



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 22, 2018 – 07:34 PM EST

PDB ID : 5NZU  
EMDB ID: : EMD-3723  
Title : The structure of the COPI coat linkage II  
Authors : Dodonova, S.O.; Aderhold, P.; Kopp, J.; Ganeva, I.; Roehling, S.; Hagen, W.J.H.; Sinning, I.; Wieland, F.; Briggs, J.A.G.  
Deposited on : 2017-05-15  
Resolution : 15.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

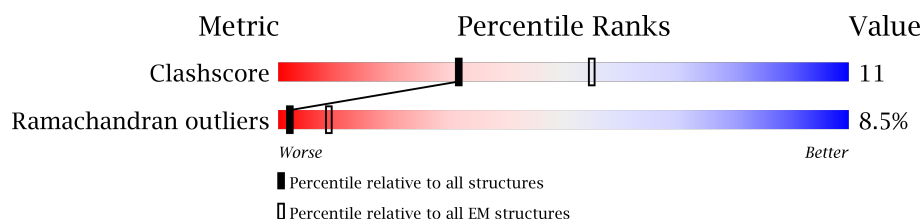
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 15.00 Å.

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

























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1-A	1262	48% 14% • 36%
1	2-A	1262	48% 14% • 36%
1	3-A	1262	48% 14% • 36%
2	1-B	968	66% 13% • 17%
2	2-B	968	66% 13% •• 17%
2	3-B	968	67% 13% • 17%
3	1-C	905	77% 14% • 7%
3	2-C	905	77% 14% • 7%
3	3-C	905	77% 14% • 7%
4	1-D	511	78% 5% • 16%
4	2-D	511	78% 5% • 16%

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Mol	Chain	Length	Quality of chain
4	3-D	511	
5	1-F	181	
5	1-M	181	
5	1-R	181	
5	2-F	181	
5	2-M	181	
5	2-R	181	
5	3-F	181	
5	3-M	181	
5	3-R	181	
6	1-G	874	
6	1-K	874	
6	2-G	874	
6	2-K	874	
6	3-G	874	
6	3-K	874	
7	1-L	177	
7	1-Z	177	
7	2-L	177	
7	2-Z	177	
7	3-L	177	
7	3-Z	177	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 59913 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1-A	813	Total	C	N	O	0	0
			3251	1626	813	812		
1	2-A	813	Total	C	N	O	0	0
			3251	1626	813	812		
1	3-A	813	Total	C	N	O	0	0
			3251	1626	813	812		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1225	LEU	-	expression tag	UNP Q8CIE6
A	1226	GLU	-	expression tag	UNP Q8CIE6
A	1227	VAL	-	expression tag	UNP Q8CIE6
A	1228	LEU	-	expression tag	UNP Q8CIE6
A	1229	PHE	-	expression tag	UNP Q8CIE6
A	1230	GLN	-	expression tag	UNP Q8CIE6
A	1231	GLY	-	expression tag	UNP Q8CIE6
A	1232	PRO	-	expression tag	UNP Q8CIE6
A	1233	SER	-	expression tag	UNP Q8CIE6
A	1234	ALA	-	expression tag	UNP Q8CIE6
A	1235	TRP	-	expression tag	UNP Q8CIE6
A	1236	SER	-	expression tag	UNP Q8CIE6
A	1237	HIS	-	expression tag	UNP Q8CIE6
A	1238	PRO	-	expression tag	UNP Q8CIE6
A	1239	GLN	-	expression tag	UNP Q8CIE6
A	1240	PHE	-	expression tag	UNP Q8CIE6
A	1241	GLU	-	expression tag	UNP Q8CIE6
A	1242	LYS	-	expression tag	UNP Q8CIE6
A	1243	GLY	-	expression tag	UNP Q8CIE6
A	1244	GLY	-	expression tag	UNP Q8CIE6
A	1245	GLY	-	expression tag	UNP Q8CIE6
A	1246	SER	-	expression tag	UNP Q8CIE6
A	1247	GLY	-	expression tag	UNP Q8CIE6
A	1248	GLY	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	GLY	-	expression tag	UNP Q8CIE6
A	1250	SER	-	expression tag	UNP Q8CIE6
A	1251	GLY	-	expression tag	UNP Q8CIE6
A	1252	GLY	-	expression tag	UNP Q8CIE6
A	1253	SER	-	expression tag	UNP Q8CIE6
A	1254	ALA	-	expression tag	UNP Q8CIE6
A	1255	TRP	-	expression tag	UNP Q8CIE6
A	1256	SER	-	expression tag	UNP Q8CIE6
A	1257	HIS	-	expression tag	UNP Q8CIE6
A	1258	PRO	-	expression tag	UNP Q8CIE6
A	1259	GLN	-	expression tag	UNP Q8CIE6
A	1260	PHE	-	expression tag	UNP Q8CIE6
A	1261	GLU	-	expression tag	UNP Q8CIE6
A	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 2 is a protein called Coatomer subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1-B	800	Total	C	N	O	0	0
			3198	1600	800	798		
2	2-B	800	Total	C	N	O	0	0
			3198	1600	800	798		
2	3-B	800	Total	C	N	O	0	0
			3198	1600	800	798		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9JIF7
B	2	HIS	-	expression tag	UNP Q9JIF7
B	3	HIS	-	expression tag	UNP Q9JIF7
B	4	HIS	-	expression tag	UNP Q9JIF7
B	5	HIS	-	expression tag	UNP Q9JIF7
B	6	HIS	-	expression tag	UNP Q9JIF7
B	7	HIS	-	expression tag	UNP Q9JIF7
B	8	GLU	-	expression tag	UNP Q9JIF7
B	9	ASN	-	expression tag	UNP Q9JIF7
B	10	LEU	-	expression tag	UNP Q9JIF7
B	11	TYR	-	expression tag	UNP Q9JIF7
B	12	PHE	-	expression tag	UNP Q9JIF7
B	13	GLN	-	expression tag	UNP Q9JIF7
B	14	GLY	-	expression tag	UNP Q9JIF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	HIS	-	expression tag	UNP Q9JIF7

- Molecule 3 is a protein called Coatomer subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1-C	843	Total	C	N	O	0	0
			3371	1686	843	842		
3	2-C	843	Total	C	N	O	0	0
			3371	1686	843	842		
3	3-C	843	Total	C	N	O	0	0
			3371	1686	843	842		

- Molecule 4 is a protein called Coatomer subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	1-D	427	Total	C	N	O	0	0
			1707	854	427	426		
4	2-D	427	Total	C	N	O	0	0
			1707	854	427	426		
4	3-D	427	Total	C	N	O	0	0
			1707	854	427	426		

- Molecule 5 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	1-F	159	Total	C	N	O	0	0
			635	318	159	158		
5	2-F	159	Total	C	N	O	0	0
			635	318	159	158		
5	3-F	159	Total	C	N	O	0	0
			635	318	159	158		
5	1-R	159	Total	C	N	O	0	0
			635	318	159	158		
5	2-R	159	Total	C	N	O	0	0
			635	318	159	158		
5	3-R	159	Total	C	N	O	0	0
			635	318	159	158		
5	1-M	159	Total	C	N	O	0	0
			635	318	159	158		
5	2-M	159	Total	C	N	O	0	0
			635	318	159	158		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	3-M	159	Total	C	N	O	0	0
			635	318	159	158		

- Molecule 6 is a protein called Coatomer subunit gamma-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1-G	798	Total	C	N	O	0	0
			3190	1596	798	796		
6	2-G	798	Total	C	N	O	0	0
			3190	1596	798	796		
6	3-G	798	Total	C	N	O	0	0
			3190	1596	798	796		
6	1-K	560	Total	C	N	O	0	0
			2239	1120	560	559		
6	2-K	560	Total	C	N	O	0	0
			2239	1120	560	559		
6	3-K	560	Total	C	N	O	0	0
			2239	1120	560	559		

- Molecule 7 is a protein called Coatomer subunit zeta-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	1-Z	139	Total	C	N	O	0	0
			555	278	139	138		
7	2-Z	139	Total	C	N	O	0	0
			555	278	139	138		
7	3-Z	139	Total	C	N	O	0	0
			555	278	139	138		
7	1-L	139	Total	C	N	O	0	0
			555	278	139	138		
7	2-L	139	Total	C	N	O	0	0
			555	278	139	138		
7	3-L	139	Total	C	N	O	0	0
			555	278	139	138		





K1	S9	A10	P22	V36	D37	K61	Q62	Q63	P64	V67	Y73	V77	W78	F87	H92	H103	E104	Y105	P106	W107	R125	T132	G133	P145	R168	K169	K170	P174	G175	A176	R182	G183	I184	T185	G186	V187	G191	A195	K198
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GLY	SER	GLN	LYS	GLN	THR	GLY	P587	G753	I592	I491	I341	D205
THR	ALA	THR	PHE	LYS	THR	THR	R598	Q754	I593	V491	R342	R206
TYR	GLU	TYR	GLU	ILE	LYS	GLY	V599	K755	I594	K492	R343	G207
ALA	ASP	ALA	VAL	CYS	ILE	TRP	I495	S756	I595	I496	I344	H214
ARG	PHE	ARG	VAL	GLY	PHE	GLY	R496	G766	I596	R497	D345	P215
THR	VAL	THR	LYS	THR	PHE	ASP	P594	L767	I597	S497	S349	T216
THR	THR	THR	LYS	THR	VAL	ASP	T595	D768	I598	A498	V354	H217
ALA	PRO	ALA	PHE	ALA	ALA	ALA	E596	D769	H502	H502	H218	P218
THR	PRO	THR	ARG	THR	THR	GLU	F597	E783	K503	G360	V221	V221
LYS	LYS	ALA	ILE	GLY	LYS	GLN	F599	P786	A504	S361	R227	R227
GLY	THR	LEU	LEU	THR	THR	ASP	K600	D787	A507	R362	Q226	Q226
PRO	CYS	PRO	LEU	VAL	GLU	GLU	L601	I788	R508	R363	V229	V229
CYS	VAL	CYS	VAL	THR	THR	ASP	A602	D789	H509	P364		
ALA	THR	ALA	THR	THR	THR	GLY	E610	G796	A510	N371	E236	E236
PRO	GLN	PRO	LEU	LEU	GLY	THR	V611	P797	V511	R372	S237	S237
THR	ILE	THR	VAL	VAL	THR	VAL	L612	P798	G514	A373	V240	V240
TYR	THR	TYR	VAL	THR	THR	GLU		A799	H515	A383	E241	E241
ASP	ASP	ASP	VAL	THR	THR	ALA	V615	G799	H516	S384	V242	V242
MET	MET	ILE	ASP	ASP	THR	PRO	K619	P800	K517	D243	D243	D243
HIS	HIS	LEU	ASN	ASN	ASN	GLY	R620	I801	A518	D392	T244	T244
ASN	VAL	VAL	VAL	ASN	SER	GLY	V621	R802	D519	K398	C245	C245
ARG	LEU	ARG	GLN	ARG	GLN	LEU	G622	P803	G522			
LEU	LEU	LEU	LEU	LEU	LEU	GLY	Q623	L804	V527	S402		
THR	THR	THR	THR	THR	THR	GLU	S624	D805	V528	K411	V252	V252
ILE	ILE	ILE	ALA	ALA	ALA	VAL		L810	V529	R412		
CYS	ALA	ALA	GLY	GLY	GLY	LEU	K631	R811	K531	S413	P259	P259
ALA	LEU	LEU	LEU	LEU	LEU	LYS	G632	G812	S532	R423	K271	K271
ASN	ASN	ASN	ILE	ILE	ILE	GLY	V642	SER	G533	N424	S272	S272
PHE	ASN	PHE	THR	THR	THR	GLU	K643	GLY	V543	R425		
THR	THR	THR	ALA	ALA	ALA	GLY	D644	GLY	G546	L429	M278	M278
ARG	ARG	ARG	VAL	VAL	VAL	THR		SER	T554	D430	R281	R281
GLY	GLY	GLY	THR	THR	THR	ALA	I660	GLY	T555	T282	T282	T282
LYS	LYS	LYS	ALA	ALA	ALA	ARG		THR	G556	H433	G283	G283
VAL	VAL	VAL	LEU	LEU	LEU	LEU	K671	ILE	R562	L436	D290	D290
GLY	GLY	GLY	THR	THR	THR	GLY	G673	SER	T563	I444	G313	G313
CYS	CYS	CYS	LEU	LEU	LEU	ASP	M674	LYS	L564	I452	F317	F317
PRO	PRO	PRO	MET	MET	MET	LEU	E679	GLY	D565	N452		
LEU	LEU	LEU	ILE	ILE	ILE	GLY		THR	L566	C453		
ARG	ARG	ARG	ILE	ILE	ILE	LEU	M666	GLY	V570	D454	R321	R321
ALA	ALA	ALA	THR	THR	THR	PRO		ALA	T571	F457	R322	R322
LEU	LEU	LEU	GLN	GLN	GLN	LEU	D728	LEU	H572	R323	R323	R323
LYS	LYS	LYS	LYS	LYS	LYS	GLY		ALA	G573	P324	P324	P324
THR	THR	THR	LEU	LEU	LEU	ASP	G731	ASP	N573	L466	A325	A325
VAL	VAL	VAL	CYS	CYS	CYS	VAL		THR	K574	L466		
PRO	PRO	PRO	TYR	TYR	TYR	PRO	A736	ILE	G575	Q479	H329	H329
LYS	LYS	LYS	GLN	GLN	GLN	LYS		THR	R583	K480	G330	G330
GLY	GLY	GLY	THR	THR	THR	LEU	G740	ILE	E584	R481		
THR	THR	THR	LEU	LEU	LEU	GLY		THR	C585	K487	R338	R338
LEU	LEU	LEU	VAL	VAL	VAL	THR	L749	SER		K487	R339	R339
GLN	GLN	GLN	ASP	ASP	ASP	GLY		VAL	R586	I488	F340	F340

● Molecule 2: Coatomer subunit beta

Chain 1-B: 

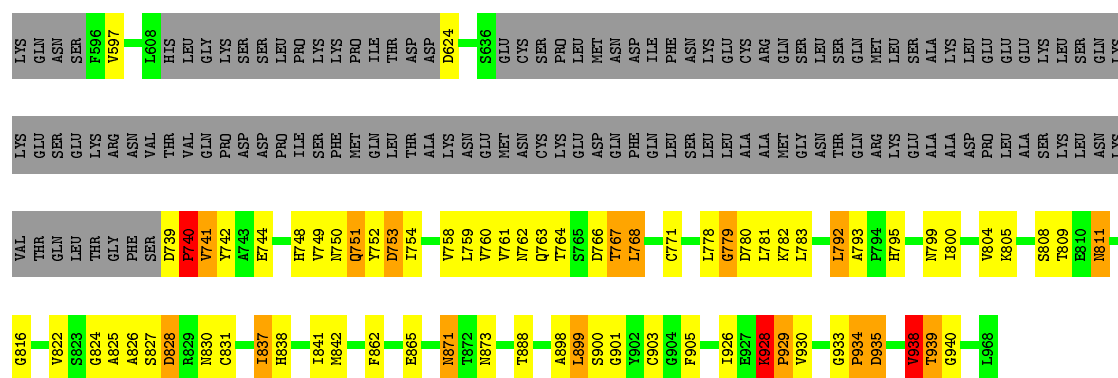
66%

13%

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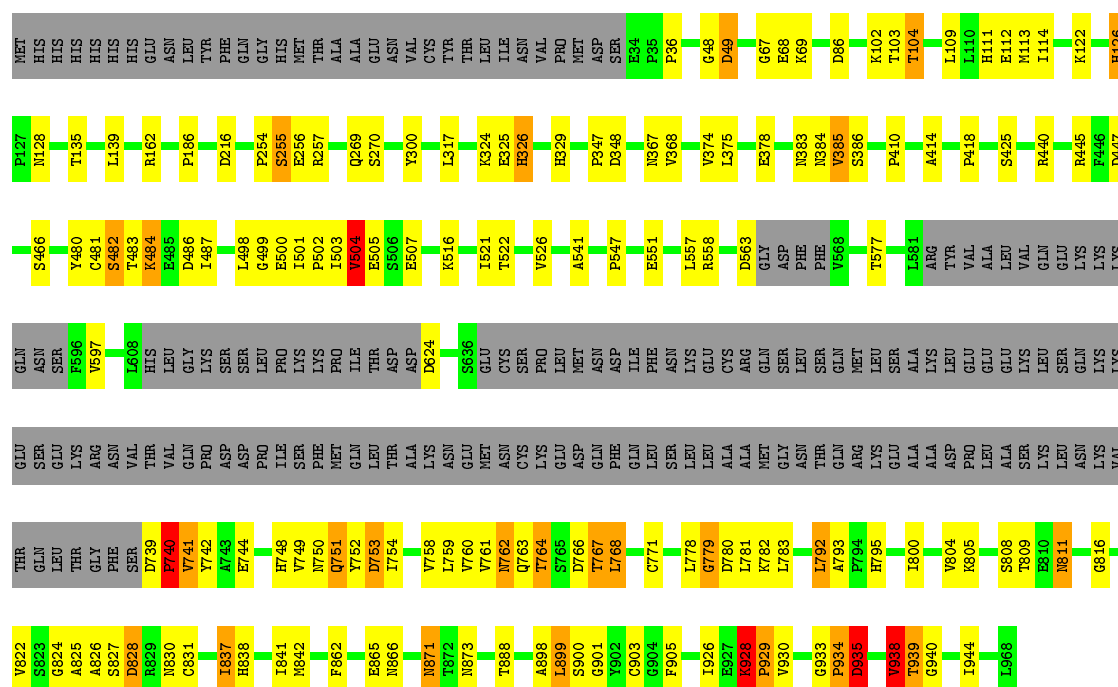
17%

MET	HIS	HIS	HIS	HIS	HIS	GLY	MET	E34	G43	L109	P127	D447
HIS	THR	THR	THR	THR	THR	GLU	SER	P35	D49	L110	M128	S466
VAL	THR	THR	THR	THR	THR	VAL	ASN	P36	G67	H111	T135	
ALA	THR	THR	THR	THR	THR	ALA	THR		E68	E112	L139	Y480
GLY	THR	THR	THR	THR	THR	GLY	PRO		K69	M113	R162	C481
ASN	THR	THR	THR	THR	THR	THR	GLY	D86	T103	I114	P186	S482
LEU	THR	THR	THR	THR	THR	LEU	ASP	K102	T104		D216	T483
THR	THR	THR	THR	THR	THR	THR	THR	S386			P186	R484
PHE	THR	THR	THR	THR	THR	THR	THR	P410			D216	D486
GLN	THR	THR	THR	THR	THR	GLN	THR		L581			I487
GLY	THR	THR	THR	THR	THR	GLY	THR	A414	ARG		P254	L488
HIS	THR	THR	THR	THR	THR	HIS	THR	P418	TYR		S255	G499
MET	THR	THR	THR	THR	THR	MET	THR		VAL		E256	G499
ALA	THR	THR	THR	THR	THR	ALA	THR	S425	ALA		R257	E505
VAL	THR	THR	THR	THR	THR	VAL	THR		LEU			E506
ALA	THR	THR	THR	THR	THR	ALA	THR	R440	GLN		L267	P502
GLY	THR	THR	THR	THR	THR	GLY	THR	R445	THR		L268	I503
ASN	THR	THR	THR	THR	THR	ASN	THR	F446	GLY		Q269	R504
THR	THR	THR	THR	THR	THR	THR	THR		VAL		S270	Q269
LEU	THR	THR	THR	THR	THR	LEU	THR		CYS			E507
ILE	THR	THR	THR	THR	THR	ILE	THR		TYR		L317	I504
VAL	THR	THR	THR	THR	THR	VAL	THR		ASN		K324	R505
PRO	THR	THR	THR	THR	THR	PRO	THR		PRO		E325	T522
MET	THR	THR	THR	THR	THR	MET	THR		THR		H329	V526
ASP	THR	THR	THR	THR	THR	ASP	THR		THR		P347	A541
SER	THR	THR	THR	THR	THR	SER	THR		THR		D348	P547
E34	THR	THR	THR	THR	THR	E34	THR		THR		L349	
P35	THR	THR	THR	THR	THR	P35	THR		THR		N367	E551
P36	THR	THR	THR	THR	THR	P36	THR		THR		V368	
G43	THR	THR	THR	THR	THR	G43	THR		THR		V374	L557
D49	THR	THR	THR	THR	THR	D49	THR		THR		L375	R588
G67	THR	THR	THR	THR	THR	G67	THR		THR		E378	D663
K69	THR	THR	THR	THR	THR	K69	THR		THR		N383	ASP
D86	THR	THR	THR	THR	THR	D86	THR		THR		N384	PHE
K102	THR	THR	THR	THR	THR	K102	THR		THR		S386	V588
T103	THR	THR	THR	THR	THR	T103	THR		THR		P410	T577
T104	THR	THR	THR	THR	THR	T104	THR		THR		A414	L581
L109	THR	THR	THR	THR	THR	L109	THR		THR		P418	ARG
L110	THR	THR	THR	THR	THR	L110	THR		THR		E112	TYR
H111	THR	THR	THR	THR	THR	H111	THR		THR		S425	VAL
M113	THR	THR	THR	THR	THR	M113	THR		THR		R440	VAL
I114	THR	THR	THR	THR	THR	I114	THR		THR		R445	GLN
K122	THR	THR	THR	THR	THR	K122	THR		THR		F446	GLY
H126	THR	THR	THR	THR	THR	H126	THR		THR			LYS



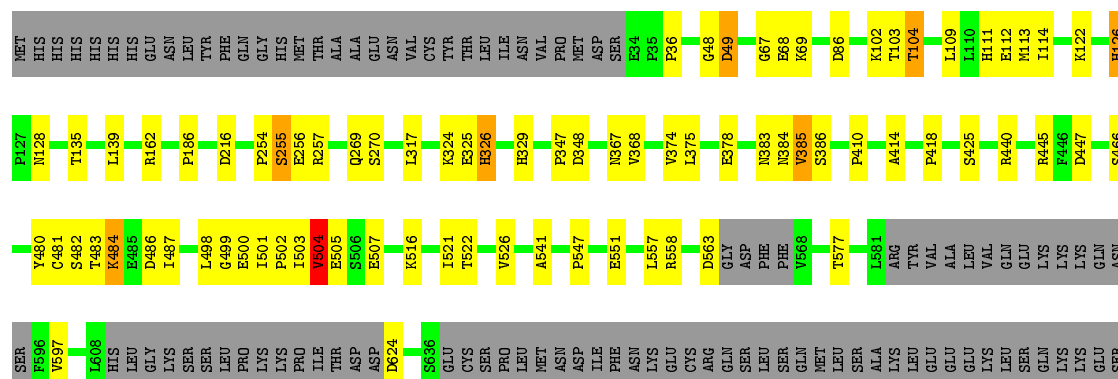
• Molecule 2: Coatomer subunit beta

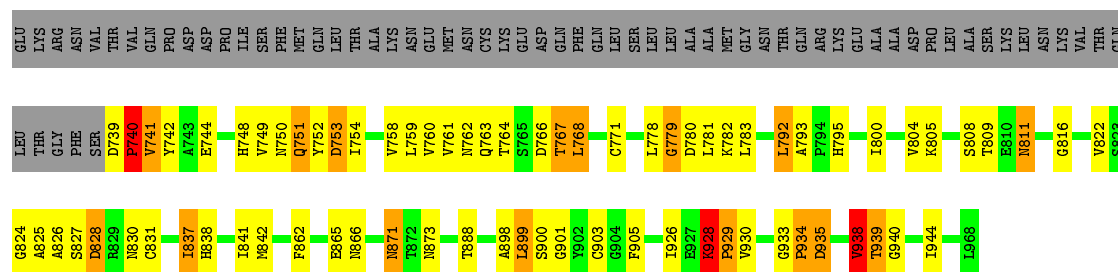
Chain 2-B: 66% 13% 17%



• Molecule 2: Coatomer subunit beta

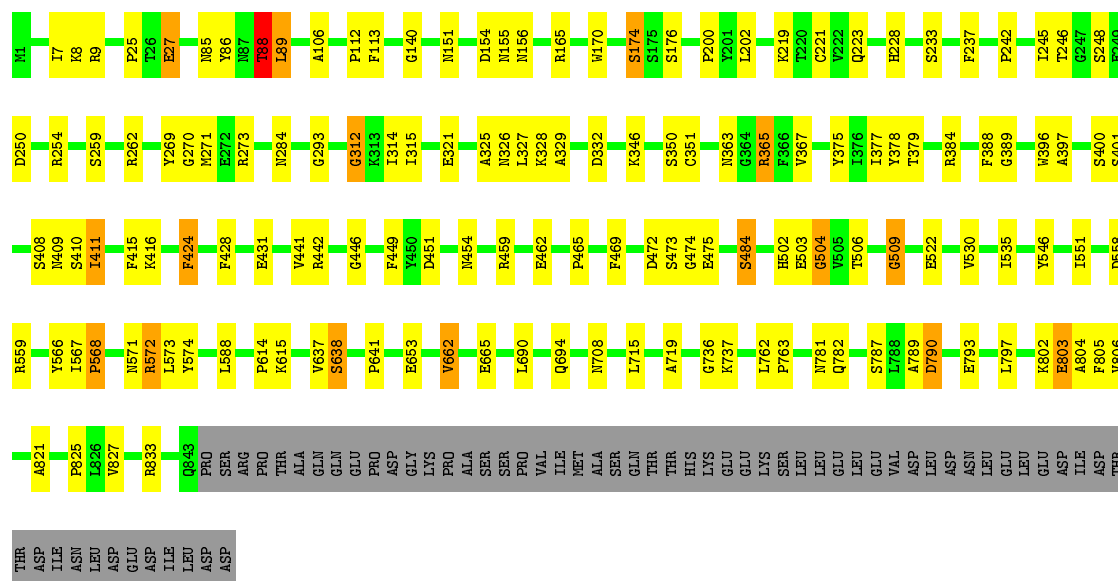
Chain 3-B: 67% 13% 17%





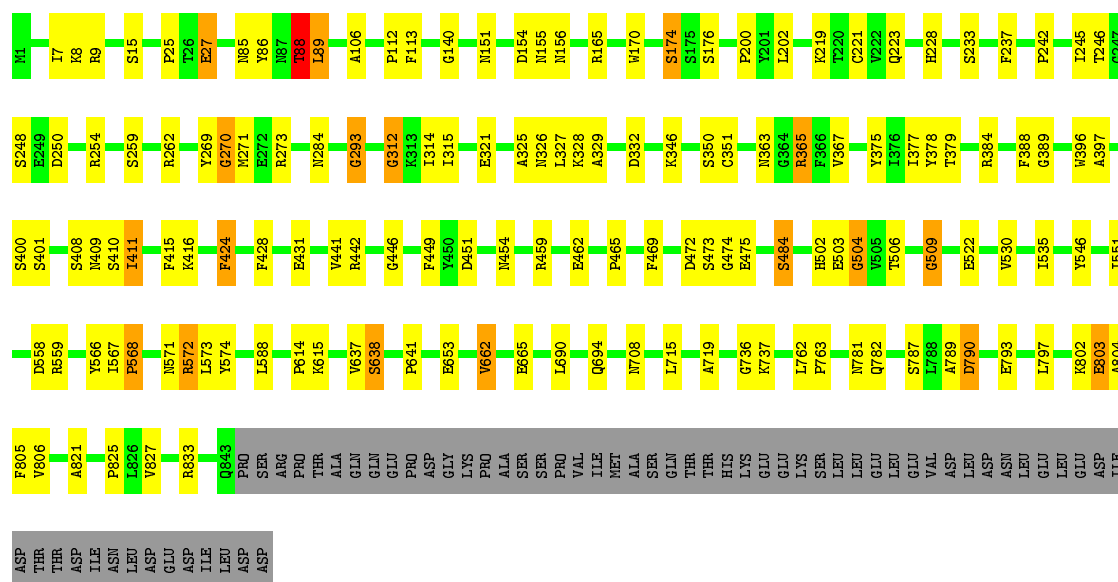
• Molecule 3: Coatomer subunit beta'

Chain 1-C: 77% 14% 7%



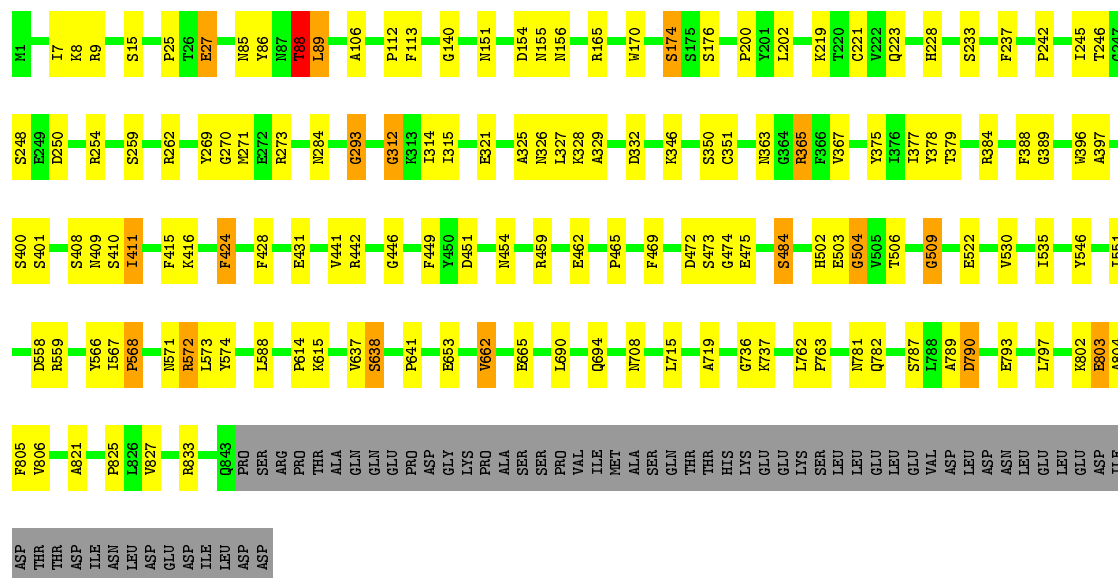
• Molecule 3: Coatomer subunit beta'

Chain 2-C: 77% 14% 7%

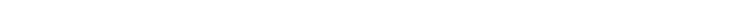


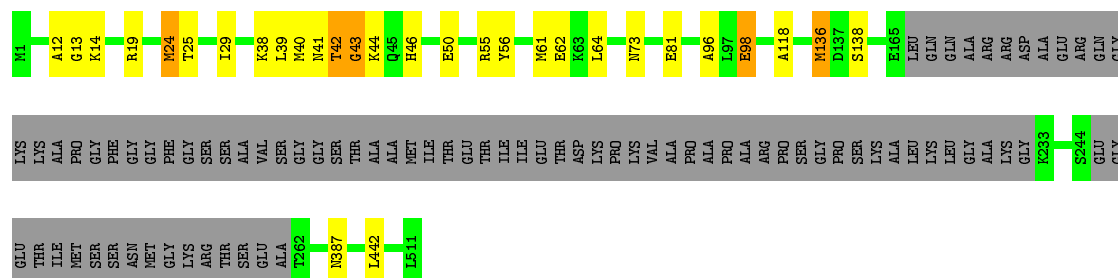
- Molecule 3: Coatomer subunit beta'

Chain 3-C:  77% 14% 7%



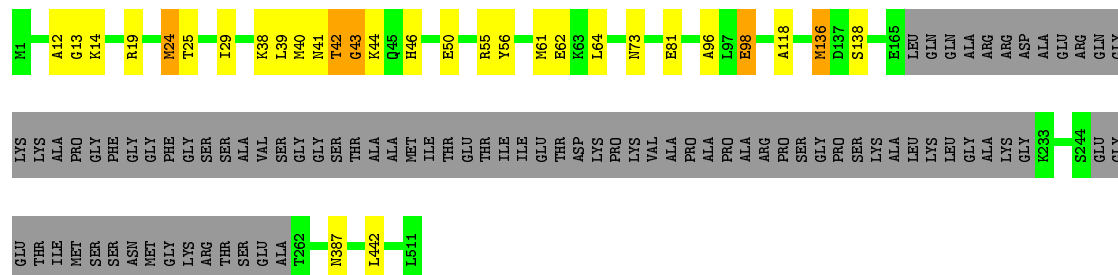
- Molecule 4: Coatomer subunit delta

Chain 1-D:  78% 5% • 16%



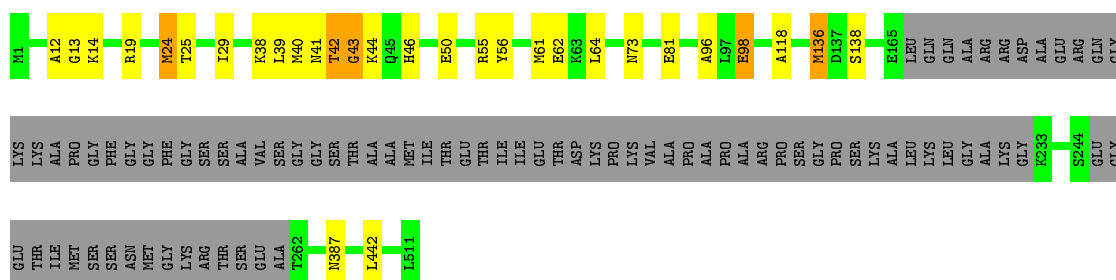
- Molecule 4: Coatomer subunit delta

Chain 2-D:  78% 5% • 16%



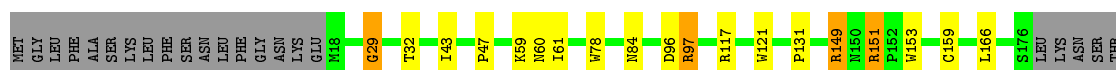
- Molecule 4: Coatomer subunit delta

Chain 3-D:  78% 5% • 16%



- Molecule 5: ADP-ribosylation factor 1

Chain 1-F: 77% 8% 12%



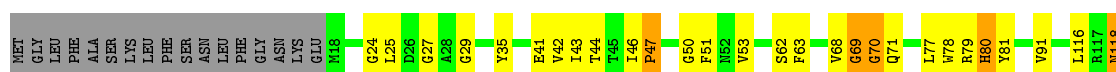
- Molecule 5: ADP-ribosylation factor 1

Chain 1-R: 55% 27% 7% 12%



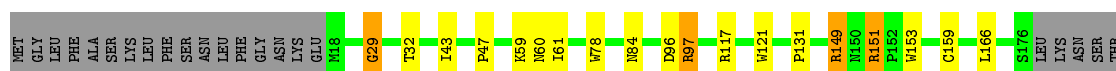
- Molecule 5: ADP-ribosylation factor 1

Chain 1-M: 64% 20% 12%



- Molecule 5: ADP-ribosylation factor 1

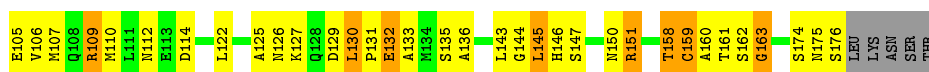
Chain 2-F: 77% 8% 12%



- Molecule 5: ADP-ribosylation factor 1

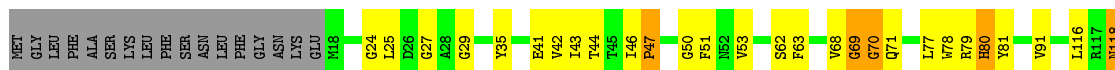
Chain 2-R: 54% 27% 7% 12%





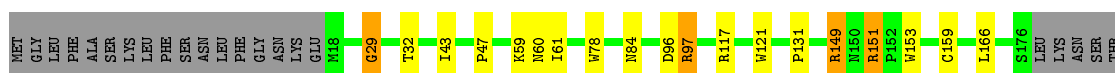
- Molecule 5: ADP-ribosylation factor 1

Chain 2-M: 64% 20% 12%



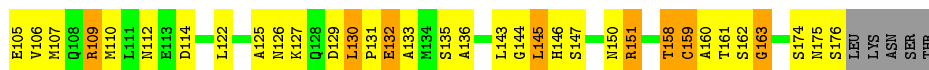
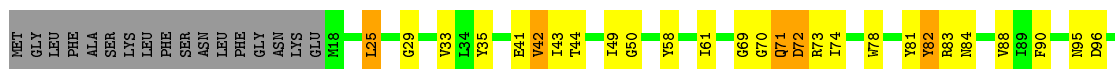
- Molecule 5: ADP-ribosylation factor 1

Chain 3-F: 77% 8% 12%



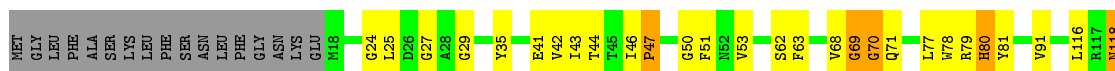
- Molecule 5: ADP-ribosylation factor 1

Chain 3-R: 54% 27% 7% 12%



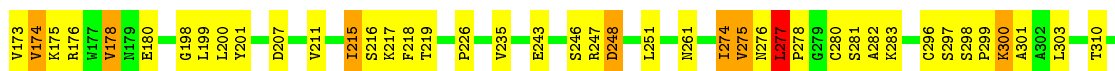
- Molecule 5: ADP-ribosylation factor 1

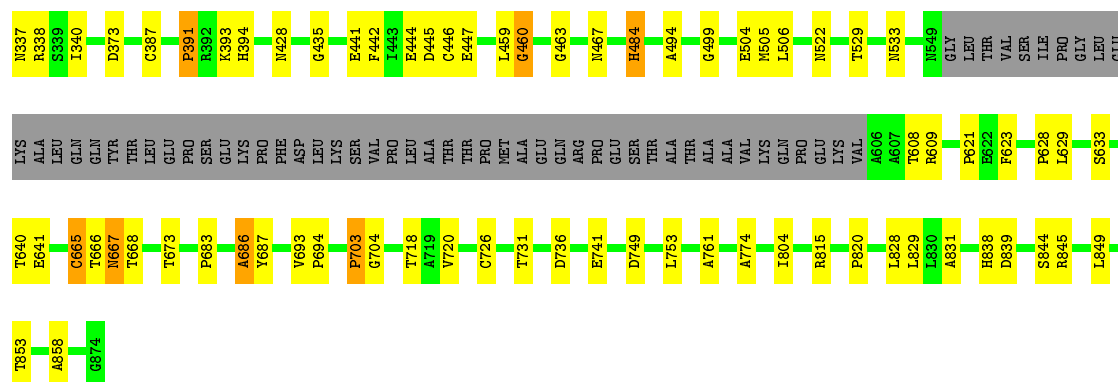
Chain 3-M: 64% 20% 12%



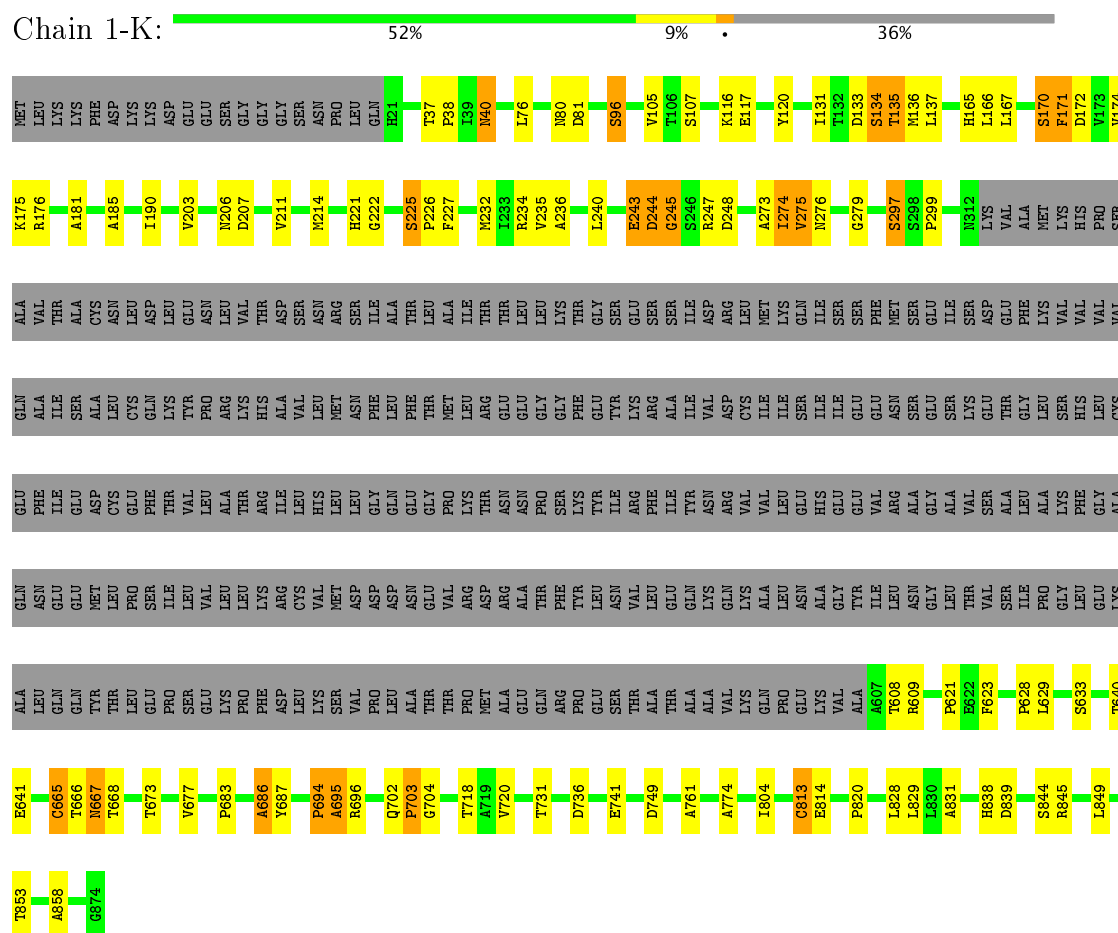
- Molecule 6: Coatomer subunit gamma-1

Chain 1-G: 75% 14% 9%

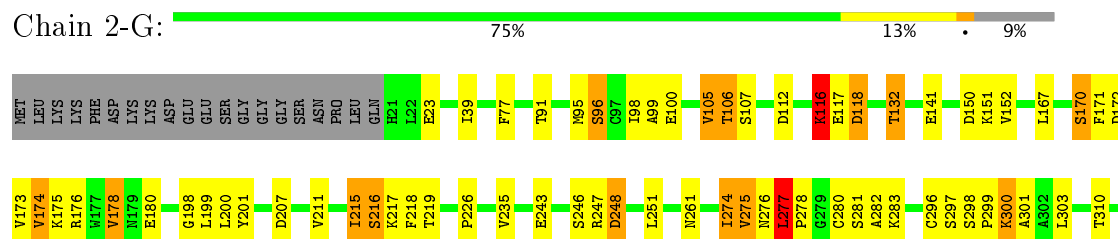




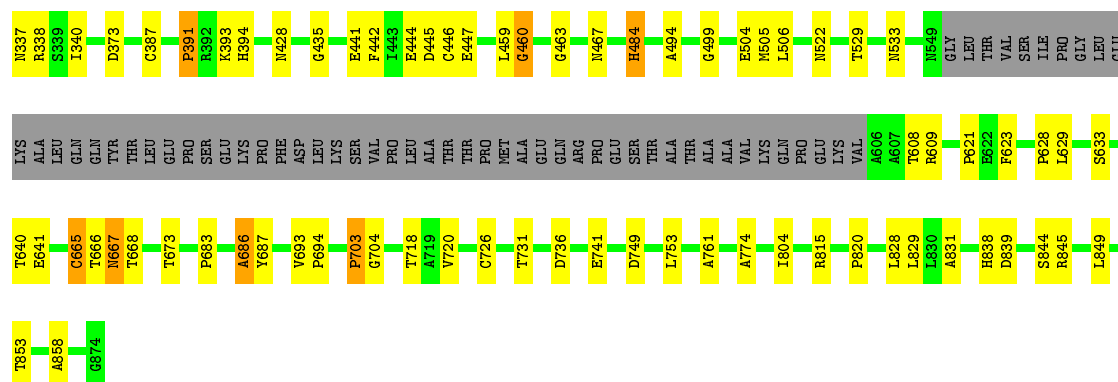
• Molecule 6: Coatomer subunit gamma-1



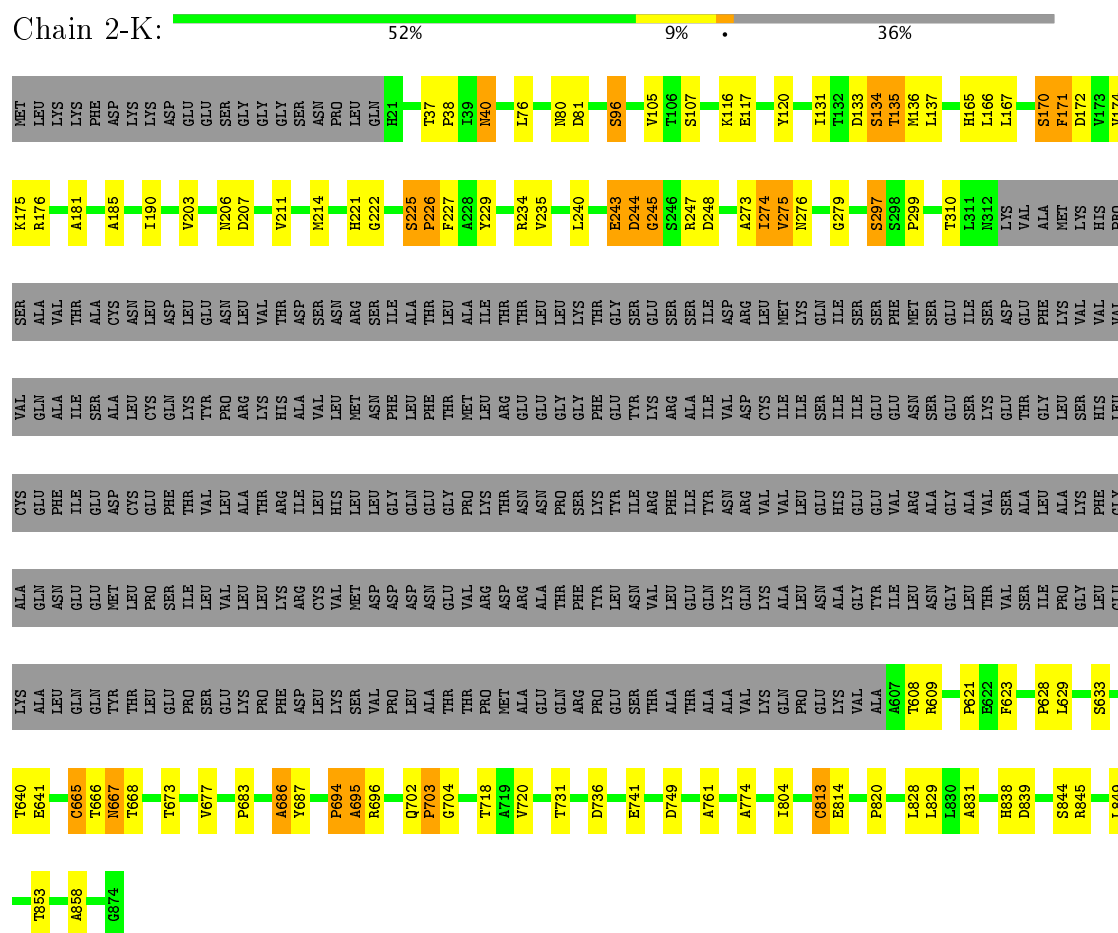
• Molecule 6: Coatomer subunit gamma-1



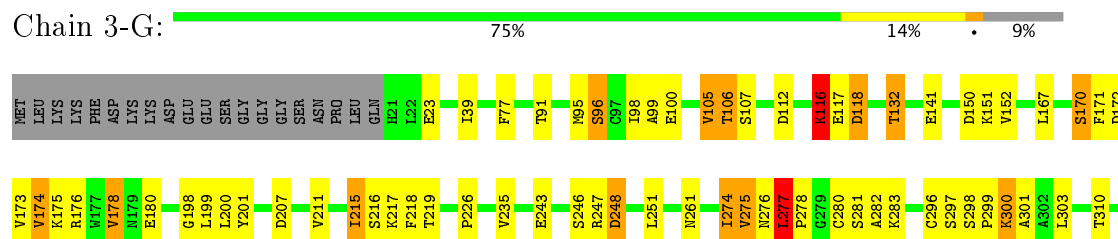


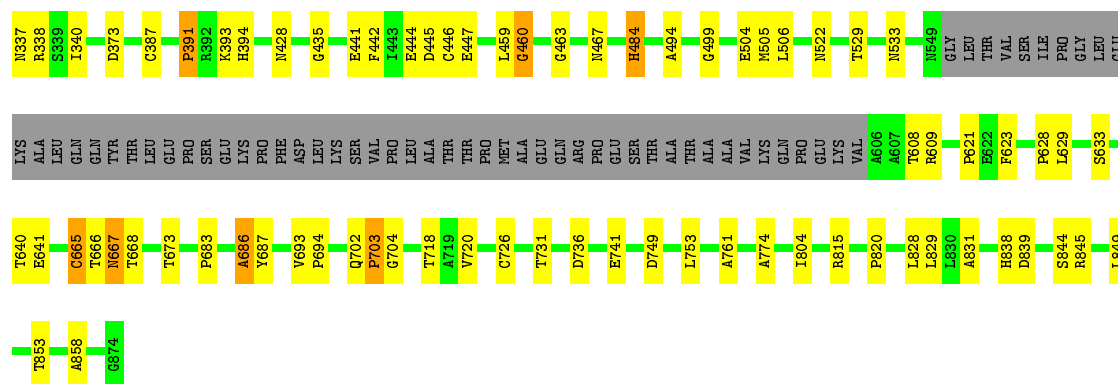


• Molecule 6: Coatomer subunit gamma-1

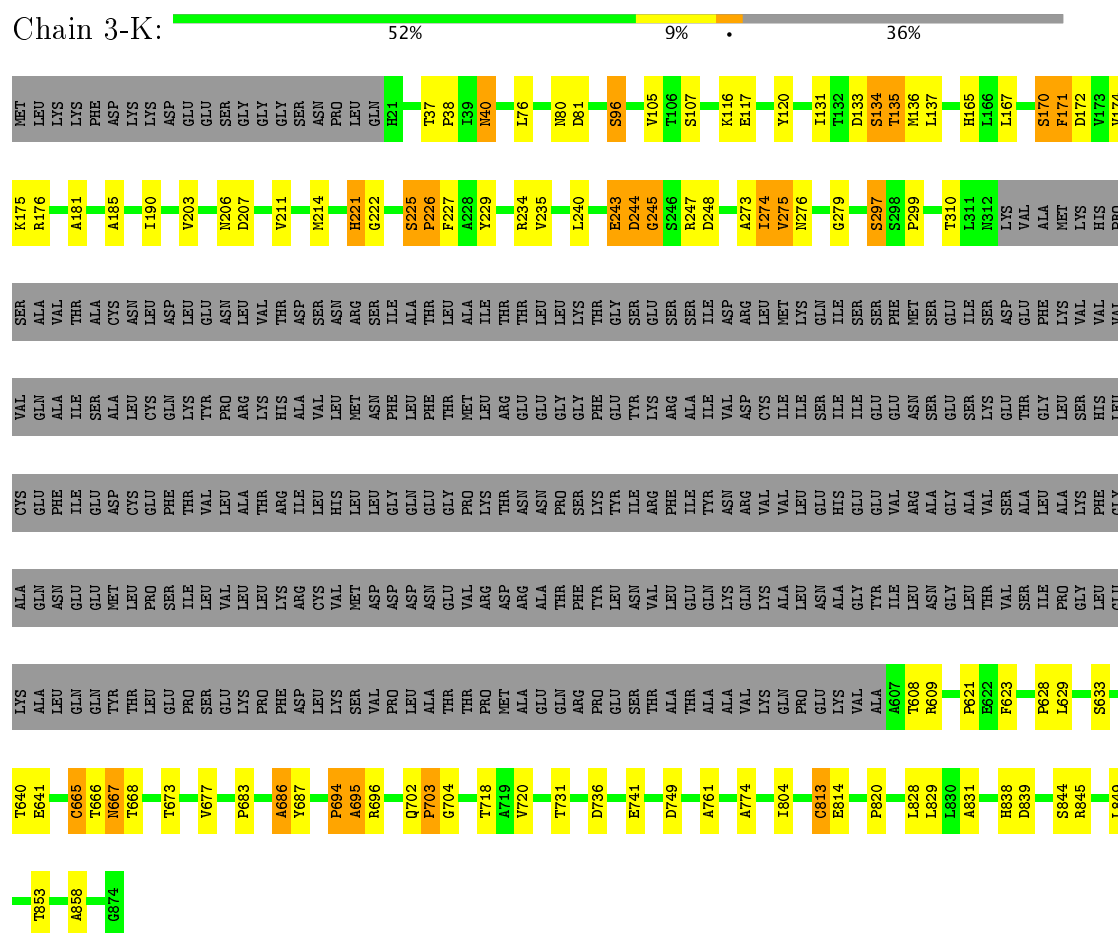


• Molecule 6: Coatomer subunit gamma-1

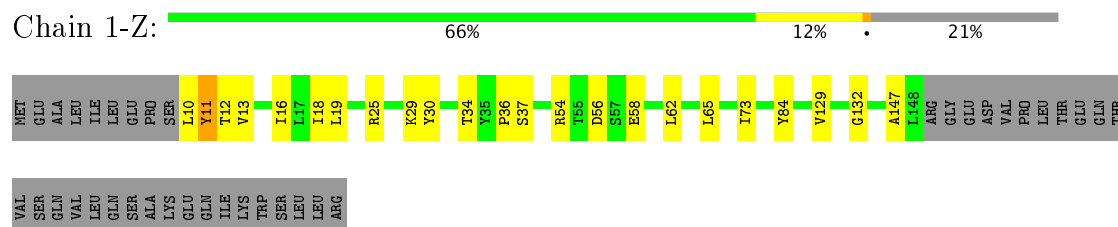




• Molecule 6: Coatomer subunit gamma-1

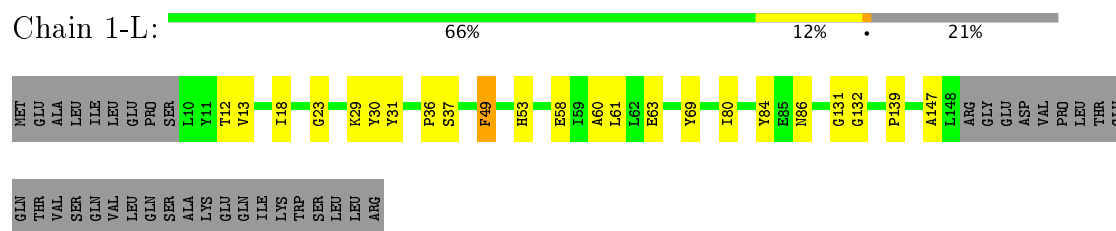


• Molecule 7: Coatomer subunit zeta-1



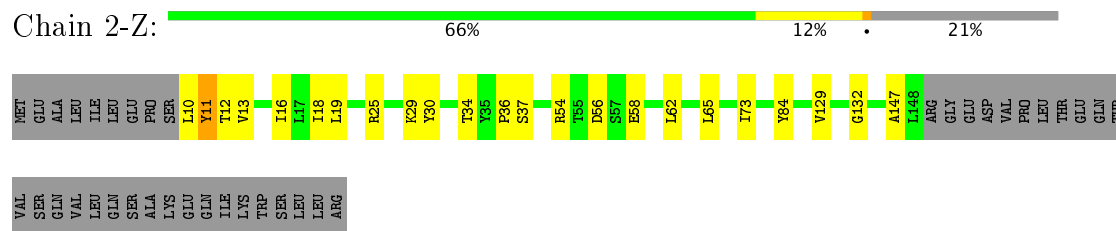
## • Molecule 7: Coatomer subunit zeta-1

Chain 1-L:



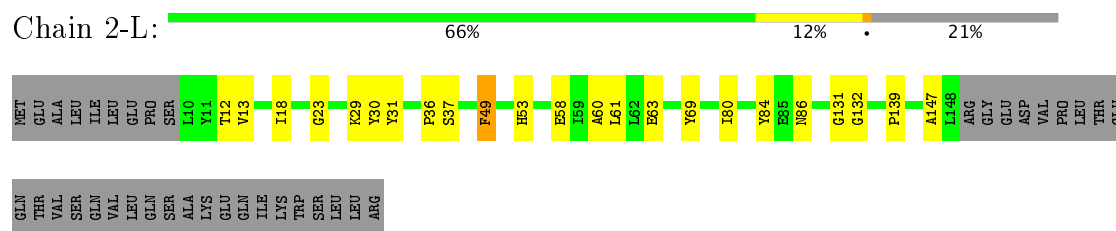
## • Molecule 7: Coatomer subunit zeta-1

Chain 2-Z:



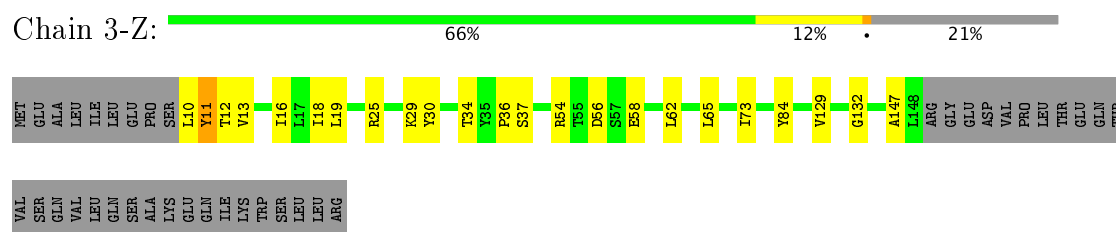
## • Molecule 7: Coatomer subunit zeta-1

Chain 2-L:



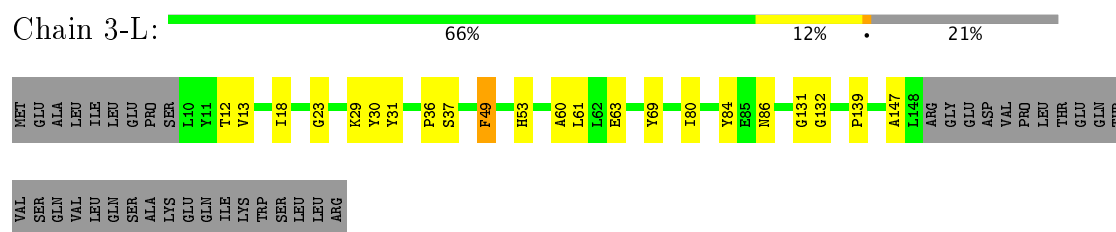
## • Molecule 7: Coatomer subunit zeta-1

Chain 3-Z:



## • Molecule 7: Coatomer subunit zeta-1

Chain 3-L:



## 4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	3312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF-determination for each individual tilt image was performed using CTFFIND4. Strip-based CTF-correction and tomogram reconstruction was performed in Imod.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

## 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	1-A	1.56	15/3250 (0.5%)	1.81	76/4061 (1.9%)
1	2-A	1.56	15/3250 (0.5%)	1.81	75/4061 (1.8%)
1	3-A	1.56	15/3250 (0.5%)	1.81	74/4061 (1.8%)
2	1-B	1.71	20/3193 (0.6%)	1.55	45/3983 (1.1%)
2	2-B	1.71	19/3193 (0.6%)	1.55	46/3983 (1.2%)
2	3-B	1.71	18/3193 (0.6%)	1.55	45/3983 (1.1%)
3	1-C	1.76	22/3370 (0.7%)	1.70	60/4211 (1.4%)
3	2-C	1.76	23/3370 (0.7%)	1.70	60/4211 (1.4%)
3	3-C	1.76	23/3370 (0.7%)	1.70	60/4211 (1.4%)
4	1-D	1.29	3/1704 (0.2%)	1.24	10/2124 (0.5%)
4	2-D	1.29	3/1704 (0.2%)	1.24	10/2124 (0.5%)
4	3-D	1.29	3/1704 (0.2%)	1.24	10/2124 (0.5%)
5	1-F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	1-M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	1-R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
5	2-F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	2-M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	2-R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
5	3-F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	3-M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	3-R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
6	1-G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	1-K	1.72	9/2237 (0.4%)	1.69	43/2793 (1.5%)
6	2-G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	2-K	1.72	9/2237 (0.4%)	1.69	43/2793 (1.5%)
6	3-G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	3-K	1.72	9/2237 (0.4%)	1.69	44/2793 (1.6%)
7	1-L	2.05	3/554 (0.5%)	1.72	8/691 (1.2%)
7	1-Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
7	2-L	2.05	3/554 (0.5%)	1.72	8/691 (1.2%)
7	2-Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
7	3-L	2.05	3/554 (0.5%)	1.72	7/691 (1.0%)
7	3-Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
All	All	1.66	302/59856 (0.5%)	1.65	991/74727 (1.3%)

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
2	1-B	0	3
2	2-B	0	3
2	3-B	0	3
All	All	0	9

All (302) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	940	GLY	N-CA	-7.79	1.34	1.46
2	3-B	940	GLY	N-CA	-7.76	1.34	1.46
2	2-B	940	GLY	N-CA	-7.75	1.34	1.46
5	1-R	29	GLY	CA-C	-7.64	1.39	1.51
5	2-R	29	GLY	CA-C	-7.62	1.39	1.51
5	3-R	29	GLY	CA-C	-7.58	1.39	1.51
5	1-R	35	TYR	CA-C	-7.35	1.33	1.52
5	2-R	35	TYR	CA-C	-7.34	1.33	1.52
5	3-R	35	TYR	CA-C	-7.33	1.33	1.52
1	2-A	191	GLY	CA-C	-7.05	1.40	1.51
1	3-A	191	GLY	CA-C	-7.05	1.40	1.51
1	1-A	191	GLY	CA-C	-7.03	1.40	1.51
3	2-C	572	ARG	CA-C	-6.61	1.35	1.52
3	3-C	572	ARG	CA-C	-6.60	1.35	1.52
3	1-C	572	ARG	CA-C	-6.59	1.35	1.52
2	1-B	418	PRO	CA-C	-6.59	1.39	1.52
2	2-B	418	PRO	CA-C	-6.58	1.39	1.52
6	1-K	235	VAL	N-CA	-6.57	1.33	1.46
1	3-A	594	PRO	CA-C	-6.57	1.39	1.52
1	2-A	594	PRO	CA-C	-6.57	1.39	1.52
1	1-A	594	PRO	CA-C	-6.56	1.39	1.52
6	1-G	215	ILE	CA-C	-6.56	1.35	1.52
2	3-B	418	PRO	CA-C	-6.55	1.39	1.52
6	3-G	215	ILE	CA-C	-6.54	1.35	1.52
6	2-K	235	VAL	N-CA	-6.54	1.33	1.46
6	2-G	215	ILE	CA-C	-6.53	1.35	1.52
6	3-K	235	VAL	N-CA	-6.51	1.33	1.46
4	3-D	55	ARG	CA-C	-6.45	1.36	1.52
4	2-D	55	ARG	CA-C	-6.44	1.36	1.52
1	1-A	612	LEU	N-CA	-6.43	1.33	1.46
1	2-A	612	LEU	N-CA	-6.43	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-D	55	ARG	CA-C	-6.42	1.36	1.52
1	3-A	612	LEU	N-CA	-6.39	1.33	1.46
1	1-A	766	GLY	CA-C	-6.37	1.41	1.51
6	1-G	839	ASP	CA-C	-6.35	1.36	1.52
5	3-R	109	ARG	CA-C	-6.35	1.36	1.52
6	2-G	839	ASP	CA-C	-6.34	1.36	1.52
1	3-A	766	GLY	CA-C	-6.34	1.41	1.51
6	1-K	839	ASP	CA-C	-6.34	1.36	1.52
5	2-R	109	ARG	CA-C	-6.34	1.36	1.52
6	3-G	839	ASP	CA-C	-6.32	1.36	1.52
6	2-K	211	VAL	CA-C	-6.32	1.36	1.52
6	2-K	839	ASP	CA-C	-6.31	1.36	1.52
5	1-R	109	ARG	CA-C	-6.31	1.36	1.52
6	3-K	839	ASP	CA-C	-6.31	1.36	1.52
1	2-A	766	GLY	CA-C	-6.31	1.41	1.51
6	3-K	211	VAL	CA-C	-6.29	1.36	1.52
6	1-K	211	VAL	CA-C	-6.28	1.36	1.52
6	3-K	214	MET	CA-C	-6.24	1.36	1.52
6	2-K	214	MET	CA-C	-6.22	1.36	1.52
6	1-K	214	MET	CA-C	-6.21	1.36	1.52
7	2-Z	19	LEU	N-CA	-6.21	1.33	1.46
7	3-Z	19	LEU	N-CA	-6.20	1.33	1.46
7	1-Z	19	LEU	N-CA	-6.19	1.33	1.46
3	1-C	293	GLY	CA-C	-6.17	1.42	1.51
3	3-C	293	GLY	CA-C	-6.17	1.42	1.51
3	3-C	416	LYS	CA-C	-6.16	1.36	1.52
3	2-C	293	GLY	CA-C	-6.16	1.42	1.51
3	2-C	416	LYS	CA-C	-6.16	1.36	1.52
3	1-C	416	LYS	CA-C	-6.12	1.37	1.52
3	2-C	378	TYR	CA-C	-6.12	1.37	1.52
3	1-C	378	TYR	CA-C	-6.10	1.37	1.52
5	2-M	29	GLY	CA-C	-6.10	1.42	1.51
3	3-C	378	TYR	CA-C	-6.10	1.37	1.52
5	3-M	29	GLY	CA-C	-6.09	1.42	1.51
5	1-M	29	GLY	CA-C	-6.05	1.42	1.51
7	1-L	23	GLY	CA-C	-6.04	1.42	1.51
1	1-A	596	GLU	N-CA	-6.04	1.34	1.46
5	2-M	47	PRO	CA-C	-6.04	1.40	1.52
5	1-M	70	GLY	CA-C	-6.03	1.42	1.51
5	3-M	47	PRO	CA-C	-6.03	1.40	1.52
5	3-M	70	GLY	CA-C	-6.02	1.42	1.51
5	1-M	47	PRO	CA-C	-6.02	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	596	GLU	N-CA	-6.01	1.34	1.46
6	1-G	774	ALA	N-CA	-6.01	1.34	1.46
1	2-A	596	GLU	N-CA	-6.01	1.34	1.46
6	2-G	774	ALA	N-CA	-6.01	1.34	1.46
5	2-M	70	GLY	CA-C	-6.00	1.42	1.51
6	3-K	774	ALA	N-CA	-5.98	1.34	1.46
7	2-L	23	GLY	CA-C	-5.97	1.42	1.51
3	2-C	641	PRO	CA-C	-5.97	1.41	1.52
7	3-L	23	GLY	CA-C	-5.97	1.42	1.51
6	1-K	774	ALA	N-CA	-5.96	1.34	1.46
2	1-B	762	ASN	CA-C	-5.96	1.37	1.52
6	3-G	774	ALA	N-CA	-5.96	1.34	1.46
6	2-K	774	ALA	N-CA	-5.96	1.34	1.46
2	3-B	762	ASN	CA-C	-5.95	1.37	1.52
2	2-B	762	ASN	CA-C	-5.92	1.37	1.52
3	3-C	641	PRO	CA-C	-5.91	1.41	1.52
3	1-C	641	PRO	CA-C	-5.91	1.41	1.52
3	3-C	384	ARG	CA-C	-5.87	1.37	1.52
3	1-C	384	ARG	CA-C	-5.86	1.37	1.52
3	2-C	384	ARG	CA-C	-5.85	1.37	1.52
6	2-K	105	VAL	N-CA	-5.79	1.34	1.46
2	3-B	940	GLY	CA-C	-5.79	1.42	1.51
2	2-B	126	HIS	CA-C	-5.78	1.38	1.52
2	1-B	126	HIS	CA-C	-5.77	1.38	1.52
6	1-K	105	VAL	N-CA	-5.77	1.34	1.46
6	3-K	105	VAL	N-CA	-5.77	1.34	1.46
2	2-B	940	GLY	CA-C	-5.76	1.42	1.51
2	3-B	126	HIS	CA-C	-5.75	1.38	1.52
2	1-B	940	GLY	CA-C	-5.75	1.42	1.51
3	2-C	377	ILE	CA-C	-5.72	1.38	1.52
3	3-C	377	ILE	CA-C	-5.71	1.38	1.52
3	1-C	377	ILE	CA-C	-5.70	1.38	1.52
5	1-F	29	GLY	N-CA	-5.65	1.37	1.46
5	3-F	29	GLY	N-CA	-5.64	1.37	1.46
5	2-F	29	GLY	N-CA	-5.63	1.37	1.46
3	1-C	245	ILE	N-CA	-5.61	1.35	1.46
3	3-C	245	ILE	N-CA	-5.60	1.35	1.46
1	1-A	660	ILE	CA-C	-5.58	1.38	1.52
1	3-A	660	ILE	CA-C	-5.58	1.38	1.52
3	2-C	245	ILE	N-CA	-5.58	1.35	1.46
1	2-A	660	ILE	CA-C	-5.57	1.38	1.52
6	1-G	235	VAL	N-CA	-5.56	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	3-G	235	VAL	N-CA	-5.55	1.35	1.46
2	2-B	378	GLU	CA-C	-5.54	1.38	1.52
6	2-G	235	VAL	N-CA	-5.54	1.35	1.46
2	3-B	378	GLU	CA-C	-5.53	1.38	1.52
1	3-A	679	GLU	CA-C	-5.53	1.38	1.52
3	2-C	568	PRO	CA-C	-5.53	1.41	1.52
3	3-C	568	PRO	CA-C	-5.53	1.41	1.52
6	2-G	442	PHE	CA-C	-5.52	1.38	1.52
1	1-A	679	GLU	CA-C	-5.52	1.38	1.52
6	3-G	442	PHE	CA-C	-5.52	1.38	1.52
1	2-A	679	GLU	CA-C	-5.51	1.38	1.52
2	1-B	378	GLU	CA-C	-5.51	1.38	1.52
7	2-Z	65	LEU	N-CA	-5.51	1.35	1.46
7	1-Z	65	LEU	N-CA	-5.51	1.35	1.46
1	1-A	360	GLY	CA-C	-5.51	1.43	1.51
3	1-C	568	PRO	CA-C	-5.50	1.41	1.52
6	1-G	442	PHE	CA-C	-5.50	1.38	1.52
6	3-K	165	HIS	CA-C	-5.48	1.38	1.52
6	1-K	165	HIS	CA-C	-5.48	1.38	1.52
6	1-K	203	VAL	N-CA	-5.48	1.35	1.46
6	3-K	203	VAL	N-CA	-5.48	1.35	1.46
2	3-B	753	ASP	N-CA	-5.47	1.35	1.46
7	3-Z	65	LEU	N-CA	-5.47	1.35	1.46
6	2-K	165	HIS	CA-C	-5.46	1.38	1.52
1	2-A	360	GLY	CA-C	-5.46	1.43	1.51
1	3-A	595	THR	N-CA	-5.46	1.35	1.46
1	3-A	360	GLY	CA-C	-5.46	1.43	1.51
2	1-B	753	ASP	N-CA	-5.45	1.35	1.46
6	2-K	203	VAL	N-CA	-5.45	1.35	1.46
2	2-B	753	ASP	N-CA	-5.44	1.35	1.46
1	1-A	600	LYS	CA-C	-5.44	1.38	1.52
1	2-A	600	LYS	CA-C	-5.44	1.38	1.52
6	2-G	180	GLU	N-CA	-5.43	1.35	1.46
1	1-A	599	PHE	N-CA	-5.43	1.35	1.46
1	3-A	599	PHE	N-CA	-5.43	1.35	1.46
3	1-C	449	PHE	CA-C	-5.43	1.38	1.52
1	3-A	600	LYS	CA-C	-5.42	1.38	1.52
3	2-C	449	PHE	CA-C	-5.42	1.38	1.52
3	3-C	449	PHE	CA-C	-5.41	1.38	1.52
2	1-B	749	VAL	CA-C	-5.40	1.39	1.52
1	2-A	599	PHE	N-CA	-5.40	1.35	1.46
5	2-R	90	PHE	N-CA	-5.40	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	595	THR	N-CA	-5.39	1.35	1.46
1	1-A	595	THR	N-CA	-5.39	1.35	1.46
6	3-G	112	ASP	CA-C	-5.39	1.39	1.52
6	1-G	112	ASP	CA-C	-5.38	1.39	1.52
6	3-G	180	GLU	N-CA	-5.38	1.35	1.46
2	3-B	749	VAL	CA-C	-5.38	1.39	1.52
6	1-G	180	GLU	N-CA	-5.38	1.35	1.46
6	2-G	112	ASP	CA-C	-5.38	1.39	1.52
2	1-B	938	VAL	CA-C	-5.37	1.39	1.52
4	3-D	56	TYR	CA-C	-5.36	1.39	1.52
4	1-D	56	TYR	CA-C	-5.36	1.39	1.52
2	3-B	938	VAL	CA-C	-5.36	1.39	1.52
1	2-A	612	LEU	CA-C	-5.36	1.39	1.52
5	3-R	90	PHE	N-CA	-5.36	1.35	1.46
5	1-R	90	PHE	N-CA	-5.36	1.35	1.46
2	2-B	749	VAL	CA-C	-5.35	1.39	1.52
3	1-C	8	LYS	CA-C	-5.35	1.39	1.52
2	2-B	938	VAL	CA-C	-5.35	1.39	1.52
4	2-D	56	TYR	CA-C	-5.35	1.39	1.52
1	1-A	612	LEU	CA-C	-5.35	1.39	1.52
1	3-A	612	LEU	CA-C	-5.35	1.39	1.52
4	2-D	81	GLU	CA-C	-5.34	1.39	1.52
2	2-B	783	LEU	CA-C	-5.34	1.39	1.52
4	3-D	81	GLU	CA-C	-5.34	1.39	1.52
3	3-C	312	GLY	CA-C	-5.34	1.43	1.51
3	2-C	312	GLY	CA-C	-5.34	1.43	1.51
4	1-D	81	GLU	CA-C	-5.33	1.39	1.52
5	3-R	107	MET	CA-C	-5.33	1.39	1.52
2	2-B	754	ILE	N-CA	-5.33	1.35	1.46
3	3-C	223	GLN	CA-C	-5.32	1.39	1.52
3	2-C	223	GLN	CA-C	-5.32	1.39	1.52
7	3-Z	19	LEU	CA-C	-5.32	1.39	1.52
5	1-R	107	MET	CA-C	-5.31	1.39	1.52
3	1-C	315	ILE	N-CA	-5.31	1.35	1.46
2	3-B	783	LEU	CA-C	-5.31	1.39	1.52
1	1-A	283	GLY	CA-C	-5.31	1.43	1.51
5	2-R	107	MET	CA-C	-5.31	1.39	1.52
3	1-C	223	GLN	CA-C	-5.31	1.39	1.52
2	1-B	783	LEU	CA-C	-5.30	1.39	1.52
3	2-C	8	LYS	CA-C	-5.30	1.39	1.52
1	3-A	283	GLY	CA-C	-5.30	1.43	1.51
3	3-C	315	ILE	N-CA	-5.30	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-C	8	LYS	CA-C	-5.30	1.39	1.52
1	2-A	283	GLY	CA-C	-5.30	1.43	1.51
7	2-Z	19	LEU	CA-C	-5.29	1.39	1.52
2	3-B	754	ILE	N-CA	-5.29	1.35	1.46
7	1-Z	19	LEU	CA-C	-5.29	1.39	1.52
2	1-B	754	ILE	N-CA	-5.29	1.35	1.46
3	1-C	312	GLY	CA-C	-5.29	1.43	1.51
2	1-B	368	VAL	N-CA	-5.28	1.35	1.46
7	2-L	49	PHE	CA-C	-5.28	1.39	1.52
3	1-C	85	ASN	N-CA	-5.27	1.35	1.46
1	3-A	610	GLU	N-CA	-5.27	1.35	1.46
3	3-C	415	PHE	CA-C	-5.26	1.39	1.52
7	1-L	49	PHE	CA-C	-5.26	1.39	1.52
3	2-C	85	ASN	N-CA	-5.26	1.35	1.46
3	3-C	85	ASN	N-CA	-5.26	1.35	1.46
1	2-A	610	GLU	N-CA	-5.26	1.35	1.46
1	1-A	610	GLU	N-CA	-5.26	1.35	1.46
2	1-B	759	LEU	N-CA	-5.26	1.35	1.46
7	3-L	49	PHE	CA-C	-5.25	1.39	1.52
2	3-B	368	VAL	N-CA	-5.25	1.35	1.46
3	1-C	415	PHE	CA-C	-5.25	1.39	1.52
2	2-B	368	VAL	N-CA	-5.25	1.35	1.46
2	2-B	759	LEU	N-CA	-5.24	1.35	1.46
3	2-C	315	ILE	N-CA	-5.24	1.35	1.46
3	3-C	736	GLY	CA-C	-5.24	1.43	1.51
3	1-C	736	GLY	CA-C	-5.24	1.43	1.51
3	2-C	736	GLY	CA-C	-5.24	1.43	1.51
5	2-R	105	GLU	CA-C	-5.24	1.39	1.52
2	3-B	440	ARG	CA-C	-5.23	1.39	1.52
2	2-B	440	ARG	CA-C	-5.23	1.39	1.52
3	2-C	415	PHE	CA-C	-5.23	1.39	1.52
2	3-B	759	LEU	N-CA	-5.22	1.35	1.46
2	1-B	440	ARG	CA-C	-5.22	1.39	1.52
5	1-R	105	GLU	CA-C	-5.21	1.39	1.52
3	2-C	379	THR	N-CA	-5.20	1.35	1.46
5	3-R	105	GLU	CA-C	-5.20	1.39	1.52
2	2-B	750	ASN	N-CA	-5.19	1.35	1.46
2	1-B	750	ASN	N-CA	-5.19	1.35	1.46
3	1-C	379	THR	N-CA	-5.18	1.35	1.46
6	3-G	499	GLY	CA-C	-5.18	1.43	1.51
2	3-B	750	ASN	N-CA	-5.18	1.35	1.46
3	3-C	379	THR	N-CA	-5.16	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1-G	499	GLY	CA-C	-5.16	1.43	1.51
2	1-B	375	LEU	CA-C	-5.15	1.39	1.52
1	2-A	631	LYS	N-CA	-5.14	1.36	1.46
2	3-B	375	LEU	CA-C	-5.13	1.39	1.52
3	3-C	573	LEU	CA-C	-5.13	1.39	1.52
2	2-B	317	LEU	CA-C	-5.13	1.39	1.52
3	1-C	367	VAL	CA-C	-5.12	1.39	1.52
5	1-R	33	VAL	N-CA	-5.12	1.36	1.46
1	3-A	631	LYS	N-CA	-5.12	1.36	1.46
6	2-G	460	GLY	CA-C	-5.12	1.43	1.51
5	2-R	110	MET	CA-C	-5.12	1.39	1.52
3	1-C	573	LEU	CA-C	-5.12	1.39	1.52
6	1-G	174	VAL	CA-C	-5.12	1.39	1.52
5	1-R	110	MET	CA-C	-5.12	1.39	1.52
5	2-M	35	TYR	CA-C	-5.12	1.39	1.52
6	2-G	174	VAL	CA-C	-5.12	1.39	1.52
6	3-G	174	VAL	CA-C	-5.12	1.39	1.52
3	2-C	367	VAL	CA-C	-5.11	1.39	1.52
2	1-B	317	LEU	CA-C	-5.11	1.39	1.52
3	3-C	367	VAL	CA-C	-5.11	1.39	1.52
6	3-G	460	GLY	CA-C	-5.11	1.43	1.51
5	3-R	33	VAL	N-CA	-5.10	1.36	1.46
5	3-M	35	TYR	CA-C	-5.10	1.39	1.52
2	3-B	317	LEU	CA-C	-5.10	1.39	1.52
1	1-A	631	LYS	N-CA	-5.10	1.36	1.46
5	1-M	35	TYR	CA-C	-5.10	1.39	1.52
3	2-C	573	LEU	CA-C	-5.10	1.39	1.52
6	2-G	499	GLY	CA-C	-5.10	1.43	1.51
5	2-R	33	VAL	N-CA	-5.09	1.36	1.46
5	3-R	110	MET	CA-C	-5.09	1.39	1.52
2	2-B	375	LEU	CA-C	-5.08	1.39	1.52
7	3-L	139	PRO	CA-C	-5.08	1.42	1.52
6	1-G	460	GLY	CA-C	-5.07	1.43	1.51
7	2-L	139	PRO	CA-C	-5.07	1.42	1.52
5	2-R	96	ASP	CA-C	-5.06	1.39	1.52
6	3-K	234	ARG	CA-C	-5.05	1.39	1.52
3	3-C	535	ILE	N-CA	-5.05	1.36	1.46
6	3-G	91	THR	N-CA	-5.05	1.36	1.46
6	2-G	91	THR	N-CA	-5.04	1.36	1.46
5	3-R	106	VAL	N-CA	-5.04	1.36	1.46
2	1-B	374	VAL	N-CA	-5.04	1.36	1.46
6	1-K	234	ARG	CA-C	-5.04	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-L	139	PRO	CA-C	-5.04	1.42	1.52
3	1-C	314	ILE	CA-C	-5.04	1.39	1.52
3	3-C	314	ILE	CA-C	-5.03	1.39	1.52
5	1-R	96	ASP	CA-C	-5.03	1.39	1.52
6	1-G	91	THR	N-CA	-5.03	1.36	1.46
5	1-R	106	VAL	N-CA	-5.03	1.36	1.46
5	3-R	96	ASP	CA-C	-5.03	1.39	1.52
2	1-B	349	LEU	CA-C	-5.02	1.40	1.52
6	2-K	234	ARG	CA-C	-5.02	1.40	1.52
2	3-B	374	VAL	N-CA	-5.02	1.36	1.46
3	2-C	535	ILE	N-CA	-5.01	1.36	1.46
3	1-C	535	ILE	N-CA	-5.01	1.36	1.46
3	3-C	588	LEU	N-CA	-5.01	1.36	1.46
2	2-B	300	TYR	CA-C	-5.01	1.40	1.52
2	2-B	374	VAL	N-CA	-5.01	1.36	1.46
5	2-R	106	VAL	N-CA	-5.00	1.36	1.46
2	1-B	799	ASN	CA-C	-5.00	1.40	1.52
3	2-C	314	ILE	CA-C	-5.00	1.40	1.52
3	2-C	588	LEU	N-CA	-5.00	1.36	1.46

All (991) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	343	GLN	N-CA-C	-9.88	84.32	111.00
1	1-A	343	GLN	N-CA-C	-9.86	84.38	111.00
1	3-A	343	GLN	N-CA-C	-9.86	84.38	111.00
6	3-K	117	GLU	C-N-CA	9.77	146.12	121.70
6	2-K	117	GLU	C-N-CA	9.76	146.10	121.70
6	1-K	117	GLU	C-N-CA	9.74	146.05	121.70
2	1-B	326	HIS	N-CA-C	-9.60	85.09	111.00
2	3-B	326	HIS	N-CA-C	-9.58	85.14	111.00
2	2-B	326	HIS	N-CA-C	-9.57	85.15	111.00
6	1-G	96	SER	N-CA-C	9.11	135.59	111.00
6	2-G	96	SER	N-CA-C	9.10	135.57	111.00
6	3-G	96	SER	N-CA-C	9.09	135.55	111.00
2	2-B	940	GLY	N-CA-C	-9.04	90.49	113.10
2	3-B	940	GLY	N-CA-C	-9.03	90.52	113.10
2	1-B	940	GLY	N-CA-C	-9.02	90.55	113.10
3	2-C	416	LYS	N-CA-C	-8.88	87.02	111.00
3	1-C	416	LYS	N-CA-C	-8.88	87.03	111.00
3	3-C	416	LYS	N-CA-C	-8.88	87.04	111.00
2	3-B	760	VAL	N-CA-C	-8.57	87.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	760	VAL	N-CA-C	-8.57	87.87	111.00
1	1-A	229	VAL	N-CA-C	-8.56	87.88	111.00
1	2-A	229	VAL	N-CA-C	-8.56	87.88	111.00
2	2-B	760	VAL	N-CA-C	-8.56	87.90	111.00
1	3-A	229	VAL	N-CA-C	-8.55	87.92	111.00
4	1-D	61	MET	N-CA-C	-8.53	87.97	111.00
4	3-D	61	MET	N-CA-C	-8.53	87.98	111.00
2	2-B	67	GLY	N-CA-C	-8.53	91.79	113.10
2	1-B	67	GLY	N-CA-C	-8.52	91.80	113.10
4	2-D	61	MET	N-CA-C	-8.52	88.00	111.00
2	3-B	67	GLY	N-CA-C	-8.51	91.82	113.10
5	1-R	150	ASN	C-N-CA	8.42	142.75	121.70
5	2-R	150	ASN	C-N-CA	8.41	142.72	121.70
5	3-R	150	ASN	C-N-CA	8.39	142.67	121.70
1	1-A	740	GLY	N-CA-C	-8.38	92.15	113.10
1	3-A	740	GLY	N-CA-C	-8.37	92.17	113.10
1	2-A	740	GLY	N-CA-C	-8.36	92.21	113.10
5	2-F	59	LYS	C-N-CA	8.30	142.45	121.70
5	3-F	59	LYS	C-N-CA	8.28	142.40	121.70
5	1-F	59	LYS	C-N-CA	8.27	142.38	121.70
1	2-A	631	LYS	N-CA-C	-8.21	88.84	111.00
1	3-A	631	LYS	N-CA-C	-8.20	88.85	111.00
1	1-A	631	LYS	N-CA-C	-8.20	88.86	111.00
5	2-R	122	LEU	N-CA-C	-8.19	88.90	111.00
5	3-R	122	LEU	N-CA-C	-8.18	88.91	111.00
5	1-R	122	LEU	N-CA-C	-8.17	88.94	111.00
1	1-A	491	VAL	C-N-CA	8.16	142.09	121.70
1	2-A	491	VAL	C-N-CA	8.16	142.09	121.70
1	3-A	491	VAL	C-N-CA	8.16	142.09	121.70
2	3-B	759	LEU	N-CA-C	-8.08	89.19	111.00
2	2-B	759	LEU	N-CA-C	-8.07	89.21	111.00
2	1-B	759	LEU	N-CA-C	-8.06	89.23	111.00
1	2-A	504	ALA	N-CA-C	-8.00	89.40	111.00
1	3-A	504	ALA	N-CA-C	-7.99	89.42	111.00
1	1-A	504	ALA	N-CA-C	-7.99	89.44	111.00
4	2-D	56	TYR	N-CA-C	-7.92	89.60	111.00
4	3-D	56	TYR	N-CA-C	-7.91	89.66	111.00
4	1-D	56	TYR	N-CA-C	-7.90	89.66	111.00
1	3-A	789	ASP	N-CA-C	-7.90	89.67	111.00
1	1-A	789	ASP	N-CA-C	-7.90	89.67	111.00
1	2-A	789	ASP	N-CA-C	-7.88	89.71	111.00
6	3-G	829	LEU	N-CA-C	-7.84	89.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2-G	829	LEU	N-CA-C	-7.82	89.89	111.00
6	1-K	829	LEU	N-CA-C	-7.82	89.90	111.00
6	3-K	829	LEU	N-CA-C	-7.81	89.91	111.00
6	2-K	829	LEU	N-CA-C	-7.81	89.92	111.00
6	1-G	829	LEU	N-CA-C	-7.80	89.93	111.00
1	1-A	779	ASP	N-CA-C	-7.78	90.01	111.00
1	2-A	371	ASN	N-CA-C	-7.77	90.02	111.00
1	1-A	371	ASN	N-CA-C	-7.77	90.03	111.00
1	2-A	779	ASP	N-CA-C	-7.77	90.03	111.00
1	3-A	371	ASN	N-CA-C	-7.77	90.03	111.00
1	3-A	779	ASP	N-CA-C	-7.76	90.05	111.00
5	3-R	144	GLY	N-CA-C	-7.74	93.76	113.10
5	1-R	144	GLY	N-CA-C	-7.74	93.76	113.10
5	2-R	144	GLY	N-CA-C	-7.73	93.77	113.10
3	2-C	441	VAL	N-CA-C	-7.67	90.29	111.00
3	3-C	441	VAL	N-CA-C	-7.67	90.30	111.00
1	2-A	803	PRO	N-CA-C	7.67	132.03	112.10
3	1-C	441	VAL	N-CA-C	-7.67	90.31	111.00
1	1-A	803	PRO	N-CA-C	7.66	132.01	112.10
1	3-A	803	PRO	N-CA-C	7.66	132.00	112.10
1	2-A	321	ARG	N-CA-C	-7.63	90.39	111.00
2	2-B	255	SER	C-N-CA	7.63	140.78	121.70
1	3-A	321	ARG	N-CA-C	-7.63	90.40	111.00
2	2-B	750	ASN	N-CA-C	-7.62	90.42	111.00
2	3-B	255	SER	C-N-CA	7.62	140.75	121.70
2	1-B	750	ASN	N-CA-C	-7.62	90.43	111.00
1	1-A	321	ARG	N-CA-C	-7.62	90.44	111.00
2	1-B	255	SER	C-N-CA	7.62	140.74	121.70
2	3-B	750	ASN	N-CA-C	-7.61	90.45	111.00
5	2-M	41	GLU	C-N-CA	7.59	140.67	121.70
5	3-M	41	GLU	C-N-CA	7.57	140.63	121.70
5	1-M	41	GLU	C-N-CA	7.57	140.62	121.70
5	1-R	159	CYS	N-CA-C	-7.55	90.61	111.00
5	2-F	97	ARG	N-CA-C	-7.54	90.64	111.00
5	2-R	159	CYS	N-CA-C	-7.54	90.63	111.00
5	1-F	97	ARG	N-CA-C	-7.54	90.66	111.00
5	3-F	97	ARG	N-CA-C	-7.53	90.67	111.00
1	3-A	622	GLY	N-CA-C	-7.53	94.28	113.10
1	1-A	622	GLY	N-CA-C	-7.53	94.28	113.10
1	2-A	622	GLY	N-CA-C	-7.53	94.28	113.10
5	3-R	159	CYS	N-CA-C	-7.52	90.69	111.00
5	1-F	61	ILE	N-CA-C	-7.49	90.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2-F	61	ILE	N-CA-C	-7.48	90.80	111.00
6	1-G	117	GLU	N-CA-C	-7.47	90.83	111.00
5	3-F	61	ILE	N-CA-C	-7.46	90.84	111.00
4	3-D	118	ALA	N-CA-C	-7.46	90.87	111.00
6	2-G	117	GLU	N-CA-C	-7.45	90.88	111.00
4	1-D	118	ALA	N-CA-C	-7.45	90.90	111.00
4	2-D	118	ALA	N-CA-C	-7.45	90.90	111.00
6	3-G	117	GLU	N-CA-C	-7.45	90.90	111.00
1	2-A	198	LYS	N-CA-C	-7.43	90.93	111.00
1	1-A	198	LYS	N-CA-C	-7.43	90.95	111.00
1	3-A	198	LYS	N-CA-C	-7.43	90.95	111.00
3	1-C	559	ARG	N-CA-C	-7.32	91.23	111.00
3	1-C	221	CYS	N-CA-C	-7.32	91.25	111.00
3	2-C	559	ARG	N-CA-C	-7.32	91.24	111.00
4	1-D	136	MET	N-CA-C	-7.31	91.25	111.00
3	3-C	559	ARG	N-CA-C	-7.31	91.26	111.00
4	2-D	136	MET	N-CA-C	-7.30	91.28	111.00
3	3-C	221	CYS	N-CA-C	-7.30	91.29	111.00
4	3-D	136	MET	N-CA-C	-7.29	91.30	111.00
3	2-C	221	CYS	N-CA-C	-7.28	91.35	111.00
6	1-G	693	VAL	C-N-CA	-7.27	91.48	122.00
6	2-G	693	VAL	C-N-CA	-7.26	91.49	122.00
6	3-G	693	VAL	C-N-CA	-7.26	91.52	122.00
1	1-A	338	ASP	N-CA-C	-7.25	91.42	111.00
2	1-B	749	VAL	N-CA-C	-7.25	91.42	111.00
2	2-B	749	VAL	N-CA-C	-7.25	91.42	111.00
1	2-A	338	ASP	N-CA-C	-7.25	91.43	111.00
2	3-B	749	VAL	N-CA-C	-7.24	91.45	111.00
1	3-A	338	ASP	N-CA-C	-7.23	91.47	111.00
2	2-B	761	VAL	N-CA-C	-7.19	91.60	111.00
1	1-A	519	ASP	N-CA-C	-7.18	91.60	111.00
2	3-B	761	VAL	N-CA-C	-7.18	91.60	111.00
1	2-A	519	ASP	N-CA-C	-7.18	91.62	111.00
2	1-B	761	VAL	N-CA-C	-7.18	91.62	111.00
1	3-A	519	ASP	N-CA-C	-7.17	91.63	111.00
2	2-B	837	ILE	N-CA-C	-7.16	91.67	111.00
2	3-B	837	ILE	N-CA-C	-7.15	91.69	111.00
2	1-B	837	ILE	N-CA-C	-7.14	91.72	111.00
5	3-M	69	GLY	N-CA-C	-7.12	95.30	113.10
2	2-B	269	GLN	N-CA-C	-7.11	91.81	111.00
5	2-M	69	GLY	N-CA-C	-7.10	95.34	113.10
5	1-M	69	GLY	N-CA-C	-7.10	95.35	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	269	GLN	N-CA-C	-7.10	91.84	111.00
2	3-B	269	GLN	N-CA-C	-7.10	91.84	111.00
2	1-B	48	GLY	N-CA-C	-7.08	95.41	113.10
5	2-F	121	TRP	N-CA-C	7.07	130.09	111.00
5	1-F	121	TRP	N-CA-C	7.07	130.08	111.00
2	2-B	48	GLY	N-CA-C	-7.07	95.43	113.10
2	3-B	48	GLY	N-CA-C	-7.07	95.44	113.10
5	3-F	121	TRP	N-CA-C	7.06	130.07	111.00
6	3-K	244	ASP	N-CA-C	-7.05	91.98	111.00
6	1-K	244	ASP	N-CA-C	-7.04	91.98	111.00
2	3-B	49	ASP	N-CA-C	-7.04	91.99	111.00
6	2-K	244	ASP	N-CA-C	-7.04	91.99	111.00
2	1-B	49	ASP	N-CA-C	-7.03	92.03	111.00
2	2-B	49	ASP	N-CA-C	-7.02	92.03	111.00
2	1-B	811	ASN	N-CA-C	-7.02	92.05	111.00
6	1-G	609	ARG	C-N-CA	7.02	139.24	121.70
2	3-B	811	ASN	N-CA-C	-7.02	92.06	111.00
2	2-B	811	ASN	N-CA-C	-7.01	92.06	111.00
1	2-A	339	ARG	N-CA-C	-7.01	92.07	111.00
6	3-G	609	ARG	C-N-CA	7.00	139.21	121.70
6	2-G	609	ARG	C-N-CA	7.00	139.21	121.70
6	2-K	609	ARG	C-N-CA	7.00	139.21	121.70
1	3-A	339	ARG	N-CA-C	-7.00	92.10	111.00
6	3-K	609	ARG	C-N-CA	7.00	139.19	121.70
1	1-A	339	ARG	N-CA-C	-6.99	92.13	111.00
6	1-K	609	ARG	C-N-CA	6.99	139.18	121.70
2	2-B	871	ASN	N-CA-C	-6.95	92.24	111.00
2	1-B	871	ASN	N-CA-C	-6.94	92.26	111.00
2	3-B	871	ASN	N-CA-C	-6.94	92.26	111.00
1	1-A	243	ASP	N-CA-C	-6.90	92.38	111.00
1	3-A	36	TRP	N-CA-C	-6.89	92.40	111.00
1	1-A	36	TRP	N-CA-C	-6.88	92.42	111.00
1	2-A	240	TRP	C-N-CA	6.88	138.90	121.70
1	3-A	243	ASP	N-CA-C	-6.88	92.44	111.00
1	2-A	36	TRP	N-CA-C	-6.87	92.44	111.00
1	2-A	243	ASP	N-CA-C	-6.87	92.46	111.00
1	1-A	240	TRP	C-N-CA	6.86	138.86	121.70
1	3-A	240	TRP	C-N-CA	6.86	138.85	121.70
1	3-A	236	GLU	N-CA-C	-6.81	92.62	111.00
1	1-A	236	GLU	N-CA-C	-6.80	92.64	111.00
1	2-A	236	GLU	N-CA-C	-6.80	92.65	111.00
3	1-C	653	GLU	N-CA-C	-6.79	92.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-C	653	GLU	N-CA-C	-6.79	92.66	111.00
3	3-C	653	GLU	N-CA-C	-6.78	92.69	111.00
1	2-A	430	ASP	N-CA-C	-6.76	92.75	111.00
1	1-A	430	ASP	N-CA-C	-6.75	92.77	111.00
1	1-A	528	ILE	N-CA-C	-6.75	92.77	111.00
1	2-A	528	ILE	N-CA-C	-6.75	92.77	111.00
1	3-A	528	ILE	N-CA-C	-6.75	92.77	111.00
1	3-A	430	ASP	N-CA-C	-6.75	92.79	111.00
3	1-C	27	GLU	N-CA-C	-6.74	92.81	111.00
3	3-C	27	GLU	N-CA-C	-6.74	92.81	111.00
3	2-C	27	GLU	N-CA-C	-6.73	92.82	111.00
1	3-A	766	GLY	N-CA-C	-6.70	96.36	113.10
1	2-A	766	GLY	N-CA-C	-6.69	96.37	113.10
1	1-A	766	GLY	N-CA-C	-6.68	96.39	113.10
6	2-G	828	LEU	N-CA-C	-6.68	92.97	111.00
6	1-G	828	LEU	N-CA-C	-6.67	92.98	111.00
6	1-K	828	LEU	N-CA-C	-6.67	92.99	111.00
6	3-G	828	LEU	N-CA-C	-6.67	93.00	111.00
6	1-K	629	LEU	C-N-CA	6.66	138.36	121.70
6	2-K	828	LEU	N-CA-C	-6.66	93.01	111.00
6	2-G	629	LEU	C-N-CA	6.66	138.34	121.70
6	2-K	629	LEU	C-N-CA	6.65	138.32	121.70
6	3-K	629	LEU	C-N-CA	6.65	138.32	121.70
6	3-K	828	LEU	N-CA-C	-6.65	93.05	111.00
6	1-G	629	LEU	C-N-CA	6.64	138.31	121.70
6	3-G	629	LEU	C-N-CA	6.64	138.30	121.70
5	1-F	159	CYS	N-CA-C	-6.62	93.11	111.00
5	2-F	159	CYS	N-CA-C	-6.62	93.12	111.00
5	3-F	159	CYS	N-CA-C	-6.62	93.13	111.00
3	3-C	379	THR	N-CA-C	-6.60	93.18	111.00
7	1-Z	11	TYR	N-CA-C	-6.59	93.21	111.00
3	1-C	379	THR	N-CA-C	-6.59	93.22	111.00
7	2-Z	11	TYR	N-CA-C	-6.59	93.22	111.00
7	3-Z	11	TYR	N-CA-C	-6.59	93.22	111.00
3	2-C	379	THR	N-CA-C	-6.58	93.22	111.00
7	2-Z	62	LEU	N-CA-C	-6.58	93.23	111.00
1	1-A	457	PHE	N-CA-C	-6.57	93.26	111.00
1	2-A	457	PHE	N-CA-C	-6.57	93.26	111.00
2	2-B	740	PRO	N-CA-C	-6.57	95.02	112.10
7	1-Z	62	LEU	N-CA-C	-6.56	93.28	111.00
2	3-B	740	PRO	N-CA-C	-6.56	95.03	112.10
1	1-A	242	VAL	N-CA-C	-6.56	93.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	740	PRO	N-CA-C	-6.55	95.06	112.10
7	3-Z	62	LEU	N-CA-C	-6.55	93.31	111.00
6	2-K	667	ASN	N-CA-C	-6.55	93.31	111.00
1	3-A	457	PHE	N-CA-C	-6.55	93.31	111.00
6	3-K	667	ASN	N-CA-C	-6.55	93.31	111.00
4	2-D	14	LYS	C-N-CA	6.55	138.07	121.70
4	1-D	14	LYS	C-N-CA	6.55	138.07	121.70
6	1-G	667	ASN	N-CA-C	-6.54	93.33	111.00
6	1-K	667	ASN	N-CA-C	-6.54	93.34	111.00
6	2-G	667	ASN	N-CA-C	-6.54	93.34	111.00
4	3-D	14	LYS	C-N-CA	6.54	138.04	121.70
1	2-A	242	VAL	N-CA-C	-6.54	93.35	111.00
6	3-G	667	ASN	N-CA-C	-6.53	93.36	111.00
1	3-A	242	VAL	N-CA-C	-6.53	93.36	111.00
2	3-B	792	LEU	N-CA-C	-6.49	93.47	111.00
5	1-M	155	ILE	N-CA-C	-6.49	93.47	111.00
5	3-M	155	ILE	N-CA-C	-6.49	93.48	111.00
5	2-M	155	ILE	N-CA-C	-6.49	93.49	111.00
1	1-A	105	TYR	N-CA-C	-6.48	93.50	111.00
2	2-B	792	LEU	N-CA-C	-6.48	93.50	111.00
1	3-A	105	TYR	N-CA-C	-6.48	93.51	111.00
2	1-B	792	LEU	N-CA-C	-6.47	93.52	111.00
1	2-A	105	TYR	N-CA-C	-6.47	93.54	111.00
6	2-K	849	LEU	N-CA-C	-6.45	93.57	111.00
4	3-D	19	ARG	C-N-CA	6.45	137.81	121.70
6	3-K	849	LEU	N-CA-C	-6.44	93.60	111.00
4	1-D	19	ARG	C-N-CA	6.44	137.80	121.70
6	2-G	849	LEU	N-CA-C	-6.44	93.62	111.00
6	1-K	849	LEU	N-CA-C	-6.43	93.63	111.00
4	2-D	19	ARG	C-N-CA	6.43	137.78	121.70
6	3-G	849	LEU	N-CA-C	-6.43	93.64	111.00
1	1-A	589	VAL	N-CA-C	-6.43	93.65	111.00
1	2-A	317	PHE	C-N-CA	6.43	137.77	121.70
6	1-G	849	LEU	N-CA-C	-6.42	93.66	111.00
1	2-A	589	VAL	N-CA-C	-6.42	93.67	111.00
1	3-A	317	PHE	C-N-CA	6.41	137.73	121.70
1	1-A	317	PHE	C-N-CA	6.41	137.73	121.70
1	3-A	589	VAL	N-CA-C	-6.41	93.69	111.00
2	1-B	754	ILE	N-CA-C	-6.40	93.73	111.00
2	2-B	754	ILE	N-CA-C	-6.40	93.72	111.00
2	3-B	754	ILE	N-CA-C	-6.39	93.76	111.00
3	1-C	546	TYR	N-CA-C	-6.38	93.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1-G	484	HIS	N-CA-C	-6.38	93.78	111.00
6	2-G	484	HIS	N-CA-C	-6.38	93.78	111.00
3	2-C	546	TYR	N-CA-C	-6.37	93.79	111.00
3	1-C	154	ASP	N-CA-C	-6.37	93.80	111.00
6	3-G	484	HIS	N-CA-C	-6.37	93.80	111.00
3	3-C	546	TYR	N-CA-C	-6.37	93.81	111.00
4	3-D	29	ILE	N-CA-C	-6.37	93.81	111.00
4	1-D	29	ILE	N-CA-C	-6.36	93.82	111.00
3	3-C	154	ASP	N-CA-C	-6.36	93.82	111.00
6	1-G	150	ASP	C-N-CA	6.36	137.60	121.70
2	2-B	414	ALA	C-N-CA	6.36	137.59	121.70
3	2-C	154	ASP	N-CA-C	-6.36	93.84	111.00
6	3-G	150	ASP	C-N-CA	6.36	137.59	121.70
6	2-G	150	ASP	C-N-CA	6.34	137.56	121.70
7	3-Z	29	LYS	N-CA-C	-6.34	93.87	111.00
4	2-D	29	ILE	N-CA-C	-6.34	93.87	111.00
2	1-B	414	ALA	C-N-CA	6.34	137.55	121.70
6	2-K	838	HIS	C-N-CA	6.34	137.56	121.70
6	1-K	838	HIS	C-N-CA	6.34	137.54	121.70
6	1-K	206	ASN	N-CA-C	-6.33	93.90	111.00
6	1-G	838	HIS	C-N-CA	6.33	137.53	121.70
5	2-M	149	ARG	N-CA-C	-6.33	93.91	111.00
2	3-B	414	ALA	C-N-CA	6.33	137.52	121.70
6	3-G	704	GLY	N-CA-C	-6.33	97.29	113.10
6	1-G	704	GLY	N-CA-C	-6.32	97.29	113.10
7	1-Z	29	LYS	N-CA-C	-6.32	93.92	111.00
6	1-K	117	GLU	CA-C-N	-6.32	103.29	117.20
6	2-G	838	HIS	C-N-CA	6.32	137.51	121.70
6	3-K	704	GLY	N-CA-C	-6.32	97.29	113.10
5	3-M	149	ARG	N-CA-C	-6.32	93.93	111.00
6	3-K	206	ASN	N-CA-C	-6.32	93.93	111.00
7	2-Z	29	LYS	N-CA-C	-6.32	93.95	111.00
6	2-K	206	ASN	N-CA-C	-6.32	93.95	111.00
5	1-M	149	ARG	N-CA-C	-6.31	93.95	111.00
6	3-G	838	HIS	C-N-CA	6.31	137.49	121.70
6	2-K	704	GLY	N-CA-C	-6.31	97.32	113.10
6	3-K	838	HIS	C-N-CA	6.31	137.48	121.70
6	1-K	704	GLY	N-CA-C	-6.31	97.33	113.10
6	2-G	704	GLY	N-CA-C	-6.31	97.33	113.10
6	2-K	117	GLU	CA-C-N	-6.30	103.33	117.20
6	3-K	96	SER	N-CA-C	6.30	128.01	111.00
1	1-A	768	ASP	C-N-CA	6.30	137.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3-K	117	GLU	CA-C-N	-6.30	103.34	117.20
6	2-K	96	SER	N-CA-C	6.30	128.00	111.00
1	3-A	768	ASP	C-N-CA	6.30	137.44	121.70
1	2-A	768	ASP	C-N-CA	6.29	137.44	121.70
6	1-K	96	SER	N-CA-C	6.29	127.99	111.00
3	2-C	155	ASN	C-N-CA	6.28	137.41	121.70
1	1-A	73	TYR	N-CA-C	-6.28	94.06	111.00
3	3-C	155	ASN	C-N-CA	6.28	137.39	121.70
1	2-A	73	TYR	N-CA-C	-6.27	94.06	111.00
1	3-A	73	TYR	N-CA-C	-6.27	94.06	111.00
5	3-M	62	SER	C-N-CA	6.26	137.36	121.70
3	1-C	155	ASN	C-N-CA	6.25	137.33	121.70
2	2-B	816	GLY	N-CA-C	-6.25	97.47	113.10
5	1-M	62	SER	C-N-CA	6.25	137.32	121.70
6	2-G	665	CYS	N-CA-C	6.24	127.86	111.00
6	1-G	665	CYS	N-CA-C	6.24	127.85	111.00
6	3-G	665	CYS	N-CA-C	6.24	127.84	111.00
5	2-M	62	SER	C-N-CA	6.24	137.29	121.70
2	3-B	816	GLY	N-CA-C	-6.23	97.52	113.10
2	1-B	816	GLY	N-CA-C	-6.23	97.52	113.10
3	2-C	113	PHE	N-CA-C	6.23	127.81	111.00
3	1-C	113	PHE	N-CA-C	6.21	127.78	111.00
3	3-C	113	PHE	N-CA-C	6.20	127.75	111.00
3	2-C	736	GLY	N-CA-C	-6.19	97.62	113.10
3	3-C	736	GLY	N-CA-C	-6.19	97.62	113.10
3	1-C	546	TYR	O-C-N	6.19	132.60	122.70
3	1-C	736	GLY	N-CA-C	-6.19	97.63	113.10
3	2-C	546	TYR	O-C-N	6.19	132.60	122.70
6	2-G	277	LEU	C-N-CA	-6.19	96.02	122.00
6	3-G	277	LEU	C-N-CA	-6.19	96.01	122.00
6	1-G	277	LEU	C-N-CA	-6.18	96.02	122.00
7	3-L	30	TYR	N-CA-C	-6.18	94.30	111.00
3	3-C	546	TYR	O-C-N	6.18	132.59	122.70
7	1-L	30	TYR	N-CA-C	-6.17	94.34	111.00
2	3-B	933	GLY	C-N-CA	-6.17	96.09	122.00
2	2-B	933	GLY	C-N-CA	-6.17	96.11	122.00
2	1-B	933	GLY	C-N-CA	-6.16	96.12	122.00
7	2-L	30	TYR	N-CA-C	-6.16	94.37	111.00
3	2-C	85	ASN	N-CA-C	-6.16	94.38	111.00
6	3-K	665	CYS	N-CA-C	6.16	127.62	111.00
6	1-K	665	CYS	N-CA-C	6.15	127.61	111.00
6	2-K	665	CYS	N-CA-C	6.15	127.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3-R	42	VAL	C-N-CA	6.15	137.08	121.70
5	2-R	42	VAL	C-N-CA	6.14	137.06	121.70
3	3-C	85	ASN	N-CA-C	-6.14	94.42	111.00
7	3-Z	25	ARG	N-CA-C	-6.14	94.43	111.00
7	1-Z	25	ARG	N-CA-C	-6.13	94.44	111.00
3	1-C	85	ASN	N-CA-C	-6.13	94.44	111.00
7	2-Z	25	ARG	N-CA-C	-6.13	94.45	111.00
5	1-R	42	VAL	C-N-CA	6.13	137.02	121.70
1	2-A	511	ILE	N-CA-C	-6.11	94.52	111.00
2	1-B	905	PHE	C-N-CA	6.10	136.96	121.70
1	1-A	511	ILE	N-CA-C	-6.10	94.53	111.00
3	2-C	546	TYR	CA-C-N	-6.10	103.78	117.20
3	1-C	396	TRP	N-CA-C	-6.10	94.54	111.00
3	3-C	315	ILE	N-CA-C	-6.09	94.54	111.00
3	3-C	546	TYR	CA-C-N	-6.09	103.80	117.20
3	1-C	315	ILE	N-CA-C	-6.08	94.57	111.00
2	2-B	905	PHE	C-N-CA	6.08	136.91	121.70
3	2-C	315	ILE	N-CA-C	-6.08	94.58	111.00
1	3-A	511	ILE	N-CA-C	-6.08	94.58	111.00
2	3-B	905	PHE	C-N-CA	6.08	136.90	121.70
3	2-C	396	TRP	N-CA-C	-6.08	94.58	111.00
7	3-Z	30	TYR	N-CA-C	-6.08	94.58	111.00
3	1-C	546	TYR	CA-C-N	-6.08	103.83	117.20
5	2-R	58	TYR	N-CA-C	-6.08	94.59	111.00
3	3-C	396	TRP	N-CA-C	-6.08	94.59	111.00
5	1-R	58	TYR	N-CA-C	-6.08	94.60	111.00
3	3-C	170	TRP	C-N-CA	6.08	136.89	121.70
7	1-Z	30	TYR	N-CA-C	-6.07	94.61	111.00
5	3-R	58	TYR	N-CA-C	-6.07	94.61	111.00
3	1-C	170	TRP	C-N-CA	6.07	136.86	121.70
6	1-G	207	ASP	N-CA-C	6.06	127.37	111.00
7	1-Z	129	VAL	N-CA-C	-6.06	94.64	111.00
3	2-C	170	TRP	C-N-CA	6.06	136.84	121.70
6	2-G	207	ASP	N-CA-C	6.05	127.34	111.00
7	2-Z	129	VAL	N-CA-C	-6.05	94.66	111.00
7	2-Z	30	TYR	N-CA-C	-6.05	94.67	111.00
7	3-Z	129	VAL	N-CA-C	-6.05	94.67	111.00
3	3-C	551	ILE	N-CA-C	-6.05	94.67	111.00
6	3-G	207	ASP	N-CA-C	6.05	127.33	111.00
2	3-B	385	VAL	C-N-CA	6.04	136.80	121.70
2	2-B	385	VAL	C-N-CA	6.04	136.79	121.70
7	3-L	80	ILE	C-N-CA	6.04	134.98	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-C	551	ILE	N-CA-C	-6.04	94.70	111.00
3	2-C	551	ILE	N-CA-C	-6.04	94.70	111.00
7	2-L	80	ILE	C-N-CA	6.03	134.97	122.30
4	1-D	50	GLU	N-CA-C	-6.03	94.72	111.00
7	1-L	80	ILE	C-N-CA	6.03	134.96	122.30
4	2-D	50	GLU	N-CA-C	-6.03	94.73	111.00
2	1-B	385	VAL	C-N-CA	6.02	136.76	121.70
4	3-D	50	GLU	N-CA-C	-6.02	94.76	111.00
3	3-C	424	PHE	N-CA-C	-6.01	94.76	111.00
3	1-C	424	PHE	N-CA-C	-6.01	94.76	111.00
6	1-K	731	THR	N-CA-C	-6.01	94.76	111.00
6	2-G	731	THR	N-CA-C	-6.01	94.76	111.00
6	1-G	731	THR	N-CA-C	-6.01	94.78	111.00
3	2-C	424	PHE	N-CA-C	-6.01	94.78	111.00
6	3-G	731	THR	N-CA-C	-6.01	94.78	111.00
6	2-K	731	THR	N-CA-C	-6.00	94.79	111.00
3	3-C	504	GLY	N-CA-C	6.00	128.10	113.10
6	2-K	80	ASN	N-CA-C	-6.00	94.81	111.00
5	1-M	53	VAL	N-CA-C	-5.99	94.82	111.00
6	3-K	731	THR	N-CA-C	-5.99	94.82	111.00
5	3-M	53	VAL	N-CA-C	-5.99	94.82	111.00
5	2-R	71	GLN	N-CA-C	-5.99	94.83	111.00
6	2-G	640	THR	N-CA-C	-5.99	94.84	111.00
3	1-C	504	GLY	N-CA-C	5.98	128.06	113.10
6	1-G	640	THR	N-CA-C	-5.98	94.84	111.00
5	1-R	71	GLN	N-CA-C	-5.98	94.86	111.00
6	3-K	80	ASN	N-CA-C	-5.98	94.85	111.00
5	3-R	71	GLN	N-CA-C	-5.98	94.86	111.00
1	1-A	599	PHE	CA-C-N	5.98	130.35	117.20
3	1-C	174	SER	N-CA-C	-5.98	94.86	111.00
6	3-G	640	THR	N-CA-C	-5.98	94.86	111.00
3	1-C	245	ILE	N-CA-C	-5.97	94.87	111.00
1	2-A	599	PHE	CA-C-N	5.97	130.34	117.20
3	3-C	245	ILE	N-CA-C	-5.97	94.87	111.00
6	3-K	640	THR	N-CA-C	-5.97	94.87	111.00
5	2-M	53	VAL	N-CA-C	-5.97	94.88	111.00
6	1-K	640	THR	N-CA-C	-5.97	94.88	111.00
3	2-C	245	ILE	N-CA-C	-5.97	94.88	111.00
3	2-C	504	GLY	N-CA-C	5.97	128.02	113.10
6	1-K	80	ASN	N-CA-C	-5.97	94.89	111.00
1	2-A	554	THR	N-CA-C	5.97	127.11	111.00
6	2-K	640	THR	N-CA-C	-5.97	94.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	554	THR	N-CA-C	5.96	127.10	111.00
1	3-A	599	PHE	CA-C-N	5.96	130.32	117.20
1	1-A	554	THR	N-CA-C	5.96	127.09	111.00
6	1-K	736	ASP	N-CA-C	-5.96	94.92	111.00
6	2-G	736	ASP	N-CA-C	-5.95	94.92	111.00
3	3-C	174	SER	N-CA-C	-5.95	94.92	111.00
3	2-C	174	SER	N-CA-C	-5.95	94.93	111.00
6	3-G	736	ASP	N-CA-C	-5.95	94.94	111.00
6	3-G	506	LEU	N-CA-C	5.95	127.06	111.00
6	1-K	222	GLY	N-CA-C	-5.95	98.24	113.10
3	2-C	151	ASN	N-CA-C	-5.94	94.95	111.00
6	3-K	736	ASP	N-CA-C	-5.94	94.95	111.00
5	1-R	96	ASP	N-CA-C	-5.94	94.96	111.00
6	1-G	736	ASP	N-CA-C	-5.94	94.96	111.00
6	2-K	736	ASP	N-CA-C	-5.94	94.96	111.00
5	3-R	96	ASP	N-CA-C	-5.94	94.96	111.00
3	3-C	151	ASN	N-CA-C	-5.94	94.96	111.00
6	1-G	506	LEU	N-CA-C	5.94	127.03	111.00
1	2-A	392	ASP	N-CA-C	-5.94	94.97	111.00
3	3-C	88	THR	N-CA-C	-5.94	94.97	111.00
6	3-K	222	GLY	N-CA-C	-5.94	98.26	113.10
5	2-R	96	ASP	N-CA-C	-5.93	94.97	111.00
6	2-K	222	GLY	N-CA-C	-5.93	98.27	113.10
3	2-C	88	THR	N-CA-C	-5.93	94.99	111.00
6	2-G	506	LEU	N-CA-C	5.93	127.01	111.00
6	2-K	240	LEU	C-N-CA	5.93	136.51	121.70
2	3-B	795	HIS	C-N-CA	5.93	136.51	121.70
3	1-C	151	ASN	N-CA-C	-5.92	95.00	111.00
1	1-A	392	ASP	N-CA-C	-5.92	95.01	111.00
1	3-A	392	ASP	N-CA-C	-5.92	95.01	111.00
3	1-C	88	THR	N-CA-C	-5.92	95.01	111.00
7	1-L	61	LEU	C-N-CA	-5.92	106.90	121.70
6	1-K	240	LEU	C-N-CA	5.91	136.47	121.70
7	2-L	61	LEU	C-N-CA	-5.91	106.93	121.70
7	3-L	61	LEU	C-N-CA	-5.91	106.94	121.70
2	1-B	928	LYS	N-CA-C	5.90	126.94	111.00
2	1-B	795	HIS	C-N-CA	5.90	136.44	121.70
2	2-B	928	LYS	N-CA-C	5.89	126.92	111.00
6	3-K	858	ALA	N-CA-C	-5.89	95.09	111.00
2	2-B	795	HIS	C-N-CA	5.89	136.42	121.70
2	3-B	928	LYS	N-CA-C	5.89	126.90	111.00
6	2-K	858	ALA	N-CA-C	-5.89	95.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3-K	240	LEU	C-N-CA	5.88	136.41	121.70
6	2-G	858	ALA	N-CA-C	-5.88	95.12	111.00
6	3-G	858	ALA	N-CA-C	-5.88	95.13	111.00
6	1-K	858	ALA	N-CA-C	-5.88	95.13	111.00
6	1-G	858	ALA	N-CA-C	-5.87	95.14	111.00
6	3-G	300	LYS	N-CA-C	-5.85	95.20	111.00
6	1-G	300	LYS	N-CA-C	-5.85	95.21	111.00
6	2-G	300	LYS	N-CA-C	-5.84	95.23	111.00
1	1-A	496	TRP	N-CA-C	-5.83	95.25	111.00
1	3-A	429	LEU	N-CA-C	-5.83	95.25	111.00
1	3-A	496	TRP	N-CA-C	-5.83	95.25	111.00
1	3-A	325	ALA	N-CA-C	5.83	126.74	111.00
1	2-A	496	TRP	N-CA-C	-5.83	95.26	111.00
3	2-C	446	GLY	N-CA-C	-5.83	98.53	113.10
3	3-C	446	GLY	N-CA-C	-5.83	98.54	113.10
3	1-C	446	GLY	N-CA-C	-5.82	98.54	113.10
6	1-K	695	ALA	N-CA-C	-5.82	95.28	111.00
1	1-A	325	ALA	N-CA-C	5.82	126.72	111.00
1	2-A	325	ALA	N-CA-C	5.82	126.72	111.00
1	2-A	429	LEU	N-CA-C	-5.82	95.29	111.00
6	2-K	695	ALA	N-CA-C	-5.82	95.29	111.00
1	1-A	429	LEU	N-CA-C	-5.82	95.30	111.00
6	3-K	695	ALA	N-CA-C	-5.81	95.31	111.00
6	3-K	845	ARG	N-CA-C	-5.81	95.31	111.00
6	1-K	845	ARG	N-CA-C	-5.79	95.36	111.00
6	2-G	845	ARG	N-CA-C	-5.79	95.38	111.00
6	2-K	845	ARG	N-CA-C	-5.79	95.38	111.00
6	3-G	845	ARG	N-CA-C	-5.78	95.38	111.00
6	1-G	845	ARG	N-CA-C	-5.78	95.40	111.00
2	3-B	325	GLU	C-N-CA	5.78	136.14	121.70
2	2-B	325	GLU	C-N-CA	5.77	136.13	121.70
4	2-D	98	GLU	N-CA-C	-5.77	95.41	111.00
2	1-B	748	HIS	N-CA-C	-5.77	95.42	111.00
6	3-K	749	ASP	N-CA-C	-5.77	95.42	111.00
2	1-B	325	GLU	C-N-CA	5.77	136.12	121.70
4	1-D	98	GLU	N-CA-C	-5.77	95.42	111.00
6	1-K	749	ASP	N-CA-C	-5.77	95.42	111.00
6	2-K	749	ASP	N-CA-C	-5.77	95.42	111.00
6	1-G	749	ASP	N-CA-C	-5.77	95.43	111.00
6	3-G	749	ASP	N-CA-C	-5.77	95.43	111.00
4	3-D	98	GLU	N-CA-C	-5.76	95.44	111.00
6	2-G	749	ASP	N-CA-C	-5.76	95.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	748	HIS	N-CA-C	-5.76	95.45	111.00
2	2-B	410	PRO	N-CA-C	-5.76	97.13	112.10
2	2-B	748	HIS	N-CA-C	-5.76	95.45	111.00
1	2-A	509	HIS	N-CA-C	-5.75	95.46	111.00
5	3-R	61	ILE	N-CA-C	-5.75	95.48	111.00
5	1-R	61	ILE	N-CA-C	-5.75	95.48	111.00
3	1-C	530	VAL	N-CA-C	-5.75	95.49	111.00
2	1-B	410	PRO	N-CA-C	-5.74	97.17	112.10
2	3-B	410	PRO	N-CA-C	-5.74	97.17	112.10
1	1-A	509	HIS	N-CA-C	-5.74	95.50	111.00
6	2-K	40	ASN	N-CA-C	-5.74	95.50	111.00
6	1-K	40	ASN	N-CA-C	-5.74	95.50	111.00
1	2-A	507	ALA	N-CA-C	-5.74	95.50	111.00
3	2-C	530	VAL	N-CA-C	-5.74	95.50	111.00
1	3-A	509	HIS	N-CA-C	-5.74	95.50	111.00
5	2-R	61	ILE	N-CA-C	-5.74	95.51	111.00
3	3-C	530	VAL	N-CA-C	-5.74	95.51	111.00
2	3-B	804	VAL	N-CA-C	-5.73	95.54	111.00
6	3-K	40	ASN	N-CA-C	-5.72	95.55	111.00
1	1-A	507	ALA	N-CA-C	-5.72	95.56	111.00
2	1-B	804	VAL	N-CA-C	-5.71	95.57	111.00
6	1-G	95	MET	N-CA-C	5.71	126.42	111.00
6	2-G	95	MET	N-CA-C	5.71	126.42	111.00
6	3-G	178	VAL	N-CA-C	5.71	126.42	111.00
6	2-G	178	VAL	N-CA-C	5.71	126.42	111.00
1	3-A	507	ALA	N-CA-C	-5.70	95.60	111.00
6	3-G	95	MET	N-CA-C	5.70	126.40	111.00
2	2-B	804	VAL	N-CA-C	-5.70	95.61	111.00
6	1-G	178	VAL	N-CA-C	5.70	126.38	111.00
4	1-D	24	MET	C-N-CA	5.70	135.94	121.70
1	2-A	67	VAL	N-CA-C	-5.69	95.63	111.00
1	3-A	77	VAL	N-CA-C	-5.69	95.63	111.00
1	2-A	77	VAL	N-CA-C	-5.69	95.64	111.00
4	2-D	24	MET	C-N-CA	5.69	135.92	121.70
1	1-A	67	VAL	N-CA-C	-5.69	95.64	111.00
1	1-A	77	VAL	N-CA-C	-5.69	95.65	111.00
6	1-K	853	THR	N-CA-C	-5.68	95.65	111.00
2	2-B	841	ILE	N-CA-C	5.68	126.35	111.00
1	3-A	67	VAL	N-CA-C	-5.68	95.65	111.00
2	3-B	841	ILE	N-CA-C	5.67	126.32	111.00
1	3-A	522	CYS	N-CA-C	-5.67	95.69	111.00
2	1-B	841	ILE	N-CA-C	5.67	126.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-D	24	MET	C-N-CA	5.67	135.87	121.70
6	2-K	853	THR	N-CA-C	-5.67	95.70	111.00
5	3-F	151	ARG	N-CA-C	-5.67	95.70	111.00
1	1-A	522	CYS	N-CA-C	-5.66	95.71	111.00
1	2-A	522	CYS	N-CA-C	-5.66	95.72	111.00
5	2-F	151	ARG	N-CA-C	-5.66	95.72	111.00
6	3-K	853	THR	N-CA-C	-5.66	95.72	111.00
1	1-A	87	PHE	N-CA-C	-5.66	95.73	111.00
5	1-F	151	ARG	N-CA-C	-5.65	95.73	111.00
6	1-G	853	THR	N-CA-C	-5.65	95.73	111.00
1	2-A	87	PHE	N-CA-C	-5.65	95.73	111.00
3	1-C	411	ILE	N-CA-C	-5.65	95.74	111.00
6	2-G	853	THR	N-CA-C	-5.65	95.74	111.00
5	2-R	41	GLU	C-N-CA	5.65	135.83	121.70
6	3-G	853	THR	N-CA-C	-5.65	95.75	111.00
2	1-B	414	ALA	O-C-N	5.64	131.73	122.70
2	2-B	926	ILE	N-CA-C	5.64	126.24	111.00
1	3-A	87	PHE	N-CA-C	-5.64	95.76	111.00
5	3-R	41	GLU	C-N-CA	5.64	135.81	121.70
1	1-A	324	PRO	C-N-CA	5.64	135.80	121.70
3	2-C	411	ILE	N-CA-C	-5.64	95.78	111.00
2	3-B	414	ALA	O-C-N	5.64	131.72	122.70
3	3-C	411	ILE	N-CA-C	-5.64	95.78	111.00
2	1-B	926	ILE	N-CA-C	5.63	126.21	111.00
2	3-B	926	ILE	N-CA-C	5.63	126.22	111.00
3	1-C	442	ARG	N-CA-C	-5.63	95.79	111.00
5	1-R	41	GLU	C-N-CA	5.63	135.78	121.70
2	2-B	414	ALA	O-C-N	5.63	131.71	122.70
1	2-A	324	PRO	C-N-CA	5.63	135.76	121.70
3	2-C	442	ARG	N-CA-C	-5.62	95.81	111.00
1	3-A	324	PRO	C-N-CA	5.62	135.76	121.70
1	3-A	611	VAL	CA-C-N	-5.62	104.83	117.20
1	1-A	611	VAL	CA-C-N	-5.62	104.83	117.20
1	2-A	227	ARG	N-CA-C	-5.62	95.82	111.00
1	1-A	227	ARG	N-CA-C	-5.62	95.83	111.00
3	3-C	442	ARG	N-CA-C	-5.62	95.84	111.00
5	3-R	151	ARG	N-CA-C	5.61	126.16	111.00
1	1-A	621	VAL	C-N-CA	5.61	134.08	122.30
1	3-A	227	ARG	N-CA-C	-5.61	95.86	111.00
1	2-A	611	VAL	CA-C-N	-5.60	104.88	117.20
7	2-Z	58	GLU	N-CA-C	-5.60	95.88	111.00
7	3-Z	58	GLU	N-CA-C	-5.60	95.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1-Z	58	GLU	N-CA-C	-5.60	95.89	111.00
5	2-R	151	ARG	N-CA-C	5.60	126.11	111.00
5	1-R	151	ARG	N-CA-C	5.59	126.11	111.00
3	2-C	9	ARG	N-CA-C	-5.59	95.90	111.00
5	1-R	88	VAL	N-CA-C	5.59	126.09	111.00
1	2-A	621	VAL	C-N-CA	5.59	134.03	122.30
5	2-R	88	VAL	N-CA-C	5.59	126.08	111.00
5	3-R	88	VAL	N-CA-C	5.59	126.08	111.00
1	1-A	423	ARG	C-N-CA	5.58	135.66	121.70
3	1-C	9	ARG	N-CA-C	-5.58	95.94	111.00
1	3-A	621	VAL	C-N-CA	5.58	134.02	122.30
1	3-A	423	ARG	C-N-CA	5.58	135.64	121.70
3	3-C	9	ARG	N-CA-C	-5.58	95.94	111.00
1	2-A	423	ARG	C-N-CA	5.57	135.63	121.70
2	3-B	800	ILE	N-CA-C	-5.57	95.97	111.00
2	2-B	800	ILE	N-CA-C	-5.56	95.99	111.00
1	3-A	487	LYS	C-N-CA	5.56	135.60	121.70
1	2-A	487	LYS	C-N-CA	5.56	135.59	121.70
1	1-A	487	LYS	C-N-CA	5.55	135.59	121.70
3	1-C	662	VAL	N-CA-C	-5.55	96.01	111.00
5	2-M	63	PHE	N-CA-C	5.55	125.98	111.00
5	3-M	63	PHE	N-CA-C	5.55	125.98	111.00
2	1-B	800	ILE	N-CA-C	-5.55	96.03	111.00
5	1-M	148	ILE	C-N-CA	5.54	135.56	121.70
3	2-C	662	VAL	N-CA-C	-5.54	96.03	111.00
3	3-C	246	THR	C-N-CA	5.54	133.94	122.30
5	2-M	148	ILE	C-N-CA	5.54	135.55	121.70
3	3-C	662	VAL	N-CA-C	-5.54	96.04	111.00
5	1-M	63	PHE	N-CA-C	5.54	125.95	111.00
1	1-A	78	TRP	N-CA-C	-5.54	96.05	111.00
5	3-M	154	PHE	N-CA-C	-5.54	96.05	111.00
5	3-M	148	ILE	C-N-CA	5.53	135.53	121.70
3	1-C	246	THR	C-N-CA	5.53	133.92	122.30
1	2-A	78	TRP	N-CA-C	-5.53	96.07	111.00
1	2-A	574	LYS	C-N-CA	5.53	133.91	122.30
6	3-K	279	GLY	N-CA-C	-5.53	99.28	113.10
3	3-C	202	LEU	N-CA-C	-5.53	96.08	111.00
6	1-K	279	GLY	N-CA-C	-5.52	99.30	113.10
5	1-M	154	PHE	N-CA-C	-5.52	96.09	111.00
3	2-C	202	LEU	N-CA-C	-5.52	96.09	111.00
1	3-A	78	TRP	N-CA-C	-5.52	96.09	111.00
1	1-A	574	LYS	C-N-CA	5.52	133.88	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2-K	279	GLY	N-CA-C	-5.52	99.31	113.10
3	1-C	89	LEU	N-CA-C	-5.51	96.11	111.00
2	1-B	828	ASP	N-CA-C	-5.51	96.12	111.00
2	3-B	828	ASP	N-CA-C	-5.51	96.12	111.00
6	3-G	132	THR	N-CA-C	5.51	125.88	111.00
2	2-B	828	ASP	N-CA-C	-5.51	96.12	111.00
5	2-M	154	PHE	N-CA-C	-5.51	96.12	111.00
3	1-C	202	LEU	N-CA-C	-5.51	96.13	111.00
3	2-C	202	LEU	O-C-N	5.51	131.51	122.70
3	2-C	246	THR	C-N-CA	5.51	133.86	122.30
3	2-C	365	ARG	N-CA-C	5.50	125.86	111.00
3	2-C	472	ASP	N-CA-C	-5.50	96.14	111.00
7	2-Z	16	ILE	N-CA-C	-5.50	96.14	111.00
3	3-C	89	LEU	N-CA-C	-5.50	96.14	111.00
6	1-G	132	THR	N-CA-C	5.50	125.85	111.00
3	2-C	89	LEU	N-CA-C	-5.50	96.15	111.00
6	2-G	132	THR	N-CA-C	5.50	125.85	111.00
6	3-G	831	ALA	C-N-CA	5.50	133.85	122.30
6	2-G	831	ALA	C-N-CA	5.50	133.85	122.30
1	3-A	574	LYS	C-N-CA	5.50	133.85	122.30
6	2-K	831	ALA	C-N-CA	5.50	133.84	122.30
3	3-C	202	LEU	O-C-N	5.50	131.50	122.70
3	3-C	365	ARG	N-CA-C	5.50	125.84	111.00
3	3-C	472	ASP	N-CA-C	-5.50	96.16	111.00
7	1-Z	16	ILE	N-CA-C	-5.49	96.17	111.00
3	1-C	365	ARG	N-CA-C	5.49	125.83	111.00
1	2-A	132	THR	N-CA-C	-5.49	96.18	111.00
1	3-A	736	ALA	N-CA-C	5.49	125.82	111.00
3	1-C	202	LEU	O-C-N	5.49	131.48	122.70
6	3-K	831	ALA	C-N-CA	5.49	133.83	122.30
3	2-C	327	LEU	N-CA-C	-5.49	96.18	111.00
1	3-A	516	ARG	C-N-CA	5.49	135.42	121.70
7	3-Z	16	ILE	N-CA-C	-5.49	96.19	111.00
6	3-K	673	THR	N-CA-C	-5.48	96.19	111.00
1	1-A	736	ALA	N-CA-C	5.48	125.80	111.00
3	1-C	472	ASP	N-CA-C	-5.48	96.20	111.00
6	1-G	116	LYS	N-CA-C	5.48	125.80	111.00
6	2-G	673	THR	N-CA-C	-5.48	96.20	111.00
6	1-K	673	THR	N-CA-C	-5.48	96.21	111.00
6	2-G	116	LYS	N-CA-C	5.48	125.79	111.00
6	1-G	831	ALA	C-N-CA	5.48	133.80	122.30
6	2-K	673	THR	N-CA-C	-5.48	96.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-C	327	LEU	N-CA-C	-5.48	96.21	111.00
6	1-K	831	ALA	C-N-CA	5.48	133.80	122.30
1	2-A	736	ALA	N-CA-C	5.48	125.78	111.00
2	1-B	256	GLU	N-CA-C	5.47	125.78	111.00
3	1-C	327	LEU	N-CA-C	-5.47	96.22	111.00
6	1-G	673	THR	N-CA-C	-5.47	96.22	111.00
1	3-A	587	PRO	N-CA-C	5.47	126.33	112.10
6	3-G	116	LYS	N-CA-C	5.47	125.78	111.00
7	1-L	29	LYS	N-CA-C	-5.47	96.23	111.00
6	3-G	673	THR	N-CA-C	-5.47	96.22	111.00
1	2-A	516	ARG	C-N-CA	5.47	135.38	121.70
1	1-A	132	THR	N-CA-C	-5.47	96.23	111.00
7	2-L	29	LYS	N-CA-C	-5.47	96.23	111.00
1	3-A	132	THR	N-CA-C	-5.47	96.24	111.00
7	3-L	29	LYS	N-CA-C	-5.47	96.24	111.00
1	1-A	516	ARG	C-N-CA	5.46	135.35	121.70
1	2-A	587	PRO	N-CA-C	5.46	126.30	112.10
2	3-B	256	GLU	N-CA-C	5.46	125.74	111.00
1	1-A	587	PRO	N-CA-C	5.45	126.28	112.10
3	3-C	202	LEU	CA-C-N	-5.45	105.20	117.20
2	1-B	103	THR	C-N-CA	5.45	135.33	121.70
2	2-B	256	GLU	N-CA-C	5.45	125.72	111.00
2	1-B	758	VAL	N-CA-C	-5.45	96.29	111.00
2	2-B	103	THR	C-N-CA	5.45	135.32	121.70
3	2-C	202	LEU	CA-C-N	-5.45	105.22	117.20
6	1-G	459	LEU	C-N-CA	5.44	133.73	122.30
2	2-B	758	VAL	N-CA-C	-5.44	96.30	111.00
2	3-B	103	THR	C-N-CA	5.44	135.29	121.70
2	1-B	257	ARG	N-CA-C	5.44	125.68	111.00
2	3-B	758	VAL	N-CA-C	-5.44	96.32	111.00
2	3-B	257	ARG	N-CA-C	5.43	125.67	111.00
2	2-B	257	ARG	N-CA-C	5.43	125.65	111.00
2	2-B	939	THR	N-CA-C	-5.42	96.36	111.00
6	2-G	459	LEU	C-N-CA	5.42	133.68	122.30
2	1-B	939	THR	N-CA-C	-5.42	96.37	111.00
3	1-C	202	LEU	CA-C-N	-5.42	105.28	117.20
2	3-B	939	THR	N-CA-C	-5.41	96.39	111.00
1	2-A	533	GLY	N-CA-C	-5.41	99.59	113.10
1	3-A	656	GLY	N-CA-C	-5.41	99.59	113.10
2	2-B	482	SER	N-CA-C	5.40	125.58	111.00
6	2-G	274	ILE	N-CA-C	5.40	125.58	111.00
6	2-G	844	SER	N-CA-C	-5.40	96.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	533	GLY	N-CA-C	-5.40	99.61	113.10
6	3-G	459	LEU	C-N-CA	5.40	133.63	122.30
1	3-A	533	GLY	N-CA-C	-5.40	99.61	113.10
6	1-K	814	GLU	N-CA-C	-5.39	96.44	111.00
6	3-G	844	SER	N-CA-C	-5.39	96.44	111.00
6	1-G	844	SER	N-CA-C	-5.39	96.45	111.00
1	2-A	444	ILE	N-CA-C	-5.39	96.45	111.00
6	3-G	274	ILE	N-CA-C	5.39	125.55	111.00
7	2-L	60	ALA	C-N-CA	5.39	135.17	121.70
2	1-B	482	SER	N-CA-C	5.39	125.55	111.00
1	2-A	656	GLY	N-CA-C	-5.39	99.64	113.10
6	2-K	844	SER	N-CA-C	-5.39	96.46	111.00
1	3-A	444	ILE	N-CA-C	-5.39	96.46	111.00
7	3-L	60	ALA	C-N-CA	5.39	135.17	121.70
6	1-K	844	SER	N-CA-C	-5.38	96.46	111.00
6	2-K	814	GLU	N-CA-C	-5.38	96.46	111.00
2	3-B	482	SER	N-CA-C	5.38	125.53	111.00
1	1-A	444	ILE	N-CA-C	-5.38	96.47	111.00
7	1-L	60	ALA	C-N-CA	5.38	135.15	121.70
6	3-K	814	GLU	N-CA-C	-5.38	96.48	111.00
1	1-A	656	GLY	N-CA-C	-5.38	99.66	113.10
6	1-G	274	ILE	N-CA-C	5.38	125.52	111.00
6	3-K	844	SER	N-CA-C	-5.37	96.50	111.00
2	3-B	744	GLU	N-CA-C	-5.36	96.52	111.00
2	2-B	744	GLU	N-CA-C	-5.36	96.53	111.00
5	2-M	91	VAL	C-N-CA	5.36	135.09	121.70
3	1-C	262	ARG	N-CA-C	-5.35	96.55	111.00
3	2-C	262	ARG	N-CA-C	-5.35	96.55	111.00
2	1-B	744	GLU	N-CA-C	-5.35	96.56	111.00
5	1-M	91	VAL	C-N-CA	5.35	135.07	121.70
5	3-M	91	VAL	C-N-CA	5.35	135.07	121.70
1	1-A	272	SER	N-CA-C	5.34	125.43	111.00
1	2-A	272	SER	N-CA-C	5.34	125.41	111.00
3	3-C	262	ARG	N-CA-C	-5.34	96.59	111.00
1	3-A	272	SER	N-CA-C	5.33	125.39	111.00
2	2-B	763	GLN	C-N-CA	5.33	135.01	121.70
3	3-C	378	TYR	O-C-N	5.33	131.22	122.70
3	1-C	509	GLY	N-CA-C	-5.32	99.80	113.10
3	2-C	509	GLY	N-CA-C	-5.31	99.81	113.10
1	1-A	329	HIS	N-CA-C	-5.31	96.66	111.00
3	3-C	106	ALA	N-CA-C	-5.31	96.67	111.00
7	2-L	13	VAL	N-CA-C	-5.31	96.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	329	HIS	N-CA-C	-5.31	96.67	111.00
1	2-A	329	HIS	N-CA-C	-5.31	96.67	111.00
1	3-A	630	GLN	N-CA-C	-5.31	96.67	111.00
3	3-C	378	TYR	CA-C-N	-5.30	105.53	117.20
3	1-C	106	ALA	N-CA-C	-5.30	96.68	111.00
3	2-C	378	TYR	CA-C-N	-5.30	105.53	117.20
1	1-A	630	GLN	N-CA-C	-5.30	96.69	111.00
1	3-A	383	ALA	C-N-CA	5.30	134.96	121.70
3	1-C	378	TYR	CA-C-N	-5.30	105.55	117.20
2	3-B	763	GLN	C-N-CA	5.30	134.94	121.70
6	3-G	686	ALA	N-CA-C	5.30	125.30	111.00
1	2-A	630	GLN	N-CA-C	-5.29	96.70	111.00
1	2-A	383	ALA	C-N-CA	5.29	134.94	121.70
3	2-C	106	ALA	N-CA-C	-5.29	96.71	111.00
7	3-L	13	VAL	N-CA-C	-5.29	96.71	111.00
1	1-A	383	ALA	C-N-CA	5.29	134.92	121.70
7	1-L	13	VAL	N-CA-C	-5.29	96.73	111.00
3	2-C	378	TYR	O-C-N	5.29	131.16	122.70
6	1-G	686	ALA	N-CA-C	5.28	125.26	111.00
6	2-G	686	ALA	N-CA-C	5.28	125.26	111.00
3	3-C	509	GLY	N-CA-C	-5.28	99.90	113.10
1	1-A	402	SER	N-CA-C	-5.28	96.75	111.00
2	1-B	763	GLN	C-N-CA	5.28	134.89	121.70
1	2-A	340	PHE	C-N-CA	5.28	134.90	121.70
5	3-F	166	LEU	C-N-CA	5.28	134.89	121.70
3	1-C	378	TYR	O-C-N	5.27	131.14	122.70
6	1-K	686	ALA	N-CA-C	5.27	125.23	111.00
6	3-K	686	ALA	N-CA-C	5.27	125.23	111.00
6	2-K	686	ALA	N-CA-C	5.27	125.23	111.00
5	2-F	166	LEU	C-N-CA	5.27	134.87	121.70
6	2-K	131	ILE	N-CA-C	5.26	125.21	111.00
1	2-A	402	SER	N-CA-C	-5.26	96.79	111.00
5	1-F	166	LEU	C-N-CA	5.26	134.85	121.70
6	3-K	131	ILE	N-CA-C	5.26	125.21	111.00
1	3-A	340	PHE	C-N-CA	5.26	134.85	121.70
1	3-A	402	SER	N-CA-C	-5.26	96.80	111.00
1	1-A	340	PHE	C-N-CA	5.25	134.83	121.70
6	1-K	131	ILE	N-CA-C	5.25	125.18	111.00
5	2-F	60	ASN	CA-C-N	-5.24	105.66	117.20
6	2-K	120	TYR	CA-C-N	-5.24	105.66	117.20
3	3-C	237	PHE	N-CA-C	-5.24	96.84	111.00
6	1-K	120	TYR	CA-C-N	-5.24	105.67	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3-F	60	ASN	CA-C-N	-5.24	105.68	117.20
3	1-C	237	PHE	N-CA-C	-5.24	96.87	111.00
6	2-K	297	SER	N-CA-C	5.24	125.13	111.00
6	3-K	120	TYR	CA-C-N	-5.23	105.69	117.20
5	1-F	60	ASN	CA-C-N	-5.23	105.70	117.20
6	3-G	838	HIS	CA-C-N	-5.23	105.70	117.20
6	3-K	297	SER	N-CA-C	5.22	125.10	111.00
6	3-K	247	ARG	N-CA-C	-5.22	96.91	111.00
6	1-G	838	HIS	CA-C-N	-5.22	105.72	117.20
6	1-K	247	ARG	N-CA-C	-5.22	96.92	111.00
3	2-C	237	PHE	N-CA-C	-5.21	96.92	111.00
6	1-K	297	SER	N-CA-C	5.21	125.07	111.00
5	2-R	25	LEU	CA-C-N	-5.21	105.73	117.20
6	2-K	838	HIS	CA-C-N	-5.21	105.74	117.20
2	1-B	822	VAL	N-CA-C	-5.21	96.94	111.00
3	1-C	574	TYR	N-CA-C	-5.21	96.94	111.00
6	3-K	838	HIS	CA-C-N	-5.21	105.74	117.20
1	1-A	570	VAL	CA-C-N	5.21	128.66	117.20
6	1-G	683	PRO	N-CA-C	5.21	125.64	112.10
3	2-C	574	TYR	N-CA-C	-5.21	96.94	111.00
6	2-G	838	HIS	CA-C-N	-5.21	105.75	117.20
6	3-G	683	PRO	N-CA-C	5.20	125.63	112.10
5	1-R	25	LEU	CA-C-N	-5.20	105.76	117.20
1	2-A	570	VAL	CA-C-N	5.20	128.64	117.20
6	2-K	247	ARG	N-CA-C	-5.20	96.96	111.00
5	3-R	25	LEU	CA-C-N	-5.20	105.76	117.20
6	1-K	838	HIS	CA-C-N	-5.20	105.77	117.20
1	3-A	570	VAL	CA-C-N	5.20	128.63	117.20
3	3-C	574	TYR	N-CA-C	-5.20	96.97	111.00
6	2-G	683	PRO	N-CA-C	5.19	125.60	112.10
2	2-B	822	VAL	N-CA-C	-5.19	96.98	111.00
6	2-K	683	PRO	N-CA-C	5.19	125.60	112.10
2	3-B	822	VAL	N-CA-C	-5.19	96.98	111.00
6	1-K	176	ARG	C-N-CA	5.19	134.67	121.70
1	3-A	245	CYS	N-CA-C	-5.19	96.99	111.00
1	1-A	436	LEU	N-CA-C	-5.19	96.99	111.00
6	1-K	683	PRO	N-CA-C	5.18	125.57	112.10
1	2-A	245	CYS	N-CA-C	-5.18	97.01	111.00
3	3-C	254	ARG	N-CA-C	-5.18	97.01	111.00
6	2-K	176	ARG	C-N-CA	5.17	134.63	121.70
1	3-A	436	LEU	N-CA-C	-5.17	97.03	111.00
1	2-A	436	LEU	N-CA-C	-5.17	97.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-C	474	GLY	C-N-CA	5.17	134.63	121.70
6	3-K	683	PRO	N-CA-C	5.17	125.54	112.10
3	1-C	254	ARG	N-CA-C	-5.17	97.05	111.00
2	3-B	504	VAL	N-CA-C	5.17	124.95	111.00
3	2-C	474	GLY	C-N-CA	5.17	134.61	121.70
1	1-A	245	CYS	N-CA-C	-5.16	97.06	111.00
6	1-G	39	ILE	N-CA-C	-5.16	97.06	111.00
3	2-C	254	ARG	N-CA-C	-5.16	97.06	111.00
3	1-C	588	LEU	N-CA-C	-5.16	97.07	111.00
2	2-B	504	VAL	N-CA-C	5.16	124.93	111.00
3	2-C	588	LEU	N-CA-C	-5.16	97.07	111.00
6	3-G	39	ILE	N-CA-C	-5.16	97.08	111.00
5	3-R	146	HIS	C-N-CA	5.16	134.59	121.70
6	3-K	176	ARG	C-N-CA	5.15	134.59	121.70
3	2-C	469	PHE	N-CA-C	-5.15	97.09	111.00
3	1-C	474	GLY	C-N-CA	5.15	134.57	121.70
5	2-F	96	ASP	N-CA-C	-5.15	97.10	111.00
6	2-G	39	ILE	N-CA-C	-5.15	97.11	111.00
3	3-C	588	LEU	N-CA-C	-5.15	97.10	111.00
5	1-F	96	ASP	N-CA-C	-5.14	97.11	111.00
6	2-G	296	CYS	C-N-CA	5.14	134.56	121.70
3	3-C	469	PHE	N-CA-C	-5.14	97.11	111.00
5	3-F	96	ASP	N-CA-C	-5.14	97.11	111.00
2	1-B	504	VAL	N-CA-C	5.14	124.88	111.00
7	1-L	18	ILE	O-C-N	5.14	130.93	122.70
6	1-G	296	CYS	C-N-CA	5.14	134.55	121.70
3	1-C	469	PHE	N-CA-C	-5.14	97.13	111.00
1	3-A	221	VAL	N-CA-C	-5.13	97.14	111.00
1	1-A	221	VAL	N-CA-C	-5.13	97.15	111.00
1	2-A	221	VAL	N-CA-C	-5.13	97.16	111.00
5	2-R	146	HIS	C-N-CA	5.12	134.51	121.70
2	3-B	782	LYS	N-CA-C	-5.12	97.18	111.00
6	3-G	296	CYS	C-N-CA	5.12	134.50	121.70
2	1-B	782	LYS	N-CA-C	-5.12	97.18	111.00
6	3-G	703	PRO	C-N-CA	5.12	133.04	122.30
3	1-C	155	ASN	CA-C-N	-5.11	105.95	117.20
5	1-R	146	HIS	C-N-CA	5.11	134.48	121.70
6	2-K	703	PRO	C-N-CA	5.11	133.03	122.30
7	3-L	18	ILE	O-C-N	5.11	130.88	122.70
6	2-G	703	PRO	C-N-CA	5.11	133.03	122.30
3	1-C	802	LYS	N-CA-C	5.11	124.79	111.00
3	2-C	802	LYS	CA-C-N	5.11	128.43	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-C	155	ASN	CA-C-N	-5.11	105.97	117.20
3	3-C	802	LYS	N-CA-C	5.11	124.79	111.00
2	2-B	782	LYS	N-CA-C	-5.10	97.22	111.00
1	3-A	515	ASN	N-CA-C	-5.10	97.22	111.00
3	2-C	803	GLU	N-CA-C	5.10	124.77	111.00
3	3-C	827	VAL	C-N-CA	5.10	134.45	121.70
6	1-G	703	PRO	C-N-CA	5.10	133.00	122.30
1	2-A	515	ASN	N-CA-C	-5.10	97.24	111.00
3	2-C	155	ASN	CA-C-N	-5.10	105.98	117.20
1	1-A	515	ASN	N-CA-C	-5.09	97.25	111.00
3	3-C	803	GLU	N-CA-C	5.09	124.75	111.00
6	1-K	703	PRO	C-N-CA	5.09	133.00	122.30
5	3-R	29	GLY	N-CA-C	-5.09	100.37	113.10
3	3-C	7	ILE	N-CA-C	-5.09	97.26	111.00
3	1-C	802	LYS	CA-C-N	5.09	128.40	117.20
3	1-C	314	ILE	N-CA-C	-5.09	97.27	111.00
6	1-G	804	ILE	N-CA-C	5.09	124.73	111.00
3	2-C	827	VAL	C-N-CA	5.08	134.41	121.70
3	1-C	803	GLU	N-CA-C	5.08	124.73	111.00
3	3-C	314	ILE	N-CA-C	-5.08	97.28	111.00
3	3-C	802	LYS	CA-C-N	5.08	128.38	117.20
3	1-C	7	ILE	N-CA-C	-5.08	97.28	111.00
3	2-C	802	LYS	N-CA-C	5.08	124.72	111.00
6	2-G	804	ILE	N-CA-C	5.08	124.72	111.00
3	1-C	827	VAL	C-N-CA	5.08	134.40	121.70
5	1-R	29	GLY	N-CA-C	-5.08	100.40	113.10
6	3-K	703	PRO	C-N-CA	5.08	132.97	122.30
7	1-Z	18	ILE	CA-C-N	-5.08	106.03	117.20
6	3-G	804	ILE	N-CA-C	5.08	124.71	111.00
5	2-R	29	GLY	N-CA-C	-5.08	100.41	113.10
7	3-Z	18	ILE	CA-C-N	-5.08	106.03	117.20
3	1-C	567	ILE	N-CA-C	-5.07	97.30	111.00
1	2-A	37	ASP	N-CA-C	-5.07	97.30	111.00
3	2-C	314	ILE	N-CA-C	-5.07	97.30	111.00
1	1-A	37	ASP	N-CA-C	-5.07	97.31	111.00
6	2-G	435	GLY	C-N-CA	5.07	134.38	121.70
7	2-Z	56	ASP	N-CA-C	-5.07	97.31	111.00
7	1-Z	56	ASP	N-CA-C	-5.07	97.31	111.00
6	2-G	141	GLU	N-CA-C	5.07	124.69	111.00
7	2-L	18	ILE	O-C-N	5.07	130.81	122.70
6	3-K	804	ILE	N-CA-C	5.07	124.69	111.00
3	2-C	7	ILE	N-CA-C	-5.07	97.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3-G	141	GLU	N-CA-C	5.07	124.68	111.00
7	3-Z	56	ASP	N-CA-C	-5.07	97.32	111.00
6	1-G	141	GLU	N-CA-C	5.07	124.68	111.00
6	3-K	120	TYR	C-N-CA	5.07	134.36	121.70
6	1-G	435	GLY	C-N-CA	5.06	134.36	121.70
6	1-K	120	TYR	C-N-CA	5.06	134.36	121.70
6	3-G	435	GLY	C-N-CA	5.06	134.35	121.70
6	1-G	118	ASP	CA-C-N	-5.06	106.07	117.20
3	3-C	567	ILE	N-CA-C	-5.06	97.34	111.00
6	3-G	118	ASP	CA-C-N	-5.06	106.07	117.20
6	1-K	804	ILE	N-CA-C	5.06	124.65	111.00
1	1-A	543	TYR	N-CA-C	-5.05	97.36	111.00
1	2-A	543	TYR	N-CA-C	-5.05	97.35	111.00
3	2-C	567	ILE	N-CA-C	-5.05	97.35	111.00
6	2-K	804	ILE	N-CA-C	5.05	124.64	111.00
1	3-A	37	ASP	N-CA-C	-5.05	97.36	111.00
3	2-C	790	ASP	CA-C-N	5.05	131.24	117.10
1	2-A	562	ARG	N-CA-C	-5.05	97.36	111.00
6	2-G	118	ASP	CA-C-N	-5.05	106.09	117.20
7	2-Z	18	ILE	CA-C-N	-5.05	106.09	117.20
1	1-A	562	ARG	N-CA-C	-5.05	97.38	111.00
1	3-A	562	ARG	N-CA-C	-5.04	97.39	111.00
3	1-C	790	ASP	CA-C-N	5.04	131.22	117.10
6	1-K	813	CYS	N-CA-C	5.04	124.60	111.00
6	2-G	815	ARG	N-CA-C	-5.04	97.40	111.00
1	3-A	543	TYR	N-CA-C	-5.04	97.39	111.00
6	3-G	815	ARG	N-CA-C	-5.04	97.40	111.00
6	1-G	815	ARG	N-CA-C	-5.04	97.40	111.00
3	3-C	790	ASP	CA-C-N	5.03	131.18	117.10
6	2-K	120	TYR	C-N-CA	5.03	134.27	121.70
6	2-K	813	CYS	N-CA-C	5.03	124.57	111.00
3	3-C	397	ALA	N-CA-C	-5.02	97.44	111.00
6	3-K	813	CYS	N-CA-C	5.02	124.56	111.00
1	2-A	249	TYR	N-CA-C	-5.02	97.45	111.00
1	3-A	249	TYR	N-CA-C	-5.02	97.45	111.00
1	2-A	428	VAL	N-CA-C	-5.01	97.46	111.00
6	3-K	221	HIS	C-N-CA	5.01	132.83	122.30
1	1-A	428	VAL	N-CA-C	-5.01	97.47	111.00
1	1-A	249	TYR	N-CA-C	-5.01	97.48	111.00
1	1-A	568	ILE	N-CA-C	-5.00	97.49	111.00
7	2-L	58	GLU	N-CA-C	-5.00	97.49	111.00
1	1-A	391	TYR	N-CA-C	-5.00	97.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	2-B	935	ASP	N-CA-C	5.00	124.51	111.00
3	2-C	397	ALA	N-CA-C	-5.00	97.49	111.00
3	1-C	397	ALA	N-CA-C	-5.00	97.50	111.00
7	1-L	58	GLU	N-CA-C	-5.00	97.50	111.00
1	2-A	424	ASN	N-CA-C	5.00	124.50	111.00
1	3-A	413	SER	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-B	898	ALA	Peptide
2	1-B	903	CYS	Peptide
2	1-B	938	VAL	Mainchain
2	2-B	898	ALA	Peptide
2	2-B	903	CYS	Peptide
2	2-B	938	VAL	Mainchain
2	3-B	898	ALA	Peptide
2	3-B	903	CYS	Peptide
2	3-B	938	VAL	Mainchain

## 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	1-A	3251	0	869	36	0
1	2-A	3251	0	869	37	0
1	3-A	3251	0	869	36	0
2	1-B	3198	0	810	56	0
2	2-B	3198	0	810	56	0
2	3-B	3198	0	810	54	0
3	1-C	3371	0	919	21	0
3	2-C	3371	0	919	23	0
3	3-C	3371	0	919	23	0
4	1-D	1707	0	450	9	0
4	2-D	1707	0	450	9	0
4	3-D	1707	0	450	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1-F	635	0	181	3	0
5	1-M	635	0	181	19	0
5	1-R	635	0	181	38	0
5	2-F	635	0	181	3	0
5	2-M	635	0	181	20	0
5	2-R	635	0	181	38	0
5	3-F	635	0	181	3	0
5	3-M	635	0	181	19	0
5	3-R	635	0	181	35	0
6	1-G	3190	0	822	59	0
6	1-K	2239	0	572	37	0
6	2-G	3190	0	822	59	0
6	2-K	2239	0	572	38	0
6	3-G	3190	0	822	57	0
6	3-K	2239	0	572	36	0
7	1-L	555	0	148	2	0
7	1-Z	555	0	147	14	0
7	2-L	555	0	148	2	0
7	2-Z	555	0	147	14	0
7	3-L	555	0	148	2	0
7	3-Z	555	0	147	14	0
All	All	59913	0	15840	824	0

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 11.

All (824) 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)
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.47
6:K:107:SER:N	5:M:50:GLY:HA3	1.28	1.47
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.47
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.45
6:G:107:SER:H	5:R:50:GLY:CA	1.31	1.44
6:G:107:SER:H	5:R:50:GLY:CA	1.31	1.43
6:K:107:SER:N	5:M:50:GLY:HA3	1.28	1.42
6:G:107:SER:H	5:R:50:GLY:CA	1.31	1.42
6:K:107:SER:N	5:M:50:GLY:HA3	1.28	1.39
6:K:167:LEU:CA	6:K:170:SER:O	1.73	1.36
6:K:167:LEU:CA	6:K:170:SER:O	1.73	1.36
6:K:167:LEU:CA	6:K:170:SER:O	1.73	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.30
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.29
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.27
3:C:269:TYR:O	3:C:271:MET:N	1.68	1.26
3:C:269:TYR:O	3:C:271:MET:N	1.68	1.25
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.24
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.24
6:K:107:SER:H	5:M:50:GLY:CA	1.53	1.22
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.22
3:C:269:TYR:O	3:C:271:MET:N	1.68	1.21
5:R:71:GLN:O	5:R:74:ILE:N	1.74	1.21
5:R:143:LEU:C	5:R:145:LEU:H	1.23	1.20
6:K:107:SER:H	5:M:50:GLY:CA	1.53	1.20
6:K:107:SER:H	5:M:50:GLY:CA	1.53	1.20
2:B:778:LEU:O	2:B:809:THR:O	1.58	1.20
5:R:71:GLN:O	5:R:74:ILE:N	1.74	1.20
2:B:778:LEU:O	2:B:809:THR:O	1.58	1.19
5:R:143:LEU:C	5:R:145:LEU:H	1.23	1.19
5:R:71:GLN:O	5:R:74:ILE:N	1.74	1.18
2:B:778:LEU:O	2:B:809:THR:O	1.58	1.18
4:D:13:GLY:HA2	4:D:38:LYS:CA	1.74	1.18
4:D:13:GLY:HA2	4:D:38:LYS:CA	1.74	1.17
4:D:13:GLY:HA2	4:D:38:LYS:CA	1.75	1.16
2:B:781:LEU:O	2:B:808:SER:O	1.63	1.16
6:G:167:LEU:CA	6:G:170:SER:O	1.95	1.15
6:G:167:LEU:CA	6:G:170:SER:O	1.95	1.14
5:R:143:LEU:C	5:R:145:LEU:H	1.23	1.14
6:G:167:LEU:CA	6:G:170:SER:O	1.95	1.14
2:B:781:LEU:O	2:B:808:SER:O	1.63	1.14
6:K:190:ILE:CA	6:K:225:SER:CA	2.26	1.14
6:K:190:ILE:CA	6:K:225:SER:CA	2.26	1.13
5:R:143:LEU:C	5:R:145:LEU:N	1.99	1.13
6:K:190:ILE:CA	6:K:225:SER:CA	2.26	1.13
2:B:781:LEU:O	2:B:808:SER:O	1.63	1.10
5:R:143:LEU:C	5:R:145:LEU:N	1.99	1.08
7:Z:11:TYR:CA	7:Z:132:GLY:HA3	1.84	1.07
2:B:778:LEU:O	2:B:809:THR:C	1.91	1.07
5:R:159:CYS:O	5:R:162:SER:N	1.88	1.07
2:B:778:LEU:O	2:B:809:THR:C	1.91	1.06
7:L:31:TYR:CA	7:L:131:GLY:O	2.03	1.06
7:Z:11:TYR:CA	7:Z:132:GLY:HA3	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:11:TYR:CA	7:Z:132:GLY:HA3	1.84	1.06
7:L:31:TYR:CA	7:L:131:GLY:O	2.03	1.06
2:B:778:LEU:O	2:B:809:THR:C	1.91	1.05
5:R:143:LEU:C	5:R:145:LEU:N	1.99	1.05
2:B:526:VAL:CA	2:B:597:VAL:CA	2.35	1.05
2:B:526:VAL:CA	2:B:597:VAL:CA	2.35	1.05
7:L:31:TYR:CA	7:L:131:GLY:O	2.03	1.05
5:R:159:CYS:O	5:R:162:SER:N	1.88	1.05
5:R:159:CYS:O	5:R:162:SER:N	1.88	1.04
2:B:526:VAL:CA	2:B:597:VAL:CA	2.35	1.03
6:G:276:ASN:O	6:G:281:SER:O	1.75	1.03
6:G:276:ASN:O	6:G:281:SER:O	1.75	1.03
6:G:276:ASN:O	6:G:281:SER:O	1.75	1.03
7:Z:12:THR:H	7:Z:132:GLY:CA	1.72	1.03
7:Z:12:THR:H	7:Z:132:GLY:CA	1.72	1.02
7:Z:12:THR:H	7:Z:132:GLY:CA	1.72	1.02
5:R:130:LEU:O	5:R:132:GLU:N	1.92	1.01
5:R:130:LEU:O	5:R:132:GLU:N	1.92	1.01
5:R:130:LEU:O	5:R:132:GLU:N	1.92	1.00
5:R:126:ASN:CA	5:R:158:THR:O	2.10	1.00
5:R:126:ASN:CA	5:R:158:THR:O	2.10	0.99
6:K:677:VAL:O	6:K:694:PRO:CA	2.11	0.99
6:K:677:VAL:O	6:K:694:PRO:CA	2.11	0.98
5:R:126:ASN:CA	5:R:158:THR:O	2.10	0.98
7:Z:11:TYR:CA	7:Z:132:GLY:CA	2.41	0.97
6:K:677:VAL:O	6:K:694:PRO:CA	2.11	0.97
7:Z:11:TYR:CA	7:Z:132:GLY:CA	2.41	0.97
6:K:167:LEU:C	6:K:170:SER:O	2.03	0.97
6:K:190:ILE:C	6:K:225:SER:CA	2.34	0.96
6:K:190:ILE:C	6:K:225:SER:CA	2.34	0.96
2:B:778:LEU:C	2:B:809:THR:O	2.04	0.95
2:B:541:ALA:CA	2:B:624:ASP:N	2.29	0.95
6:K:167:LEU:C	6:K:170:SER:O	2.03	0.95
2:B:778:LEU:C	2:B:809:THR:O	2.04	0.95
6:K:167:LEU:C	6:K:170:SER:O	2.03	0.95
2:B:766:ASP:O	2:B:768:LEU:N	2.00	0.95
2:B:778:LEU:C	2:B:809:THR:O	2.04	0.95
2:B:541:ALA:CA	2:B:624:ASP:N	2.29	0.95
2:B:541:ALA:CA	2:B:624:ASP:N	2.29	0.95
6:K:190:ILE:C	6:K:225:SER:CA	2.34	0.95
7:Z:12:THR:N	7:Z:132:GLY:CA	2.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:11:TYR:CA	7:Z:132:GLY:CA	2.41	0.94
2:B:766:ASP:O	2:B:768:LEU:N	2.00	0.94
6:G:107:SER:N	5:R:50:GLY:CA	2.05	0.94
7:Z:12:THR:N	7:Z:132:GLY:CA	2.30	0.94
7:Z:12:THR:N	7:Z:132:GLY:CA	2.30	0.94
2:B:824:GLY:CA	2:B:830:ASN:O	2.16	0.93
2:B:766:ASP:O	2:B:768:LEU:N	2.00	0.93
2:B:824:GLY:CA	2:B:830:ASN:O	2.16	0.93
2:B:824:GLY:CA	2:B:830:ASN:O	2.16	0.93
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.92
7:Z:12:THR:N	7:Z:132:GLY:O	2.02	0.92
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.92
6:K:107:SER:CA	5:M:50:GLY:HA3	2.00	0.92
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.91
7:Z:12:THR:N	7:Z:132:GLY:O	2.02	0.91
5:R:125:ALA:O	5:R:158:THR:O	1.89	0.91
5:R:125:ALA:O	5:R:158:THR:O	1.89	0.91
5:R:125:ALA:O	5:R:158:THR:O	1.88	0.90
6:K:107:SER:CA	5:M:50:GLY:HA3	2.00	0.90
7:Z:12:THR:N	7:Z:132:GLY:O	2.02	0.90
6:K:107:SER:CA	5:M:50:GLY:HA3	2.00	0.89
2:B:767:THR:CA	2:B:792:LEU:H	1.85	0.89
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.89
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.89
2:B:767:THR:CA	2:B:792:LEU:H	1.85	0.89
2:B:781:LEU:CA	2:B:805:LYS:O	2.22	0.88
6:G:198:GLY:O	6:G:201:TYR:N	2.07	0.88
2:B:767:THR:CA	2:B:792:LEU:H	1.85	0.88
6:K:167:LEU:O	6:K:170:SER:O	1.92	0.88
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.88
6:G:198:GLY:O	6:G:201:TYR:N	2.07	0.87
6:G:198:GLY:O	6:G:201:TYR:N	2.07	0.87
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.87
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.87
6:G:107:SER:N	5:R:50:GLY:CA	2.05	0.87
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.86
6:K:190:ILE:O	6:K:225:SER:CA	2.23	0.86
6:K:107:SER:N	5:M:50:GLY:CA	2.24	0.86
6:K:190:ILE:O	6:K:225:SER:CA	2.23	0.86
2:B:781:LEU:CA	2:B:805:LYS:O	2.22	0.86
2:B:781:LEU:CA	2:B:805:LYS:O	2.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:167:LEU:O	6:K:170:SER:O	1.92	0.86
2:B:483:THR:O	2:B:487:ILE:N	2.09	0.86
6:K:190:ILE:O	6:K:225:SER:CA	2.23	0.86
6:K:167:LEU:O	6:K:170:SER:O	1.92	0.86
6:G:107:SER:N	5:R:50:GLY:CA	2.05	0.85
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.85
6:G:107:SER:H	5:R:50:GLY:C	1.79	0.85
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.85
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.85
6:K:190:ILE:CA	6:K:225:SER:N	2.40	0.85
5:R:78:TRP:O	5:R:81:TYR:O	1.95	0.85
6:G:107:SER:H	5:R:50:GLY:C	1.79	0.85
2:B:483:THR:O	2:B:487:ILE:N	2.09	0.85
2:B:739:ASP:O	2:B:740:PRO:O	1.96	0.84
6:G:301:ALA:C	6:G:303:LEU:H	1.79	0.84
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.84
6:G:106:THR:C	5:R:50:GLY:HA3	1.98	0.84
5:R:78:TRP:O	5:R:81:TYR:O	1.95	0.84
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.84
6:K:190:ILE:CA	6:K:225:SER:N	2.40	0.84
2:B:483:THR:O	2:B:487:ILE:N	2.09	0.84
1:A:214:HIS:O	1:A:217:MET:N	2.10	0.84
2:B:739:ASP:O	2:B:740:PRO:O	1.96	0.84
6:G:106:THR:C	5:R:50:GLY:HA3	1.98	0.84
6:G:301:ALA:C	6:G:303:LEU:H	1.79	0.84
5:R:78:TRP:O	5:R:81:TYR:O	1.95	0.84
2:B:739:ASP:O	2:B:740:PRO:O	1.96	0.84
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.84
6:K:190:ILE:CA	6:K:225:SER:N	2.40	0.84
6:K:107:SER:N	5:M:50:GLY:CA	2.24	0.83
6:G:301:ALA:C	6:G:303:LEU:H	1.79	0.83
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.83
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.83
2:B:824:GLY:HA2	2:B:830:ASN:O	1.78	0.83
2:B:824:GLY:HA2	2:B:830:ASN:O	1.78	0.83
1:A:214:HIS:O	1:A:217:MET:N	2.11	0.83
1:A:214:HIS:O	1:A:217:MET:N	2.10	0.83
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.83
5:R:130:LEU:C	5:R:132:GLU:H	1.82	0.83
6:G:107:SER:H	5:R:50:GLY:C	1.79	0.82
4:D:41:ASN:O	4:D:43:GLY:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:106:THR:C	5:R:50:GLY:HA3	1.98	0.82
5:R:130:LEU:C	5:R:132:GLU:H	1.82	0.82
4:D:41:ASN:O	4:D:43:GLY:N	2.12	0.82
6:K:107:SER:N	5:M:50:GLY:CA	2.24	0.81
4:D:41:ASN:O	4:D:43:GLY:N	2.12	0.81
5:M:79:ARG:O	5:M:81:TYR:N	2.13	0.81
2:B:767:THR:C	2:B:792:LEU:H	1.84	0.81
2:B:483:THR:O	2:B:484:LYS:C	2.18	0.81
2:B:824:GLY:HA2	2:B:830:ASN:O	1.78	0.81
2:B:483:THR:O	2:B:484:LYS:C	2.18	0.81
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.81
2:B:767:THR:C	2:B:792:LEU:H	1.84	0.81
5:R:130:LEU:C	5:R:132:GLU:H	1.82	0.81
7:Z:13:VAL:H	7:Z:132:GLY:HA2	1.46	0.81
2:B:483:THR:O	2:B:484:LYS:C	2.18	0.81
2:B:767:THR:C	2:B:792:LEU:H	1.84	0.81
7:Z:13:VAL:H	7:Z:132:GLY:HA2	1.46	0.81
5:M:79:ARG:O	5:M:81:TYR:N	2.13	0.80
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.80
7:Z:11:TYR:C	7:Z:132:GLY:HA3	2.02	0.80
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.80
7:Z:11:TYR:C	7:Z:132:GLY:HA3	2.02	0.80
7:Z:11:TYR:C	7:Z:132:GLY:HA3	2.02	0.80
5:M:79:ARG:O	5:M:81:TYR:N	2.13	0.80
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.80
4:D:13:GLY:CA	4:D:38:LYS:CA	2.60	0.79
7:Z:13:VAL:H	7:Z:132:GLY:HA2	1.46	0.79
7:Z:12:THR:H	7:Z:132:GLY:C	1.86	0.79
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.79
6:G:277:LEU:O	6:G:280:CYS:N	2.16	0.79
6:G:277:LEU:O	6:G:280:CYS:N	2.16	0.79
7:Z:12:THR:H	7:Z:132:GLY:C	1.86	0.79
2:B:483:THR:O	2:B:486:ASP:N	2.17	0.78
2:B:740:PRO:O	2:B:741:VAL:C	2.18	0.78
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.78
7:Z:12:THR:H	7:Z:132:GLY:C	1.86	0.78
2:B:483:THR:O	2:B:486:ASP:N	2.17	0.77
2:B:483:THR:O	2:B:486:ASP:N	2.17	0.77
4:D:13:GLY:CA	4:D:38:LYS:CA	2.60	0.77
4:D:13:GLY:CA	4:D:38:LYS:CA	2.60	0.77
3:C:637:VAL:O	3:C:638:SER:O	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:740:PRO:O	2:B:741:VAL:C	2.18	0.77
6:G:105:VAL:O	6:G:107:SER:N	2.17	0.77
6:G:105:VAL:O	6:G:107:SER:N	2.17	0.76
6:G:277:LEU:O	6:G:280:CYS:N	2.16	0.76
7:Z:12:THR:H	7:Z:132:GLY:HA2	1.51	0.76
7:Z:12:THR:H	7:Z:132:GLY:HA2	1.51	0.76
3:C:637:VAL:O	3:C:638:SER:O	2.03	0.76
2:B:766:ASP:C	2:B:768:LEU:H	1.89	0.76
6:G:105:VAL:O	6:G:107:SER:N	2.17	0.75
7:Z:12:THR:N	7:Z:132:GLY:HA3	2.00	0.75
3:C:637:VAL:O	3:C:638:SER:O	2.03	0.75
2:B:740:PRO:O	2:B:741:VAL:C	2.18	0.75
7:Z:12:THR:H	7:Z:132:GLY:HA2	1.51	0.75
2:B:766:ASP:C	2:B:768:LEU:H	1.89	0.74
1:A:800:PRO:O	3:C:805:PHE:O	2.05	0.74
7:Z:12:THR:N	7:Z:132:GLY:HA3	2.00	0.74
2:B:766:ASP:C	2:B:768:LEU:H	1.89	0.74
7:Z:12:THR:N	7:Z:132:GLY:HA3	2.00	0.74
5:M:77:LEU:O	5:M:80:HIS:N	2.20	0.74
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.74
1:A:800:PRO:O	3:C:805:PHE:O	2.05	0.74
5:M:77:LEU:O	5:M:80:HIS:N	2.20	0.74
1:A:800:PRO:O	3:C:805:PHE:O	2.05	0.74
5:M:77:LEU:O	5:M:80:HIS:N	2.21	0.74
6:G:301:ALA:C	6:G:303:LEU:N	2.41	0.74
6:G:215:ILE:O	6:G:219:THR:N	2.22	0.73
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.73
6:G:215:ILE:O	6:G:219:THR:N	2.22	0.73
5:R:143:LEU:O	5:R:145:LEU:N	2.22	0.73
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.73
5:R:174:SER:O	5:R:176:SER:N	2.21	0.73
5:R:174:SER:O	5:R:176:SER:N	2.21	0.73
5:R:174:SER:O	5:R:176:SER:N	2.21	0.72
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.72
6:G:215:ILE:O	6:G:219:THR:N	2.22	0.72
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.72
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.72
2:B:928:LYS:O	2:B:934:PRO:O	2.08	0.72
5:R:143:LEU:O	5:R:145:LEU:N	2.22	0.71
2:B:928:LYS:O	2:B:934:PRO:O	2.08	0.71
2:B:928:LYS:O	2:B:934:PRO:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:301:ALA:C	6:G:303:LEU:N	2.41	0.71
5:R:143:LEU:O	5:R:145:LEU:N	2.22	0.71
6:G:301:ALA:C	6:G:303:LEU:N	2.41	0.71
5:F:29:GLY:HA2	5:F:32:THR:H	1.56	0.71
6:G:247:ARG:O	6:G:248:ASP:C	2.24	0.71
1:A:801:ILE:O	3:C:805:PHE:N	2.24	0.71
7:Z:12:THR:N	7:Z:132:GLY:C	2.44	0.70
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.70
3:C:269:TYR:C	3:C:271:MET:N	2.44	0.70
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.70
6:G:215:ILE:O	6:G:217:LYS:N	2.25	0.70
6:G:167:LEU:C	6:G:170:SER:O	2.30	0.70
6:G:215:ILE:O	6:G:217:LYS:N	2.25	0.70
7:Z:12:THR:N	7:Z:132:GLY:C	2.44	0.70
6:G:167:LEU:C	6:G:170:SER:O	2.30	0.70
1:A:801:ILE:O	3:C:805:PHE:N	2.24	0.70
5:F:29:GLY:HA2	5:F:32:THR:H	1.56	0.70
4:D:41:ASN:C	4:D:43:GLY:H	1.95	0.70
6:G:337:ASN:O	6:G:340:ILE:N	2.25	0.70
5:F:29:GLY:HA2	5:F:32:THR:H	1.56	0.69
6:G:247:ARG:O	6:G:248:ASP:C	2.24	0.69
6:K:133:ASP:O	6:K:134:SER:O	2.10	0.69
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.69
6:K:133:ASP:O	6:K:134:SER:O	2.10	0.69
6:G:215:ILE:O	6:G:217:LYS:N	2.25	0.69
1:A:801:ILE:O	3:C:805:PHE:N	2.24	0.69
6:G:172:ASP:O	6:G:175:LYS:N	2.26	0.69
6:G:337:ASN:O	6:G:340:ILE:N	2.25	0.69
6:G:167:LEU:C	6:G:170:SER:O	2.30	0.69
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.69
4:D:41:ASN:C	4:D:43:GLY:H	1.95	0.69
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.68
6:G:247:ARG:O	6:G:248:ASP:C	2.24	0.68
6:K:133:ASP:O	6:K:134:SER:O	2.10	0.68
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.68
6:G:247:ARG:O	6:G:248:ASP:O	2.12	0.68
6:G:172:ASP:O	6:G:175:LYS:N	2.26	0.68
6:G:172:ASP:O	6:G:175:LYS:N	2.26	0.68
7:Z:10:LEU:O	7:Z:11:TYR:C	2.32	0.68
6:G:337:ASN:O	6:G:340:ILE:N	2.25	0.68
6:K:107:SER:CA	5:M:50:GLY:O	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:ASN:C	4:D:43:GLY:H	1.95	0.67
6:G:247:ARG:O	6:G:248:ASP:O	2.12	0.67
6:G:247:ARG:O	6:G:248:ASP:O	2.12	0.67
7:Z:10:LEU:O	7:Z:11:TYR:C	2.32	0.67
7:Z:10:LEU:O	7:Z:11:TYR:O	2.13	0.67
6:K:107:SER:CA	5:M:50:GLY:O	2.43	0.67
7:Z:10:LEU:O	7:Z:11:TYR:O	2.13	0.67
2:B:779:GLY:O	2:B:808:SER:O	2.14	0.66
6:G:277:LEU:CA	6:G:280:CYS:CA	2.74	0.66
6:G:277:LEU:CA	6:G:280:CYS:CA	2.74	0.66
7:Z:12:THR:N	7:Z:132:GLY:C	2.44	0.66
2:B:779:GLY:O	2:B:808:SER:O	2.14	0.66
6:K:107:SER:CA	5:M:50:GLY:O	2.43	0.66
7:Z:10:LEU:O	7:Z:11:TYR:C	2.32	0.66
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.66
2:B:766:ASP:C	2:B:768:LEU:N	2.45	0.66
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.66
7:Z:10:LEU:O	7:Z:11:TYR:O	2.13	0.66
2:B:929:PRO:CA	2:B:935:ASP:O	2.44	0.66
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.66
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.66
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.66
2:B:779:GLY:O	2:B:808:SER:O	2.14	0.66
2:B:929:PRO:CA	2:B:935:ASP:O	2.44	0.66
2:B:929:PRO:CA	2:B:935:ASP:O	2.44	0.66
5:R:71:GLN:C	5:R:74:ILE:H	2.00	0.66
2:B:563:ASP:C	2:B:577:THR:C	2.55	0.66
6:G:277:LEU:CA	6:G:280:CYS:CA	2.74	0.66
6:K:135:THR:C	6:K:137:LEU:H	2.00	0.65
4:D:39:LEU:C	4:D:41:ASN:H	2.00	0.65
5:R:71:GLN:O	5:R:74:ILE:CA	2.44	0.65
2:B:563:ASP:C	2:B:577:THR:C	2.55	0.65
4:D:39:LEU:C	4:D:41:ASN:H	2.00	0.65
2:B:112:GLU:O	2:B:114:ILE:N	2.30	0.65
4:D:39:LEU:C	4:D:41:ASN:H	2.00	0.65
6:G:167:LEU:O	6:G:170:SER:O	2.15	0.64
5:R:71:GLN:C	5:R:74:ILE:H	2.00	0.64
5:R:71:GLN:O	5:R:74:ILE:CA	2.44	0.64
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.64
6:G:167:LEU:O	6:G:170:SER:O	2.15	0.64
5:R:71:GLN:C	5:R:74:ILE:H	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLU:O	2:B:114:ILE:N	2.30	0.64
2:B:563:ASP:C	2:B:577:THR:C	2.55	0.64
2:B:824:GLY:HA3	2:B:830:ASN:O	1.96	0.64
6:G:167:LEU:O	6:G:170:SER:O	2.15	0.64
2:B:112:GLU:O	2:B:114:ILE:N	2.30	0.64
6:K:243:GLU:O	6:K:245:GLY:N	2.31	0.64
6:K:135:THR:C	6:K:137:LEU:H	2.00	0.64
2:B:766:ASP:O	2:B:792:LEU:O	2.16	0.64
5:R:71:GLN:O	5:R:74:ILE:CA	2.44	0.63
6:K:243:GLU:O	6:K:245:GLY:N	2.31	0.63
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.63
6:K:243:GLU:O	6:K:245:GLY:N	2.31	0.63
5:M:116:LEU:O	5:M:118:ASN:N	2.32	0.63
2:B:766:ASP:O	2:B:792:LEU:O	2.16	0.63
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.63
2:B:766:ASP:C	2:B:768:LEU:N	2.45	0.63
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.63
2:B:739:ASP:O	2:B:740:PRO:C	2.38	0.63
6:K:135:THR:C	6:K:137:LEU:H	2.00	0.63
5:M:116:LEU:O	5:M:118:ASN:N	2.32	0.63
5:M:24:GLY:O	5:M:68:VAL:O	2.17	0.63
2:B:824:GLY:HA3	2:B:830:ASN:O	1.96	0.62
1:A:227:ARG:O	1:A:245:CYS:O	2.18	0.62
2:B:766:ASP:O	2:B:792:LEU:O	2.16	0.62
1:A:803:PRO:N	3:C:803:GLU:H	1.97	0.62
5:M:24:GLY:O	5:M:68:VAL:O	2.17	0.62
1:A:803:PRO:N	3:C:803:GLU:H	1.97	0.62
6:K:107:SER:CA	5:M:50:GLY:CA	2.75	0.62
1:A:227:ARG:O	1:A:245:CYS:O	2.18	0.62
6:G:172:ASP:O	6:G:173:VAL:C	2.36	0.62
5:M:116:LEU:O	5:M:118:ASN:N	2.32	0.62
1:A:803:PRO:N	3:C:803:GLU:H	1.97	0.62
2:B:824:GLY:HA3	2:B:830:ASN:O	1.96	0.61
2:B:739:ASP:O	2:B:740:PRO:C	2.38	0.61
5:R:71:GLN:O	5:R:72:ASP:C	2.39	0.61
5:M:24:GLY:O	5:M:68:VAL:O	2.17	0.61
5:R:71:GLN:O	5:R:72:ASP:C	2.39	0.61
1:A:227:ARG:O	1:A:245:CYS:O	2.17	0.61
6:K:107:SER:CA	5:M:50:GLY:CA	2.75	0.61
2:B:779:GLY:N	2:B:809:THR:O	2.22	0.61
5:R:69:GLY:C	5:R:71:GLN:H	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:172:ASP:O	6:G:173:VAL:C	2.36	0.60
5:R:71:GLN:O	5:R:72:ASP:C	2.39	0.60
3:C:269:TYR:O	3:C:271:MET:CA	2.49	0.60
5:R:69:GLY:C	5:R:71:GLN:H	2.04	0.60
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.60
6:K:135:THR:O	6:K:137:LEU:N	2.34	0.60
3:C:269:TYR:O	3:C:271:MET:CA	2.49	0.60
6:K:135:THR:O	6:K:137:LEU:N	2.35	0.60
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.60
6:G:215:ILE:C	6:G:217:LYS:H	2.05	0.60
6:G:215:ILE:C	6:G:217:LYS:N	2.55	0.60
6:G:215:ILE:C	6:G:217:LYS:H	2.05	0.60
6:G:215:ILE:C	6:G:217:LYS:N	2.55	0.60
5:R:69:GLY:C	5:R:71:GLN:H	2.04	0.60
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.60
5:R:159:CYS:O	5:R:162:SER:CA	2.50	0.59
5:R:82:TYR:O	5:R:83:ARG:C	2.39	0.59
2:B:740:PRO:O	2:B:742:TYR:N	2.35	0.59
3:C:269:TYR:C	3:C:271:MET:H	2.02	0.59
2:B:557:LEU:O	2:B:558:ARG:C	2.41	0.59
2:B:563:ASP:C	2:B:577:THR:CA	2.71	0.59
5:R:159:CYS:O	5:R:162:SER:CA	2.50	0.59
2:B:739:ASP:O	2:B:740:PRO:C	2.38	0.59
2:B:557:LEU:O	2:B:558:ARG:C	2.41	0.59
2:B:563:ASP:C	2:B:577:THR:CA	2.71	0.59
5:M:128:GLN:H	5:M:159:CYS:CA	2.16	0.59
2:B:740:PRO:O	2:B:742:TYR:N	2.35	0.59
6:K:135:THR:O	6:K:137:LEU:N	2.35	0.59
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.59
5:R:159:CYS:O	5:R:162:SER:CA	2.50	0.59
6:G:215:ILE:O	6:G:218:PHE:N	2.36	0.59
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.59
2:B:563:ASP:C	2:B:577:THR:CA	2.71	0.59
5:M:128:GLN:H	5:M:159:CYS:CA	2.16	0.59
6:G:215:ILE:O	6:G:218:PHE:N	2.36	0.58
6:G:215:ILE:O	6:G:218:PHE:N	2.36	0.58
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.58
2:B:740:PRO:O	2:B:742:TYR:N	2.35	0.58
3:C:269:TYR:O	3:C:271:MET:CA	2.49	0.58
6:G:215:ILE:C	6:G:217:LYS:H	2.05	0.58
6:G:337:ASN:O	6:G:338:ARG:C	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:VAL:CA	2:B:597:VAL:N	2.67	0.58
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.58
3:C:269:TYR:C	3:C:271:MET:H	2.02	0.58
6:G:172:ASP:O	6:G:173:VAL:C	2.36	0.58
6:G:337:ASN:O	6:G:338:ARG:C	2.39	0.58
6:K:107:SER:CA	5:M:50:GLY:CA	2.75	0.58
5:M:128:GLN:H	5:M:159:CYS:CA	2.16	0.58
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.58
6:G:337:ASN:O	6:G:338:ARG:C	2.39	0.58
2:B:766:ASP:C	2:B:768:LEU:N	2.45	0.58
2:B:779:GLY:N	2:B:809:THR:O	2.22	0.58
2:B:504:VAL:O	2:B:507:GLU:N	2.37	0.58
6:G:277:LEU:CA	6:G:280:CYS:C	2.72	0.58
2:B:563:ASP:C	2:B:577:THR:O	2.43	0.57
6:G:277:LEU:CA	6:G:280:CYS:C	2.72	0.57
2:B:563:ASP:C	2:B:577:THR:O	2.43	0.57
2:B:563:ASP:C	2:B:577:THR:O	2.43	0.57
5:R:82:TYR:O	5:R:83:ARG:C	2.39	0.57
3:C:269:TYR:C	3:C:271:MET:H	2.02	0.57
2:B:504:VAL:O	2:B:507:GLU:N	2.37	0.57
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.57
6:G:387:CYS:O	6:G:391:PRO:CA	2.53	0.57
6:G:215:ILE:C	6:G:217:LYS:N	2.55	0.57
6:G:387:CYS:O	6:G:391:PRO:CA	2.53	0.57
6:G:277:LEU:CA	6:G:280:CYS:C	2.72	0.57
2:B:526:VAL:CA	2:B:597:VAL:N	2.67	0.57
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.57
2:B:504:VAL:O	2:B:507:GLU:N	2.37	0.57
2:B:526:VAL:CA	2:B:597:VAL:N	2.67	0.57
6:G:387:CYS:O	6:G:391:PRO:CA	2.53	0.57
6:G:198:GLY:C	6:G:201:TYR:H	2.07	0.56
2:B:767:THR:CA	2:B:792:LEU:N	2.65	0.56
2:B:779:GLY:HA2	2:B:811:ASN:H	1.70	0.56
5:R:82:TYR:O	5:R:83:ARG:C	2.39	0.56
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.56
2:B:899:LEU:O	2:B:900:SER:C	2.44	0.56
2:B:899:LEU:O	2:B:900:SER:C	2.44	0.56
2:B:541:ALA:N	2:B:624:ASP:N	2.53	0.56
2:B:541:ALA:N	2:B:624:ASP:N	2.53	0.56
6:K:135:THR:C	6:K:137:LEU:N	2.58	0.56
6:K:274:ILE:O	6:K:276:ASN:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:274:ILE:O	6:K:276:ASN:N	2.39	0.56
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.56
2:B:102:LYS:C	2:B:104:THR:H	2.09	0.56
2:B:779:GLY:HA2	2:B:811:ASN:H	1.70	0.56
6:G:277:LEU:CA	6:G:280:CYS:N	2.69	0.56
2:B:557:LEU:O	2:B:558:ARG:C	2.41	0.56
6:G:277:LEU:CA	6:G:280:CYS:N	2.69	0.56
6:G:277:LEU:CA	6:G:280:CYS:N	2.69	0.56
2:B:541:ALA:N	2:B:624:ASP:N	2.53	0.55
6:K:107:SER:H	5:M:50:GLY:HA3	0.67	0.55
6:K:274:ILE:O	6:K:276:ASN:N	2.39	0.55
6:G:106:THR:CA	5:R:50:GLY:HA3	2.36	0.55
2:B:899:LEU:O	2:B:900:SER:C	2.44	0.55
6:G:726:CYS:O	6:G:753:LEU:O	2.25	0.55
3:C:506:THR:C	3:C:509:GLY:H	2.10	0.55
3:C:506:THR:C	3:C:509:GLY:H	2.10	0.55
6:G:106:THR:CA	5:R:50:GLY:HA3	2.36	0.55
2:B:779:GLY:HA2	2:B:811:ASN:H	1.70	0.55
3:C:375:TYR:O	3:C:388:PHE:CA	2.56	0.54
6:G:198:GLY:C	6:G:200:LEU:N	2.58	0.54
3:C:506:THR:C	3:C:509:GLY:H	2.10	0.54
2:B:102:LYS:C	2:B:104:THR:H	2.09	0.54
6:K:135:THR:C	6:K:137:LEU:N	2.58	0.54
2:B:767:THR:CA	2:B:792:LEU:N	2.65	0.54
1:A:496:TRP:CA	1:A:502:HIS:H	2.20	0.54
3:C:375:TYR:O	3:C:388:PHE:CA	2.55	0.54
6:K:665:CYS:O	6:K:703:PRO:CA	2.55	0.54
6:G:726:CYS:O	6:G:753:LEU:O	2.25	0.54
6:G:726:CYS:O	6:G:753:LEU:O	2.25	0.54
2:B:767:THR:CA	2:B:792:LEU:N	2.65	0.54
5:M:47:PRO:C	5:M:69:GLY:HA3	2.29	0.54
6:G:247:ARG:O	6:G:251:LEU:N	2.37	0.54
2:B:102:LYS:C	2:B:104:THR:H	2.09	0.54
3:C:375:TYR:O	3:C:388:PHE:CA	2.55	0.54
6:K:665:CYS:O	6:K:703:PRO:CA	2.55	0.53
6:G:106:THR:CA	5:R:50:GLY:HA3	2.36	0.53
6:K:665:CYS:O	6:K:703:PRO:CA	2.55	0.53
5:R:69:GLY:O	5:R:71:GLN:N	2.34	0.53
5:R:71:GLN:C	5:R:73:ARG:N	2.60	0.53
1:A:496:TRP:CA	1:A:502:HIS:H	2.20	0.53
5:M:25:LEU:C	5:M:69:GLY:HA2	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:78:TRP:O	5:M:79:ARG:C	2.46	0.53
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.53
5:R:71:GLN:C	5:R:73:ARG:N	2.60	0.53
5:M:25:LEU:C	5:M:69:GLY:HA2	2.29	0.53
5:M:25:LEU:C	5:M:69:GLY:HA2	2.28	0.53
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.53
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.53
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.53
4:D:41:ASN:C	4:D:43:GLY:N	2.60	0.53
6:G:665:CYS:O	6:G:703:PRO:CA	2.57	0.53
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.53
3:C:174:SER:C	3:C:176:SER:H	2.12	0.53
6:G:665:CYS:O	6:G:703:PRO:CA	2.57	0.53
6:G:247:ARG:O	6:G:251:LEU:N	2.37	0.53
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.53
5:M:47:PRO:C	5:M:69:GLY:HA3	2.29	0.53
6:G:247:ARG:O	6:G:251:LEU:N	2.37	0.53
3:C:174:SER:C	3:C:176:SER:H	2.12	0.53
6:G:665:CYS:O	6:G:703:PRO:CA	2.57	0.53
2:B:112:GLU:C	2:B:114:ILE:H	2.12	0.53
3:C:174:SER:C	3:C:176:SER:H	2.12	0.53
5:M:47:PRO:C	5:M:69:GLY:HA3	2.29	0.53
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.52
5:R:135:SER:O	5:R:136:ALA:C	2.48	0.52
2:B:112:GLU:C	2:B:114:ILE:H	2.12	0.52
6:G:198:GLY:C	6:G:200:LEU:N	2.58	0.52
6:G:198:GLY:C	6:G:201:TYR:H	2.07	0.52
6:G:198:GLY:C	6:G:201:TYR:H	2.07	0.52
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.52
6:G:198:GLY:C	6:G:200:LEU:N	2.58	0.52
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.52
1:A:496:TRP:CA	1:A:502:HIS:H	2.20	0.52
5:R:69:GLY:O	5:R:71:GLN:N	2.34	0.52
6:G:274:ILE:O	6:G:275:VAL:C	2.48	0.52
5:M:78:TRP:O	5:M:79:ARG:C	2.46	0.52
2:B:112:GLU:C	2:B:114:ILE:H	2.12	0.52
5:R:69:GLY:O	5:R:71:GLN:N	2.34	0.52
1:A:802:MET:O	3:C:804:ALA:CA	2.58	0.52
2:B:483:THR:O	2:B:484:LYS:O	2.28	0.52
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.52
2:B:767:THR:CA	2:B:793:ALA:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:274:ILE:O	6:G:275:VAL:C	2.48	0.52
6:G:666:THR:O	6:G:668:THR:N	2.43	0.52
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.52
1:A:802:MET:O	3:C:804:ALA:CA	2.58	0.52
6:G:666:THR:O	6:G:668:THR:N	2.43	0.52
5:R:71:GLN:C	5:R:73:ARG:N	2.60	0.52
7:Z:11:TYR:C	7:Z:132:GLY:CA	2.69	0.52
1:A:802:MET:O	3:C:804:ALA:CA	2.58	0.51
6:G:274:ILE:O	6:G:275:VAL:C	2.48	0.51
2:B:767:THR:CA	2:B:793:ALA:N	2.73	0.51
6:G:198:GLY:O	6:G:199:LEU:C	2.49	0.51
5:R:135:SER:O	5:R:136:ALA:C	2.48	0.51
2:B:483:THR:O	2:B:484:LYS:O	2.28	0.51
5:R:135:SER:O	5:R:136:ALA:C	2.48	0.51
5:R:71:GLN:O	5:R:73:ARG:N	2.43	0.51
3:C:375:TYR:N	3:C:389:GLY:O	2.41	0.51
5:R:71:GLN:O	5:R:73:ARG:N	2.43	0.51
2:B:767:THR:CA	2:B:793:ALA:N	2.73	0.51
6:G:666:THR:O	6:G:668:THR:N	2.43	0.51
2:B:767:THR:O	2:B:768:LEU:C	2.49	0.51
6:G:666:THR:O	6:G:667:ASN:C	2.49	0.51
6:G:172:ASP:C	6:G:175:LYS:H	2.14	0.51
6:G:198:GLY:O	6:G:199:LEU:C	2.49	0.51
5:R:127:LYS:H	5:R:159:CYS:CA	2.24	0.51
5:M:77:LEU:O	5:M:80:HIS:CA	2.59	0.51
5:R:127:LYS:H	5:R:159:CYS:CA	2.24	0.51
2:B:324:LYS:C	2:B:326:HIS:H	2.15	0.51
5:R:71:GLN:O	5:R:73:ARG:N	2.43	0.50
2:B:767:THR:O	2:B:768:LEU:C	2.49	0.50
5:M:77:LEU:O	5:M:80:HIS:CA	2.59	0.50
2:B:483:THR:O	2:B:484:LYS:O	2.28	0.50
2:B:324:LYS:C	2:B:326:HIS:H	2.15	0.50
2:B:767:THR:O	2:B:768:LEU:C	2.49	0.50
6:G:666:THR:O	6:G:667:ASN:C	2.49	0.50
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.50
3:C:459:ARG:CA	3:C:509:GLY:HA3	2.42	0.50
6:G:211:VAL:O	6:G:215:ILE:N	2.45	0.50
5:M:77:LEU:O	5:M:80:HIS:CA	2.59	0.50
3:C:459:ARG:CA	3:C:509:GLY:HA3	2.42	0.50
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.50
5:M:173:LEU:C	5:M:175:ASN:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.50
5:M:173:LEU:C	5:M:175:ASN:H	2.15	0.50
5:M:78:TRP:O	5:M:79:ARG:C	2.46	0.50
6:G:198:GLY:O	6:G:199:LEU:C	2.49	0.50
5:R:127:LYS:H	5:R:159:CYS:CA	2.24	0.50
6:G:211:VAL:O	6:G:215:ILE:N	2.45	0.50
5:R:69:GLY:C	5:R:71:GLN:N	2.65	0.50
5:F:149:ARG:C	5:F:151:ARG:H	2.16	0.49
5:R:69:GLY:C	5:R:71:GLN:N	2.65	0.49
6:G:277:LEU:C	6:G:280:CYS:N	2.66	0.49
2:B:928:LYS:C	2:B:934:PRO:O	2.51	0.49
5:R:130:LEU:C	5:R:132:GLU:N	2.51	0.49
5:R:130:LEU:C	5:R:132:GLU:N	2.51	0.49
6:G:211:VAL:O	6:G:215:ILE:N	2.45	0.49
4:D:42:THR:O	4:D:43:GLY:C	2.50	0.49
6:G:277:LEU:C	6:G:280:CYS:N	2.66	0.49
6:G:277:LEU:CA	6:G:280:CYS:H	2.26	0.49
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.49
6:G:172:ASP:C	6:G:175:LYS:H	2.14	0.49
6:G:172:ASP:C	6:G:175:LYS:H	2.14	0.49
6:G:666:THR:O	6:G:667:ASN:C	2.49	0.49
2:B:928:LYS:C	2:B:934:PRO:O	2.51	0.49
3:C:568:PRO:C	3:C:571:ASN:H	2.16	0.49
6:K:135:THR:C	6:K:137:LEU:N	2.58	0.49
2:B:324:LYS:C	2:B:326:HIS:H	2.15	0.49
6:G:246:SER:C	6:G:248:ASP:N	2.66	0.49
6:G:277:LEU:CA	6:G:280:CYS:H	2.26	0.49
2:B:928:LYS:C	2:B:934:PRO:O	2.51	0.49
4:D:42:THR:O	4:D:43:GLY:C	2.50	0.49
6:G:726:CYS:O	6:G:753:LEU:N	2.44	0.49
6:K:172:ASP:O	6:K:175:LYS:N	2.46	0.49
3:C:459:ARG:CA	3:C:509:GLY:HA3	2.42	0.48
4:D:41:ASN:C	4:D:43:GLY:N	2.60	0.48
6:G:246:SER:C	6:G:248:ASP:N	2.66	0.48
3:C:568:PRO:C	3:C:571:ASN:H	2.16	0.48
5:R:69:GLY:C	5:R:71:GLN:N	2.65	0.48
6:K:172:ASP:O	6:K:175:LYS:N	2.46	0.48
6:K:274:ILE:O	6:K:275:VAL:C	2.52	0.48
5:M:173:LEU:C	5:M:175:ASN:H	2.15	0.48
6:G:726:CYS:O	6:G:753:LEU:N	2.44	0.48
4:D:42:THR:O	4:D:43:GLY:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:568:PRO:C	3:C:571:ASN:H	2.16	0.48
6:G:441:GLU:O	6:G:444:GLU:O	2.32	0.48
6:K:666:THR:O	6:K:668:THR:N	2.47	0.48
6:G:441:GLU:O	6:G:444:GLU:O	2.32	0.48
6:G:107:SER:CA	5:R:50:GLY:HA3	2.24	0.48
6:K:172:ASP:O	6:K:175:LYS:N	2.46	0.48
6:G:277:LEU:C	6:G:280:CYS:N	2.66	0.48
5:F:149:ARG:C	5:F:151:ARG:H	2.15	0.48
6:G:277:LEU:CA	6:G:280:CYS:H	2.26	0.48
5:F:149:ARG:C	5:F:151:ARG:H	2.16	0.48
6:K:666:THR:O	6:K:668:THR:N	2.47	0.48
4:D:39:LEU:C	4:D:41:ASN:N	2.66	0.48
2:B:767:THR:CA	2:B:792:LEU:C	2.83	0.47
3:C:637:VAL:O	3:C:638:SER:C	2.52	0.47
6:G:441:GLU:O	6:G:444:GLU:O	2.32	0.47
2:B:767:THR:CA	2:B:792:LEU:C	2.83	0.47
6:G:301:ALA:O	6:G:303:LEU:N	2.48	0.47
4:D:39:LEU:C	4:D:41:ASN:N	2.66	0.47
3:C:375:TYR:N	3:C:389:GLY:O	2.41	0.47
6:G:301:ALA:O	6:G:303:LEU:N	2.47	0.47
6:K:666:THR:O	6:K:668:THR:N	2.47	0.47
2:B:767:THR:CA	2:B:792:LEU:C	2.83	0.47
6:G:726:CYS:O	6:G:753:LEU:N	2.44	0.47
6:G:116:LYS:O	6:G:118:ASP:N	2.48	0.47
2:B:779:GLY:N	2:B:809:THR:O	2.22	0.47
4:D:39:LEU:C	4:D:41:ASN:N	2.66	0.47
5:M:173:LEU:C	5:M:175:ASN:N	2.68	0.47
6:G:460:GLY:HA2	6:G:494:ALA:CA	2.44	0.47
3:C:637:VAL:O	3:C:638:SER:C	2.52	0.47
6:K:274:ILE:O	6:K:275:VAL:C	2.52	0.47
5:M:173:LEU:C	5:M:175:ASN:N	2.68	0.47
5:R:159:CYS:C	5:R:161:THR:N	2.68	0.47
6:G:246:SER:C	6:G:248:ASP:N	2.66	0.47
6:K:274:ILE:O	6:K:275:VAL:C	2.52	0.47
6:G:116:LYS:O	6:G:118:ASP:N	2.48	0.47
6:G:116:LYS:O	6:G:118:ASP:N	2.48	0.47
6:G:665:CYS:O	6:G:703:PRO:N	2.48	0.47
3:C:233:SER:H	3:C:248:SER:CA	2.29	0.47
3:C:86:TYR:C	3:C:88:THR:H	2.19	0.46
6:G:460:GLY:HA2	6:G:494:ALA:CA	2.44	0.46
3:C:637:VAL:O	3:C:638:SER:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:233:SER:H	3:C:248:SER:CA	2.28	0.46
5:M:173:LEU:C	5:M:175:ASN:N	2.68	0.46
6:G:665:CYS:O	6:G:703:PRO:N	2.48	0.46
6:G:665:CYS:O	6:G:703:PRO:N	2.48	0.46
6:G:460:GLY:HA2	6:G:494:ALA:CA	2.44	0.46
2:B:842:MET:O	2:B:888:THR:O	2.34	0.46
6:K:243:GLU:C	6:K:245:GLY:N	2.69	0.46
3:C:233:SER:H	3:C:248:SER:CA	2.28	0.46
6:G:301:ALA:O	6:G:303:LEU:N	2.48	0.46
6:K:244:ASP:O	6:K:245:GLY:C	2.54	0.46
6:K:665:CYS:O	6:K:702:GLN:C	2.54	0.46
7:Z:11:TYR:C	7:Z:132:GLY:CA	2.69	0.46
6:G:107:SER:CA	5:R:50:GLY:HA3	2.24	0.46
6:K:666:THR:O	6:K:667:ASN:C	2.53	0.46
3:C:269:TYR:O	3:C:270:GLY:C	2.48	0.46
6:K:665:CYS:O	6:K:702:GLN:O	2.34	0.46
2:B:842:MET:O	2:B:888:THR:O	2.34	0.46
6:G:298:SER:O	6:G:300:LYS:N	2.49	0.46
2:B:751:GLN:C	2:B:753:ASP:H	2.19	0.46
6:K:665:CYS:O	6:K:702:GLN:C	2.54	0.46
6:K:243:GLU:C	6:K:245:GLY:N	2.69	0.46
6:K:665:CYS:O	6:K:702:GLN:C	2.54	0.46
6:K:135:THR:O	6:K:136:MET:C	2.54	0.45
2:B:842:MET:O	2:B:888:THR:O	2.34	0.45
6:K:135:THR:O	6:K:136:MET:C	2.54	0.45
6:K:666:THR:O	6:K:667:ASN:C	2.53	0.45
6:G:172:ASP:C	6:G:174:VAL:N	2.66	0.45
6:K:665:CYS:O	6:K:702:GLN:O	2.34	0.45
6:K:695:ALA:O	6:K:696:ARG:C	2.55	0.45
3:C:375:TYR:N	3:C:389:GLY:O	2.41	0.45
6:G:172:ASP:C	6:G:174:VAL:N	2.66	0.45
3:C:86:TYR:C	3:C:88:THR:H	2.19	0.45
5:R:159:CYS:C	5:R:161:THR:N	2.68	0.45
2:B:751:GLN:C	2:B:753:ASP:H	2.20	0.45
2:B:751:GLN:C	2:B:753:ASP:H	2.19	0.45
5:F:29:GLY:CA	5:F:32:THR:H	2.26	0.45
6:K:133:ASP:O	6:K:134:SER:C	2.53	0.45
6:K:244:ASP:O	6:K:245:GLY:C	2.54	0.45
6:K:665:CYS:O	6:K:702:GLN:O	2.34	0.45
3:C:86:TYR:C	3:C:88:THR:H	2.19	0.45
6:K:243:GLU:C	6:K:245:GLY:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:298:SER:O	6:G:300:LYS:N	2.50	0.45
2:B:778:LEU:O	2:B:809:THR:CA	2.65	0.44
6:K:666:THR:O	6:K:667:ASN:C	2.53	0.44
7:Z:11:TYR:C	7:Z:132:GLY:CA	2.69	0.44
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.44
6:K:695:ALA:O	6:K:696:ARG:C	2.55	0.44
6:K:107:SER:H	5:M:50:GLY:HA3	0.67	0.44
5:R:159:CYS:C	5:R:161:THR:N	2.68	0.44
6:K:273:ALA:C	6:K:275:VAL:H	2.21	0.44
6:K:273:ALA:C	6:K:275:VAL:H	2.21	0.44
6:G:298:SER:O	6:G:300:LYS:N	2.50	0.44
1:A:749:LEU:O	1:A:753:GLY:HA2	2.18	0.44
3:C:715:LEU:O	3:C:719:ALA:N	2.51	0.44
6:K:166:LEU:O	6:K:170:SER:N	2.42	0.44
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.44
5:F:29:GLY:CA	5:F:32:THR:H	2.26	0.44
6:K:181:ALA:O	6:K:185:ALA:N	2.51	0.44
6:K:181:ALA:O	6:K:185:ALA:N	2.51	0.44
7:L:49:PHE:O	7:L:53:HIS:N	2.51	0.44
6:K:181:ALA:O	6:K:185:ALA:N	2.51	0.43
7:L:49:PHE:O	7:L:53:HIS:N	2.51	0.43
6:G:176:ARG:C	6:G:178:VAL:H	2.21	0.43
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.43
6:K:171:PHE:O	6:K:174:VAL:N	2.52	0.43
6:K:695:ALA:O	6:K:696:ARG:C	2.55	0.43
1:A:749:LEU:O	1:A:753:GLY:HA2	2.18	0.43
6:K:273:ALA:C	6:K:275:VAL:H	2.21	0.43
6:G:176:ARG:C	6:G:178:VAL:H	2.21	0.43
3:C:484:SER:CA	3:C:522:GLU:H	2.32	0.43
6:G:529:THR:O	6:G:533:ASN:N	2.52	0.43
6:K:171:PHE:O	6:K:174:VAL:N	2.52	0.43
6:G:529:THR:O	6:G:533:ASN:N	2.52	0.43
6:K:171:PHE:O	6:K:174:VAL:N	2.52	0.43
5:R:143:LEU:CA	5:R:145:LEU:H	2.20	0.43
6:G:274:ILE:O	6:G:275:VAL:O	2.37	0.43
6:G:274:ILE:O	6:G:275:VAL:O	2.37	0.43
5:F:29:GLY:CA	5:F:32:THR:H	2.26	0.43
7:L:49:PHE:O	7:L:53:HIS:N	2.51	0.43
3:C:715:LEU:O	3:C:719:ALA:N	2.51	0.43
6:G:529:THR:O	6:G:533:ASN:N	2.52	0.43
2:B:135:THR:O	2:B:139:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLU:C	2:B:114:ILE:N	2.73	0.43
6:K:226:PRO:O	6:K:229:TYR:N	2.51	0.43
6:K:244:ASP:O	6:K:245:GLY:C	2.54	0.43
5:R:70:GLY:O	5:R:72:ASP:N	2.52	0.43
6:G:107:SER:N	5:R:50:GLY:O	2.52	0.43
6:K:133:ASP:O	6:K:134:SER:C	2.53	0.43
3:C:484:SER:CA	3:C:522:GLU:H	2.32	0.43
3:C:484:SER:CA	3:C:522:GLU:H	2.32	0.42
6:G:274:ILE:O	6:G:275:VAL:O	2.37	0.42
5:R:109:ARG:C	5:R:112:ASN:H	2.23	0.42
4:D:41:ASN:C	4:D:43:GLY:N	2.60	0.42
6:G:107:SER:CA	5:R:50:GLY:CA	2.92	0.42
3:C:690:LEU:O	3:C:694:GLN:N	2.53	0.42
6:K:135:THR:O	6:K:136:MET:C	2.54	0.42
6:G:107:SER:CA	5:R:50:GLY:HA3	2.24	0.42
5:R:70:GLY:O	5:R:72:ASP:N	2.52	0.42
5:R:109:ARG:C	5:R:112:ASN:H	2.23	0.42
2:B:779:GLY:O	2:B:808:SER:C	2.58	0.42
2:B:112:GLU:C	2:B:114:ILE:N	2.72	0.42
4:D:62:GLU:C	4:D:64:LEU:H	2.23	0.42
2:B:135:THR:O	2:B:139:LEU:N	2.52	0.42
6:K:166:LEU:O	6:K:170:SER:N	2.42	0.42
6:K:226:PRO:O	6:K:229:TYR:N	2.51	0.42
2:B:267:LEU:C	2:B:269:GLN:H	2.24	0.41
5:R:70:GLY:O	5:R:72:ASP:N	2.52	0.41
6:K:232:MET:O	6:K:236:ALA:N	2.53	0.41
2:B:482:SER:C	2:B:484:LYS:N	2.71	0.41
3:C:690:LEU:O	3:C:694:GLN:N	2.53	0.41
2:B:779:GLY:O	2:B:808:SER:C	2.58	0.41
6:G:172:ASP:C	6:G:174:VAL:N	2.66	0.41
6:G:176:ARG:C	6:G:178:VAL:H	2.21	0.41
5:R:143:LEU:CA	5:R:145:LEU:H	2.20	0.41
3:C:690:LEU:O	3:C:694:GLN:N	2.53	0.41
5:M:27:GLY:H	5:M:46:ILE:CA	2.34	0.41
2:B:866:ASN:O	2:B:944:ILE:O	2.39	0.41
2:B:135:THR:O	2:B:139:LEU:N	2.52	0.41
5:R:109:ARG:C	5:R:112:ASN:H	2.23	0.41
6:G:107:SER:N	5:R:50:GLY:O	2.52	0.41
6:G:107:SER:CA	5:R:50:GLY:CA	2.92	0.41
2:B:778:LEU:O	2:B:809:THR:CA	2.65	0.41
3:C:715:LEU:O	3:C:719:ALA:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:27:GLY:H	5:M:46:ILE:CA	2.34	0.41
2:B:779:GLY:O	2:B:808:SER:C	2.58	0.41
3:C:15:SER:H	3:C:293:GLY:HA2	1.86	0.41
6:G:215:ILE:O	6:G:216:SER:C	2.60	0.41
2:B:112:GLU:C	2:B:114:ILE:N	2.73	0.41
3:C:566:TYR:CA	3:C:572:ARG:O	2.69	0.41
1:A:373:ALA:C	1:A:375:ASN:N	2.75	0.41
2:B:122:LYS:O	2:B:126:HIS:N	2.55	0.40
6:G:277:LEU:C	6:G:280:CYS:H	2.24	0.40
3:C:566:TYR:CA	3:C:572:ARG:O	2.69	0.40
5:M:79:ARG:O	5:M:81:TYR:O	2.39	0.40
1:A:9:SER:N	1:A:313:GLY:HA3	2.36	0.40
2:B:767:THR:CA	2:B:793:ALA:CA	2.99	0.40
1:A:9:SER:N	1:A:313:GLY:HA3	2.36	0.40
2:B:767:THR:CA	2:B:793:ALA:CA	2.99	0.40
6:G:702:GLN:O	6:G:703:PRO:C	2.60	0.40
5:R:25:LEU:C	5:R:70:GLY:H	2.24	0.40
1:A:598:LYS:O	1:A:602:ALA:N	2.54	0.40
2:B:866:ASN:O	2:B:944:ILE:O	2.39	0.40
3:C:566:TYR:CA	3:C:572:ARG:O	2.69	0.40
2:B:122:LYS:O	2:B:126:HIS:N	2.54	0.40
4:D:62:GLU:C	4:D:64:LEU:H	2.23	0.40
5:R:160:ALA:C	5:R:163:GLY:H	2.24	0.40
2:B:122:LYS:O	2:B:126:HIS:N	2.54	0.40
5:M:79:ARG:O	5:M:81:TYR:O	2.39	0.40
5:R:160:ALA:C	5:R:163:GLY:H	2.24	0.40
2:B:482:SER:C	2:B:484:LYS:N	2.71	0.40
5:R:25:LEU:C	5:R:70:GLY:H	2.24	0.40
1:A:598:LYS:O	1:A:602:ALA:N	2.54	0.40
2:B:762:ASN:C	2:B:764:THR:H	2.18	0.40
5:M:27:GLY:H	5:M:46:ILE:CA	2.34	0.40
3:C:15:SER:H	3:C:293:GLY:HA2	1.86	0.40
4:D:62:GLU:C	4:D:64:LEU:H	2.23	0.40

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	1-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0	6
1	2-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0	6
1	3-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0	6
2	1-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	1	14
2	2-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	1	14
2	3-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	1	14
3	1-C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1	16
3	2-C	841/905 (93%)	682 (81%)	90 (11%)	69 (8%)	1	16
3	3-C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1	16
4	1-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	4	33
4	2-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	4	33
4	3-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	4	33
5	1-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	2	24
5	1-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0	8
5	1-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	7
5	2-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	2	24
5	2-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0	8
5	2-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	7
5	3-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	2	24
5	3-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0	8
5	3-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	7
6	1-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1	20
6	1-K	556/874 (64%)	475 (85%)	43 (8%)	38 (7%)	1	20
6	2-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1	20
6	2-K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	3-G	794/874 (91%)	679 (86%)	60 (8%)	55 (7%)	1	20
6	3-K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1	19
7	1-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	21
7	1-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	26
7	2-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	21
7	2-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	26
7	3-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	21
7	3-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	26
All	All	14874/18873 (79%)	12224 (82%)	1379 (9%)	1271 (8%)	2	15

All (1271) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	63	GLN
1	1-A	64	PRO
1	1-A	92	HIS
1	1-A	106	PRO
1	1-A	125	ARG
1	1-A	169	LYS
1	1-A	174	PRO
1	1-A	187	VAL
1	1-A	215	PRO
1	1-A	237	SER
1	1-A	250	ASN
1	1-A	252	VAL
1	1-A	271	LYS
1	1-A	278	MET
1	1-A	281	ARG
1	1-A	324	PRO
1	1-A	325	ALA
1	1-A	341	LEU
1	1-A	343	GLN
1	1-A	384	SER
1	1-A	454	ASP
1	1-A	457	PHE
1	1-A	466	LEU
1	1-A	479	GLN
1	1-A	492	LYS
1	1-A	566	LEU

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Mol	Chain	Res	Type
1	1-A	583	ARG
1	1-A	584	GLU
1	1-A	592	ILE
1	1-A	593	ASP
1	1-A	619	LYS
1	1-A	642	VAL
1	1-A	671	LYS
1	1-A	728	ASP
1	1-A	779	ASP
1	1-A	788	ILE
1	1-A	796	GLN
1	1-A	797	PRO
1	1-A	798	PRO
1	1-A	803	PRO
1	1-A	805	ASP
1	1-A	811	LEU
2	1-B	36	PRO
2	1-B	68	GLU
2	1-B	109	LEU
2	1-B	111	HIS
2	1-B	113	MET
2	1-B	254	PRO
2	1-B	255	SER
2	1-B	329	HIS
2	1-B	348	ASP
2	1-B	367	ASN
2	1-B	385	VAL
2	1-B	386	SER
2	1-B	466	SER
2	1-B	480	TYR
2	1-B	484	LYS
2	1-B	500	GLU
2	1-B	501	ILE
2	1-B	502	PRO
2	1-B	503	ILE
2	1-B	505	GLU
2	1-B	521	ILE
2	1-B	522	THR
2	1-B	547	PRO
2	1-B	767	THR
2	1-B	771	CYS
2	1-B	826	ALA

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Mol	Chain	Res	Type
2	1-B	831	CYS
2	1-B	865	GLU
2	1-B	899	LEU
2	1-B	929	PRO
2	1-B	930	VAL
2	1-B	934	PRO
2	1-B	935	ASP
2	1-B	938	VAL
3	1-C	27	GLU
3	1-C	89	LEU
3	1-C	200	PRO
3	1-C	228	HIS
3	1-C	270	GLY
3	1-C	273	ARG
3	1-C	325	ALA
3	1-C	326	ASN
3	1-C	328	LYS
3	1-C	329	ALA
3	1-C	332	ASP
3	1-C	350	SER
3	1-C	363	ASN
3	1-C	365	ARG
3	1-C	400	SER
3	1-C	410	SER
3	1-C	411	ILE
3	1-C	424	PHE
3	1-C	451	ASP
3	1-C	462	GLU
3	1-C	475	GLU
3	1-C	484	SER
3	1-C	502	HIS
3	1-C	614	PRO
3	1-C	615	LYS
3	1-C	638	SER
3	1-C	762	LEU
3	1-C	781	ASN
3	1-C	782	GLN
3	1-C	789	ALA
3	1-C	790	ASP
3	1-C	806	VAL
3	1-C	825	PRO
3	1-C	833	ARG

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Mol	Chain	Res	Type
4	1-D	12	ALA
4	1-D	44	LYS
4	1-D	73	ASN
4	1-D	96	ALA
5	1-F	97	ARG
5	1-F	117	ARG
5	1-F	131	PRO
6	1-G	77	PHE
6	1-G	100	GLU
6	1-G	106	THR
6	1-G	132	THR
6	1-G	151	LYS
6	1-G	171	PHE
6	1-G	243	GLU
6	1-G	261	ASN
6	1-G	275	VAL
6	1-G	277	LEU
6	1-G	283	LYS
6	1-G	299	PRO
6	1-G	373	ASP
6	1-G	394	HIS
6	1-G	446	CYS
6	1-G	484	HIS
6	1-G	608	THR
6	1-G	621	PRO
6	1-G	686	ALA
6	1-G	741	GLU
5	1-R	42	VAL
5	1-R	43	ILE
5	1-R	130	LEU
5	1-R	131	PRO
5	1-R	145	LEU
5	1-R	147	SER
5	1-R	151	ARG
5	1-R	175	ASN
7	1-Z	36	PRO
7	1-Z	37	SER
7	1-Z	84	TYR
6	1-K	134	SER
6	1-K	135	THR
6	1-K	170	SER
6	1-K	171	PHE

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Mol	Chain	Res	Type
6	1-K	207	ASP
6	1-K	221	HIS
6	1-K	225	SER
6	1-K	226	PRO
6	1-K	227	PHE
6	1-K	243	GLU
6	1-K	275	VAL
6	1-K	299	PRO
6	1-K	608	THR
6	1-K	621	PRO
6	1-K	741	GLU
6	1-K	813	CYS
7	1-L	37	SER
7	1-L	84	TYR
7	1-L	147	ALA
5	1-M	42	VAL
5	1-M	43	ILE
5	1-M	44	THR
5	1-M	51	PHE
5	1-M	71	GLN
5	1-M	80	HIS
5	1-M	118	ASN
5	1-M	149	ARG
1	2-A	63	GLN
1	2-A	64	PRO
1	2-A	92	HIS
1	2-A	106	PRO
1	2-A	125	ARG
1	2-A	169	LYS
1	2-A	174	PRO
1	2-A	187	VAL
1	2-A	215	PRO
1	2-A	237	SER
1	2-A	250	ASN
1	2-A	252	VAL
1	2-A	271	LYS
1	2-A	278	MET
1	2-A	281	ARG
1	2-A	324	PRO
1	2-A	325	ALA
1	2-A	341	LEU
1	2-A	343	GLN

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Mol	Chain	Res	Type
1	2-A	384	SER
1	2-A	454	ASP
1	2-A	457	PHE
1	2-A	466	LEU
1	2-A	479	GLN
1	2-A	492	LYS
1	2-A	566	LEU
1	2-A	583	ARG
1	2-A	584	GLU
1	2-A	592	ILE
1	2-A	593	ASP
1	2-A	619	LYS
1	2-A	642	VAL
1	2-A	671	LYS
1	2-A	728	ASP
1	2-A	779	ASP
1	2-A	788	ILE
1	2-A	796	GLN
1	2-A	797	PRO
1	2-A	798	PRO
1	2-A	803	PRO
1	2-A	805	ASP
1	2-A	811	LEU
2	2-B	36	PRO
2	2-B	68	GLU
2	2-B	109	LEU
2	2-B	111	HIS
2	2-B	113	MET
2	2-B	254	PRO
2	2-B	255	SER
2	2-B	329	HIS
2	2-B	348	ASP
2	2-B	367	ASN
2	2-B	385	VAL
2	2-B	386	SER
2	2-B	466	SER
2	2-B	480	TYR
2	2-B	484	LYS
2	2-B	500	GLU
2	2-B	501	ILE
2	2-B	502	PRO
2	2-B	503	ILE

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Mol	Chain	Res	Type
2	2-B	505	GLU
2	2-B	521	ILE
2	2-B	522	THR
2	2-B	547	PRO
2	2-B	767	THR
2	2-B	771	CYS
2	2-B	826	ALA
2	2-B	831	CYS
2	2-B	865	GLU
2	2-B	899	LEU
2	2-B	929	PRO
2	2-B	930	VAL
2	2-B	934	PRO
2	2-B	935	ASP
2	2-B	938	VAL
3	2-C	27	GLU
3	2-C	89	LEU
3	2-C	200	PRO
3	2-C	228	HIS
3	2-C	270	GLY
3	2-C	273	ARG
3	2-C	325	ALA
3	2-C	326	ASN
3	2-C	328	LYS
3	2-C	329	ALA
3	2-C	332	ASP
3	2-C	350	SER
3	2-C	363	ASN
3	2-C	365	ARG
3	2-C	400	SER
3	2-C	410	SER
3	2-C	411	ILE
3	2-C	424	PHE
3	2-C	451	ASP
3	2-C	462	GLU
3	2-C	475	GLU
3	2-C	484	SER
3	2-C	502	HIS
3	2-C	614	PRO
3	2-C	615	LYS
3	2-C	638	SER
3	2-C	762	LEU

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Mol	Chain	Res	Type
3	2-C	781	ASN
3	2-C	782	GLN
3	2-C	789	ALA
3	2-C	790	ASP
3	2-C	806	VAL
3	2-C	825	PRO
3	2-C	833	ARG
4	2-D	12	ALA
4	2-D	44	LYS
4	2-D	73	ASN
4	2-D	96	ALA
5	2-F	97	ARG
5	2-F	117	ARG
5	2-F	131	PRO
6	2-G	77	PHE
6	2-G	100	GLU
6	2-G	106	THR
6	2-G	132	THR
6	2-G	151	LYS
6	2-G	171	PHE
6	2-G	243	GLU
6	2-G	261	ASN
6	2-G	275	VAL
6	2-G	277	LEU
6	2-G	283	LYS
6	2-G	299	PRO
6	2-G	373	ASP
6	2-G	394	HIS
6	2-G	446	CYS
6	2-G	484	HIS
6	2-G	608	THR
6	2-G	621	PRO
6	2-G	686	ALA
6	2-G	741	GLU
5	2-R	42	VAL
5	2-R	43	ILE
5	2-R	130	LEU
5	2-R	131	PRO
5	2-R	145	LEU
5	2-R	147	SER
5	2-R	151	ARG
5	2-R	175	ASN

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Mol	Chain	Res	Type
7	2-Z	36	PRO
7	2-Z	37	SER
7	2-Z	84	TYR
6	2-K	134	SER
6	2-K	135	THR
6	2-K	170	SER
6	2-K	171	PHE
6	2-K	207	ASP
6	2-K	221	HIS
6	2-K	225	SER
6	2-K	226	PRO
6	2-K	227	PHE
6	2-K	243	GLU
6	2-K	275	VAL
6	2-K	299	PRO
6	2-K	608	THR
6	2-K	621	PRO
6	2-K	741	GLU
6	2-K	813	CYS
7	2-L	37	SER
7	2-L	84	TYR
7	2-L	147	ALA
5	2-M	42	VAL
5	2-M	43	ILE
5	2-M	44	THR
5	2-M	51	PHE
5	2-M	71	GLN
5	2-M	80	HIS
5	2-M	118	ASN
5	2-M	149	ARG
1	3-A	63	GLN
1	3-A	64	PRO
1	3-A	92	HIS
1	3-A	106	PRO
1	3-A	169	LYS
1	3-A	174	PRO
1	3-A	187	VAL
1	3-A	215	PRO
1	3-A	237	SER
1	3-A	250	ASN
1	3-A	252	VAL
1	3-A	271	LYS

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Mol	Chain	Res	Type
1	3-A	278	MET
1	3-A	281	ARG
1	3-A	324	PRO
1	3-A	325	ALA
1	3-A	341	LEU
1	3-A	343	GLN
1	3-A	384	SER
1	3-A	454	ASP
1	3-A	457	PHE
1	3-A	466	LEU
1	3-A	479	GLN
1	3-A	492	LYS
1	3-A	566	LEU
1	3-A	583	ARG
1	3-A	584	GLU
1	3-A	592	ILE
1	3-A	593	ASP
1	3-A	619	LYS
1	3-A	642	VAL
1	3-A	671	LYS
1	3-A	728	ASP
1	3-A	779	ASP
1	3-A	788	ILE
1	3-A	796	GLN
1	3-A	797	PRO
1	3-A	798	PRO
1	3-A	803	PRO
1	3-A	805	ASP
1	3-A	811	LEU
2	3-B	36	PRO
2	3-B	68	GLU
2	3-B	109	LEU
2	3-B	111	HIS
2	3-B	113	MET
2	3-B	254	PRO
2	3-B	255	SER
2	3-B	329	HIS
2	3-B	348	ASP
2	3-B	367	ASN
2	3-B	385	VAL
2	3-B	386	SER
2	3-B	466	SER

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Mol	Chain	Res	Type
2	3-B	480	TYR
2	3-B	484	LYS
2	3-B	500	GLU
2	3-B	501	ILE
2	3-B	502	PRO
2	3-B	503	ILE
2	3-B	505	GLU
2	3-B	521	ILE
2	3-B	522	THR
2	3-B	547	PRO
2	3-B	767	THR
2	3-B	771	CYS
2	3-B	826	ALA
2	3-B	831	CYS
2	3-B	865	GLU
2	3-B	899	LEU
2	3-B	929	PRO
2	3-B	930	VAL
2	3-B	934	PRO
2	3-B	935	ASP
2	3-B	938	VAL
3	3-C	27	GLU
3	3-C	89	LEU
3	3-C	200	PRO
3	3-C	228	HIS
3	3-C	270	GLY
3	3-C	273	ARG
3	3-C	325	ALA
3	3-C	326	ASN
3	3-C	328	LYS
3	3-C	329	ALA
3	3-C	332	ASP
3	3-C	350	SER
3	3-C	363	ASN
3	3-C	365	ARG
3	3-C	400	SER
3	3-C	410	SER
3	3-C	411	ILE
3	3-C	424	PHE
3	3-C	451	ASP
3	3-C	462	GLU
3	3-C	475	GLU

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Mol	Chain	Res	Type
3	3-C	484	SER
3	3-C	502	HIS
3	3-C	614	PRO
3	3-C	615	LYS
3	3-C	638	SER
3	3-C	762	LEU
3	3-C	781	ASN
3	3-C	782	GLN
3	3-C	789	ALA
3	3-C	790	ASP
3	3-C	806	VAL
3	3-C	825	PRO
3	3-C	833	ARG
4	3-D	12	ALA
4	3-D	44	LYS
4	3-D	73	ASN
4	3-D	96	ALA
5	3-F	97	ARG
5	3-F	117	ARG
5	3-F	131	PRO
6	3-G	77	PHE
6	3-G	100	GLU
6	3-G	106	THR
6	3-G	132	THR
6	3-G	151	LYS
6	3-G	171	PHE
6	3-G	243	GLU
6	3-G	261	ASN
6	3-G	275	VAL
6	3-G	277	LEU
6	3-G	283	LYS
6	3-G	299	PRO
6	3-G	373	ASP
6	3-G	394	HIS
6	3-G	446	CYS
6	3-G	484	HIS
6	3-G	608	THR
6	3-G	621	PRO
6	3-G	686	ALA
6	3-G	741	GLU
5	3-R	42	VAL
5	3-R	43	ILE

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Mol	Chain	Res	Type
5	3-R	130	LEU
5	3-R	131	PRO
5	3-R	145	LEU
5	3-R	147	SER
5	3-R	151	ARG
5	3-R	175	ASN
7	3-Z	36	PRO
7	3-Z	37	SER
7	3-Z	84	TYR
6	3-K	134	SER
6	3-K	135	THR
6	3-K	170	SER
6	3-K	171	PHE
6	3-K	207	ASP
6	3-K	221	HIS
6	3-K	225	SER
6	3-K	226	PRO
6	3-K	227	PHE
6	3-K	243	GLU
6	3-K	275	VAL
6	3-K	299	PRO
6	3-K	608	THR
6	3-K	621	PRO
6	3-K	741	GLU
6	3-K	813	CYS
7	3-L	37	SER
7	3-L	84	TYR
7	3-L	147	ALA
5	3-M	42	VAL
5	3-M	43	ILE
5	3-M	44	THR
5	3-M	51	PHE
5	3-M	71	GLN
5	3-M	80	HIS
5	3-M	118	ASN
5	3-M	149	ARG
1	1-A	10	ALA
1	1-A	185	THR
1	1-A	282	THR
1	1-A	290	ASP
1	1-A	345	ASP
1	1-A	373	ALA

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Mol	Chain	Res	Type
1	1-A	425	ARG
1	1-A	498	ALA
1	1-A	546	SER
1	1-A	564	LEU
1	1-A	572	ARG
1	1-A	622	GLY
1	1-A	624	SER
1	1-A	632	LYS
1	1-A	672	ASN
1	1-A	787	ASP
1	1-A	800	PRO
2	1-B	49	ASP
2	1-B	69	LYS
2	1-B	162	ARG
2	1-B	186	PRO
2	1-B	383	ASN
2	1-B	445	ARG
2	1-B	498	LEU
2	1-B	499	GLY
2	1-B	551	GLU
2	1-B	740	PRO
2	1-B	741	VAL
2	1-B	751	GLN
2	1-B	764	THR
2	1-B	828	ASP
2	1-B	838	HIS
2	1-B	862	PHE
2	1-B	873	ASN
2	1-B	939	THR
3	1-C	88	THR
3	1-C	219	LYS
3	1-C	428	PHE
3	1-C	465	PRO
3	1-C	503	GLU
3	1-C	504	GLY
3	1-C	558	ASP
3	1-C	665	GLU
3	1-C	787	SER
3	1-C	793	GLU
3	1-C	797	LEU
4	1-D	24	MET
4	1-D	25	THR

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Mol	Chain	Res	Type
4	1-D	42	THR
4	1-D	98	GLU
4	1-D	136	MET
4	1-D	387	ASN
4	1-D	442	LEU
6	1-G	96	SER
6	1-G	98	ILE
6	1-G	105	VAL
6	1-G	116	LYS
6	1-G	216	SER
6	1-G	278	PRO
6	1-G	310	THR
6	1-G	463	GLY
6	1-G	467	ASN
6	1-G	522	ASN
6	1-G	633	SER
6	1-G	718	THR
5	1-R	72	ASP
5	1-R	82	TYR
5	1-R	84	ASN
5	1-R	95	ASN
5	1-R	132	GLU
5	1-R	133	ALA
7	1-Z	73	ILE
6	1-K	38	PRO
6	1-K	116	LYS
6	1-K	245	GLY
6	1-K	297	SER
6	1-K	633	SER
6	1-K	686	ALA
6	1-K	718	THR
7	1-L	12	THR
7	1-L	69	TYR
7	1-L	132	GLY
5	1-M	70	GLY
5	1-M	129	ASP
5	1-M	164	GLU
1	2-A	10	ALA
1	2-A	185	THR
1	2-A	282	THR
1	2-A	290	ASP
1	2-A	345	ASP

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Mol	Chain	Res	Type
1	2-A	373	ALA
1	2-A	425	ARG
1	2-A	498	ALA
1	2-A	546	SER
1	2-A	564	LEU
1	2-A	572	ARG
1	2-A	622	GLY
1	2-A	624	SER
1	2-A	632	LYS
1	2-A	672	ASN
1	2-A	787	ASP
1	2-A	800	PRO
2	2-B	49	ASP
2	2-B	69	LYS
2	2-B	162	ARG
2	2-B	186	PRO
2	2-B	383	ASN
2	2-B	445	ARG
2	2-B	498	LEU
2	2-B	499	GLY
2	2-B	551	GLU
2	2-B	740	PRO
2	2-B	741	VAL
2	2-B	751	GLN
2	2-B	764	THR
2	2-B	828	ASP
2	2-B	838	HIS
2	2-B	862	PHE
2	2-B	873	ASN
2	2-B	939	THR
3	2-C	88	THR
3	2-C	219	LYS
3	2-C	428	PHE
3	2-C	465	PRO
3	2-C	503	GLU
3	2-C	504	GLY
3	2-C	558	ASP
3	2-C	665	GLU
3	2-C	787	SER
3	2-C	793	GLU
3	2-C	797	LEU
4	2-D	24	MET

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Mol	Chain	Res	Type
4	2-D	25	THR
4	2-D	42	THR
4	2-D	98	GLU
4	2-D	136	MET
4	2-D	387	ASN
4	2-D	442	LEU
6	2-G	96	SER
6	2-G	98	ILE
6	2-G	105	VAL
6	2-G	116	LYS
6	2-G	216	SER
6	2-G	278	PRO
6	2-G	310	THR
6	2-G	463	GLY
6	2-G	467	ASN
6	2-G	522	ASN
6	2-G	633	SER
6	2-G	718	THR
5	2-R	72	ASP
5	2-R	82	TYR
5	2-R	84	ASN
5	2-R	95	ASN
5	2-R	132	GLU
5	2-R	133	ALA
7	2-Z	73	ILE
6	2-K	38	PRO
6	2-K	116	LYS
6	2-K	245	GLY
6	2-K	297	SER
6	2-K	633	SER
6	2-K	686	ALA
6	2-K	718	THR
7	2-L	12	THR
7	2-L	69	TYR
7	2-L	132	GLY
5	2-M	70	GLY
5	2-M	129	ASP
5	2-M	164	GLU
1	3-A	10	ALA
1	3-A	125	ARG
1	3-A	185	THR
1	3-A	282	THR

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Mol	Chain	Res	Type
1	3-A	290	ASP
1	3-A	345	ASP
1	3-A	373	ALA
1	3-A	425	ARG
1	3-A	498	ALA
1	3-A	546	SER
1	3-A	564	LEU
1	3-A	572	ARG
1	3-A	622	GLY
1	3-A	624	SER
1	3-A	632	LYS
1	3-A	672	ASN
1	3-A	787	ASP
1	3-A	800	PRO
2	3-B	49	ASP
2	3-B	69	LYS
2	3-B	162	ARG
2	3-B	186	PRO
2	3-B	383	ASN
2	3-B	445	ARG
2	3-B	498	LEU
2	3-B	499	GLY
2	3-B	551	GLU
2	3-B	740	PRO
2	3-B	741	VAL
2	3-B	751	GLN
2	3-B	764	THR
2	3-B	828	ASP
2	3-B	838	HIS
2	3-B	862	PHE
2	3-B	873	ASN
2	3-B	939	THR
3	3-C	88	THR
3	3-C	219	LYS
3	3-C	428	PHE
3	3-C	465	PRO
3	3-C	503	GLU
3	3-C	504	GLY
3	3-C	558	ASP
3	3-C	665	GLU
3	3-C	787	SER
3	3-C	793	GLU

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Mol	Chain	Res	Type
3	3-C	797	LEU
4	3-D	24	MET
4	3-D	25	THR
4	3-D	42	THR
4	3-D	98	GLU
4	3-D	136	MET
4	3-D	387	ASN
4	3-D	442	LEU
6	3-G	96	SER
6	3-G	98	ILE
6	3-G	105	VAL
6	3-G	116	LYS
6	3-G	216	SER
6	3-G	278	PRO
6	3-G	310	THR
6	3-G	463	GLY
6	3-G	467	ASN
6	3-G	522	ASN
6	3-G	633	SER
6	3-G	718	THR
5	3-R	72	ASP
5	3-R	82	TYR
5	3-R	84	ASN
5	3-R	95	ASN
5	3-R	132	GLU
5	3-R	133	ALA
7	3-Z	73	ILE
6	3-K	38	PRO
6	3-K	116	LYS
6	3-K	245	GLY
6	3-K	297	SER
6	3-K	633	SER
6	3-K	686	ALA
6	3-K	718	THR
7	3-L	12	THR
7	3-L	69	TYR
7	3-L	132	GLY
5	3-M	70	GLY
5	3-M	129	ASP
5	3-M	164	GLU
1	1-A	61	LYS
1	1-A	62	GLN

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Mol	Chain	Res	Type
1	1-A	168	ARG
1	1-A	176	ALA
1	1-A	183	GLY
1	1-A	218	PRO
1	1-A	251	ASN
1	1-A	323	ARG
1	1-A	340	PHE
1	1-A	349	SER
1	1-A	362	LYS
1	1-A	433	HIS
1	1-A	481	ARG
1	1-A	527	ASN
1	1-A	555	THR
1	1-A	585	CYS
1	1-A	686	ASN
1	1-A	731	GLY
1	1-A	755	LYS
2	1-B	216	ASP
2	1-B	779	GLY
2	1-B	871	ASN
3	1-C	140	GLY
3	1-C	156	ASN
3	1-C	250	ASP
3	1-C	259	SER
3	1-C	351	CYS
3	1-C	408	SER
3	1-C	454	ASN
3	1-C	708	ASN
3	1-C	763	PRO
4	1-D	46	HIS
4	1-D	138	SER
5	1-F	47	PRO
5	1-F	84	ASN
5	1-F	149	ARG
6	1-G	170	SER
6	1-G	282	ALA
6	1-G	297	SER
6	1-G	391	PRO
6	1-G	393	LYS
6	1-G	445	ASP
6	1-G	447	GLU
6	1-G	504	GLU

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Mol	Chain	Res	Type
6	1-G	505	MET
6	1-G	628	PRO
6	1-G	641	GLU
6	1-G	687	TYR
6	1-G	720	VAL
6	1-G	761	ALA
5	1-R	114	ASP
7	1-Z	147	ALA
6	1-K	96	SER
6	1-K	248	ASP
6	1-K	628	PRO
6	1-K	641	GLU
6	1-K	687	TYR
6	1-K	720	VAL
6	1-K	761	ALA
7	1-L	36	PRO
5	1-M	127	LYS
5	1-M	135	SER
5	1-M	165	GLY
1	2-A	61	LYS
1	2-A	62	GLN
1	2-A	168	ARG
1	2-A	176	ALA
1	2-A	183	GLY
1	2-A	218	PRO
1	2-A	251	ASN
1	2-A	323	ARG
1	2-A	340	PHE
1	2-A	349	SER
1	2-A	362	LYS
1	2-A	433	HIS
1	2-A	481	ARG
1	2-A	527	ASN
1	2-A	555	THR
1	2-A	585	CYS
1	2-A	686	ASN
1	2-A	731	GLY
1	2-A	755	LYS
2	2-B	216	ASP
2	2-B	779	GLY
2	2-B	871	ASN
3	2-C	140	GLY

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Mol	Chain	Res	Type
3	2-C	156	ASN
3	2-C	250	ASP
3	2-C	259	SER
3	2-C	351	CYS
3	2-C	408	SER
3	2-C	454	ASN
3	2-C	708	ASN
3	2-C	763	PRO
4	2-D	46	HIS
4	2-D	138	SER
5	2-F	47	PRO
5	2-F	84	ASN
5	2-F	149	ARG
6	2-G	170	SER
6	2-G	282	ALA
6	2-G	297	SER
6	2-G	391	PRO
6	2-G	393	LYS
6	2-G	445	ASP
6	2-G	447	GLU
6	2-G	504	GLU
6	2-G	505	MET
6	2-G	628	PRO
6	2-G	641	GLU
6	2-G	687	TYR
6	2-G	720	VAL
6	2-G	761	ALA
5	2-R	114	ASP
7	2-Z	147	ALA
6	2-K	96	SER
6	2-K	248	ASP
6	2-K	628	PRO
6	2-K	641	GLU
6	2-K	687	TYR
6	2-K	720	VAL
6	2-K	761	ALA
7	2-L	36	PRO
5	2-M	127	LYS
5	2-M	135	SER
5	2-M	165	GLY
1	3-A	61	LYS
1	3-A	62	GLN

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Mol	Chain	Res	Type
1	3-A	168	ARG
1	3-A	176	ALA
1	3-A	183	GLY
1	3-A	218	PRO
1	3-A	251	ASN
1	3-A	323	ARG
1	3-A	340	PHE
1	3-A	349	SER
1	3-A	362	LYS
1	3-A	433	HIS
1	3-A	481	ARG
1	3-A	527	ASN
1	3-A	555	THR
1	3-A	585	CYS
1	3-A	686	ASN
1	3-A	731	GLY
1	3-A	755	LYS
2	3-B	216	ASP
2	3-B	779	GLY
2	3-B	871	ASN
3	3-C	140	GLY
3	3-C	156	ASN
3	3-C	250	ASP
3	3-C	259	SER
3	3-C	351	CYS
3	3-C	408	SER
3	3-C	454	ASN
3	3-C	708	ASN
3	3-C	763	PRO
4	3-D	46	HIS
4	3-D	138	SER
5	3-F	47	PRO
5	3-F	84	ASN
5	3-F	149	ARG
6	3-G	170	SER
6	3-G	282	ALA
6	3-G	297	SER
6	3-G	391	PRO
6	3-G	393	LYS
6	3-G	445	ASP
6	3-G	447	GLU
6	3-G	504	GLU

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Mol	Chain	Res	Type
6	3-G	505	MET
6	3-G	628	PRO
6	3-G	641	GLU
6	3-G	687	TYR
6	3-G	720	VAL
6	3-G	761	ALA
5	3-R	114	ASP
7	3-Z	147	ALA
6	3-K	96	SER
6	3-K	248	ASP
6	3-K	628	PRO
6	3-K	641	GLU
6	3-K	687	TYR
6	3-K	720	VAL
6	3-K	761	ALA
7	3-L	36	PRO
5	3-M	127	LYS
5	3-M	135	SER
5	3-M	165	GLY
1	1-A	73	TYR
1	1-A	103	HIS
1	1-A	170	LYS
1	1-A	205	ASP
1	1-A	236	GLU
1	1-A	330	GLY
1	1-A	398	LYS
1	1-A	411	LYS
1	1-A	424	ASN
1	1-A	488	ILE
1	1-A	556	GLY
1	1-A	783	GLU
1	1-A	786	PRO
1	1-A	801	ILE
2	1-B	128	ASN
2	1-B	384	ASN
2	1-B	425	SER
2	1-B	447	ASP
2	1-B	481	CYS
2	1-B	504	VAL
2	1-B	752	TYR
2	1-B	768	LEU
2	1-B	780	ASP

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Mol	Chain	Res	Type
2	1-B	827	SER
2	1-B	837	ILE
2	1-B	901	GLY
2	1-B	928	LYS
3	1-C	165	ARG
3	1-C	321	GLU
3	1-C	346	LYS
3	1-C	401	SER
3	1-C	409	ASN
3	1-C	431	GLU
3	1-C	662	VAL
3	1-C	821	ALA
5	1-F	153	TRP
6	1-G	23	GLU
6	1-G	226	PRO
6	1-G	428	ASN
6	1-G	623	PHE
5	1-R	44	THR
5	1-R	129	ASP
5	1-R	158	THR
7	1-Z	34	THR
6	1-K	76	LEU
6	1-K	623	PHE
7	1-L	86	ASN
5	1-M	119	ALA
5	1-M	133	ALA
1	2-A	73	TYR
1	2-A	103	HIS
1	2-A	170	LYS
1	2-A	205	ASP
1	2-A	236	GLU
1	2-A	330	GLY
1	2-A	398	LYS
1	2-A	411	LYS
1	2-A	424	ASN
1	2-A	488	ILE
1	2-A	556	GLY
1	2-A	783	GLU
1	2-A	786	PRO
1	2-A	801	ILE
2	2-B	128	ASN
2	2-B	384	ASN

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Mol	Chain	Res	Type
2	2-B	425	SER
2	2-B	447	ASP
2	2-B	481	CYS
2	2-B	504	VAL
2	2-B	752	TYR
2	2-B	768	LEU
2	2-B	780	ASP
2	2-B	827	SER
2	2-B	837	ILE
2	2-B	901	GLY
2	2-B	928	LYS
3	2-C	165	ARG
3	2-C	321	GLU
3	2-C	346	LYS
3	2-C	401	SER
3	2-C	409	ASN
3	2-C	431	GLU
3	2-C	662	VAL
3	2-C	821	ALA
5	2-F	153	TRP
6	2-G	23	GLU
6	2-G	226	PRO
6	2-G	428	ASN
6	2-G	623	PHE
5	2-R	44	THR
5	2-R	129	ASP
7	2-Z	34	THR
6	2-K	76	LEU
6	2-K	623	PHE
7	2-L	86	ASN
5	2-M	119	ALA
5	2-M	133	ALA
1	3-A	73	TYR
1	3-A	103	HIS
1	3-A	170	LYS
1	3-A	205	ASP
1	3-A	236	GLU
1	3-A	330	GLY
1	3-A	398	LYS
1	3-A	411	LYS
1	3-A	424	ASN
1	3-A	488	ILE

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Mol	Chain	Res	Type
1	3-A	556	GLY
1	3-A	783	GLU
1	3-A	786	PRO
1	3-A	801	ILE
2	3-B	128	ASN
2	3-B	384	ASN
2	3-B	425	SER
2	3-B	447	ASP
2	3-B	481	CYS
2	3-B	504	VAL
2	3-B	752	TYR
2	3-B	768	LEU
2	3-B	780	ASP
2	3-B	827	SER
2	3-B	837	ILE
2	3-B	901	GLY
2	3-B	928	LYS
3	3-C	165	ARG
3	3-C	321	GLU
3	3-C	346	LYS
3	3-C	401	SER
3	3-C	409	ASN
3	3-C	431	GLU
3	3-C	662	VAL
3	3-C	821	ALA
5	3-F	153	TRP
6	3-G	23	GLU
6	3-G	226	PRO
6	3-G	428	ASN
6	3-G	623	PHE
5	3-R	44	THR
5	3-R	129	ASP
7	3-Z	34	THR
6	3-K	76	LEU
6	3-K	623	PHE
7	3-L	86	ASN
5	3-M	119	ALA
5	3-M	133	ALA
1	1-A	182	ARG
1	1-A	195	ALA
1	1-A	364	PRO
1	1-A	452	ASN

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Mol	Chain	Res	Type
1	1-A	517	LYS
1	1-A	531	LYS
1	1-A	621	VAL
1	1-A	644	ASP
1	1-A	810	LEU
2	1-B	270	SER
2	1-B	347	PRO
2	1-B	825	ALA
3	1-C	242	PRO
3	1-C	284	ASN
3	1-C	473	SER
3	1-C	737	LYS
4	1-D	40	MET
4	1-D	43	GLY
5	1-F	78	TRP
6	1-G	99	ALA
6	1-G	248	ASP
6	1-K	40	ASN
6	1-K	81	ASP
7	1-L	63	GLU
5	1-M	151	ARG
1	2-A	182	ARG
1	2-A	195	ALA
1	2-A	364	PRO
1	2-A	452	ASN
1	2-A	517	LYS
1	2-A	531	LYS
1	2-A	621	VAL
1	2-A	644	ASP
1	2-A	810	LEU
2	2-B	270	SER
2	2-B	347	PRO
2	2-B	825	ALA
3	2-C	242	PRO
3	2-C	284	ASN
3	2-C	473	SER
3	2-C	737	LYS
4	2-D	40	MET
4	2-D	43	GLY
5	2-F	78	TRP
6	2-G	99	ALA
6	2-G	248	ASP

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Mol	Chain	Res	Type
5	2-R	158	THR
6	2-K	40	ASN
6	2-K	81	ASP
7	2-L	63	GLU
5	2-M	151	ARG
1	3-A	182	ARG
1	3-A	195	ALA
1	3-A	364	PRO
1	3-A	452	ASN
1	3-A	517	LYS
1	3-A	531	LYS
1	3-A	621	VAL
1	3-A	644	ASP
1	3-A	810	LEU
2	3-B	270	SER
2	3-B	347	PRO
2	3-B	825	ALA
3	3-C	242	PRO
3	3-C	284	ASN
3	3-C	473	SER
3	3-C	737	LYS
4	3-D	40	MET
4	3-D	43	GLY
5	3-F	78	TRP
6	3-G	99	ALA
6	3-G	248	ASP
5	3-R	158	THR
6	3-K	40	ASN
6	3-K	81	ASP
7	3-L	63	GLU
5	3-M	151	ARG
1	1-A	643	LYS
1	1-A	802	MET
2	1-B	86	ASP
2	1-B	104	THR
3	1-C	25	PRO
6	1-G	152	VAL
5	1-R	49	ILE
7	1-Z	54	ARG
6	1-K	37	THR
6	1-K	694	PRO
1	2-A	643	LYS

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Mol	Chain	Res	Type
1	2-A	802	MET
2	2-B	86	ASP
2	2-B	104	THR
3	2-C	25	PRO
6	2-G	152	VAL
5	2-R	49	ILE
7	2-Z	54	ARG
6	2-K	37	THR
6	2-K	310	THR
6	2-K	694	PRO
1	3-A	643	LYS
1	3-A	802	MET
2	3-B	86	ASP
2	3-B	104	THR
3	3-C	25	PRO
6	3-G	152	VAL
5	3-R	49	ILE
7	3-Z	54	ARG
6	3-K	310	THR
6	3-K	694	PRO
3	1-C	312	GLY
6	1-K	274	ILE
3	2-C	312	GLY
6	2-K	274	ILE
3	3-C	312	GLY
6	3-K	37	THR
6	3-K	274	ILE
1	1-A	22	PRO
1	1-A	503	VAL
1	1-A	615	VAL
3	1-C	112	PRO
5	1-R	163	GLY
5	1-M	148	ILE
1	2-A	22	PRO
1	2-A	503	VAL
1	2-A	615	VAL
3	2-C	112	PRO
5	2-R	163	GLY
5	2-M	148	ILE
1	3-A	22	PRO
1	3-A	503	VAL
1	3-A	615	VAL

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Mol	Chain	Res	Type
3	3-C	112	PRO
5	3-R	163	GLY
5	3-M	148	ILE
1	1-A	133	GLY
1	1-A	259	PRO
5	1-F	43	ILE
6	1-G	820	PRO
6	1-K	820	PRO
1	2-A	133	GLY
1	2-A	259	PRO
5	2-F	43	ILE
6	2-G	820	PRO
6	2-K	820	PRO
1	3-A	133	GLY
1	3-A	259	PRO
5	3-F	43	ILE
6	3-G	820	PRO
6	3-K	820	PRO
6	1-G	694	PRO
1	2-A	575	GLY
6	2-G	694	PRO
1	3-A	575	GLY
6	3-G	694	PRO
1	1-A	575	GLY
2	1-B	516	LYS
2	2-B	516	LYS
2	3-B	516	LYS

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.