Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 05:12 pm GMT

PDB ID	:	5NZV
EMDB ID	:	EMD-3724
Title	:	The structure of the COPI coat linkage IV
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	:	17.30 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:

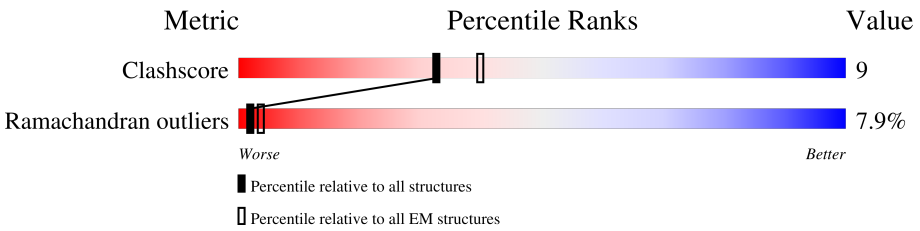
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 17.30 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	A	1262	7%, 73%, 14%, •, 11%
1	H	1262	39%, 73%, 14%, •, 11%
2	E	308	7%, 93%, •, 5%
2	O	308	19%, 93%, •, 5%
3	B	968	15%, 66%, 13%, • •, 17%
3	I	968	49%, 66%, 14%, •, 17%
4	C	905	18%, 77%, 14%, •, 7%
4	J	905	33%, 77%, 15%, •, 7%
5	D	511	13%, 78%, 5%, •, 16%

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Mol	Chain	Length	Quality of chain
5	N	511	14% 29% 5% 65%
6	F	181	6% 77% 8% 12%
6	M	181	27% 64% 20% 12%
6	P	181	30% 77% 8% 12%
6	R	181	49% 55% 27% 7% 12%
6	T	181	41% 64% 20% 12%
7	G	874	36% 75% 14% 9%
7	K	874	26% 52% 9% 36%
7	Q	874	25% 52% 10% 36%
8	L	177	31% 66% 12% 21%
8	S	177	31% 66% 12% 21%
8	U	177	29% 66% 12% 21%
8	Z	177	23% 66% 12% 21%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 39958 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	A	1126	4503	2252	1126	1125	0	0
1	H	1126	4503	2252	1126	1125	0	0

There are 76 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
A	1249	GLY	-	expression tag	UNP Q8CIE6
A	1250	SER	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
H	1225	LEU	-	expression tag	UNP Q8CIE6
H	1226	GLU	-	expression tag	UNP Q8CIE6
H	1227	VAL	-	expression tag	UNP Q8CIE6
H	1228	LEU	-	expression tag	UNP Q8CIE6
H	1229	PHE	-	expression tag	UNP Q8CIE6
H	1230	GLN	-	expression tag	UNP Q8CIE6
H	1231	GLY	-	expression tag	UNP Q8CIE6
H	1232	PRO	-	expression tag	UNP Q8CIE6
H	1233	SER	-	expression tag	UNP Q8CIE6
H	1234	ALA	-	expression tag	UNP Q8CIE6
H	1235	TRP	-	expression tag	UNP Q8CIE6
H	1236	SER	-	expression tag	UNP Q8CIE6
H	1237	HIS	-	expression tag	UNP Q8CIE6
H	1238	PRO	-	expression tag	UNP Q8CIE6
H	1239	GLN	-	expression tag	UNP Q8CIE6
H	1240	PHE	-	expression tag	UNP Q8CIE6
H	1241	GLU	-	expression tag	UNP Q8CIE6
H	1242	LYS	-	expression tag	UNP Q8CIE6
H	1243	GLY	-	expression tag	UNP Q8CIE6
H	1244	GLY	-	expression tag	UNP Q8CIE6
H	1245	GLY	-	expression tag	UNP Q8CIE6
H	1246	SER	-	expression tag	UNP Q8CIE6
H	1247	GLY	-	expression tag	UNP Q8CIE6
H	1248	GLY	-	expression tag	UNP Q8CIE6
H	1249	GLY	-	expression tag	UNP Q8CIE6
H	1250	SER	-	expression tag	UNP Q8CIE6
H	1251	GLY	-	expression tag	UNP Q8CIE6
H	1252	GLY	-	expression tag	UNP Q8CIE6
H	1253	SER	-	expression tag	UNP Q8CIE6
H	1254	ALA	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1255	TRP	-	expression tag	UNP Q8CIE6
H	1256	SER	-	expression tag	UNP Q8CIE6
H	1257	HIS	-	expression tag	UNP Q8CIE6
H	1258	PRO	-	expression tag	UNP Q8CIE6
H	1259	GLN	-	expression tag	UNP Q8CIE6
H	1260	PHE	-	expression tag	UNP Q8CIE6
H	1261	GLU	-	expression tag	UNP Q8CIE6
H	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	E	292	1169	584	292	293	0	0
2	O	292	1169	584	292	293	0	0

- Molecule 3 is a protein called Coatomer subunit beta.

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

There are 30 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
I	1	MET	-	initiating methionine	UNP Q9JIF7
I	2	HIS	-	expression tag	UNP Q9JIF7
I	3	HIS	-	expression tag	UNP Q9JIF7
I	4	HIS	-	expression tag	UNP Q9JIF7
I	5	HIS	-	expression tag	UNP Q9JIF7
I	6	HIS	-	expression tag	UNP Q9JIF7
I	7	HIS	-	expression tag	UNP Q9JIF7
I	8	GLU	-	expression tag	UNP Q9JIF7
I	9	ASN	-	expression tag	UNP Q9JIF7
I	10	LEU	-	expression tag	UNP Q9JIF7
I	11	TYR	-	expression tag	UNP Q9JIF7
I	12	PHE	-	expression tag	UNP Q9JIF7
I	13	GLN	-	expression tag	UNP Q9JIF7
I	14	GLY	-	expression tag	UNP Q9JIF7
I	15	HIS	-	expression tag	UNP Q9JIF7

- Molecule 4 is a protein called Coatomer subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	C	843	3371	1686	843	842	0	0
4	J	843	3371	1686	843	842	0	0

- Molecule 5 is a protein called Coatomer subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	D	427	1707	854	427	426	0	0
5	N	177	706	354	177	175	0	0

- Molecule 6 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	159	635	318	159	158	0	0
6	R	159	635	318	159	158	0	0
6	M	159	635	318	159	158	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	P	159	635	318	159	158	0	0
6	T	159	635	318	159	158	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	798	3190	1596	798	796	0	0
7	K	560	2239	1120	560	559	0	0
7	Q	560	2239	1120	560	559	0	0

- Molecule 8 is a protein called Coatomer subunit zeta-1.

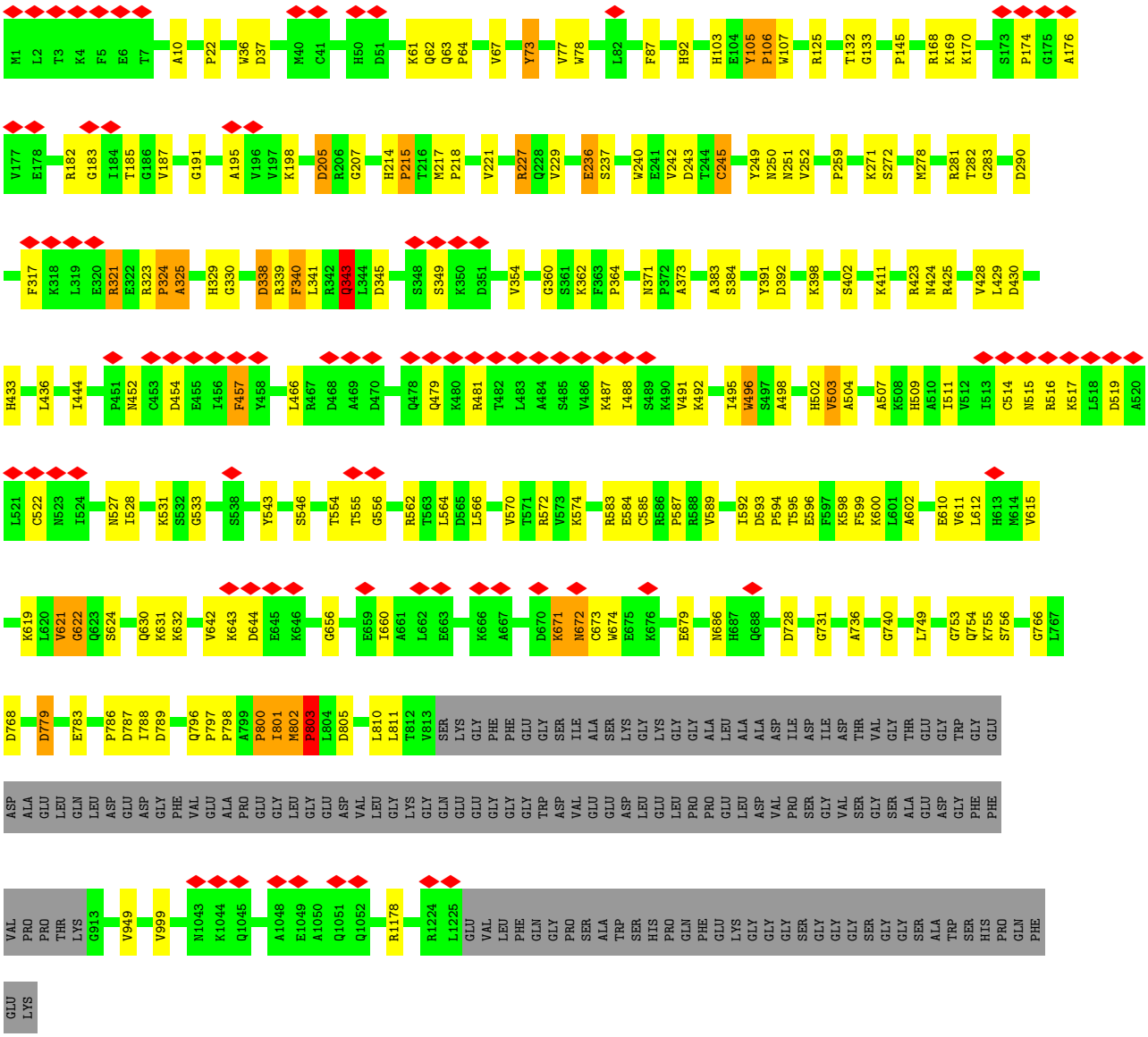
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	Z	139	555	278	139	138	0	0
8	L	139	555	278	139	138	0	0
8	U	139	555	278	139	138	0	0
8	S	139	555	278	139	138	0	0

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.

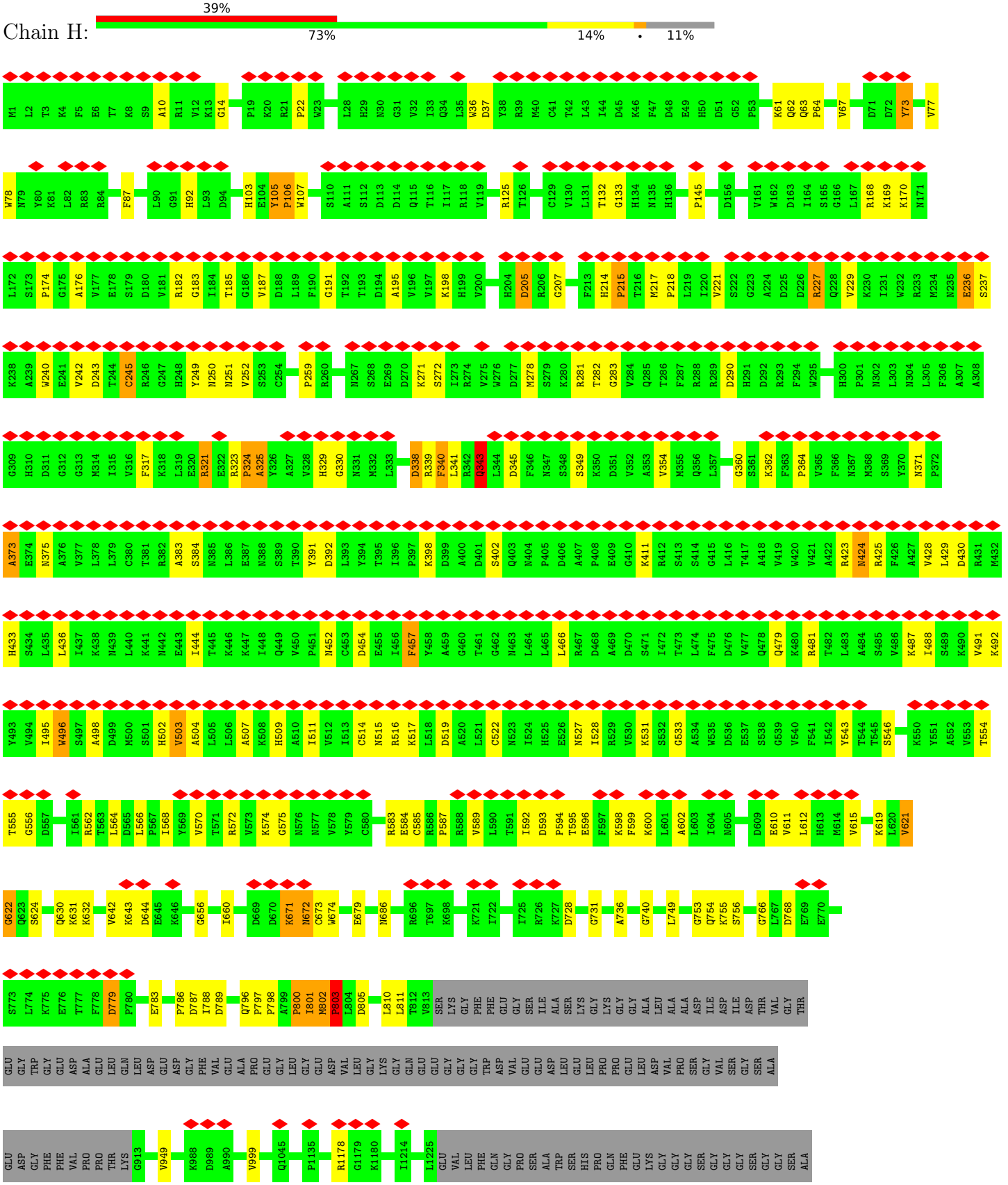
- Molecule 1: Coatomer subunit alpha

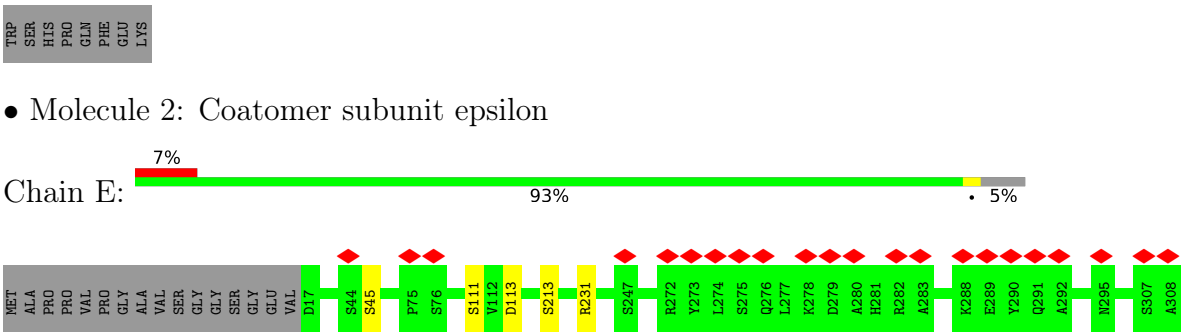
Chain A: 7% 73% 14% 11%

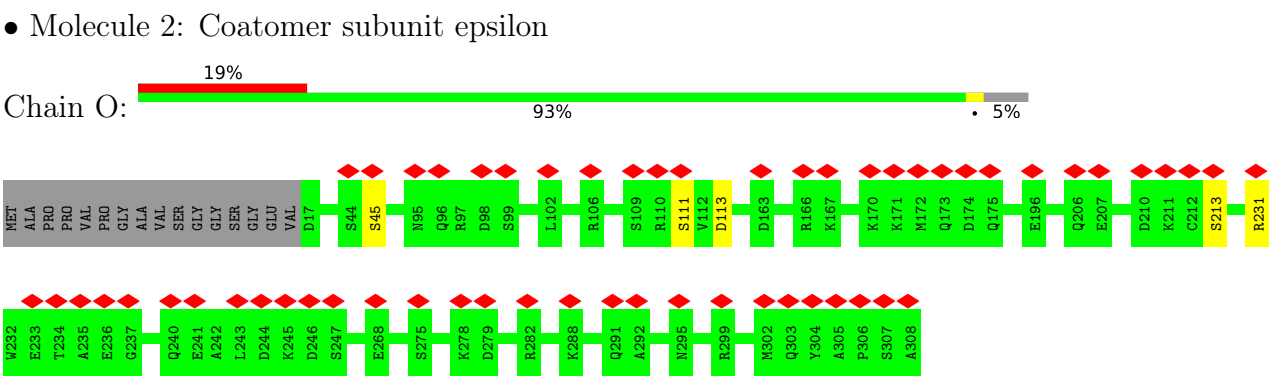


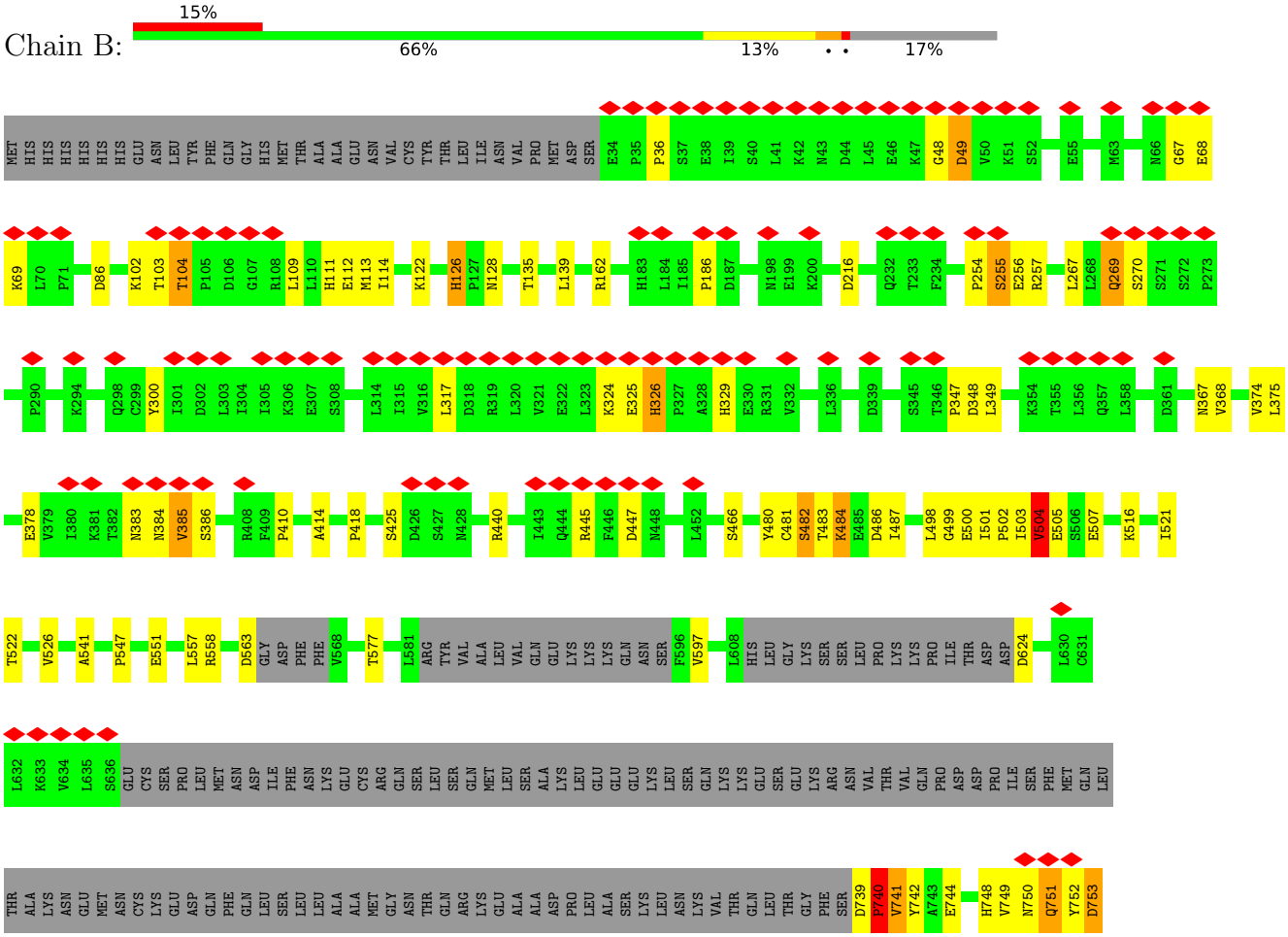
- Molecule 1: Coatomer subunit alpha

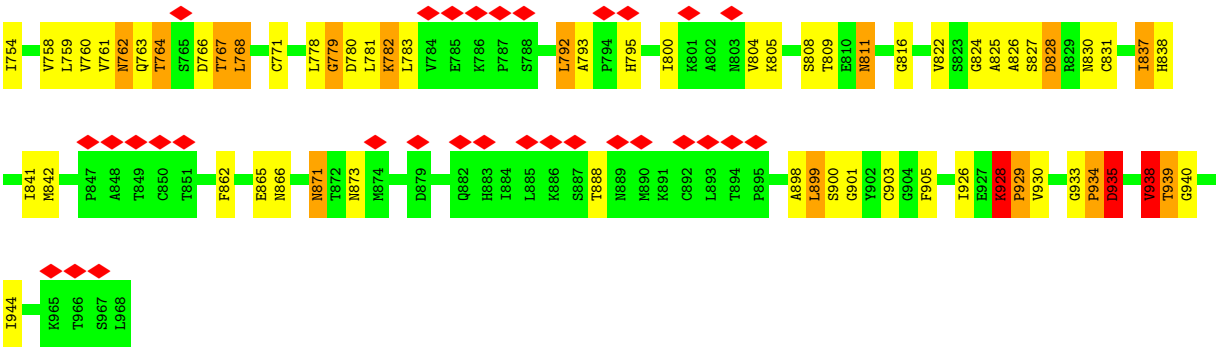
Chain H:




TRP SER HIS PRO GLN PHE GLU LYS
• Molecule 2: Coatomer subunit epsilon
Chain E:
7%
93%
• 5%
MET ALA PRO PRO VAL PRO GLY ALA VAL SER GLY GLY SER GLY GLU VAL D17 S44 S45 P75 S76 S111 V112 D113 S213 R231 S247 R272 Y273 L274 S275 Q276 L277 K278 D279 A280 H281 R282 A283 K288 E289 Y290 Q291 A292 N295 S307 A308

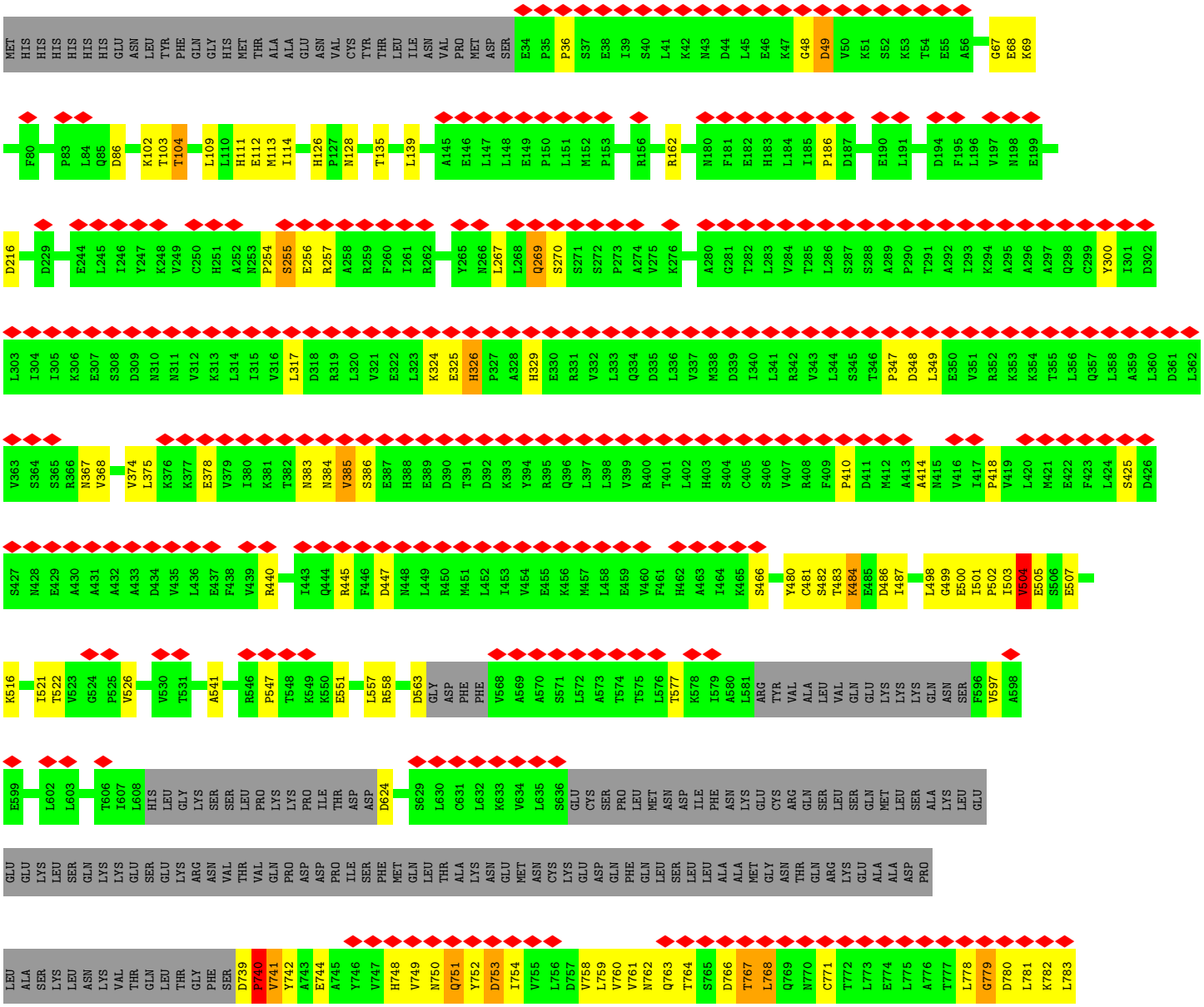

• Molecule 2: Coatomer subunit epsilon
Chain O:
19%
93%
• 5%
MET ALA PRO PRO VAL PRO GLY ALA VAL SER GLY GLY SER GLY GLU VAL D17 S44 S45 N95 Q96 R97 D98 S99 L102 R106 S109 R110 S111 V112 D113 D163 R166 K167 K170 K171 M172 Q173 D174 Q175 E196 Q206 E207 D210 K211 C212 S213 R231
W232 E233 T234 A235 E236 G237 Q240 E241 A242 L243 D244 K245 D246 S247 E268 S275 K278 D279 R282 K288 Q291 A292 N295 R299 M302 Q303 Y304 A305 P306 S307 A308

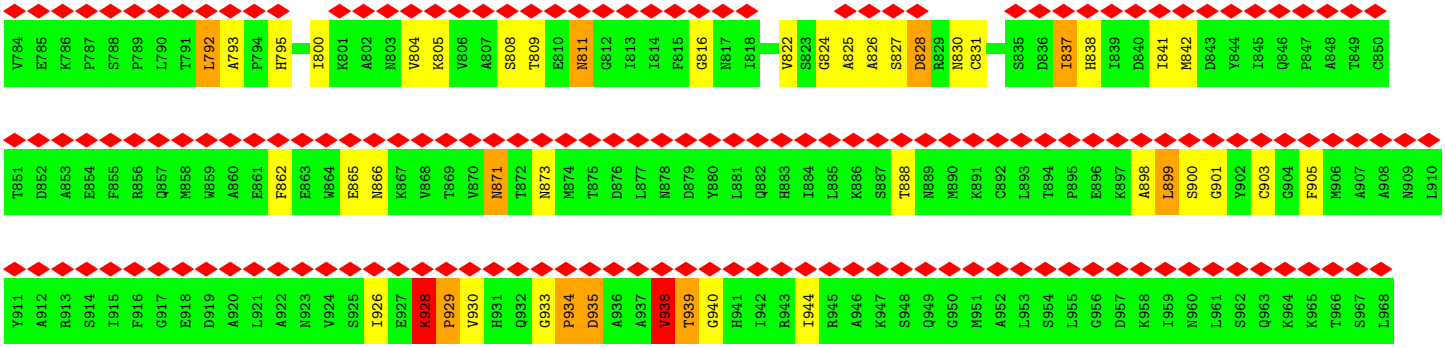

• Molecule 3: Coatomer subunit beta
Chain B:
15%
66%
13%
• •
17%
MET HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY HIS MET THR ALA ALA GLU ASN VAL CYS TYR THR LEU ILE ASN VAL PRO MET ASP SER E34 P35 P36 S37 E38 I39 S40 L41 K42 N43 D44 L45 E46 K47 G48 D49 V50 K51 S52 E55 M63 N66 G67 E68
K69 L70 P71 D86 K102 T103 T104 P105 D106 G107 R108 L109 L110 H111 E112 M113 I114 K122 H126 P127 N128 T135 L139 R162 H183 L184 I185 P186 D187 N198 E199 K200 D216 Q232 T233 F234 P254 S255 E256 R257 L267 L268 Q269 S270 S271 S272 P273
P290 K294 Q298 C299 Y300 I301 D302 L303 I304 I305 K306 E307 S308 L314 I315 V316 L317 D318 R319 L320 V321 E322 L323 K324 E325 H326 P327 A328 H329 E330 R331 V332 L336 D339 S345 T346 P347 D348 L349 K354 T355 L356 Q357 L358 D361 N367 V368 V374 L375
E378 V379 I380 K381 T382 N383 N384 V385 S386 R408 F409 P410 A414 P418 S425 D426 S427 N428 R440 I443 Q444 R445 F446 D447 N448 L452 S466 Y480 C481 S482 T483 K484 E485 D486 I487 L498 G499 E500 I501 P502 I503 W504 E505 S506 E507 K516 I521
T522 V526 A541 P547 E551 L557 R558 D563 GLY ASP PHE PHE V568 T577 L581 ARG TYR VAL ALA LEU VAL GLN GLU LYS LYS LYS GLN ASN SER F596 V597 L608 HIS LEU GLY LYS SER SER LEU PRO LYS LYS PRO ILE THR ASP ASP D624 L630 C631
L632 K633 V634 L635 S636 GLU CYS SER PRO LEU MET ASN ASP ILE PHE ASN LYS GLU CYS ARG GLN SER LEU SER GLN MET LEU SER ALA LYS LEU GLU GLU GLU GLU LYS LEU SER SER GLN LYS LYS GLU SER GLU LYS ARG ASN VAL THR VAL GLN PRO ASP ASP PRO ILE SER PHE MET GLN LEU
THR ALA LYS ASN GLU MET ASN CYS LYS GLU ASP GLN PHE GLN LEU SER LEU LEU ALA ALA MET GLY ASN THR GLN ARG LYS GLU ALA ALA ASP PRO LEU ALA SER LYS LYS LEU ASN LYS VAL THR GLN LEU THR GLY PHE SER D739 P740 V741 Y742 A743 E744 H748 V749 N750 Q751 Y752 D753



- Molecule 3: Coatomer subunit beta

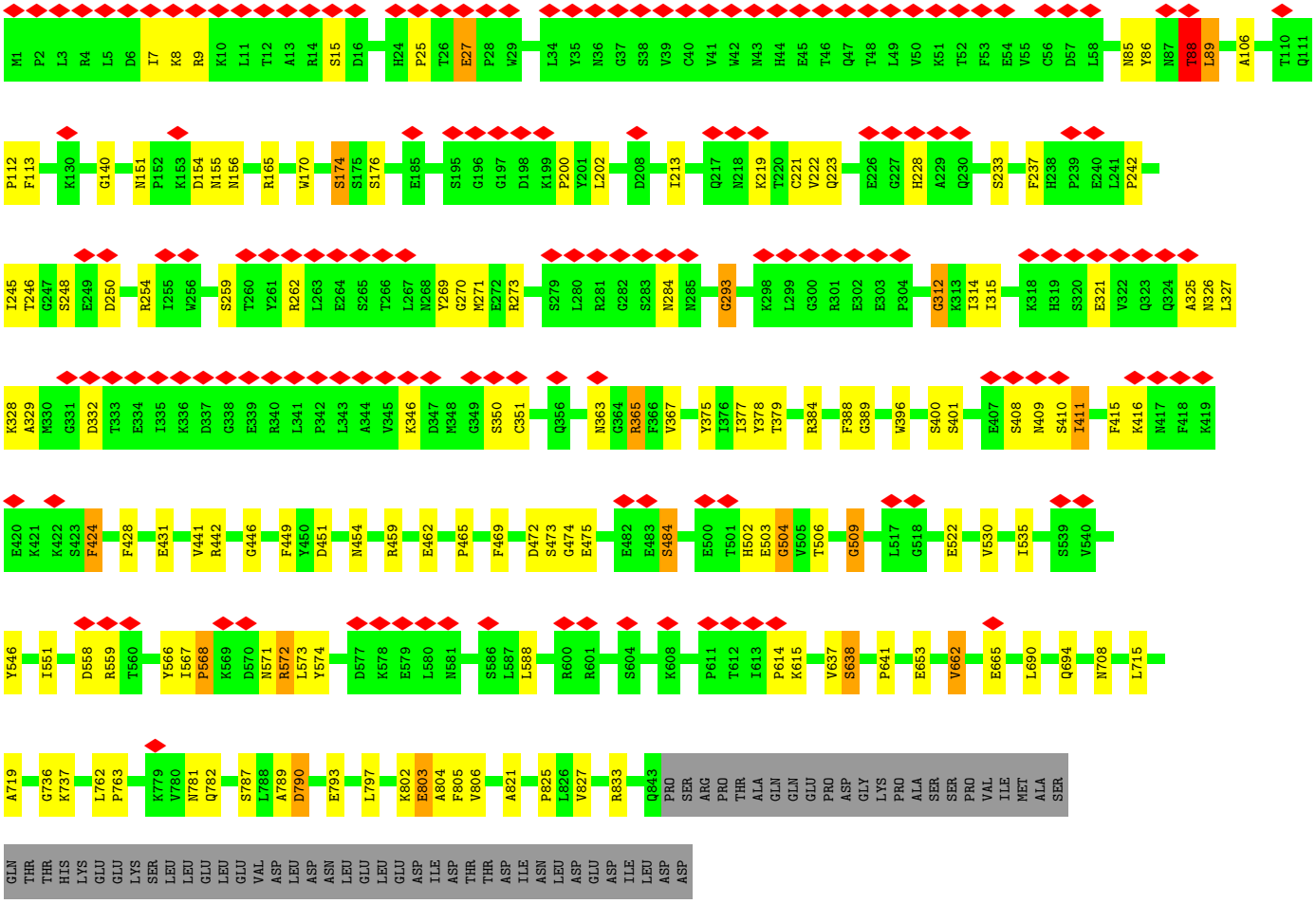
Chain I:





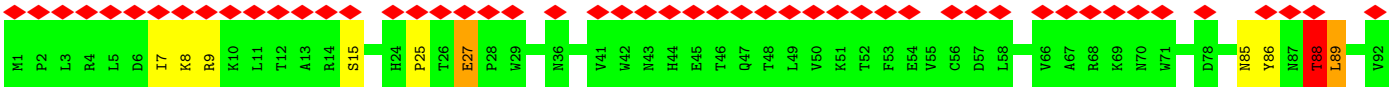
- Molecule 4: Coatomer subunit beta'

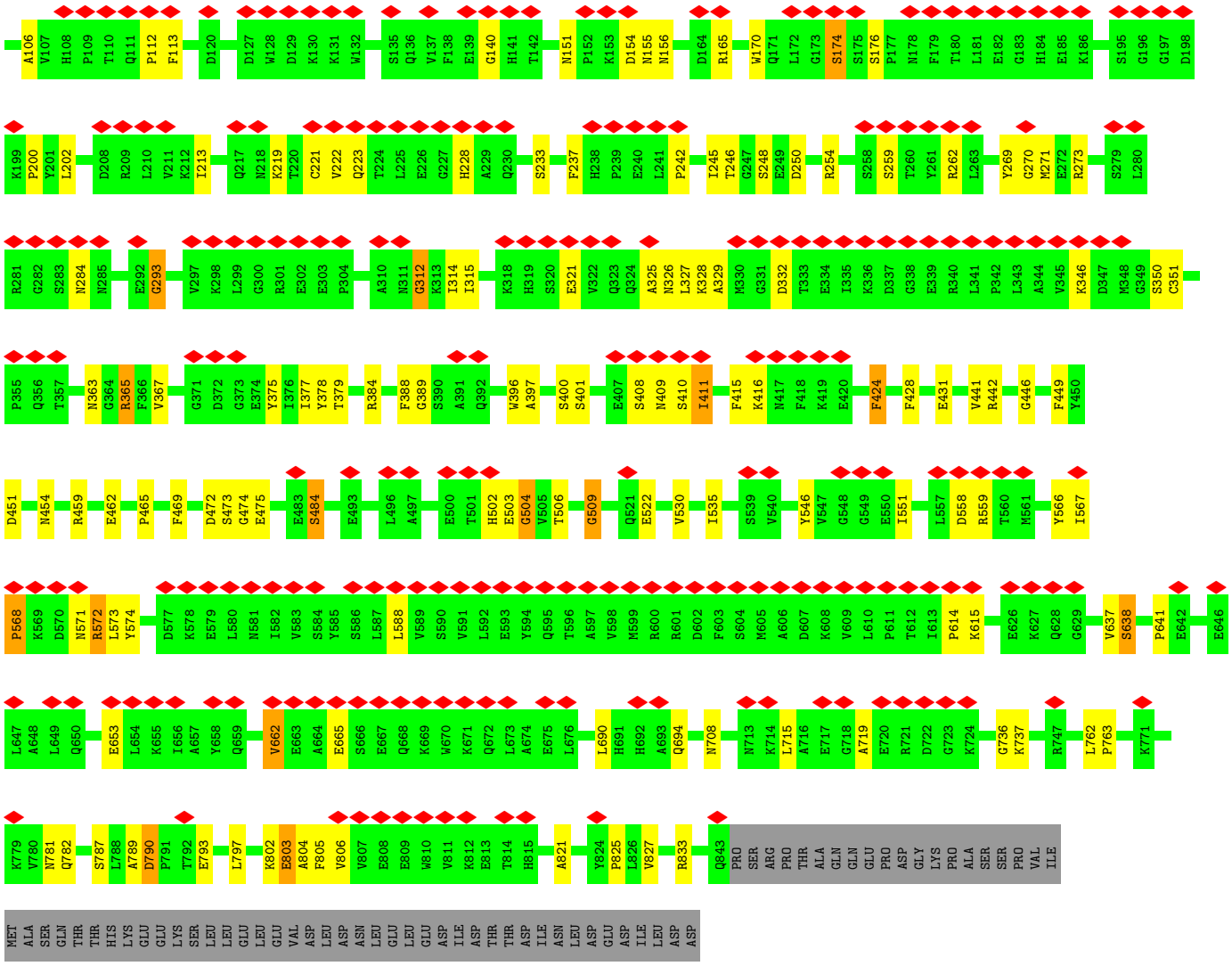
Chain C:



- Molecule 4: Coatomer subunit beta'

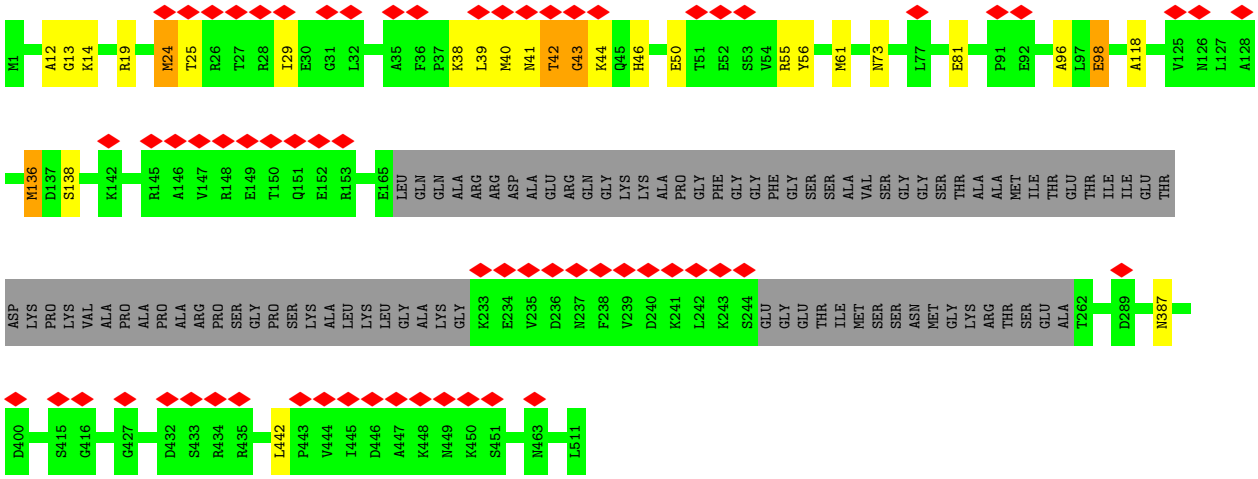
Chain J:





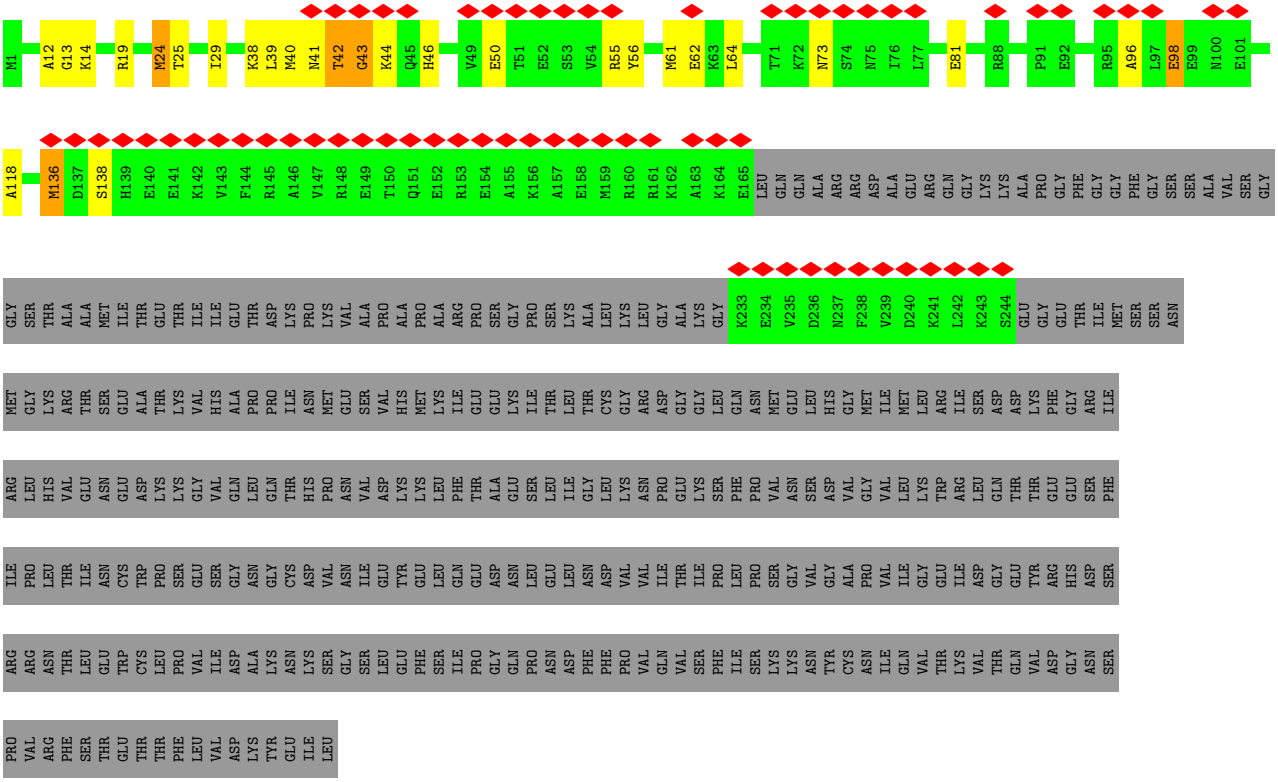
- Molecule 5: Coatomer subunit delta

Chain D:



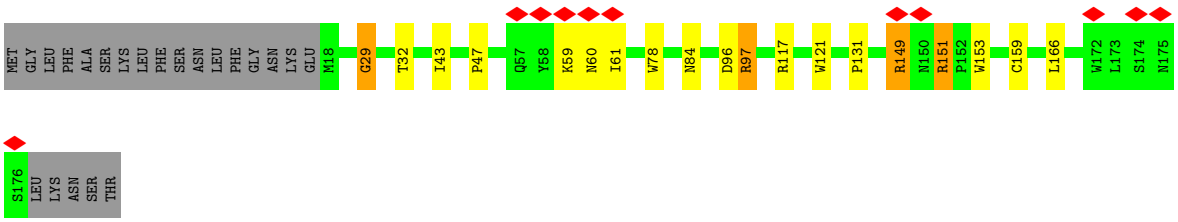
- Molecule 5: Coatomer subunit delta

Chain N:



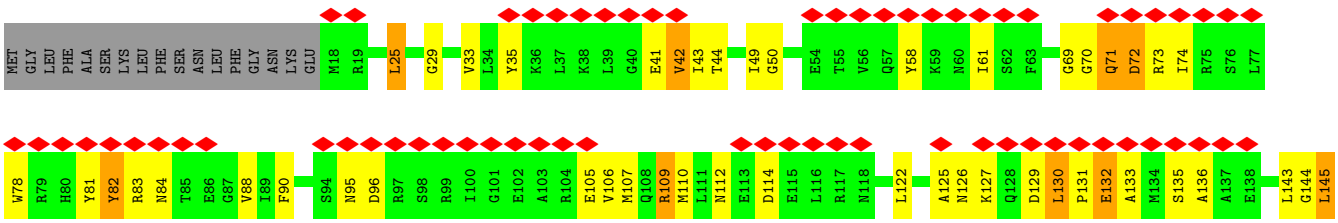
- Molecule 6: ADP-ribosylation factor 1

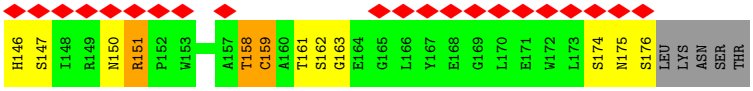
Chain F:



- Molecule 6: ADP-ribosylation factor 1

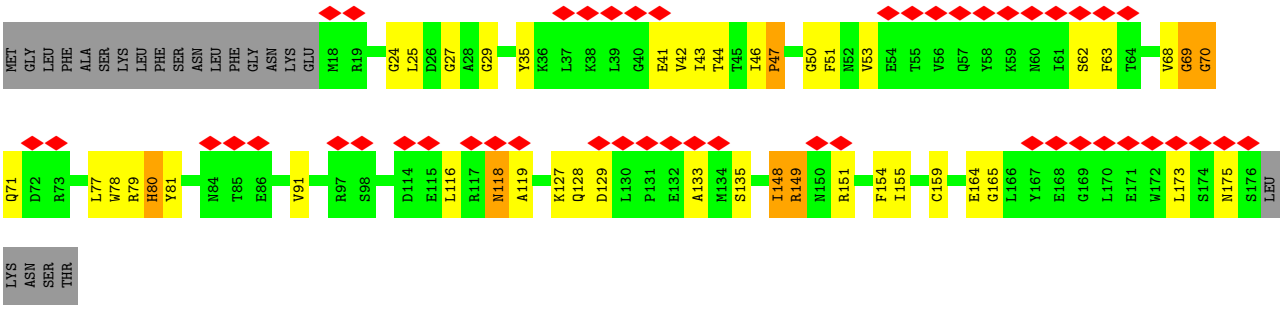
Chain R:





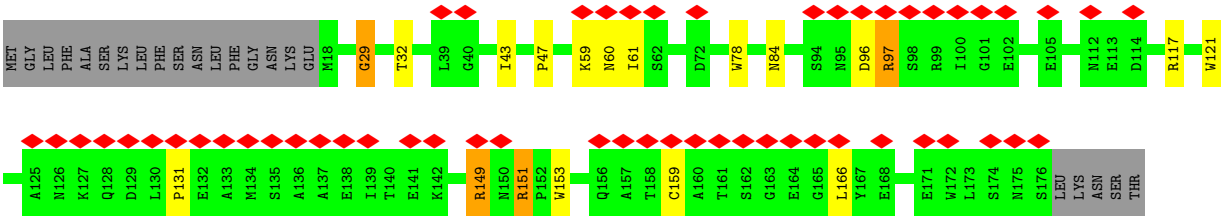
- Molecule 6: ADP-ribosylation factor 1

Chain M:



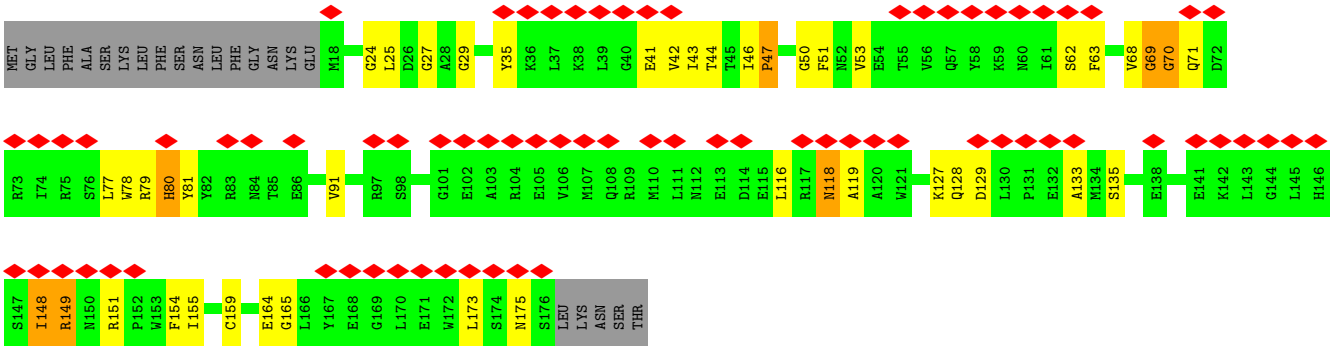
- Molecule 6: ADP-ribosylation factor 1

Chain P:



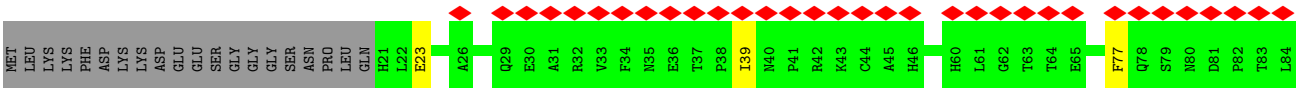
- Molecule 6: ADP-ribosylation factor 1

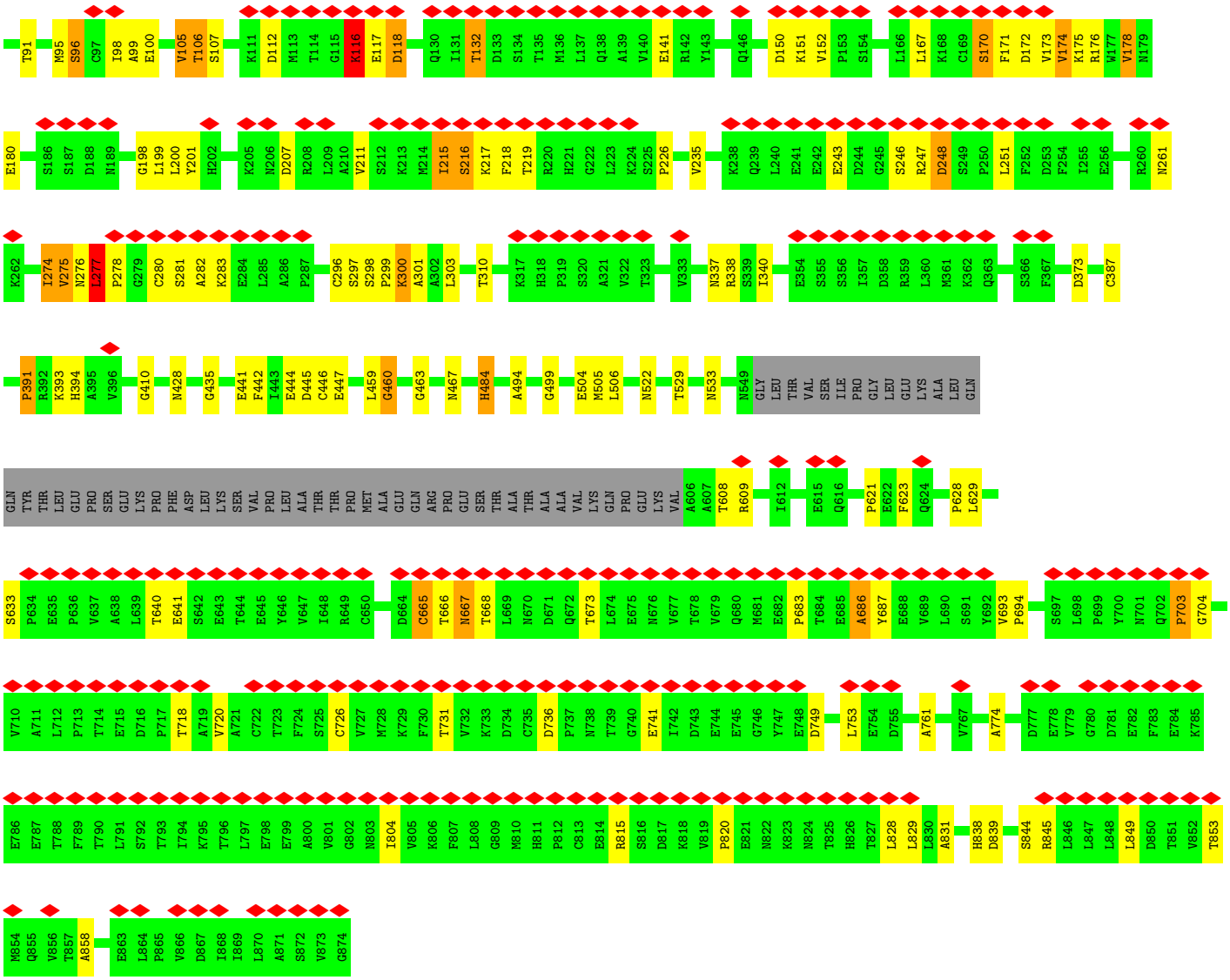
Chain T:



- Molecule 7: Coatomer subunit gamma-1

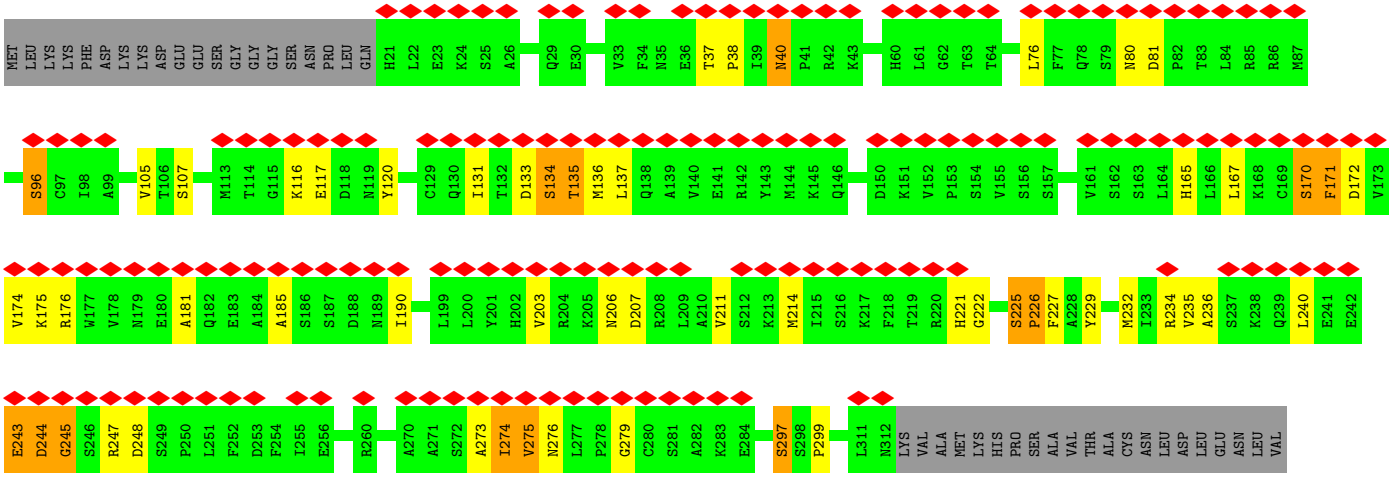
Chain G:

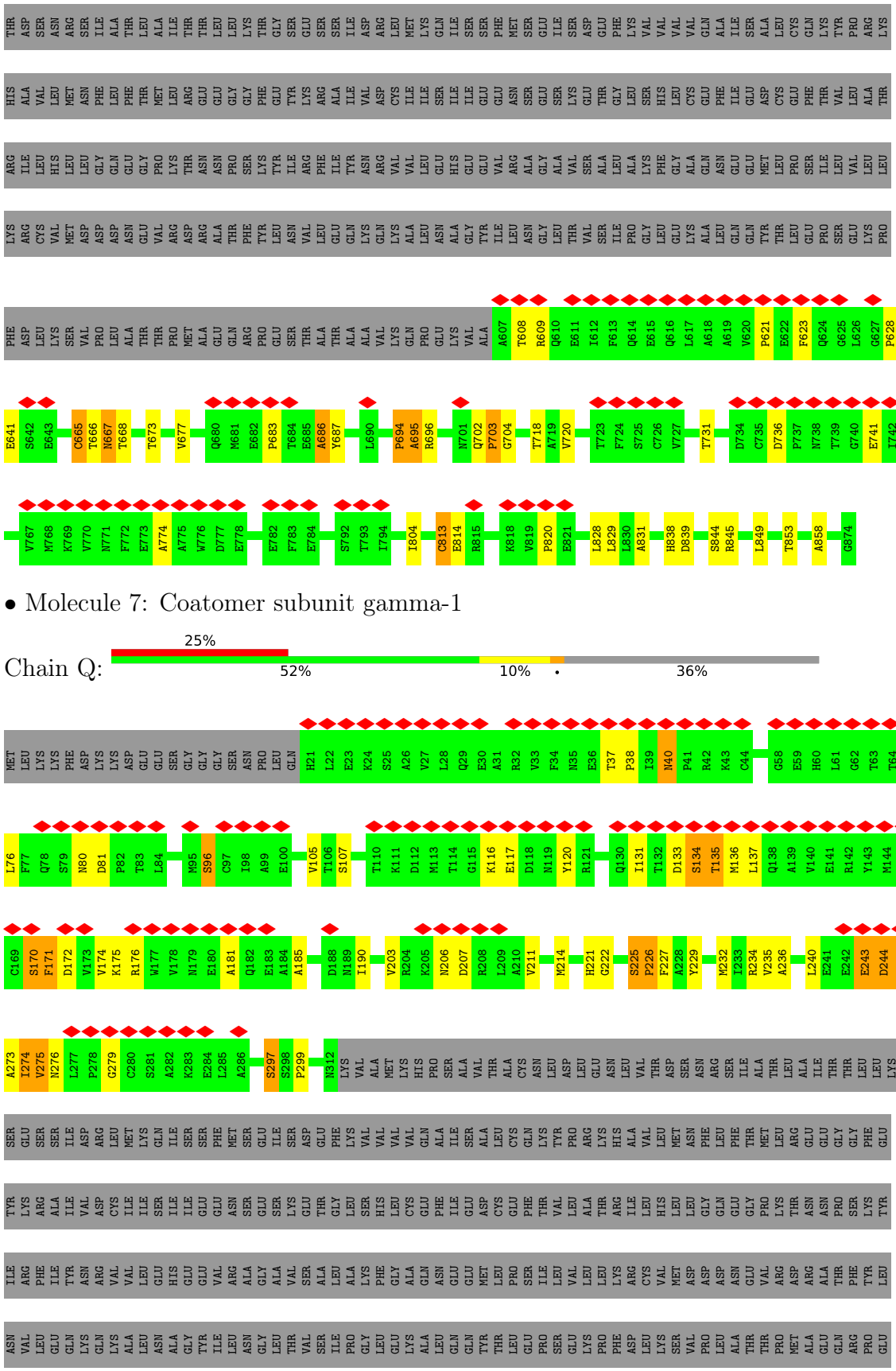




- Molecule 7: Coatomer subunit gamma-1

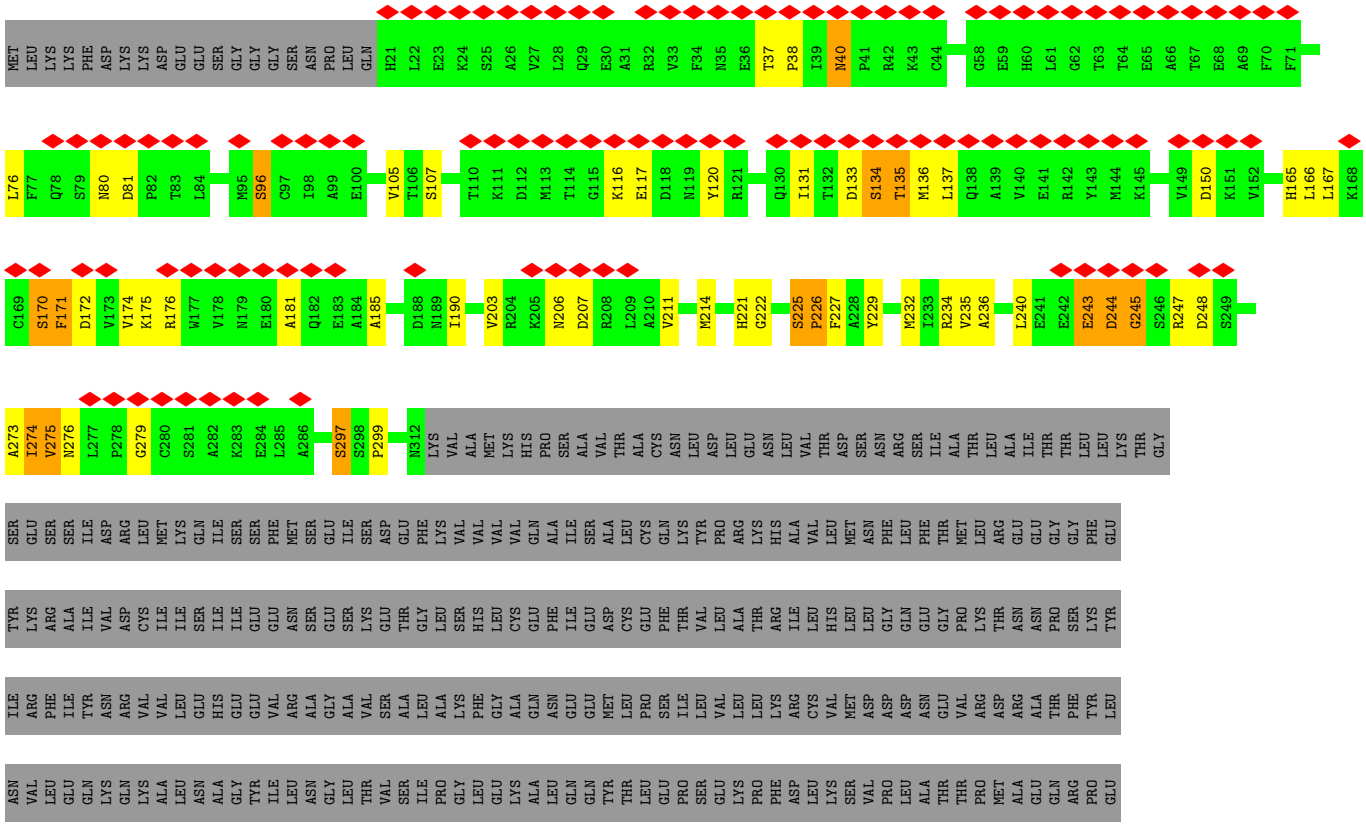
Chain K:

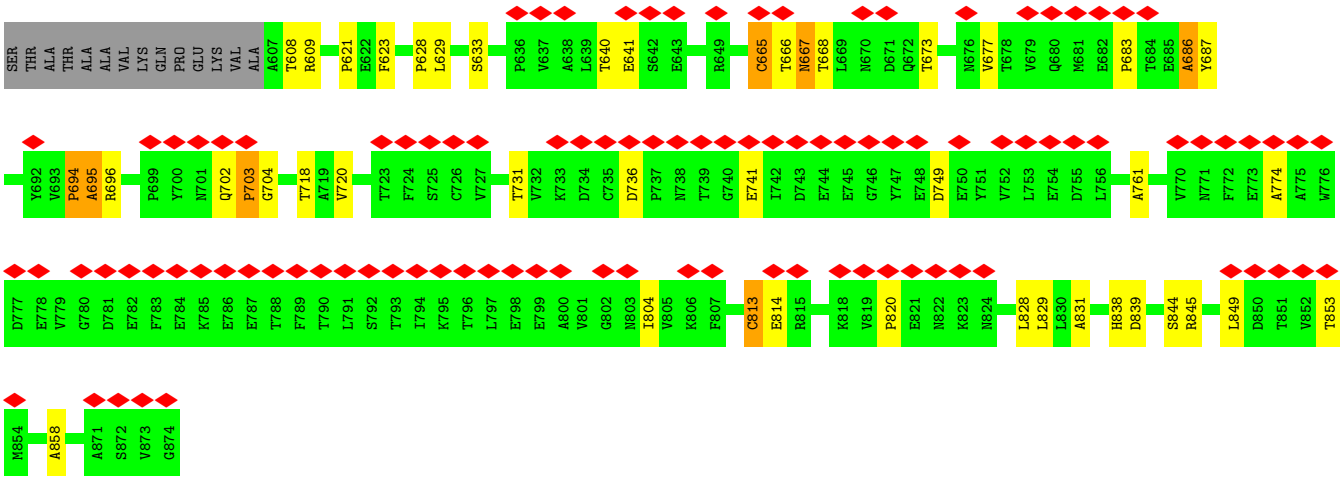




- Molecule 7: Coatomer subunit gamma-1

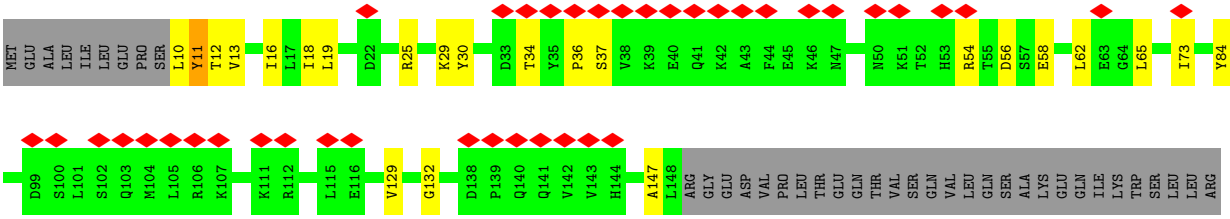
Chain Q:





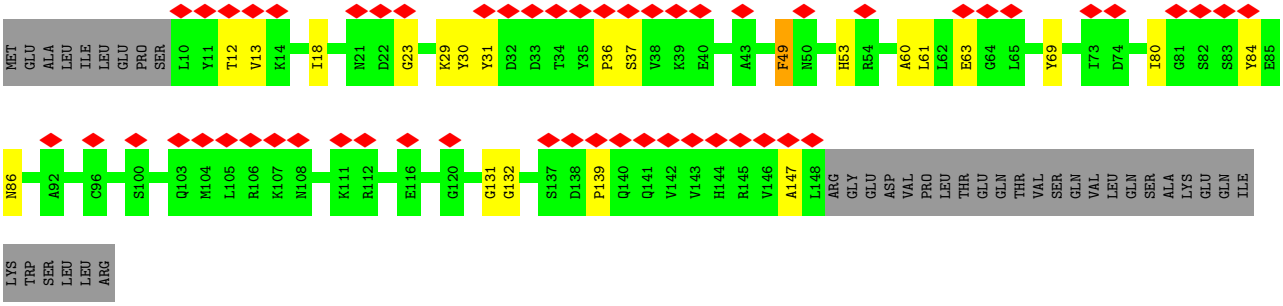
- Molecule 8: Coatomer subunit zeta-1

Chain Z:



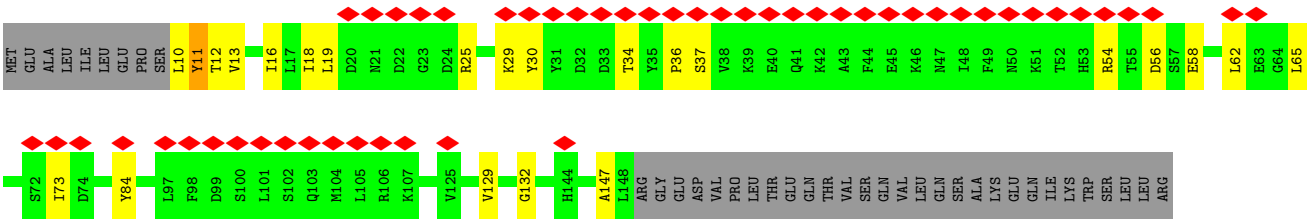
- Molecule 8: Coatomer subunit zeta-1

Chain L:



- Molecule 8: Coatomer subunit zeta-1

Chain U:



• Molecule 8: Coatomer subunit zeta-1

Chain S: 31% 66% 12% • 21%

MET GLU ALA LEU ILE LEU GLU PRO SER L10 Y11 T12 V13 I18 N21 D22 G23 K29 Y30 Y31 D32 D33 T34 Y35 P36 S37 V38 K39 E40 Q41 K42 A43 F44 E45 K46 F49 N50 K51 T52 H53 R54 E58 I59 A60 L61 L62 E63 Y69 S72 I73 D74 I80

Y84 E85 N86 C96 D99 S100 L101 S102 Q103 M104 L105 R106 K107 N108 V109 E110 K111 R112 A113 L114 L115 E116 G131 G132 D138 P139 Q140 Q141 V142 V143 H144 R145 V146 A147 L148 ARG GLY GLU ASP VAL PRO LEU THR GLU GLN THR VAL SER GLN VAL LEU GLN SER ALA LYS

GLU GLN ILE LYS TRP SER LEU LEU ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	1640	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	0.190	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	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	A	1.41	16/4501 (0.4%)	1.59	75/5623 (1.3%)
1	H	1.41	16/4501 (0.4%)	1.59	77/5623 (1.4%)
2	E	0.91	0/1168	0.63	0/1457
2	O	0.91	0/1168	0.63	0/1457
3	B	1.71	20/3193 (0.6%)	1.55	46/3983 (1.2%)
3	I	1.71	20/3193 (0.6%)	1.55	45/3983 (1.1%)
4	C	1.76	22/3370 (0.7%)	1.70	59/4211 (1.4%)
4	J	1.76	22/3370 (0.7%)	1.70	60/4211 (1.4%)
5	D	1.28	3/1704 (0.2%)	1.24	10/2124 (0.5%)
5	N	1.67	3/704 (0.4%)	1.65	10/877 (1.1%)
6	F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
6	M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
6	P	1.57	1/634 (0.2%)	1.71	9/791 (1.1%)
6	R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
6	T	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
7	G	1.62	11/3188 (0.3%)	1.59	46/3982 (1.2%)
7	K	1.72	9/2237 (0.4%)	1.69	43/2793 (1.5%)
7	Q	1.72	9/2237 (0.4%)	1.69	44/2793 (1.6%)
8	L	2.05	3/554 (0.5%)	1.72	7/691 (1.0%)
8	S	2.05	3/554 (0.5%)	1.72	8/691 (1.2%)
8	U	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
8	Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
All	All	1.61	183/39920 (0.5%)	1.58	603/49836 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	3
3	I	0	3
All	All	0	6

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	940	GLY	N-CA	-7.79	1.34	1.46
3	B	940	GLY	N-CA	-7.78	1.34	1.46
6	R	29	GLY	CA-C	-7.66	1.39	1.51
6	R	35	TYR	CA-C	-7.33	1.33	1.52
1	A	191	GLY	CA-C	-7.05	1.40	1.51
1	H	191	GLY	CA-C	-7.01	1.40	1.51
4	J	572	ARG	CA-C	-6.61	1.35	1.52
4	C	572	ARG	CA-C	-6.60	1.35	1.52
1	H	594	PRO	CA-C	-6.59	1.39	1.52
3	I	418	PRO	CA-C	-6.58	1.39	1.52
3	B	418	PRO	CA-C	-6.57	1.39	1.52
7	G	215	ILE	CA-C	-6.57	1.35	1.52
7	Q	235	VAL	N-CA	-6.57	1.33	1.46
7	K	235	VAL	N-CA	-6.56	1.33	1.46
1	A	594	PRO	CA-C	-6.55	1.39	1.52
1	A	612	LEU	N-CA	-6.46	1.33	1.46
1	H	612	LEU	N-CA	-6.43	1.33	1.46
5	D	55	ARG	CA-C	-6.41	1.36	1.52
1	H	766	GLY	CA-C	-6.40	1.41	1.51
5	N	55	ARG	CA-C	-6.39	1.36	1.52
1	A	766	GLY	CA-C	-6.39	1.41	1.51
7	Q	839	ASP	CA-C	-6.34	1.36	1.52
6	R	109	ARG	CA-C	-6.32	1.36	1.52
7	K	839	ASP	CA-C	-6.32	1.36	1.52
7	G	839	ASP	CA-C	-6.32	1.36	1.52
7	Q	211	VAL	CA-C	-6.29	1.36	1.52
7	K	211	VAL	CA-C	-6.27	1.36	1.52
8	Z	19	LEU	N-CA	-6.24	1.33	1.46
7	Q	214	MET	CA-C	-6.23	1.36	1.52
7	K	214	MET	CA-C	-6.21	1.36	1.52
8	U	19	LEU	N-CA	-6.19	1.33	1.46
4	C	293	GLY	CA-C	-6.16	1.42	1.51
4	J	293	GLY	CA-C	-6.14	1.42	1.51
4	C	378	TYR	CA-C	-6.12	1.37	1.52
4	C	416	LYS	CA-C	-6.09	1.37	1.52
4	J	378	TYR	CA-C	-6.09	1.37	1.52
4	J	416	LYS	CA-C	-6.09	1.37	1.52
6	M	29	GLY	CA-C	-6.07	1.42	1.51
6	T	29	GLY	CA-C	-6.04	1.42	1.51
6	T	70	GLY	CA-C	-6.04	1.42	1.51
6	M	70	GLY	CA-C	-6.03	1.42	1.51
8	S	23	GLY	CA-C	-6.02	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	23	GLY	CA-C	-6.02	1.42	1.51
6	M	47	PRO	CA-C	-6.02	1.40	1.52
1	A	596	GLU	N-CA	-6.01	1.34	1.46
6	T	47	PRO	CA-C	-6.01	1.40	1.52
7	G	774	ALA	N-CA	-6.01	1.34	1.46
1	H	596	GLU	N-CA	-5.99	1.34	1.46
7	Q	774	ALA	N-CA	-5.97	1.34	1.46
3	I	762	ASN	CA-C	-5.96	1.37	1.52
7	K	774	ALA	N-CA	-5.96	1.34	1.46
3	B	762	ASN	CA-C	-5.96	1.37	1.52
4	J	641	PRO	CA-C	-5.94	1.41	1.52
4	C	641	PRO	CA-C	-5.90	1.41	1.52
4	C	384	ARG	CA-C	-5.88	1.37	1.52
4	J	384	ARG	CA-C	-5.86	1.37	1.52
7	Q	105	VAL	N-CA	-5.82	1.34	1.46
3	I	940	GLY	CA-C	-5.77	1.42	1.51
7	K	105	VAL	N-CA	-5.76	1.34	1.46
3	I	126	HIS	CA-C	-5.76	1.38	1.52
3	B	126	HIS	CA-C	-5.75	1.38	1.52
3	B	940	GLY	CA-C	-5.73	1.42	1.51
6	F	29	GLY	N-CA	-5.71	1.37	1.46
4	J	377	ILE	CA-C	-5.69	1.38	1.52
4	C	377	ILE	CA-C	-5.67	1.38	1.52
6	P	29	GLY	N-CA	-5.62	1.37	1.46
4	C	245	ILE	N-CA	-5.61	1.35	1.46
1	A	660	ILE	CA-C	-5.60	1.38	1.52
4	J	245	ILE	N-CA	-5.59	1.35	1.46
1	H	660	ILE	CA-C	-5.59	1.38	1.52
7	G	235	VAL	N-CA	-5.57	1.35	1.46
4	J	568	PRO	CA-C	-5.53	1.41	1.52
4	C	568	PRO	CA-C	-5.52	1.41	1.52
3	B	378	GLU	CA-C	-5.52	1.38	1.52
1	A	679	GLU	CA-C	-5.52	1.38	1.52
8	Z	65	LEU	N-CA	-5.51	1.35	1.46
3	I	378	GLU	CA-C	-5.51	1.38	1.52
1	A	360	GLY	CA-C	-5.51	1.43	1.51
1	H	679	GLU	CA-C	-5.51	1.38	1.52
1	H	360	GLY	CA-C	-5.50	1.43	1.51
7	G	442	PHE	CA-C	-5.50	1.38	1.52
8	U	65	LEU	N-CA	-5.50	1.35	1.46
7	K	165	HIS	CA-C	-5.49	1.38	1.52
3	B	753	ASP	N-CA	-5.47	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	165	HIS	CA-C	-5.46	1.38	1.52
7	Q	203	VAL	N-CA	-5.46	1.35	1.46
7	K	203	VAL	N-CA	-5.46	1.35	1.46
4	C	449	PHE	CA-C	-5.45	1.38	1.52
1	H	600	LYS	CA-C	-5.45	1.38	1.52
1	A	600	LYS	CA-C	-5.44	1.38	1.52
3	I	753	ASP	N-CA	-5.43	1.35	1.46
1	H	599	PHE	N-CA	-5.42	1.35	1.46
4	J	449	PHE	CA-C	-5.42	1.38	1.52
3	I	749	VAL	CA-C	-5.41	1.38	1.52
7	G	112	ASP	CA-C	-5.41	1.38	1.52
1	H	595	THR	N-CA	-5.41	1.35	1.46
3	B	749	VAL	CA-C	-5.40	1.39	1.52
7	G	180	GLU	N-CA	-5.40	1.35	1.46
5	N	56	TYR	CA-C	-5.40	1.39	1.52
1	A	599	PHE	N-CA	-5.38	1.35	1.46
1	A	612	LEU	CA-C	-5.37	1.39	1.52
3	B	938	VAL	CA-C	-5.37	1.39	1.52
6	R	90	PHE	N-CA	-5.37	1.35	1.46
3	I	938	VAL	CA-C	-5.37	1.39	1.52
1	A	595	THR	N-CA	-5.36	1.35	1.46
1	H	612	LEU	CA-C	-5.36	1.39	1.52
4	C	8	LYS	CA-C	-5.35	1.39	1.52
4	J	8	LYS	CA-C	-5.35	1.39	1.52
5	D	56	TYR	CA-C	-5.34	1.39	1.52
1	H	283	GLY	CA-C	-5.34	1.43	1.51
4	J	315	ILE	N-CA	-5.33	1.35	1.46
5	N	81	GLU	CA-C	-5.33	1.39	1.52
3	B	783	LEU	CA-C	-5.32	1.39	1.52
5	D	81	GLU	CA-C	-5.32	1.39	1.52
8	U	19	LEU	CA-C	-5.32	1.39	1.52
6	R	107	MET	CA-C	-5.32	1.39	1.52
4	C	312	GLY	CA-C	-5.31	1.43	1.51
1	A	283	GLY	CA-C	-5.31	1.43	1.51
4	C	223	GLN	CA-C	-5.30	1.39	1.52
3	I	783	LEU	CA-C	-5.30	1.39	1.52
4	C	85	ASN	N-CA	-5.29	1.35	1.46
3	I	754	ILE	N-CA	-5.29	1.35	1.46
3	I	368	VAL	N-CA	-5.29	1.35	1.46
3	B	368	VAL	N-CA	-5.28	1.35	1.46
4	J	223	GLN	CA-C	-5.28	1.39	1.52
4	C	315	ILE	N-CA	-5.27	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	754	ILE	N-CA	-5.27	1.35	1.46
3	I	759	LEU	N-CA	-5.27	1.35	1.46
4	J	415	PHE	CA-C	-5.27	1.39	1.52
8	L	49	PHE	CA-C	-5.26	1.39	1.52
1	H	610	GLU	N-CA	-5.26	1.35	1.46
8	Z	19	LEU	CA-C	-5.26	1.39	1.52
4	J	312	GLY	CA-C	-5.26	1.43	1.51
1	A	610	GLU	N-CA	-5.26	1.35	1.46
4	J	736	GLY	CA-C	-5.25	1.43	1.51
4	C	415	PHE	CA-C	-5.25	1.39	1.52
8	S	49	PHE	CA-C	-5.25	1.39	1.52
4	J	85	ASN	N-CA	-5.24	1.35	1.46
3	I	440	ARG	CA-C	-5.24	1.39	1.52
3	B	759	LEU	N-CA	-5.23	1.35	1.46
3	B	440	ARG	CA-C	-5.22	1.39	1.52
4	C	736	GLY	CA-C	-5.22	1.43	1.51
4	C	379	THR	N-CA	-5.20	1.35	1.46
6	R	105	GLU	CA-C	-5.20	1.39	1.52
3	I	750	ASN	N-CA	-5.20	1.35	1.46
3	B	750	ASN	N-CA	-5.19	1.35	1.46
3	I	375	LEU	CA-C	-5.16	1.39	1.52
4	J	379	THR	N-CA	-5.16	1.36	1.46
7	G	499	GLY	CA-C	-5.15	1.43	1.51
4	C	367	VAL	CA-C	-5.13	1.39	1.52
3	B	317	LEU	CA-C	-5.13	1.39	1.52
6	R	33	VAL	N-CA	-5.13	1.36	1.46
4	C	573	LEU	CA-C	-5.12	1.39	1.52
3	B	375	LEU	CA-C	-5.12	1.39	1.52
7	G	174	VAL	CA-C	-5.12	1.39	1.52
4	J	367	VAL	CA-C	-5.11	1.39	1.52
6	T	35	TYR	CA-C	-5.11	1.39	1.52
4	J	573	LEU	CA-C	-5.11	1.39	1.52
7	G	460	GLY	CA-C	-5.10	1.43	1.51
1	H	631	LYS	N-CA	-5.09	1.36	1.46
6	M	35	TYR	CA-C	-5.09	1.39	1.52
3	I	317	LEU	CA-C	-5.08	1.39	1.52
6	R	110	MET	CA-C	-5.08	1.39	1.52
1	A	631	LYS	N-CA	-5.08	1.36	1.46
3	B	374	VAL	N-CA	-5.07	1.36	1.46
3	I	374	VAL	N-CA	-5.06	1.36	1.46
7	Q	234	ARG	CA-C	-5.06	1.39	1.52
6	R	96	ASP	CA-C	-5.05	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	314	ILE	CA-C	-5.05	1.39	1.52
4	C	314	ILE	CA-C	-5.05	1.39	1.52
1	H	14	GLY	CA-C	-5.04	1.43	1.51
8	S	139	PRO	CA-C	-5.04	1.42	1.52
3	B	349	LEU	CA-C	-5.03	1.39	1.52
3	I	300	TYR	CA-C	-5.03	1.39	1.52
8	L	139	PRO	CA-C	-5.02	1.42	1.52
7	K	234	ARG	CA-C	-5.02	1.40	1.52
3	B	300	TYR	CA-C	-5.02	1.40	1.52
7	G	91	THR	N-CA	-5.01	1.36	1.46
6	R	106	VAL	N-CA	-5.01	1.36	1.46
4	J	535	ILE	N-CA	-5.01	1.36	1.46
1	A	631	LYS	CA-C	-5.00	1.40	1.52
3	I	349	LEU	CA-C	-5.00	1.40	1.52
4	C	535	ILE	N-CA	-5.00	1.36	1.46

All (603) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	343	GLN	N-CA-C	-9.87	84.34	111.00
1	H	343	GLN	N-CA-C	-9.86	84.39	111.00
7	Q	117	GLU	C-N-CA	9.72	146.01	121.70
7	K	117	GLU	C-N-CA	9.71	145.98	121.70
3	I	326	HIS	N-CA-C	-9.60	85.09	111.00
3	B	326	HIS	N-CA-C	-9.59	85.09	111.00
7	G	96	SER	N-CA-C	9.11	135.59	111.00
3	B	940	GLY	N-CA-C	-9.03	90.53	113.10
3	I	940	GLY	N-CA-C	-9.02	90.55	113.10
4	C	416	LYS	N-CA-C	-8.88	87.02	111.00
4	J	416	LYS	N-CA-C	-8.88	87.03	111.00
3	B	760	VAL	N-CA-C	-8.57	87.85	111.00
3	I	760	VAL	N-CA-C	-8.57	87.85	111.00
1	H	229	VAL	N-CA-C	-8.55	87.91	111.00
1	A	229	VAL	N-CA-C	-8.55	87.92	111.00
5	D	61	MET	N-CA-C	-8.54	87.93	111.00
5	N	61	MET	N-CA-C	-8.52	87.98	111.00
3	B	67	GLY	N-CA-C	-8.52	91.80	113.10
3	I	67	GLY	N-CA-C	-8.52	91.80	113.10
6	R	150	ASN	C-N-CA	8.42	142.75	121.70
1	A	740	GLY	N-CA-C	-8.39	92.13	113.10
1	H	740	GLY	N-CA-C	-8.38	92.15	113.10
6	P	59	LYS	C-N-CA	8.26	142.36	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	59	LYS	C-N-CA	8.25	142.33	121.70
1	A	631	LYS	N-CA-C	-8.22	88.82	111.00
1	H	631	LYS	N-CA-C	-8.20	88.86	111.00
1	H	491	VAL	C-N-CA	8.17	142.12	121.70
6	R	122	LEU	N-CA-C	-8.16	88.96	111.00
1	A	491	VAL	C-N-CA	8.14	142.06	121.70
3	I	759	LEU	N-CA-C	-8.07	89.21	111.00
3	B	759	LEU	N-CA-C	-8.06	89.23	111.00
1	A	504	ALA	N-CA-C	-7.98	89.46	111.00
1	H	504	ALA	N-CA-C	-7.98	89.46	111.00
1	A	789	ASP	N-CA-C	-7.91	89.64	111.00
5	D	56	TYR	N-CA-C	-7.91	89.64	111.00
5	N	56	TYR	N-CA-C	-7.91	89.66	111.00
1	H	789	ASP	N-CA-C	-7.89	89.71	111.00
7	K	829	LEU	N-CA-C	-7.83	89.87	111.00
7	Q	829	LEU	N-CA-C	-7.81	89.91	111.00
7	G	829	LEU	N-CA-C	-7.79	89.96	111.00
1	A	779	ASP	N-CA-C	-7.79	89.98	111.00
1	H	371	ASN	N-CA-C	-7.78	90.00	111.00
1	H	779	ASP	N-CA-C	-7.77	90.03	111.00
1	A	371	ASN	N-CA-C	-7.76	90.03	111.00
6	R	144	GLY	N-CA-C	-7.72	93.79	113.10
4	J	441	VAL	N-CA-C	-7.68	90.26	111.00
4	C	441	VAL	N-CA-C	-7.68	90.27	111.00
1	A	803	PRO	N-CA-C	7.67	132.05	112.10
1	H	803	PRO	N-CA-C	7.67	132.03	112.10
1	A	321	ARG	N-CA-C	-7.62	90.41	111.00
3	B	750	ASN	N-CA-C	-7.62	90.43	111.00
3	I	750	ASN	N-CA-C	-7.62	90.43	111.00
1	H	321	ARG	N-CA-C	-7.61	90.44	111.00
3	I	255	SER	C-N-CA	7.61	140.72	121.70
3	B	255	SER	C-N-CA	7.60	140.69	121.70
6	M	41	GLU	C-N-CA	7.58	140.65	121.70
6	T	41	GLU	C-N-CA	7.56	140.60	121.70
6	P	97	ARG	N-CA-C	-7.55	90.62	111.00
6	F	97	ARG	N-CA-C	-7.54	90.63	111.00
6	R	159	CYS	N-CA-C	-7.54	90.64	111.00
1	H	622	GLY	N-CA-C	-7.53	94.28	113.10
1	A	622	GLY	N-CA-C	-7.53	94.28	113.10
6	P	61	ILE	N-CA-C	-7.49	90.77	111.00
6	F	61	ILE	N-CA-C	-7.48	90.80	111.00
7	G	117	GLU	N-CA-C	-7.48	90.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	118	ALA	N-CA-C	-7.45	90.89	111.00
5	N	118	ALA	N-CA-C	-7.44	90.91	111.00
1	H	198	LYS	N-CA-C	-7.43	90.95	111.00
1	A	198	LYS	N-CA-C	-7.42	90.97	111.00
4	J	559	ARG	N-CA-C	-7.33	91.20	111.00
4	J	221	CYS	N-CA-C	-7.33	91.21	111.00
4	C	221	CYS	N-CA-C	-7.33	91.22	111.00
4	C	559	ARG	N-CA-C	-7.33	91.22	111.00
5	D	136	MET	N-CA-C	-7.31	91.26	111.00
5	N	136	MET	N-CA-C	-7.31	91.26	111.00
3	B	749	VAL	N-CA-C	-7.26	91.39	111.00
1	H	338	ASP	N-CA-C	-7.26	91.40	111.00
7	G	693	VAL	C-N-CA	-7.25	91.53	122.00
1	A	338	ASP	N-CA-C	-7.25	91.42	111.00
3	I	749	VAL	N-CA-C	-7.24	91.45	111.00
1	A	519	ASP	N-CA-C	-7.20	91.57	111.00
1	H	519	ASP	N-CA-C	-7.18	91.61	111.00
3	I	761	VAL	N-CA-C	-7.18	91.61	111.00
3	B	761	VAL	N-CA-C	-7.17	91.64	111.00
3	I	837	ILE	N-CA-C	-7.15	91.69	111.00
3	B	837	ILE	N-CA-C	-7.14	91.71	111.00
6	T	69	GLY	N-CA-C	-7.12	95.31	113.10
3	B	269	GLN	N-CA-C	-7.10	91.82	111.00
6	M	69	GLY	N-CA-C	-7.10	95.36	113.10
3	I	269	GLN	N-CA-C	-7.09	91.86	111.00
3	B	48	GLY	N-CA-C	-7.08	95.39	113.10
3	I	48	GLY	N-CA-C	-7.07	95.42	113.10
6	F	121	TRP	N-CA-C	7.06	130.06	111.00
6	P	121	TRP	N-CA-C	7.06	130.06	111.00
7	K	244	ASP	N-CA-C	-7.05	91.96	111.00
3	B	49	ASP	N-CA-C	-7.04	92.01	111.00
7	Q	244	ASP	N-CA-C	-7.04	92.00	111.00
7	G	609	ARG	C-N-CA	7.02	139.25	121.70
3	I	811	ASN	N-CA-C	-7.02	92.05	111.00
3	I	49	ASP	N-CA-C	-7.01	92.06	111.00
3	B	811	ASN	N-CA-C	-7.01	92.07	111.00
1	A	339	ARG	N-CA-C	-7.00	92.10	111.00
7	K	609	ARG	C-N-CA	6.99	139.18	121.70
1	H	339	ARG	N-CA-C	-6.99	92.14	111.00
7	Q	609	ARG	C-N-CA	6.99	139.16	121.70
3	B	871	ASN	N-CA-C	-6.94	92.27	111.00
3	I	871	ASN	N-CA-C	-6.93	92.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	243	ASP	N-CA-C	-6.90	92.38	111.00
1	H	36	TRP	N-CA-C	-6.90	92.38	111.00
1	A	36	TRP	N-CA-C	-6.89	92.40	111.00
1	A	243	ASP	N-CA-C	-6.89	92.40	111.00
1	H	240	TRP	C-N-CA	6.88	138.90	121.70
1	A	240	TRP	C-N-CA	6.87	138.88	121.70
1	H	236	GLU	N-CA-C	-6.81	92.61	111.00
4	C	653	GLU	N-CA-C	-6.80	92.64	111.00
1	A	236	GLU	N-CA-C	-6.79	92.66	111.00
4	J	653	GLU	N-CA-C	-6.79	92.67	111.00
1	H	430	ASP	N-CA-C	-6.77	92.72	111.00
1	H	528	ILE	N-CA-C	-6.76	92.76	111.00
1	A	528	ILE	N-CA-C	-6.75	92.77	111.00
1	A	430	ASP	N-CA-C	-6.74	92.80	111.00
4	C	27	GLU	N-CA-C	-6.74	92.80	111.00
4	J	27	GLU	N-CA-C	-6.74	92.81	111.00
1	H	766	GLY	N-CA-C	-6.69	96.38	113.10
7	Q	629	LEU	C-N-CA	6.68	138.41	121.70
1	A	766	GLY	N-CA-C	-6.68	96.41	113.10
7	G	828	LEU	N-CA-C	-6.67	92.98	111.00
7	K	629	LEU	C-N-CA	6.67	138.38	121.70
7	K	828	LEU	N-CA-C	-6.67	92.98	111.00
7	Q	828	LEU	N-CA-C	-6.66	93.02	111.00
6	F	159	CYS	N-CA-C	-6.63	93.10	111.00
7	G	629	LEU	C-N-CA	6.63	138.28	121.70
6	P	159	CYS	N-CA-C	-6.63	93.10	111.00
8	U	11	TYR	N-CA-C	-6.60	93.19	111.00
8	Z	11	TYR	N-CA-C	-6.59	93.19	111.00
4	C	379	THR	N-CA-C	-6.59	93.21	111.00
4	J	379	THR	N-CA-C	-6.58	93.22	111.00
1	A	457	PHE	N-CA-C	-6.57	93.26	111.00
8	Z	62	LEU	N-CA-C	-6.57	93.26	111.00
3	I	740	PRO	N-CA-C	-6.57	95.02	112.10
1	H	457	PHE	N-CA-C	-6.57	93.27	111.00
1	H	242	VAL	N-CA-C	-6.56	93.29	111.00
8	U	62	LEU	N-CA-C	-6.56	93.30	111.00
1	A	242	VAL	N-CA-C	-6.55	93.31	111.00
5	N	14	LYS	C-N-CA	6.55	138.07	121.70
7	Q	667	ASN	N-CA-C	-6.55	93.32	111.00
7	K	667	ASN	N-CA-C	-6.55	93.32	111.00
7	G	667	ASN	N-CA-C	-6.55	93.32	111.00
3	B	740	PRO	N-CA-C	-6.54	95.09	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	14	LYS	C-N-CA	6.54	138.05	121.70
6	T	155	ILE	N-CA-C	-6.50	93.44	111.00
6	M	155	ILE	N-CA-C	-6.49	93.48	111.00
3	B	792	LEU	N-CA-C	-6.48	93.50	111.00
1	A	105	TYR	N-CA-C	-6.48	93.51	111.00
1	H	105	TYR	N-CA-C	-6.47	93.53	111.00
3	I	792	LEU	N-CA-C	-6.46	93.55	111.00
5	N	19	ARG	C-N-CA	6.45	137.82	121.70
7	Q	849	LEU	N-CA-C	-6.44	93.61	111.00
1	A	317	PHE	C-N-CA	6.42	137.76	121.70
1	A	589	VAL	N-CA-C	-6.42	93.66	111.00
7	K	849	LEU	N-CA-C	-6.42	93.66	111.00
1	H	317	PHE	C-N-CA	6.42	137.76	121.70
1	H	589	VAL	N-CA-C	-6.42	93.66	111.00
5	D	19	ARG	C-N-CA	6.42	137.75	121.70
7	G	849	LEU	N-CA-C	-6.41	93.70	111.00
3	B	754	ILE	N-CA-C	-6.40	93.71	111.00
3	I	754	ILE	N-CA-C	-6.40	93.72	111.00
7	G	484	HIS	N-CA-C	-6.39	93.75	111.00
4	C	154	ASP	N-CA-C	-6.38	93.77	111.00
7	G	150	ASP	C-N-CA	6.38	137.65	121.70
4	J	546	TYR	N-CA-C	-6.37	93.80	111.00
4	C	546	TYR	N-CA-C	-6.37	93.81	111.00
5	N	29	ILE	N-CA-C	-6.36	93.82	111.00
4	J	154	ASP	N-CA-C	-6.36	93.83	111.00
5	D	29	ILE	N-CA-C	-6.35	93.84	111.00
7	Q	206	ASN	N-CA-C	-6.35	93.86	111.00
7	Q	838	HIS	C-N-CA	6.34	137.56	121.70
7	K	206	ASN	N-CA-C	-6.34	93.89	111.00
7	K	117	GLU	CA-C-N	-6.33	103.26	117.20
7	K	838	HIS	C-N-CA	6.33	137.54	121.70
7	G	838	HIS	C-N-CA	6.33	137.53	121.70
7	Q	117	GLU	CA-C-N	-6.33	103.27	117.20
3	B	414	ALA	C-N-CA	6.33	137.53	121.70
8	U	29	LYS	N-CA-C	-6.33	93.91	111.00
7	G	704	GLY	N-CA-C	-6.33	97.29	113.10
3	I	414	ALA	C-N-CA	6.32	137.51	121.70
6	T	149	ARG	N-CA-C	-6.32	93.93	111.00
8	Z	29	LYS	N-CA-C	-6.32	93.93	111.00
7	Q	704	GLY	N-CA-C	-6.32	97.31	113.10
1	H	768	ASP	C-N-CA	6.31	137.48	121.70
7	Q	96	SER	N-CA-C	6.31	128.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	704	GLY	N-CA-C	-6.30	97.34	113.10
6	M	149	ARG	N-CA-C	-6.30	93.98	111.00
1	A	768	ASP	C-N-CA	6.30	137.45	121.70
7	K	96	SER	N-CA-C	6.28	127.96	111.00
1	A	73	TYR	N-CA-C	-6.28	94.05	111.00
1	H	73	TYR	N-CA-C	-6.27	94.06	111.00
4	C	155	ASN	C-N-CA	6.26	137.35	121.70
4	J	155	ASN	C-N-CA	6.26	137.34	121.70
6	M	62	SER	C-N-CA	6.25	137.34	121.70
6	T	62	SER	C-N-CA	6.25	137.32	121.70
3	I	816	GLY	N-CA-C	-6.24	97.50	113.10
7	G	665	CYS	N-CA-C	6.24	127.84	111.00
4	C	113	PHE	N-CA-C	6.24	127.84	111.00
3	B	816	GLY	N-CA-C	-6.23	97.52	113.10
4	J	113	PHE	N-CA-C	6.22	127.79	111.00
4	J	736	GLY	N-CA-C	-6.21	97.58	113.10
4	J	546	TYR	O-C-N	6.19	132.61	122.70
7	G	277	LEU	C-N-CA	-6.19	96.01	122.00
8	S	30	TYR	N-CA-C	-6.18	94.32	111.00
4	C	736	GLY	N-CA-C	-6.17	97.67	113.10
3	I	933	GLY	C-N-CA	-6.17	96.09	122.00
8	L	30	TYR	N-CA-C	-6.17	94.35	111.00
7	Q	665	CYS	N-CA-C	6.16	127.64	111.00
4	C	546	TYR	O-C-N	6.16	132.55	122.70
3	B	933	GLY	C-N-CA	-6.15	96.16	122.00
4	J	85	ASN	N-CA-C	-6.15	94.39	111.00
7	K	665	CYS	N-CA-C	6.15	127.60	111.00
8	Z	25	ARG	N-CA-C	-6.14	94.41	111.00
8	U	25	ARG	N-CA-C	-6.13	94.44	111.00
4	C	85	ASN	N-CA-C	-6.12	94.46	111.00
3	I	905	PHE	C-N-CA	6.11	136.98	121.70
6	R	42	VAL	C-N-CA	6.10	136.95	121.70
4	C	315	ILE	N-CA-C	-6.10	94.54	111.00
4	J	396	TRP	N-CA-C	-6.09	94.54	111.00
1	H	511	ILE	N-CA-C	-6.09	94.55	111.00
4	C	396	TRP	N-CA-C	-6.09	94.56	111.00
3	B	905	PHE	C-N-CA	6.09	136.92	121.70
4	J	546	TYR	CA-C-N	-6.09	103.80	117.20
1	A	511	ILE	N-CA-C	-6.09	94.56	111.00
6	R	58	TYR	N-CA-C	-6.08	94.59	111.00
8	Z	30	TYR	N-CA-C	-6.07	94.60	111.00
4	J	315	ILE	N-CA-C	-6.07	94.60	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	207	ASP	N-CA-C	6.07	127.39	111.00
8	U	30	TYR	N-CA-C	-6.07	94.62	111.00
4	J	170	TRP	C-N-CA	6.06	136.85	121.70
4	C	546	TYR	CA-C-N	-6.06	103.87	117.20
4	C	170	TRP	C-N-CA	6.05	136.84	121.70
8	Z	129	VAL	N-CA-C	-6.05	94.68	111.00
4	C	551	ILE	N-CA-C	-6.04	94.69	111.00
8	U	129	VAL	N-CA-C	-6.04	94.70	111.00
3	B	385	VAL	C-N-CA	6.04	136.79	121.70
8	L	80	ILE	C-N-CA	6.04	134.97	122.30
3	I	385	VAL	C-N-CA	6.03	136.78	121.70
5	D	50	GLU	N-CA-C	-6.03	94.73	111.00
4	J	551	ILE	N-CA-C	-6.03	94.73	111.00
5	N	50	GLU	N-CA-C	-6.03	94.73	111.00
4	C	424	PHE	N-CA-C	-6.02	94.75	111.00
7	G	731	THR	N-CA-C	-6.01	94.77	111.00
4	J	424	PHE	N-CA-C	-6.01	94.77	111.00
7	Q	731	THR	N-CA-C	-6.01	94.77	111.00
4	J	504	GLY	N-CA-C	6.00	128.11	113.10
7	K	731	THR	N-CA-C	-6.00	94.80	111.00
6	T	53	VAL	N-CA-C	-6.00	94.81	111.00
8	S	80	ILE	C-N-CA	5.99	134.89	122.30
4	J	245	ILE	N-CA-C	-5.99	94.83	111.00
4	C	245	ILE	N-CA-C	-5.99	94.84	111.00
4	J	174	SER	N-CA-C	-5.98	94.84	111.00
6	R	71	GLN	N-CA-C	-5.98	94.85	111.00
6	M	53	VAL	N-CA-C	-5.98	94.85	111.00
1	A	599	PHE	CA-C-N	5.98	130.35	117.20
4	C	504	GLY	N-CA-C	5.97	128.03	113.10
7	Q	80	ASN	N-CA-C	-5.97	94.88	111.00
4	C	174	SER	N-CA-C	-5.97	94.88	111.00
7	G	640	THR	N-CA-C	-5.97	94.88	111.00
1	H	599	PHE	CA-C-N	5.97	130.33	117.20
7	Q	640	THR	N-CA-C	-5.97	94.88	111.00
7	K	80	ASN	N-CA-C	-5.97	94.89	111.00
7	K	640	THR	N-CA-C	-5.96	94.90	111.00
7	Q	736	ASP	N-CA-C	-5.96	94.90	111.00
1	A	554	THR	N-CA-C	5.96	127.10	111.00
7	G	736	ASP	N-CA-C	-5.96	94.92	111.00
7	K	736	ASP	N-CA-C	-5.95	94.93	111.00
7	K	222	GLY	N-CA-C	-5.95	98.23	113.10
1	H	554	THR	N-CA-C	5.95	127.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	222	GLY	N-CA-C	-5.95	98.23	113.10
6	R	96	ASP	N-CA-C	-5.94	94.96	111.00
7	G	506	LEU	N-CA-C	5.94	127.03	111.00
4	C	151	ASN	N-CA-C	-5.94	94.97	111.00
8	S	61	LEU	C-N-CA	-5.93	106.87	121.70
1	H	392	ASP	N-CA-C	-5.93	94.99	111.00
4	J	151	ASN	N-CA-C	-5.93	95.00	111.00
8	L	61	LEU	C-N-CA	-5.92	106.90	121.70
1	A	392	ASP	N-CA-C	-5.92	95.02	111.00
4	J	88	THR	N-CA-C	-5.91	95.04	111.00
4	C	88	THR	N-CA-C	-5.91	95.04	111.00
7	Q	240	LEU	C-N-CA	5.91	136.48	121.70
3	B	928	LYS	N-CA-C	5.91	126.95	111.00
3	I	928	LYS	N-CA-C	5.91	126.95	111.00
7	K	240	LEU	C-N-CA	5.90	136.46	121.70
3	B	795	HIS	C-N-CA	5.89	136.42	121.70
3	I	795	HIS	C-N-CA	5.89	136.42	121.70
7	G	858	ALA	N-CA-C	-5.88	95.11	111.00
7	K	858	ALA	N-CA-C	-5.88	95.12	111.00
7	Q	858	ALA	N-CA-C	-5.88	95.12	111.00
1	A	496	TRP	N-CA-C	-5.84	95.23	111.00
7	G	300	LYS	N-CA-C	-5.84	95.23	111.00
1	H	496	TRP	N-CA-C	-5.84	95.24	111.00
4	J	446	GLY	N-CA-C	-5.83	98.53	113.10
7	Q	695	ALA	N-CA-C	-5.82	95.29	111.00
7	K	695	ALA	N-CA-C	-5.82	95.29	111.00
1	H	325	ALA	N-CA-C	5.82	126.71	111.00
1	H	429	LEU	N-CA-C	-5.82	95.29	111.00
1	A	429	LEU	N-CA-C	-5.82	95.29	111.00
4	C	446	GLY	N-CA-C	-5.82	98.56	113.10
1	A	325	ALA	N-CA-C	5.82	126.70	111.00
7	K	845	ARG	N-CA-C	-5.80	95.34	111.00
3	I	325	GLU	C-N-CA	5.78	136.15	121.70
3	B	748	HIS	N-CA-C	-5.78	95.40	111.00
7	Q	845	ARG	N-CA-C	-5.78	95.40	111.00
3	B	325	GLU	C-N-CA	5.77	136.13	121.70
3	I	748	HIS	N-CA-C	-5.77	95.42	111.00
7	G	845	ARG	N-CA-C	-5.77	95.42	111.00
5	D	98	GLU	N-CA-C	-5.77	95.42	111.00
7	G	749	ASP	N-CA-C	-5.77	95.43	111.00
5	N	98	GLU	N-CA-C	-5.77	95.43	111.00
7	K	749	ASP	N-CA-C	-5.76	95.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	530	VAL	N-CA-C	-5.76	95.46	111.00
7	Q	749	ASP	N-CA-C	-5.76	95.46	111.00
3	B	410	PRO	N-CA-C	-5.75	97.14	112.10
1	H	509	HIS	N-CA-C	-5.75	95.48	111.00
1	A	509	HIS	N-CA-C	-5.75	95.48	111.00
4	C	530	VAL	N-CA-C	-5.75	95.49	111.00
6	R	61	ILE	N-CA-C	-5.75	95.48	111.00
3	I	410	PRO	N-CA-C	-5.74	97.18	112.10
7	Q	40	ASN	N-CA-C	-5.74	95.51	111.00
7	K	40	ASN	N-CA-C	-5.72	95.55	111.00
1	A	507	ALA	N-CA-C	-5.72	95.56	111.00
3	B	804	VAL	N-CA-C	-5.72	95.56	111.00
7	G	95	MET	N-CA-C	5.72	126.44	111.00
1	H	507	ALA	N-CA-C	-5.71	95.59	111.00
5	D	24	MET	C-N-CA	5.70	135.96	121.70
3	I	804	VAL	N-CA-C	-5.70	95.60	111.00
1	H	77	VAL	N-CA-C	-5.70	95.61	111.00
1	A	67	VAL	N-CA-C	-5.70	95.62	111.00
7	G	178	VAL	N-CA-C	5.69	126.37	111.00
5	N	24	MET	C-N-CA	5.69	135.93	121.70
7	K	853	THR	N-CA-C	-5.69	95.63	111.00
7	Q	853	THR	N-CA-C	-5.69	95.64	111.00
1	H	67	VAL	N-CA-C	-5.68	95.67	111.00
1	A	77	VAL	N-CA-C	-5.68	95.67	111.00
1	A	522	CYS	N-CA-C	-5.68	95.67	111.00
1	A	87	PHE	N-CA-C	-5.67	95.68	111.00
3	I	841	ILE	N-CA-C	5.67	126.32	111.00
3	I	414	ALA	O-C-N	5.67	131.77	122.70
3	B	841	ILE	N-CA-C	5.67	126.30	111.00
3	B	414	ALA	O-C-N	5.66	131.76	122.70
1	A	324	PRO	C-N-CA	5.66	135.84	121.70
7	G	853	THR	N-CA-C	-5.66	95.73	111.00
6	F	151	ARG	N-CA-C	-5.66	95.73	111.00
1	H	522	CYS	N-CA-C	-5.66	95.73	111.00
4	J	411	ILE	N-CA-C	-5.65	95.73	111.00
6	P	151	ARG	N-CA-C	-5.65	95.74	111.00
4	C	411	ILE	N-CA-C	-5.65	95.75	111.00
1	H	87	PHE	N-CA-C	-5.64	95.76	111.00
1	H	324	PRO	C-N-CA	5.64	135.80	121.70
4	J	442	ARG	N-CA-C	-5.63	95.80	111.00
1	A	227	ARG	N-CA-C	-5.63	95.81	111.00
1	H	227	ARG	N-CA-C	-5.63	95.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	611	VAL	CA-C-N	-5.62	104.83	117.20
3	I	926	ILE	N-CA-C	5.62	126.18	111.00
3	B	926	ILE	N-CA-C	5.62	126.18	111.00
4	C	442	ARG	N-CA-C	-5.62	95.82	111.00
6	R	41	GLU	C-N-CA	5.62	135.75	121.70
1	A	611	VAL	CA-C-N	-5.62	104.84	117.20
6	R	151	ARG	N-CA-C	5.61	126.14	111.00
1	A	621	VAL	C-N-CA	5.61	134.07	122.30
1	H	621	VAL	C-N-CA	5.60	134.07	122.30
8	U	58	GLU	N-CA-C	-5.60	95.88	111.00
4	J	9	ARG	N-CA-C	-5.59	95.90	111.00
1	A	423	ARG	C-N-CA	5.59	135.67	121.70
6	R	88	VAL	N-CA-C	5.59	126.09	111.00
8	Z	58	GLU	N-CA-C	-5.58	95.92	111.00
1	A	487	LYS	C-N-CA	5.58	135.64	121.70
4	C	9	ARG	N-CA-C	-5.57	95.96	111.00
1	H	423	ARG	C-N-CA	5.57	135.63	121.70
3	B	800	ILE	N-CA-C	-5.57	95.97	111.00
4	C	662	VAL	N-CA-C	-5.56	95.99	111.00
6	M	148	ILE	C-N-CA	5.55	135.57	121.70
1	H	487	LYS	C-N-CA	5.55	135.57	121.70
6	T	63	PHE	N-CA-C	5.55	125.98	111.00
1	H	78	TRP	N-CA-C	-5.54	96.03	111.00
1	A	78	TRP	N-CA-C	-5.54	96.04	111.00
4	C	246	THR	C-N-CA	5.54	133.93	122.30
4	J	662	VAL	N-CA-C	-5.54	96.05	111.00
7	Q	279	GLY	N-CA-C	-5.54	99.26	113.10
6	M	63	PHE	N-CA-C	5.53	125.94	111.00
6	T	148	ILE	C-N-CA	5.53	135.53	121.70
3	I	800	ILE	N-CA-C	-5.53	96.07	111.00
3	I	828	ASP	N-CA-C	-5.52	96.09	111.00
4	C	202	LEU	O-C-N	5.52	131.53	122.70
4	J	89	LEU	N-CA-C	-5.52	96.10	111.00
6	T	154	PHE	N-CA-C	-5.52	96.10	111.00
1	A	574	LYS	C-N-CA	5.51	133.88	122.30
3	B	828	ASP	N-CA-C	-5.51	96.11	111.00
4	C	202	LEU	N-CA-C	-5.51	96.11	111.00
6	M	154	PHE	N-CA-C	-5.51	96.11	111.00
7	K	279	GLY	N-CA-C	-5.51	99.32	113.10
4	J	246	THR	C-N-CA	5.51	133.88	122.30
4	C	89	LEU	N-CA-C	-5.50	96.14	111.00
4	J	202	LEU	N-CA-C	-5.50	96.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	574	LYS	C-N-CA	5.50	133.85	122.30
7	K	831	ALA	C-N-CA	5.50	133.84	122.30
4	C	365	ARG	N-CA-C	5.49	125.83	111.00
7	G	132	THR	N-CA-C	5.49	125.83	111.00
4	J	472	ASP	N-CA-C	-5.49	96.17	111.00
4	C	327	LEU	N-CA-C	-5.49	96.19	111.00
4	J	365	ARG	N-CA-C	5.49	125.81	111.00
7	G	673	THR	N-CA-C	-5.48	96.19	111.00
8	Z	16	ILE	N-CA-C	-5.48	96.19	111.00
1	A	736	ALA	N-CA-C	5.48	125.80	111.00
7	G	116	LYS	N-CA-C	5.48	125.80	111.00
4	J	202	LEU	O-C-N	5.48	131.47	122.70
7	G	831	ALA	C-N-CA	5.48	133.81	122.30
4	C	472	ASP	N-CA-C	-5.48	96.21	111.00
1	H	516	ARG	C-N-CA	5.48	135.40	121.70
3	I	256	GLU	N-CA-C	5.48	125.79	111.00
7	K	673	THR	N-CA-C	-5.48	96.22	111.00
1	H	736	ALA	N-CA-C	5.47	125.78	111.00
4	J	327	LEU	N-CA-C	-5.47	96.22	111.00
8	U	16	ILE	N-CA-C	-5.47	96.22	111.00
7	Q	831	ALA	C-N-CA	5.47	133.79	122.30
1	H	132	THR	N-CA-C	-5.47	96.22	111.00
7	Q	673	THR	N-CA-C	-5.47	96.22	111.00
1	A	132	THR	N-CA-C	-5.47	96.23	111.00
3	B	256	GLU	N-CA-C	5.47	125.77	111.00
8	S	29	LYS	N-CA-C	-5.47	96.24	111.00
1	A	587	PRO	N-CA-C	5.46	126.31	112.10
8	L	29	LYS	N-CA-C	-5.46	96.25	111.00
1	H	587	PRO	N-CA-C	5.46	126.31	112.10
3	B	103	THR	C-N-CA	5.46	135.35	121.70
3	I	103	THR	C-N-CA	5.45	135.33	121.70
3	I	257	ARG	N-CA-C	5.45	125.72	111.00
3	I	758	VAL	N-CA-C	-5.45	96.29	111.00
3	B	257	ARG	N-CA-C	5.45	125.70	111.00
1	A	516	ARG	C-N-CA	5.44	135.31	121.70
3	B	758	VAL	N-CA-C	-5.44	96.32	111.00
4	C	202	LEU	CA-C-N	-5.43	105.25	117.20
7	G	459	LEU	C-N-CA	5.43	133.71	122.30
3	B	939	THR	N-CA-C	-5.43	96.35	111.00
3	I	939	THR	N-CA-C	-5.41	96.39	111.00
1	A	533	GLY	N-CA-C	-5.40	99.59	113.10
4	J	202	LEU	CA-C-N	-5.40	105.32	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	814	GLU	N-CA-C	-5.40	96.42	111.00
7	K	814	GLU	N-CA-C	-5.39	96.44	111.00
1	H	656	GLY	N-CA-C	-5.39	99.62	113.10
3	B	482	SER	N-CA-C	5.39	125.55	111.00
3	I	482	SER	N-CA-C	5.39	125.55	111.00
7	K	844	SER	N-CA-C	-5.39	96.46	111.00
1	H	533	GLY	N-CA-C	-5.39	99.63	113.10
1	A	444	ILE	N-CA-C	-5.38	96.46	111.00
8	L	60	ALA	C-N-CA	5.38	135.16	121.70
7	G	844	SER	N-CA-C	-5.38	96.47	111.00
1	A	656	GLY	N-CA-C	-5.38	99.64	113.10
1	H	444	ILE	N-CA-C	-5.38	96.47	111.00
8	S	60	ALA	C-N-CA	5.38	135.15	121.70
7	G	274	ILE	N-CA-C	5.38	125.52	111.00
7	Q	844	SER	N-CA-C	-5.37	96.49	111.00
6	M	91	VAL	C-N-CA	5.36	135.11	121.70
4	C	262	ARG	N-CA-C	-5.35	96.55	111.00
3	I	744	GLU	N-CA-C	-5.35	96.56	111.00
3	B	744	GLU	N-CA-C	-5.34	96.58	111.00
1	A	272	SER	N-CA-C	5.34	125.42	111.00
1	H	272	SER	N-CA-C	5.34	125.42	111.00
4	J	262	ARG	N-CA-C	-5.34	96.58	111.00
6	T	91	VAL	C-N-CA	5.34	135.05	121.70
1	H	329	HIS	N-CA-C	-5.32	96.62	111.00
4	J	378	TYR	CA-C-N	-5.32	105.51	117.20
1	H	630	GLN	N-CA-C	-5.31	96.66	111.00
4	C	509	GLY	N-CA-C	-5.31	99.82	113.10
1	A	329	HIS	N-CA-C	-5.31	96.67	111.00
4	J	509	GLY	N-CA-C	-5.31	99.84	113.10
4	J	106	ALA	N-CA-C	-5.30	96.68	111.00
4	J	378	TYR	O-C-N	5.30	131.19	122.70
4	C	106	ALA	N-CA-C	-5.30	96.69	111.00
1	A	630	GLN	N-CA-C	-5.30	96.70	111.00
1	A	383	ALA	C-N-CA	5.29	134.94	121.70
8	S	13	VAL	N-CA-C	-5.29	96.70	111.00
7	G	686	ALA	N-CA-C	5.29	125.28	111.00
4	C	378	TYR	CA-C-N	-5.29	105.57	117.20
8	L	13	VAL	N-CA-C	-5.29	96.72	111.00
7	Q	686	ALA	N-CA-C	5.29	125.27	111.00
3	I	763	GLN	C-N-CA	5.28	134.90	121.70
1	H	383	ALA	C-N-CA	5.28	134.90	121.70
1	A	402	SER	N-CA-C	-5.28	96.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	763	GLN	C-N-CA	5.28	134.89	121.70
1	H	340	PHE	C-N-CA	5.27	134.88	121.70
7	Q	131	ILE	N-CA-C	5.27	125.23	111.00
1	H	402	SER	N-CA-C	-5.26	96.79	111.00
7	K	686	ALA	N-CA-C	5.26	125.20	111.00
1	A	340	PHE	C-N-CA	5.26	134.84	121.70
7	K	131	ILE	N-CA-C	5.26	125.19	111.00
4	C	378	TYR	O-C-N	5.25	131.10	122.70
6	F	166	LEU	C-N-CA	5.24	134.81	121.70
4	J	237	PHE	N-CA-C	-5.24	96.84	111.00
4	C	237	PHE	N-CA-C	-5.24	96.85	111.00
7	K	120	TYR	CA-C-N	-5.24	105.67	117.20
7	Q	120	TYR	CA-C-N	-5.24	105.68	117.20
6	F	60	ASN	CA-C-N	-5.23	105.69	117.20
6	P	166	LEU	C-N-CA	5.22	134.76	121.70
6	P	60	ASN	CA-C-N	-5.22	105.71	117.20
7	G	838	HIS	CA-C-N	-5.22	105.72	117.20
7	K	297	SER	N-CA-C	5.22	125.09	111.00
1	A	570	VAL	CA-C-N	5.22	128.68	117.20
7	K	247	ARG	N-CA-C	-5.21	96.92	111.00
3	B	822	VAL	N-CA-C	-5.21	96.93	111.00
4	J	574	TYR	N-CA-C	-5.21	96.93	111.00
7	Q	297	SER	N-CA-C	5.21	125.07	111.00
1	H	570	VAL	CA-C-N	5.21	128.66	117.20
6	R	25	LEU	CA-C-N	-5.21	105.74	117.20
7	G	683	PRO	N-CA-C	5.21	125.64	112.10
7	Q	247	ARG	N-CA-C	-5.21	96.94	111.00
4	C	574	TYR	N-CA-C	-5.21	96.95	111.00
7	K	176	ARG	C-N-CA	5.20	134.70	121.70
1	H	436	LEU	N-CA-C	-5.20	96.96	111.00
3	I	822	VAL	N-CA-C	-5.20	96.97	111.00
7	K	838	HIS	CA-C-N	-5.20	105.77	117.20
1	A	436	LEU	N-CA-C	-5.19	96.98	111.00
7	Q	838	HIS	CA-C-N	-5.19	105.78	117.20
7	K	683	PRO	N-CA-C	5.19	125.59	112.10
7	Q	176	ARG	C-N-CA	5.18	134.65	121.70
4	C	254	ARG	N-CA-C	-5.18	97.02	111.00
1	H	245	CYS	N-CA-C	-5.17	97.03	111.00
4	J	588	LEU	N-CA-C	-5.17	97.05	111.00
7	Q	683	PRO	N-CA-C	5.17	125.53	112.10
4	J	254	ARG	N-CA-C	-5.16	97.06	111.00
1	A	245	CYS	N-CA-C	-5.16	97.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	39	ILE	N-CA-C	-5.16	97.07	111.00
8	L	18	ILE	O-C-N	5.16	130.95	122.70
4	C	474	GLY	C-N-CA	5.15	134.58	121.70
3	I	504	VAL	N-CA-C	5.15	124.91	111.00
3	B	504	VAL	N-CA-C	5.14	124.89	111.00
4	C	469	PHE	N-CA-C	-5.14	97.11	111.00
4	C	588	LEU	N-CA-C	-5.14	97.11	111.00
6	F	96	ASP	N-CA-C	-5.14	97.11	111.00
4	J	469	PHE	N-CA-C	-5.14	97.11	111.00
4	J	474	GLY	C-N-CA	5.14	134.56	121.70
6	P	96	ASP	N-CA-C	-5.14	97.12	111.00
8	S	18	ILE	O-C-N	5.14	130.92	122.70
7	G	296	CYS	C-N-CA	5.13	134.54	121.70
1	H	221	VAL	N-CA-C	-5.13	97.15	111.00
3	I	782	LYS	N-CA-C	-5.12	97.17	111.00
4	J	802	LYS	N-CA-C	5.12	124.83	111.00
3	B	782	LYS	N-CA-C	-5.12	97.17	111.00
1	A	221	VAL	N-CA-C	-5.12	97.18	111.00
4	C	802	LYS	N-CA-C	5.12	124.82	111.00
4	J	155	ASN	CA-C-N	-5.11	105.95	117.20
4	C	155	ASN	CA-C-N	-5.11	105.96	117.20
7	G	703	PRO	C-N-CA	5.11	133.03	122.30
7	K	703	PRO	C-N-CA	5.11	133.02	122.30
1	H	515	ASN	N-CA-C	-5.10	97.22	111.00
4	J	827	VAL	C-N-CA	5.10	134.45	121.70
4	J	803	GLU	N-CA-C	5.10	124.77	111.00
4	C	7	ILE	N-CA-C	-5.10	97.24	111.00
1	A	515	ASN	N-CA-C	-5.09	97.25	111.00
4	C	314	ILE	N-CA-C	-5.09	97.25	111.00
7	G	804	ILE	N-CA-C	5.09	124.75	111.00
4	J	802	LYS	CA-C-N	5.09	128.40	117.20
7	Q	703	PRO	C-N-CA	5.09	132.99	122.30
4	C	802	LYS	CA-C-N	5.09	128.40	117.20
8	U	18	ILE	CA-C-N	-5.09	106.00	117.20
4	C	803	GLU	N-CA-C	5.09	124.74	111.00
6	R	146	HIS	C-N-CA	5.09	134.42	121.70
4	C	827	VAL	C-N-CA	5.09	134.42	121.70
4	J	314	ILE	N-CA-C	-5.08	97.28	111.00
1	H	37	ASP	N-CA-C	-5.08	97.28	111.00
4	J	7	ILE	N-CA-C	-5.08	97.28	111.00
1	A	37	ASP	N-CA-C	-5.07	97.30	111.00
8	Z	56	ASP	N-CA-C	-5.07	97.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	141	GLU	N-CA-C	5.07	124.68	111.00
6	R	29	GLY	N-CA-C	-5.07	100.44	113.10
7	K	120	TYR	C-N-CA	5.07	134.36	121.70
1	H	543	TYR	N-CA-C	-5.07	97.33	111.00
7	G	435	GLY	C-N-CA	5.06	134.36	121.70
4	J	567	ILE	N-CA-C	-5.06	97.33	111.00
8	U	56	ASP	N-CA-C	-5.06	97.33	111.00
8	Z	18	ILE	CA-C-N	-5.06	106.07	117.20
4	C	567	ILE	N-CA-C	-5.06	97.34	111.00
7	Q	120	TYR	C-N-CA	5.05	134.34	121.70
7	Q	804	ILE	N-CA-C	5.05	124.65	111.00
7	G	118	ASP	CA-C-N	-5.05	106.08	117.20
4	C	790	ASP	CA-C-N	5.05	131.24	117.10
7	K	813	CYS	N-CA-C	5.05	124.63	111.00
1	A	543	TYR	N-CA-C	-5.04	97.38	111.00
1	A	562	ARG	N-CA-C	-5.04	97.38	111.00
7	K	804	ILE	N-CA-C	5.04	124.62	111.00
7	Q	813	CYS	N-CA-C	5.04	124.61	111.00
4	J	790	ASP	CA-C-N	5.04	131.21	117.10
1	H	562	ARG	N-CA-C	-5.04	97.40	111.00
7	G	815	ARG	N-CA-C	-5.03	97.41	111.00
1	H	568	ILE	N-CA-C	-5.02	97.44	111.00
1	A	249	TYR	N-CA-C	-5.02	97.45	111.00
4	J	397	ALA	N-CA-C	-5.02	97.45	111.00
1	A	428	VAL	N-CA-C	-5.02	97.46	111.00
1	A	391	TYR	N-CA-C	-5.01	97.47	111.00
1	H	249	TYR	N-CA-C	-5.01	97.47	111.00
8	S	58	GLU	N-CA-C	-5.01	97.48	111.00
7	G	410	GLY	N-CA-C	-5.01	100.58	113.10
7	Q	150	ASP	C-N-CA	5.01	134.22	121.70
1	H	428	VAL	N-CA-C	-5.00	97.49	111.00
1	H	391	TYR	N-CA-C	-5.00	97.49	111.00
3	B	935	ASP	N-CA-C	5.00	124.50	111.00
1	H	424	ASN	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
3	I	898	ALA	Peptide
3	I	903	CYS	Peptide
3	I	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	A	4503	0	1194	36	0
1	H	4503	0	1194	37	0
2	E	1169	0	303	0	0
2	O	1169	0	303	0	0
3	B	3198	0	810	57	0
3	I	3198	0	810	55	0
4	C	3371	0	919	24	0
4	J	3371	0	919	24	0
5	D	1707	0	450	8	0
5	N	706	0	182	9	0
6	F	635	0	181	3	0
6	M	635	0	181	19	0
6	P	635	0	181	3	0
6	R	635	0	181	35	0
6	T	635	0	181	20	0
7	G	3190	0	822	58	0
7	K	2239	0	572	37	0
7	Q	2239	0	572	39	0
8	L	555	0	148	2	0
8	S	555	0	148	2	0
8	U	555	0	147	15	0
8	Z	555	0	147	14	0
All	All	39958	0	10545	467	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 9.

All (467) 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)
7:G:107:SER:N	6:R:50:GLY:HA3	1.16	1.48
7:G:107:SER:H	6:R:50:GLY:CA	1.31	1.44
7:K:107:SER:N	6:M:50:GLY:HA3	1.28	1.44
7:Q:107:SER:N	6:T:50:GLY:HA3	1.28	1.43
7:Q:167:LEU:CA	7:Q:170:SER:O	1.73	1.35
7:K:167:LEU:CA	7:K:170:SER:O	1.73	1.33
1:H:145:PRO:CA	1:H:215:PRO:O	1.80	1.29
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.27
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.25
4:C:269:TYR:O	4:C:271:MET:N	1.68	1.25
4:J:269:TYR:O	4:J:271:MET:N	1.68	1.23
1:H:503:VAL:O	1:H:514:CYS:O	1.53	1.22
7:Q:107:SER:H	6:T:50:GLY:CA	1.53	1.21
6:R:71:GLN:O	6:R:74:ILE:N	1.74	1.21
7:K:107:SER:H	6:M:50:GLY:CA	1.53	1.20
3:I:778:LEU:O	3:I:809:THR:O	1.58	1.20
6:R:143:LEU:C	6:R:145:LEU:H	1.23	1.20
3:B:778:LEU:O	3:B:809:THR:O	1.58	1.19
5:N:13:GLY:HA2	5:N:38:LYS:CA	1.74	1.18
3:B:781:LEU:O	3:B:808:SER:O	1.63	1.16
5:D:13:GLY:HA2	5:D:38:LYS:CA	1.74	1.16
7:G:167:LEU:CA	7:G:170:SER:O	1.95	1.14
3:I:781:LEU:O	3:I:808:SER:O	1.63	1.13
7:Q:190:ILE:CA	7:Q:225:SER:CA	2.26	1.13
6:R:143:LEU:C	6:R:145:LEU:N	1.99	1.12
7:K:190:ILE:CA	7:K:225:SER:CA	2.26	1.12
3:I:778:LEU:O	3:I:809:THR:C	1.91	1.08
8:Z:11:TYR:CA	8:Z:132:GLY:HA3	1.84	1.07
3:B:778:LEU:O	3:B:809:THR:C	1.91	1.06
8:U:11:TYR:CA	8:U:132:GLY:HA3	1.84	1.06
8:S:31:TYR:CA	8:S:131:GLY:O	2.03	1.06
6:R:159:CYS:O	6:R:162:SER:N	1.88	1.05
8:L:31:TYR:CA	8:L:131:GLY:O	2.03	1.05
3:B:526:VAL:CA	3:B:597:VAL:CA	2.35	1.04
3:I:526:VAL:CA	3:I:597:VAL:CA	2.35	1.04
8:Z:12:THR:H	8:Z:132:GLY:CA	1.72	1.03
6:R:130:LEU:O	6:R:132:GLU:N	1.92	1.02
8:U:12:THR:H	8:U:132:GLY:CA	1.72	1.02
7:G:276:ASN:O	7:G:281:SER:O	1.75	1.02
6:R:126:ASN:CA	6:R:158:THR:O	2.10	0.99
7:Q:677:VAL:O	7:Q:694:PRO:CA	2.11	0.98
7:K:677:VAL:O	7:K:694:PRO:CA	2.11	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:167:LEU:C	7:Q:170:SER:O	2.03	0.97
7:K:167:LEU:C	7:K:170:SER:O	2.03	0.96
3:I:541:ALA:CA	3:I:624:ASP:N	2.29	0.96
8:Z:11:TYR:CA	8:Z:132:GLY:CA	2.41	0.96
3:I:778:LEU:C	3:I:809:THR:O	2.04	0.95
3:B:541:ALA:CA	3:B:624:ASP:N	2.29	0.95
8:Z:12:THR:N	8:Z:132:GLY:CA	2.30	0.95
7:K:190:ILE:C	7:K:225:SER:CA	2.34	0.95
7:Q:190:ILE:C	7:Q:225:SER:CA	2.34	0.95
3:B:778:LEU:C	3:B:809:THR:O	2.04	0.95
8:U:12:THR:N	8:U:132:GLY:CA	2.30	0.94
8:U:11:TYR:CA	8:U:132:GLY:CA	2.41	0.94
3:B:824:GLY:CA	3:B:830:ASN:O	2.16	0.93
3:B:766:ASP:O	3:B:768:LEU:N	2.00	0.93
3:I:766:ASP:O	3:I:768:LEU:N	2.00	0.93
3:I:824:GLY:CA	3:I:830:ASN:O	2.16	0.93
8:Z:12:THR:N	8:Z:132:GLY:O	2.02	0.92
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.92
1:H:495:ILE:O	1:H:502:HIS:O	1.87	0.91
6:R:125:ALA:O	6:R:158:THR:O	1.89	0.91
7:K:107:SER:CA	6:M:50:GLY:HA3	2.00	0.91
7:Q:107:SER:CA	6:T:50:GLY:HA3	2.00	0.90
1:H:105:TYR:O	1:H:106:PRO:C	2.08	0.89
8:U:12:THR:N	8:U:132:GLY:O	2.02	0.89
3:B:767:THR:CA	3:B:792:LEU:H	1.85	0.89
3:I:767:THR:CA	3:I:792:LEU:H	1.85	0.89
3:I:781:LEU:CA	3:I:805:LYS:O	2.22	0.88
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.88
7:Q:167:LEU:O	7:Q:170:SER:O	1.92	0.87
1:H:105:TYR:O	1:H:107:TRP:N	2.06	0.87
7:G:198:GLY:O	7:G:201:TYR:N	2.07	0.87
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.87
7:K:167:LEU:O	7:K:170:SER:O	1.92	0.86
7:Q:107:SER:N	6:T:50:GLY:CA	2.24	0.86
3:B:781:LEU:CA	3:B:805:LYS:O	2.22	0.86
7:G:107:SER:N	6:R:50:GLY:CA	2.05	0.86
7:Q:190:ILE:O	7:Q:225:SER:CA	2.23	0.86
7:K:190:ILE:O	7:K:225:SER:CA	2.23	0.85
1:H:503:VAL:O	1:H:514:CYS:C	2.15	0.85
1:H:671:LYS:O	1:H:674:TRP:N	2.08	0.85
6:R:78:TRP:O	6:R:81:TYR:O	1.95	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:190:ILE:CA	7:K:225:SER:N	2.40	0.85
3:I:483:THR:O	3:I:487:ILE:N	2.09	0.85
7:G:107:SER:H	6:R:50:GLY:C	1.79	0.84
7:G:301:ALA:C	7:G:303:LEU:H	1.79	0.84
1:H:214:HIS:O	1:H:217:MET:N	2.11	0.84
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.84
7:G:106:THR:C	6:R:50:GLY:HA3	1.98	0.84
3:B:483:THR:O	3:B:487:ILE:N	2.09	0.84
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.84
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.84
7:Q:190:ILE:CA	7:Q:225:SER:N	2.40	0.84
1:H:671:LYS:O	1:H:673:CYS:N	2.11	0.84
3:B:824:GLY:HA2	3:B:830:ASN:O	1.78	0.83
3:B:739:ASP:O	3:B:740:PRO:O	1.96	0.83
7:K:107:SER:N	6:M:50:GLY:CA	2.24	0.83
3:I:824:GLY:HA2	3:I:830:ASN:O	1.78	0.83
1:A:214:HIS:O	1:A:217:MET:N	2.11	0.83
3:I:739:ASP:O	3:I:740:PRO:O	1.95	0.83
5:N:41:ASN:O	5:N:43:GLY:N	2.12	0.82
3:I:483:THR:O	3:I:484:LYS:C	2.18	0.82
3:B:483:THR:O	3:B:484:LYS:C	2.18	0.81
3:B:767:THR:C	3:B:792:LEU:H	1.84	0.81
3:I:767:THR:C	3:I:792:LEU:H	1.84	0.81
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.81
6:R:130:LEU:C	6:R:132:GLU:H	1.82	0.81
5:D:41:ASN:O	5:D:43:GLY:N	2.12	0.81
6:T:79:ARG:O	6:T:81:TYR:N	2.13	0.81
8:Z:13:VAL:H	8:Z:132:GLY:HA2	1.46	0.81
6:M:79:ARG:O	6:M:81:TYR:N	2.13	0.80
1:H:496:TRP:CA	1:H:502:HIS:CA	2.59	0.80
8:U:11:TYR:C	8:U:132:GLY:HA3	2.02	0.80
5:D:13:GLY:CA	5:D:38:LYS:CA	2.60	0.80
1:H:749:LEU:O	1:H:753:GLY:N	2.15	0.80
8:Z:11:TYR:C	8:Z:132:GLY:HA3	2.02	0.79
8:U:13:VAL:H	8:U:132:GLY:HA2	1.46	0.79
8:U:12:THR:H	8:U:132:GLY:C	1.86	0.79
3:I:740:PRO:O	3:I:741:VAL:C	2.18	0.78
3:B:483:THR:O	3:B:486:ASP:N	2.17	0.78
3:I:483:THR:O	3:I:486:ASP:N	2.17	0.78
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.78
8:Z:12:THR:H	8:Z:132:GLY:C	1.86	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:13:GLY:CA	5:N:38:LYS:CA	2.60	0.77
8:U:12:THR:N	8:U:132:GLY:HA3	2.00	0.77
3:B:766:ASP:C	3:B:768:LEU:H	1.89	0.77
7:G:277:LEU:O	7:G:280:CYS:N	2.16	0.76
8:Z:12:THR:N	8:Z:132:GLY:HA3	2.00	0.76
4:J:637:VAL:O	4:J:638:SER:O	2.03	0.76
4:C:637:VAL:O	4:C:638:SER:O	2.03	0.76
3:B:740:PRO:O	3:B:741:VAL:C	2.18	0.75
7:G:105:VAL:O	7:G:107:SER:N	2.17	0.75
8:Z:12:THR:H	8:Z:132:GLY:HA2	1.51	0.75
6:M:77:LEU:O	6:M:80:HIS:N	2.20	0.74
3:I:766:ASP:C	3:I:768:LEU:H	1.89	0.74
6:T:77:LEU:O	6:T:80:HIS:N	2.20	0.74
1:H:671:LYS:O	1:H:672:ASN:C	2.26	0.73
1:H:800:PRO:O	4:J:805:PHE:O	2.05	0.73
7:G:301:ALA:C	7:G:303:LEU:N	2.41	0.73
6:R:143:LEU:O	6:R:145:LEU:N	2.22	0.72
6:R:174:SER:O	6:R:176:SER:N	2.21	0.72
1:A:800:PRO:O	4:C:805:PHE:O	2.05	0.72
8:U:12:THR:H	8:U:132:GLY:HA2	1.51	0.72
7:G:215:ILE:O	7:G:219:THR:N	2.22	0.72
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.71
3:I:928:LYS:O	3:I:934:PRO:O	2.08	0.71
6:P:29:GLY:HA2	6:P:32:THR:H	1.56	0.71
6:F:29:GLY:HA2	6:F:32:THR:H	1.56	0.71
8:Z:12:THR:N	8:Z:132:GLY:C	2.44	0.71
1:H:671:LYS:C	1:H:673:CYS:N	2.39	0.71
1:H:801:ILE:O	4:J:805:PHE:N	2.24	0.70
5:N:41:ASN:C	5:N:43:GLY:H	1.95	0.70
1:H:496:TRP:CA	1:H:502:HIS:N	2.54	0.70
1:A:801:ILE:O	4:C:805:PHE:N	2.24	0.70
3:B:928:LYS:O	3:B:934:PRO:O	2.08	0.70
7:G:215:ILE:O	7:G:217:LYS:N	2.25	0.70
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.70
7:G:337:ASN:O	7:G:340:ILE:N	2.25	0.69
3:I:766:ASP:C	3:I:768:LEU:N	2.45	0.69
7:G:247:ARG:O	7:G:248:ASP:C	2.24	0.69
1:H:214:HIS:O	1:H:217:MET:CA	2.40	0.69
8:U:12:THR:N	8:U:132:GLY:C	2.44	0.69
7:G:167:LEU:C	7:G:170:SER:O	2.30	0.69
4:J:269:TYR:C	4:J:271:MET:N	2.44	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:41:ASN:C	5:D:43:GLY:H	1.95	0.69
7:K:133:ASP:O	7:K:134:SER:O	2.10	0.69
7:Q:133:ASP:O	7:Q:134:SER:O	2.10	0.69
7:G:172:ASP:O	7:G:175:LYS:N	2.26	0.68
8:U:10:LEU:O	8:U:11:TYR:C	2.32	0.68
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.68
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.68
7:G:247:ARG:O	7:G:248:ASP:O	2.12	0.68
8:Z:10:LEU:O	8:Z:11:TYR:C	2.32	0.68
7:Q:107:SER:CA	6:T:50:GLY:O	2.43	0.67
7:K:107:SER:CA	6:M:50:GLY:O	2.43	0.67
8:U:10:LEU:O	8:U:11:TYR:O	2.13	0.67
3:I:929:PRO:CA	3:I:935:ASP:O	2.44	0.66
8:Z:10:LEU:O	8:Z:11:TYR:O	2.13	0.66
1:H:214:HIS:O	1:H:217:MET:O	2.14	0.66
3:B:779:GLY:O	3:B:808:SER:O	2.14	0.66
3:I:779:GLY:O	3:I:808:SER:O	2.13	0.66
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.66
4:C:269:TYR:C	4:C:271:MET:N	2.44	0.66
6:R:71:GLN:C	6:R:74:ILE:H	2.00	0.66
3:B:929:PRO:CA	3:B:935:ASP:O	2.44	0.66
7:G:277:LEU:CA	7:G:280:CYS:CA	2.73	0.65
1:H:749:LEU:O	1:H:753:GLY:CA	2.44	0.65
7:G:167:LEU:O	7:G:170:SER:O	2.15	0.65
3:I:563:ASP:C	3:I:577:THR:C	2.55	0.65
5:N:39:LEU:C	5:N:41:ASN:H	2.00	0.65
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.65
6:R:71:GLN:O	6:R:74:ILE:CA	2.44	0.65
3:I:112:GLU:O	3:I:114:ILE:N	2.30	0.65
3:B:112:GLU:O	3:B:114:ILE:N	2.30	0.64
3:B:563:ASP:C	3:B:577:THR:C	2.55	0.64
3:B:766:ASP:C	3:B:768:LEU:N	2.45	0.64
5:D:39:LEU:C	5:D:41:ASN:H	2.00	0.64
3:I:766:ASP:O	3:I:792:LEU:O	2.16	0.64
7:Q:135:THR:C	7:Q:137:LEU:H	2.00	0.64
7:K:135:THR:C	7:K:137:LEU:H	2.00	0.63
7:K:243:GLU:O	7:K:245:GLY:N	2.31	0.63
6:M:116:LEU:O	6:M:118:ASN:N	2.32	0.63
1:A:803:PRO:N	4:C:803:GLU:H	1.97	0.63
3:B:766:ASP:O	3:B:792:LEU:O	2.16	0.63
7:Q:243:GLU:O	7:Q:245:GLY:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:824:GLY:HA3	3:B:830:ASN:O	1.96	0.63
1:H:754:GLN:C	1:H:756:SER:H	2.02	0.63
6:T:116:LEU:O	6:T:118:ASN:N	2.32	0.63
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.62
6:M:24:GLY:O	6:M:68:VAL:O	2.17	0.62
7:Q:107:SER:CA	6:T:50:GLY:CA	2.75	0.62
1:H:227:ARG:O	1:H:245:CYS:O	2.18	0.62
6:T:24:GLY:O	6:T:68:VAL:O	2.17	0.62
3:I:824:GLY:HA3	3:I:830:ASN:O	1.96	0.62
1:A:227:ARG:O	1:A:245:CYS:O	2.18	0.61
7:K:107:SER:CA	6:M:50:GLY:CA	2.75	0.61
1:H:803:PRO:N	4:J:803:GLU:H	1.97	0.61
4:C:269:TYR:O	4:C:271:MET:CA	2.49	0.61
4:J:269:TYR:O	4:J:271:MET:CA	2.49	0.61
3:B:739:ASP:O	3:B:740:PRO:C	2.38	0.61
6:R:71:GLN:O	6:R:72:ASP:C	2.39	0.61
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.60
6:R:69:GLY:C	6:R:71:GLN:H	2.04	0.60
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.60
3:I:739:ASP:O	3:I:740:PRO:C	2.38	0.60
7:K:135:THR:O	7:K:137:LEU:N	2.35	0.60
7:G:172:ASP:O	7:G:173:VAL:C	2.36	0.60
7:Q:135:THR:O	7:Q:137:LEU:N	2.35	0.60
3:I:563:ASP:C	3:I:577:THR:CA	2.71	0.59
1:H:214:HIS:O	1:H:217:MET:C	2.40	0.59
7:G:215:ILE:O	7:G:218:PHE:N	2.36	0.59
1:H:205:ASP:H	1:H:207:GLY:H	1.49	0.59
3:B:557:LEU:O	3:B:558:ARG:C	2.41	0.59
3:I:557:LEU:O	3:I:558:ARG:C	2.41	0.59
6:R:159:CYS:O	6:R:162:SER:CA	2.50	0.59
6:T:128:GLN:H	6:T:159:CYS:CA	2.16	0.59
3:B:563:ASP:C	3:B:577:THR:CA	2.71	0.59
3:B:740:PRO:O	3:B:742:TYR:N	2.35	0.59
6:M:128:GLN:H	6:M:159:CYS:CA	2.16	0.59
7:G:215:ILE:C	7:G:217:LYS:H	2.05	0.58
7:G:215:ILE:C	7:G:217:LYS:N	2.55	0.58
3:B:526:VAL:CA	3:B:597:VAL:N	2.67	0.58
3:I:740:PRO:O	3:I:742:TYR:N	2.35	0.58
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.58
7:G:337:ASN:O	7:G:338:ARG:C	2.39	0.58
3:I:779:GLY:N	3:I:809:THR:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:277:LEU:CA	7:G:280:CYS:C	2.72	0.58
6:R:82:TYR:O	6:R:83:ARG:C	2.39	0.58
3:I:504:VAL:O	3:I:507:GLU:N	2.37	0.57
3:B:504:VAL:O	3:B:507:GLU:N	2.37	0.57
3:B:563:ASP:C	3:B:577:THR:O	2.43	0.57
3:I:563:ASP:C	3:I:577:THR:O	2.43	0.57
3:I:526:VAL:CA	3:I:597:VAL:N	2.67	0.57
8:Z:11:TYR:C	8:Z:132:GLY:CA	2.69	0.57
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.57
1:H:671:LYS:C	1:H:673:CYS:H	2.06	0.56
3:B:541:ALA:N	3:B:624:ASP:N	2.53	0.56
7:G:387:CYS:O	7:G:391:PRO:CA	2.53	0.56
1:H:754:GLN:O	1:H:756:SER:N	2.38	0.56
3:B:899:LEU:O	3:B:900:SER:C	2.43	0.56
7:G:277:LEU:CA	7:G:280:CYS:N	2.69	0.56
7:K:274:ILE:O	7:K:276:ASN:N	2.39	0.56
3:I:779:GLY:HA2	3:I:811:ASN:H	1.70	0.56
4:J:269:TYR:C	4:J:271:MET:H	2.02	0.56
3:I:899:LEU:O	3:I:900:SER:C	2.44	0.56
3:B:779:GLY:HA2	3:B:811:ASN:H	1.70	0.56
4:C:269:TYR:C	4:C:271:MET:H	2.02	0.56
7:Q:274:ILE:O	7:Q:276:ASN:N	2.39	0.56
4:C:506:THR:C	4:C:509:GLY:H	2.10	0.55
8:U:11:TYR:C	8:U:132:GLY:CA	2.69	0.55
6:R:69:GLY:O	6:R:71:GLN:N	2.34	0.55
3:I:541:ALA:N	3:I:624:ASP:N	2.53	0.55
4:J:506:THR:C	4:J:509:GLY:H	2.10	0.55
7:G:198:GLY:C	7:G:201:TYR:H	2.07	0.55
3:B:102:LYS:C	3:B:104:THR:H	2.09	0.54
7:K:135:THR:C	7:K:137:LEU:N	2.58	0.54
7:Q:665:CYS:O	7:Q:703:PRO:CA	2.55	0.54
1:A:496:TRP:CA	1:A:502:HIS:H	2.20	0.54
3:I:102:LYS:C	3:I:104:THR:H	2.10	0.54
7:G:106:THR:CA	6:R:50:GLY:HA3	2.36	0.54
7:G:198:GLY:C	7:G:200:LEU:N	2.58	0.54
7:G:726:CYS:O	7:G:753:LEU:O	2.25	0.54
4:J:174:SER:C	4:J:176:SER:H	2.12	0.54
7:Q:107:SER:H	6:T:50:GLY:HA3	0.67	0.54
7:K:665:CYS:O	7:K:703:PRO:CA	2.56	0.54
4:C:375:TYR:O	4:C:388:PHE:CA	2.56	0.54
1:H:343:GLN:CA	1:H:354:VAL:H	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.53
6:M:25:LEU:C	6:M:69:GLY:HA2	2.29	0.53
3:I:112:GLU:C	3:I:114:ILE:H	2.12	0.53
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.53
3:B:767:THR:CA	3:B:792:LEU:N	2.65	0.53
6:T:78:TRP:O	6:T:79:ARG:C	2.46	0.53
6:T:47:PRO:C	6:T:69:GLY:HA3	2.29	0.53
4:J:375:TYR:O	4:J:388:PHE:CA	2.56	0.53
1:H:321:ARG:H	1:H:338:ASP:CA	2.22	0.53
1:H:754:GLN:C	1:H:756:SER:N	2.62	0.53
4:C:174:SER:C	4:C:176:SER:H	2.12	0.52
3:B:112:GLU:C	3:B:114:ILE:H	2.12	0.52
7:G:247:ARG:O	7:G:251:LEU:N	2.37	0.52
6:R:71:GLN:C	6:R:73:ARG:N	2.60	0.52
6:M:47:PRO:C	6:M:69:GLY:HA3	2.29	0.52
7:G:666:THR:O	7:G:668:THR:N	2.43	0.52
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.52
3:I:767:THR:CA	3:I:793:ALA:N	2.73	0.52
1:H:802:MET:O	4:J:804:ALA:CA	2.58	0.52
6:T:25:LEU:C	6:T:69:GLY:HA2	2.29	0.52
1:A:802:MET:O	4:C:804:ALA:CA	2.58	0.52
7:G:274:ILE:O	7:G:275:VAL:C	2.48	0.52
7:G:665:CYS:O	7:G:703:PRO:CA	2.57	0.52
1:H:343:GLN:N	1:H:354:VAL:H	2.06	0.52
3:B:767:THR:CA	3:B:793:ALA:N	2.73	0.52
1:H:495:ILE:O	1:H:502:HIS:C	2.49	0.52
1:H:496:TRP:CA	1:H:502:HIS:H	2.20	0.52
3:I:767:THR:CA	3:I:792:LEU:N	2.65	0.51
7:Q:135:THR:C	7:Q:137:LEU:N	2.58	0.51
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.51
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.51
3:B:767:THR:O	3:B:768:LEU:C	2.49	0.51
6:M:77:LEU:O	6:M:80:HIS:CA	2.59	0.51
6:R:71:GLN:O	6:R:73:ARG:N	2.43	0.51
6:R:135:SER:O	6:R:136:ALA:C	2.48	0.51
3:B:483:THR:O	3:B:484:LYS:O	2.28	0.51
6:T:77:LEU:O	6:T:80:HIS:CA	2.59	0.51
5:N:41:ASN:C	5:N:43:GLY:N	2.60	0.51
7:G:666:THR:O	7:G:667:ASN:C	2.49	0.51
6:R:69:GLY:C	6:R:71:GLN:N	2.65	0.51
6:R:127:LYS:H	6:R:159:CYS:CA	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:173:LEU:C	6:M:175:ASN:H	2.15	0.50
6:M:78:TRP:O	6:M:79:ARG:C	2.46	0.50
3:I:483:THR:O	3:I:484:LYS:O	2.28	0.50
7:G:172:ASP:C	7:G:175:LYS:H	2.14	0.50
7:G:211:VAL:O	7:G:215:ILE:N	2.45	0.50
4:J:459:ARG:CA	4:J:509:GLY:HA3	2.42	0.50
3:I:324:LYS:C	3:I:326:HIS:H	2.15	0.50
4:C:459:ARG:CA	4:C:509:GLY:HA3	2.42	0.49
3:B:324:LYS:C	3:B:326:HIS:H	2.15	0.49
3:B:928:LYS:C	3:B:934:PRO:O	2.51	0.49
7:G:198:GLY:O	7:G:199:LEU:C	2.49	0.49
3:I:928:LYS:C	3:I:934:PRO:O	2.51	0.49
4:C:568:PRO:C	4:C:571:ASN:H	2.16	0.49
6:T:173:LEU:C	6:T:175:ASN:H	2.15	0.49
3:I:767:THR:O	3:I:768:LEU:C	2.49	0.49
7:G:277:LEU:C	7:G:280:CYS:N	2.66	0.48
7:Q:172:ASP:O	7:Q:175:LYS:N	2.46	0.48
7:G:277:LEU:CA	7:G:280:CYS:H	2.26	0.48
4:J:568:PRO:C	4:J:571:ASN:H	2.16	0.48
7:G:246:SER:C	7:G:248:ASP:N	2.66	0.48
4:J:375:TYR:N	4:J:389:GLY:O	2.41	0.48
7:G:441:GLU:O	7:G:444:GLU:O	2.32	0.48
7:G:107:SER:CA	6:R:50:GLY:HA3	2.24	0.48
5:D:39:LEU:C	5:D:41:ASN:N	2.66	0.48
5:D:42:THR:O	5:D:43:GLY:C	2.50	0.48
7:G:460:GLY:HA2	7:G:494:ALA:CA	2.44	0.48
7:K:172:ASP:O	7:K:175:LYS:N	2.46	0.48
3:I:767:THR:CA	3:I:792:LEU:C	2.83	0.48
4:J:637:VAL:O	4:J:638:SER:C	2.52	0.48
4:C:637:VAL:O	4:C:638:SER:C	2.52	0.47
7:Q:666:THR:O	7:Q:668:THR:N	2.47	0.47
6:F:149:ARG:C	6:F:151:ARG:H	2.15	0.47
6:T:173:LEU:C	6:T:175:ASN:N	2.68	0.47
5:N:42:THR:O	5:N:43:GLY:C	2.50	0.47
7:K:666:THR:O	7:K:668:THR:N	2.47	0.47
3:B:767:THR:CA	3:B:792:LEU:C	2.83	0.47
7:G:116:LYS:O	7:G:118:ASP:N	2.48	0.47
7:G:301:ALA:O	7:G:303:LEU:N	2.48	0.47
6:M:173:LEU:C	6:M:175:ASN:N	2.68	0.47
7:K:666:THR:O	7:K:667:ASN:C	2.53	0.47
7:Q:274:ILE:O	7:Q:275:VAL:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:666:THR:O	7:Q:667:ASN:C	2.53	0.47
6:P:149:ARG:C	6:P:151:ARG:H	2.16	0.47
7:K:274:ILE:O	7:K:275:VAL:C	2.52	0.46
7:Q:244:ASP:O	7:Q:245:GLY:C	2.54	0.46
7:G:665:CYS:O	7:G:703:PRO:N	2.48	0.46
6:R:159:CYS:C	6:R:161:THR:N	2.68	0.46
7:K:665:CYS:O	7:K:702:GLN:C	2.54	0.46
3:B:842:MET:O	3:B:888:THR:O	2.34	0.46
7:K:135:THR:O	7:K:136:MET:C	2.54	0.46
7:K:665:CYS:O	7:K:702:GLN:O	2.34	0.46
4:J:86:TYR:C	4:J:88:THR:H	2.19	0.46
4:C:233:SER:H	4:C:248:SER:CA	2.28	0.46
3:I:842:MET:O	3:I:888:THR:O	2.34	0.46
4:J:233:SER:H	4:J:248:SER:CA	2.29	0.46
7:Q:243:GLU:C	7:Q:245:GLY:N	2.69	0.45
7:K:244:ASP:O	7:K:245:GLY:C	2.54	0.45
3:B:751:GLN:C	3:B:753:ASP:H	2.19	0.45
7:Q:665:CYS:O	7:Q:702:GLN:C	2.54	0.45
7:K:695:ALA:O	7:K:696:ARG:C	2.55	0.45
7:Q:135:THR:O	7:Q:136:MET:C	2.54	0.45
4:C:86:TYR:C	4:C:88:THR:H	2.19	0.45
7:G:172:ASP:C	7:G:174:VAL:N	2.66	0.45
7:G:298:SER:O	7:G:300:LYS:N	2.50	0.45
7:Q:166:LEU:O	7:Q:170:SER:N	2.42	0.45
7:K:243:GLU:C	7:K:245:GLY:N	2.69	0.45
7:Q:665:CYS:O	7:Q:702:GLN:O	2.34	0.45
7:K:273:ALA:C	7:K:275:VAL:H	2.21	0.45
1:H:321:ARG:N	1:H:338:ASP:O	2.50	0.45
5:D:41:ASN:C	5:D:43:GLY:N	2.60	0.44
4:C:375:TYR:N	4:C:389:GLY:O	2.41	0.44
7:G:726:CYS:O	7:G:753:LEU:N	2.44	0.44
3:I:751:GLN:C	3:I:753:ASP:H	2.19	0.44
7:G:176:ARG:C	7:G:178:VAL:H	2.21	0.44
7:K:226:PRO:O	7:K:229:TYR:N	2.51	0.43
8:L:49:PHE:O	8:L:53:HIS:N	2.51	0.43
6:F:29:GLY:CA	6:F:32:THR:H	2.26	0.43
7:K:181:ALA:O	7:K:185:ALA:N	2.51	0.43
1:H:749:LEU:O	1:H:753:GLY:HA2	2.18	0.43
5:N:39:LEU:C	5:N:41:ASN:N	2.66	0.43
7:Q:273:ALA:C	7:Q:275:VAL:H	2.21	0.43
7:Q:695:ALA:O	7:Q:696:ARG:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:778:LEU:O	3:I:809:THR:CA	2.65	0.43
7:Q:171:PHE:O	7:Q:174:VAL:N	2.52	0.43
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.43
4:C:484:SER:CA	4:C:522:GLU:H	2.32	0.43
4:C:715:LEU:O	4:C:719:ALA:N	2.51	0.43
7:K:171:PHE:O	7:K:174:VAL:N	2.52	0.43
7:Q:133:ASP:O	7:Q:134:SER:C	2.53	0.43
7:Q:181:ALA:O	7:Q:185:ALA:N	2.51	0.43
6:P:29:GLY:CA	6:P:32:THR:H	2.26	0.43
7:G:274:ILE:O	7:G:275:VAL:O	2.37	0.43
7:K:107:SER:H	6:M:50:GLY:HA3	0.67	0.43
1:A:749:LEU:O	1:A:753:GLY:HA2	2.18	0.42
4:J:484:SER:CA	4:J:522:GLU:H	2.32	0.42
3:B:482:SER:C	3:B:484:LYS:N	2.71	0.42
7:G:107:SER:N	6:R:50:GLY:O	2.52	0.42
8:S:49:PHE:O	8:S:53:HIS:N	2.51	0.42
7:G:529:THR:O	7:G:533:ASN:N	2.52	0.42
7:Q:226:PRO:O	7:Q:229:TYR:N	2.51	0.42
6:R:70:GLY:O	6:R:72:ASP:N	2.52	0.42
4:J:715:LEU:O	4:J:719:ALA:N	2.51	0.42
4:J:690:LEU:O	4:J:694:GLN:N	2.53	0.42
3:B:779:GLY:O	3:B:808:SER:C	2.58	0.42
4:C:690:LEU:O	4:C:694:GLN:N	2.53	0.42
3:I:779:GLY:O	3:I:808:SER:C	2.58	0.42
3:B:267:LEU:C	3:B:269:GLN:H	2.24	0.42
3:I:267:LEU:C	3:I:269:GLN:H	2.23	0.42
7:K:232:MET:O	7:K:236:ALA:N	2.53	0.41
3:I:866:ASN:O	3:I:944:ILE:O	2.39	0.41
5:N:62:GLU:C	5:N:64:LEU:H	2.23	0.41
8:U:12:THR:N	8:U:132:GLY:HA2	2.20	0.41
6:R:109:ARG:C	6:R:112:ASN:H	2.23	0.41
7:Q:232:MET:O	7:Q:236:ALA:N	2.53	0.41
3:B:112:GLU:C	3:B:114:ILE:N	2.72	0.41
3:B:135:THR:O	3:B:139:LEU:N	2.52	0.41
6:M:27:GLY:H	6:M:46:ILE:CA	2.34	0.41
3:I:135:THR:O	3:I:139:LEU:N	2.52	0.41
3:B:767:THR:CA	3:B:793:ALA:CA	2.99	0.41
3:B:866:ASN:O	3:B:944:ILE:O	2.39	0.41
3:B:762:ASN:C	3:B:764:THR:H	2.18	0.41
7:G:215:ILE:O	7:G:216:SER:C	2.60	0.41
1:H:598:LYS:O	1:H:602:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:112:GLU:C	3:I:114:ILE:N	2.72	0.41
3:I:767:THR:CA	3:I:793:ALA:CA	2.99	0.41
4:J:213:ILE:O	4:J:222:VAL:N	2.54	0.41
1:A:598:LYS:O	1:A:602:ALA:N	2.54	0.41
3:B:122:LYS:O	3:B:126:HIS:N	2.54	0.41
4:J:15:SER:H	4:J:293:GLY:HA2	1.86	0.40
4:J:566:TYR:CA	4:J:572:ARG:O	2.69	0.40
4:C:15:SER:H	4:C:293:GLY:HA2	1.86	0.40
4:C:213:ILE:O	4:C:222:VAL:N	2.54	0.40
3:B:782:LYS:N	3:B:805:LYS:O	2.55	0.40
6:R:25:LEU:C	6:R:70:GLY:H	2.24	0.40
6:T:79:ARG:O	6:T:81:TYR:O	2.39	0.40
4:C:566:TYR:CA	4:C:572:ARG:O	2.69	0.40
1:H:373:ALA:C	1:H:375:ASN:N	2.75	0.40
6:T:27:GLY:H	6:T:46:ILE:CA	2.34	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	A	1122/1262 (89%)	891 (79%)	120 (11%)	111 (10%)	0 9
1	H	1122/1262 (89%)	891 (79%)	119 (11%)	112 (10%)	0 9
2	E	290/308 (94%)	276 (95%)	9 (3%)	5 (2%)	9 42
2	O	290/308 (94%)	276 (95%)	9 (3%)	5 (2%)	9 42
3	B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
3	I	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 10
4	C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1 12
4	J	841/905 (93%)	680 (81%)	92 (11%)	69 (8%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	421/511 (82%)	386 (92%)	20 (5%)	15 (4%)	3	25
5	N	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1	13
6	F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1	18
6	M	157/181 (87%)	127 (81%)	12 (8%)	18 (12%)	0	6
6	P	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1	18
6	R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	5
6	T	157/181 (87%)	127 (81%)	12 (8%)	18 (12%)	0	6
7	G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1	15
7	K	556/874 (64%)	475 (85%)	43 (8%)	38 (7%)	1	15
7	Q	556/874 (64%)	475 (85%)	43 (8%)	38 (7%)	1	15
8	L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
8	S	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	16
8	U	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
8	Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	19
All	All	9919/12143 (82%)	8263 (83%)	872 (9%)	784 (8%)	2	13

All (784) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	64	PRO
1	A	92	HIS
1	A	106	PRO
1	A	125	ARG
1	A	169	LYS
1	A	174	PRO
1	A	187	VAL
1	A	215	PRO
1	A	237	SER
1	A	250	ASN
1	A	252	VAL
1	A	271	LYS
1	A	278	MET
1	A	281	ARG
1	A	324	PRO
1	A	325	ALA
1	A	341	LEU

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Mol	Chain	Res	Type
1	A	343	GLN
1	A	384	SER
1	A	454	ASP
1	A	457	PHE
1	A	466	LEU
1	A	479	GLN
1	A	492	LYS
1	A	566	LEU
1	A	583	ARG
1	A	584	GLU
1	A	592	ILE
1	A	593	ASP
1	A	619	LYS
1	A	642	VAL
1	A	671	LYS
1	A	728	ASP
1	A	779	ASP
1	A	788	ILE
1	A	796	GLN
1	A	797	PRO
1	A	798	PRO
1	A	803	PRO
1	A	805	ASP
1	A	811	LEU
1	A	949	VAL
1	A	999	VAL
2	E	111	SER
2	E	231	ARG
3	B	36	PRO
3	B	68	GLU
3	B	109	LEU
3	B	111	HIS
3	B	113	MET
3	B	254	PRO
3	B	255	SER
3	B	329	HIS
3	B	348	ASP
3	B	367	ASN
3	B	385	VAL
3	B	386	SER
3	B	466	SER
3	B	480	TYR

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

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Mol	Chain	Res	Type
4	C	502	HIS
4	C	614	PRO
4	C	615	LYS
4	C	638	SER
4	C	762	LEU
4	C	781	ASN
4	C	782	GLN
4	C	789	ALA
4	C	790	ASP
4	C	806	VAL
4	C	825	PRO
4	C	833	ARG
5	D	12	ALA
5	D	44	LYS
5	D	73	ASN
5	D	96	ALA
6	F	97	ARG
6	F	117	ARG
6	F	131	PRO
7	G	77	PHE
7	G	100	GLU
7	G	106	THR
7	G	132	THR
7	G	151	LYS
7	G	171	PHE
7	G	243	GLU
7	G	261	ASN
7	G	275	VAL
7	G	277	LEU
7	G	283	LYS
7	G	299	PRO
7	G	373	ASP
7	G	394	HIS
7	G	446	CYS
7	G	484	HIS
7	G	608	THR
7	G	621	PRO
7	G	686	ALA
7	G	741	GLU
6	R	42	VAL
6	R	43	ILE
6	R	130	LEU

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Mol	Chain	Res	Type
6	R	131	PRO
6	R	145	LEU
6	R	147	SER
6	R	151	ARG
6	R	175	ASN
8	Z	36	PRO
8	Z	37	SER
8	Z	84	TYR
7	K	134	SER
7	K	135	THR
7	K	170	SER
7	K	171	PHE
7	K	207	ASP
7	K	221	HIS
7	K	225	SER
7	K	226	PRO
7	K	227	PHE
7	K	243	GLU
7	K	275	VAL
7	K	299	PRO
7	K	608	THR
7	K	621	PRO
7	K	741	GLU
7	K	813	CYS
8	L	37	SER
8	L	84	TYR
8	L	147	ALA
6	M	42	VAL
6	M	43	ILE
6	M	44	THR
6	M	51	PHE
6	M	71	GLN
6	M	80	HIS
6	M	118	ASN
6	M	149	ARG
1	H	63	GLN
1	H	64	PRO
1	H	92	HIS
1	H	106	PRO
1	H	125	ARG
1	H	169	LYS
1	H	174	PRO

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Mol	Chain	Res	Type
1	H	187	VAL
1	H	215	PRO
1	H	237	SER
1	H	250	ASN
1	H	252	VAL
1	H	271	LYS
1	H	278	MET
1	H	281	ARG
1	H	324	PRO
1	H	325	ALA
1	H	341	LEU
1	H	343	GLN
1	H	384	SER
1	H	454	ASP
1	H	457	PHE
1	H	466	LEU
1	H	479	GLN
1	H	492	LYS
1	H	566	LEU
1	H	583	ARG
1	H	584	GLU
1	H	592	ILE
1	H	593	ASP
1	H	619	LYS
1	H	642	VAL
1	H	671	LYS
1	H	728	ASP
1	H	779	ASP
1	H	788	ILE
1	H	796	GLN
1	H	797	PRO
1	H	798	PRO
1	H	803	PRO
1	H	805	ASP
1	H	811	LEU
1	H	949	VAL
1	H	999	VAL
2	O	111	SER
2	O	231	ARG
3	I	36	PRO
3	I	68	GLU
3	I	109	LEU

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Mol	Chain	Res	Type
3	I	111	HIS
3	I	113	MET
3	I	254	PRO
3	I	255	SER
3	I	329	HIS
3	I	348	ASP
3	I	367	ASN
3	I	385	VAL
3	I	386	SER
3	I	466	SER
3	I	480	TYR
3	I	484	LYS
3	I	500	GLU
3	I	501	ILE
3	I	502	PRO
3	I	503	ILE
3	I	505	GLU
3	I	521	ILE
3	I	522	THR
3	I	547	PRO
3	I	767	THR
3	I	771	CYS
3	I	826	ALA
3	I	831	CYS
3	I	865	GLU
3	I	899	LEU
3	I	929	PRO
3	I	930	VAL
3	I	934	PRO
3	I	935	ASP
3	I	938	VAL
4	J	27	GLU
4	J	89	LEU
4	J	200	PRO
4	J	228	HIS
4	J	270	GLY
4	J	273	ARG
4	J	325	ALA
4	J	326	ASN
4	J	328	LYS
4	J	329	ALA
4	J	332	ASP

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Mol	Chain	Res	Type
4	J	350	SER
4	J	363	ASN
4	J	365	ARG
4	J	400	SER
4	J	410	SER
4	J	411	ILE
4	J	424	PHE
4	J	451	ASP
4	J	462	GLU
4	J	475	GLU
4	J	484	SER
4	J	502	HIS
4	J	614	PRO
4	J	615	LYS
4	J	638	SER
4	J	762	LEU
4	J	781	ASN
4	J	782	GLN
4	J	789	ALA
4	J	790	ASP
4	J	806	VAL
4	J	825	PRO
4	J	833	ARG
5	N	12	ALA
5	N	44	LYS
5	N	73	ASN
5	N	96	ALA
6	P	97	ARG
6	P	117	ARG
6	P	131	PRO
8	U	36	PRO
8	U	37	SER
8	U	84	TYR
7	Q	134	SER
7	Q	135	THR
7	Q	170	SER
7	Q	171	PHE
7	Q	207	ASP
7	Q	221	HIS
7	Q	225	SER
7	Q	226	PRO
7	Q	227	PHE

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Mol	Chain	Res	Type
7	Q	243	GLU
7	Q	275	VAL
7	Q	299	PRO
7	Q	608	THR
7	Q	621	PRO
7	Q	686	ALA
7	Q	741	GLU
7	Q	813	CYS
8	S	37	SER
8	S	84	TYR
8	S	147	ALA
6	T	42	VAL
6	T	43	ILE
6	T	44	THR
6	T	51	PHE
6	T	71	GLN
6	T	80	HIS
6	T	118	ASN
6	T	149	ARG
1	A	10	ALA
1	A	185	THR
1	A	282	THR
1	A	290	ASP
1	A	345	ASP
1	A	373	ALA
1	A	425	ARG
1	A	498	ALA
1	A	546	SER
1	A	564	LEU
1	A	572	ARG
1	A	622	GLY
1	A	624	SER
1	A	632	LYS
1	A	672	ASN
1	A	787	ASP
1	A	800	PRO
1	A	1178	ARG
3	B	49	ASP
3	B	69	LYS
3	B	162	ARG
3	B	186	PRO
3	B	383	ASN

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Mol	Chain	Res	Type
3	B	445	ARG
3	B	498	LEU
3	B	499	GLY
3	B	551	GLU
3	B	740	PRO
3	B	741	VAL
3	B	751	GLN
3	B	764	THR
3	B	828	ASP
3	B	838	HIS
3	B	862	PHE
3	B	873	ASN
3	B	939	THR
4	C	88	THR
4	C	219	LYS
4	C	428	PHE
4	C	465	PRO
4	C	503	GLU
4	C	504	GLY
4	C	558	ASP
4	C	665	GLU
4	C	787	SER
4	C	793	GLU
4	C	797	LEU
5	D	24	MET
5	D	25	THR
5	D	42	THR
5	D	98	GLU
5	D	136	MET
5	D	387	ASN
5	D	442	LEU
7	G	96	SER
7	G	98	ILE
7	G	105	VAL
7	G	116	LYS
7	G	216	SER
7	G	278	PRO
7	G	310	THR
7	G	463	GLY
7	G	467	ASN
7	G	522	ASN
7	G	633	SER

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Mol	Chain	Res	Type
7	G	718	THR
6	R	72	ASP
6	R	82	TYR
6	R	84	ASN
6	R	95	ASN
6	R	132	GLU
6	R	133	ALA
8	Z	73	ILE
7	K	38	PRO
7	K	116	LYS
7	K	245	GLY
7	K	297	SER
7	K	633	SER
7	K	686	ALA
7	K	718	THR
8	L	12	THR
8	L	69	TYR
8	L	132	GLY
6	M	70	GLY
6	M	129	ASP
6	M	164	GLU
1	H	10	ALA
1	H	185	THR
1	H	282	THR
1	H	290	ASP
1	H	345	ASP
1	H	373	ALA
1	H	425	ARG
1	H	498	ALA
1	H	546	SER
1	H	564	LEU
1	H	572	ARG
1	H	622	GLY
1	H	624	SER
1	H	632	LYS
1	H	672	ASN
1	H	787	ASP
1	H	800	PRO
1	H	1178	ARG
3	I	49	ASP
3	I	69	LYS
3	I	162	ARG

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Mol	Chain	Res	Type
3	I	186	PRO
3	I	383	ASN
3	I	445	ARG
3	I	498	LEU
3	I	499	GLY
3	I	551	GLU
3	I	740	PRO
3	I	741	VAL
3	I	751	GLN
3	I	764	THR
3	I	828	ASP
3	I	838	HIS
3	I	862	PHE
3	I	873	ASN
3	I	939	THR
4	J	88	THR
4	J	219	LYS
4	J	428	PHE
4	J	465	PRO
4	J	503	GLU
4	J	504	GLY
4	J	558	ASP
4	J	665	GLU
4	J	787	SER
4	J	793	GLU
4	J	797	LEU
5	N	24	MET
5	N	25	THR
5	N	42	THR
5	N	98	GLU
5	N	136	MET
8	U	73	ILE
7	Q	38	PRO
7	Q	116	LYS
7	Q	245	GLY
7	Q	297	SER
7	Q	633	SER
7	Q	718	THR
8	S	12	THR
8	S	69	TYR
8	S	132	GLY
6	T	70	GLY

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Mol	Chain	Res	Type
6	T	129	ASP
6	T	164	GLU
1	A	61	LYS
1	A	62	GLN
1	A	168	ARG
1	A	176	ALA
1	A	183	GLY
1	A	218	PRO
1	A	251	ASN
1	A	323	ARG
1	A	340	PHE
1	A	349	SER
1	A	362	LYS
1	A	433	HIS
1	A	481	ARG
1	A	527	ASN
1	A	555	THR
1	A	585	CYS
1	A	686	ASN
1	A	731	GLY
1	A	755	LYS
3	B	216	ASP
3	B	779	GLY
3	B	871	ASN
4	C	140	GLY
4	C	156	ASN
4	C	250	ASP
4	C	259	SER
4	C	351	CYS
4	C	408	SER
4	C	454	ASN
4	C	708	ASN
4	C	763	PRO
5	D	46	HIS
5	D	138	SER
6	F	47	PRO
6	F	84	ASN
6	F	149	ARG
7	G	170	SER
7	G	282	ALA
7	G	297	SER
7	G	391	PRO

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Mol	Chain	Res	Type
7	G	393	LYS
7	G	445	ASP
7	G	447	GLU
7	G	504	GLU
7	G	505	MET
7	G	628	PRO
7	G	641	GLU
7	G	687	TYR
7	G	720	VAL
7	G	761	ALA
6	R	114	ASP
8	Z	147	ALA
7	K	96	SER
7	K	248	ASP
7	K	628	PRO
7	K	641	GLU
7	K	687	TYR
7	K	720	VAL
7	K	761	ALA
8	L	36	PRO
6	M	127	LYS
6	M	135	SER
6	M	165	GLY
1	H	61	LYS
1	H	62	GLN
1	H	168	ARG
1	H	176	ALA
1	H	183	GLY
1	H	218	PRO
1	H	251	ASN
1	H	323	ARG
1	H	340	PHE
1	H	349	SER
1	H	362	LYS
1	H	433	HIS
1	H	481	ARG
1	H	527	ASN
1	H	555	THR
1	H	585	CYS
1	H	686	ASN
1	H	731	GLY
1	H	755	LYS

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Mol	Chain	Res	Type
3	I	216	ASP
3	I	779	GLY
3	I	871	ASN
4	J	140	GLY
4	J	156	ASN
4	J	250	ASP
4	J	259	SER
4	J	351	CYS
4	J	408	SER
4	J	454	ASN
4	J	708	ASN
4	J	763	PRO
5	N	46	HIS
5	N	138	SER
6	P	47	PRO
6	P	84	ASN
6	P	149	ARG
8	U	147	ALA
7	Q	96	SER
7	Q	248	ASP
7	Q	628	PRO
7	Q	641	GLU
7	Q	687	TYR
7	Q	720	VAL
7	Q	761	ALA
8	S	36	PRO
6	T	127	LYS
6	T	135	SER
6	T	165	GLY
1	A	73	TYR
1	A	103	HIS
1	A	170	LYS
1	A	205	ASP
1	A	236	GLU
1	A	330	GLY
1	A	398	LYS
1	A	411	LYS
1	A	424	ASN
1	A	488	ILE
1	A	556	GLY
1	A	783	GLU
1	A	786	PRO

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Mol	Chain	Res	Type
1	A	801	ILE
2	E	113	ASP
3	B	128	ASN
3	B	384	ASN
3	B	425	SER
3	B	447	ASP
3	B	481	CYS
3	B	504	VAL
3	B	752	TYR
3	B	768	LEU
3	B	780	ASP
3	B	827	SER
3	B	837	ILE
3	B	901	GLY
3	B	928	LYS
4	C	165	ARG
4	C	321	GLU
4	C	346	LYS
4	C	401	SER
4	C	409	ASN
4	C	431	GLU
4	C	662	VAL
4	C	821	ALA
6	F	153	TRP
7	G	23	GLU
7	G	428	ASN
7	G	623	PHE
6	R	44	THR
6	R	129	ASP
6	R	158	THR
8	Z	34	THR
7	K	76	LEU
7	K	623	PHE
8	L	86	ASN
6	M	119	ALA
6	M	133	ALA
1	H	73	TYR
1	H	103	HIS
1	H	170	LYS
1	H	205	ASP
1	H	236	GLU
1	H	330	GLY

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Mol	Chain	Res	Type
1	H	398	LYS
1	H	411	LYS
1	H	424	ASN
1	H	488	ILE
1	H	556	GLY
1	H	783	GLU
1	H	786	PRO
1	H	801	ILE
2	O	113	ASP
3	I	128	ASN
3	I	384	ASN
3	I	425	SER
3	I	447	ASP
3	I	481	CYS
3	I	504	VAL
3	I	752	TYR
3	I	768	LEU
3	I	780	ASP
3	I	827	SER
3	I	837	ILE
3	I	901	GLY
3	I	928	LYS
4	J	165	ARG
4	J	321	GLU
4	J	346	LYS
4	J	401	SER
4	J	409	ASN
4	J	431	GLU
4	J	662	VAL
4	J	821	ALA
6	P	153	TRP
8	U	34	THR
7	Q	76	LEU
7	Q	623	PHE
8	S	86	ASN
6	T	119	ALA
6	T	133	ALA
1	A	182	ARG
1	A	195	ALA
1	A	364	PRO
1	A	452	ASN
1	A	517	LYS

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Mol	Chain	Res	Type
1	A	531	LYS
1	A	621	VAL
1	A	644	ASP
1	A	810	LEU
3	B	270	SER
3	B	347	PRO
3	B	825	ALA
4	C	242	PRO
4	C	284	ASN
4	C	473	SER
4	C	737	LYS
5	D	40	MET
5	D	43	GLY
6	F	78	TRP
7	G	99	ALA
7	G	226	PRO
7	G	248	ASP
7	K	40	ASN
7	K	81	ASP
8	L	63	GLU
6	M	151	ARG
1	H	182	ARG
1	H	195	ALA
1	H	364	PRO
1	H	452	ASN
1	H	517	LYS
1	H	531	LYS
1	H	621	VAL
1	H	644	ASP
1	H	810	LEU
3	I	270	SER
3	I	347	PRO
3	I	825	ALA
4	J	242	PRO
4	J	284	ASN
4	J	473	SER
4	J	737	LYS
5	N	40	MET
5	N	43	GLY
6	P	78	TRP
7	Q	40	ASN
7	Q	81	ASP

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Mol	Chain	Res	Type
8	S	63	GLU
6	T	151	ARG
1	A	643	LYS
1	A	802	MET
3	B	86	ASP
3	B	104	THR
4	C	25	PRO
7	G	152	VAL
6	R	49	ILE
8	Z	54	ARG
7	K	37	THR
7	K	694	PRO
1	H	643	LYS
1	H	802	MET
3	I	86	ASP
3	I	104	THR
4	J	25	PRO
8	U	54	ARG
7	Q	37	THR
7	Q	694	PRO
4	C	312	GLY
7	K	274	ILE
4	J	312	GLY
7	Q	274	ILE
1	A	22	PRO
1	A	503	VAL
1	A	615	VAL
2	E	213	SER
4	C	112	PRO
6	R	163	GLY
6	M	148	ILE
1	H	22	PRO
1	H	503	VAL
1	H	615	VAL
2	O	213	SER
4	J	112	PRO
6	T	148	ILE
1	A	133	GLY
1	A	259	PRO
6	F	43	ILE
7	G	820	PRO
7	K	820	PRO

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Mol	Chain	Res	Type
1	H	133	GLY
1	H	259	PRO
6	P	43	ILE
7	Q	820	PRO
7	G	694	PRO
2	E	45	SER
3	B	516	LYS
1	H	575	GLY
2	O	45	SER
3	I	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)

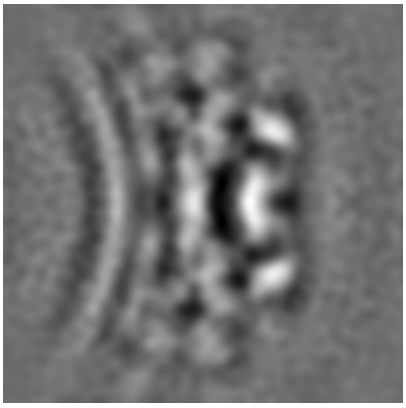
This section contains visualisations of the EMDB entry EMD-3724. These allow visual inspection of the internal detail of the map and identification of artifacts.

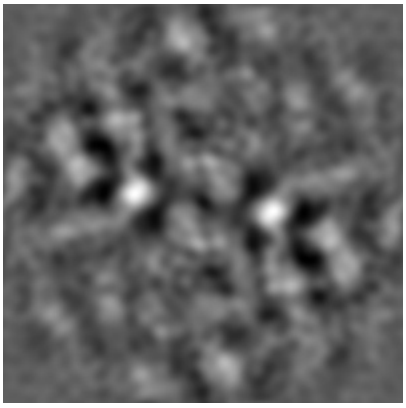
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map

X


Y

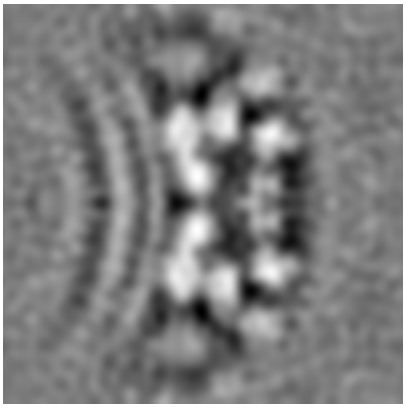

Z

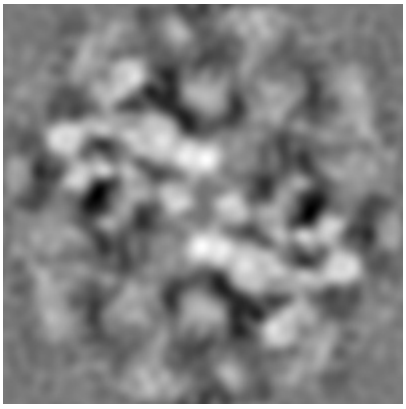
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 106


Y Index: 106

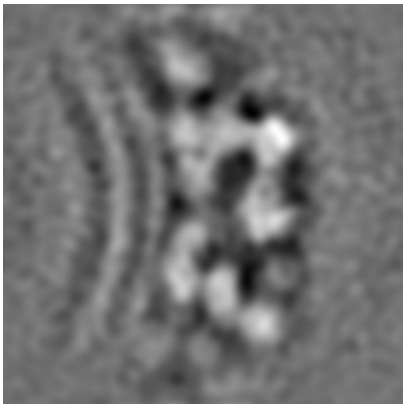

Z Index: 106

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

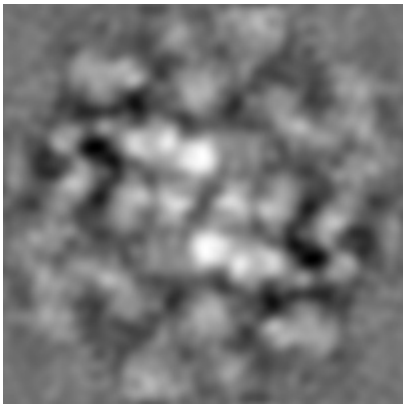
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 106



Y Index: 100



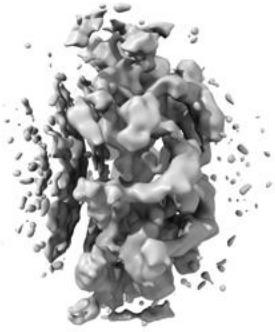
Z Index: 101

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

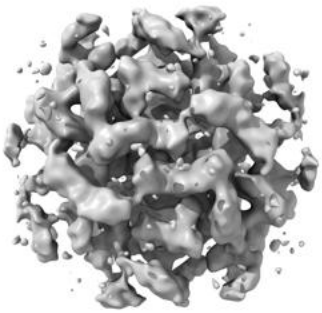
6.4 Orthogonal surface views (i)

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.

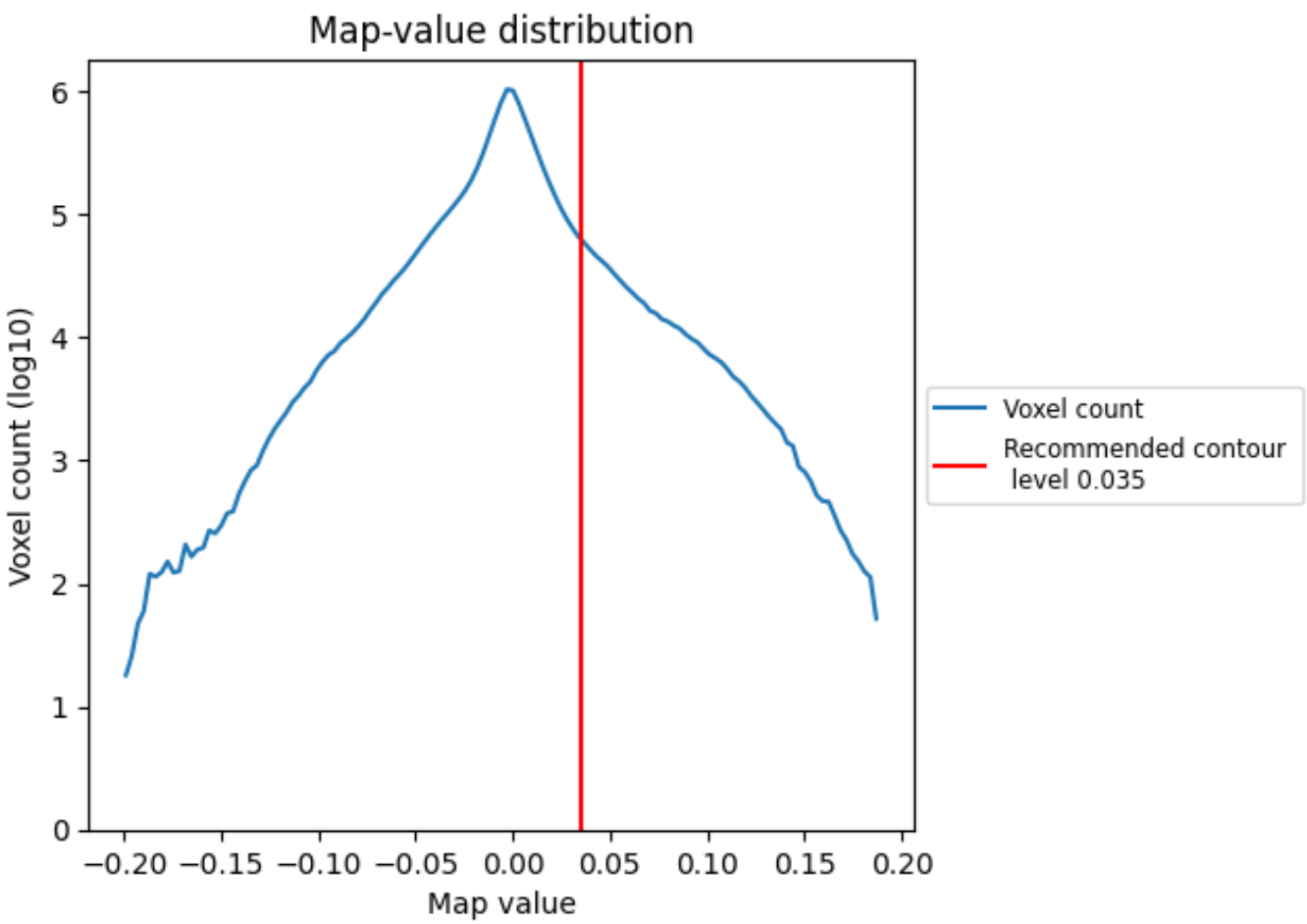
6.5 Mask visualisation (i)

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

7 Map analysis (i)

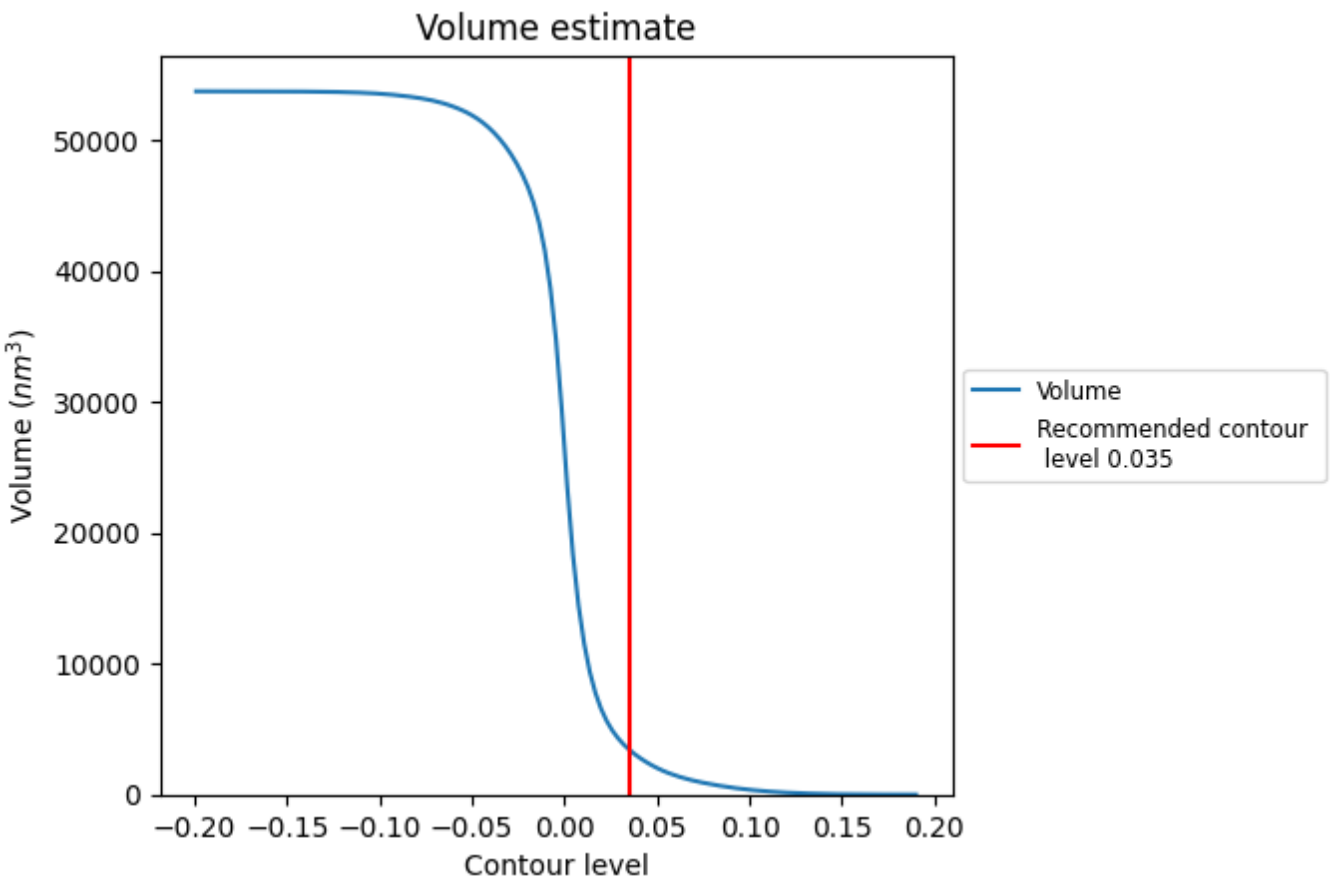
This section contains the results of statistical analysis of the map.

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.

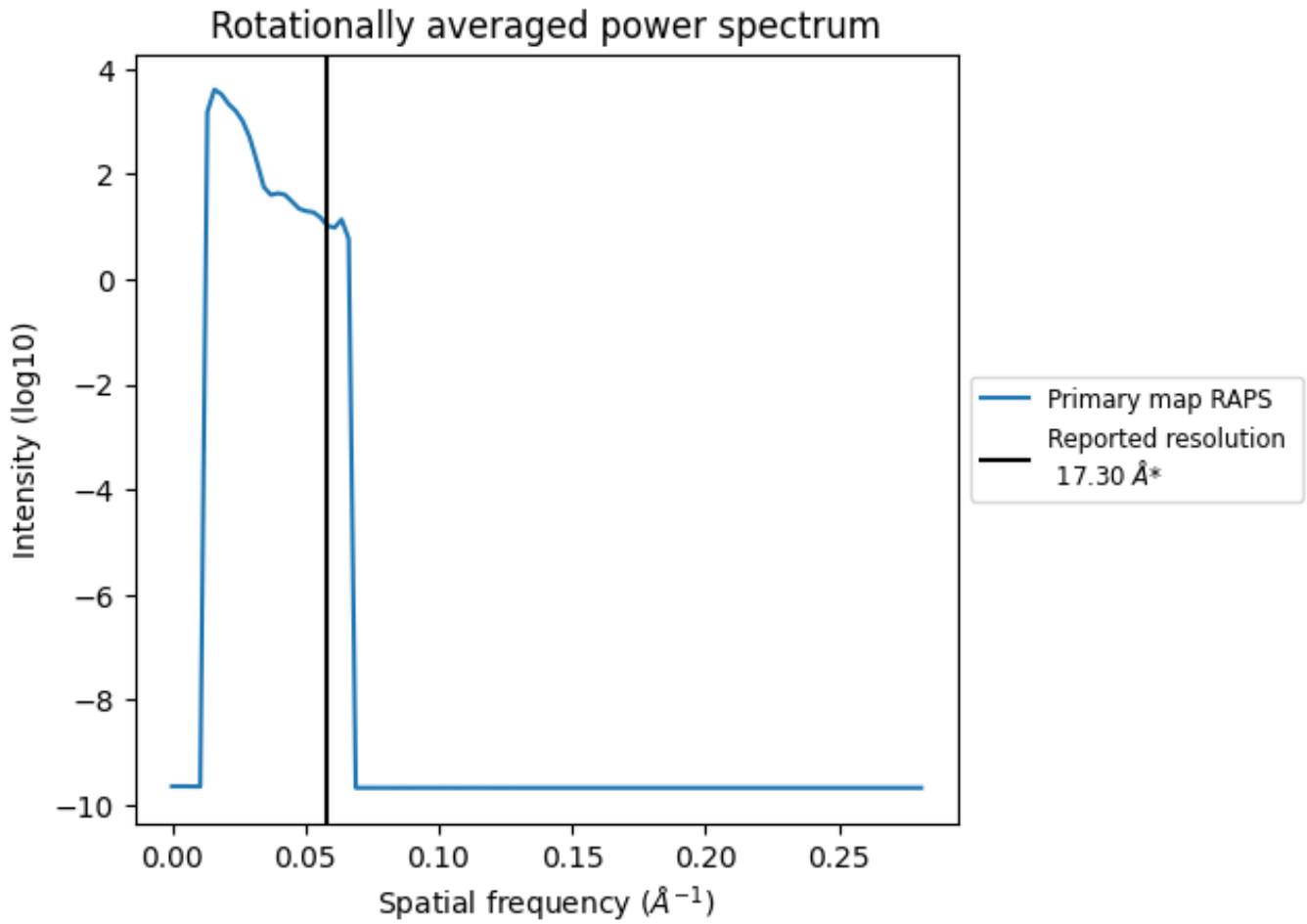
7.2 Volume estimate (i)



The volume at the recommended contour level is 3439 nm^3; this corresponds to an approximate mass of 3106 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)

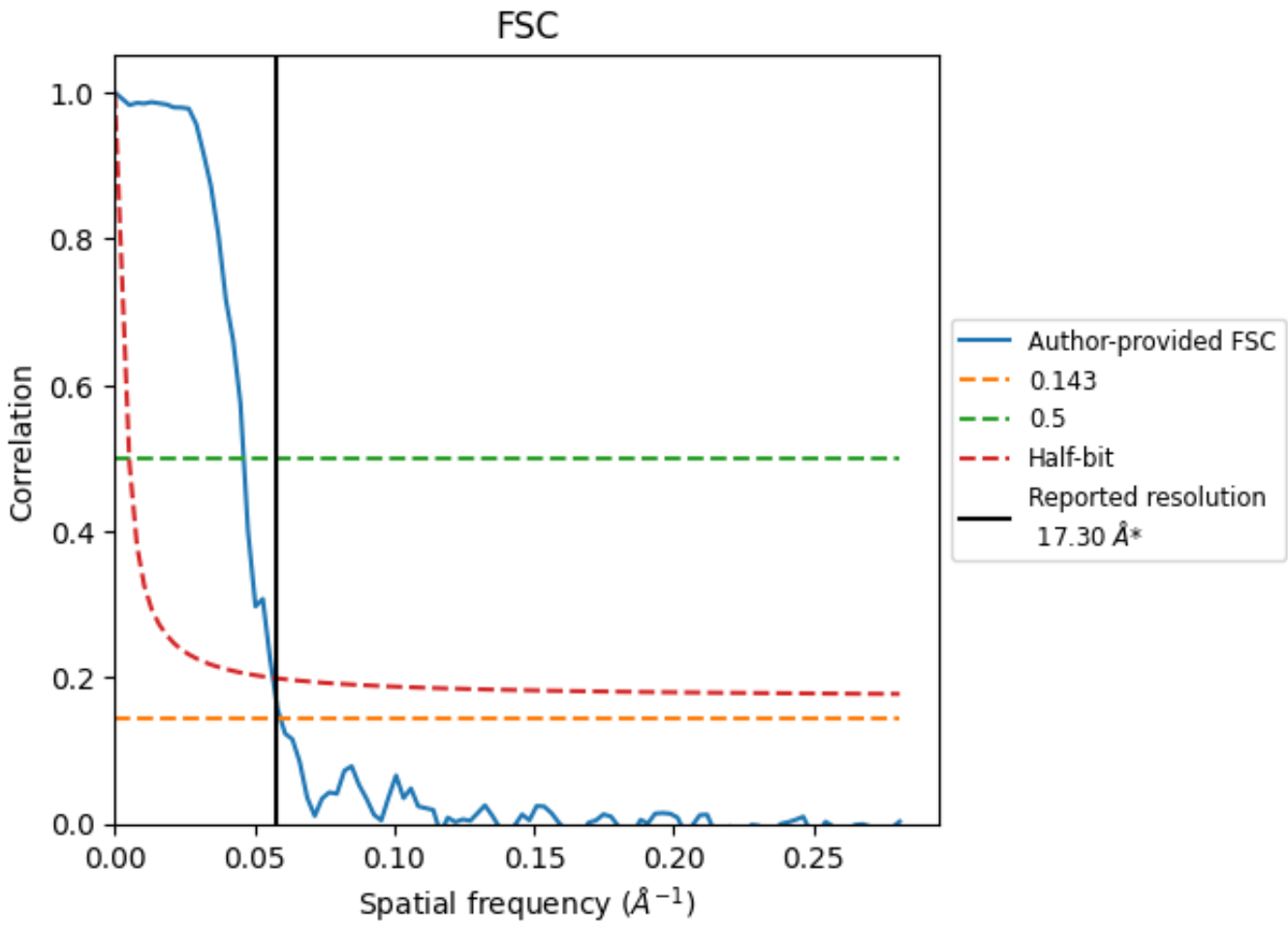


*Reported resolution corresponds to spatial frequency of 0.058 Å^{-1}

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 0.058 Å^{-1}

8.2 Resolution estimates (i)

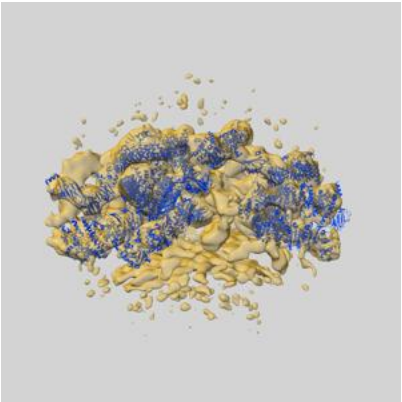
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	17.30	-	-
Author-provided FSC curve	16.86	21.65	17.67
Unmasked-calculated*	-	-	-

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

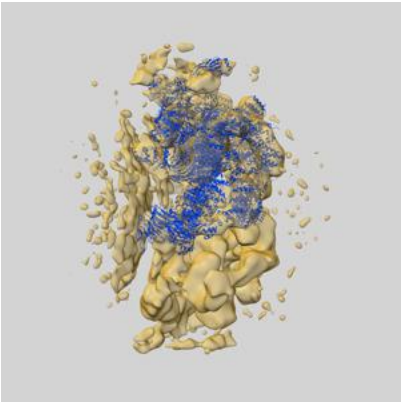
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3724 and PDB model 5NZV. Per-residue inclusion information can be found in section 3 on page 9.

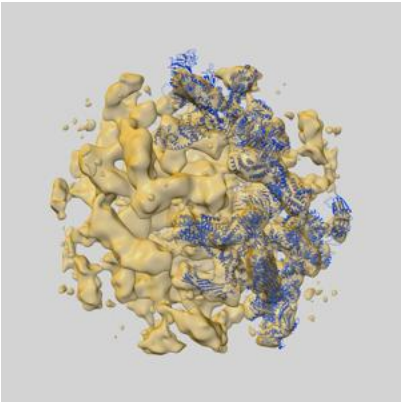
9.1 Map-model overlay (i)



X



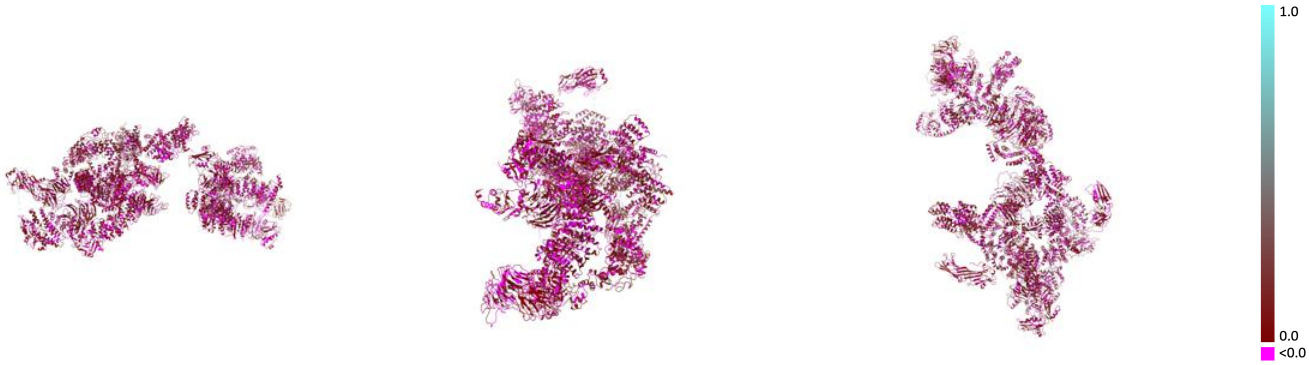
Y



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.

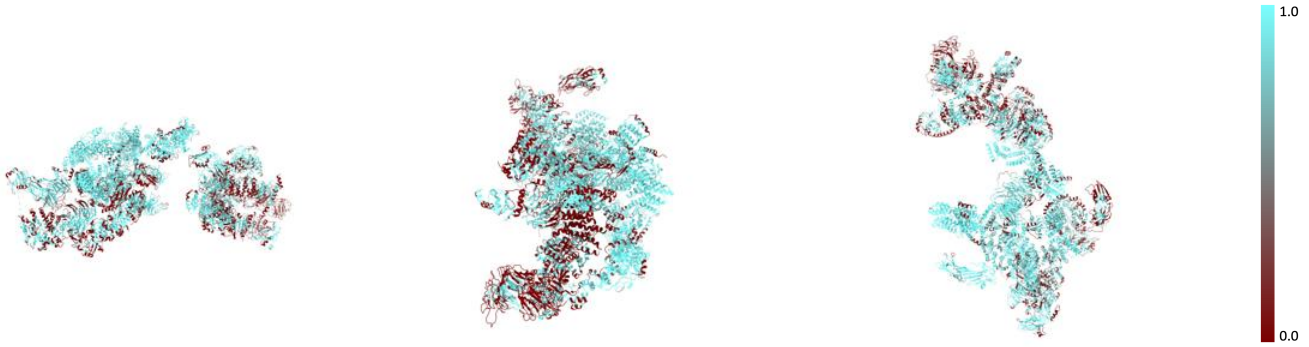
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

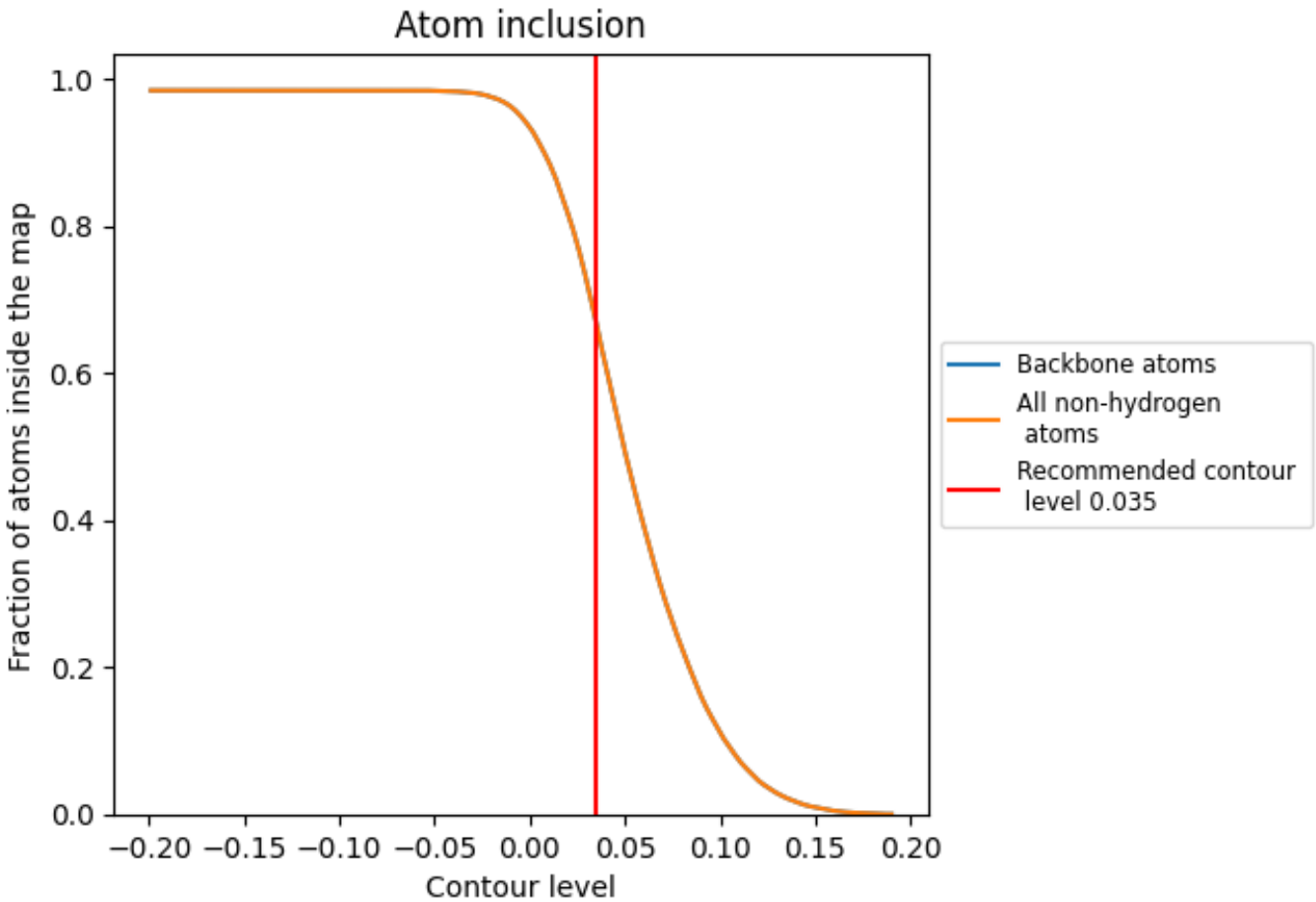
9.3 Atom inclusion mapped to coordinate model (i)



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, 67% of all backbone atoms, 67% 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	Q-score
All	0.6677	0.0620
A	0.9061	0.0780
B	0.8002	0.0730
C	0.7843	0.0790
D	0.8278	0.0730
E	0.9162	0.0920
F	0.9307	0.0660
G	0.5781	0.0480
H	0.5563	0.0460
I	0.3852	0.0440
J	0.6170	0.0610
K	0.5587	0.0640
L	0.5928	0.0520
M	0.6772	0.0670
N	0.5977	0.0550
O	0.7853	0.0570
P	0.6205	0.0640
Q	0.5757	0.0600
R	0.4268	0.0720
S	0.5982	0.0460
T	0.5024	0.0490
U	0.5964	0.0740
Z	0.6757	0.0480