



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

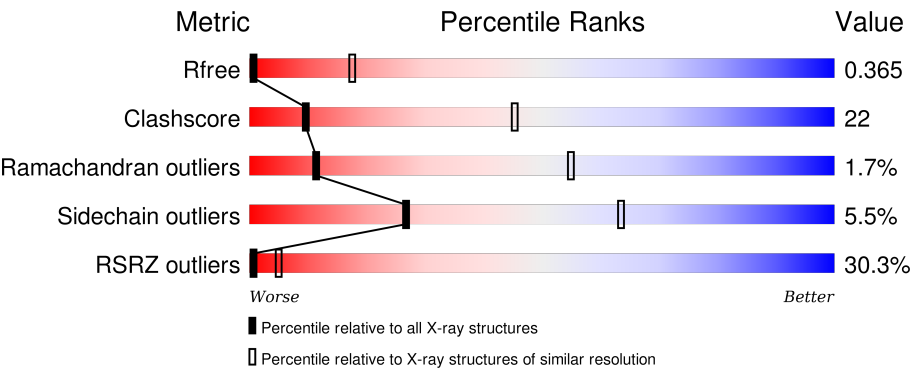
# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	213	<div><div>17%</div><div><div></div><div>81%</div><div>16%</div><div>..</div></div></div>
1	G	213	<div><div>33%</div><div><div></div><div>76%</div><div>21%</div><div>..</div></div></div>
1	K	213	<div><div>30%</div><div><div></div><div>82%</div><div>15%</div><div>..</div></div></div>
1	L	213	<div><div>38%</div><div><div></div><div>77%</div><div>20%</div><div>..</div></div></div>
1	P	213	<div><div>18%</div><div><div></div><div>82%</div><div>15%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	Q	213	
2	E	229	
2	H	229	
2	I	229	
2	M	229	
2	O	229	
2	R	229	
3	A	211	
3	B	211	
3	C	211	
3	D	211	
3	J	211	
3	N	211	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 28972 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2G12 IgG dimer light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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.

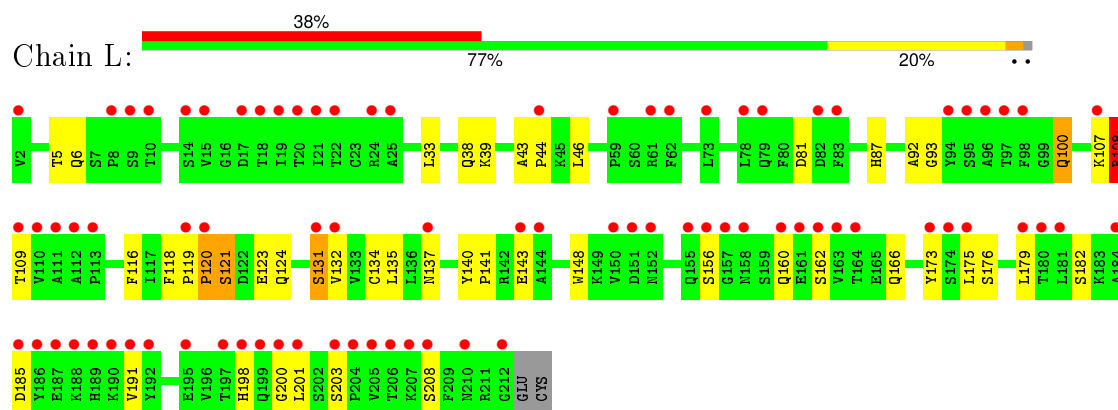
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	B	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	C	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	D	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	J	207	Total	C	N	O	S	0	0	0
			1660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



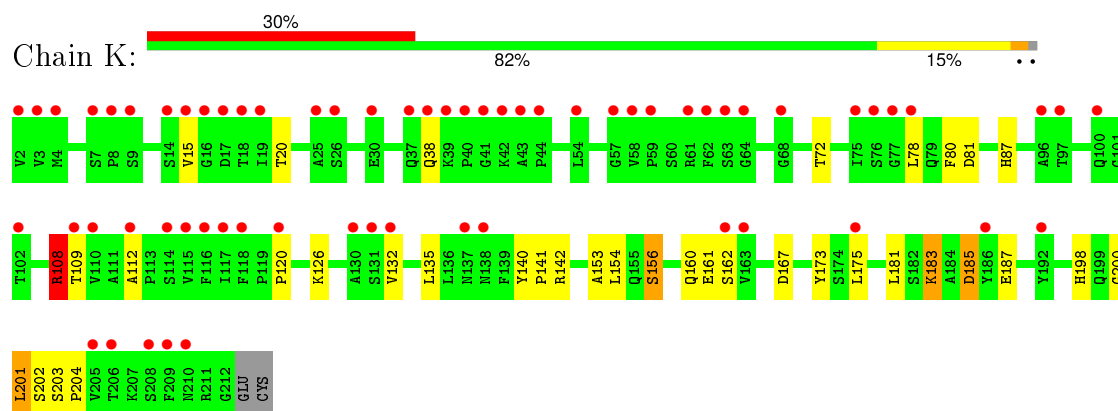
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

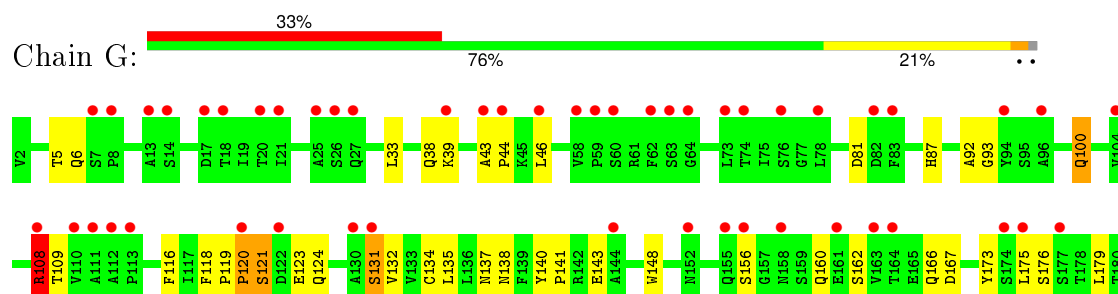
#### • Molecule 1: 2G12 IgG dimer light chain

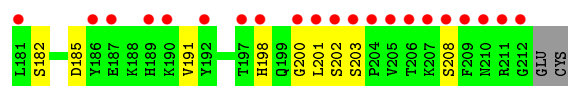


#### • Molecule 1: 2G12 IgG dimer light chain

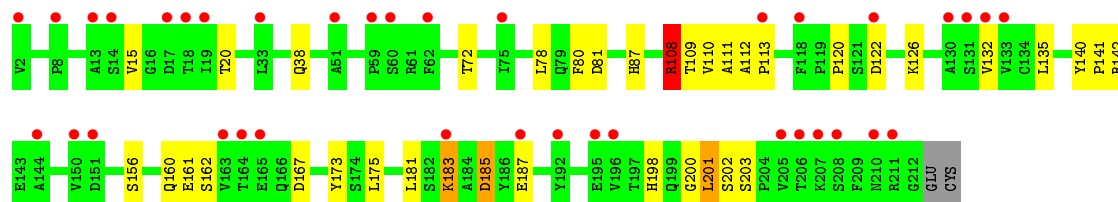
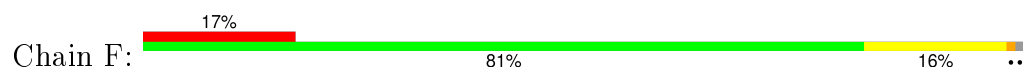


#### • Molecule 1: 2G12 IgG dimer light chain

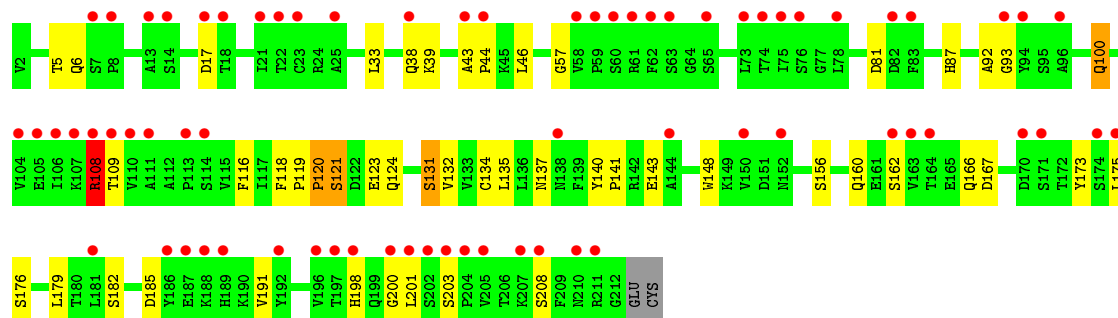
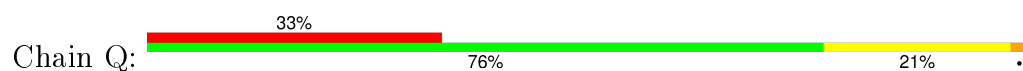




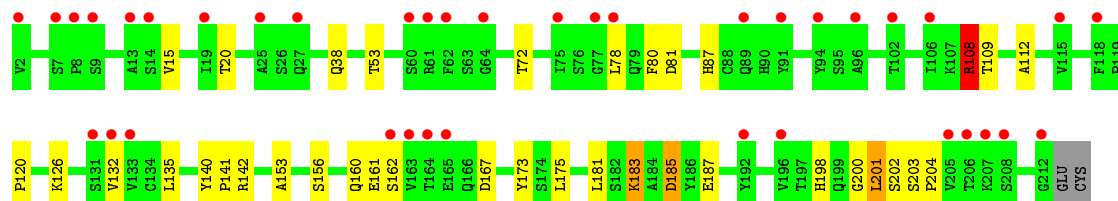
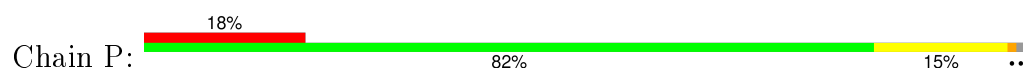
- Molecule 1: 2G12 IgG dimer light chain



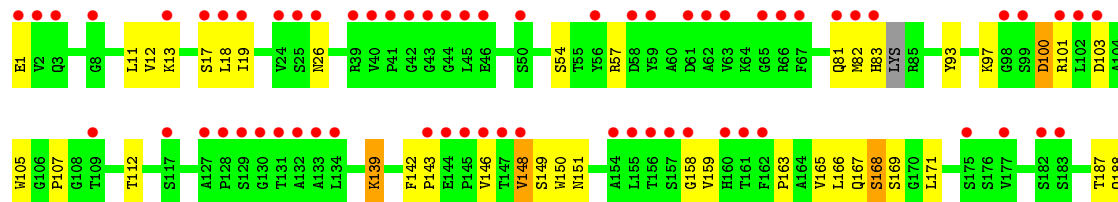
- Molecule 1: 2G12 IgG dimer light chain

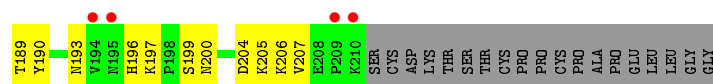


- Molecule 1: 2G12 IgG dimer light chain

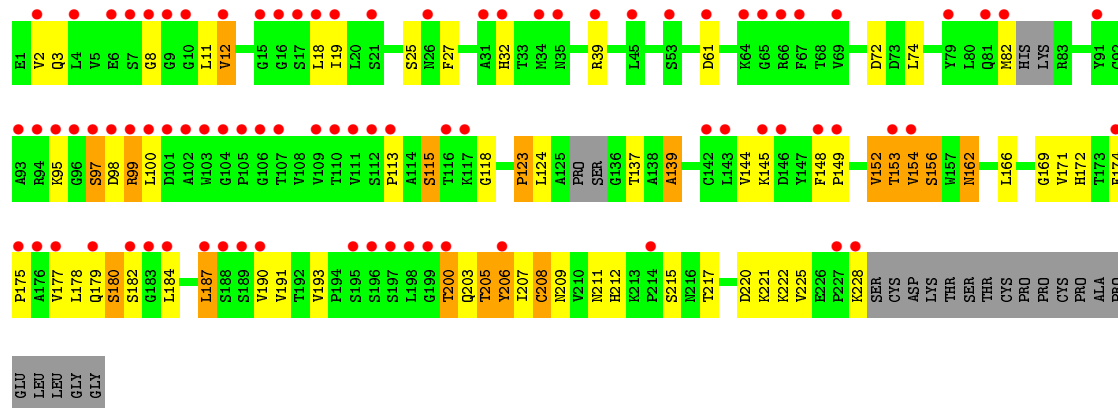
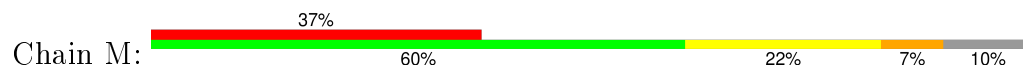


- Molecule 2: Hepatitis B virus receptor binding protein

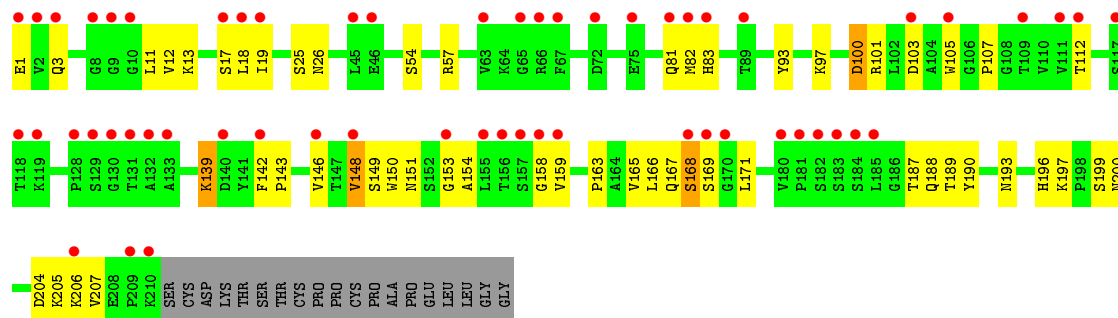




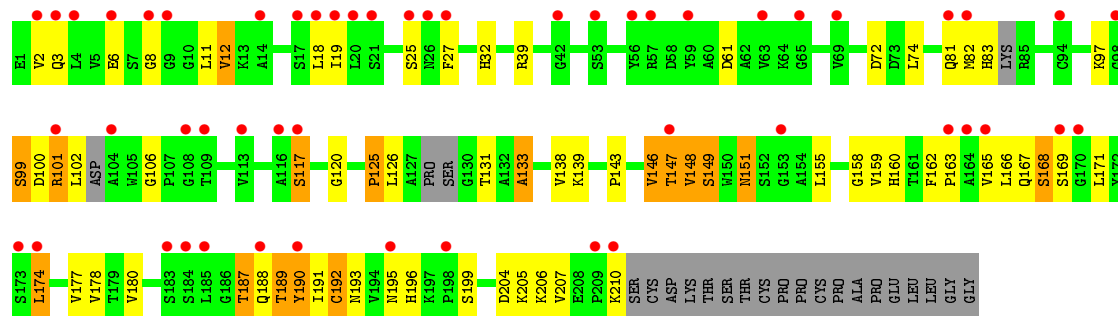
• Molecule 2: Hepatitis B virus receptor binding protein



• Molecule 2: Hepatitis B virus receptor binding protein

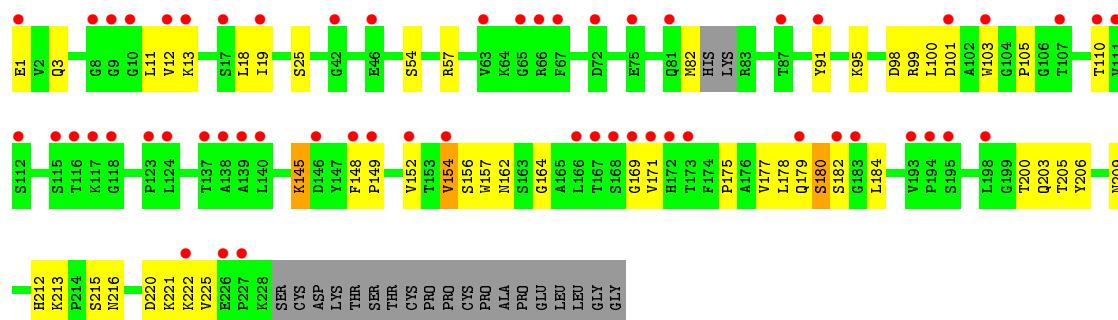


• Molecule 2: Hepatitis B virus receptor binding protein

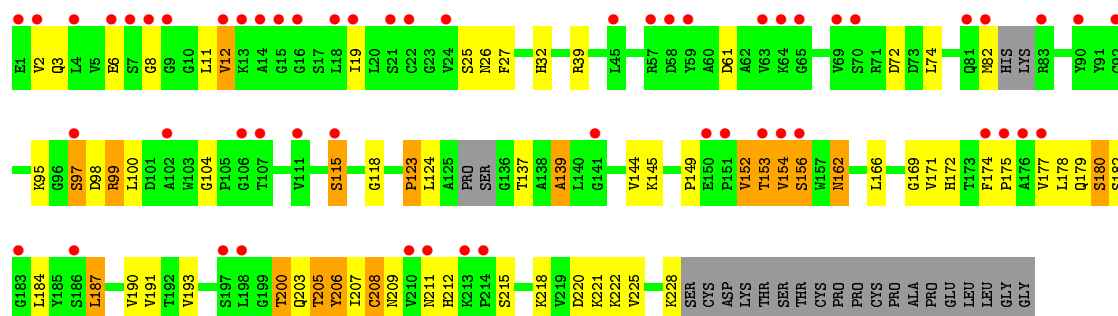


• Molecule 2: Hepatitis B virus receptor binding protein

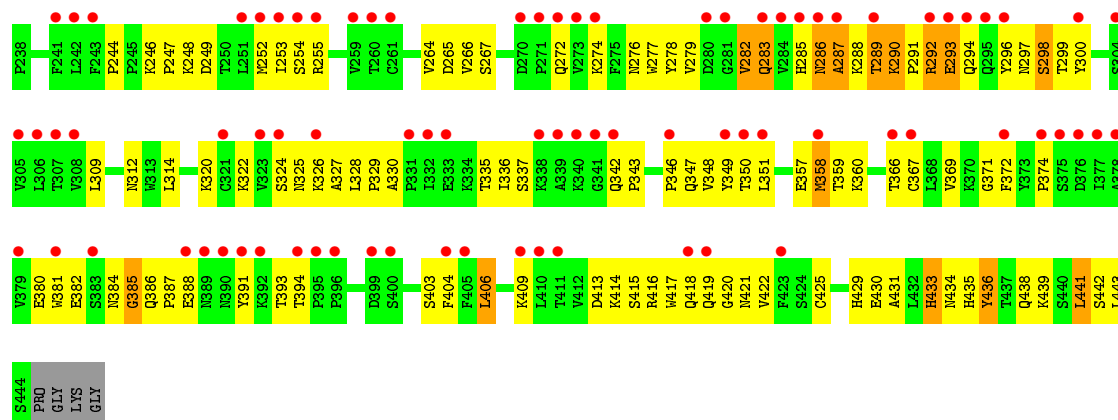
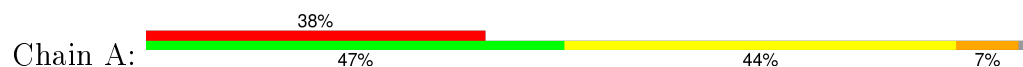




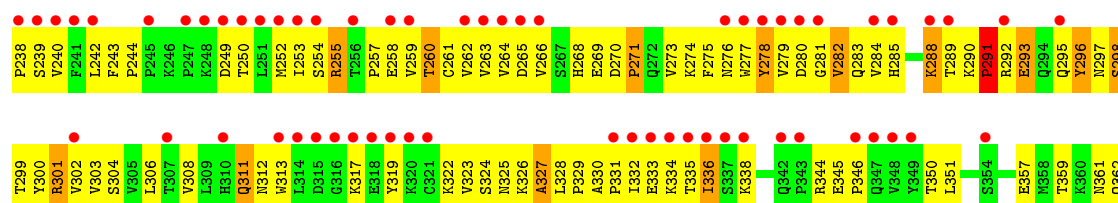
- Molecule 2: Hepatitis B virus receptor binding protein

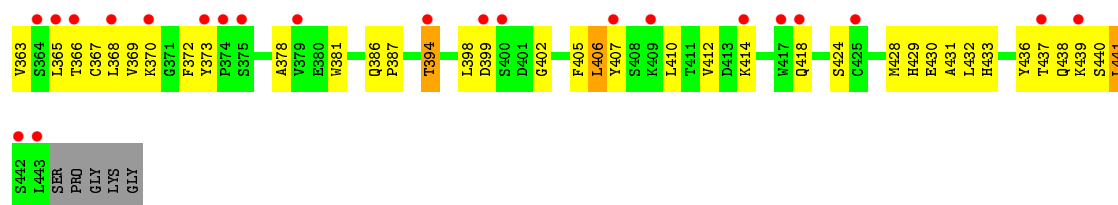


- Molecule 3: 2G12 IgG dimer heavy chain

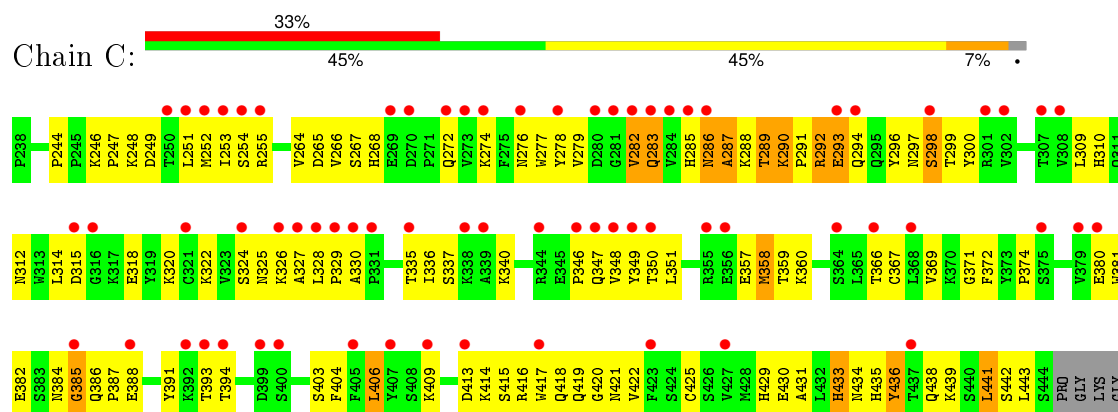


- Molecule 3: 2G12 IgG dimer heavy chain

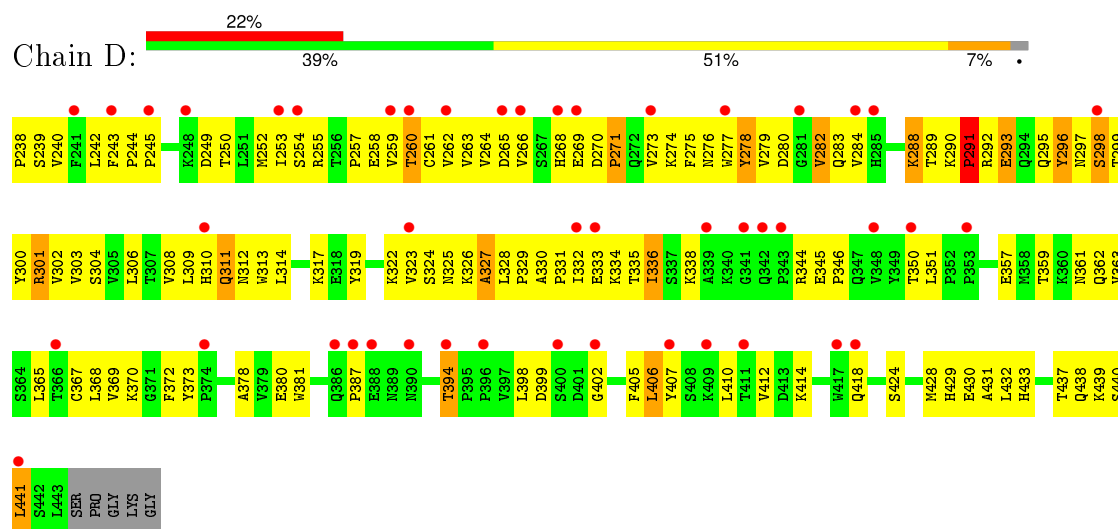




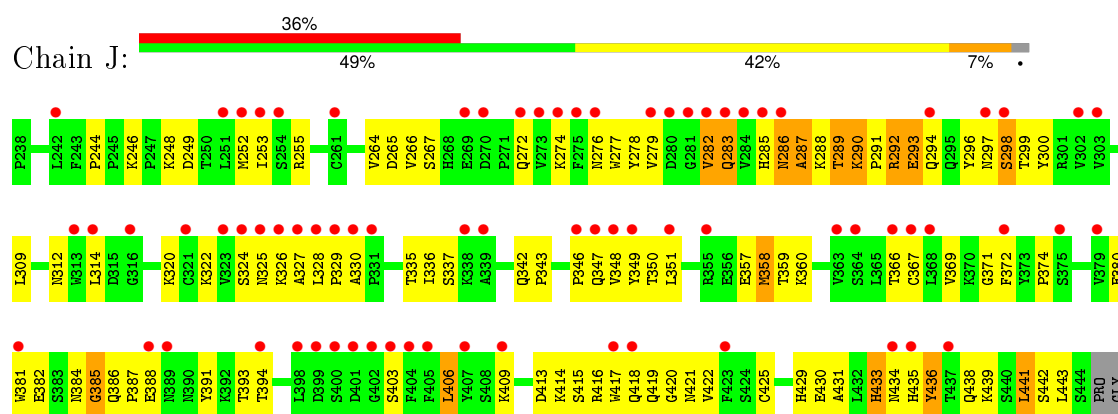
• Molecule 3: 2G12 IgG dimer heavy chain



• Molecule 3: 2G12 IgG dimer heavy chain



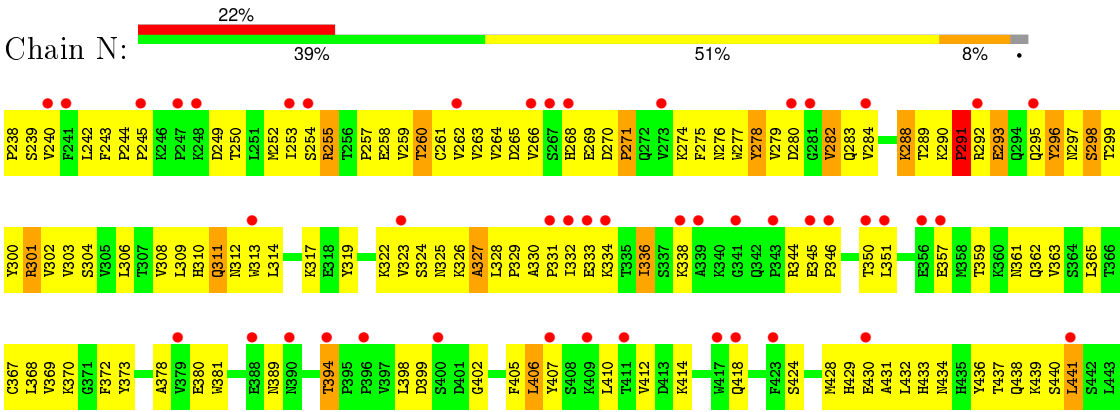
• Molecule 3: 2G12 IgG dimer heavy chain



LYS

GLY

• Molecule 3: 2G12 IgG dimer heavy chain



SER

PRO

GLY

LYS

GLY

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	374.73 Å   374.73 Å   64.45 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	64.91 – 6.50 64.91 – 5.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (64.91-6.50) 99.9 (64.91-5.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 6.17 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.381   ,   0.366 0.379   ,   0.365	Depositor DCC
$R_{free}$ test set	511 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	243.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.14 , 258.7	EDS
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	26 of 13592 reflections (0.191%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	28972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	481.0	wwPDB-VP

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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	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(°)	Ideal(°)
1	F	108	ARG	NE-CZ-NH2	-13.67	113.46	120.30
1	P	108	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	K	108	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	L	108	ARG	NE-CZ-NH2	-12.31	114.15	120.30
1	L	108	ARG	NE-CZ-NH1	12.09	126.34	120.30
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(°)	Ideal(°)
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

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
1:F:201:LEU:HD13	2:O:99:ARG:CG	1.48	1.27
2:I:148:VAL:C	2:I:149:SER:N	1.86	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
1:F:112:ALA:CB	2:O:99:ARG:HG2	1.74	1.14
2:O:11:LEU:HD11	2:R:178:LEU:HD21	1.24	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:F:112:ALA:HB2	2:O:99:ARG:HA	1.22	1.12
1:K:202:SER:HB2	3:A:296:TYR:O	1.47	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
1:P:203:SER:HB2	3:J:298:SER:CB	1.84	1.07
2:I:117:SER:HB2	3:D:282:VAL:HG12	1.30	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
3:C:252:MET:C	3:N:253:ILE:CD1	2.29	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
2:E:166:LEU:HD21	2:I:11:LEU:CD1	1.91	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:C:294:GLN:CG	2:O:1:GLU:O	2.08	0.99
3:B:266:VAL:HB	3:B:300:TYR:HB2	1.44	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
3:C:252:MET:O	3:N:253:ILE:HD13	1.66	0.96
1:K:156:SER:CB	3:B:333:GLU:CD	2.34	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
1:F:201:LEU:HD11	2:O:99:ARG:HD3	0.92	0.91
2:M:115:SER:H	3:B:282:VAL:CG1	1.82	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: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
2:M:115:SER:N	3:B:282:VAL:CG1	2.33	0.89
3:C:282:VAL:O	3:C:283:GLN:HB2	1.72	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
1:K:108:ARG:HD3	1:K:109:THR:O	1.74	0.88
3:J:282:VAL:O	3:J:283:GLN:HB2	1.72	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
2:O:178:LEU:CD2	2:R:11:LEU:HD11	2.01	0.88
1:F:108:ARG:HD3	1:F:109:THR:O	1.74	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
1:F:20:THR:HG23	1:F:72:THR:CG2	2.04	0.87
3:A:282:VAL:O	3:A:283:GLN:HB2	1.72	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
1:P:108:ARG:HD3	1:P:109:THR:O	1.74	0.85
2:E:81:GLN:HE21	2:E:83:HIS:HE1	1.23	0.85
2:E:166:LEU:CD2	2:I:11:LEU:HD11	2.01	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:GLN:HE21	2:H:83:HIS:HE1	1.23	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
3:C:253:ILE:HD13	3:N:310:HIS:NE2	1.93	0.84
2:M:217:THR:OG1	3:B:285:HIS:CD2	2.31	0.84
3:C:253:ILE:HG22	3:N:310:HIS:CE1	2.13	0.83
3:D:328:LEU:HD21	3:D:332:ILE:HG13	1.59	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
1:Q:6:GLN:H	1:Q:100:GLN:HE22	1.27	0.82
3:A:346:PRO:HB3	3:A:372:PHE:HB3	1.60	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
2:H:206:LYS:HA	2:H:207:VAL:N	1.95	0.81
3:B:291:PRO:HB3	3:B:304:SER:HA	1.60	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:314:LEU:HD22	3:J:430:GLU:HG3	1.62	0.81
3:J:346:PRO:HB3	3:J:372:PHE:HB3	1.60	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
1:G:118:PHE:HE1	2:I:133:ALA:O	1.65	0.79
3:A:291:PRO:C	3:A:292:ARG:HD2	2.03	0.79
1:Q:108:ARG:HD3	1:Q:109:THR:O	1.83	0.79
1:G:108:ARG:HD3	1:G:109:THR:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:291:PRO:C	3:J:292:ARG:HD2	2.03	0.78
1:Q:118:PHE:HE1	2:R:139:ALA:O	1.65	0.78
1:L:108:ARG:HD3	1:L:109:THR:O	1.83	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:C:268:HIS:HB3	1:Q:57:GLY:HA2	1.66	0.77
3:B:429:HIS:HD2	3:B:431:ALA:H	1.31	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
3:C:253:ILE:CD1	3:N:310:HIS:HE2	1.98	0.76
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
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:D:328:LEU:HD12	3:D:329:PRO:HD2	1.69	0.74
3:J:292:ARG:O	3:J:293:GLU:HB3	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:365:LEU:HD12	3:B:410:LEU:HD23	1.69	0.74
1:G:198:HIS:CD2	1:G:200:GLY:H	2.04	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:N:266:VAL:HB	3:N:300:TYR:CB	2.16	0.74
3:J:429:HIS:CD2	3:J:431:ALA:H	2.05	0.74
3:A:272:GLN:NE2	3:A:326:LYS:HD2	2.01	0.74
1:F:112:ALA:HB3	2:O:99:ARG:CA	2.03	0.74
3:A:429:HIS:CD2	3:A:431:ALA:H	2.05	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: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:A:422:VAL:HG22	3:A:442:SER:OG	1.92	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:F:112:ALA:CB	2:O:99:ARG:HA	2.01	0.69
3:J:422:VAL:HG22	3:J:442:SER:OG	1.92	0.69
1:G:137:ASN:OD1	2:I:160:HIS:CD2	2.46	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:PRO:O	2:H:196:HIS:HE1	1.75	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: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
3:A:252:MET:HB2	3:A:255:ARG:HG3	1.75	0.69
1:L:137:ASN:OD1	2:M:172:HIS:CD2	2.46	0.68
2:R:145:LYS:HE2	2:R:179:GLN:HE22	1.58	0.68
2:E:143:PRO:O	2:E:196:HIS:HE1	1.75	0.68
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.58	0.68
1:K:112:ALA:HB1	1:K:201:LEU:HD13	1.73	0.68
1:F:110:VAL:CB	2:O:100:LEU:HD12	2.19	0.68
3:C:253:ILE:CG2	3:N:310:HIS:NE2	2.32	0.68
1:G:160:GLN:HB3	2:I:165:VAL:HG11	1.74	0.68
1:F:198:HIS:HD2	1:F:200:GLY:H	1.39	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
2:I:139:LYS:HE2	2:I:167:GLN:HE22	1.58	0.68
2:H:81:GLN:NE2	2:H:83:HIS:HE1	1.91	0.68
3:B:270:ASP:N	3:B:271:PRO:HD3	2.09	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
1:Q:160:GLN:HB3	2:R:177:VAL:HG11	1.74	0.67
3:D:270:ASP:N	3:D:271:PRO:HD3	2.09	0.67
2:E:11:LEU:HD12	2:I:166:LEU:HD21	1.70	0.67
3:C:429:HIS:HD2	3:C:431:ALA:H	1.42	0.67
1:F:112:ALA:HB1	1:F:201:LEU:HD13	1.73	0.67
2:O:11:LEU:HD12	2:R:178:LEU:HD21	1.70	0.67
1:F:20:THR:CG2	1:F:72:THR:HG23	2.24	0.67
1:P:20:THR:CG2	1:P:72:THR:HG23	2.24	0.67
3:J:418:GLN:HA	3:J:443:LEU:CD2	2.24	0.67
3:C:418:GLN:HA	3:C:443:LEU:CD2	2.24	0.66
3:A:418:GLN:HA	3:A:443:LEU:CD2	2.24	0.66
3:A:325:ASN:ND2	3:A:327:ALA:HB3	2.10	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: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:E:12:VAL:HG11	2:E:82:MET:CE	2.26	0.65
1:K:20:THR:CG2	1:K:72:THR:HG23	2.24	0.65
2:H:12:VAL:HG11	2:H:82:MET:CE	2.26	0.65
1:Q:160:GLN:CD	2:R:177:VAL:HG11	2.17	0.65
3:J:325:ASN:ND2	3:J:327:ALA:HB3	2.10	0.65
2:E:11:LEU:HD11	2:I:166:LEU:CG	2.27	0.65
3:A:429:HIS:HD2	3:A:431:ALA:H	1.43	0.65
2:O:11:LEU:HD11	2:R:178:LEU:CG	2.27	0.65
1:P:153:ALA:HA	3:N:330:ALA:HB2	1.77	0.65
1:L:160:GLN:CD	2:M:177:VAL:HG11	2.17	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:D:290:LYS:HE3	3:D:292:ARG:HH22	1.61	0.64
3:A:328:LEU:HG	3:A:330:ALA:O	1.98	0.64
3:J:328:LEU:HG	3:J:330:ALA:O	1.98	0.64
3:D:330:ALA:HB1	3:D:331:PRO:HD2	1.79	0.64
3:N:290:LYS:HE3	3:N:292:ARG:HH22	1.61	0.64
1:G:160:GLN:CD	2:I:165:VAL:HG11	2.17	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: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
1:Q:132:VAL:HG22	1:Q:179:LEU:HB3	1.80	0.64
2:O:12:VAL:HG11	2:O:82:MET:HE3	1.79	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
2:R:154:VAL:C	2:R:156:SER:CA	2.64	0.63
1:G:132:VAL:HG22	1:G:179:LEU:HB3	1.79	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
3:N:330:ALA:HB1	3:N:331:PRO:HD2	1.80	0.63
1:G:162:SER:OG	2:I:163:PRO:HD2	1.99	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
1:Q:100:GLN:H	1:Q:100:GLN:CD	2.02	0.62
2:I:81:GLN:NE2	2:I:83:HIS:HE1	1.98	0.62
3:C:288:LYS:HD2	3:C:288:LYS:H	1.63	0.62
1:Q:118:PHE:CZ	2:R:139:ALA:O	2.52	0.62
1:L:118:PHE:CZ	2:M:139:ALA:O	2.52	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
2:I:12:VAL:HG11	2:I:82:MET:HE3	1.82	0.62
2:R:115:SER:HB2	3:N:282:VAL:HG12	1.81	0.62
1:L:5:THR:HA	1:L:100:GLN:HE22	1.64	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:Q:118:PHE:HB2	2:R:124:LEU:HD22	1.83	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:121:SER:CB	2:R:123:PRO:HD2	2.31	0.60
3:C:435:HIS:CE1	3:N:254:SER:OG	2.53	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: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
3:B:406:LEU:HD12	3:B: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
1:G:121:SER:CB	2:I:125:PRO:HD2	2.32	0.60
3:C:417:TRP:CH2	3:C:441:LEU:HD22	2.37	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: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
3:D:406:LEU:C	3:D:406:LEU:HD12	2.22	0.59
3:D:274:LYS:HE2	3:D:276:ASN:HD21	1.67	0.59
1:L:135:LEU:HD22	2:M:190:VAL:HG21	1.84	0.59
1:L:160:GLN:CD	2:M:177:VAL:CG1	2.70	0.59
3:B:274:LYS:HE2	3:B:276:ASN:HD21	1.67	0.59
1:G:135:LEU:HD22	2:I:177:VAL:HG21	1.84	0.59
2:M:203:GLN:OE1	2:M:205:THR:N	2.36	0.59
2:E:150:TRP:C	2:E:151:ASN:N	2.55	0.59
3:C:433:HIS:ND1	3:C:434:ASN:OD1	2.35	0.59
3:C:417:TRP:HH2	3:C:441:LEU:HD22	1.67	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
2:R:203:GLN:OE1	2:R:205:THR:N	2.36	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
3:C:252:MET:CA	3:N:253:ILE:HG12	2.33	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
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)
1:F:202:SER:O	3:C:297:ASN:O	2.17	0.59
3:B:266:VAL:CB	3:B:300:TYR:HB2	2.28	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
1:G:46:LEU:HD22	2:E:103:ASP:HA	1.84	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
1:L:118:PHE:CD1	2:M:124:LEU:HB3	2.38	0.58
3:A:286:ASN:O	3:A:287:ALA:HB2	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
3:N:269:GLU:O	3:N:269:GLU:HG2	2.03	0.58
1:Q:135:LEU:HD22	2:R:190:VAL:HG21	1.84	0.58
1:Q:118:PHE:CD1	2:R:124:LEU:HB3	2.38	0.58
3:N:279:VAL:HG23	3:N:279:VAL:O	2.03	0.58
3:C:421:ASN:HD22	3:C:421:ASN:N	2.00	0.58
1:L:160:GLN:CB	2:M:177:VAL:HG11	2.33	0.58
1:G:166:GLN:HG3	1:G:173:TYR:CZ	2.39	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
1:Q:46:LEU:HD22	2:O:101:ASP:HA	1.84	0.58
3:N:424:SER:OG	3:N:438:GLN:HG2	2.04	0.58
3:A:433:HIS:ND1	3:A:434:ASN:OD1	2.36	0.58
1:P:183:LYS:O	1:P:187:GLU:HG3	2.04	0.58
3:A:384:ASN:O	3:A:386:GLN:N	2.31	0.58
2:O:145:LYS:HE2	2:O:179:GLN:OE1	2.03	0.58
3:B:279:VAL:HG23	3:B:279:VAL:O	2.04	0.58
1:K:154:LEU:N	3:B:330:ALA:HB3	2.19	0.58
3:D:288:LYS:HE2	3:D:306:LEU:HD11	1.86	0.58
3:D:279:VAL:HG23	3:D:279:VAL:O	2.04	0.57
3:B:296:TYR:CE1	3:B:301:ARG:HD3	2.38	0.57
3:J:415:SER:O	3:J:419:GLN:HG3	2.04	0.57
3:N:257:PRO:HB2	3:N:308:VAL:HB	1.85	0.57
1:L:166:GLN:HG3	1:L:173:TYR:CZ	2.38	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:Q:5:THR:HA	1:Q:100:GLN:NE2	2.19	0.57

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:265:ASP:HA	3:B:299:THR:HB	1.86	0.56
3:D:439:LYS:HE3	3:D:440:SER:O	2.05	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
2:E:158:GLY:O	2:E:159:VAL:N	2.38	0.56
3:C:320:LYS:HG3	3:C:335:THR:HG22	1.87	0.56
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
3:B:288:LYS:HE2	3:B:306:LEU:HD11	1.86	0.56
3:A:328:LEU:HD12	3:A:329:PRO:HD2	1.88	0.56
1:F:203:SER:CB	3:C:298:SER:CA	2.84	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:G:118:PHE:CB	2:I:126:LEU:HD22	2.36	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: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
2:M:166:LEU:HD21	2:M:191:VAL:HG21	1.87	0.56
2:I:155:LEU:HD21	2:I:178:VAL:HG21	1.87	0.56
1:F:38:GLN:NE2	2:I:39:ARG:HD2	2.20	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
1:G:135:LEU:CD2	2:I:177:VAL:HG21	2.36	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
2:O:203:GLN:HB2	2:O:206:TYR:CZ	2.42	0.55
3:N:439:LYS:HE3	3:N:440:SER:O	2.05	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:O:169:GLY:O	2:O:171:VAL:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:118:PHE:CB	2:M:124:LEU:HD22	2.35	0.55
2:H:188:GLN:HB2	2:H:190:TYR:CZ	2.42	0.55
2:E:12:VAL:HG11	2:E:82:MET:HE1	1.89	0.55
2:I:151:ASN:N	2:I:151:ASN:OD1	2.38	0.55
1:F:202:SER:O	3:C:296:TYR:C	2.45	0.55
3:B:325:ASN:ND2	3:B:326:LYS:H	2.04	0.55
1:K:204:PRO:HD3	3:A:297:ASN:HB2	1.88	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
1:K:153:ALA:HB1	3:B:331:PRO:HD2	1.89	0.54
3:A:289:THR:O	3:A:290:LYS:HB2	2.07	0.54
1:F:38:GLN:HE22	2:I:39:ARG:HD2	1.72	0.54
2:O:13:LYS:HD3	2:O:148:PHE:CE1	2.42	0.54
2:E:165:VAL:HG11	1:F:160:GLN:CD	2.27	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
1:P:38:GLN:HE22	2:R:39:ARG:HD2	1.72	0.54
2:I:180:VAL:HG11	2:I:190:TYR:CE1	2.43	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:N:238:PRO:CG	3:N:328:LEU:HD13	2.37	0.54
3:D:238:PRO:CG	3:D:328:LEU:HD13	2.37	0.54
3:J:414:LYS:O	3:J:418:GLN:HG3	2.07	0.54
3:C:414:LYS:HE2	3:C:418:GLN:NE2	2.22	0.54
3:B:275:PHE:HE1	3:B:302:VAL:HG12	1.72	0.54
2:M:193:VAL:HG11	2:M:206:TYR:CE1	2.43	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:A:414:LYS:O	3:A:418:GLN:HG3	2.08	0.54
3:A:414:LYS:HE2	3:A:418:GLN:NE2	2.22	0.54
2:H:13:LYS:HD3	2:H:142:PHE:CE1	2.42	0.54
1:F:15:VAL:HG21	1:F:80:PHE:CZ	2.42	0.54
3:C:253:ILE:HD13	3:N:255:ARG:O	2.08	0.54
3:B:322:LYS:HE3	3:B:333:GLU:OE2	2.08	0.54
3:B:238:PRO:CG	3:B:328:LEU:HD13	2.37	0.54
2:E:13:LYS:HD3	2:E:142:PHE:CE1	2.42	0.54
3:D:322:LYS:HE3	3:D:333:GLU:OE2	2.08	0.54
2:R:193:VAL:HG11	2:R:206:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:240:VAL:O	3:B:334:LYS:HE3	2.08	0.54
3:N:322:LYS:HE3	3:N:333:GLU:OE2	2.08	0.54
2:E:190:TYR:O	2:E:207:VAL:N	2.41	0.54
2:E:206:LYS:CA	2:E:207:VAL:N	2.67	0.54
3:N:240:VAL:O	3:N:334:LYS:HE3	2.08	0.54
3:B:351:LEU:C	3:B:441:LEU:HD11	2.28	0.54
1:P:203:SER:HA	3:J:297:ASN:HB2	1.90	0.54
3:B:262:VAL:HG13	3:B:303:VAL:HG22	1.90	0.54
2:O:222:LYS:CA	2:O:225:VAL:N	2.67	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:I:117:SER:HB2	3:D:282:VAL:HG11	1.85	0.54
3:A:418:GLN:HA	3:A:443:LEU:HD22	1.90	0.54
2:R:149:PRO:O	2:R:212:HIS:HE1	1.92	0.53
1:K:38:GLN:HE22	2:M:39:ARG:HD2	1.72	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:418:GLN:HA	3:C: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
2:H:190:TYR:O	2:H:207:VAL:N	2.41	0.53
2:O:212:HIS:HD2	2:O:215:SER:OG	1.92	0.53
3:D:351:LEU:C	3:D:441:LEU:HD11	2.28	0.53
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.91	0.53
3:C:285:HIS:O	3:C:286:ASN:HB2	2.08	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
3:D:275:PHE:HE1	3:D:302:VAL:HG12	1.72	0.53
2:H:57:ARG:NH1	2:M:72:ASP:OD2	2.37	0.53
2:O:206:TYR:O	2:O:225:VAL:N	2.41	0.53
1:G:93:GLY:O	2:E:97:LYS:HE2	2.09	0.53
2:E:196:HIS:HD2	2:E:199:SER:OG	1.92	0.53
3:D:240:VAL:O	3:D:334:LYS:HE3	2.08	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
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
3:C:351:LEU:HB2	3:C:366:THR:HB	1.90	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:J:285:HIS:O	3:J:286:ASN:HB2	2.09	0.52
2:H:196:HIS:HD2	2:H:199:SER:OG	1.92	0.52
1:L:175:LEU:C	2:M:174:PHE:CE2	2.82	0.52
3:A:351:LEU:HB2	3:A:366:THR:HB	1.90	0.52
1:Q:116:PHE:CG	2:R:139:ALA:HB3	2.44	0.52
1:F:110:VAL:HB	2:O:100:LEU:CD1	2.23	0.52
3:A:393:THR:HG22	3:A:394:THR:O	2.10	0.52
3:N:262:VAL:HG13	3:N:303:VAL:HG22	1.90	0.52
1:G:116:PHE:CG	2:I:133:ALA:HB3	2.44	0.52
1:Q:175:LEU:C	2:R:174:PHE:CE2	2.82	0.52
3:D:312:ASN:ND2	3:D:317:LYS:HD2	2.24	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
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:C:393:THR:HG22	3:C:394:THR:O	2.10	0.52
3:N:297:ASN:O	3:N:298:SER:HB3	2.09	0.52
1:L:175:LEU:CA	2:M:174:PHE:HE2	2.23	0.52
3:J:351:LEU:HB2	3:J:366:THR:HB	1.90	0.52
3:B:297:ASN:O	3:B:298:SER:HB3	2.09	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:B:312:ASN:ND2	3:B:317:LYS:HD2	2.24	0.52
1:Q:121:SER:HB2	2:R:123:PRO:HD2	1.92	0.52
3:C:294:GLN:NE2	2:O:1:GLU:O	2.43	0.52
1:P:120:PRO:HD3	1:P:132:VAL:HG22	1.91	0.52
1:L:44:PRO:HG2	2:H:105:TRP:CE3	2.45	0.52
3:D:378:ALA:HB3	3:D:428:MET:HB2	1.92	0.52
1:L:121:SER:HB2	2:M:123:PRO:HD2	1.92	0.52
3:A:285:HIS:O	3:A:286:ASN:HB2	2.08	0.52
3:D:249:ASP:O	3:D:257:PRO:HG3	2.10	0.52
3:A:436:TYR:C	3:A:436:TYR:CD1	2.84	0.52
3:N:296:TYR:HE1	3:N:301:ARG:HD3	1.74	0.51
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
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
1:G:44:PRO:HG2	2:E:105:TRP:CE3	2.45	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:N:325:ASN:ND2	3:N:326:LYS:N	2.59	0.51
3:D:325:ASN:ND2	3:D:326:LYS:N	2.58	0.51
3:D:289:THR:HG22	3:D:290:LYS:N	2.21	0.51
2:I:196:HIS:CD2	2:I:199:SER:OG	2.64	0.51
3:N:378:ALA:HB3	3:N:428:MET:HB2	1.92	0.51
2:M:212:HIS:CD2	2:M:215:SER:OG	2.64	0.51
3:B:325:ASN:ND2	3:B:326:LYS:N	2.59	0.51
3:J:350:THR:HB	3:J:441:LEU:CG	2.40	0.51
1:G:175:LEU:CA	2:I:162:PHE:HE2	2.23	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:G:198:HIS:HD2	1:G:200:GLY:H	1.53	0.51
1:F:120:PRO:HD3	1:F:132:VAL:HG22	1.91	0.51
3:D:266:VAL:CB	3:D:300:TYR:HB2	2.28	0.51
3:C:283:GLN:C	3:C:285:HIS:N	2.63	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:D:296:TYR:HE1	3:D:301:ARG:HD3	1.74	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
2:E:188:GLN:HA	2:E:189:THR:N	2.24	0.51
3:C:429:HIS:O	3:C:435:HIS:HA	2.11	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
3:A:418:GLN:C	3:A:420:GLY:H	2.15	0.51
2:H:12:VAL:HG11	2:H:82:MET:HE1	1.91	0.51
2:M:203:GLN:O	2:M:205:THR:HA	2.11	0.51
2:M:144:VAL:HG11	2:M:152:VAL:HG11	1.93	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
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:D:261:CYS:HB2	3:D:277:TRP:CZ2	2.47	0.50
3:N:278:TYR:N	3:N:278:TYR:CD1	2.79	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:C:253:ILE:HD12	3:N:310:HIS:CD2	2.47	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:B:291:PRO:HB3	3:B:304:SER:CA	2.37	0.50
3:J:360:LYS:O	3:J:414:LYS:HD2	2.11	0.50
3:C:360:LYS:O	3:C:414:LYS:HD2	2.11	0.50
3:N:261:CYS:HB2	3:N:277:TRP:CZ2	2.47	0.50
3:C:268:HIS:HB3	1:Q:57:GLY:CA	2.39	0.50
3:A:429:HIS:O	3:A:435:HIS:HA	2.11	0.50
1:Q:162:SER:OG	2:R:175:PRO:CD	2.59	0.50
3:C:409:LYS:HB2	3:D:407:TYR:OH	2.12	0.50
3:B:249:ASP:O	3:B:257:PRO:HG3	2.11	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:K:154:LEU:N	3:B:330:ALA:CB	2.70	0.50
3:D:406:LEU:O	3:D:406:LEU:HD12	2.12	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
1:Q:6:GLN:N	1:Q:100:GLN:HE22	2.02	0.50
1:L:124:GLN:NE2	1:L:131:SER:OG	2.40	0.50
1:G:124:GLN:NE2	1:G:131:SER:OG	2.40	0.50
3:C:253:ILE:HD11	3:N:255:ARG:H	1.76	0.50
3:C:380:GLU:O	3:C:425:CYS:HA	2.12	0.50
3:A:283:GLN:C	3:A:285:HIS:N	2.62	0.50
3:C:418:GLN:C	3:C:420:GLY:H	2.15	0.50
3:A:246:LYS:HB2	3:A:249:ASP:OD2	2.12	0.50
3:C:253:ILE:HB	3:N:310:HIS:CD2	2.47	0.50
3:C:294:GLN:O	3:C:300:TYR:CD1	2.65	0.50
3:J:429:HIS:O	3:J:435:HIS:HA	2.11	0.50
3:J:380:GLU:O	3:J:425:CYS:HA	2.12	0.50
3:A:409:LYS:HB2	3:B:407:TYR:OH	2.12	0.50
3:D:250:THR:HG22	3:D:257:PRO:HB3	1.94	0.50
3:B:250:THR:HG22	3:B:257:PRO:HB3	1.94	0.50
3:A:294:GLN:O	3:A:300:TYR:CD1	2.65	0.50
1:G:121:SER:HB2	2:I:125:PRO:HD2	1.92	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:N:250:THR:HG22	3:N:257:PRO:HB3	1.94	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: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:B:289:THR:HG22	3:B:290:LYS:N	2.21	0.49
3:B:278:TYR:N	3:B:278:TYR:CD1	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:380:GLU:O	3:A:425:CYS:HA	2.12	0.49
3:A:357:GLU:C	3:A:359:THR:H	2.15	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:N:332:ILE:CG2	3:N:333:GLU:N	2.74	0.49
3:B:292:ARG:O	3:B:293:GLU:HB3	2.12	0.49
2:O:203:GLN:O	2:O:205:THR:HA	2.13	0.49
3:A:360:LYS:O	3:A:414:LYS:HD2	2.11	0.49
3:A:350:THR:HB	3:A:441:LEU:CG	2.40	0.49
3:J:294:GLN:O	3:J:300:TYR:CD1	2.65	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:C:266:VAL:O	3:C:300:TYR:HB2	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:D:249:ASP:C	3:D:257:PRO:HG3	2.32	0.49
3:C:246:LYS:HB2	3:C:249:ASP:OD2	2.12	0.49
3:J:409:LYS:HB2	3:N:407:TYR:OH	2.12	0.49
3:B:369:VAL:O	3:B:405:PHE:HA	2.12	0.49
3:J:277:TRP:O	3:J:283:GLN:HB3	2.13	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:D:398:LEU:HD11	3:D:402:GLY:HA2	1.95	0.49
3:C:277:TRP:O	3:C:283:GLN:HB3	2.13	0.49
3:J:278:TYR:HB2	3:J:320:LYS:HB3	1.95	0.49
3:A:248:LYS:O	3:A:255:ARG:HD3	2.13	0.49
3:B:406:LEU:HD12	3:B:406:LEU:O	2.12	0.49
3:A:266:VAL:O	3:A:300:TYR:HB2	2.13	0.49
3:J:266:VAL:O	3:J:300:TYR:HB2	2.13	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
2:E:188:GLN:O	2:E:189:THR:HA	2.12	0.48
3:A:384:ASN:OD1	3:A:385:GLY:N	2.41	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
2:O:11:LEU:HD11	2:R:178:LEU:HD11	1.95	0.48
3:C:283:GLN:CD	3:C:287:ALA:HB2	2.34	0.48
3:C:278:TYR:HB2	3:C:320:LYS:HB3	1.94	0.48
3:N:398:LEU:HD11	3:N:402:GLY:HA2	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
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:N:259:VAL:HG23	3:N:308:VAL:CG2	2.43	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:C:248:LYS:O	3:C:255:ARG:HD3	2.13	0.48
3:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	0.48
1:F:108:ARG:HD2	1:F:140:TYR:CB	2.43	0.48
3:C:346:PRO:CB	3:C:372:PHE:HB3	2.39	0.48
3:J:346:PRO:CB	3:J:372:PHE:HB3	2.39	0.48
3:J:248:LYS:O	3:J:255:ARG:HD3	2.13	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:J:358:MET:O	3:J:414:LYS:HE3	2.14	0.48
3:D:259:VAL:HG23	3:D:308:VAL:CG2	2.43	0.48
3:B:259:VAL:HG23	3:B:308:VAL:CG2	2.43	0.48
1:K:156:SER:HB3	3:B:333:GLU:CD	2.22	0.48
1:G:176:SER:N	2:I:162:PHE:CE2	2.81	0.48
2:R:118:GLY:HA2	2:R:212:HIS:HD2	1.77	0.48
3:D:350:THR:HB	3:D:441:LEU:HG	1.95	0.48
2:E:57:ARG:NH1	2:I:72:ASP:OD2	2.37	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:C:252:MET:CA	3:N:253:ILE:HD13	2.36	0.48
2:H:57:ARG:HH22	2:M: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
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:C:253:ILE:CG2	3:N:310:HIS:CG	2.96	0.47
1:L:6:GLN:N	1:L:100:GLN:HE22	2.02	0.47
1:G:162:SER:OG	2:I:163:PRO:O	2.28	0.47
3:B:368:LEU:HD12	3:B:369:VAL:H	1.79	0.47
2:H:188:GLN:O	2:H:189:THR:HA	2.13	0.47
3:A:292:ARG:O	3:A:293:GLU:CB	2.58	0.47
3:J:414:LYS:HG2	3:J:418:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:350:THR:HB	3:N:441:LEU:HG	1.95	0.47
3:D:368:LEU:HD12	3:D:369:VAL:H	1.79	0.47
2:M:2:VAL:HG13	2:M:27:PHE:CD2	2.49	0.47
3:A:388:GLU:OE2	3:A:416:ARG:NH2	2.42	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:B:244:PRO:HB3	3:B:336:ILE:HD11	1.95	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
2:M:212:HIS:HD2	2:M:215:SER:OG	1.97	0.47
3:J:384:ASN:OD1	3:J:385:GLY:N	2.41	0.47
3:C:289:THR:CG2	3:C:290:LYS:N	2.78	0.47
2:M:118:GLY:HA2	2:M:212:HIS:HD2	1.77	0.47
3:A:414:LYS:HG2	3:A:418:GLN:NE2	2.29	0.47
3:C:414:LYS:HG2	3:C:418:GLN:NE2	2.29	0.47
1:G:176:SER:HB3	2:I:162:PHE:CD1	2.50	0.47
3:C:384:ASN:OD1	3:C:385:GLY:N	2.41	0.47
3:D:275:PHE:HZ	3:D:302:VAL:O	1.98	0.47
3:D:312:ASN:HB3	3:D:319:TYR:OH	2.14	0.47
3:N:432:LEU:HD22	3:N:437:THR:HB	1.97	0.47
3:N:368:LEU:HD12	3:N:369:VAL:H	1.80	0.47
2:M:32:HIS:HD2	2:M:95:LYS:O	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: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
2:I:196:HIS:HD2	2:I:199:SER:OG	1.97	0.47
3:N:312:ASN:HB3	3:N:319:TYR:OH	2.14	0.47
3:B:432:LEU:HD22	3:B:437:THR:HB	1.97	0.47
3:A:388:GLU:HA	3:A:388:GLU:OE1	2.14	0.47
2:R:208:CYS:SG	2:R:221:LYS:HB3	2.55	0.47
3:J:388:GLU:OE1	3:J:388:GLU:HA	2.14	0.47
3:B:278:TYR:CE2	3:B:284:VAL:HG22	2.50	0.47
3:N:275:PHE:HZ	3:N:302:VAL:O	1.97	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:D:278:TYR:CE2	3:D:284:VAL:HG22	2.50	0.47
3:B:261:CYS:HB2	3:B:277:TRP:CH2	2.50	0.47
1:K:154:LEU:H	3:B:330:ALA:HB3	1.77	0.46
3:C:288:LYS:CD	3:C:288:LYS:H	2.27	0.46
3:N:291:PRO:CB	3:N:304:SER:HA	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:212:HIS:HD2	2:R:215:SER:OG	1.97	0.46
3:N:261:CYS:HB2	3:N:277:TRP:CH2	2.50	0.46
3:C:438:GLN:O	3:C:439:LYS:HD3	2.15	0.46
2:I:32:HIS:HD2	2:I:97:LYS:O	1.97	0.46
3:C:388:GLU:HA	3:C:388:GLU:OE1	2.14	0.46
1:P:202:SER:HB2	3:J:296:TYR:O	2.14	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:P:153:ALA:CB	3:N:330:ALA:HB1	2.45	0.46
1:L:6:GLN:H	1:L:100:GLN:NE2	2.03	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:A:371:GLY:HA2	3:A:403:SER:OG	2.15	0.46
3:N:322:LYS:HG3	3:N:333:GLU:HG2	1.97	0.46
2:E:18:LEU:N	2:E:82:MET:HE2	2.30	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
3:J:286:ASN:O	3:J:287:ALA:CB	2.63	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
1:Q:176:SER:HB3	2:R:174:PHE:CD1	2.50	0.46
3:D:361:ASN:ND2	3:D:362:GLN:HG3	2.31	0.46
3:N:300:TYR:O	3:N:301:ARG:HB2	2.16	0.46
3:B:311:GLN:N	3:B:311:GLN:NE2	2.53	0.46
3:D:311:GLN:NE2	3:D:311:GLN:N	2.53	0.46
3:N:279:VAL:O	3:N:282:VAL:HG22	2.15	0.46
3:B:344:ARG:O	3:B:372:PHE:HA	2.16	0.46
3:B:275:PHE:HZ	3:B:302:VAL:O	1.98	0.46
2:M:208:CYS:SG	2:M:221:LYS:HB3	2.55	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:N:344:ARG:O	3:N:372:PHE:HA	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
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:D:279:VAL:O	3:D:282:VAL:HG22	2.15	0.46
3:A:346:PRO:CB	3:A:372:PHE:HB3	2.39	0.46
2:O:12:VAL:HG11	2:O:82:MET:HE1	1.98	0.46
3:N:406:LEU:CD1	3:N:406:LEU:C	2.85	0.46
3:D:242:LEU:HD13	3:D:336:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:99:SER:C	2:I:101:ARG:H	2.19	0.46
3:B:279:VAL:O	3:B:282:VAL:HG22	2.15	0.46
3:A:296:TYR:HB3	3:A:297:ASN:H	1.56	0.46
3:D:300:TYR:O	3:D:301:ARG:HB2	2.16	0.46
1:P:153:ALA:CB	3:N:330:ALA:CB	2.94	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
3:A:265:ASP:HA	3:A:299:THR:HB	1.98	0.46
1:L:121:SER:CB	1:L:121:SER:HG	2.17	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
3:N:279:VAL:O	3:N:280:ASP:HB2	2.16	0.45
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	0.45
3:N:439:LYS:HA	3:N:439:LYS:HD2	1.81	0.45
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:N:361:ASN:ND2	3:N:362:GLN:HG3	2.31	0.45
3:C:253:ILE:CB	3:N:310:HIS:CD2	3.00	0.45
3:J:296:TYR:HB3	3:J:297:ASN:H	1.56	0.45
2:H:11:LEU:HD21	2:M:179:GLN:O	2.16	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
1:F:141:PRO:O	1:F:198:HIS:HE1	2.00	0.45
3:D:406:LEU:C	3:D:406:LEU:CD1	2.84	0.45
1:L:176:SER:HB3	2:M:174:PHE:CD1	2.50	0.45
3:A:421:ASN:ND2	3:A:421:ASN:N	2.64	0.45
2:M:97:SER:C	2:M:99:ARG:H	2.19	0.45
1:Q:121:SER:HG	1:Q:121:SER:CB	2.17	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:G:118:PHE:CG	2:I:126:LEU:HB3	2.52	0.45
3:A:286:ASN:O	3:A:287:ALA:CB	2.63	0.45
3:D:326:LYS:C	3:D:328:LEU:H	2.20	0.45
3:C:374:PRO:O	3:C:429:HIS:HE1	2.00	0.45
1:K:141:PRO:O	1:K:198:HIS:HE1	2.00	0.45
3:D:308:VAL:HG11	3:D:313:TRP:HB2	1.97	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
2:I:192:CYS:SG	2:I:205:LYS:HB3	2.55	0.45
3:C:292:ARG:O	3:C:293:GLU:CB	2.58	0.45
3:C:265:ASP:HA	3:C:299:THR:HB	1.98	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:C:278:TYR:CD1	3:C:278:TYR:N	2.85	0.45
3:N:238:PRO:CB	3:N:328:LEU:HD13	2.47	0.45
1:G:92:ALA:O	2:E:97:LYS:CE	2.64	0.45
3:D:345:GLU:HA	3:D:431:ALA:HB3	1.99	0.45
3:J:374:PRO:O	3:J:429:HIS:HE1	2.00	0.45
3:D:269:GLU:C	3:D:271:PRO:HD3	2.36	0.45
2:M:18:LEU:HB2	2:M:82:MET:HE1	1.99	0.45
3:B:361:ASN:ND2	3:B:362:GLN:HG3	2.31	0.45
3:J:278:TYR:CD1	3:J:278:TYR:N	2.85	0.45
3:D:238:PRO:CB	3:D:328:LEU:HD13	2.47	0.45
3:B:323:VAL:HG12	3:B:324:SER:N	2.32	0.45
3:B:300:TYR:O	3:B:301:ARG:CB	2.64	0.45
1:Q:118:PHE:CG	2:R:124:LEU:HB3	2.52	0.45
3:B:406:LEU:C	3:B:406:LEU:CD1	2.84	0.45
2:M:200:THR:HB	2:M:203:GLN:N	2.32	0.45
3:D:432:LEU:HD11	3:D:437:THR:HG22	1.98	0.45
3:B:238:PRO:CB	3:B:328:LEU:HD13	2.47	0.45
3:D:279:VAL:O	3:D:280:ASP:HB2	2.17	0.45
3:B:301:ARG:HG2	3:B:303:VAL:HG23	1.99	0.45
3:D:300:TYR:O	3:D:301:ARG:CB	2.65	0.45
1:Q:116:PHE:CG	2:R:139:ALA:CB	3.00	0.45
1:L:92:ALA:O	2:H:97:LYS:CE	2.64	0.45
3:B:269:GLU:C	3:B:271:PRO:HD3	2.36	0.45
2:H:165:VAL:CG1	1:K:160:GLN:CD	2.86	0.45
3:A:244:PRO:HB3	3:A:336:ILE:HD13	1.99	0.45
3:C:244:PRO:HB3	3:C:336:ILE:HD13	1.99	0.45
3:D:323:VAL:HG12	3:D:324:SER:N	2.32	0.45
1:P:204:PRO:HD3	3:J:297:ASN:HB2	1.99	0.45
3:D:301:ARG:HG2	3:D:303:VAL:HG23	1.99	0.45
3:D:290:LYS:HE3	3:D:292:ARG:HH12	1.82	0.45
3:J:292:ARG:O	3:J:293:GLU:CB	2.58	0.45
3:J:421:ASN:N	3:J:421:ASN:ND2	2.64	0.45
3:B:265:ASP:HA	3:B:299:THR:CB	2.47	0.45
3:J:388:GLU:OE2	3:J:416:ARG:NH2	2.42	0.45
2:E:19:ILE:HD13	2:I:19:ILE:O	2.16	0.45
3:N:300:TYR:O	3:N:301:ARG:CB	2.65	0.44
3:N:326:LYS:C	3:N:328:LEU:H	2.20	0.44
3:J:266:VAL:HB	3:J:300:TYR:HB2	1.98	0.44
2:E:163:PRO:HD2	1:F:162:SER:OG	2.16	0.44
3:C:347:GLN:NE2	3:C:349:TYR:OH	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:265:ASP:HA	3:J:299:THR:HB	1.98	0.44
1:F:112:ALA:HB3	2:O:99:ARG:HB3	0.48	0.44
2:O:11:LEU:HD21	2:R:179:GLN:O	2.17	0.44
3:D:296:TYR:HB3	3:D:297:ASN:H	1.34	0.44
1:P:153:ALA:CA	3:N:330:ALA:HB2	2.45	0.44
2:R:115:SER:H	3:N:282:VAL:HG12	1.82	0.44
1:P:141:PRO:O	1:P:198:HIS:HE1	2.00	0.44
3:B:239:SER:HB3	3:B:264:VAL:CG2	2.48	0.44
3:C:296:TYR:HB3	3:C:297:ASN:H	1.56	0.44
3:B:326:LYS:C	3:B:328:LEU:H	2.20	0.44
3:N:311:GLN:N	3:N:311:GLN:NE2	2.53	0.44
1:G:116:PHE:CG	2:I:133:ALA:CB	3.00	0.44
3:N:290:LYS:HE3	3:N:292:ARG:HH12	1.82	0.44
3:A:291:PRO:O	3:A:292:ARG:HD2	2.17	0.44
3:N:265:ASP:HA	3:N:299:THR:CB	2.47	0.44
2:O:177:VAL:CG1	1:P:160:GLN:CD	2.86	0.44
2:H:19:ILE:HD13	2:M:19:ILE:O	2.16	0.44
2:E:11:LEU:HD21	2:I:167:GLN:O	2.16	0.44
3:C:266:VAL:HB	3:C:300:TYR:HB2	1.98	0.44
1:L:118:PHE:CG	2:M:124:LEU:HB3	2.52	0.44
2:H:18:LEU:N	2:H:82:MET:HE2	2.32	0.44
2:R:200:THR:HB	2:R:203:GLN:N	2.32	0.44
3:B:258:GLU:HA	3:B:308:VAL:HG23	1.99	0.44
3:N:242:LEU:HD13	3:N:336:ILE:HG22	1.97	0.44
3:B:296:TYR:HB3	3:B:297:ASN:H	1.34	0.44
3:J:288:LYS:H	3:J:288:LYS:CD	2.27	0.44
3:A:278:TYR:N	3:A:278:TYR:CD1	2.85	0.44
3:D:258:GLU:HA	3:D:308:VAL:HG23	1.99	0.44
3:N:239:SER:HB3	3:N:264:VAL:CG2	2.47	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:J:347:GLN:NE2	3:J:349:TYR:OH	2.50	0.44
3:D:239:SER:HB3	3:D: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
2:I:18:LEU:HB2	2:I:82:MET:HE1	1.99	0.44
3:D:439:LYS:HD2	3:D:439:LYS:HA	1.82	0.44
2:R:206:TYR:O	2:R:225:VAL:N	2.51	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
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)
3:C:436:TYR:CD2	3:N:434:ASN:OD1	2.71	0.44
2:I:187:THR:HB	2:I:188:GLN:N	2.32	0.44
3:N:258:GLU:HA	3:N:308:VAL:HG23	1.99	0.44
2:E:165:VAL:CG1	1:F:160:GLN:CD	2.86	0.44
2:I:190:TYR:O	2:I:207:VAL:N	2.51	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
2:M:115:SER:HB2	3:B:282:VAL:HG11	1.58	0.43
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
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
1:L:116:PHE:CG	2:M:139:ALA:CB	3.00	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
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
3:C:294:GLN:HG3	2:O:1:GLU:HB2	1.65	0.43
1:Q:160:GLN:NE2	2:R:177:VAL:HG12	2.31	0.43
3:A:348:VAL:O	3:A:439:LYS:HG3	2.19	0.43
2:E:19:ILE:CD1	2:I:19:ILE:O	2.67	0.43
3:C:293:GLU:OE1	2:O:1:GLU:CG	2.66	0.43
3:N:301:ARG:HG2	3:N:303:VAL:HG23	1.99	0.43
3:C:278:TYR:HA	3:C:282:VAL:O	2.18	0.43
3:J:278:TYR:HA	3:J:282:VAL:O	2.18	0.43
3:C:388:GLU:OE2	3:C:416:ARG:NH2	2.42	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:A:347:GLN:NE2	3:A:349:TYR:OH	2.51	0.43
1:P:142:ARG:HD3	1:P:173:TYR:CE2	2.54	0.43
1:F:113:PRO:O	2:O:99:ARG:HD2	2.17	0.43
3:B:266:VAL:HB	3:B:300:TYR:CD2	2.54	0.43
3:N:296:TYR:HB3	3:N:297:ASN:H	1.34	0.43
3:B:386:GLN:HA	3:B:387:PRO:HD3	1.76	0.43
2:O:11:LEU:HD11	2:R:178:LEU:CD1	2.49	0.43
3:C:436:TYR:CE1	3:N:436:TYR:O	2.72	0.43
3:C:282:VAL:O	3:C:283:GLN:CB	2.52	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:287:ALA:O	3:C:288:LYS:C	2.56	0.43
2:M:206:TYR:O	2:M:225:VAL:N	2.51	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
3:D:338:LYS:NZ	3:D:430:GLU:OE2	2.52	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:C:253:ILE:CD1	3:N:310:HIS:CD2	3.02	0.43
2:M:115:SER:H	3:B:282:VAL:CB	2.30	0.43
2:H:11:LEU:HD11	2:M:178:LEU:CD1	2.49	0.43
3:B:290:LYS:HE3	3:B:292:ARG:HH12	1.82	0.43
3:D:368:LEU:HD12	3:D:369:VAL:N	2.34	0.43
3:N:238:PRO:HB2	3:N:328:LEU:HD13	2.01	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
2:R:222:LYS:HA	2:R:225:VAL:N	2.34	0.43
2:O:19:ILE:CD1	2:R:19:ILE:O	2.67	0.43
2:I:192:CYS:SG	2:I:192:CYS:O	2.77	0.43
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:C:391:TYR:CD2	3:C:391:TYR:C	2.92	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
3:C:328:LEU:HA	3:C:329:PRO:HD3	1.94	0.42
2:M:222:LYS:HA	2:M:225:VAL:N	2.34	0.42
1:K:15:VAL:HG21	1:K:80:PHE:CE2	2.54	0.42
3:B:368:LEU:HD12	3:B:369:VAL:N	2.34	0.42
3:J:287:ALA:O	3:J:288:LYS:C	2.56	0.42
1:Q:108:ARG:HD2	1:Q:140:TYR:CB	2.50	0.42
3:D:278:TYR:HE2	3:D:284:VAL:HG22	1.83	0.42
3:N:368:LEU:HD12	3:N:369:VAL:N	2.34	0.42
2:E:11:LEU:HD11	2:I:166:LEU:CD1	2.49	0.42
1:K:156:SER:HB2	3:B:333:GLU:CD	2.18	0.42
3:N:266:VAL:HB	3:N:300:TYR:CD2	2.54	0.42
3:C:283:GLN:C	3:C:285:HIS:H	2.23	0.42
1:K:38:GLN:OE1	1:K:87:HIS:HE1	2.03	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
3:B:414:LYS:O	3:B:418:GLN:HG3	2.19	0.42
3:N:357:GLU:C	3:N:359:THR:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:GLN:NE2	2:E:93:TYR:OH	2.48	0.42
3:A:391:TYR:CD2	3:A:391:TYR:C	2.92	0.42
1:P:153:ALA:HB1	3:N:330:ALA:HB1	2.02	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
3:D:266:VAL:HB	3:D:300:TYR:CD2	2.54	0.42
3:C:433:HIS:CE1	3:N:380:GLU:OE1	2.73	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:P:15:VAL:HG21	1:P:80:PHE:CE2	2.54	0.42
1:F:15:VAL:HG21	1:F: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
2:H:19:ILE:CD1	2:M:8:GLY:HA3	2.49	0.42
1:F:142:ARG:HD3	1:F:173:TYR:CE2	2.54	0.42
1:K:161:GLU:HG2	1:K:175:LEU:HD21	2.01	0.42
3:B:357:GLU:C	3:B:359:THR:H	2.23	0.42
3:N:291:PRO:O	3:N:292:ARG:HB3	2.19	0.42
3:D:291:PRO:O	3:D:292:ARG:HB3	2.19	0.42
2:R:12:VAL:HG11	2:R:82:MET:HE1	1.99	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
2:M:3:GLN:HB2	2:M:25:SER:HB2	2.02	0.42
1:K:142:ARG:HD3	1:K:173:TYR:CE2	2.54	0.42
3:B:291:PRO:O	3:B:292:ARG:HB3	2.19	0.42
1:L:100:GLN:CD	1:L:100:GLN:N	2.71	0.42
1:G:141:PRO:O	1:G:198:HIS:HE1	2.02	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:B:338:LYS:NZ	3:B:430:GLU:OE2	2.52	0.42
3:J:391:TYR:CD2	3:J:391:TYR:C	2.93	0.42
3:B:238:PRO:HB2	3:B:328:LEU:HD13	2.01	0.42
1:K:108:ARG:HD2	1:K:140:TYR:CG	2.55	0.42
3:C:372:PHE:O	3:C:404:PHE:N	2.44	0.42
1:Q:141:PRO:O	1:Q:198:HIS:HE1	2.02	0.42
3:A:328:LEU:HD12	3:A:329:PRO:CD	2.50	0.42
3:D:350:THR:HB	3:D:441:LEU:CD1	2.50	0.42
3:A:367:CYS:HB2	3:A:381:TRP:CH2	2.55	0.42
1:F:20:THR:CG2	1:F:72:THR:CG2	2.86	0.41
3:A:283:GLN:C	3:A:285:HIS:H	2.23	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
3:J:348:VAL:O	3:J:439:LYS:HG3	2.19	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: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:Q:100:GLN:CD	1:Q:100:GLN:N	2.72	0.41
1:G:100:GLN:N	1:G:100:GLN:CD	2.71	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:C:434:ASN:HA	3:N:252:MET:HE3	2.00	0.41
1:F:108:ARG:HD2	1:F:140:TYR:CG	2.55	0.41
1:P:108:ARG:HD2	1:P:140:TYR:CG	2.55	0.41
3:N:325:ASN:HD22	3:N:326:LYS:N	2.15	0.41
2:M:217:THR:HG1	3:B:285:HIS:CD2	2.36	0.41
3:D:325:ASN:HD22	3:D:326:LYS:N	2.15	0.41
1:L:160:GLN:NE2	2:M:177:VAL:HG12	2.31	0.41
1:L:141:PRO:O	1:L:198:HIS:HE1	2.02	0.41
2:I:151:ASN:N	2:I:191:ILE:O	2.53	0.41
3:A:342:GLN:HA	3:A:343:PRO:HD3	1.83	0.41
3:B:325:ASN:HD22	3:B:326:LYS:N	2.15	0.41
1:Q:108:ARG:CD	1:Q:109:THR:O	2.62	0.41
1:L:108:ARG:HD2	1:L:140:TYR:CB	2.50	0.41
3:J:328:LEU:HD12	3:J:329:PRO:CD	2.50	0.41
3:C:328:LEU:HD12	3:C:329:PRO:CD	2.50	0.41
3:A:246:LYS:HA	3:A:247:PRO:HD3	1.94	0.41
2:E:19:ILE:CD1	2:I:8:GLY:HA3	2.49	0.41
1:L:38:GLN:OE1	1:L:87:HIS:HE1	2.04	0.41
3:J:309:LEU:O	3:J:312:ASN:N	2.51	0.41
3:J:367:CYS:HB2	3:J:381:TRP:CH2	2.55	0.41
3:J:274:LYS:HE2	3:J:324:SER:HB2	2.02	0.41
3:C:367:CYS:HB2	3:C:381:TRP:CH2	2.55	0.41
1:P:108:ARG:HD2	1:P:140:TYR:HB3	2.03	0.41
1:G:108:ARG:HD2	1:G:140:TYR:CB	2.49	0.41
3:B:276:ASN:HB3	3:B:278:TYR:CE1	2.56	0.41
1:G:38:GLN:OE1	1:G:87:HIS:HE1	2.04	0.41
2:R:3:GLN:HB2	2:R:25:SER:HB2	2.02	0.41
2:O:54:SER:HB2	2:R:74:LEU:HD12	2.02	0.41
3:A:274:LYS:HE2	3:A:324:SER:HB2	2.02	0.41
1:K:20:THR:CG2	1:K:72:THR:CG2	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:283:GLN:C	3:J:285:HIS:H	2.23	0.41
3:B:273:VAL:HB	3:B:302:VAL:HG21	2.03	0.41
1:G:175:LEU:CA	2:I:162:PHE:CE2	3.03	0.41
3:C:386:GLN:HG3	3:C:387:PRO:HD2	2.02	0.41
1:Q:38:GLN:OE1	1:Q:87:HIS:HE1	2.04	0.41
3:J:369:VAL:HB	3:J:406:LEU:HD12	2.02	0.41
1:L:143:GLU:CD	1:L:143:GLU:H	2.24	0.41
1:G:134:CYS:HB2	1:G:148:TRP:CH2	2.56	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: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:154:VAL:CA	2:M:156:SER:N	2.79	0.41
1:K:204:PRO:HD2	3:A:298:SER:OG	2.21	0.41
3:C:382:GLU:OE1	3:N:433:HIS:CE1	2.74	0.41
3:C:286:ASN:HB3	3:C:287:ALA:H	1.63	0.41
1:F:108:ARG:HD2	1:F:140:TYR:HB3	2.03	0.41
3:D:268:HIS:O	3:D:271:PRO:CG	2.68	0.41
3:A:328:LEU:HA	3:A:329:PRO:HD3	1.94	0.41
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.41
1:Q:175:LEU:CA	2:R:174:PHE:CE2	3.03	0.41
1:L:175:LEU:CA	2:M:174:PHE:CE2	3.03	0.41
1:F:38:GLN:OE1	1:F:87:HIS:HE1	2.03	0.41
2:R:162:ASN:N	2:R:207:ILE:O	2.53	0.41
3:N:350:THR:HB	3:N:441:LEU:CD1	2.50	0.41
3:J:336:ILE:HG12	3:J:337:SER:N	2.35	0.41
1:Q:134:CYS:HB2	1:Q:148:TRP:CH2	2.56	0.41
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.56	0.41
3:C:274:LYS:HE2	3:C:324:SER:HB2	2.02	0.41
3:B:367:CYS:HB2	3:B:381:TRP:CZ2	2.56	0.41
1:Q:143:GLU:H	1:Q:143:GLU:CD	2.24	0.41
2:R:154:VAL:CA	2:R:156:SER:N	2.79	0.41
2:O:18:LEU:N	2:O:82:MET:HE2	2.36	0.41
1:Q:162:SER:OG	2:R:175:PRO:O	2.28	0.41
3:J:386:GLN:HA	3:J:387:PRO:HD3	1.88	0.41
3:B:350:THR:HB	3:B:441:LEU:HD12	2.03	0.41
2:I:205:LYS:HA	2:I:205:LYS:HD3	1.97	0.41
3:N:367:CYS:HB2	3:N:381:TRP:CZ2	2.56	0.41
2:H:54:SER:HB2	2:M:74:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:309:LEU:O	3:A:312:ASN:N	2.51	0.41
3:N:310:HIS:O	3:N:314:LEU:HG	2.22	0.40
3:C:248:LYS:NZ	3:C:380:GLU:OE2	2.47	0.40
3:A:386:GLN:HG3	3:A:387:PRO:HD2	2.02	0.40
3:N:308:VAL:HG12	3:N:309:LEU:N	2.36	0.40
3:N:350:THR:HB	3:N:441:LEU:CG	2.51	0.40
3:J:342:GLN:HA	3:J:343:PRO:HD3	1.83	0.40
2:R:187:LEU:HD12	2:R:187:LEU:C	2.41	0.40
2:M:187:LEU:HD12	2:M:187:LEU:C	2.41	0.40
2:I:6:GLU:OE1	2:I:106:GLY:HA3	2.22	0.40
3:D:270:ASP:N	3:D:271:PRO:CD	2.82	0.40
3:N:276:ASN:HB3	3:N:278:TYR:CE1	2.56	0.40
3:D:276:ASN:HB3	3:D:278:TYR:CE1	2.56	0.40
3:B:350:THR:HB	3:B:441:LEU:CG	2.51	0.40
3:D:350:THR:HB	3:D:441:LEU:CG	2.51	0.40
3:D:350:THR:HB	3:D:441:LEU:HD12	2.03	0.40
3:D:273:VAL:HB	3:D:302:VAL:HG21	2.03	0.40
3:C:336:ILE:HG12	3:C:337:SER:N	2.35	0.40
3:J:282:VAL:O	3:J:283:GLN:CB	2.52	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
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: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:C:310:HIS:CD2	3:N:253:ILE:HD13	2.44	0.40
2:E:206:LYS:O	2:E:207:VAL:HA	2.22	0.40
3:A:252:MET:HB2	3:A:255:ARG:CG	2.49	0.40
3:D:245:PRO:HB3	3:D:258:GLU:H	1.87	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:B:335:THR:O	3:B:336:ILE:HB	2.21	0.40
2:I:174:LEU:HD12	2:I:174:LEU:C	2.41	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:H:165:VAL:HG11	1:K:160:GLN:OE1	2.21	0.40
2:E:165:VAL:HG11	1:F:160:GLN:OE1	2.21	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: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 ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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	29
3	B	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
3	C	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	29
3	D	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	29
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
All	All	3605/3918 (92%)	3348 (93%)	194 (5%)	63 (2%)	11	55

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 ⓘ

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%)	35	69
1	G	182/184 (99%)	172 (94%)	10 (6%)	27	63
1	K	182/184 (99%)	174 (96%)	8 (4%)	35	69
1	L	182/184 (99%)	172 (94%)	10 (6%)	27	63
1	P	182/184 (99%)	174 (96%)	8 (4%)	35	69
1	Q	182/184 (99%)	172 (94%)	10 (6%)	27	63
2	E	176/192 (92%)	167 (95%)	9 (5%)	29	66
2	H	175/192 (91%)	166 (95%)	9 (5%)	29	66
2	I	172/192 (90%)	157 (91%)	15 (9%)	13	45
2	M	172/192 (90%)	157 (91%)	15 (9%)	13	45
2	O	174/192 (91%)	165 (95%)	9 (5%)	29	65
2	R	172/192 (90%)	156 (91%)	16 (9%)	11	42
3	A	193/196 (98%)	187 (97%)	6 (3%)	47	77
3	B	192/196 (98%)	180 (94%)	12 (6%)	22	59
3	C	193/196 (98%)	187 (97%)	6 (3%)	47	77
3	D	192/196 (98%)	180 (94%)	12 (6%)	22	59
3	J	193/196 (98%)	187 (97%)	6 (3%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	192/196 (98%)	180 (94%)	12 (6%)	22	59
All	All	3288/3432 (96%)	3107 (94%)	181 (6%)	27	63

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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	F	211/213 (99%)	0.99	37 (17%) 2 7	467, 467, 467, 467	0
1	G	211/213 (99%)	1.67	71 (33%) 0 4	526, 526, 526, 526	0
1	K	211/213 (99%)	1.56	64 (30%) 1 5	487, 487, 487, 487	0
1	L	211/213 (99%)	1.89	82 (38%) 0 4	547, 547, 547, 547	0
1	P	211/213 (99%)	0.98	38 (18%) 2 7	467, 467, 467, 467	0
1	Q	211/213 (99%)	1.64	70 (33%) 0 4	527, 527, 527, 527	0
2	E	210/229 (91%)	1.39	57 (27%) 1 5	407, 407, 407, 407	0
2	H	209/229 (91%)	1.73	69 (33%) 0 4	427, 427, 427, 427	0
2	I	206/229 (89%)	1.27	52 (25%) 1 5	456, 456, 456, 456	0
2	M	206/229 (89%)	2.04	84 (40%) 0 4	477, 477, 477, 477	0
2	O	208/229 (90%)	1.40	57 (27%) 1 5	407, 407, 407, 407	0
2	R	206/229 (89%)	1.39	55 (26%) 1 5	457, 457, 457, 457	0
3	A	207/211 (98%)	1.92	81 (39%) 0 4	516, 516, 516, 516	0
3	B	206/211 (97%)	2.11	83 (40%) 0 4	520, 520, 520, 520	0
3	C	207/211 (98%)	1.79	69 (33%) 0 4	485, 485, 485, 485	0
3	D	206/211 (97%)	1.24	46 (22%) 1 6	489, 489, 489, 489	0
3	J	207/211 (98%)	1.83	75 (36%) 0 4	490, 490, 490, 490	0
3	N	206/211 (97%)	1.35	47 (22%) 1 6	494, 494, 494, 494	0
All	All	3750/3918 (95%)	1.57	1137 (30%) 1 5	407, 487, 547, 547	0

All (1137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	254	SER	13.1
3	C	348	VAL	12.6
1	G	208	SER	11.2

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Mol	Chain	Res	Type	RSRZ
1	K	38	GLN	10.6
3	B	238	PRO	9.9
1	L	189	HIS	9.8
1	Q	208	SER	9.7
3	B	253	ILE	9.1
3	A	253	ILE	9.0
1	L	174	SER	9.0
3	C	349	TYR	8.9
3	C	254	SER	8.9
2	M	198	LEU	8.7
2	H	146	VAL	8.6
2	H	3	GLN	8.5
1	Q	163	VAL	8.5
2	M	8	GLY	8.5
2	H	131	THR	8.4
1	P	8	PRO	8.3
2	O	116	THR	8.3
2	M	94	ARG	8.3
1	L	206	THR	8.2
3	D	254	SER	8.1
3	C	281	GLY	8.0
3	N	332	ILE	8.0
2	R	175	PRO	8.0
3	J	284	VAL	7.9
3	B	334	LYS	7.9
3	B	240	VAL	7.8
3	J	330	ALA	7.8
2	H	102	LEU	7.8
1	K	8	PRO	7.7
3	A	331	PRO	7.7
3	B	332	ILE	7.6
3	B	281	GLY	7.6
3	J	348	VAL	7.6
3	C	326	LYS	7.6
2	M	10	GLY	7.6
1	G	44	PRO	7.6
3	C	399	ASP	7.5
3	J	281	GLY	7.5
1	P	164	THR	7.4
1	G	202	SER	7.4
1	K	14	SER	7.4
1	Q	62	PHE	7.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	J	399	ASP	7.3
2	H	45	LEU	7.2
3	C	284	VAL	7.2
1	G	203	SER	7.2
1	K	17	ASP	7.2
3	A	388	GLU	7.1
3	B	336	ILE	7.1
3	D	341	GLY	7.1
1	L	78	LEU	7.1
1	Q	197	THR	7.1
3	A	284	VAL	7.1
3	J	349	TYR	7.1
1	L	184	ALA	7.1
3	A	272	GLN	7.0
3	B	337	SER	7.0
3	B	316	GLY	7.0
2	H	130	GLY	6.9
3	C	339	ALA	6.8
1	Q	44	PRO	6.8
1	F	164	THR	6.8
2	I	164	ALA	6.8
2	M	188	SER	6.7
2	R	198	LEU	6.6
3	B	443	LEU	6.6
1	L	198	HIS	6.6
2	M	183	GLY	6.6
2	M	175	PRO	6.6
1	L	163	VAL	6.6
1	L	197	THR	6.6
1	L	164	THR	6.6
1	F	205	VAL	6.6
1	P	163	VAL	6.5
2	H	145	PRO	6.5
1	Q	59	PRO	6.5
3	B	333	GLU	6.5
3	B	247	PRO	6.4
3	J	323	VAL	6.4
3	J	329	PRO	6.4
1	L	188	LYS	6.4
3	J	338	LYS	6.4
3	B	241	PHE	6.3
1	G	62	PHE	6.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	338	LYS	6.3
2	M	199	GLY	6.3
1	L	200	GLY	6.2
2	H	144	GLU	6.2
3	A	339	ALA	6.2
2	M	9	GLY	6.1
3	A	252	MET	6.1
1	L	205	VAL	6.1
3	B	250	THR	6.0
3	B	254	SER	6.0
2	M	110	THR	6.0
1	K	75	ILE	6.0
2	H	101	ARG	6.0
3	J	254	SER	6.0
1	G	59	PRO	6.0
3	J	285	HIS	6.0
1	L	157	GLY	5.9
1	K	76	SER	5.9
1	G	206	THR	5.9
3	A	390	ASN	5.9
3	C	282	VAL	5.9
3	A	285	HIS	5.9
3	J	364	SER	5.9
3	B	442	SER	5.8
3	C	379	VAL	5.8
3	A	350	THR	5.8
1	L	112	ALA	5.8
2	H	148	VAL	5.8
2	H	40	VAL	5.8
1	Q	202	SER	5.8
3	J	379	VAL	5.8
3	J	282	VAL	5.8
1	Q	108	ARG	5.7
1	Q	189	HIS	5.7
3	A	379	VAL	5.7
3	D	253	ILE	5.7
2	H	58	ASP	5.7
1	L	156	SER	5.7
3	B	417	TRP	5.7
2	O	10	GLY	5.6
2	M	97	SER	5.6
1	G	163	VAL	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Q	201	LEU	5.6
2	M	182	SER	5.6
3	J	298	SER	5.5
3	J	339	ALA	5.5
1	L	158	ASN	5.5
1	G	187	GLU	5.5
1	K	44	PRO	5.5
2	M	154	VAL	5.5
3	A	375	SER	5.5
3	B	239	SER	5.5
1	F	8	PRO	5.5
3	J	261	CYS	5.5
2	E	133	ALA	5.4
2	R	176	ALA	5.4
3	J	388	GLU	5.4
2	R	14	ALA	5.3
1	Q	164	THR	5.3
3	N	253	ILE	5.3
1	Q	60	SER	5.3
1	Q	111	ALA	5.3
3	B	289	THR	5.3
3	J	253	ILE	5.3
1	L	204	PRO	5.3
2	H	44	GLY	5.2
3	C	298	SER	5.2
1	G	21	ILE	5.2
1	L	190	LYS	5.2
1	Q	152	ASN	5.2
2	M	228	LYS	5.2
3	B	368	LEU	5.2
3	C	253	ILE	5.2
1	G	14	SER	5.2
2	E	83	HIS	5.2
2	R	57	ARG	5.2
3	A	419	GLN	5.2
3	B	321	CYS	5.2
1	G	201	LEU	5.2
2	O	154	VAL	5.2
2	R	154	VAL	5.2
3	N	241	PHE	5.2
2	M	146	ASP	5.1
2	M	93	ALA	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	N	333	GLU	5.1
3	J	328	LEU	5.1
2	H	62	ALA	5.1
1	K	96	ALA	5.1
3	B	335	THR	5.1
2	E	118	THR	5.1
2	M	101	ASP	5.0
2	R	214	PRO	5.0
2	M	107	THR	5.0
3	C	302	VAL	5.0
2	O	148	PHE	5.0
3	B	348	VAL	5.0
3	C	273	VAL	5.0
1	K	102	THR	4.9
3	A	293	GLU	4.9
3	J	366	THR	4.9
1	L	19	ILE	4.9
2	R	82	MET	4.9
3	C	327	ALA	4.9
1	G	27	GLN	4.9
3	C	252	MET	4.9
1	F	206	THR	4.9
3	A	346	PRO	4.9
3	A	306	LEU	4.9
1	L	185	ASP	4.9
2	O	118	GLY	4.9
3	J	280	ASP	4.9
1	L	132	VAL	4.9
1	F	13	ALA	4.8
3	C	330	ALA	4.8
3	D	333	GLU	4.8
1	P	206	THR	4.8
2	E	157	SER	4.8
1	Q	76	SER	4.8
3	J	400	SER	4.8
1	L	144	ALA	4.8
1	F	131	SER	4.8
1	K	115	VAL	4.8
2	M	184	LEU	4.8
2	E	156	THR	4.8
2	H	160	HIS	4.8
1	Q	58	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	148	VAL	4.8
2	H	63	VAL	4.7
3	A	349	TYR	4.7
3	A	400	SER	4.7
2	O	138	ALA	4.7
3	J	283	GLN	4.7
2	E	158	GLY	4.7
1	L	131	SER	4.7
3	C	285	HIS	4.7
3	C	283	GLN	4.7
2	E	132	ALA	4.6
2	E	140	ASP	4.6
3	C	272	GLN	4.6
3	C	366	THR	4.6
3	N	390	ASN	4.6
2	I	109	THR	4.6
2	O	117	LYS	4.6
3	N	341	GLY	4.6
3	B	379	VAL	4.6
1	G	186	TYR	4.6
2	M	106	GLY	4.6
3	A	372	PHE	4.6
2	R	19	ILE	4.6
3	J	326	LYS	4.6
3	A	270	ASP	4.6
1	G	204	PRO	4.5
3	C	347	GLN	4.5
1	L	201	LEU	4.5
2	M	96	GLY	4.5
2	E	65	GLY	4.5
2	M	176	ALA	4.5
3	J	327	ALA	4.5
3	J	324	SER	4.5
1	G	152	ASN	4.5
1	F	163	VAL	4.5
2	H	81	GLN	4.5
2	E	66	ARG	4.5
1	L	110	VAL	4.5
1	G	111	ALA	4.5
2	O	146	ASP	4.5
1	P	118	PHE	4.5
2	I	2	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	Q	171	SER	4.5
3	B	320	LYS	4.4
2	O	17	SER	4.4
3	N	350	THR	4.4
2	H	133	ALA	4.4
2	M	197	SER	4.4
2	M	214	PRO	4.4
2	O	167	THR	4.4
3	A	377	ILE	4.4
1	L	161	GLU	4.4
2	H	155	LEU	4.4
3	B	280	ASP	4.4
2	M	82	MET	4.3
1	L	151	ASP	4.3
1	L	113	PRO	4.3
1	G	25	ALA	4.3
1	G	210	ASN	4.3
1	Q	198	HIS	4.3
1	G	164	THR	4.3
2	H	39	ARG	4.3
1	G	205	VAL	4.3
3	J	276	ASN	4.3
2	E	131	THR	4.3
2	O	46	GLU	4.3
1	Q	174	SER	4.3
2	E	17	SER	4.3
2	E	9	GLY	4.3
2	H	195	ASN	4.2
2	R	153	THR	4.2
2	M	79	TYR	4.2
2	R	211	ASN	4.2
1	Q	203	SER	4.2
3	N	273	VAL	4.2
3	B	266	VAL	4.2
3	B	315	ASP	4.2
1	K	114	SER	4.2
1	P	132	VAL	4.2
1	P	62	PHE	4.2
2	O	198	LEU	4.2
3	C	329	PRO	4.2
2	I	26	ASN	4.2
2	O	115	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	O	139	ALA	4.1
2	O	193	VAL	4.1
1	F	14	SER	4.1
2	O	9	GLY	4.1
1	K	42	LYS	4.1
1	L	62	PHE	4.1
1	L	155	GLN	4.1
3	B	338	LYS	4.1
2	M	177	VAL	4.1
2	H	66	ARG	4.1
2	H	154	ALA	4.1
3	A	395	PRO	4.1
2	M	104	GLY	4.1
2	H	147	THR	4.1
1	L	111	ALA	4.1
1	G	144	ALA	4.1
3	D	241	PHE	4.1
1	L	18	THR	4.1
1	G	26	SER	4.1
2	M	32	HIS	4.1
2	E	129	SER	4.1
3	N	346	PRO	4.1
2	M	95	LYS	4.1
1	L	20	THR	4.1
1	L	152	ASN	4.0
1	G	197	THR	4.0
2	H	156	THR	4.0
2	I	14	ALA	4.0
1	G	175	LEU	4.0
2	H	65	GLY	4.0
3	N	248	LYS	4.0
1	P	205	VAL	4.0
3	C	278	TYR	4.0
3	A	292	ARG	4.0
1	Q	7	SER	4.0
2	I	183	SER	4.0
1	G	113	PRO	4.0
1	Q	21	ILE	4.0
2	M	149	PRO	4.0
1	Q	43	ALA	4.0
1	Q	104	VAL	4.0
1	L	44	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
3	B	400	SER	4.0
2	E	10	GLY	3.9
2	R	197	SER	3.9
3	J	347	GLN	3.9
1	L	96	ALA	3.9
3	J	403	SER	3.9
3	A	389	ASN	3.9
1	L	199	GLN	3.9
3	A	326	LYS	3.9
1	K	39	LYS	3.9
1	K	62	PHE	3.9
1	L	162	SER	3.9
2	H	24	VAL	3.9
3	A	378	ALA	3.9
1	K	163	VAL	3.9
1	Q	75	ILE	3.9
3	B	418	GLN	3.9
3	N	262	VAL	3.9
3	C	276	ASN	3.9
1	Q	144	ALA	3.9
2	R	107	THR	3.9
2	E	170	GLY	3.8
2	R	8	GLY	3.8
2	R	210	VAL	3.8
2	O	137	THR	3.8
2	M	31	ALA	3.8
3	N	356	GLU	3.8
3	N	247	PRO	3.8
2	R	92	CYS	3.8
3	A	289	THR	3.8
2	O	226	GLU	3.8
2	I	117	SER	3.8
1	Q	204	PRO	3.8
3	A	332	ILE	3.8
1	G	20	THR	3.8
1	Q	18	THR	3.7
2	O	66	ARG	3.7
2	E	119	LYS	3.7
3	C	331	PRO	3.7
2	E	112	THR	3.7
3	B	242	LEU	3.7
1	K	118	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	110	VAL	3.7
1	Q	14	SER	3.7
2	R	111	VAL	3.7
1	Q	162	SER	3.7
2	H	99	SER	3.7
1	K	37	GLN	3.7
3	B	366	THR	3.7
1	K	117	ILE	3.7
1	G	63	SER	3.7
3	J	363	VAL	3.7
1	K	116	PHE	3.7
1	Q	106	ILE	3.7
3	C	274	LYS	3.7
3	D	387	PRO	3.7
2	M	200	THR	3.7
3	C	364	SER	3.7
2	H	43	GLY	3.6
3	J	402	GLY	3.6
1	G	83	PHE	3.6
2	I	9	GLY	3.6
3	C	335	THR	3.6
2	H	129	SER	3.6
3	C	328	LEU	3.6
1	L	175	LEU	3.6
3	J	321	CYS	3.6
2	E	185	LEU	3.6
2	O	65	GLY	3.6
1	K	208	SER	3.6
3	B	399	ASP	3.6
3	A	286	ASN	3.6
1	G	192	TYR	3.6
1	G	198	HIS	3.6
2	H	158	GLY	3.6
1	Q	38	GLN	3.6
3	D	262	VAL	3.6
3	B	354	SER	3.6
1	G	110	VAL	3.6
1	Q	192	TYR	3.6
2	E	46	GLU	3.5
3	A	273	VAL	3.5
1	Q	114	SER	3.5
1	G	209	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	19	ILE	3.5
1	K	206	THR	3.5
1	F	196	VAL	3.5
2	I	57	ARG	3.5
1	Q	113	PRO	3.5
1	G	78	LEU	3.5
3	A	243	PHE	3.5
3	N	295	GLN	3.5
1	Q	200	GLY	3.5
2	O	67	PHE	3.5
1	K	175	LEU	3.5
2	M	196	SER	3.5
3	A	351	LEU	3.5
3	A	255	ARG	3.5
3	B	278	TYR	3.5
3	B	292	ARG	3.5
1	P	2	VAL	3.5
2	H	46	GLU	3.5
2	H	109	THR	3.5
3	A	308	VAL	3.5
2	O	110	THR	3.5
2	M	64	LYS	3.5
1	K	57	GLY	3.5
3	J	286	ASN	3.5
1	G	76	SER	3.5
2	M	116	THR	3.5
2	O	103	TRP	3.5
3	A	410	LEU	3.5
1	L	17	ASP	3.5
2	H	2	VAL	3.5
1	K	77	GLY	3.5
2	M	179	GLN	3.5
1	P	60	SER	3.5
2	M	17	SER	3.5
3	C	286	ASN	3.5
3	C	400	SER	3.5
1	K	40	PRO	3.5
1	G	96	ALA	3.4
3	J	401	ASP	3.4
1	G	161	GLU	3.4
1	G	207	LYS	3.4
1	F	17	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	210	ASN	3.4
1	Q	205	VAL	3.4
1	K	120	PRO	3.4
3	B	276	ASN	3.4
3	B	374	PRO	3.4
1	Q	13	ALA	3.4
3	J	316	GLY	3.4
2	H	83	HIS	3.4
2	E	45	LEU	3.4
1	L	2	VAL	3.4
1	L	94	TYR	3.4
2	R	9	GLY	3.4
3	D	260	THR	3.4
1	Q	170	ASP	3.4
2	O	124	LEU	3.4
3	A	383	SER	3.4
2	M	148	PHE	3.4
3	B	407	TYR	3.4
2	E	142	PHE	3.4
2	I	198	PRO	3.4
2	R	70	SER	3.4
3	A	340	LYS	3.4
3	D	418	GLN	3.4
3	N	254	SER	3.4
2	I	153	GLY	3.4
1	L	9	SER	3.4
1	G	58	VAL	3.3
2	H	157	SER	3.3
2	M	195	SER	3.3
1	P	9	SER	3.3
3	A	399	ASP	3.3
1	Q	8	PRO	3.3
2	E	159	VAL	3.3
1	G	122	ASP	3.3
3	N	394	THR	3.3
1	K	15	VAL	3.3
2	H	25	SER	3.3
2	H	143	PRO	3.3
3	D	386	GLN	3.3
3	B	331	PRO	3.3
3	B	314	LEU	3.3
2	E	18	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	J	251	LEU	3.3
3	N	281	GLY	3.3
3	N	266	VAL	3.3
1	K	2	VAL	3.3
3	B	284	VAL	3.3
2	M	187	LEU	3.3
1	K	30	GLU	3.3
2	H	182	SER	3.3
2	I	173	SER	3.3
2	H	132	ALA	3.3
2	M	112	SER	3.3
2	I	21	SER	3.3
2	M	174	PHE	3.3
1	K	9	SER	3.2
1	P	208	SER	3.2
2	M	98	ASP	3.2
2	O	183	GLY	3.2
3	N	423	PHE	3.2
1	Q	188	LYS	3.2
2	H	82	MET	3.2
1	F	75	ILE	3.2
2	I	8	GLY	3.2
1	L	79	GLN	3.2
2	O	63	VAL	3.2
1	K	109	THR	3.2
3	A	271	PRO	3.2
3	J	270	ASP	3.2
2	R	1	GLU	3.2
3	D	343	PRO	3.2
2	E	169	SER	3.2
2	R	13	LYS	3.2
2	E	130	GLY	3.2
3	C	316	GLY	3.2
2	H	13	LYS	3.2
1	P	212	GLY	3.2
3	N	343	PRO	3.2
2	E	155	LEU	3.2
2	I	185	LEU	3.2
2	R	4	LEU	3.2
3	C	307	THR	3.2
3	N	441	LEU	3.2
1	G	82	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	1	GLU	3.2
3	A	283	GLN	3.2
3	N	400	SER	3.2
2	I	25	SER	3.2
2	E	19	ILE	3.2
1	K	112	ALA	3.2
3	B	251	LEU	3.2
3	A	338	LYS	3.2
3	D	332	ILE	3.1
3	J	375	SER	3.1
2	H	194	VAL	3.1
3	D	350	THR	3.1
1	G	211	ARG	3.1
3	N	407	TYR	3.1
2	M	21	SER	3.1
3	N	292	ARG	3.1
2	M	69	VAL	3.1
3	A	323	VAL	3.1
1	L	208	SER	3.1
1	G	17	ASP	3.1
3	B	347	GLN	3.1
3	J	272	GLN	3.1
1	K	61	ARG	3.1
2	E	210	LYS	3.1
1	K	131	SER	3.1
1	K	19	ILE	3.1
2	H	19	ILE	3.1
3	B	317	LYS	3.1
3	J	302	VAL	3.1
1	P	192	TYR	3.1
2	M	105	PRO	3.1
1	Q	210	ASN	3.1
1	P	196	VAL	3.1
1	G	158	ASN	3.1
1	K	54	LEU	3.1
2	I	82	MET	3.1
3	B	313	TRP	3.1
1	K	64	GLY	3.1
1	F	207	LYS	3.1
1	L	14	SER	3.0
1	Q	25	ALA	3.0
2	M	19	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	19	ILE	3.0
3	A	381	TRP	3.0
1	Q	63	SER	3.0
2	E	103	ASP	3.0
2	M	189	SER	3.0
2	E	3	GLN	3.0
1	L	179	LEU	3.0
3	C	394	THR	3.0
3	B	262	VAL	3.0
1	K	16	GLY	3.0
2	R	186	SER	3.0
2	E	105	TRP	3.0
1	L	73	LEU	3.0
2	H	50	SER	3.0
1	F	133	VAL	3.0
2	I	20	LEU	3.0
3	C	375	SER	3.0
1	L	25	ALA	3.0
1	L	195	GLU	3.0
1	F	187	GLU	3.0
1	F	208	SER	3.0
1	G	104	VAL	3.0
3	D	259	VAL	3.0
1	K	130	ALA	3.0
1	P	131	SER	3.0
3	C	392	LYS	3.0
2	M	103	TRP	3.0
2	M	117	LYS	3.0
1	G	174	SER	3.0
3	C	407	TYR	3.0
3	A	305	VAL	3.0
3	B	285	HIS	3.0
1	G	181	LEU	3.0
2	I	163	PRO	3.0
1	L	203	SER	2.9
3	A	418	GLN	2.9
3	N	411	THR	2.9
3	B	439	LYS	2.9
1	F	59	PRO	2.9
2	O	195	SER	2.9
3	C	294	GLN	2.9
3	N	323	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	Q	23	CYS	2.9
1	L	150	VAL	2.9
1	G	130	ALA	2.9
1	L	8	PRO	2.9
2	O	168	SER	2.9
2	M	18	LEU	2.9
2	M	109	VAL	2.9
3	J	331	PRO	2.9
1	K	18	THR	2.9
3	C	368	LEU	2.9
2	E	2	VAL	2.9
2	E	63	VAL	2.9
2	E	183	SER	2.9
1	L	21	ILE	2.9
1	F	183	LYS	2.9
2	O	72	ASP	2.9
2	R	90	TYR	2.9
2	H	134	LEU	2.9
3	C	388	GLU	2.9
2	R	58	ASP	2.9
2	I	101	ARG	2.9
3	D	245	PRO	2.9
2	M	4	LEU	2.9
1	L	181	LEU	2.9
2	M	145	LYS	2.9
2	O	123	PRO	2.9
3	C	301	ARG	2.9
1	L	98	PHE	2.9
2	R	21	SER	2.9
2	M	35	ASN	2.8
2	I	17	SER	2.8
3	A	241	PHE	2.8
3	B	295	GLN	2.8
1	P	133	VAL	2.8
3	B	288	LYS	2.8
1	L	97	THR	2.8
2	M	39	ARG	2.8
2	E	128	PRO	2.8
3	J	368	LEU	2.8
2	E	182	SER	2.8
1	Q	74	THR	2.8
3	J	437	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	13	ALA	2.8
2	I	19	ILE	2.8
2	E	8	GLY	2.8
2	E	89	THR	2.8
2	I	59	TYR	2.8
3	B	349	TYR	2.8
2	H	18	LEU	2.8
2	I	116	ALA	2.8
2	O	166	LEU	2.8
3	C	280	ASP	2.8
1	G	112	ALA	2.8
1	P	61	ARG	2.8
1	G	189	HIS	2.8
1	F	18	THR	2.8
2	M	34	MET	2.8
2	O	171	VAL	2.8
2	O	194	PRO	2.8
3	B	245	PRO	2.8
3	J	279	VAL	2.8
1	K	209	PHE	2.8
3	B	364	SER	2.8
2	I	195	ASN	2.8
3	B	375	SER	2.7
3	D	323	VAL	2.7
1	F	132	VAL	2.7
2	O	8	GLY	2.7
2	H	183	SER	2.7
2	M	65	GLY	2.7
2	O	172	HIS	2.7
2	E	72	ASP	2.7
3	N	284	VAL	2.7
2	H	128	PRO	2.7
2	M	12	VAL	2.7
2	E	117	SER	2.7
1	F	165	GLU	2.7
3	C	251	LEU	2.7
2	M	190	VAL	2.7
3	N	409	LYS	2.7
3	A	295	GLN	2.7
1	L	212	GLY	2.7
1	L	180	THR	2.7
1	K	162	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	64	GLY	2.7
3	J	418	GLN	2.7
2	R	156	SER	2.7
1	K	138	ASN	2.7
1	G	8	PRO	2.7
1	L	160	GLN	2.7
1	Q	175	LEU	2.7
3	B	394	THR	2.7
2	E	181	PRO	2.7
3	B	409	LYS	2.7
3	C	293	GLU	2.7
3	C	321	CYS	2.7
1	L	143	GLU	2.7
2	E	75	GLU	2.7
3	A	251	LEU	2.7
3	A	374	PRO	2.7
3	C	324	SER	2.7
1	Q	22	THR	2.7
3	D	268	HIS	2.7
2	R	81	GLN	2.7
1	K	26	SER	2.7
2	H	175	SER	2.7
1	K	192	TYR	2.7
1	Q	94	TYR	2.7
2	M	143	LEU	2.7
3	B	258	GLU	2.7
3	C	255	ARG	2.7
3	B	437	THR	2.7
2	M	113	PRO	2.7
2	H	59	TYR	2.7
3	C	423	PHE	2.7
2	I	113	VAL	2.7
1	K	43	ALA	2.6
2	M	227	PRO	2.6
1	Q	83	PHE	2.6
1	Q	150	VAL	2.6
1	G	39	LYS	2.6
1	G	94	TYR	2.6
2	R	177	VAL	2.6
3	B	373	TYR	2.6
3	A	341	GLY	2.6
1	K	78	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	173	THR	2.6
1	Q	61	ARG	2.6
2	I	184	SER	2.6
2	E	206	LYS	2.6
2	O	19	ILE	2.6
1	L	15	VAL	2.6
1	G	43	ALA	2.6
1	F	192	TYR	2.6
2	O	111	VAL	2.6
1	G	60	SER	2.6
3	N	339	ALA	2.6
3	A	333	GLU	2.6
3	N	267	SER	2.6
1	Q	186	TYR	2.6
2	I	174	LEU	2.6
2	M	102	ALA	2.6
2	O	12	VAL	2.6
2	O	81	GLN	2.6
1	K	58	VAL	2.6
3	N	379	VAL	2.6
2	R	15	GLY	2.6
3	N	240	VAL	2.6
1	F	33	LEU	2.6
2	I	3	GLN	2.6
3	A	409	LYS	2.6
1	L	173	TYR	2.6
3	B	263	VAL	2.6
3	B	425	CYS	2.6
2	E	180	VAL	2.6
3	B	259	VAL	2.6
3	B	346	PRO	2.6
3	D	411	THR	2.6
2	E	209	PRO	2.6
2	I	65	GLY	2.6
3	N	331	PRO	2.6
1	K	25	ALA	2.6
1	F	195	GLU	2.6
1	G	200	GLY	2.6
1	G	13	ALA	2.6
1	Q	187	GLU	2.6
3	A	376	ASP	2.6
3	A	294	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	212	GLY	2.5
2	R	213	LYS	2.5
3	A	392	LYS	2.5
1	P	7	SER	2.5
2	M	67	PHE	2.5
2	O	75	GLU	2.5
3	C	405	PHE	2.5
2	E	81	GLN	2.5
3	J	346	PRO	2.5
3	J	398	LEU	2.5
2	I	42	GLY	2.5
3	C	409	LYS	2.5
2	O	149	PRO	2.5
2	I	53	SER	2.5
1	G	73	LEU	2.5
2	I	108	GLY	2.5
1	F	2	VAL	2.5
1	F	118	PHE	2.5
3	D	390	ASN	2.5
1	Q	110	VAL	2.5
1	P	27	GLN	2.5
2	M	16	GLY	2.5
3	A	394	THR	2.5
3	D	248	LYS	2.5
2	H	17	SER	2.5
1	K	132	VAL	2.5
2	E	168	SER	2.5
3	J	273	VAL	2.5
1	K	137	ASN	2.5
3	J	252	MET	2.5
3	D	353	PRO	2.5
3	J	274	LYS	2.5
3	A	242	LEU	2.5
3	J	409	LYS	2.5
1	L	207	LYS	2.5
1	P	89	GLN	2.5
3	B	307	THR	2.5
2	M	111	VAL	2.5
2	H	61	ASP	2.5
2	R	183	GLY	2.5
3	C	380	GLU	2.5
2	M	91	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	131	SER	2.5
2	I	27	PHE	2.5
3	D	342	GLN	2.5
3	D	366	THR	2.5
2	O	1	GLU	2.5
1	Q	107	LYS	2.5
1	Q	207	LYS	2.5
3	D	273	VAL	2.5
1	L	191	VAL	2.4
1	Q	78	LEU	2.4
3	J	297	ASN	2.4
3	N	351	LEU	2.4
1	G	18	THR	2.4
3	C	437	THR	2.4
1	F	113	PRO	2.4
2	I	6	GLU	2.4
3	A	391	TYR	2.4
3	B	318	GLU	2.4
3	J	242	LEU	2.4
3	J	407	TYR	2.4
2	H	103	ASP	2.4
2	O	152	VAL	2.4
2	O	182	SER	2.4
1	L	24	ARG	2.4
1	P	94	TYR	2.4
1	L	59	PRO	2.4
1	P	102	THR	2.4
3	D	339	ALA	2.4
1	G	46	LEU	2.4
3	B	264	VAL	2.4
3	D	396	PRO	2.4
2	H	209	PRO	2.4
2	R	64	LYS	2.4
3	J	313	TRP	2.4
1	F	151	ASP	2.4
1	K	41	GLY	2.4
2	E	111	VAL	2.4
1	L	22	THR	2.4
2	O	227	PRO	2.4
2	I	210	LYS	2.4
3	N	334	LYS	2.4
1	F	130	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	82	MET	2.4
1	Q	105	GLU	2.4
2	R	150	GLU	2.4
2	I	69	VAL	2.4
1	L	137	ASN	2.4
3	C	269	GLU	2.4
3	B	370	LYS	2.4
2	R	24	VAL	2.4
1	Q	211	ARG	2.4
3	D	266	VAL	2.4
2	O	222	LYS	2.4
3	J	269	GLU	2.4
3	C	427	VAL	2.4
3	B	343	PRO	2.4
2	H	42	GLY	2.4
2	R	6	GLU	2.4
3	J	417	TRP	2.4
3	A	423	PHE	2.4
3	J	404	PHE	2.4
3	N	245	PRO	2.4
1	P	77	GLY	2.4
1	L	187	GLU	2.4
3	C	356	GLU	2.4
3	D	388	GLU	2.4
1	L	120	PRO	2.4
2	O	169	GLY	2.3
3	B	252	MET	2.3
2	M	2	VAL	2.3
2	I	188	GLN	2.3
2	O	107	THR	2.3
3	D	402	GLY	2.3
3	B	319	TYR	2.3
1	L	192	TYR	2.3
1	P	78	LEU	2.3
2	O	101	ASP	2.3
3	J	314	LEU	2.3
1	L	61	ARG	2.3
1	F	51	ALA	2.3
2	R	115	SER	2.3
1	Q	181	LEU	2.3
2	H	56	TYR	2.3
2	I	81	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	261	CYS	2.3
3	D	407	TYR	2.3
1	P	14	SER	2.3
3	C	350	THR	2.3
3	A	367	CYS	2.3
1	K	97	THR	2.3
2	O	179	GLN	2.3
3	D	284	VAL	2.3
1	Q	196	VAL	2.3
3	A	307	THR	2.3
3	J	394	THR	2.3
2	R	174	PHE	2.3
2	O	13	LYS	2.3
2	O	87	THR	2.3
3	D	417	TRP	2.3
2	E	146	VAL	2.3
1	G	155	GLN	2.3
1	F	60	SER	2.3
3	A	342	GLN	2.3
3	J	367	CYS	2.3
1	P	207	LYS	2.3
2	M	81	GLN	2.3
2	I	4	LEU	2.3
2	H	127	ALA	2.3
1	K	7	SER	2.3
2	M	45	LEU	2.3
2	M	100	LEU	2.3
3	J	389	ASN	2.3
2	E	109	THR	2.3
1	P	96	ALA	2.3
3	D	374	PRO	2.3
1	P	75	ILE	2.3
2	I	169	SER	2.3
2	H	161	THR	2.3
3	A	411	THR	2.3
3	D	269	GLU	2.3
3	D	409	LYS	2.3
3	J	325	ASN	2.3
2	R	45	LEU	2.3
3	N	313	TRP	2.3
1	P	91	TYR	2.3
1	G	156	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	108	ARG	2.3
2	M	99	ARG	2.3
1	L	186	TYR	2.3
2	I	170	GLY	2.3
2	M	7	SER	2.2
1	K	205	VAL	2.2
2	O	42	GLY	2.2
1	K	100	GLN	2.2
3	J	372	PHE	2.2
3	A	321	CYS	2.2
2	I	56	TYR	2.2
2	R	59	TYR	2.2
2	M	15	GLY	2.2
2	I	18	LEU	2.2
1	F	211	ARG	2.2
3	A	296	TYR	2.2
3	C	344	ARG	2.2
1	L	119	PRO	2.2
3	B	279	VAL	2.2
3	C	270	ASP	2.2
3	N	280	ASP	2.2
2	E	184	SER	2.2
2	M	26	ASN	2.2
3	A	259	VAL	2.2
3	N	430	GLU	2.2
2	R	2	VAL	2.2
2	R	63	VAL	2.2
3	C	250	THR	2.2
1	F	150	VAL	2.2
2	R	16	GLY	2.2
3	B	265	ASP	2.2
3	B	277	TRP	2.2
2	R	7	SER	2.2
1	P	64	GLY	2.2
3	N	268	HIS	2.2
1	K	63	SER	2.2
1	Q	17	ASP	2.2
2	H	41	PRO	2.2
2	R	151	PRO	2.2
3	N	396	PRO	2.2
3	N	418	GLN	2.2
2	H	210	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	R	18	LEU	2.2
3	A	404	PHE	2.2
1	G	177	SER	2.2
1	F	144	ALA	2.2
1	P	162	SER	2.2
2	R	65	GLY	2.2
3	J	275	PHE	2.2
3	N	345	GLU	2.2
1	L	82	ASP	2.2
2	M	53	SER	2.2
2	I	98	GLY	2.2
2	R	12	VAL	2.2
3	C	417	TRP	2.2
1	Q	65	SER	2.2
3	J	355	ARG	2.2
3	C	413	ASP	2.2
2	I	94	CYS	2.2
1	K	68	GLY	2.2
3	B	249	ASP	2.2
3	N	338	LYS	2.2
3	N	388	GLU	2.2
2	I	165	VAL	2.2
3	B	342	GLN	2.2
3	D	243	PHE	2.2
3	J	381	TRP	2.2
1	K	186	TYR	2.2
1	F	122	ASP	2.2
2	H	98	GLY	2.2
3	A	304	SER	2.2
3	B	248	LYS	2.2
3	A	260	THR	2.1
2	H	117	SER	2.1
3	D	441	LEU	2.1
2	I	104	ALA	2.1
2	R	106	GLY	2.1
3	A	280	ASP	2.1
3	B	365	LEU	2.1
3	D	277	TRP	2.1
2	E	67	PHE	2.1
3	D	298	SER	2.1
1	K	3	VAL	2.1
1	Q	96	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	366	THR	2.1
3	C	308	VAL	2.1
3	D	310	HIS	2.1
2	H	162	PHE	2.1
1	P	106	ILE	2.1
1	P	165	GLU	2.1
2	H	8	GLY	2.1
2	O	140	LEU	2.1
1	L	10	THR	2.1
3	D	400	SER	2.1
1	K	59	PRO	2.1
2	M	206	TYR	2.1
2	I	209	PRO	2.1
2	M	66	ARG	2.1
2	R	141	GLY	2.1
3	B	310	HIS	2.1
3	C	393	THR	2.1
1	Q	93	GLY	2.1
3	A	287	ALA	2.1
3	A	300	TYR	2.1
3	J	351	LEU	2.1
2	R	22	CYS	2.1
3	N	417	TRP	2.1
2	O	112	SER	2.1
1	P	25	ALA	2.1
2	R	69	VAL	2.1
1	F	62	PHE	2.1
1	Q	138	ASN	2.1
2	H	177	VAL	2.1
2	I	190	TYR	2.1
3	C	355	ARG	2.1
1	G	7	SER	2.1
2	R	97	SER	2.1
1	G	190	LYS	2.1
3	D	265	ASP	2.1
2	M	6	GLU	2.1
3	B	256	THR	2.1
3	C	385	GLY	2.1
3	D	281	GLY	2.1
1	G	120	PRO	2.1
1	Q	82	ASP	2.1
3	N	357	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	91	TYR	2.1
1	L	210	ASN	2.1
2	R	102	ALA	2.1
3	A	405	PHE	2.1
2	M	61	ASP	2.1
3	C	346	PRO	2.1
1	K	4	MET	2.1
3	A	281	GLY	2.1
3	A	324	SER	2.1
1	Q	73	LEU	2.1
3	J	294	GLN	2.1
3	D	348	VAL	2.1
1	Q	109	THR	2.1
1	L	107	LYS	2.1
3	J	423	PHE	2.1
3	B	414	LYS	2.1
2	M	153	THR	2.0
3	A	396	PRO	2.0
3	J	435	HIS	2.0
3	C	315	ASP	2.0
1	L	95	SER	2.0
1	L	109	THR	2.0
2	H	26	ASN	2.0
2	H	67	PHE	2.0
3	A	358	MET	2.0
3	B	302	VAL	2.0
2	R	83	ARG	2.0
2	I	63	VAL	2.0
3	A	274	LYS	2.0
3	J	434	ASN	2.0
1	L	83	PHE	2.0
2	I	147	THR	2.0
3	D	394	THR	2.0
1	K	210	ASN	2.0
2	M	142	CYS	2.0
3	J	303	VAL	2.0
3	J	405	PHE	2.0
3	D	285	HIS	2.0
1	G	74	THR	2.0
1	P	115	VAL	2.0
2	E	153	GLY	2.0
2	E	1	GLU	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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.