41
2:R:154:VAL:CA	2:R:156:SER:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:162:SER:OG	2:R:175:PRO:O	2.28	0.41
3:A:386:GLN:HG3	3:A:387:PRO:HD2	2.02	0.40
3:C:248:LYS:NZ	3:C:380:GLU:OE2	2.47	0.40
2:I:6:GLU:OE1	2:I:106:GLY:HA3	2.22	0.40
3:J:342:GLN:HA	3:J:343:PRO:HD3	1.83	0.40
2:M:187:LEU:HD12	2:M:187:LEU:C	2.41	0.40
3:N:308:VAL:HG12	3:N:309:LEU:N	2.36	0.40
3:N:310:HIS:O	3:N:314:LEU:HG	2.22	0.40
3:N:350:THR:HB	3:N:441:LEU:CG	2.51	0.40
2:R:187:LEU:HD12	2:R:187:LEU:C	2.41	0.40
3:B:350:THR:HB	3:B:441:LEU:CG	2.51	0.40
3:C:336:ILE:HG12	3:C:337:SER:N	2.35	0.40
3:D:270:ASP:N	3:D:271:PRO:CD	2.82	0.40
3:D:273:VAL:HB	3:D:302:VAL:HG21	2.03	0.40
3:D:276:ASN:HB3	3:D:278:TYR:CE1	2.56	0.40
3:D:350:THR:HB	3:D:441:LEU:HD12	2.03	0.40
3:D:350:THR:HB	3:D:441:LEU:CG	2.51	0.40
3:N:276:ASN:HB3	3:N:278:TYR:CE1	2.56	0.40
3:B:274:LYS:HG2	3:B:275:PHE:N	2.37	0.40
3:D:308:VAL:HG12	3:D:309:LEU:N	2.36	0.40
3:D:367:CYS:HB2	3:D:381:TRP:CZ2	2.56	0.40
2:E:3:GLN:HB2	2:E:25:SER:HB2	2.04	0.40
3:J:282:VAL:O	3:J:283:GLN:CB	2.52	0.40
1:Q:176:SER:HB3	2:R:174:PHE:CZ	2.57	0.40
2:R:6:GLU:OE1	2:R:104:GLY:HA3	2.22	0.40
3:A:252:MET:HB2	3:A:255:ARG:CG	2.49	0.40
3:B:335:THR:O	3:B:336:ILE:HB	2.21	0.40
3:B:351:LEU:HB2	3:B:366:THR:HB	2.03	0.40
3:C:246:LYS:HA	3:C:247:PRO:HD3	1.94	0.40
3:C:310:HIS:CD2	3:N:253:ILE:HD13	2.44	0.40
3:D:245:PRO:HB3	3:D:258:GLU:H	1.87	0.40
2:E:206:LYS:O	2:E:207:VAL:HA	2.22	0.40
2:I:174:LEU:HD12	2:I:174:LEU:C	2.41	0.40
3:C:369:VAL:HB	3:C:406:LEU:HD12	2.02	0.40
3:D:310:HIS:O	3:D:314:LEU:HG	2.22	0.40
2:E:165:VAL:HG11	1:F:160:GLN:OE1	2.21	0.40
2:H:165:VAL:HG11	1:K:160:GLN:OE1	2.21	0.40
1:L:176:SER:HB3	2:M:174:PHE:CZ	2.57	0.40
3:N:245:PRO:HB3	3:N:258:GLU:H	1.87	0.40
2:O:3:GLN:HB2	2:O:25:SER:HB2	2.04	0.40

All (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
2:H:1:GLU:CG	3:A:294:GLN:N[5_555]	0.70	1.50
3:A:253:ILE:CG1	3:B:253:ILE:C[6_555]	0.72	1.48
3:A:252:MET:C	3:B:253:ILE:CG1[6_555]	0.74	1.46
2:E:1:GLU:CD	3:J:293:GLU:CG[3_565]	0.76	1.44
3:D:253:ILE:CA	3:J:253:ILE:CG1[3_565]	0.77	1.43
2:H:26:ASN:ND2	3:A:294:GLN:NE2[5_555]	0.86	1.34
2:E:1:GLU:CA	3:J:294:GLN:CA[3_565]	0.90	1.30
2:H:1:GLU:CA	3:A:294:GLN:CA[5_555]	0.93	1.27
3:D:252:MET:O	3:J:253:ILE:CD1[3_565]	0.98	1.22
2:H:1:GLU:CA	3:A:294:GLN:CB[5_555]	1.03	1.17
3:A:254:SER:N	3:B:253:ILE:CG2[6_555]	1.07	1.13
2:H:1:GLU:CB	3:A:294:GLN:CA[5_555]	1.11	1.09
2:E:1:GLU:CG	3:J:294:GLN:N[3_565]	1.13	1.07
2:E:1:GLU:OE2	3:J:293:GLU:CG[3_565]	1.14	1.06
3:A:253:ILE:CA	3:B:253:ILE:CB[6_555]	1.14	1.06
2:H:1:GLU:CB	3:A:294:GLN:N[5_555]	1.15	1.05
3:D:253:ILE:CG2	3:J:253:ILE:N[3_565]	1.18	1.02
2:E:1:GLU:OE2	3:J:293:GLU:CB[3_565]	1.20	1.00
2:H:1:GLU:OE1	3:A:293:GLU:CG[5_555]	1.21	0.99
2:E:153:GLY:C	3:D:269:GLU:OE2[1_556]	1.22	0.98
3:A:382:GLU:OE1	3:B:433:HIS:NE2[6_555]	1.24	0.96
3:A:253:ILE:N	3:B:253:ILE:CG1[6_555]	1.25	0.95
2:E:1:GLU:CB	3:J:293:GLU:C[3_565]	1.26	0.94
2:E:26:ASN:CG	3:J:294:GLN:NE2[3_565]	1.26	0.94
3:A:253:ILE:CG1	3:B:253:ILE:O[6_555]	1.27	0.93
2:E:1:GLU:OE1	3:J:293:GLU:CG[3_565]	1.28	0.92
3:A:252:MET:O	3:B:253:ILE:CD1[6_555]	1.31	0.89
2:H:1:GLU:CD	3:A:293:GLU:CG[5_555]	1.32	0.88
2:E:26:ASN:ND2	3:J:294:GLN:NE2[3_565]	1.32	0.88
3:A:252:MET:C	3:B:253:ILE:CD1[6_555]	1.34	0.86
2:E:1:GLU:CB	3:J:293:GLU:O[3_565]	1.34	0.86
3:A:252:MET:CA	3:B:253:ILE:CG1[6_555]	1.34	0.86
3:D:253:ILE:N	3:J:253:ILE:CG1[3_565]	1.35	0.85
3:A:252:MET:C	3:B:253:ILE:CB[6_555]	1.35	0.85
2:E:1:GLU:CB	3:J:294:GLN:N[3_565]	1.36	0.84
3:A:253:ILE:N	3:B:253:ILE:CA[6_555]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:GLU:OE2	3:A:293:GLU:OE1[5_555]	1.38	0.82
2:E:1:GLU:CD	3:J:293:GLU:CB[3_565]	1.40	0.80
2:E:1:GLU:OE2	3:J:293:GLU:CD[3_565]	1.41	0.79
3:A:253:ILE:CB	3:B:253:ILE:CA[6_555]	1.42	0.78
3:A:253:ILE:CD1	3:B:255:ARG:N[6_555]	1.42	0.78
3:D:253:ILE:CB	3:J:253:ILE:CA[3_565]	1.42	0.78
2:H:1:GLU:OE2	3:A:293:GLU:CD[5_555]	1.44	0.76
2:E:1:GLU:N	3:J:294:GLN:CA[3_565]	1.46	0.74
2:E:1:GLU:CA	3:J:294:GLN:CB[3_565]	1.47	0.73
2:E:154:ALA:N	3:D:269:GLU:OE2[1_556]	1.48	0.72
3:A:253:ILE:CA	3:B:253:ILE:CA[6_555]	1.48	0.72
3:D:253:ILE:CG2	3:J:253:ILE:C[3_565]	1.48	0.72
2:E:1:GLU:N	3:J:294:GLN:CG[3_565]	1.50	0.70
2:H:26:ASN:CG	3:A:294:GLN:NE2[5_555]	1.52	0.68
2:H:1:GLU:OE2	3:A:293:GLU:CB[5_555]	1.54	0.66
3:D:253:ILE:CB	3:J:253:ILE:N[3_565]	1.55	0.65
2:E:1:GLU:CG	3:J:293:GLU:C[3_565]	1.55	0.65
2:H:1:GLU:OE2	3:A:293:GLU:CG[5_555]	1.55	0.65
2:H:1:GLU:CB	3:A:293:GLU:C[5_555]	1.55	0.65
3:D:252:MET:SD	3:J:434:ASN:ND2[3_565]	1.56	0.64
3:D:253:ILE:CA	3:J:253:ILE:CB[3_565]	1.58	0.62
3:A:253:ILE:CG1	3:B:254:SER:N[6_555]	1.60	0.60
3:A:253:ILE:C	3:B:253:ILE:CG2[6_555]	1.60	0.60
3:A:382:GLU:CD	3:B:433:HIS:CD2[6_555]	1.63	0.57
3:D:310:HIS:CE1	3:J:253:ILE:CG2[3_565]	1.64	0.56
1:P:53:THR:OG1	3:N:389:ASN:OD1[1_556]	1.66	0.54
2:E:153:GLY:O	3:D:269:GLU:OE2[1_556]	1.67	0.53
3:A:253:ILE:CB	3:B:253:ILE:C[6_555]	1.68	0.52
2:H:1:GLU:O	3:A:294:GLN:CG[5_555]	1.68	0.52
2:H:1:GLU:CG	3:A:293:GLU:C[5_555]	1.69	0.51
2:E:1:GLU:CB	3:J:294:GLN:CA[3_565]	1.69	0.51
3:D:253:ILE:C	3:J:253:ILE:CG1[3_565]	1.69	0.51
3:A:382:GLU:OE1	3:B:433:HIS:CG[6_555]	1.70	0.50
2:H:1:GLU:CG	3:A:294:GLN:CA[5_555]	1.71	0.49
3:A:252:MET:CA	3:B:253:ILE:CD1[6_555]	1.72	0.48
2:E:153:GLY:O	3:D:269:GLU:CD[1_556]	1.73	0.47
2:E:26:ASN:CB	3:J:294:GLN:NE2[3_565]	1.73	0.47
2:H:1:GLU:CB	3:A:293:GLU:O[5_555]	1.75	0.45
2:H:1:GLU:CD	3:A:293:GLU:CB[5_555]	1.75	0.45
2:H:1:GLU:CD	3:A:293:GLU:C[5_555]	1.75	0.45
3:D:433:HIS:CD2	3:J:382:GLU:OE1[3_565]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:253:ILE:CB	3:B:253:ILE:O[6_555]	1.76	0.44
3:A:253:ILE:CG1	3:B:253:ILE:CA[6_555]	1.77	0.43
2:H:26:ASN:ND2	3:A:294:GLN:CD[5_555]	1.80	0.40
2:H:100:ASP:O	1:K:200:GLY:O[5_555]	1.80	0.40
2:E:1:GLU:CD	3:J:293:GLU:CD[3_565]	1.80	0.40
2:H:1:GLU:N	3:A:294:GLN:CG[5_555]	1.80	0.40
3:A:252:MET:N	3:B:253:ILE:CD1[6_555]	1.80	0.40
2:H:1:GLU:OE2	3:A:293:GLU:CA[5_555]	1.81	0.39
2:H:1:GLU:OE1	3:A:293:GLU:CB[5_555]	1.81	0.39
3:D:310:HIS:NE2	3:J:253:ILE:CG2[3_565]	1.82	0.38
2:H:1:GLU:CD	3:A:293:GLU:CD[5_555]	1.83	0.37
3:D:252:MET:C	3:J:253:ILE:CD1[3_565]	1.84	0.36
3:D:380:GLU:OE1	3:J:433:HIS:NE2[3_565]	1.85	0.35
2:E:1:GLU:OE2	3:J:293:GLU:OE1[3_565]	1.85	0.35
3:D:253:ILE:CG2	3:J:252:MET:C[3_565]	1.86	0.34
2:H:1:GLU:CD	3:A:293:GLU:CA[5_555]	1.86	0.34
1:L:107:LYS:CE	1:G:202:SER:OG[5_555]	1.86	0.34
2:E:1:GLU:O	3:J:294:GLN:CG[3_565]	1.87	0.33
2:E:1:GLU:OE1	3:J:293:GLU:CB[3_565]	1.87	0.33
2:H:1:GLU:N	3:A:294:GLN:CA[5_555]	1.87	0.33
3:A:252:MET:O	3:B:253:ILE:CG1[6_555]	1.88	0.32
2:E:100:ASP:O	1:P:200:GLY:O[3_565]	1.89	0.31
3:D:252:MET:C	3:J:253:ILE:CG1[3_565]	1.89	0.31
3:A:253:ILE:N	3:B:253:ILE:CG2[6_555]	1.89	0.31
3:A:253:ILE:CD1	3:B:255:ARG:O[6_555]	1.91	0.29
2:H:1:GLU:CD	3:A:294:GLN:N[5_555]	1.92	0.28
2:I:101:ARG:NE	3:D:387:PRO:CD[1_556]	1.92	0.28
2:H:1:GLU:CD	3:A:293:GLU:OE1[5_555]	1.93	0.27
3:D:253:ILE:CG1	3:J:253:ILE:N[3_565]	1.93	0.27
2:E:26:ASN:ND2	3:J:294:GLN:CD[3_565]	1.94	0.26
3:A:252:MET:C	3:B:253:ILE:CG2[6_555]	1.96	0.24
3:A:254:SER:O	3:B:311:GLN:OE1[6_555]	1.96	0.24
2:E:1:GLU:CA	3:J:294:GLN:N[3_565]	1.97	0.23
3:A:253:ILE:C	3:B:253:ILE:CB[6_555]	1.99	0.21
2:E:153:GLY:C	3:D:269:GLU:CD[1_556]	1.99	0.21
3:A:252:MET:O	3:B:253:ILE:CB[6_555]	2.01	0.19
2:H:1:GLU:CA	3:A:294:GLN:CG[5_555]	2.01	0.19
3:A:436:TYR:CE1	3:B:436:TYR:CD1[6_555]	2.01	0.19
3:D:252:MET:O	3:J:253:ILE:CG1[3_565]	2.02	0.18
3:A:434:ASN:ND2	3:B:252:MET:SD[6_555]	2.02	0.18
2:H:1:GLU:C	3:A:294:GLN:CB[5_555]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:GLU:CD	3:J:293:GLU:CA[3_565]	2.03	0.17
2:H:1:GLU:CA	3:A:294:GLN:C[5_555]	2.03	0.17
3:D:253:ILE:CA	3:J:253:ILE:CA[3_565]	2.05	0.15
3:A:253:ILE:CG2	3:B:253:ILE:O[6_555]	2.05	0.15
2:H:1:GLU:C	3:A:294:GLN:CG[5_555]	2.05	0.15
2:I:101:ARG:NE	3:D:387:PRO:CG[1_556]	2.05	0.15
2:E:1:GLU:OE2	3:J:293:GLU:CA[3_565]	2.06	0.14
2:H:1:GLU:CB	3:A:294:GLN:CB[5_555]	2.06	0.14
3:A:253:ILE:CA	3:B:253:ILE:CG2[6_555]	2.06	0.14
2:E:1:GLU:CA	3:J:294:GLN:CG[3_565]	2.07	0.13
3:A:252:MET:O	3:B:253:ILE:CG2[6_555]	2.07	0.13
2:O:164:GLY:O	3:N:269:GLU:OE2[1_556]	2.08	0.12
3:D:253:ILE:CG1	3:J:252:MET:C[3_565]	2.08	0.12
3:D:254:SER:OG	3:J:435:HIS:CE1[3_565]	2.09	0.11
2:E:1:GLU:C	3:J:294:GLN:CG[3_565]	2.12	0.08
3:D:253:ILE:CG2	3:J:252:MET:O[3_565]	2.12	0.08
2:E:1:GLU:CD	3:J:293:GLU:C[3_565]	2.14	0.06
2:H:26:ASN:CB	3:A:294:GLN:NE2[5_555]	2.14	0.06
3:A:253:ILE:CD1	3:B:252:MET:O[6_555]	2.15	0.05
2:H:101:ARG:CG	1:K:112:ALA:CB[5_555]	2.15	0.05
3:C:315:ASP:OD2	2:R:26:ASN:O[1_554]	2.16	0.04
3:A:253:ILE:N	3:B:253:ILE:N[6_555]	2.16	0.04
3:A:253:ILE:CA	3:B:253:ILE:C[6_555]	2.16	0.04
3:D:380:GLU:OE1	3:J:433:HIS:CE1[3_565]	2.16	0.04
3:A:382:GLU:OE1	3:B:433:HIS:CE1[6_555]	2.17	0.03
2:E:101:ARG:CG	1:P:201:LEU:CD1[3_565]	2.17	0.03
2:E:1:GLU:CG	3:J:294:GLN:CA[3_565]	2.17	0.03
2:E:1:GLU:CG	3:J:293:GLU:CG[3_565]	2.17	0.03
3:A:252:MET:N	3:B:253:ILE:CG1[6_555]	2.17	0.03
3:D:253:ILE:CG2	3:J:253:ILE:CB[3_565]	2.19	0.01
2:E:1:GLU:N	3:J:294:GLN:N[3_565]	2.19	0.01
2:I:101:ARG:NH2	3:D:387:PRO:CG[1_556]	2.19	0.01

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

All (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
3	B	301	ARG
3	C	283	GLN
3	C	287	ALA
3	C	289	THR
3	C	433	HIS
3	D	298	SER
3	D	301	ARG

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Mol	Chain	Res	Type
3	J	283	GLN
3	J	287	ALA
3	J	289	THR
3	J	433	HIS
3	N	298	SER
3	N	301	ARG
3	A	267	SER
3	A	298	SER
3	B	271	PRO
3	C	267	SER
3	C	298	SER
3	D	271	PRO
3	J	267	SER
3	J	298	SER
3	N	271	PRO
3	A	293	GLU
3	A	385	GLY
3	B	282	VAL
3	B	291	PRO
3	B	293	GLU
3	C	293	GLU
3	C	385	GLY
3	D	282	VAL
3	D	291	PRO
3	D	293	GLU
3	J	293	GLU
3	J	385	GLY
3	N	282	VAL
3	N	291	PRO
3	N	293	GLU
3	A	286	ASN
3	A	358	MET
3	B	283	GLN
3	B	295	GLN
3	C	286	ASN
3	C	358	MET
3	D	283	GLN
3	D	295	GLN
3	J	286	ASN
3	J	358	MET
3	N	283	GLN
3	N	295	GLN

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Mol	Chain	Res	Type
3	B	336	ILE
3	D	327	ALA
3	D	336	ILE
3	N	327	ALA
3	N	336	ILE
3	B	327	ALA
3	A	290	LYS
3	C	290	LYS
3	J	290	LYS

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	N	192/196 (98%)	180 (94%)	12 (6%)	18 43
All	All	3288/3432 (96%)	3107 (94%)	181 (6%)	21 47

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	33	LEU
1	L	39	LYS
1	L	100	GLN
1	L	108	ARG
1	L	123	GLU
1	L	156	SER
1	L	191	VAL
1	L	201	LEU
1	L	203	SER
1	L	208	SER
2	H	112	THR
2	H	139	LYS
2	H	146	VAL
2	H	171	LEU
2	H	187	THR
2	H	193	ASN
2	H	197	LYS
2	H	200	ASN
2	H	205	LYS
1	K	78	LEU
1	K	108	ARG
1	K	126	LYS
1	K	135	LEU
1	K	156	SER
1	K	181	LEU
1	K	185	ASP
1	K	201	LEU
2	M	12	VAL
2	M	97	SER
2	M	99	ARG
2	M	100	LEU
2	M	115	SER
2	M	152	VAL
2	M	153	THR
2	M	156	SER
2	M	162	ASN

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Mol	Chain	Res	Type
2	M	184	LEU
2	M	187	LEU
2	M	200	THR
2	M	205	THR
2	M	209	ASN
2	M	228	LYS
3	A	282	VAL
3	A	292	ARG
3	A	406	LEU
3	A	413	ASP
3	A	436	TYR
3	A	441	LEU
3	B	255	ARG
3	B	260	THR
3	B	278	TYR
3	B	288	LYS
3	B	291	PRO
3	B	296	TYR
3	B	311	GLN
3	B	370	LYS
3	B	394	THR
3	B	399	ASP
3	B	406	LEU
3	B	441	LEU
1	G	33	LEU
1	G	39	LYS
1	G	100	GLN
1	G	108	ARG
1	G	123	GLU
1	G	156	SER
1	G	191	VAL
1	G	201	LEU
1	G	203	SER
1	G	208	SER
2	E	112	THR
2	E	139	LYS
2	E	146	VAL
2	E	171	LEU
2	E	187	THR
2	E	193	ASN
2	E	197	LYS
2	E	200	ASN

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Mol	Chain	Res	Type
2	E	205	LYS
1	F	78	LEU
1	F	108	ARG
1	F	126	LYS
1	F	135	LEU
1	F	156	SER
1	F	181	LEU
1	F	185	ASP
1	F	201	LEU
2	I	12	VAL
2	I	99	SER
2	I	101	ARG
2	I	102	LEU
2	I	117	SER
2	I	146	VAL
2	I	147	THR
2	I	149	SER
2	I	151	ASN
2	I	171	LEU
2	I	174	LEU
2	I	187	THR
2	I	189	THR
2	I	193	ASN
2	I	210	LYS
3	C	282	VAL
3	C	292	ARG
3	C	406	LEU
3	C	413	ASP
3	C	436	TYR
3	C	441	LEU
3	D	255	ARG
3	D	260	THR
3	D	278	TYR
3	D	288	LYS
3	D	291	PRO
3	D	296	TYR
3	D	311	GLN
3	D	370	LYS
3	D	394	THR
3	D	399	ASP
3	D	406	LEU
3	D	441	LEU

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Mol	Chain	Res	Type
1	Q	33	LEU
1	Q	39	LYS
1	Q	100	GLN
1	Q	108	ARG
1	Q	123	GLU
1	Q	156	SER
1	Q	191	VAL
1	Q	201	LEU
1	Q	203	SER
1	Q	208	SER
2	O	110	THR
2	O	145	LYS
2	O	152	VAL
2	O	184	LEU
2	O	200	THR
2	O	209	ASN
2	O	213	LYS
2	O	216	ASN
2	O	221	LYS
1	P	78	LEU
1	P	108	ARG
1	P	126	LYS
1	P	135	LEU
1	P	156	SER
1	P	181	LEU
1	P	185	ASP
1	P	201	LEU
2	R	12	VAL
2	R	97	SER
2	R	99	ARG
2	R	100	LEU
2	R	115	SER
2	R	152	VAL
2	R	153	THR
2	R	156	SER
2	R	162	ASN
2	R	184	LEU
2	R	187	LEU
2	R	200	THR
2	R	205	THR
2	R	209	ASN
2	R	218	LYS

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Mol	Chain	Res	Type
2	R	228	LYS
3	J	282	VAL
3	J	292	ARG
3	J	406	LEU
3	J	413	ASP
3	J	436	TYR
3	J	441	LEU
3	N	255	ARG
3	N	260	THR
3	N	278	TYR
3	N	288	LYS
3	N	291	PRO
3	N	296	TYR
3	N	311	GLN
3	N	370	LYS
3	N	394	THR
3	N	399	ASP
3	N	406	LEU
3	N	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	87	HIS
1	L	89	GLN
1	L	100	GLN
1	L	198	HIS
2	H	32	HIS
2	H	81	GLN
2	H	83	HIS
2	H	196	HIS
1	K	87	HIS
1	K	89	GLN
1	K	90	HIS
1	K	198	HIS
1	K	210	ASN
2	M	32	HIS
2	M	81	GLN
2	M	179	GLN
2	M	212	HIS
3	A	272	GLN

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Mol	Chain	Res	Type
3	A	283	GLN
3	A	311	GLN
3	A	325	ASN
3	A	347	GLN
3	A	361	ASN
3	A	390	ASN
3	A	418	GLN
3	A	419	GLN
3	A	421	ASN
3	A	429	HIS
3	B	272	GLN
3	B	276	ASN
3	B	283	GLN
3	B	285	HIS
3	B	311	GLN
3	B	312	ASN
3	B	325	ASN
3	B	342	GLN
3	B	361	ASN
3	B	389	ASN
3	B	390	ASN
3	B	419	GLN
3	B	429	HIS
3	B	434	ASN
3	B	438	GLN
1	G	38	GLN
1	G	87	HIS
1	G	89	GLN
1	G	100	GLN
1	G	198	HIS
2	E	32	HIS
2	E	81	GLN
2	E	83	HIS
2	E	196	HIS
1	F	87	HIS
1	F	89	GLN
1	F	90	HIS
1	F	198	HIS
1	F	210	ASN
2	I	32	HIS
2	I	81	GLN
2	I	83	HIS

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Mol	Chain	Res	Type
2	I	167	GLN
2	I	196	HIS
3	C	272	GLN
3	C	283	GLN
3	C	311	GLN
3	C	325	ASN
3	C	347	GLN
3	C	361	ASN
3	C	390	ASN
3	C	418	GLN
3	C	419	GLN
3	C	421	ASN
3	C	429	HIS
3	C	435	HIS
3	D	272	GLN
3	D	276	ASN
3	D	283	GLN
3	D	286	ASN
3	D	311	GLN
3	D	312	ASN
3	D	325	ASN
3	D	342	GLN
3	D	361	ASN
3	D	389	ASN
3	D	390	ASN
3	D	419	GLN
3	D	429	HIS
3	D	434	ASN
3	D	438	GLN
1	Q	38	GLN
1	Q	87	HIS
1	Q	89	GLN
1	Q	100	GLN
1	Q	198	HIS
2	O	32	HIS
2	O	212	HIS
1	P	87	HIS
1	P	89	GLN
1	P	90	HIS
1	P	198	HIS
1	P	210	ASN
2	R	32	HIS

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Mol	Chain	Res	Type
2	R	179	GLN
2	R	212	HIS
3	J	272	GLN
3	J	283	GLN
3	J	311	GLN
3	J	325	ASN
3	J	347	GLN
3	J	361	ASN
3	J	390	ASN
3	J	418	GLN
3	J	419	GLN
3	J	421	ASN
3	J	429	HIS
3	N	272	GLN
3	N	276	ASN
3	N	283	GLN
3	N	286	ASN
3	N	312	ASN
3	N	325	ASN
3	N	342	GLN
3	N	361	ASN
3	N	389	ASN
3	N	390	ASN
3	N	419	GLN
3	N	429	HIS
3	N	434	ASN
3	N	438	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (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

All 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
1	O	127:SER	C	136:GLY	N	11.41
1	M	100:LEU	C	101:ASP	N	11.16
1	R	100:LEU	C	101:ASP	N	11.16
1	H	81:GLN	C	82:MET	N	8.84
1	E	81:GLN	C	82:MET	N	8.84
1	O	81:GLN	C	82:MET	N	8.84
1	M	81:GLN	C	82:MET	N	8.78
1	I	81:GLN	C	82:MET	N	8.78
1	R	81:GLN	C	82:MET	N	8.78
1	I	82:MET	C	83:HIS	N	7.02
1	H	82:MET	C	83:HIS	N	6.99
1	E	82:MET	C	83:HIS	N	6.99
1	E	84:LYS	C	85:ARG	N	4.06
1	H	52:SER	C	53:SER	N	3.91
1	E	52:SER	C	53:SER	N	3.91

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	52:SER	C	53:SER	N	3.91
1	M	52:SER	C	53:SER	N	3.88
1	I	52:SER	C	53:SER	N	3.88
1	R	52:SER	C	53:SER	N	3.88
1	M	203:GLN	C	205:THR	N	3.66
1	I	188:GLN	C	189:THR	N	3.66
1	R	203:GLN	C	205:THR	N	3.66
1	H	188:GLN	C	189:THR	N	3.28
1	E	188:GLN	C	189:THR	N	3.28
1	O	203:GLN	C	205:THR	N	3.28
1	M	200:THR	C	203:GLN	N	3.26
1	I	187:THR	C	188:GLN	N	3.26
1	R	200:THR	C	203:GLN	N	3.26
1	M	222:LYS	C	225:VAL	N	3.05
1	I	206:LYS	C	207:VAL	N	3.05
1	R	222:LYS	C	225:VAL	N	3.05
1	H	187:THR	C	188:GLN	N	2.93
1	E	187:THR	C	188:GLN	N	2.93
1	O	200:THR	C	203:GLN	N	2.93
1	M	157:TRP	C	162:ASN	N	2.89
1	I	150:TRP	C	151:ASN	N	2.89
1	R	157:TRP	C	162:ASN	N	2.89
1	H	206:LYS	C	207:VAL	N	2.78
1	E	206:LYS	C	207:VAL	N	2.78
1	O	222:LYS	C	225:VAL	N	2.78
1	H	150:TRP	C	151:ASN	N	2.55
1	E	150:TRP	C	151:ASN	N	2.55
1	O	157:TRP	C	162:ASN	N	2.55
1	M	169:GLY	C	171:VAL	N	2.52
1	I	158:GLY	C	159:VAL	N	2.52
1	R	169:GLY	C	171:VAL	N	2.51
1	H	158:GLY	C	159:VAL	N	2.17
1	E	158:GLY	C	159:VAL	N	2.17
1	O	169:GLY	C	171:VAL	N	2.17
1	M	180:SER	C	182:SER	N	1.98
1	I	168:SER	C	169:SER	N	1.98
1	R	180:SER	C	182:SER	N	1.98
1	H	168:SER	C	169:SER	N	1.87
1	E	168:SER	C	169:SER	N	1.87
1	O	180:SER	C	182:SER	N	1.87
1	M	154:VAL	C	156:SER	N	1.86
1	I	148:VAL	C	149:SER	N	1.86

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	154:VAL	C	156:SER	N	1.86
1	H	148:VAL	C	149:SER	N	1.72
1	E	148:VAL	C	149:SER	N	1.72
1	O	154:VAL	C	156:SER	N	1.72

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	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

All (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
1	L	174	SER	9.1
3	B	238	PRO	8.7
1	L	189	HIS	8.7
1	P	8	PRO	8.5
2	H	146	VAL	8.4
3	N	332	ILE	8.3
2	M	94	ARG	8.2
2	H	3	GLN	8.2
3	B	253	ILE	8.1
3	A	253	ILE	8.0
2	O	116	THR	8.0
2	H	131	THR	8.0
2	M	198	LEU	7.9
3	B	240	VAL	7.9
1	Q	163	VAL	7.8
3	B	332	ILE	7.8
2	M	8	GLY	7.8
3	C	254	SER	7.8
3	B	316	GLY	7.8
1	L	206	THR	7.7
3	C	349	TYR	7.6
3	D	254	SER	7.6
3	C	399	ASP	7.6
3	C	326	LYS	7.5
2	R	175	PRO	7.5
3	J	399	ASP	7.5
3	A	331	PRO	7.4
3	J	284	VAL	7.3
3	B	281	GLY	7.3
1	K	8	PRO	7.3
3	C	281	GLY	7.3
3	B	334	LYS	7.2
3	A	388	GLU	7.2
1	G	44	PRO	7.2
2	H	145	PRO	7.1
3	J	348	VAL	7.1
3	D	341	GLY	7.0
2	H	45	LEU	7.0
1	G	203	SER	6.8
3	C	284	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
3	B	247	PRO	6.8
1	Q	62	PHE	6.8
3	J	338	LYS	6.8
3	J	330	ALA	6.8
1	Q	44	PRO	6.7
1	G	202	SER	6.7
2	H	102	LEU	6.7
3	A	284	VAL	6.7
2	M	188	SER	6.7
3	B	321	CYS	6.6
3	C	338	LYS	6.6
1	L	78	LEU	6.6
2	M	10	GLY	6.6
1	P	164	THR	6.5
3	C	339	ALA	6.5
1	K	17	ASP	6.5
1	L	198	HIS	6.5
1	Q	197	THR	6.4
3	A	272	GLN	6.3
3	B	336	ILE	6.3
3	B	337	SER	6.3
3	J	349	TYR	6.3
1	G	62	PHE	6.2
3	J	281	GLY	6.2
1	L	188	LYS	6.2
3	B	241	PHE	6.2
1	L	164	THR	6.2
3	B	239	SER	6.1
1	F	205	VAL	6.1
3	J	329	PRO	6.1
1	Q	59	PRO	6.1
2	H	130	GLY	6.1
1	L	184	ALA	6.0
1	P	163	VAL	6.0
1	L	163	VAL	6.0
2	M	9	GLY	6.0
3	J	261	CYS	6.0
2	M	175	PRO	5.9
2	O	10	GLY	5.9
3	A	350	THR	5.9
1	F	164	THR	5.9
2	H	144	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
3	A	375	SER	5.8
3	J	379	VAL	5.8
1	K	76	SER	5.8
1	L	197	THR	5.8
1	L	200	GLY	5.7
3	J	285	HIS	5.7
3	A	285	HIS	5.7
1	K	75	ILE	5.7
3	B	250	THR	5.7
3	B	333	GLU	5.7
3	J	388	GLU	5.7
3	B	443	LEU	5.7
3	A	379	VAL	5.7
2	I	164	ALA	5.6
3	A	339	ALA	5.6
3	J	323	VAL	5.6
2	M	199	GLY	5.6
2	R	57	ARG	5.6
2	H	148	VAL	5.6
3	J	364	SER	5.6
3	A	252	MET	5.6
3	J	254	SER	5.6
1	G	187	GLU	5.6
1	G	206	THR	5.5
2	M	110	THR	5.5
1	G	27	GLN	5.5
2	M	183	GLY	5.5
3	C	379	VAL	5.5
3	B	254	SER	5.5
2	R	198	LEU	5.4
3	A	390	ASN	5.4
3	B	348	VAL	5.4
3	C	282	VAL	5.4
1	G	59	PRO	5.4
1	G	163	VAL	5.4
1	F	8	PRO	5.4
1	Q	108	ARG	5.4
1	K	44	PRO	5.3
2	M	107	THR	5.3
1	Q	202	SER	5.3
3	D	253	ILE	5.3
3	J	282	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	H	101	ARG	5.3
2	M	97	SER	5.3
2	H	58	ASP	5.2
1	L	205	VAL	5.2
2	E	83	HIS	5.2
1	K	14	SER	5.1
1	Q	152	ASN	5.1
1	L	156	SER	5.1
2	H	44	GLY	5.1
3	B	417	TRP	5.1
1	Q	164	THR	5.1
1	Q	189	HIS	5.1
2	H	40	VAL	5.1
3	B	442	SER	5.1
3	J	298	SER	5.0
3	B	368	LEU	5.0
1	Q	201	LEU	5.0
3	J	339	ALA	5.0
2	M	154	VAL	5.0
3	C	285	HIS	5.0
1	L	158	ASN	5.0
2	R	214	PRO	5.0
3	N	333	GLU	5.0
2	O	154	VAL	4.9
3	N	253	ILE	4.9
3	J	328	LEU	4.9
2	E	133	ALA	4.9
2	O	117	LYS	4.9
1	L	190	LYS	4.9
3	B	335	THR	4.9
1	G	14	SER	4.9
2	M	101	ASP	4.9
2	E	118	THR	4.9
3	C	302	VAL	4.9
2	O	118	GLY	4.8
3	C	298	SER	4.8
3	B	320	LYS	4.8
1	L	112	ALA	4.8
3	J	326	LYS	4.8
3	J	253	ILE	4.8
1	Q	60	SER	4.8
2	R	14	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
2	H	195	ASN	4.8
3	B	289	THR	4.8
1	Q	111	ALA	4.8
2	M	106	GLY	4.8
1	L	157	GLY	4.8
1	L	19	ILE	4.8
3	J	283	GLN	4.7
3	D	333	GLU	4.7
3	A	395	PRO	4.7
2	I	109	THR	4.7
3	A	346	PRO	4.7
3	C	252	MET	4.7
3	C	283	GLN	4.7
3	J	400	SER	4.7
1	G	21	ILE	4.7
3	J	366	THR	4.7
1	L	185	ASP	4.7
2	M	93	ALA	4.7
3	N	241	PHE	4.7
1	L	132	VAL	4.7
2	M	228	LYS	4.7
2	E	157	SER	4.7
2	R	19	ILE	4.6
1	K	102	THR	4.6
2	E	148	VAL	4.6
1	Q	58	VAL	4.6
1	L	204	PRO	4.6
2	H	160	HIS	4.6
3	C	253	ILE	4.6
2	H	62	ALA	4.6
1	K	96	ALA	4.6
2	O	138	ALA	4.6
2	R	176	ALA	4.6
3	N	341	GLY	4.5
1	G	210	ASN	4.5
3	A	419	GLN	4.5
2	E	140	ASP	4.5
1	G	204	PRO	4.5
2	O	148	PHE	4.5
1	G	201	LEU	4.5
3	A	377	ILE	4.5
2	H	133	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	186	TYR	4.5
1	F	131	SER	4.5
3	C	347	GLN	4.4
3	C	366	THR	4.4
3	A	270	ASP	4.4
3	C	327	ALA	4.4
3	A	400	SER	4.4
2	O	146	ASP	4.4
3	C	330	ALA	4.4
1	L	155	GLN	4.4
3	A	293	GLU	4.4
2	E	132	ALA	4.4
2	M	214	PRO	4.4
1	L	110	VAL	4.4
1	L	131	SER	4.4
2	M	182	SER	4.4
3	J	327	ALA	4.4
2	O	46	GLU	4.3
2	R	82	MET	4.3
3	N	350	THR	4.3
2	E	158	GLY	4.3
1	Q	174	SER	4.3
1	F	206	THR	4.3
1	F	13	ALA	4.3
1	L	161	GLU	4.3
1	G	152	ASN	4.3
2	M	96	GLY	4.3
1	K	115	VAL	4.3
2	R	211	ASN	4.3
2	M	146	ASP	4.3
2	M	177	VAL	4.3
3	J	280	ASP	4.3
3	B	379	VAL	4.3
1	L	199	GLN	4.2
3	J	324	SER	4.2
1	P	118	PHE	4.2
2	H	39	ARG	4.2
3	N	273	VAL	4.2
2	R	153	THR	4.2
3	B	280	ASP	4.2
1	L	113	PRO	4.2
3	A	306	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	147	THR	4.2
2	M	32	HIS	4.2
3	C	273	VAL	4.2
1	Q	198	HIS	4.2
2	I	2	VAL	4.2
1	P	206	THR	4.2
2	E	66	ARG	4.1
2	E	156	THR	4.1
2	I	57	ARG	4.1
2	R	154	VAL	4.1
3	A	349	TYR	4.1
2	E	119	LYS	4.1
3	N	356	GLU	4.1
1	L	151	ASP	4.1
1	F	163	VAL	4.1
2	H	81	GLN	4.1
1	Q	171	SER	4.1
3	J	321	CYS	4.1
1	L	18	THR	4.1
1	Q	76	SER	4.1
1	G	164	THR	4.1
3	B	315	ASP	4.1
1	K	42	LYS	4.1
3	A	389	ASN	4.1
3	C	329	PRO	4.1
1	P	132	VAL	4.0
1	P	62	PHE	4.0
2	M	95	LYS	4.0
2	M	176	ALA	4.0
3	J	347	GLN	4.0
1	G	111	ALA	4.0
2	M	184	LEU	4.0
2	O	139	ALA	4.0
2	O	193	VAL	4.0
3	B	400	SER	4.0
1	G	26	SER	4.0
1	Q	7	SER	4.0
2	O	17	SER	4.0
2	H	24	VAL	4.0
1	G	25	ALA	4.0
3	B	338	LYS	4.0
2	M	149	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
3	J	286	ASN	4.0
2	H	63	VAL	4.0
3	N	248	LYS	4.0
3	A	372	PHE	4.0
3	C	272	GLN	4.0
1	L	62	PHE	4.0
2	E	131	THR	4.0
2	R	210	VAL	3.9
2	R	107	THR	3.9
3	N	390	ASN	3.9
2	H	25	SER	3.9
2	H	66	ARG	3.9
1	K	62	PHE	3.9
2	H	65	GLY	3.9
2	M	82	MET	3.9
2	R	8	GLY	3.9
2	E	17	SER	3.9
3	B	331	PRO	3.9
2	E	10	GLY	3.9
3	D	241	PHE	3.9
1	K	39	LYS	3.8
3	C	274	LYS	3.8
1	P	205	VAL	3.8
1	L	201	LEU	3.8
2	M	197	SER	3.8
2	I	14	ALA	3.8
1	G	205	VAL	3.8
2	O	198	LEU	3.8
3	B	242	LEU	3.8
3	A	326	LYS	3.8
3	J	276	ASN	3.8
2	O	167	THR	3.8
2	E	65	GLY	3.8
2	O	9	GLY	3.8
3	B	266	VAL	3.8
2	E	129	SER	3.8
2	R	92	CYS	3.8
2	M	79	TYR	3.8
2	I	26	ASN	3.8
1	G	113	PRO	3.7
3	N	346	PRO	3.7
1	Q	104	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	O	226	GLU	3.7
1	L	144	ALA	3.7
3	C	331	PRO	3.7
1	Q	203	SER	3.7
1	Q	18	THR	3.7
2	H	129	SER	3.7
1	F	196	VAL	3.7
1	L	20	THR	3.7
1	G	197	THR	3.7
2	E	9	GLY	3.7
2	I	183	SER	3.7
1	G	63	SER	3.7
3	A	292	ARG	3.7
3	C	286	ASN	3.7
3	N	247	PRO	3.7
1	L	111	ALA	3.7
3	A	378	ALA	3.7
3	J	363	VAL	3.7
2	I	117	SER	3.6
1	K	163	VAL	3.6
2	H	154	ALA	3.6
3	J	403	SER	3.6
1	G	207	LYS	3.6
3	A	286	ASN	3.6
1	L	162	SER	3.6
1	K	114	SER	3.6
2	H	46	GLU	3.6
3	B	399	ASP	3.6
1	K	118	PHE	3.6
2	M	187	LEU	3.6
3	J	402	GLY	3.6
1	L	44	PRO	3.6
3	C	364	SER	3.6
2	H	158	GLY	3.6
1	F	14	SER	3.6
2	M	31	ALA	3.6
3	B	366	THR	3.6
1	G	175	LEU	3.5
1	K	175	LEU	3.5
1	G	198	HIS	3.5
2	M	104	GLY	3.5
1	L	96	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	I	173	SER	3.5
2	R	197	SER	3.5
3	D	387	PRO	3.5
2	I	9	GLY	3.5
1	G	144	ALA	3.5
2	R	111	VAL	3.5
1	K	37	GLN	3.5
3	A	289	THR	3.5
1	G	20	THR	3.5
2	H	99	SER	3.5
1	Q	106	ILE	3.5
3	N	262	VAL	3.5
3	A	332	ILE	3.5
2	E	46	GLU	3.5
2	O	115	SER	3.5
1	Q	21	ILE	3.5
3	B	418	GLN	3.5
3	C	276	ASN	3.5
1	K	110	VAL	3.5
1	L	17	ASP	3.4
1	P	9	SER	3.4
2	O	137	THR	3.4
1	L	175	LEU	3.4
1	G	83	PHE	3.4
2	H	43	GLY	3.4
3	J	401	ASP	3.4
3	A	255	ARG	3.4
2	M	148	PHE	3.4
1	Q	200	GLY	3.4
3	D	386	GLN	3.4
1	G	110	VAL	3.4
1	K	208	SER	3.4
2	R	13	LYS	3.4
1	G	58	VAL	3.4
1	K	120	PRO	3.4
2	O	65	GLY	3.4
3	B	374	PRO	3.4
2	M	17	SER	3.4
1	Q	14	SER	3.4
2	E	170	GLY	3.4
1	Q	43	ALA	3.4
1	L	152	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	410	LEU	3.4
2	H	83	HIS	3.4
2	M	116	THR	3.4
2	E	112	THR	3.4
2	R	70	SER	3.4
3	B	347	GLN	3.3
1	Q	113	PRO	3.3
2	O	66	ARG	3.3
1	L	2	VAL	3.3
1	Q	162	SER	3.3
3	C	400	SER	3.3
2	H	156	THR	3.3
1	G	209	PHE	3.3
2	R	186	SER	3.3
3	C	278	TYR	3.3
1	Q	204	PRO	3.3
2	M	200	THR	3.3
3	D	343	PRO	3.3
2	I	8	GLY	3.3
2	I	25	SER	3.3
1	F	210	ASN	3.3
2	H	155	LEU	3.3
3	B	292	ARG	3.3
3	N	394	THR	3.3
3	D	262	VAL	3.3
2	M	64	LYS	3.3
1	K	40	PRO	3.3
3	C	328	LEU	3.3
1	F	19	ILE	3.3
2	E	19	ILE	3.3
2	O	67	PHE	3.3
3	A	399	ASP	3.3
2	E	128	PRO	3.3
3	B	251	LEU	3.3
1	Q	75	ILE	3.2
1	Q	114	SER	3.2
3	A	273	VAL	3.2
3	D	332	ILE	3.2
1	G	122	ASP	3.2
1	K	116	PHE	3.2
3	N	343	PRO	3.2
2	O	124	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	351	LEU	3.2
2	R	9	GLY	3.2
3	A	340	LYS	3.2
1	Q	8	PRO	3.2
1	Q	192	TYR	3.2
3	A	383	SER	3.2
2	E	185	LEU	3.2
1	Q	205	VAL	3.2
1	L	94	TYR	3.2
2	I	153	GLY	3.2
2	M	105	PRO	3.2
1	K	77	GLY	3.2
3	B	317	LYS	3.2
2	E	45	LEU	3.2
2	H	157	SER	3.2
3	B	276	ASN	3.2
1	Q	38	GLN	3.2
1	K	61	ARG	3.2
1	Q	144	ALA	3.2
3	N	295	GLN	3.2
2	M	189	SER	3.2
1	K	206	THR	3.2
3	N	281	GLY	3.2
3	A	283	GLN	3.2
1	P	60	SER	3.1
2	M	112	SER	3.1
1	G	192	TYR	3.1
1	Q	210	ASN	3.1
2	I	198	PRO	3.1
2	H	128	PRO	3.1
3	J	251	LEU	3.1
3	J	270	ASP	3.1
2	M	179	GLN	3.1
2	O	103	TRP	3.1
3	B	354	SER	3.1
2	H	182	SER	3.1
2	R	58	ASP	3.1
2	H	2	VAL	3.1
3	B	314	LEU	3.1
1	K	117	ILE	3.1
2	M	196	SER	3.1
1	G	96	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	N	423	PHE	3.1
1	K	15	VAL	3.1
1	G	161	GLU	3.1
2	H	109	THR	3.1
1	L	79	GLN	3.1
2	M	117	LYS	3.1
1	G	76	SER	3.1
2	O	110	THR	3.1
3	A	243	PHE	3.1
1	K	30	GLU	3.1
3	B	407	TYR	3.1
3	C	321	CYS	3.1
1	F	187	GLU	3.1
2	H	143	PRO	3.1
3	B	284	VAL	3.1
2	I	21	SER	3.1
2	H	82	MET	3.1
1	F	17	ASP	3.1
1	G	78	LEU	3.1
1	K	9	SER	3.1
2	M	195	SER	3.1
2	M	174	PHE	3.1
1	K	54	LEU	3.0
1	P	196	VAL	3.0
2	M	98	ASP	3.0
2	E	159	VAL	3.0
3	A	376	ASP	3.0
1	L	179	LEU	3.0
3	N	331	PRO	3.0
3	A	308	VAL	3.0
1	L	97	THR	3.0
2	H	19	ILE	3.0
2	M	190	VAL	3.0
3	C	335	THR	3.0
2	R	1	GLU	3.0
2	R	4	LEU	3.0
3	A	338	LYS	3.0
1	G	82	ASP	3.0
1	L	195	GLU	3.0
1	K	109	THR	3.0
1	F	59	PRO	3.0
3	N	400	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	133	VAL	3.0
2	E	142	PHE	3.0
3	D	260	THR	3.0
2	H	50	SER	3.0
3	C	307	THR	3.0
3	N	254	SER	3.0
2	H	132	ALA	3.0
2	M	109	VAL	3.0
3	J	375	SER	3.0
1	G	104	VAL	3.0
2	M	19	ILE	3.0
1	K	131	SER	3.0
3	A	271	PRO	3.0
1	Q	170	ASP	3.0
1	L	9	SER	3.0
3	B	313	TRP	2.9
2	O	195	SER	2.9
2	H	194	VAL	2.9
3	C	394	THR	2.9
3	D	418	GLN	2.9
2	M	21	SER	2.9
2	I	17	SER	2.9
2	I	19	ILE	2.9
1	F	75	ILE	2.9
2	H	1	GLU	2.9
2	O	183	GLY	2.9
3	B	278	TYR	2.9
2	E	105	TRP	2.9
3	C	301	ARG	2.9
1	Q	63	SER	2.9
3	A	381	TRP	2.9
3	A	374	PRO	2.9
1	K	162	SER	2.9
1	P	208	SER	2.9
3	C	388	GLU	2.9
3	D	350	THR	2.9
3	J	331	PRO	2.9
1	K	57	GLY	2.9
3	J	302	VAL	2.9
1	G	211	ARG	2.9
2	E	210	LYS	2.9
3	B	288	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
3	J	274	LYS	2.9
1	G	17	ASP	2.9
1	K	19	ILE	2.9
2	I	101	ARG	2.9
3	N	407	TYR	2.9
3	N	284	VAL	2.9
3	D	245	PRO	2.9
2	H	13	LYS	2.9
1	G	174	SER	2.9
2	E	183	SER	2.9
2	E	18	LEU	2.9
1	F	195	GLU	2.8
1	Q	25	ALA	2.8
1	L	208	SER	2.8
3	C	368	LEU	2.8
3	N	323	VAL	2.8
3	N	266	VAL	2.8
1	K	18	THR	2.8
2	E	3	GLN	2.8
2	I	195	ASN	2.8
2	E	130	GLY	2.8
1	L	14	SER	2.8
2	E	169	SER	2.8
2	I	20	LEU	2.8
3	B	245	PRO	2.8
3	N	292	ARG	2.8
2	E	72	ASP	2.8
2	O	63	VAL	2.8
3	D	259	VAL	2.8
1	Q	23	CYS	2.8
3	N	441	LEU	2.8
1	P	19	ILE	2.8
3	C	294	GLN	2.8
2	I	163	PRO	2.8
3	C	392	LYS	2.8
1	L	203	SER	2.8
1	P	133	VAL	2.8
2	E	155	LEU	2.8
2	O	72	ASP	2.8
2	M	18	LEU	2.8
3	B	295	GLN	2.8
1	G	181	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	J	398	LEU	2.8
1	G	158	ASN	2.8
2	R	21	SER	2.8
1	F	132	VAL	2.8
2	M	39	ARG	2.8
1	F	208	SER	2.8
2	O	123	PRO	2.8
2	M	69	VAL	2.8
3	A	241	PHE	2.7
1	L	98	PHE	2.7
1	K	209	PHE	2.7
3	J	368	LEU	2.7
2	H	134	LEU	2.7
3	A	418	GLN	2.7
3	J	272	GLN	2.7
1	K	2	VAL	2.7
3	B	425	CYS	2.7
1	Q	74	THR	2.7
3	B	264	VAL	2.7
1	L	180	THR	2.7
1	P	2	VAL	2.7
2	O	168	SER	2.7
3	B	364	SER	2.7
1	P	61	ARG	2.7
2	M	103	TRP	2.7
1	L	150	VAL	2.7
2	M	35	ASN	2.7
1	F	18	THR	2.7
3	B	262	VAL	2.7
1	F	207	LYS	2.7
3	B	439	LYS	2.7
1	P	131	SER	2.7
2	H	183	SER	2.7
3	A	409	LYS	2.7
1	L	160	GLN	2.7
2	M	65	GLY	2.7
1	G	130	ALA	2.7
1	Q	13	ALA	2.7
2	I	3	GLN	2.7
2	I	82	MET	2.7
3	C	375	SER	2.7
1	P	7	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	34	MET	2.6
2	O	171	VAL	2.6
1	G	212	GLY	2.6
1	P	13	ALA	2.6
1	Q	188	LYS	2.6
1	K	16	GLY	2.6
1	K	64	GLY	2.6
3	B	285	HIS	2.6
3	J	316	GLY	2.6
2	M	113	PRO	2.6
2	R	81	GLN	2.6
3	J	346	PRO	2.6
3	D	323	VAL	2.6
3	C	407	TYR	2.6
3	N	409	LYS	2.6
3	B	258	GLU	2.6
3	N	411	THR	2.6
1	P	192	TYR	2.6
2	I	185	LEU	2.6
2	O	194	PRO	2.6
3	A	394	THR	2.6
3	C	324	SER	2.6
1	L	73	LEU	2.6
2	M	145	LYS	2.6
2	E	8	GLY	2.6
2	R	90	TYR	2.6
3	A	261	CYS	2.6
1	G	8	PRO	2.6
2	E	103	ASP	2.6
1	G	39	LYS	2.6
1	L	21	ILE	2.6
2	E	182	SER	2.6
3	A	321	CYS	2.6
3	A	323	VAL	2.6
1	K	25	ALA	2.6
3	B	349	TYR	2.6
3	C	255	ARG	2.6
1	K	130	ALA	2.6
3	J	437	THR	2.6
2	M	4	LEU	2.6
1	Q	61	ARG	2.6
3	D	284	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	8	PRO	2.5
2	E	111	VAL	2.5
2	E	146	VAL	2.5
1	K	112	ALA	2.5
1	L	143	GLU	2.5
1	K	78	LEU	2.5
1	K	138	ASN	2.5
1	Q	187	GLU	2.5
2	H	175	SER	2.5
2	O	81	GLN	2.5
3	C	316	GLY	2.5
3	J	389	ASN	2.5
1	K	43	ALA	2.5
1	Q	22	THR	2.5
3	D	353	PRO	2.5
2	E	75	GLU	2.5
2	I	65	GLY	2.5
3	B	259	VAL	2.5
1	Q	175	LEU	2.5
3	C	423	PHE	2.5
1	L	212	GLY	2.5
2	O	19	ILE	2.5
3	A	411	THR	2.5
1	K	58	VAL	2.5
2	I	113	VAL	2.5
1	Q	83	PHE	2.5
2	O	166	LEU	2.5
1	Q	150	VAL	2.5
1	K	26	SER	2.5
2	M	111	VAL	2.5
3	N	379	VAL	2.5
1	P	89	GLN	2.5
1	P	102	THR	2.5
3	A	333	GLU	2.5
3	D	268	HIS	2.5
3	C	251	LEU	2.5
3	C	250	THR	2.5
1	K	137	ASN	2.5
1	L	181	LEU	2.5
1	F	165	GLU	2.5
2	O	75	GLU	2.5
3	B	375	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	341	GLY	2.5
2	I	116	ALA	2.5
2	R	177	VAL	2.5
1	Q	94	TYR	2.5
3	B	370	LYS	2.5
3	A	305	VAL	2.5
3	B	263	VAL	2.5
3	B	394	THR	2.5
3	C	405	PHE	2.5
3	D	411	THR	2.5
3	J	418	GLN	2.5
3	N	339	ALA	2.5
2	I	174	LEU	2.5
1	L	15	VAL	2.4
1	K	132	VAL	2.4
1	F	51	ALA	2.4
2	E	117	SER	2.4
1	L	191	VAL	2.4
2	E	206	LYS	2.4
2	H	61	ASP	2.4
2	E	89	THR	2.4
2	E	63	VAL	2.4
3	D	396	PRO	2.4
3	J	252	MET	2.4
3	B	409	LYS	2.4
1	G	94	TYR	2.4
1	L	25	ALA	2.4
1	F	183	LYS	2.4
2	E	2	VAL	2.4
2	O	152	VAL	2.4
3	D	374	PRO	2.4
3	D	348	VAL	2.4
3	J	409	LYS	2.4
1	Q	186	TYR	2.4
3	B	373	TYR	2.4
3	D	269	GLU	2.4
3	A	295	GLN	2.4
3	B	318	GLU	2.4
3	D	390	ASN	2.4
2	H	18	LEU	2.4
3	A	251	LEU	2.4
3	N	245	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	248	LYS	2.4
1	L	61	ARG	2.4
2	I	27	PHE	2.4
3	N	267	SER	2.4
1	G	18	THR	2.4
2	M	143	LEU	2.4
3	D	273	VAL	2.4
1	L	173	TYR	2.4
2	R	156	SER	2.4
3	J	314	LEU	2.4
2	E	81	GLN	2.4
2	I	59	TYR	2.4
3	A	294	GLN	2.4
3	J	279	VAL	2.4
2	M	67	PHE	2.4
1	G	131	SER	2.4
3	D	342	GLN	2.4
1	G	189	HIS	2.4
2	E	153	GLY	2.4
2	R	24	VAL	2.4
2	R	213	LYS	2.4
3	B	343	PRO	2.4
3	D	366	THR	2.4
3	A	392	LYS	2.4
2	M	12	VAL	2.4
2	M	16	GLY	2.4
2	O	172	HIS	2.3
3	C	409	LYS	2.3
1	G	177	SER	2.3
2	M	102	ALA	2.3
1	F	118	PHE	2.3
2	R	18	LEU	2.3
2	O	227	PRO	2.3
2	R	64	LYS	2.3
1	Q	196	VAL	2.3
2	M	2	VAL	2.3
1	L	22	THR	2.3
1	G	64	GLY	2.3
3	C	350	THR	2.3
2	H	59	TYR	2.3
1	L	24	ARG	2.3
2	M	227	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	274	LYS	2.3
3	B	252	MET	2.3
1	Q	207	LYS	2.3
2	E	82	MET	2.3
2	I	42	GLY	2.3
1	G	112	ALA	2.3
1	Q	105	GLU	2.3
3	C	270	ASP	2.3
2	E	181	PRO	2.3
2	O	42	GLY	2.3
1	G	200	GLY	2.3
3	B	307	THR	2.3
2	R	22	CYS	2.3
3	C	380	GLU	2.3
1	Q	110	VAL	2.3
3	B	319	TYR	2.3
3	C	293	GLU	2.3
1	G	155	GLN	2.3
3	C	269	GLU	2.3
2	O	182	SER	2.3
2	R	183	GLY	2.3
2	I	53	SER	2.3
1	F	192	TYR	2.3
2	R	12	VAL	2.3
3	C	280	ASP	2.3
2	R	65	GLY	2.3
1	Q	107	LYS	2.3
2	I	184	SER	2.3
2	I	94	CYS	2.3
2	O	101	ASP	2.3
3	B	248	LYS	2.3
1	K	192	TYR	2.3
2	O	12	VAL	2.3
1	P	165	GLU	2.2
3	B	437	THR	2.2
2	O	111	VAL	2.2
2	R	15	GLY	2.2
3	A	242	LEU	2.2
2	I	165	VAL	2.2
1	K	7	SER	2.2
3	N	240	VAL	2.2
2	O	149	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	1	GLU	2.2
1	F	151	ASP	2.2
3	B	265	ASP	2.2
3	D	331	PRO	2.2
1	K	100	GLN	2.2
2	I	56	TYR	2.2
1	F	60	SER	2.2
2	E	180	VAL	2.2
2	I	108	GLY	2.2
2	H	127	ALA	2.2
1	G	73	LEU	2.2
2	E	209	PRO	2.2
3	B	346	PRO	2.2
3	C	437	THR	2.2
2	E	168	SER	2.2
3	J	367	CYS	2.2
3	N	280	ASP	2.2
1	L	137	ASN	2.2
1	P	27	GLN	2.2
3	D	339	ALA	2.2
3	J	394	THR	2.2
2	M	53	SER	2.2
1	L	207	LYS	2.2
1	G	13	ALA	2.2
1	F	130	ALA	2.2
2	H	26	ASN	2.2
2	O	169	GLY	2.2
3	A	307	THR	2.2
3	A	342	GLN	2.2
3	A	396	PRO	2.2
3	J	273	VAL	2.2
3	J	297	ASN	2.2
2	I	6	GLU	2.2
2	I	18	LEU	2.2
1	F	150	VAL	2.2
1	L	210	ASN	2.2
1	F	113	PRO	2.2
1	Q	211	ARG	2.2
2	O	222	LYS	2.2
2	R	115	SER	2.2
3	J	269	GLU	2.2
1	G	7	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	184	SER	2.2
1	F	122	ASP	2.2
1	P	25	ALA	2.2
2	I	4	LEU	2.2
2	I	209	PRO	2.2
2	I	81	GLN	2.2
2	O	173	THR	2.2
1	K	59	PRO	2.2
3	B	279	VAL	2.2
2	M	91	TYR	2.2
3	D	285	HIS	2.2
2	M	81	GLN	2.2
1	P	94	TYR	2.2
1	K	41	GLY	2.1
1	F	211	ARG	2.1
1	P	212	GLY	2.1
3	B	277	TRP	2.2
3	J	313	TRP	2.2
2	I	188	GLN	2.1
2	O	8	GLY	2.1
3	N	351	LEU	2.1
2	O	140	LEU	2.1
1	L	59	PRO	2.1
3	A	296	TYR	2.1
1	F	2	VAL	2.1
1	Q	138	ASN	2.1
2	M	26	ASN	2.1
1	L	187	GLU	2.1
1	F	33	LEU	2.1
1	Q	82	ASP	2.1
3	D	402	GLY	2.1
1	G	43	ALA	2.1
3	J	325	ASN	2.1
1	Q	181	LEU	2.1
1	P	75	ILE	2.1
3	N	345	GLU	2.1
1	P	162	SER	2.1
3	A	304	SER	2.1
2	H	209	PRO	2.1
1	Q	78	LEU	2.1
3	J	417	TRP	2.1
3	N	334	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	338	LYS	2.1
1	K	60	SER	2.1
1	G	60	SER	2.1
1	L	186	TYR	2.1
1	L	192	TYR	2.1
3	A	358	MET	2.1
3	J	303	VAL	2.1
3	J	404	PHE	2.1
1	K	210	ASN	2.1
3	J	407	TYR	2.1
2	H	103	ASP	2.1
3	D	409	LYS	2.1
1	K	97	THR	2.1
2	M	99	ARG	2.1
3	A	367	CYS	2.1
1	L	120	PRO	2.1
3	N	396	PRO	2.1
1	G	190	LYS	2.1
2	R	150	GLU	2.1
2	M	45	LEU	2.1
1	L	95	SER	2.1
2	R	50	SER	2.1
1	K	68	GLY	2.1
3	N	430	GLU	2.1
1	P	91	TYR	2.1
3	D	281	GLY	2.1
1	L	82	ASP	2.1
2	M	15	GLY	2.1
3	A	290	LYS	2.1
2	M	108	VAL	2.1
2	R	2	VAL	2.1
2	R	6	GLU	2.1
3	B	249	ASP	2.1
2	R	7	SER	2.1
1	Q	17	ASP	2.1
3	C	427	VAL	2.1
2	H	17	SER	2.1
2	O	112	SER	2.1
3	A	423	PHE	2.1
2	M	66	ARG	2.1
2	E	176	SER	2.1
2	R	106	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	R	151	PRO	2.1
3	D	407	TYR	2.1
1	L	107	LYS	2.1
1	P	64	GLY	2.1
2	H	176	SER	2.1
2	M	100	LEU	2.1
3	D	417	TRP	2.1
2	I	210	LYS	2.1
2	O	107	THR	2.0
2	I	98	GLY	2.0
3	C	346	PRO	2.0
3	C	413	ASP	2.0
2	H	162	PHE	2.0
1	P	106	ILE	2.0
3	B	310	HIS	2.0
2	R	16	GLY	2.0
3	C	288	LYS	2.0
3	J	275	PHE	2.0
2	O	179	GLN	2.0
2	H	38	ARG	2.0
2	H	98	GLY	2.0
2	O	13	LYS	2.0
3	N	357	GLU	2.0
1	P	96	ALA	2.0
2	I	170	GLY	2.0
3	N	313	TRP	2.0
2	M	153	THR	2.0
2	H	173	SER	2.0
2	I	69	VAL	2.0
3	A	404	PHE	2.0
2	I	147	THR	2.0
2	E	67	PHE	2.0
3	A	384	ASN	2.0
2	R	45	LEU	2.0
3	A	287	ALA	2.0
3	C	393	THR	2.0
1	Q	199	GLN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.