Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 04:47 pm GMT

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 EM Validation Report for a publicly released PDB entry.

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

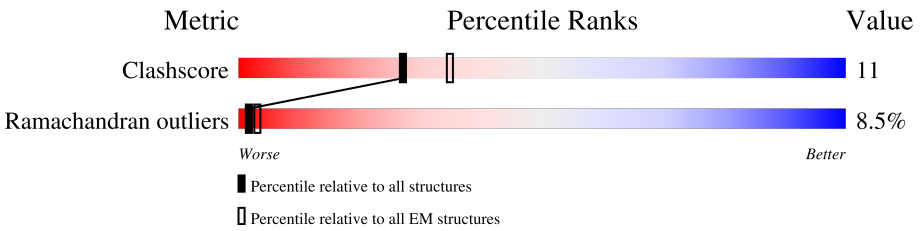
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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	158937	4297
Ramachandran outliers	154571	4023

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	1262	7%; 48%; 14%; •; 36%
1	2-A	1262	48%; 14%; •; 36%
1	3-A	1262	48%; 14%; •; 36%
2	1-B	968	12%; 66%; 13%; •; 17%
2	2-B	968	66%; 13%; • •; 17%
2	3-B	968	67%; 13%; •; 17%
3	1-C	905	8%; 77%; 14%; •; 7%
3	2-C	905	77%; 14%; •; 7%
3	3-C	905	77%; 14%; •; 7%

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Mol	Chain	Length	Quality of chain
4	1-D	511	14% 78% 5% 16%
4	2-D	511	78% 5% 16%
4	3-D	511	78% 5% 16%
5	1-F	181	77% 8% 12%
5	1-M	181	8% 64% 20% 12%
5	1-R	181	22% 55% 27% 7% 12%
5	2-F	181	77% 8% 12%
5	2-M	181	64% 20% 12%
5	2-R	181	54% 27% 7% 12%
5	3-F	181	77% 8% 12%
5	3-M	181	64% 20% 12%
5	3-R	181	54% 27% 7% 12%
6	1-G	874	25% 75% 14% 9%
6	1-K	874	6% 52% 9% 36%
6	2-G	874	75% 13% 9%
6	2-K	874	52% 9% 36%
6	3-G	874	75% 14% 9%
6	3-K	874	52% 9% 36%
7	1-L	177	13% 66% 12% 21%
7	1-Z	177	13% 66% 12% 21%
7	2-L	177	66% 12% 21%
7	2-Z	177	66% 12% 21%
7	3-L	177	66% 12% 21%
7	3-Z	177	66% 12% 21%

2 Entry composition (i)

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
			Total	C	N	O		
1	1-A	813	3251	1626	813	812	0	0
1	2-A	813	3251	1626	813	812	0	0
1	3-A	813	3251	1626	813	812	0	0

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
			Total	C	N	O		
2	1-B	800	3198	1600	800	798	0	0
2	2-B	800	3198	1600	800	798	0	0
2	3-B	800	3198	1600	800	798	0	0

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
			Total	C	N	O		
3	1-C	843	3371	1686	843	842	0	0
3	2-C	843	3371	1686	843	842	0	0
3	3-C	843	3371	1686	843	842	0	0

- Molecule 4 is a protein called Coatomer subunit delta.

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

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

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

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

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

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

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

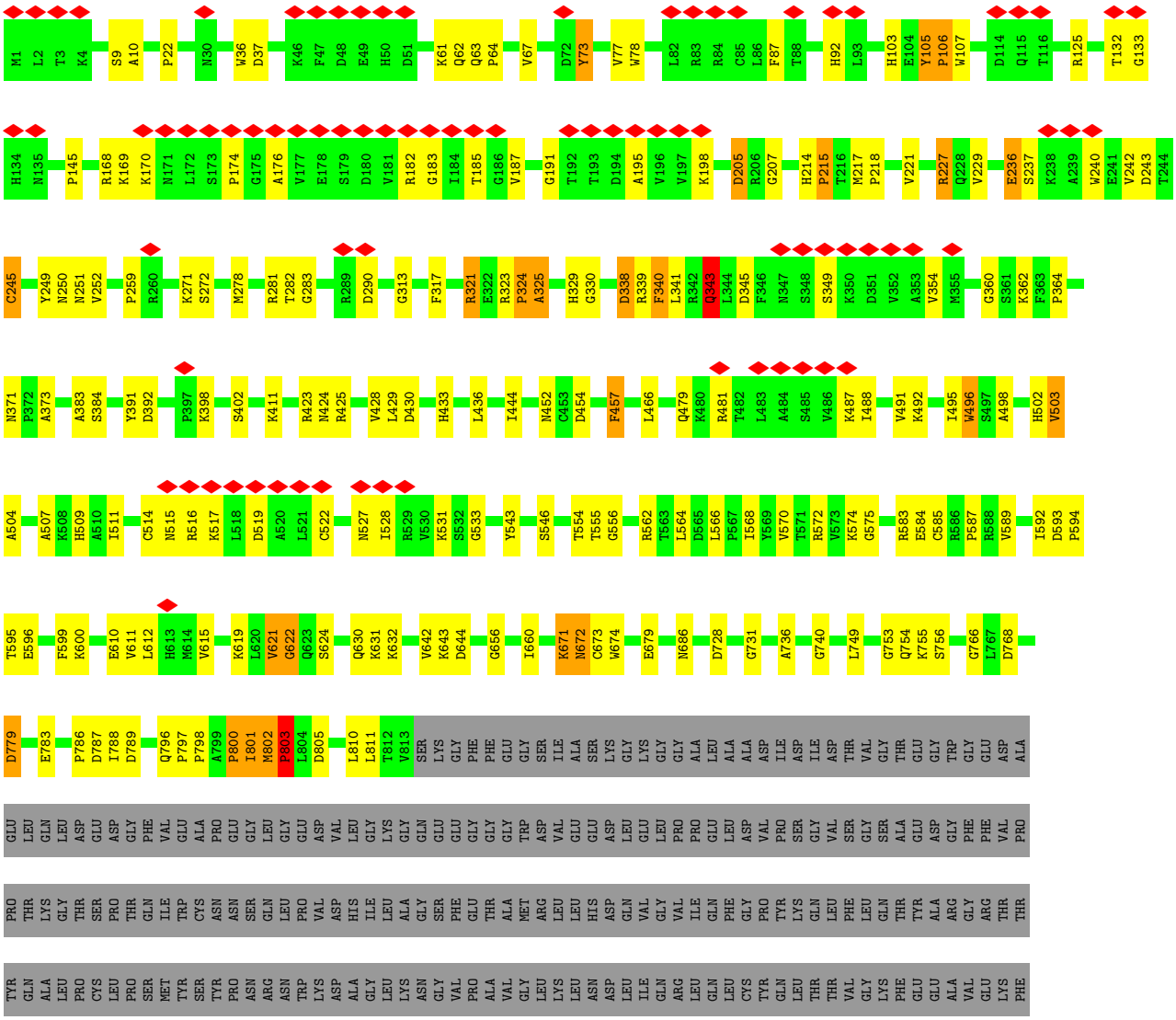
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	1-Z	139	555	278	139	138	0	0
7	2-Z	139	555	278	139	138	0	0
7	3-Z	139	555	278	139	138	0	0
7	1-L	139	555	278	139	138	0	0
7	2-L	139	555	278	139	138	0	0
7	3-L	139	555	278	139	138	0	0

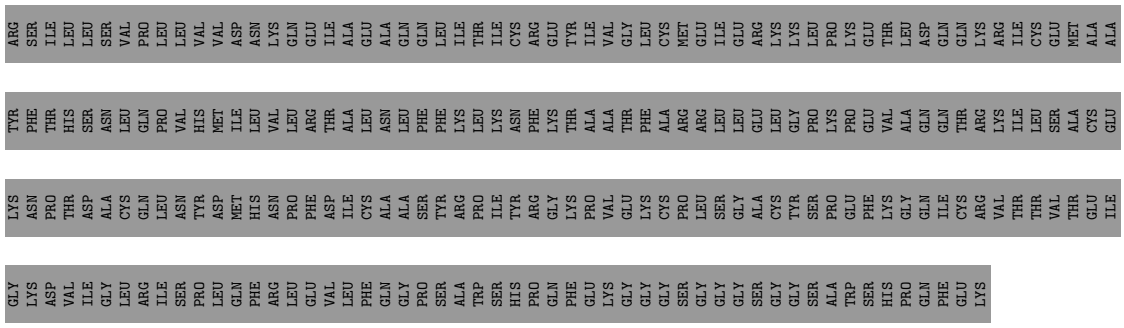
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Coatomer subunit alpha

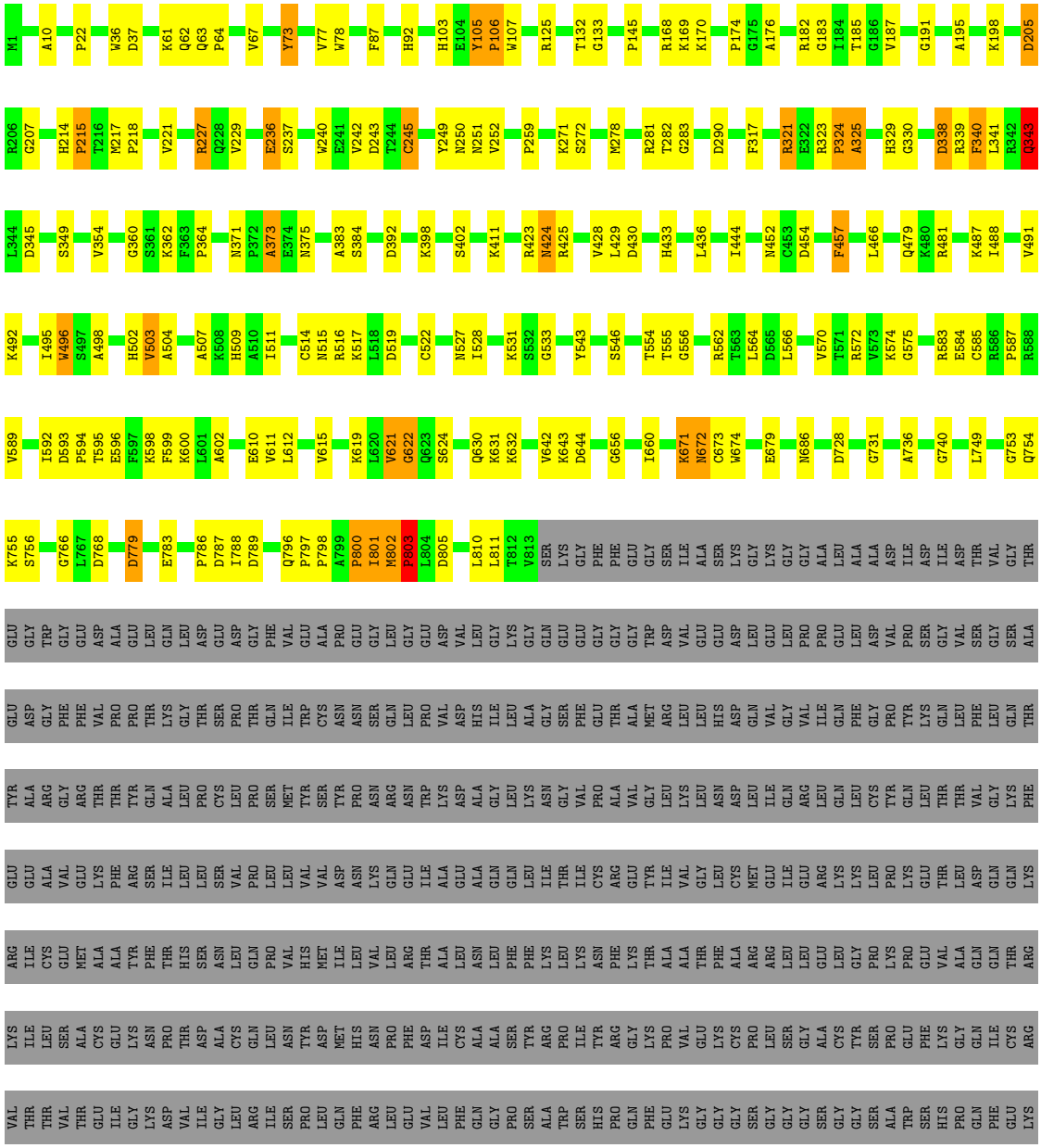
Chain 1-A:





- Molecule 1: Coatomer subunit alpha

Chain 2-A: 48% 14% • 36%



- Molecule 1: Coatomer subunit alpha

Chain 3-A: 48% 14% • 36%

M1 S9 A10 P22 W36 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

D205 R206 G207 H214 P215 T216 M217 P218 V221 R227 Q228 V229 E236 S237 W240 E241 V242 D243 T244 C245 Y249 N250 N251 V252 P259 K271 S272 M278 R281 T282 G283 D290 G313 F317 R321 E322 R323 P324 A325 H329 G330 D338 R339 E340

L341 R342 Q343 L344 D345 S349 V354 G360 S361 K362 F363 P364 N371 P372 A373 A383 S384 D392 K398 S402 K411 R412 S413 R423 N424 R425 L429 D430 H433 L436 I444 N452 C453 D454 F457 L466 Q479 K480 R481 K487 I488

V491 K492 I495 W496 S497 A498 H502 V503 A504 A507 K508 H509 A510 I511 C514 N515 R516 K517 L518 D519 C522 N527 I528 K531 S532 G533 Y543 S546 T554 T555 G556 R562 T563 L564 D565 L566 V570 T571 R572 V573 K574 G575 R583 E584 C585 R586

P587 R588 V589 I592 D593 P594 T595 E596 F597 K598 F599 K600 L601 A602 E610 V611 L612 V615 K619 L620 V621 G622 Q623 S624 Q630 K631 K632 V642 K643 D644 G656 I660 K671 N672 C673 W674 E679 N686 D728 G731 A736 G740 L749

G753 Q754 K755 S756 G766 L767 D768 D779 E783 P786 D787 I788 D789 Q796 P797 P798 A799 P800 I801 M802 P803 L804 D805 L810 L811 T812 V813 SER LYS GLY PHE PHE GLU GLY SER ILE ALA SER LYS GLY LYS GLY GLY ALA LEU ALA ALA ASP ILE ASP ILE ASP THR VAL

GLY THR GLU GLY TRP GLY GLU ASP ALA GLU LEU GLN LEU ASP GLU ASP GLY PHE VAL GLU ALA PRO GLU GLY LEU GLY GLU ASP VAL LEU GLY LYS GLY GLN GLU GLU GLY GLY GLY TRP ASP VAL GLU GLU ASP LEU GLU LEU PRO PRO GLU LEU ASP VAL PRO SER GLY VAL SER GLY

SER ALA GLU ASP GLY PHE PHE VAL PRO PRO THR THR LYS GLY THR SER PRO THR GLN ILE TRP CYS ASN ASN SER GLN LEU PRO VAL ASP HIS ILE LEU ALA GLY SER PHE GLU THR ALA MET ARG LEU LEU HIS ASP GLN VAL GLY VAL ILE GLN PHE GLY PRO TYR LYS GLN LEU PHE LEU

GLN THR TYR ALA ARG GLY ARG THR THR TYR GLN ALA LEU PRO CYS LEU PRO SER MET TYR SER TYR PRO ASN ARG ASN TRP LYS ASP ALA GLY LEU LYS ASN GLY VAL PRO ALA VAL GLY LEU LYS LEU ASN ASP LEU ILE GLN ARG LEU GLN LEU CYS TYR GLN LEU THR THR VAL GLY

LYS PHE GLU GLU ALA VAL GLU LYS PHE ARG SER ILE LEU LEU SER VAL PRO LEU LEU VAL VAL ASP ASN LYS GLN GLU ILE ALA GLU ALA GLN GLN LEU ILE THR ILE CYS ARG GLU TYR ILE VAL GLY LEU CYS MET GLU ILE GLN ARG LYS LYS LEU PRO LYS GLU THR LEU ASP GLN

GLN LYS ARG ILE CYS GLU MET ALA ALA TYR PHE THR HIS SER ASN LEU GLN PRO VAL HIS MET ILE LEU VAL LEU ARG THR ALA LEU ASN LEU PHE PHE LYS LEU LYS ASN PHE LYS THR ALA ALA THR PHE ALA ARG ARG LEU LEU GLU LEU GLY PRO LYS PRO GLU VAL ALA GLN GLN

THR ARG LYS ILE LEU SER ALA CYS GLN LEU ASN TYR ASP MET THR ASN PRO THR ASP ALA CYS ALA ALA SER TYR ARG PRO ILE TYR ARG GLY LYS PRO VAL GLU LYS CYS PRO LEU SER GLY ALA CYS TYR SER PRO GLU PHE LYS GLY GLN ILE

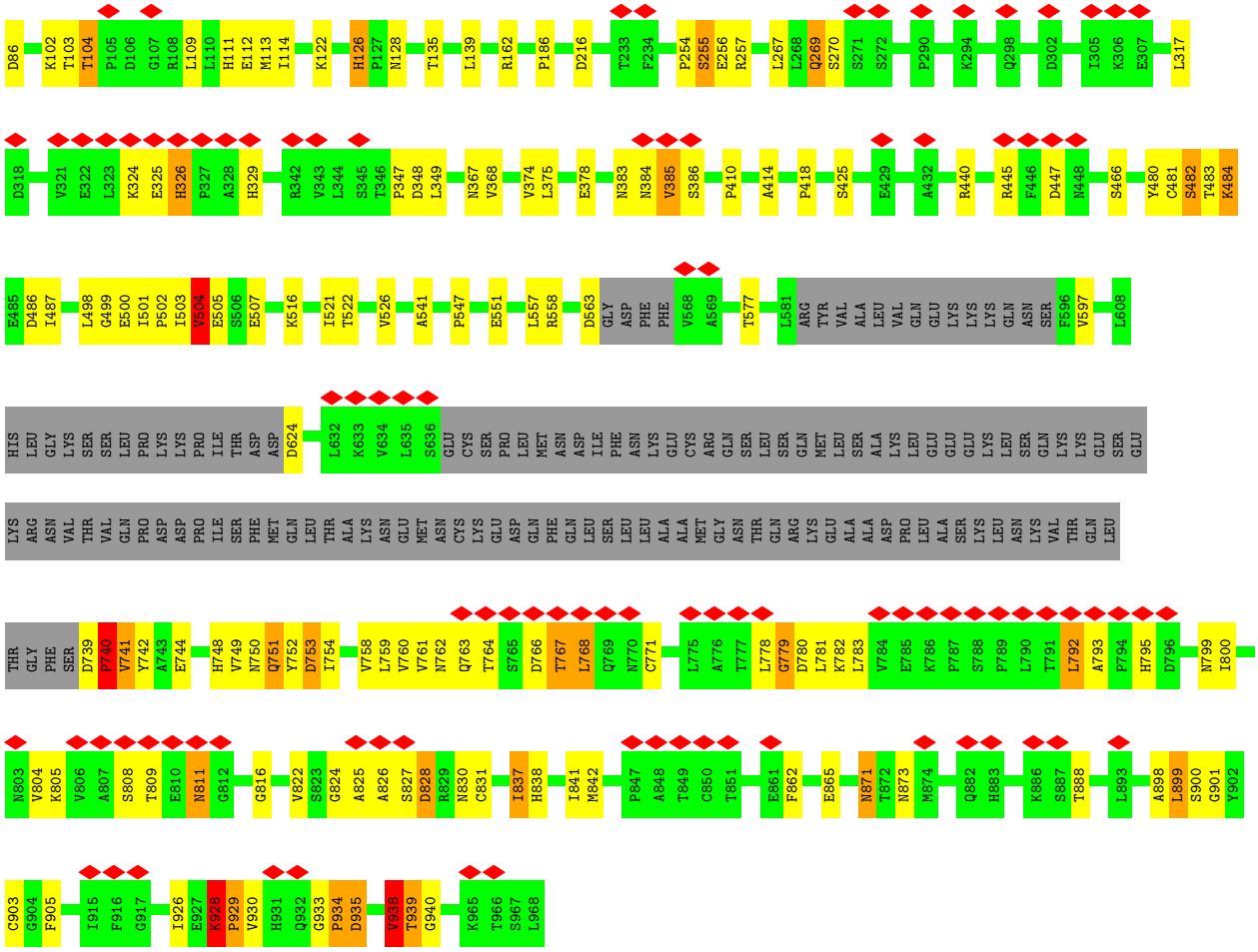
CYS ARG VAL THR THR VAL THR GLU ILE GLY LYS ASP VAL ILE GLY LEU ARG ILE SER PRO LEU GLN PHE ARG LEU GLU VAL LEU PHE GLN GLY PRO SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE

GLU LYS

• Molecule 2: Coatomer subunit beta

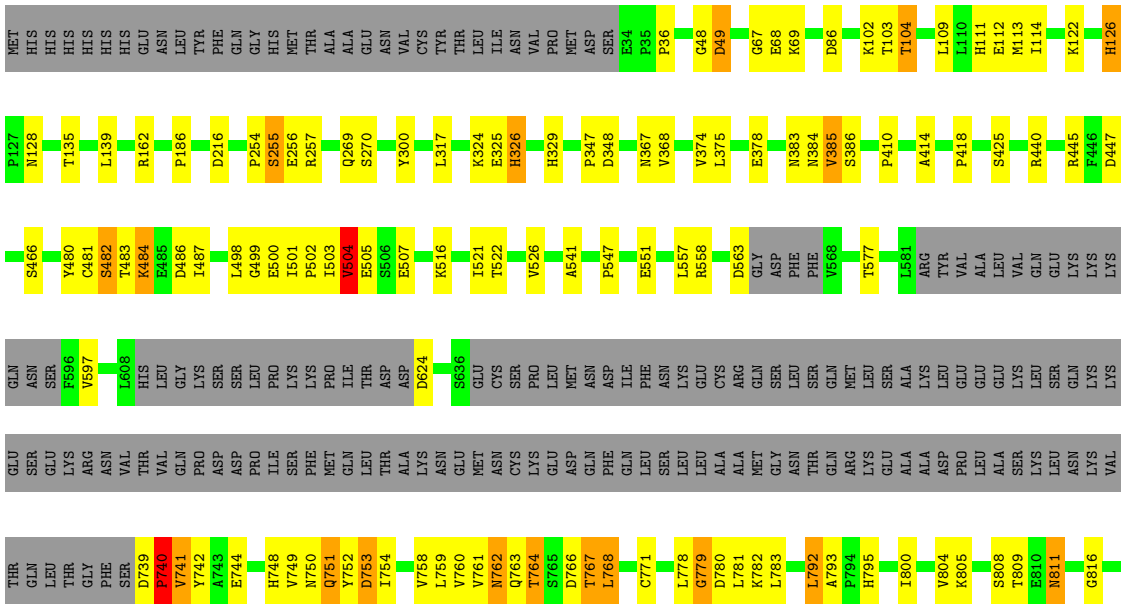
Chain 1-B: 12% 66% 13% • 17%

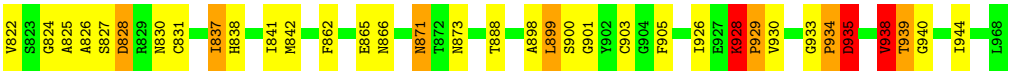
MET HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY HIS MET THR ALA ALA GLU ASN VAL CYS TYR THR LEU ILE ASN VAL PRO MET ASP SER E34 P35 P36 S37 E38 I39 S40 L41 K42 N43 D44 L45 E46 K47 G48 D49 V50 K51 S52 N66 G67 E68 K69 L70 P71



• Molecule 2: Coatomer subunit beta

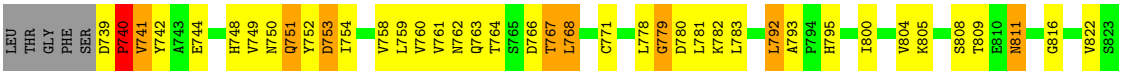
Chain 2-B: 66% 13% • • 17%

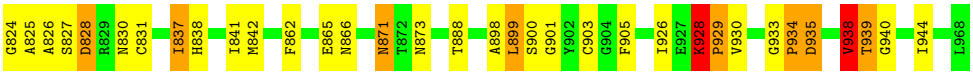




• Molecule 2: Coatomer subunit beta

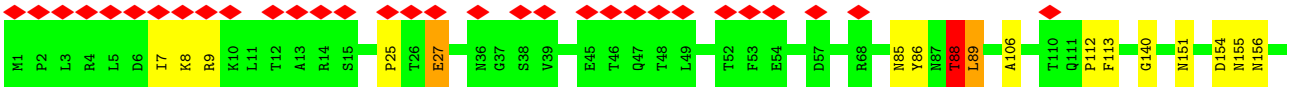
Chain 3-B:

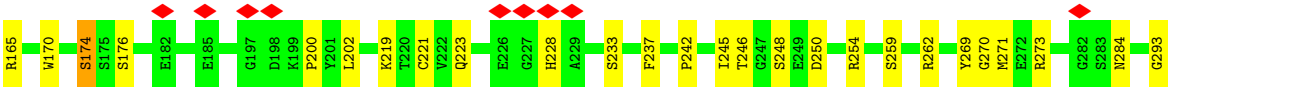


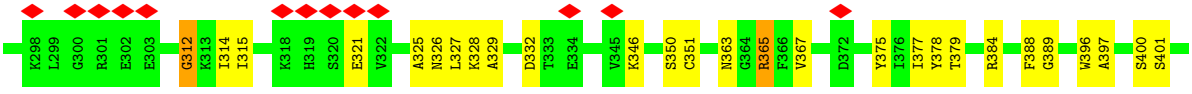


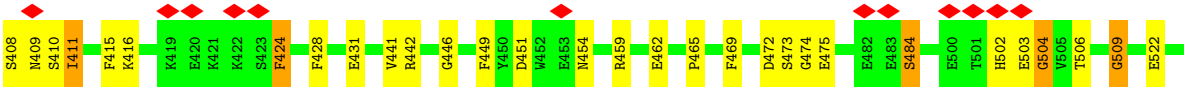
• Molecule 3: Coatomer subunit beta'

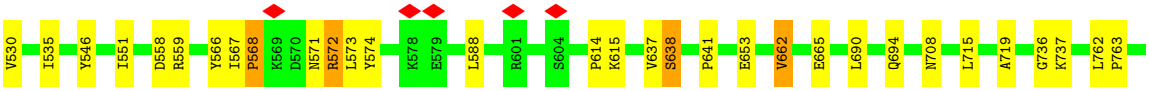
Chain 1-C:

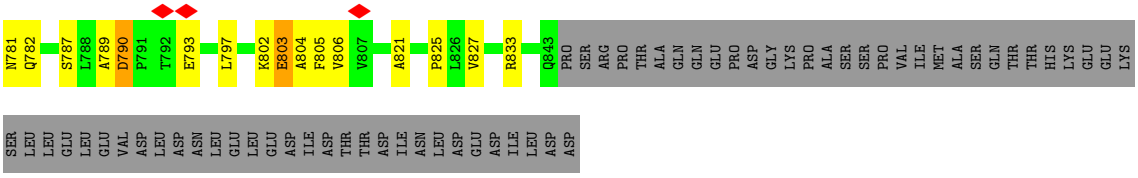






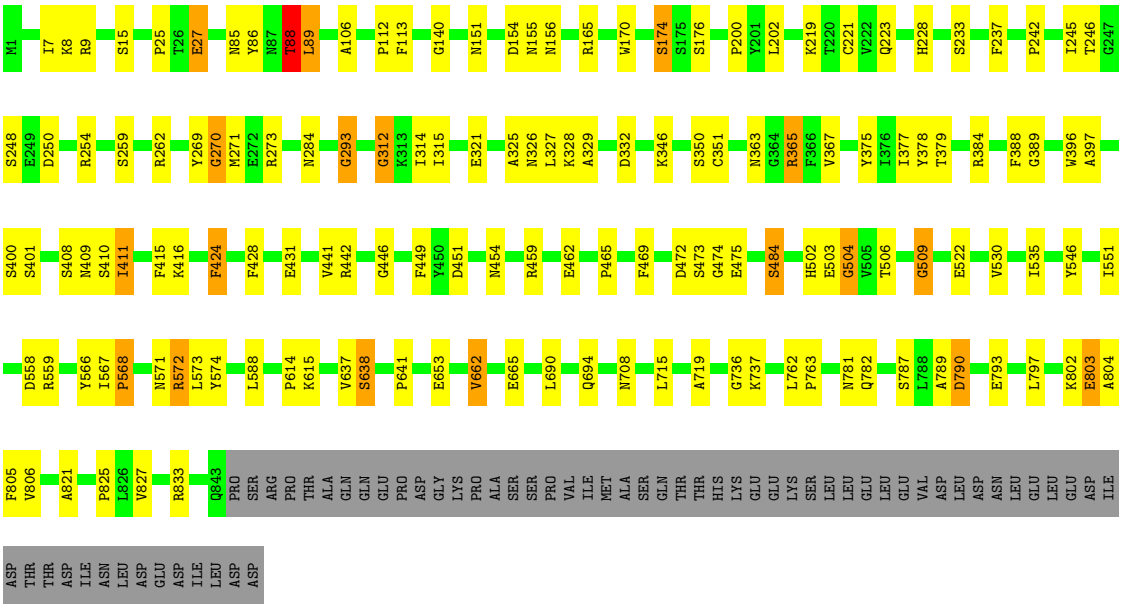






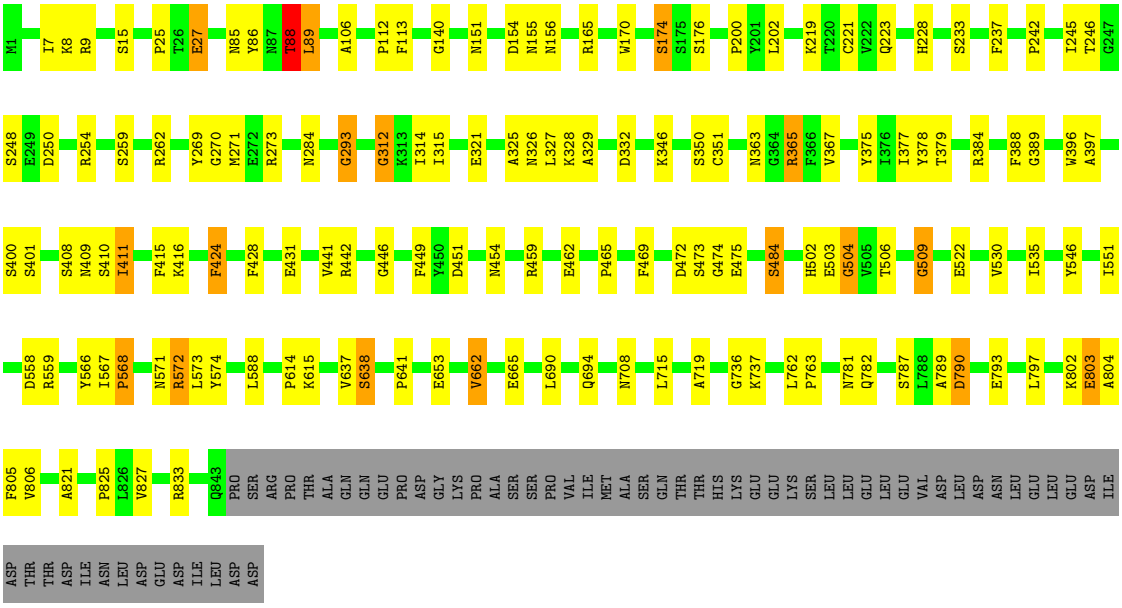
- Molecule 3: Coatomer subunit beta'

Chain 2-C:



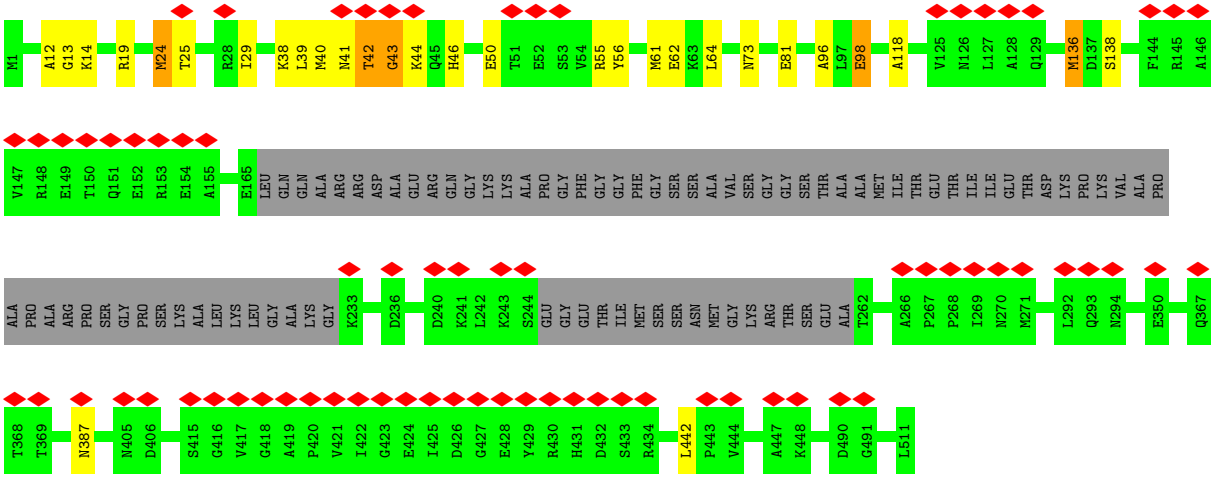
- Molecule 3: Coatomer subunit beta'

Chain 3-C:



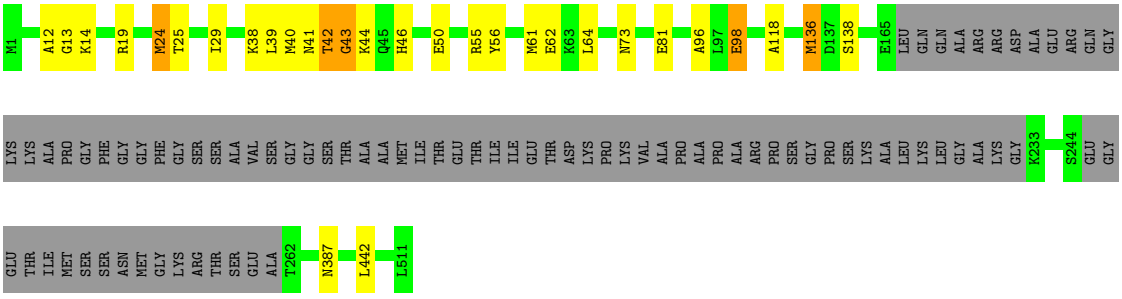
• Molecule 4: Coatomer subunit delta

Chain 1-D:



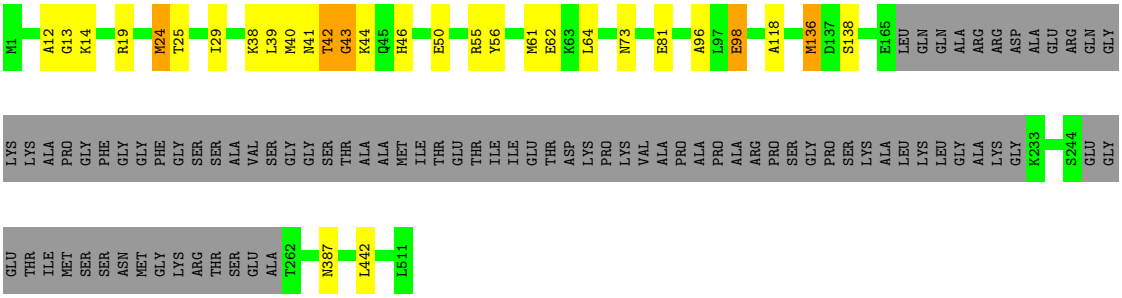
• Molecule 4: Coatomer subunit delta

Chain 2-D:



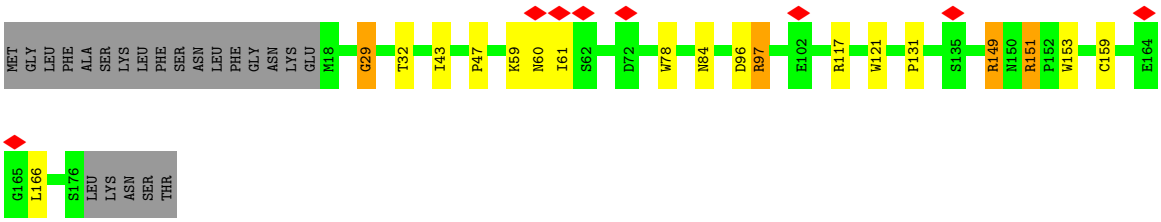
• Molecule 4: Coatomer subunit delta

Chain 3-D:



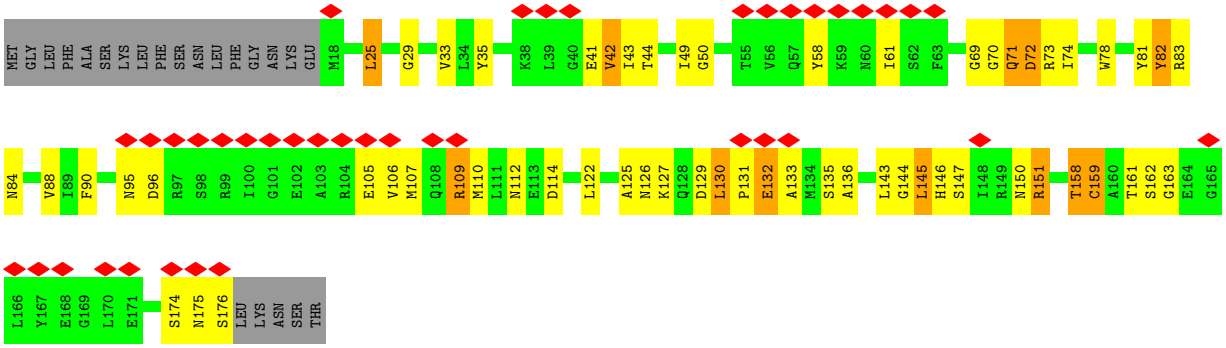
• Molecule 5: ADP-ribosylation factor 1

Chain 1-F:



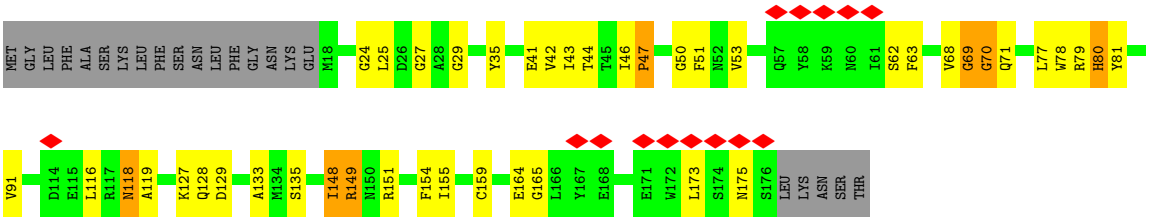
• Molecule 5: ADP-ribosylation factor 1

Chain 1-R:



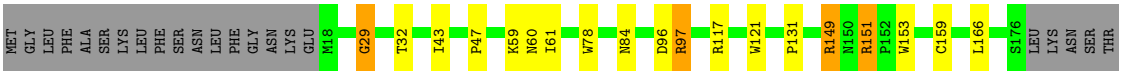
• Molecule 5: ADP-ribosylation factor 1

Chain 1-M:



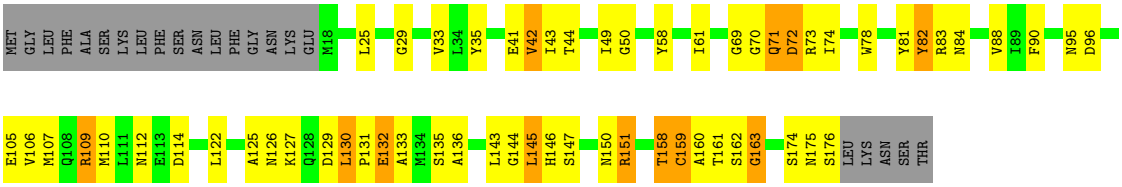
• Molecule 5: ADP-ribosylation factor 1

Chain 2-F:



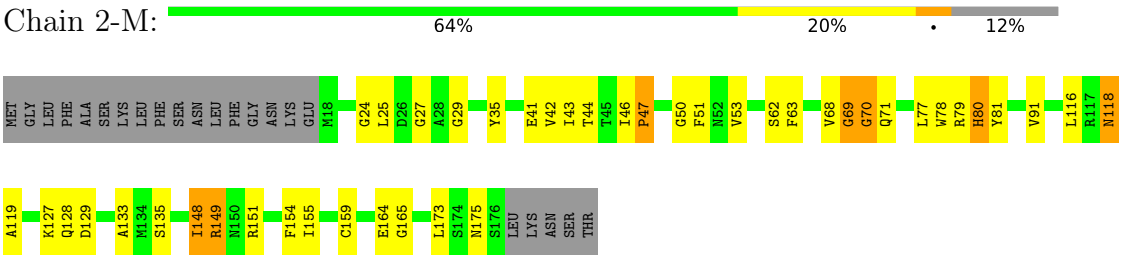
• Molecule 5: ADP-ribosylation factor 1

Chain 2-R:



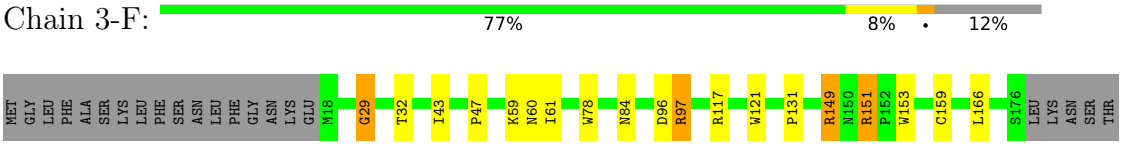
- Molecule 5: ADP-ribosylation factor 1

Chain 2-M:



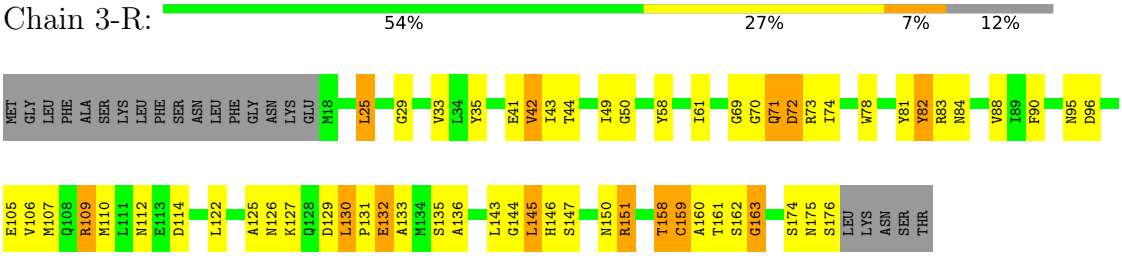
- Molecule 5: ADP-ribosylation factor 1

Chain 3-F:



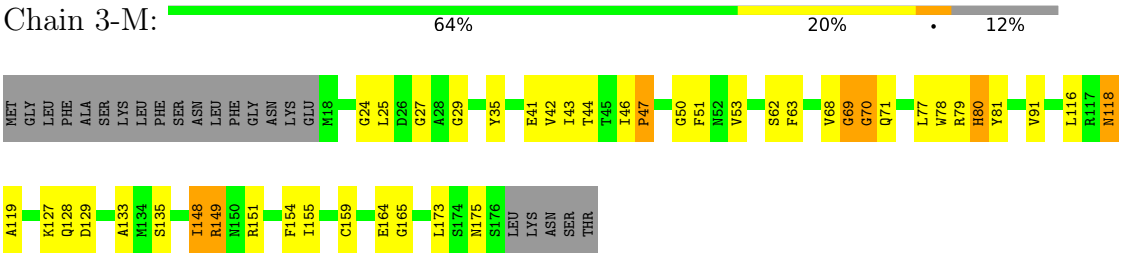
- Molecule 5: ADP-ribosylation factor 1

Chain 3-R:



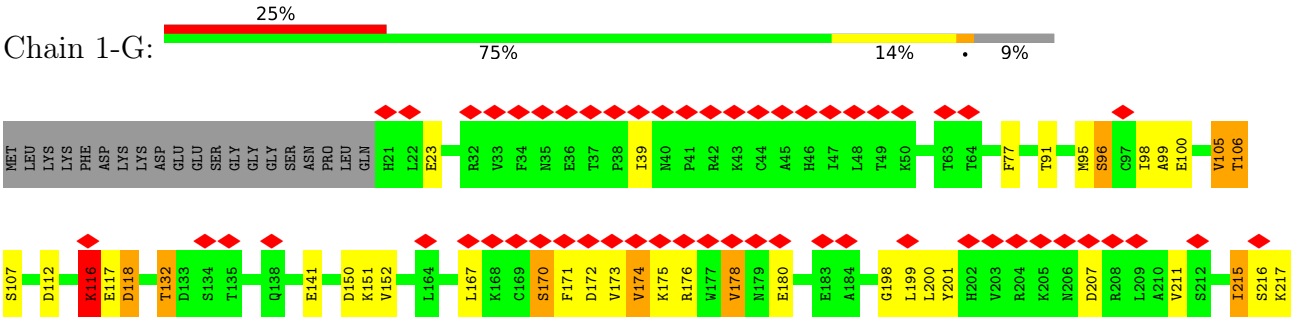
- Molecule 5: ADP-ribosylation factor 1

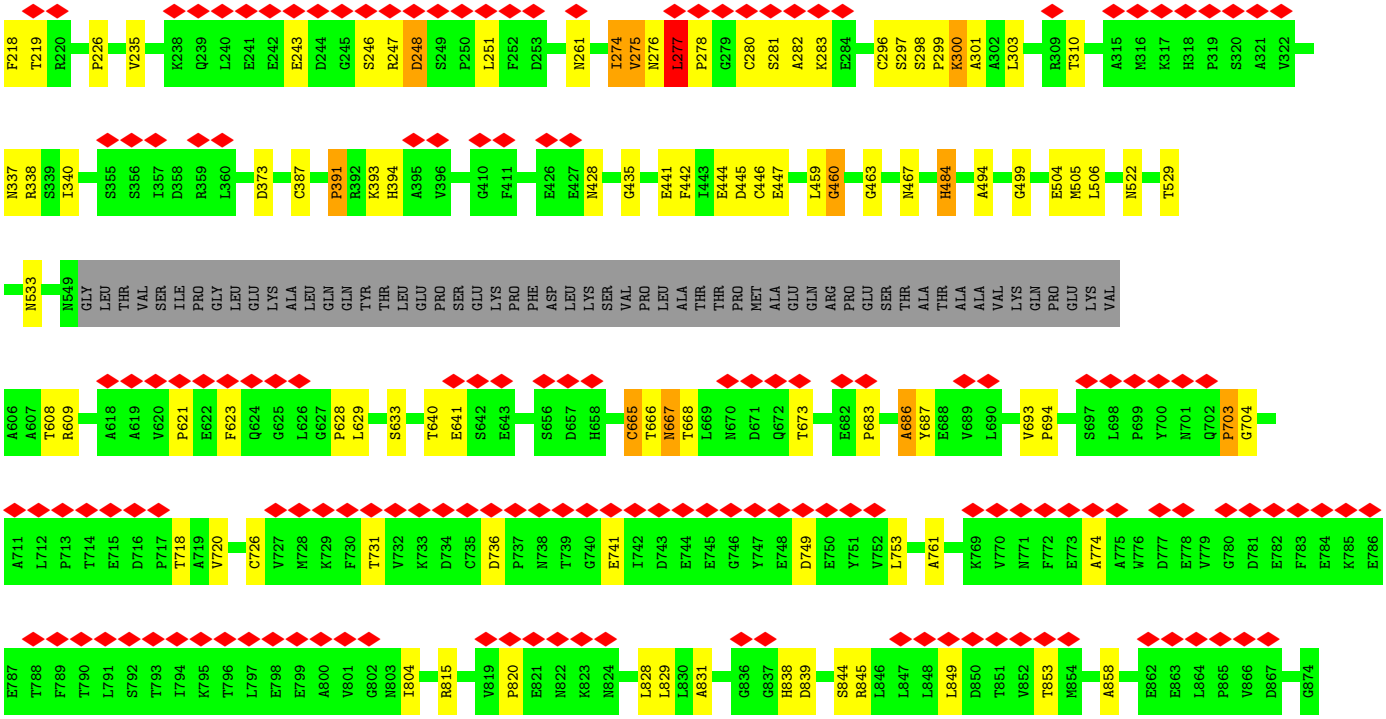
Chain 3-M:



- Molecule 6: Coatomer subunit gamma-1

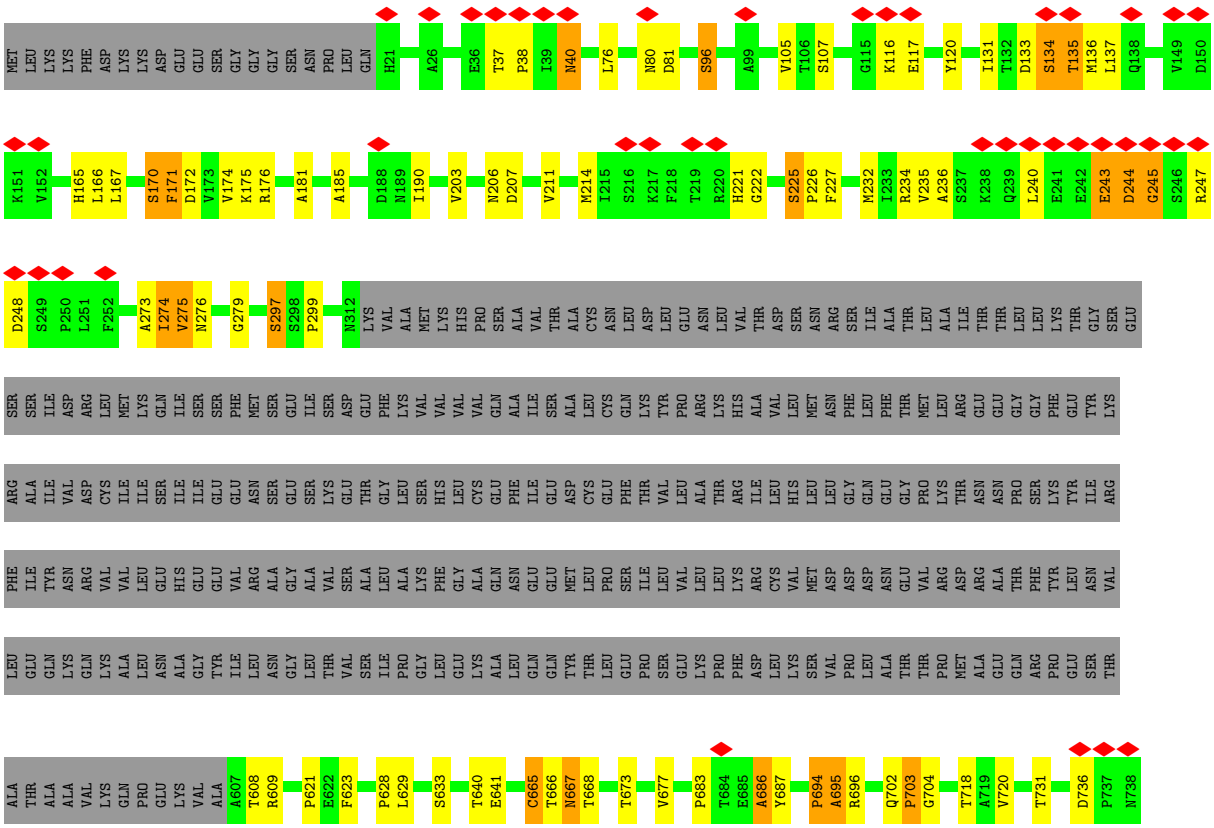
Chain 1-G:

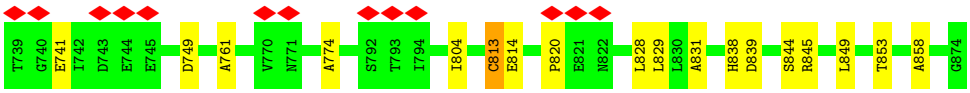




- Molecule 6: Coatomer subunit gamma-1

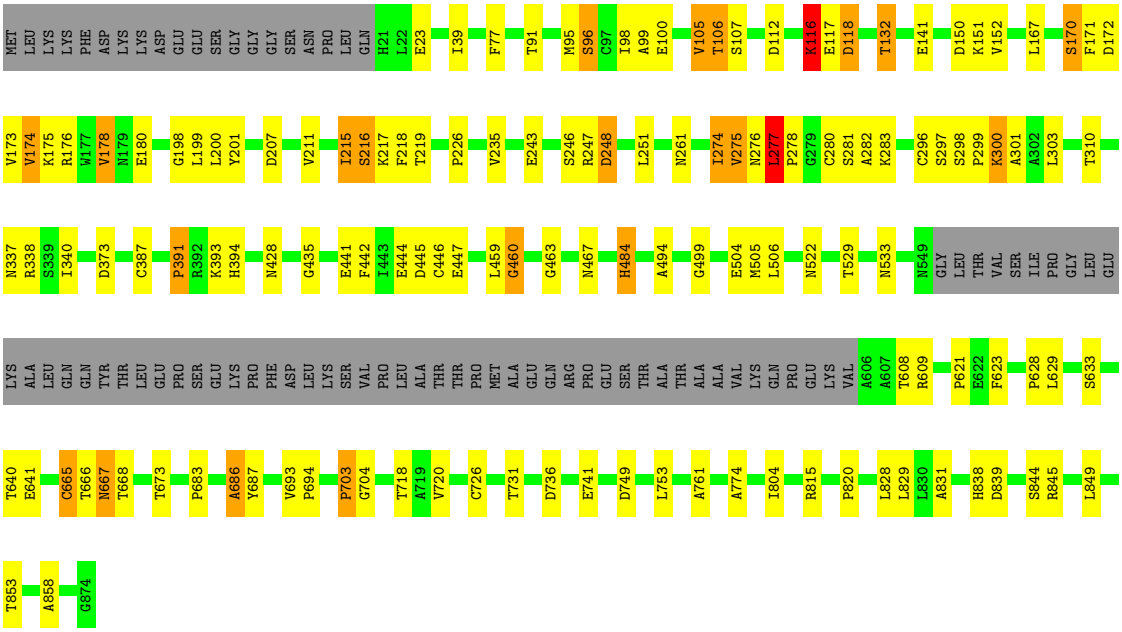
Chain 1-K:





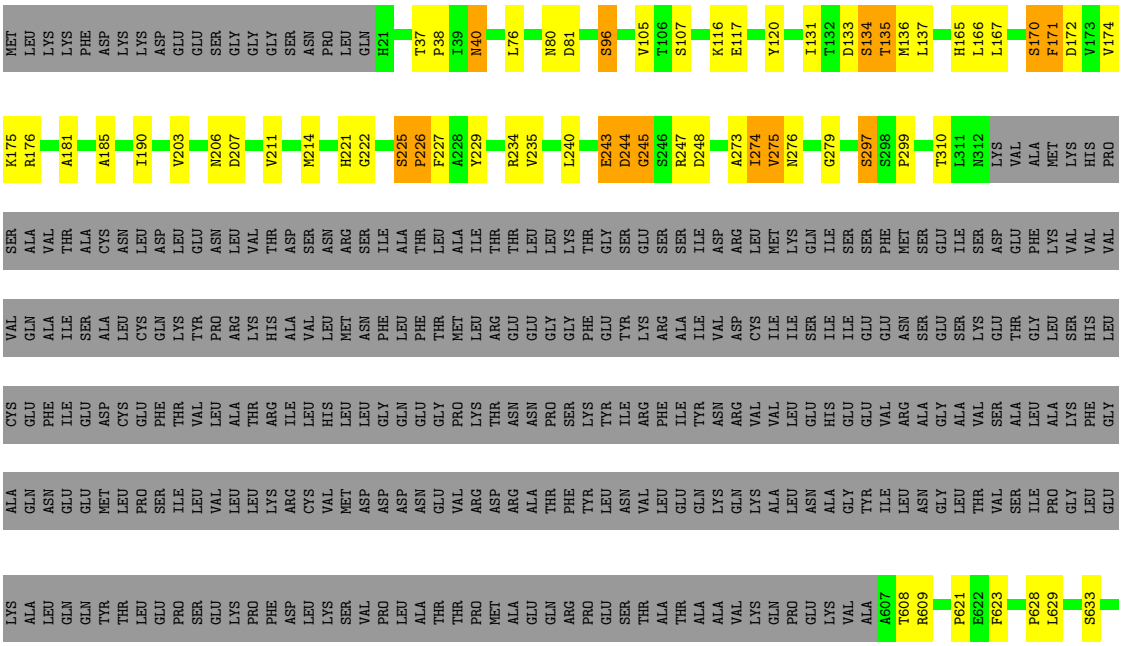
• Molecule 6: Coatomer subunit gamma-1

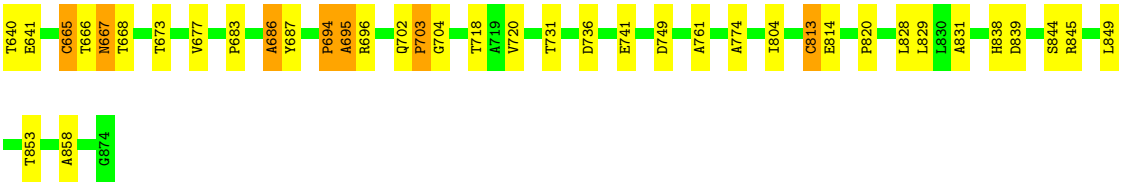
Chain 2-G: 75% 13% • 9%



• Molecule 6: Coatomer subunit gamma-1

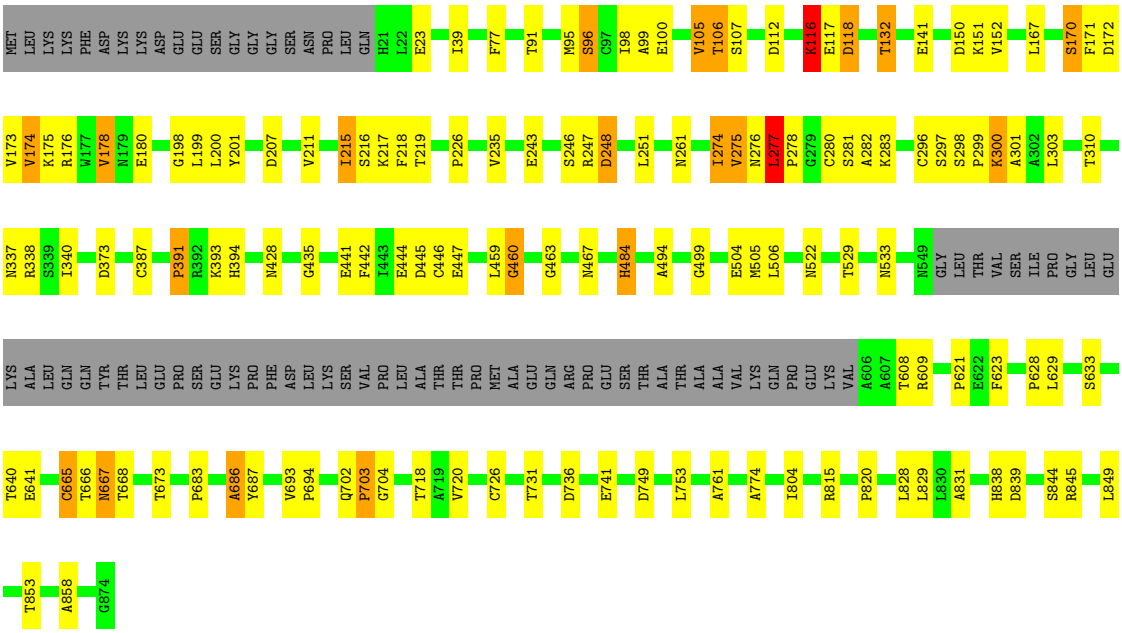
Chain 2-K: 52% 9% • 36%





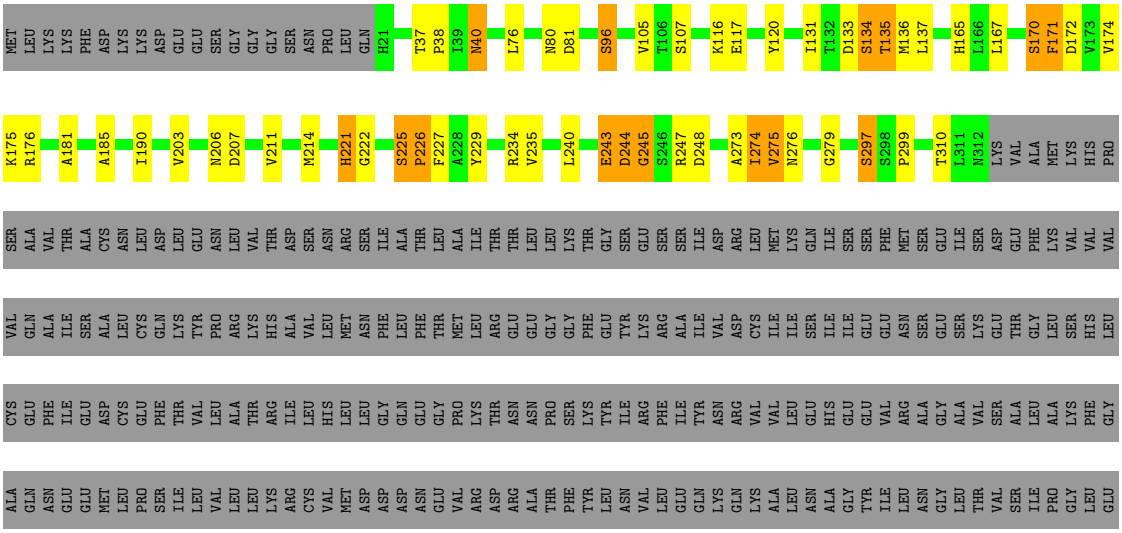
• Molecule 6: Coatomer subunit gamma-1

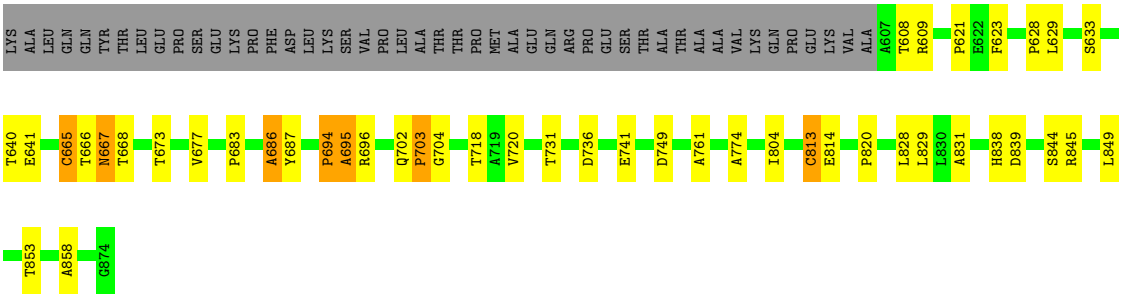
Chain 3-G:



• Molecule 6: Coatomer subunit gamma-1

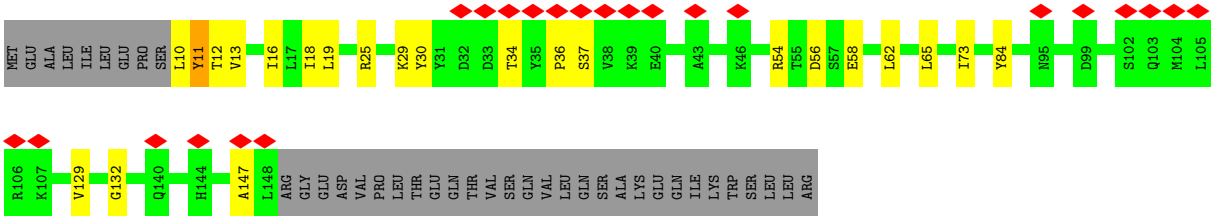
Chain 3-K:





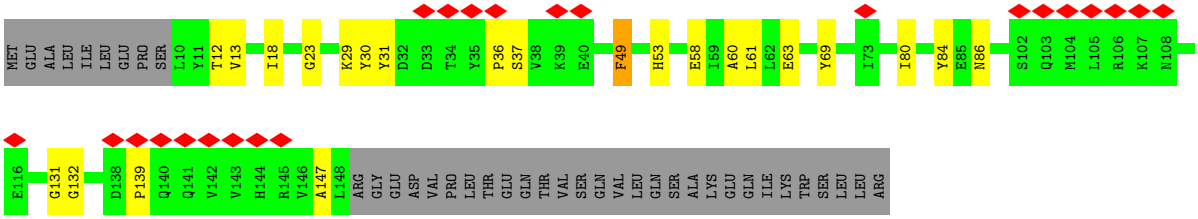
• Molecule 7: Coatomer subunit zeta-1

Chain 1-Z:



• Molecule 7: Coatomer subunit zeta-1

Chain 1-L:

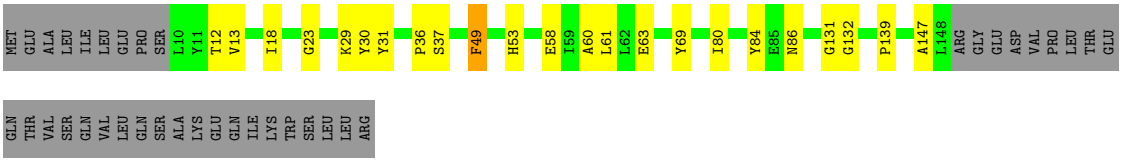


• Molecule 7: Coatomer subunit zeta-1

Chain 2-Z:

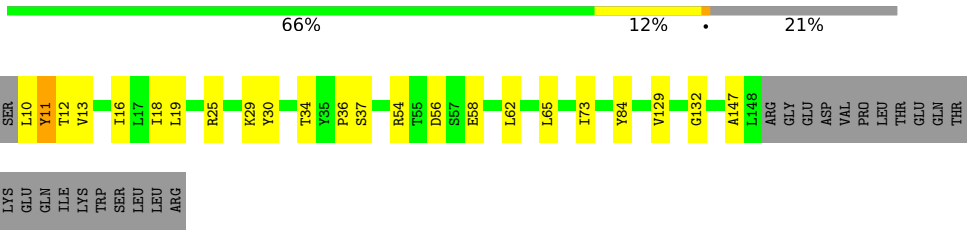
• Molecule 7: Coatomer subunit zeta-1

Chain 2-L:



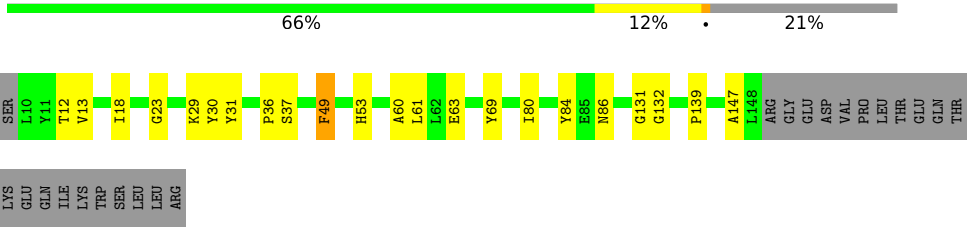
• Molecule 7: Coatomer subunit zeta-1

Chain 3-Z:



• Molecule 7: Coatomer subunit zeta-1

Chain 3-L:



4 Experimental information (i)

Property	Value	Source
EM 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 ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	377.36, 377.36, 377.36	wwPDB
Map dimensions	212, 212, 212	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.78, 1.78, 1.78	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Continued on next page...

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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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
1:A:800:PRO:O	3:C:805:PHE:O	2.05	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
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:24:GLY:O	5:M:68:VAL:O	2.17	0.63
5:M:116:LEU:O	5:M:118:ASN:N	2.32	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:82:TYR:O	5:R:83:ARG:C	2.39	0.59
5:R:159:CYS:O	5:R:162:SER:CA	2.50	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:G:106:THR:CA	5:R:50:GLY:HA3	2.36	0.55
6:K:274:ILE:O	6:K:276:ASN:N	2.39	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:71:GLN:O	5:R:73:ARG:N	2.43	0.51
5:R:135:SER:O	5:R:136:ALA:C	2.48	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: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
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:78:TRP:O	5:M:79:ARG:C	2.46	0.50
5:M:173:LEU:C	5:M:175:ASN:H	2.15	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:CA	6:G:280:CYS:H	2.26	0.49
6:G:277:LEU:C	6:G:280:CYS:N	2.66	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:R:159:CYS:C	5:R:161:THR:N	2.68	0.47
5:M:173:LEU:C	5:M:175:ASN: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
7:Z:11:TYR:C	7:Z:132:GLY:CA	2.69	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
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
7:Z:11:TYR:C	7:Z:132:GLY:CA	2.69	0.44
6:K:666:THR:O	6:K:667:ASN:C	2.53	0.44
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.44
6:K:107:SER:H	5:M:50:GLY:HA3	0.67	0.44
6:K:695:ALA:O	6:K:696:ARG:C	2.55	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
5:R:143:LEU:CA	5:R:145:LEU:H	2.20	0.43
6:K:171:PHE:O	6:K:174:VAL:N	2.52	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
5:R:70:GLY:O	5:R:72:ASP:N	2.52	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
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:R:160:ALA:C	5:R:163:GLY:H	2.24	0.40
5:M:79:ARG:O	5:M:81:TYR:O	2.39	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 5
1	2-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0 5
1	3-A	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0 5
2	1-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
2	2-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
2	3-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
3	1-C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1 12
3	2-C	841/905 (93%)	682 (81%)	90 (11%)	69 (8%)	1 12
3	3-C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1 12
4	1-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	3 25
4	2-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	3 25
4	3-D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	3 25
5	1-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 18
5	1-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 6
5	1-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 5
5	2-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 18
5	2-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 6
5	2-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 5
5	3-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 18
5	3-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 6
5	3-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 5
6	1-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1 15
6	1-K	556/874 (64%)	475 (85%)	43 (8%)	38 (7%)	1 15
6	2-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1 15
6	2-K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	3-G	794/874 (91%)	679 (86%)	60 (8%)	55 (7%)	1	15
6	3-K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1	14
7	1-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
7	1-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
7	2-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
7	2-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
7	3-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
7	3-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
All	All	14874/18873 (79%)	12224 (82%)	1379 (9%)	1271 (8%)	2	12

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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Continued from previous page...

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 (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

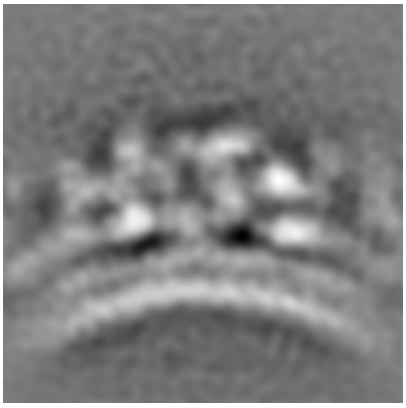
6 Map visualisation (i)

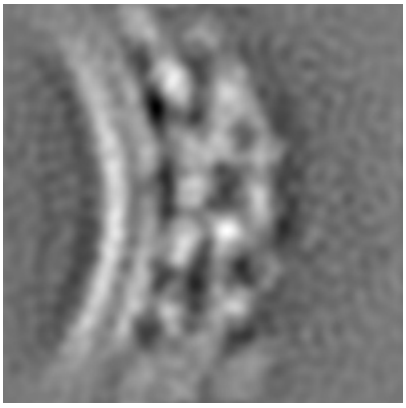
This section contains visualisations of the EMDB entry EMD-3723. These allow visual inspection of the internal detail of the map and identification of artifacts.

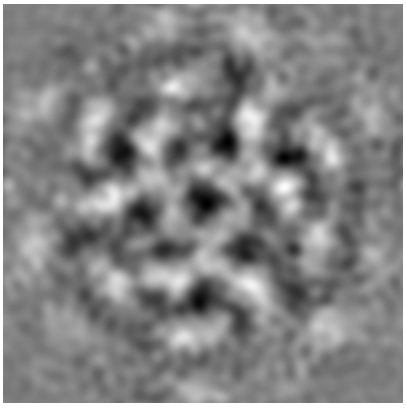
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

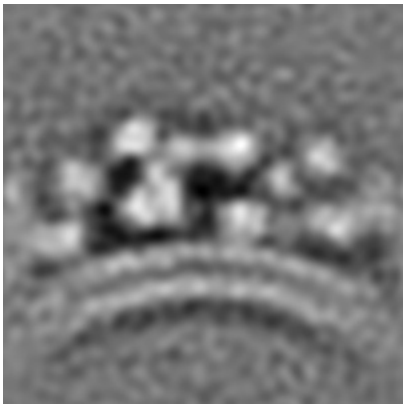

Y

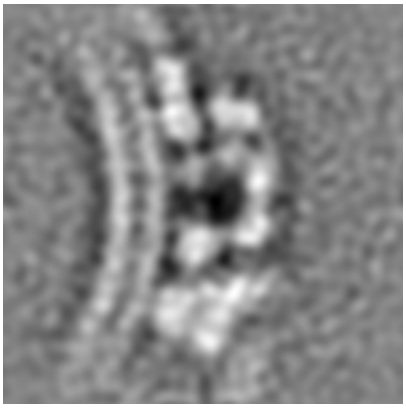

Z

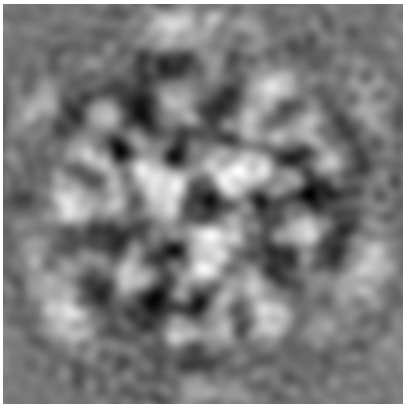
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 106

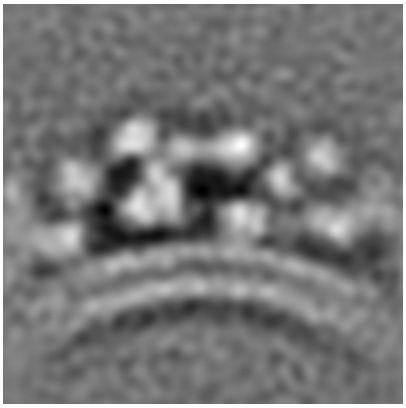

Y Index: 106


Z Index: 106

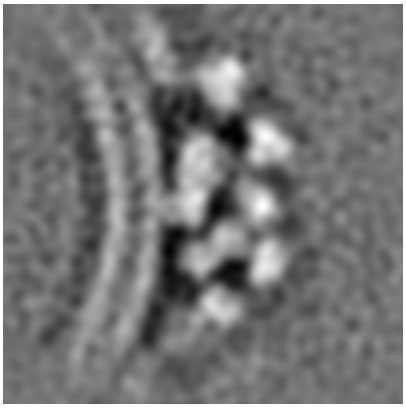
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

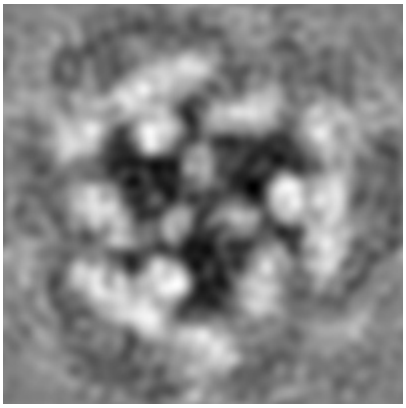
6.3.1 Primary map



X Index: 105



Y Index: 127



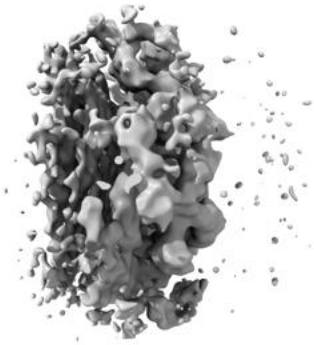
Z Index: 89

The images above show the largest variance slices of the map in three orthogonal directions.

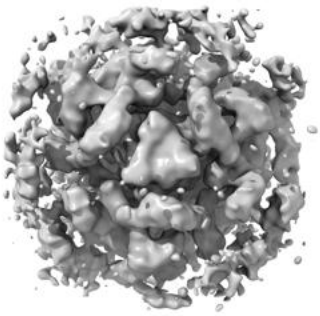
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

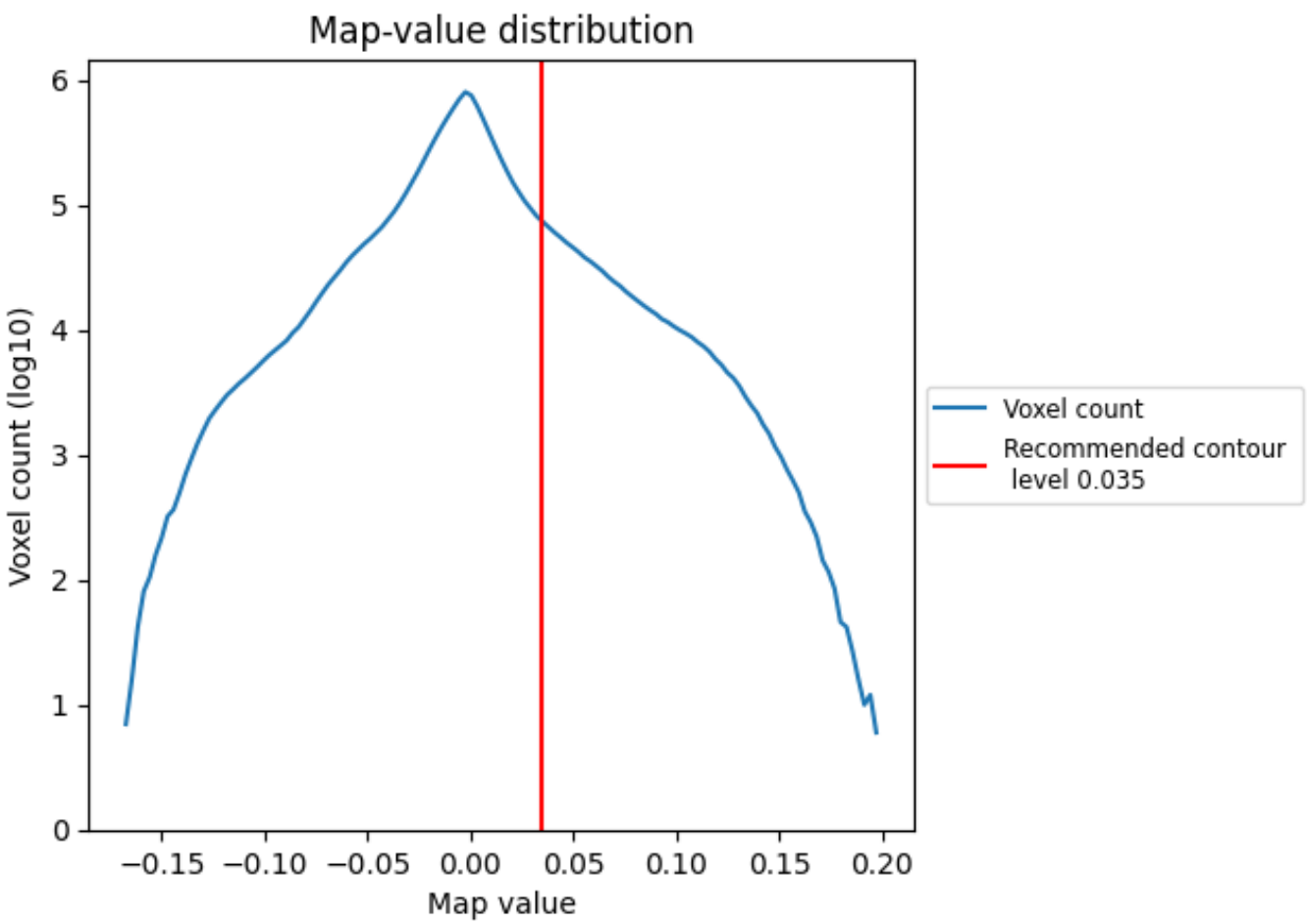
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

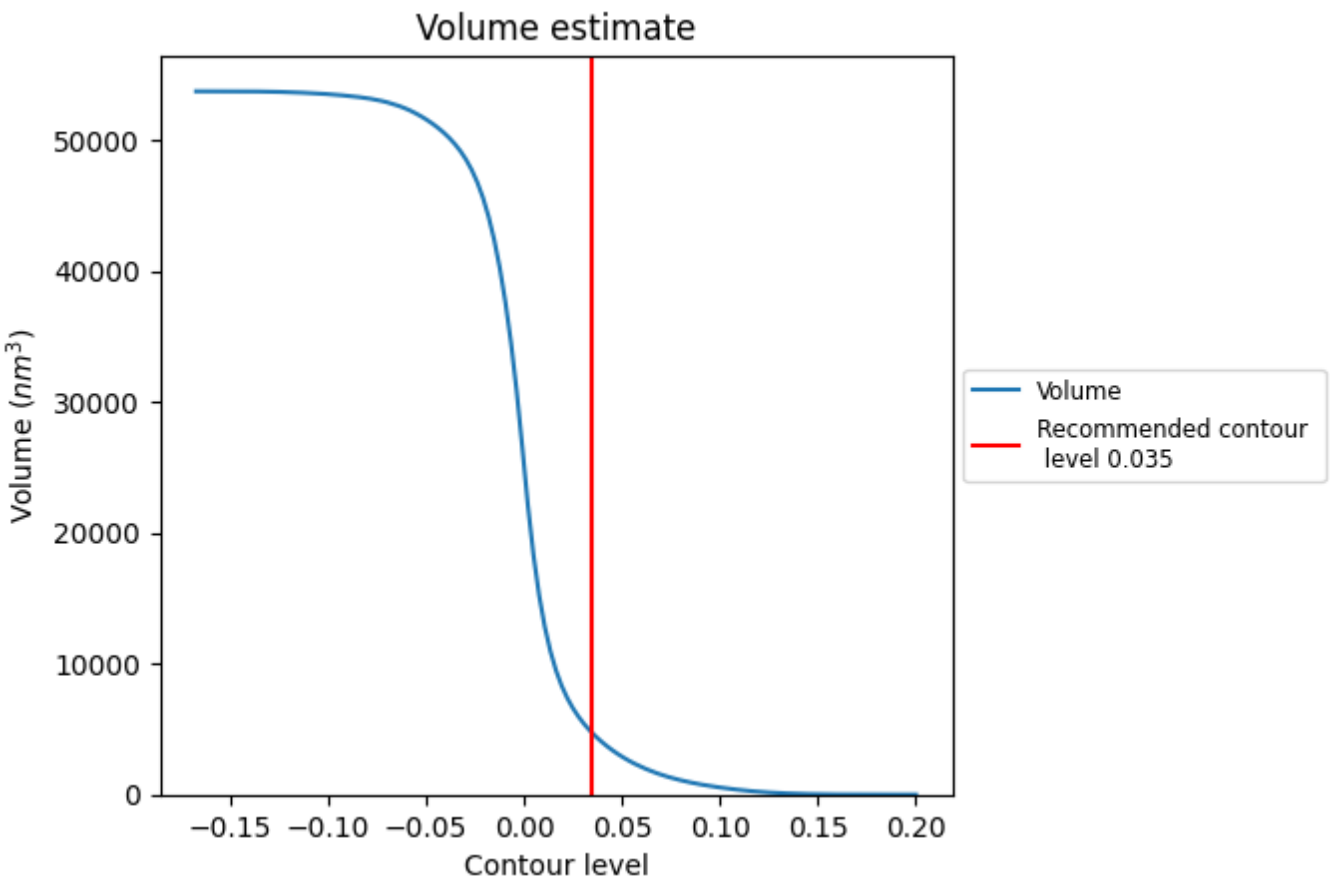
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

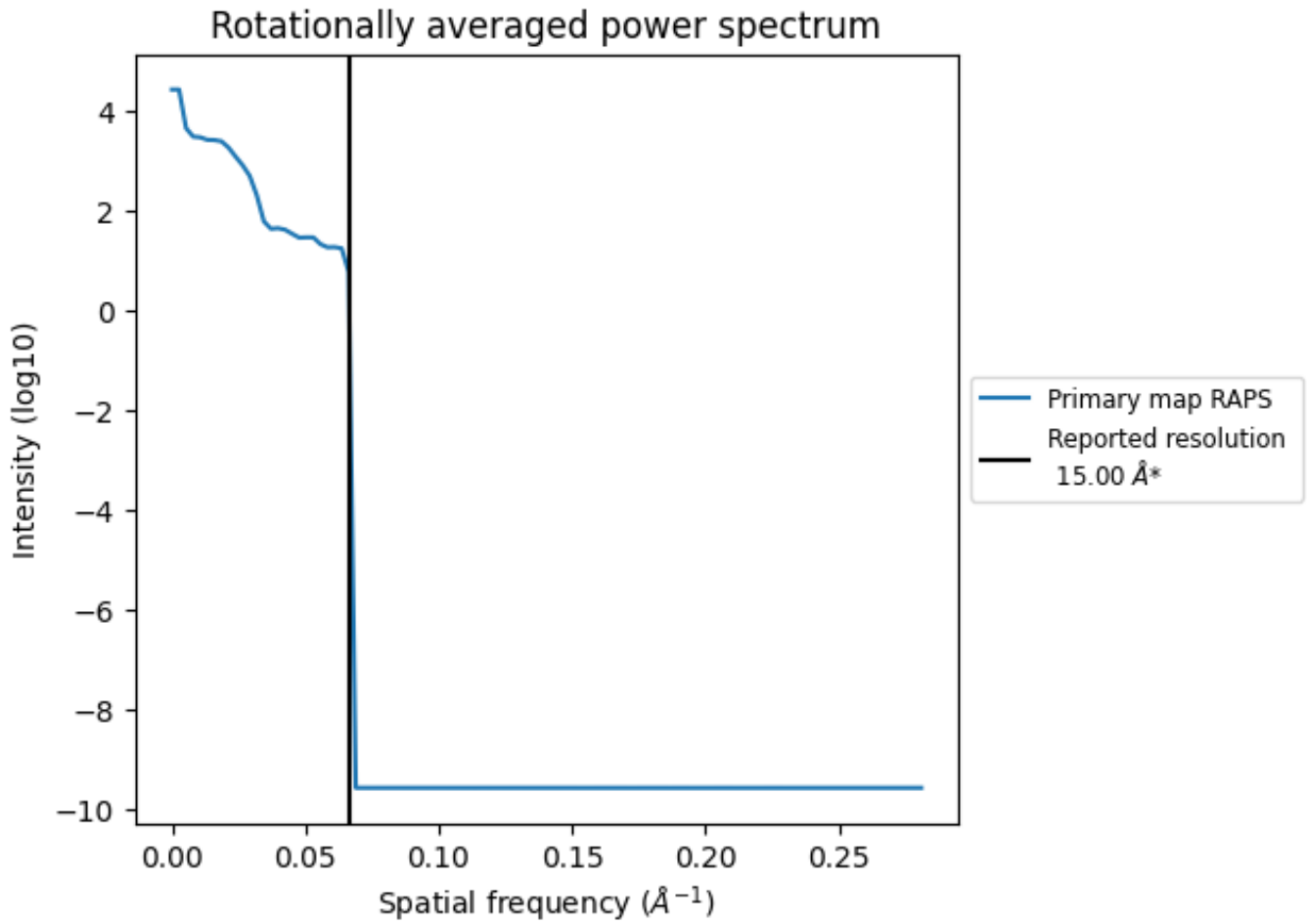
7.2 Volume estimate (i)



The volume at the recommended contour level is 4694 nm^3; this corresponds to an approximate mass of 4240 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

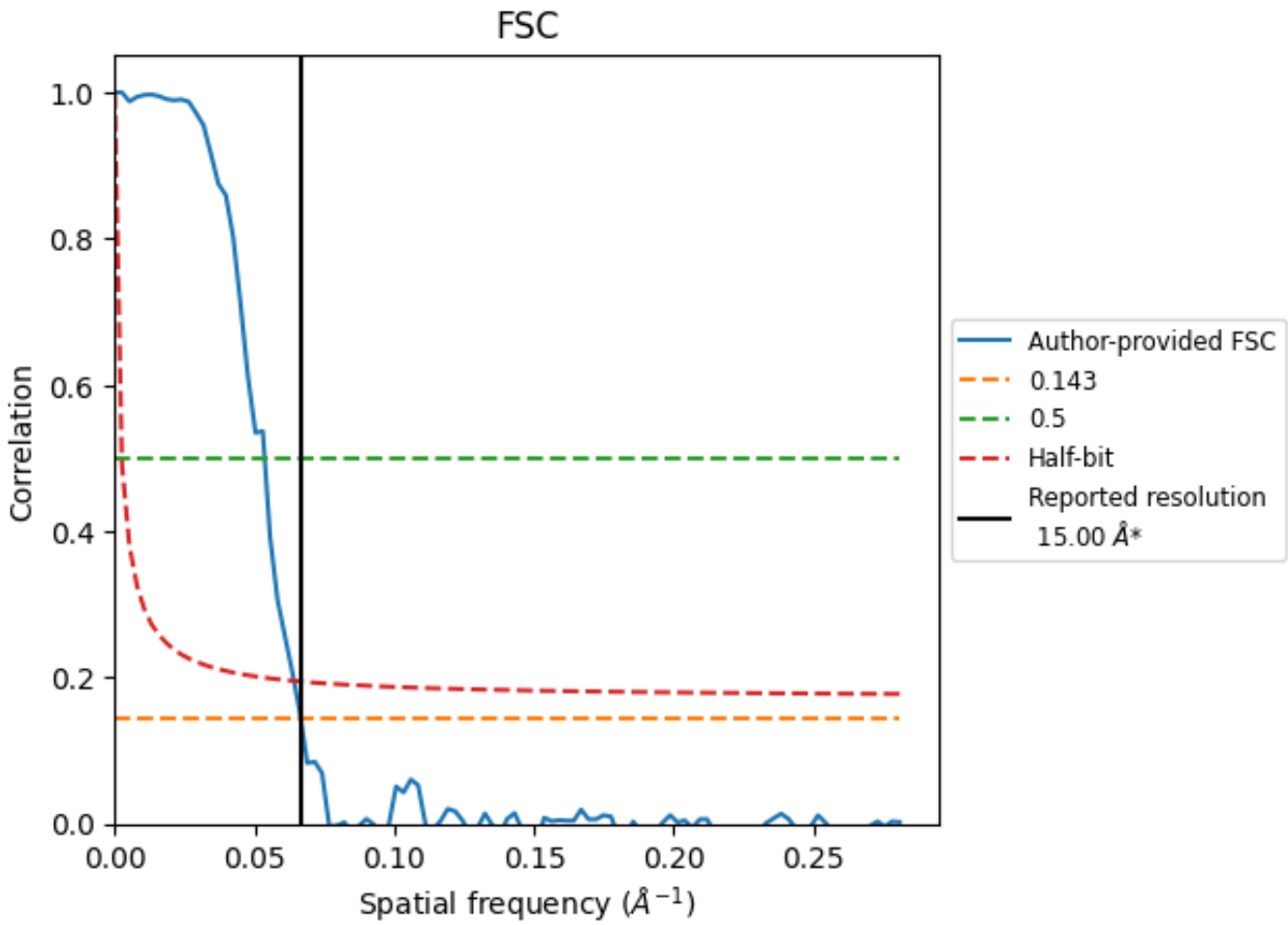


*Reported resolution corresponds to spatial frequency of 0.067 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.067 Å^{-1}

8.2 Resolution estimates (i)

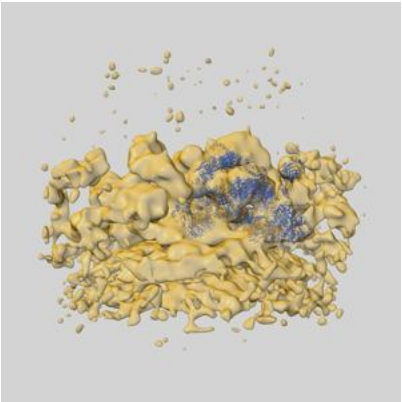
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	15.00	-	-
Author-provided FSC curve	15.02	18.62	15.58
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

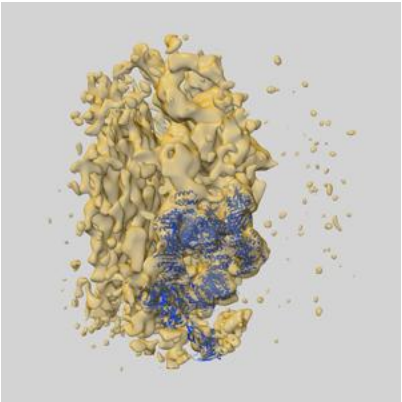
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3723 and PDB model 5NZU. Per-residue inclusion information can be found in section 3 on page 8.

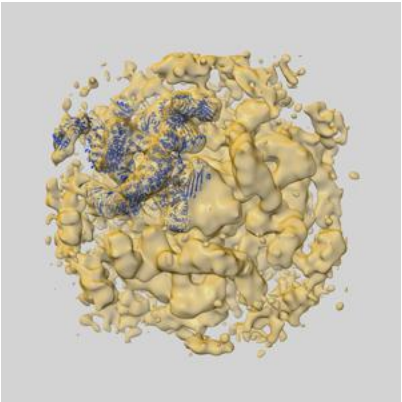
9.1 Map-model overlay (i)



X



Y



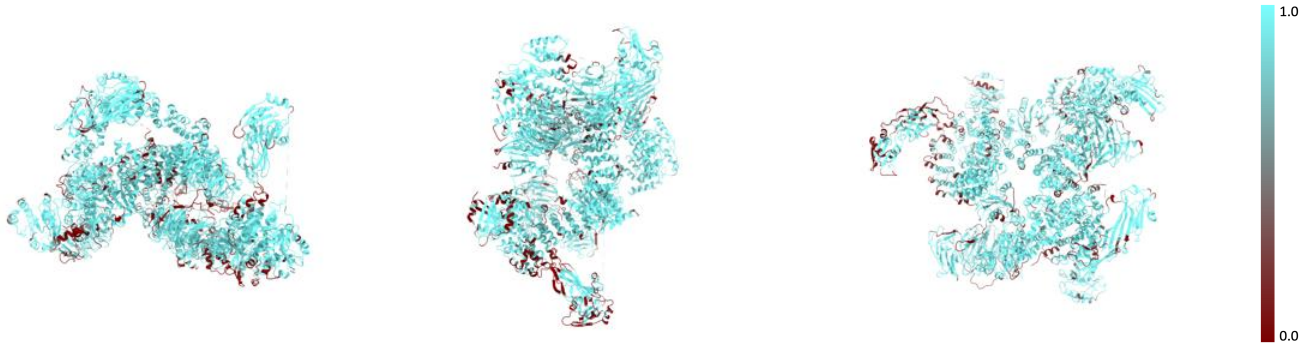
Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

This section was not generated.

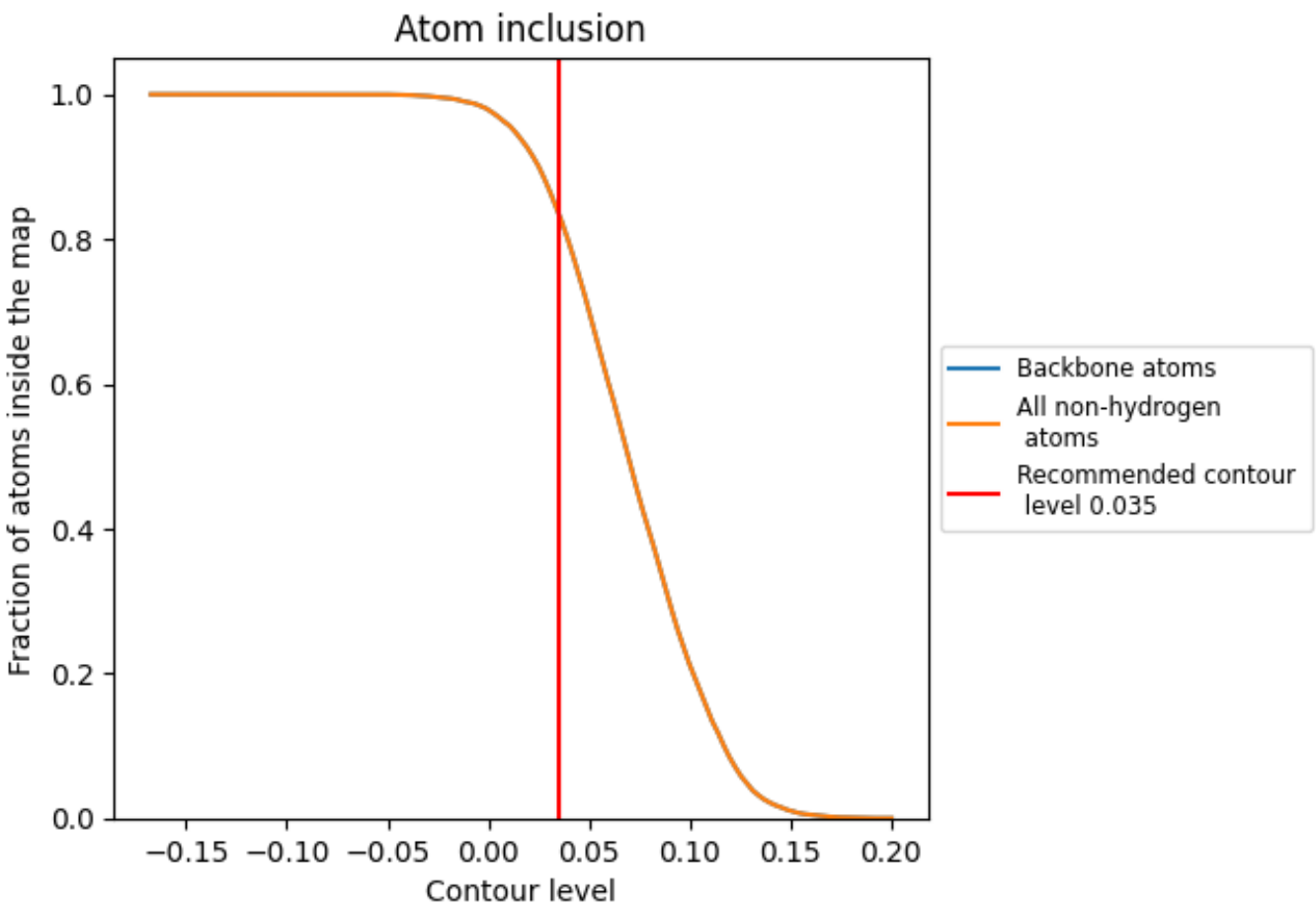
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8354
A	0.8868
B	0.8324
C	0.8959
D	0.8120
F	0.9181
G	0.7044
K	0.8781
L	0.8108
M	0.8945
R	0.7370
Z	0.8126