Full wwPDB EM Validation Report ⓘ

May 31, 2022 – 07:20 pm BST

PDB ID	:	7R4Q
EMDB ID	:	EMD-14314
Title	:	The SARS-CoV-2 spike in complex with the 1.29 neutralizing nanobody
Authors	:	Casasnovas, J.M.; Melero, R.; Arranz, R.; Fernandez, L.A.
Deposited on	:	2022-02-09
Resolution	:	3.60 Å(reported)
Based on initial models	:	6ZXN, 3TPK

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 ⓘ symbol.

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

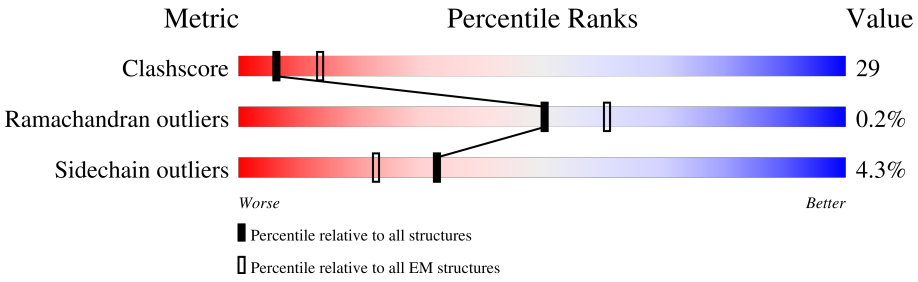
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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
Sidechain outliers	154315	3826

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	1264	28% 51% 25% 5% • 16%
1	B	1264	25% 49% 27% 5% • 17%
1	C	1264	25% 51% 25% 6% • 16%
2	D	126	44% 37% 56% • 5%
2	E	126	25% 36% 56% • 5%
3	F	2	50% 50% 50%
3	G	2	100% 100%
3	H	2	100% 100%

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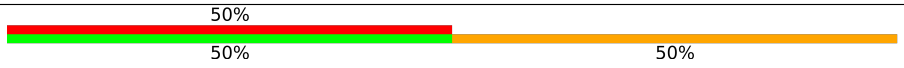
Mol	Chain	Length	Quality of chain
3	I	2	
3	J	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1307	-	-	X	-
4	NAG	B	1310	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 51957 atoms, of which 24719 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1060	Total	C	H	N	O	S	3	0
			16380	5297	8079	1383	1583	38		
1	B	1054	Total	C	H	N	O	S	3	0
			16287	5268	8034	1376	1571	38		
1	C	1060	Total	C	H	N	O	S	1	0
			16361	5292	8069	1382	1580	38		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	TYR	-	expression tag	UNP P0DTC2
A	1215	ILE	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	GLU	-	expression tag	UNP P0DTC2
A	1218	ALA	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	ASP	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLN	-	expression tag	UNP P0DTC2
A	1224	ALA	-	expression tag	UNP P0DTC2
A	1225	TYR	-	expression tag	UNP P0DTC2
A	1226	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	LYS	-	expression tag	UNP P0DTC2
A	1229	ASP	-	expression tag	UNP P0DTC2
A	1230	GLY	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	TRP	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	SER	-	expression tag	UNP P0DTC2
A	1237	THR	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	ASN	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	TYR	-	expression tag	UNP P0DTC2
A	1246	PHE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	TYR	-	expression tag	UNP P0DTC2
A	1251	LYS	-	expression tag	UNP P0DTC2
A	1252	ASP	-	expression tag	UNP P0DTC2
A	1253	ASP	-	expression tag	UNP P0DTC2
A	1254	ASP	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	LYS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	HIS	-	expression tag	UNP P0DTC2
A	1264	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	TYR	-	expression tag	UNP P0DTC2
B	1215	ILE	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	GLU	-	expression tag	UNP P0DTC2
B	1218	ALA	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	ASP	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLN	-	expression tag	UNP P0DTC2
B	1224	ALA	-	expression tag	UNP P0DTC2
B	1225	TYR	-	expression tag	UNP P0DTC2
B	1226	VAL	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	LYS	-	expression tag	UNP P0DTC2
B	1229	ASP	-	expression tag	UNP P0DTC2
B	1230	GLY	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	TRP	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	SER	-	expression tag	UNP P0DTC2
B	1237	THR	-	expression tag	UNP P0DTC2
B	1238	PHE	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	ASN	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	TYR	-	expression tag	UNP P0DTC2
B	1246	PHE	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	TYR	-	expression tag	UNP P0DTC2
B	1251	LYS	-	expression tag	UNP P0DTC2
B	1252	ASP	-	expression tag	UNP P0DTC2
B	1253	ASP	-	expression tag	UNP P0DTC2
B	1254	ASP	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	LYS	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	HIS	-	expression tag	UNP P0DTC2
B	1264	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	TYR	-	expression tag	UNP P0DTC2
C	1215	ILE	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	GLU	-	expression tag	UNP P0DTC2
C	1218	ALA	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	ASP	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLN	-	expression tag	UNP P0DTC2
C	1224	ALA	-	expression tag	UNP P0DTC2
C	1225	TYR	-	expression tag	UNP P0DTC2
C	1226	VAL	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	ASP	-	expression tag	UNP P0DTC2
C	1230	GLY	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	TRP	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	SER	-	expression tag	UNP P0DTC2
C	1237	THR	-	expression tag	UNP P0DTC2
C	1238	PHE	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	ASN	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	TYR	-	expression tag	UNP P0DTC2
C	1246	PHE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	TYR	-	expression tag	UNP P0DTC2
C	1251	LYS	-	expression tag	UNP P0DTC2
C	1252	ASP	-	expression tag	UNP P0DTC2
C	1253	ASP	-	expression tag	UNP P0DTC2
C	1254	ASP	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	LYS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	HIS	-	expression tag	UNP P0DTC2
C	1264	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Camel-derived nanobody 1.29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	120	Total	C	N	O	S	0	0
			895	554	154	184	3		

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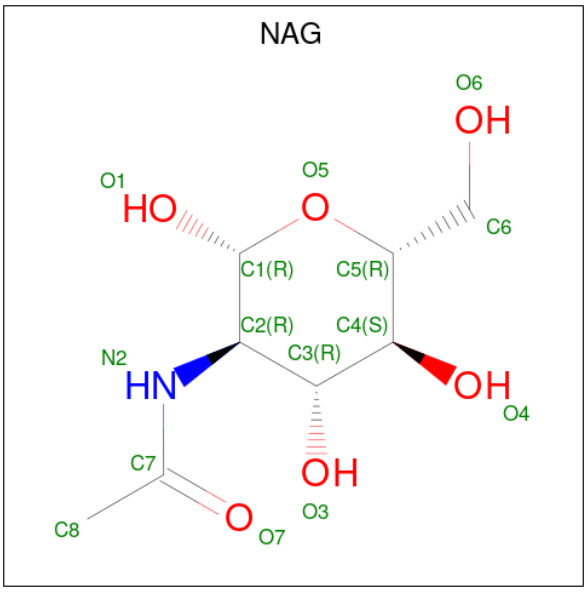
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	120	Total	C	N	O	S	0	0
			895	554	154	184	3		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	J	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0

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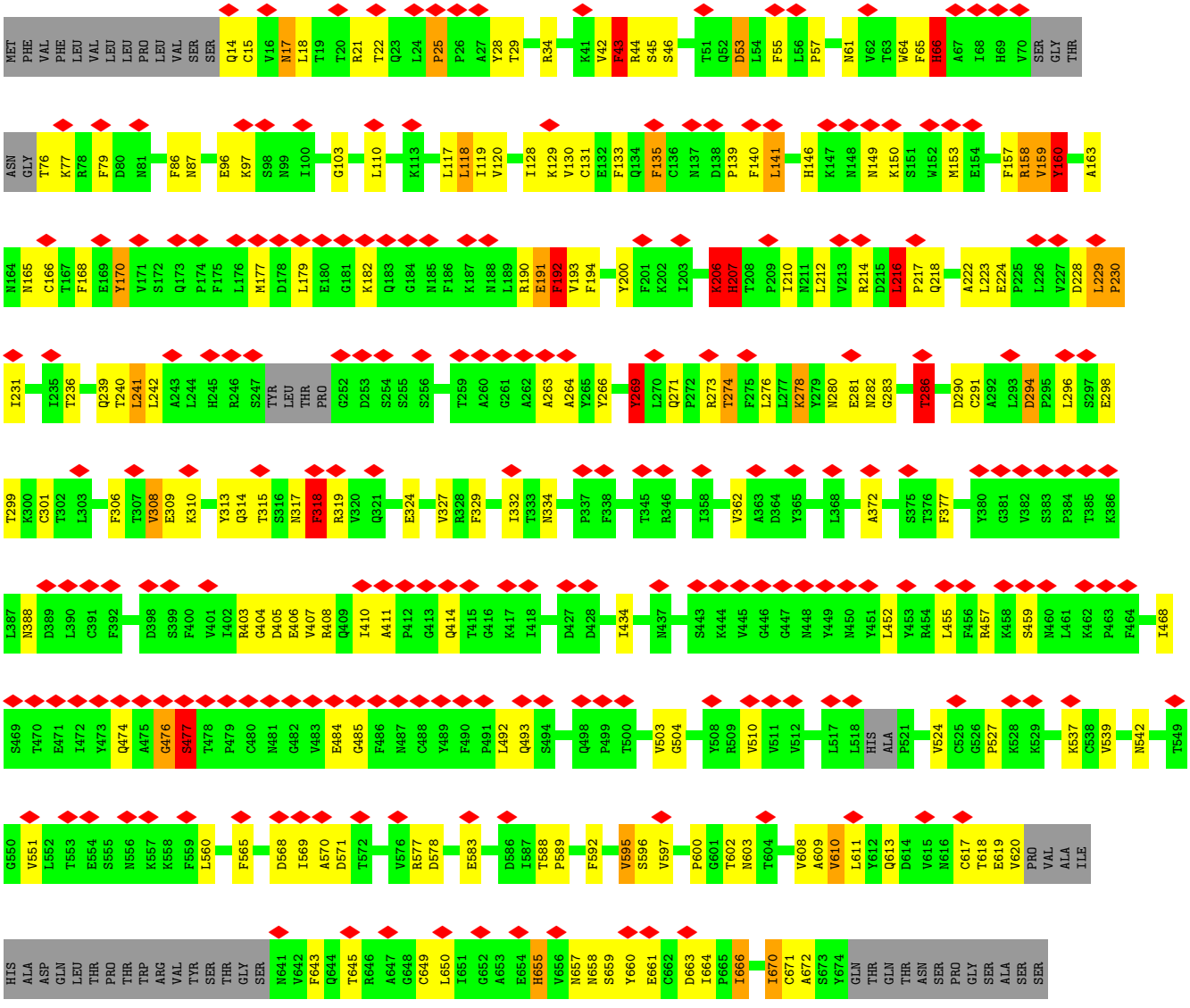
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	B	1	349	104	167	13	65	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0
4	C	1	148	48	64	6	30	0

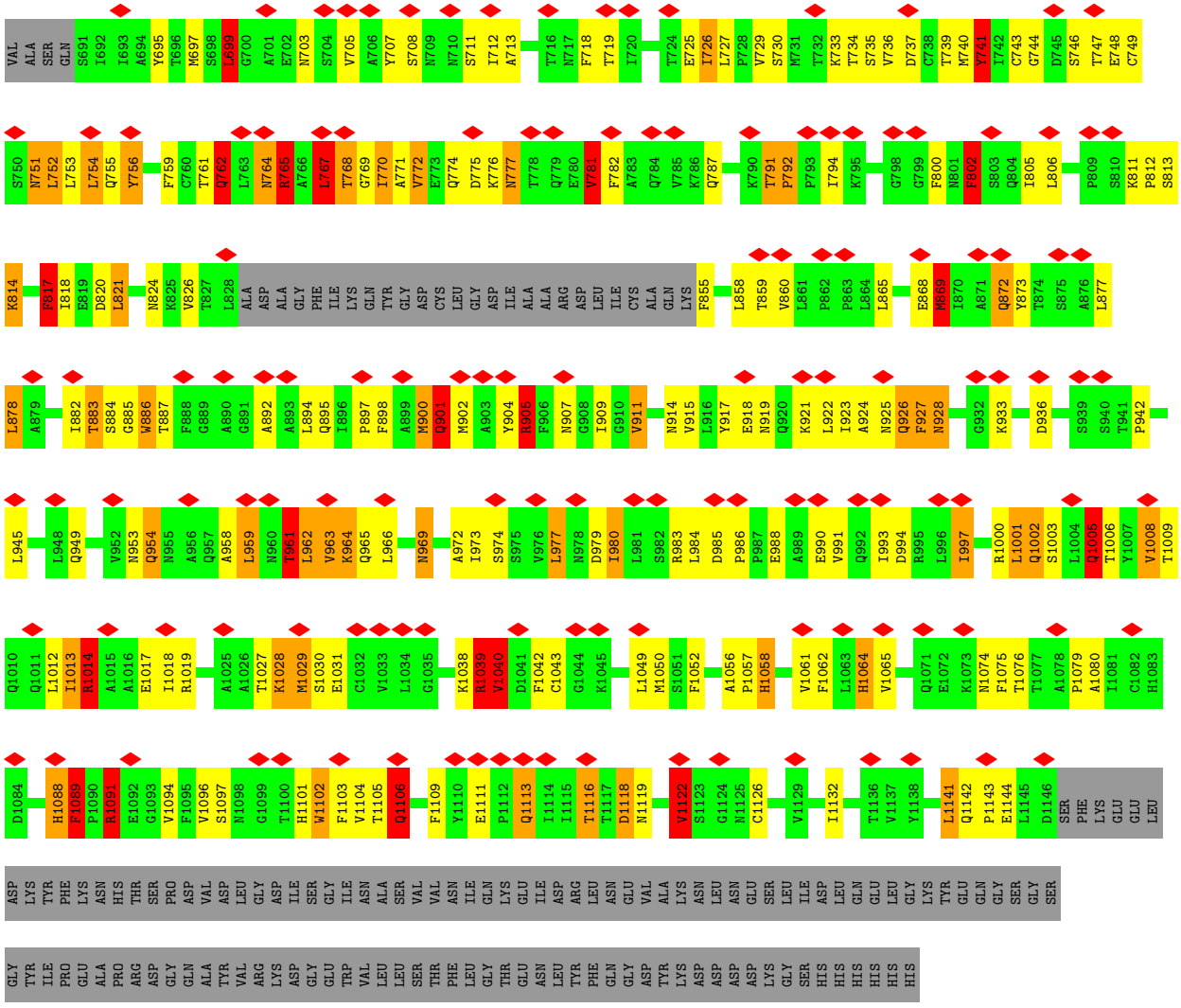
3 Residue-property plots (i)

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: Spike glycoprotein

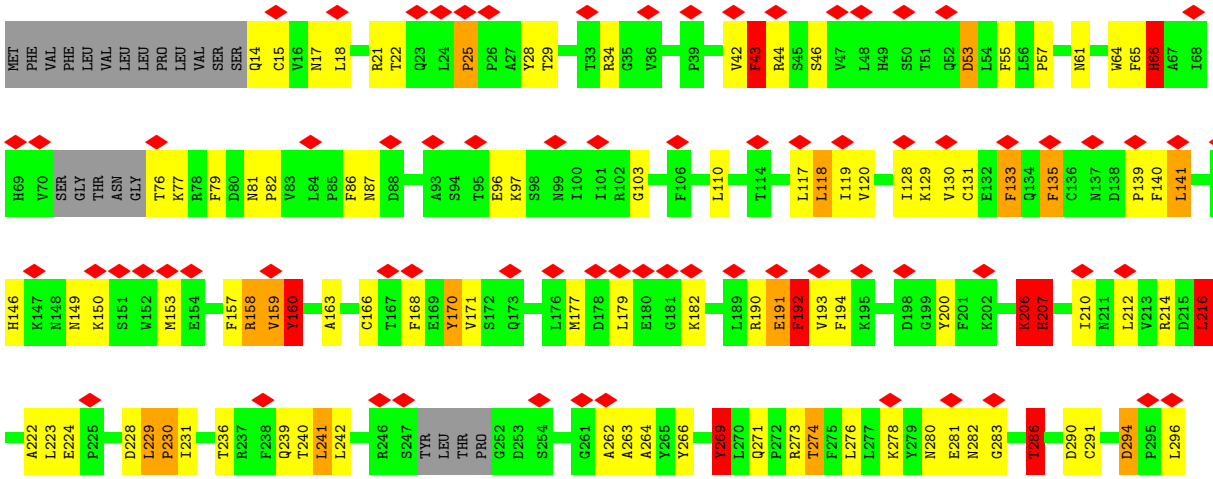
Chain A:

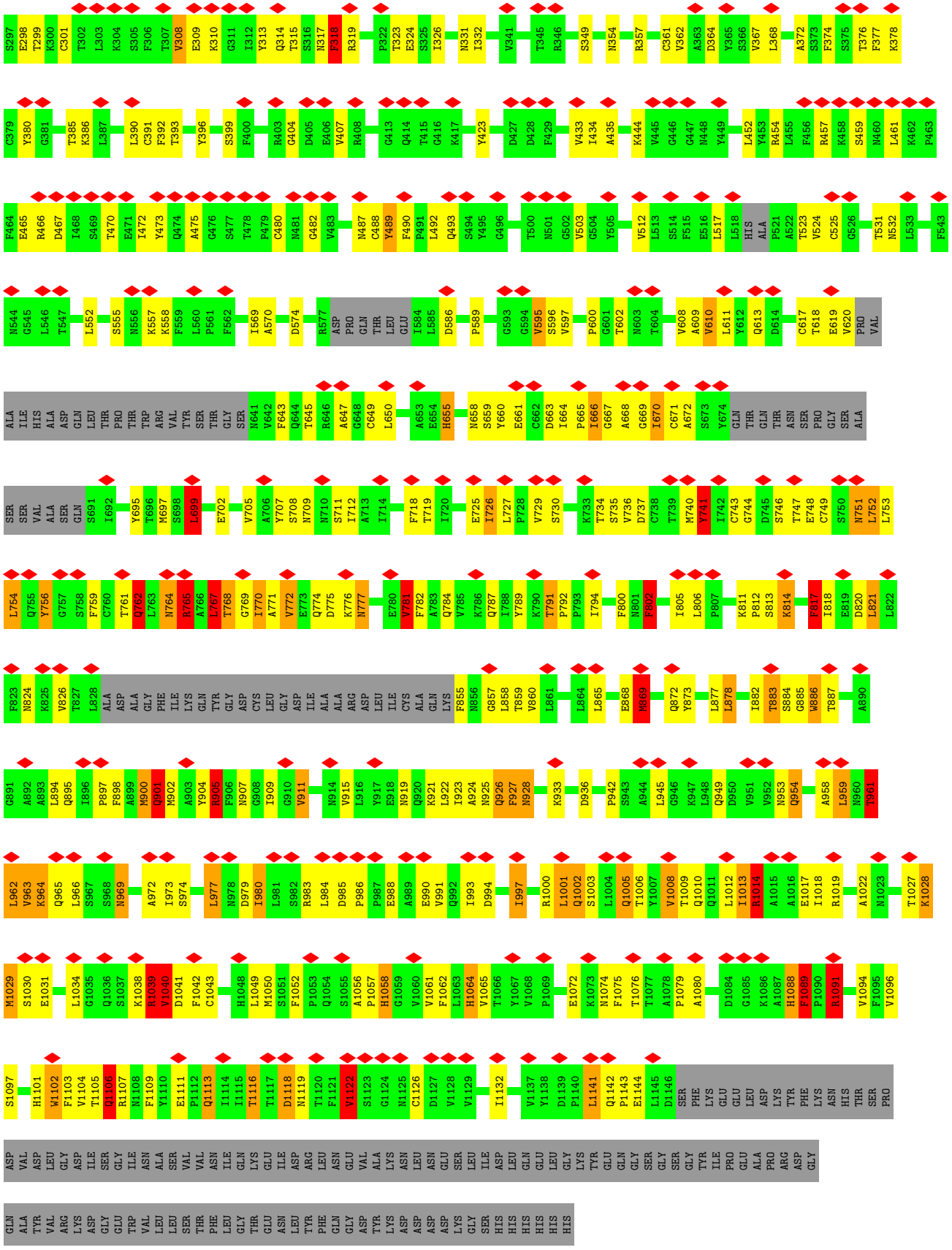




• Molecule 1: Spike glycoprotein

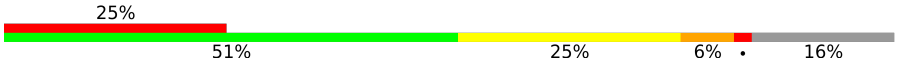
Chain B:

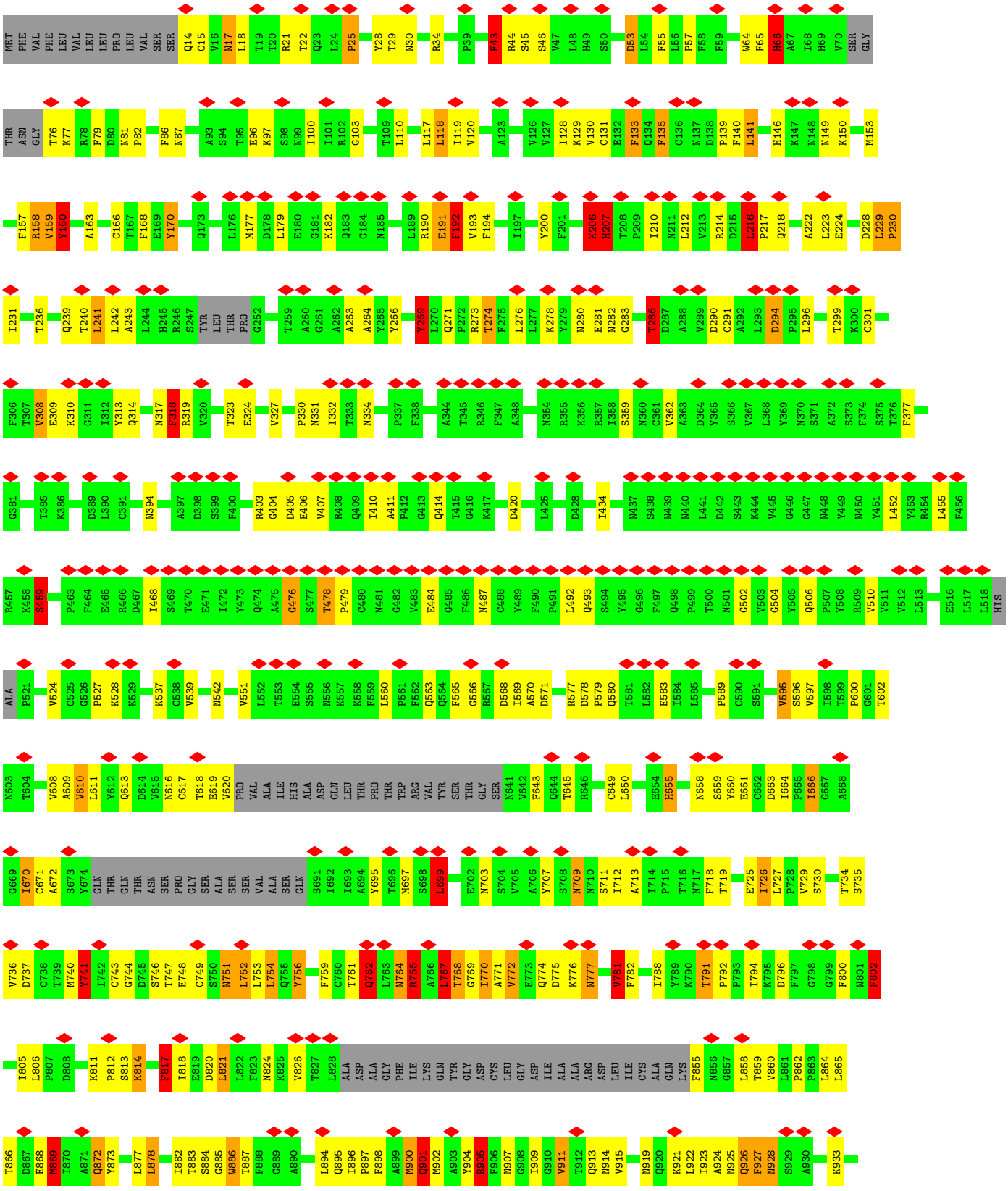




• Molecule 1: Spike glycoprotein

Chain C:


25%
51%
25%
6%
16%


MET Q14 C15
PHE V16 N17
VAL L18
PHE T19 T20
LEU R21 T22
LEU Q23 L24
LEU P25
VAL Y28 T29
PRO N30
LEU R34
SER P39 F43
SER R44 S45 S46
V47 L48
H49 S50
D53 L54
F55 L56
P57 F58
F59 W64
F65 H66
A67 I68
H69 V70
SER GLY
THR T76 K77
ASN R78 F79
GLY D80 N81
P82 F86
N87 A93
S94 T95
E96 K97
S98 N99
I100 I101
R102 G103
T109 L110
L117 L118
I119 V120
A123 V126
V127 I128
K129 V130
C131 E132
F133 Q134
F135 C136
N137 D138
P139 F140
L141 H146
K147 N148
N149 K150
M153
F157 R158
V159 Y160
A163 C166
T167 F168
E169 Y170
Q173 L176
M177 D178
L179 E180
G181 K182
Q183 G184
N185 L189
R190 E191
F192 V193
F194 I197
Y200 F201
K206 H207
T208 P209
I210 N211
L212 V213
R214 D215
L216 P217
Q218 A222
L223 E224
D228 L229
P230
I231 T236
Q239 T240
L241 L242
A243 L244
H245 R246
S247 TYR
LEU THR
PRO G252
T259 A260
G261 A262
A263 A264
Y265 Y266
Y269 L270
Q271 P272
R273 T274
F275 L276
L277 K278
Y279 N280
E281 N282
G283 T286
D287 A288
V289 D290
C291 A292
L293 D294
P295 L296
T299 K300
C301
F306 T307
V308 E309
K310 G311
I312 Y313
Q314 N317
F318 R319
V320 T323
E324 V327
P330 N331
I332 T333
N334 P337
F338 A344
T345 R346
F347 A348
N354 R355
K356 R357
I358 S359
N360 C361
V362 A363
D364 Y365
S366 V367
L368 Y369
N370 S371
A372 S373
F374 S375
T376 F377
G381 T385
K386 D389
L390 C391
N394 A397
D398 S399
F400 R403
G404 D405
E406 V407
R408 Q409
I410 A411
P412 G413
Q414 T415
G416 K417
D420 L425
D428 I434
N437 S438
N439 N440
L441 D442
S443 K444
V445 G446
G447 N448
Y449 N450
Y451 L452
Y453 R454
L455 F456
R457 K458
S459 P463
F464 E465
R466 D467
I468 S469
T470 E471
I472 Y473
Q474 A475
G476 S477
T478 P479
C480 N481
G482 V483
E484 G485
F486 N487
C488 Y489
F490 P491
L492 Q493
S494 Y495
G496 F497
Q498 P499
T500 N501
G502 V503
G504 Y505
Q506 P507
Y508 R509
V510 V511
V512 L513
E516 L517
L518 HIS
ALA P521
V524 C525
G526 P527
K528 K529
K537 C538
V539 N542
V551 L552
T553 E554
S555 N556
K557 K558
F559 L560
P561 F562
Q563 Q564
F565 G566
R567 D568
I569 A570
D571 R577
D578 P579
Q580 T581
L582 E583
I584 L585
P589 C590
S591 V595
S596 V597
I598 T599
P600 G601
T602
N603 T604
V608 A609
V610 L611
Y612 Q613
D614 V615
N616 C617
T618 E619
V620 PRO
VAL ALA
ILE HIS
ALA ASP
GLN LEU
THR PRO
THR TRP
ARG VAL
TYR SER
THR GLY
SER N641
V642 F643
Q644 T645
R646 C649
L650 E654
H655 N658
S659 Y660
E661 C662
D663 I664
P665 I666
G667 A668
G669 I670
C671 A672
S673 Y674
GLN THR
GLN THR
ASN SER
PRO GLY
SER ALA
SER SER
VAL ALA
ALA SER
GLN S691
I692 I693
A694 Y695
T696 M697
S698 L699
E702 N703
S704 V705
A706 Y707
S708 N709
N710 S711
I712 A713
I714 P715
T716 N717
F718 T719
E725 I726
L727 P728
V729 S730
T734 S735
V736 D737
C738 T739
M740 Y741
I742 C743
G744 D745
S746 T747
E748 C749
S750 N751
L752 L753
L754 Q755
Y756 F759
C760 T761
Q762 L763
N764 R765
A766 L767
T768 G769
I770 A771
V772 E773
Q774 D775
K776 N777
V781 F782
I788 Y789
K790 T791
P792 P793
I794 K795
D796 F797
G798 G799
F800 N801
F802
I805 L806
P807 D808
K811 P812
S813 K814
F817 I818
E819 D820
L821 L822
F823 N824
K825 V826
T827 L828
ALA ASP
ALA GLY
PHE ILE
LYS GLN
TYR GLY
ASP CYS
LEU GLY
ASP ILE
ALA ALA
ARG ASP
LEU ILE
CYS ALA
GLN LYS
F855 N856
G857 L858
T859 V860
L861 P862
P863 L864
L865
T866 D867
E868 M869
I870 A871
Q872 Y873
L877 L878
I882 T883
S884 G885
W886 T887
F888 G889
A890 L894
Q895 I896
P897 F898
A899 M900
Q901 M902
A903 Y904
R905 F906
N907 G908
I909 G910
V911 T912
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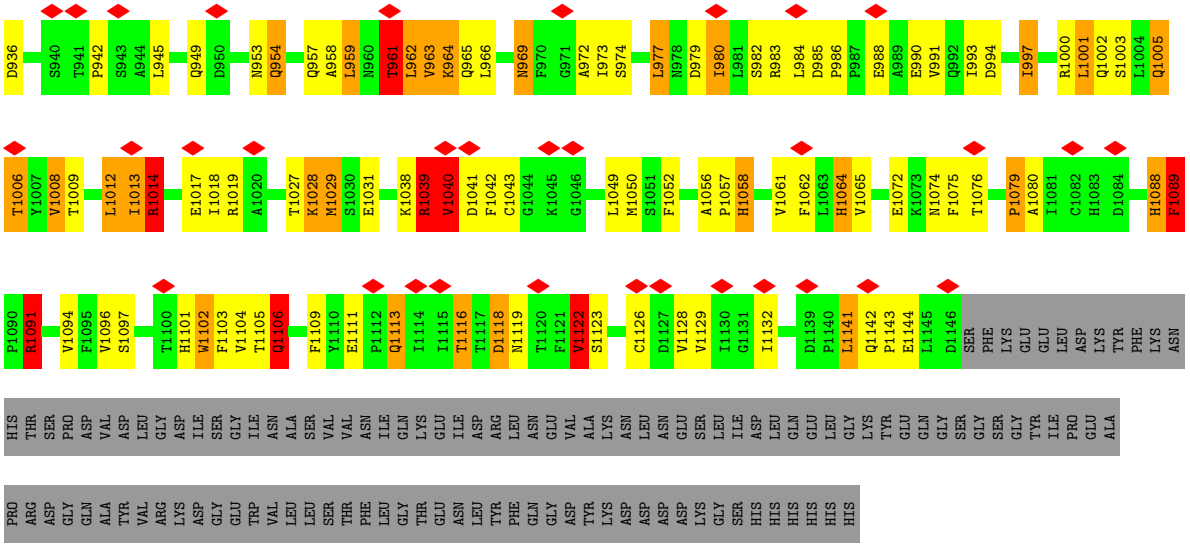
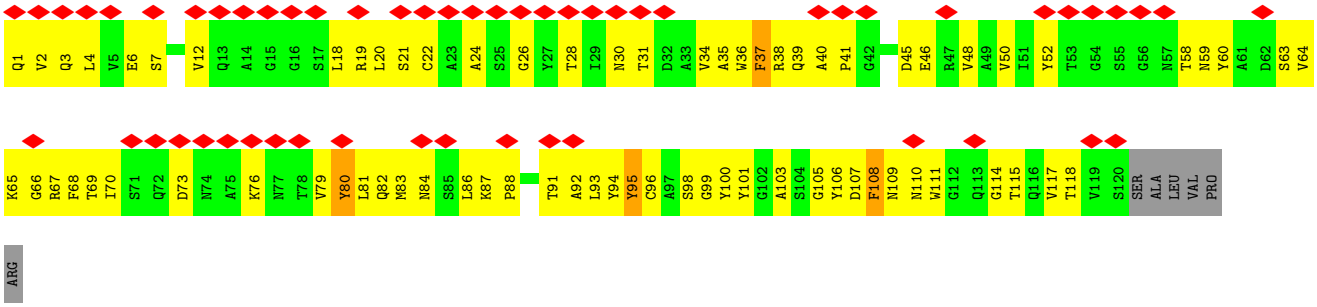
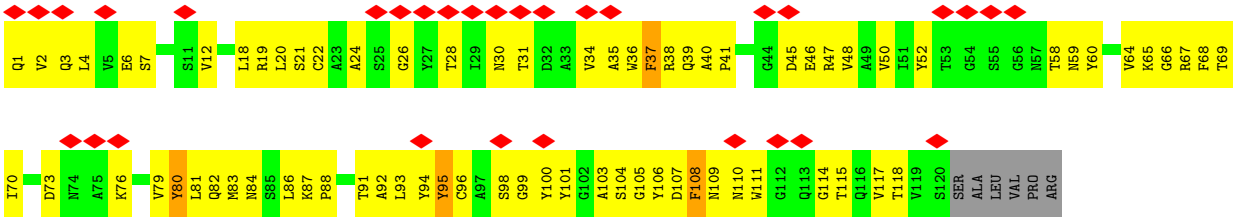
L922 I923
A924 N925
Q926 F927
N928 S929
A930 K933



• Molecule 2: Camel-derived nanobody 1.29



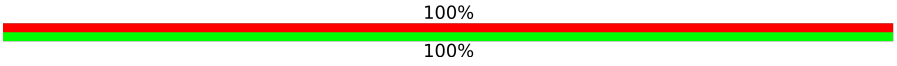
• Molecule 2: Camel-derived nanobody 1.29



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

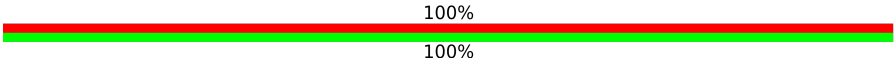
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.963	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	418.2, 418.2, 418.2	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	1.05	65/8501 (0.8%)	2.07	240/11563 (2.1%)
1	B	1.06	66/8452 (0.8%)	2.08	238/11495 (2.1%)
1	C	1.05	66/8488 (0.8%)	2.07	239/11544 (2.1%)
2	D	0.34	0/912	0.54	0/1238
2	E	0.34	0/912	0.54	0/1238
All	All	1.02	197/27265 (0.7%)	2.01	717/37078 (1.9%)

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
1	A	11	40
1	B	11	38
1	C	11	38
All	All	33	116

All (197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	PHE	CE1-CZ	-24.11	0.91	1.37
1	A	192	PHE	CE1-CZ	-24.04	0.91	1.37
1	B	192	PHE	CE1-CZ	-24.04	0.91	1.37
1	B	741	TYR	CG-CD1	-17.29	1.16	1.39
1	C	741	TYR	CG-CD1	-17.27	1.16	1.39
1	A	741	TYR	CG-CD1	-17.26	1.16	1.39
1	B	741	TYR	CD2-CE2	17.03	1.65	1.39
1	C	741	TYR	CD2-CE2	16.99	1.64	1.39
1	A	741	TYR	CD2-CE2	16.98	1.64	1.39
1	A	741	TYR	CE1-CZ	-16.46	1.17	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	741	TYR	CE1-CZ	-16.44	1.17	1.38
1	B	741	TYR	CE1-CZ	-16.44	1.17	1.38
1	B	1106	GLN	CB-CG	-15.74	1.10	1.52
1	C	1106	GLN	CB-CG	-15.74	1.10	1.52
1	A	1106	GLN	CB-CG	-15.73	1.10	1.52
1	A	741	TYR	CE2-CZ	-13.41	1.21	1.38
1	B	741	TYR	CE2-CZ	-13.37	1.21	1.38
1	C	741	TYR	CE2-CZ	-13.36	1.21	1.38
1	C	43	PHE	CE1-CZ	-12.71	1.13	1.37
1	A	43	PHE	CE1-CZ	-12.69	1.13	1.37
1	B	43	PHE	CE1-CZ	-12.68	1.13	1.37
1	A	772	VAL	CB-CG2	-12.36	1.26	1.52
1	B	772	VAL	CB-CG2	-12.36	1.26	1.52
1	C	772	VAL	CB-CG2	-12.34	1.26	1.52
1	C	911	VAL	CB-CG2	12.02	1.78	1.52
1	A	911	VAL	CB-CG2	12.01	1.78	1.52
1	B	911	VAL	CB-CG2	12.01	1.78	1.52
1	C	911	VAL	CB-CG1	-12.00	1.27	1.52
1	A	911	VAL	CB-CG1	-11.98	1.27	1.52
1	B	911	VAL	CB-CG1	-11.96	1.27	1.52
1	B	170	TYR	CG-CD2	-11.39	1.24	1.39
1	A	170	TYR	CG-CD2	-11.38	1.24	1.39
1	C	170	TYR	CG-CD2	-11.36	1.24	1.39
1	C	230	PRO	CG-CD	-11.32	1.13	1.50
1	A	230	PRO	CG-CD	-11.32	1.13	1.50
1	B	230	PRO	CG-CD	-11.32	1.13	1.50
1	B	756	TYR	CD1-CE1	-11.30	1.22	1.39
1	C	756	TYR	CD1-CE1	-11.29	1.22	1.39
1	A	756	TYR	CD1-CE1	-11.27	1.22	1.39
1	A	817	PHE	CG-CD1	-10.85	1.22	1.38
1	C	817	PHE	CG-CD1	-10.82	1.22	1.38
1	B	817	PHE	CG-CD1	-10.81	1.22	1.38
1	A	170	TYR	CD2-CE2	-9.75	1.24	1.39
1	B	43	PHE	CD1-CE1	-9.71	1.19	1.39
1	B	170	TYR	CD2-CE2	-9.69	1.24	1.39
1	C	43	PHE	CD1-CE1	-9.69	1.19	1.39
1	C	170	TYR	CD2-CE2	-9.68	1.24	1.39
1	A	43	PHE	CD1-CE1	-9.67	1.20	1.39
1	A	43	PHE	CG-CD1	-8.92	1.25	1.38
1	B	43	PHE	CG-CD1	-8.87	1.25	1.38
1	C	43	PHE	CG-CD1	-8.85	1.25	1.38
1	B	1106	GLN	CD-OE1	-8.45	1.05	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1106	GLN	CD-OE1	-8.42	1.05	1.24
1	C	1106	GLN	CD-OE1	-8.39	1.05	1.24
1	C	756	TYR	CD2-CE2	-8.33	1.26	1.39
1	A	756	TYR	CD2-CE2	-8.31	1.26	1.39
1	B	756	TYR	CD2-CE2	-8.31	1.26	1.39
1	A	308	VAL	CB-CG1	-8.14	1.35	1.52
1	C	308	VAL	CB-CG1	-8.10	1.35	1.52
1	B	308	VAL	CB-CG1	-8.09	1.35	1.52
1	A	308	VAL	CB-CG2	7.95	1.69	1.52
1	B	308	VAL	CB-CG2	7.93	1.69	1.52
1	C	308	VAL	CB-CG2	7.93	1.69	1.52
1	B	269	TYR	CG-CD1	-7.91	1.28	1.39
1	C	269	TYR	CG-CD1	-7.90	1.28	1.39
1	A	269	TYR	CG-CD1	-7.88	1.28	1.39
1	B	192	PHE	CG-CD1	-7.73	1.27	1.38
1	C	192	PHE	CG-CD1	-7.71	1.27	1.38
1	A	192	PHE	CG-CD1	-7.67	1.27	1.38
1	A	770	ILE	CB-CG2	7.54	1.76	1.52
1	B	770	ILE	CB-CG2	7.53	1.76	1.52
1	C	741	TYR	CG-CD2	7.51	1.49	1.39
1	C	770	ILE	CB-CG2	7.51	1.76	1.52
1	A	741	TYR	CG-CD2	7.51	1.49	1.39
1	B	741	TYR	CG-CD2	7.46	1.48	1.39
1	B	595	VAL	CB-CG2	7.39	1.68	1.52
1	A	595	VAL	CB-CG2	7.35	1.68	1.52
1	C	595	VAL	CB-CG2	7.34	1.68	1.52
1	C	802	PHE	CG-CD1	-7.23	1.27	1.38
1	A	595	VAL	CB-CG1	-7.22	1.37	1.52
1	C	595	VAL	CB-CG1	-7.21	1.37	1.52
1	B	595	VAL	CB-CG1	-7.20	1.37	1.52
1	A	802	PHE	CG-CD1	-7.20	1.27	1.38
1	B	802	PHE	CG-CD1	-7.17	1.27	1.38
1	A	959	LEU	CG-CD2	6.95	1.77	1.51
1	C	959	LEU	CG-CD2	6.95	1.77	1.51
1	B	959	LEU	CG-CD2	6.93	1.77	1.51
1	C	802	PHE	CG-CD2	6.86	1.49	1.38
1	B	802	PHE	CG-CD2	6.85	1.49	1.38
1	A	802	PHE	CG-CD2	6.82	1.49	1.38
1	A	28	TYR	CD1-CE1	-6.76	1.29	1.39
1	B	699	LEU	CG-CD2	6.68	1.76	1.51
1	A	699	LEU	CG-CD2	6.66	1.76	1.51
1	C	699	LEU	CG-CD2	6.66	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	TYR	CD1-CE1	-6.64	1.29	1.39
1	C	28	TYR	CD1-CE1	-6.64	1.29	1.39
1	C	909	ILE	CB-CG2	6.63	1.73	1.52
1	A	909	ILE	CB-CG2	6.63	1.73	1.52
1	B	909	ILE	CB-CG2	6.60	1.73	1.52
1	B	699	LEU	CG-CD1	-6.46	1.27	1.51
1	C	699	LEU	CG-CD1	-6.46	1.27	1.51
1	A	699	LEU	CG-CD1	-6.46	1.27	1.51
1	B	160	TYR	CG-CD1	-6.42	1.30	1.39
1	A	901	GLN	CD-NE2	-6.42	1.16	1.32
1	B	901	GLN	CD-NE2	-6.40	1.16	1.32
1	C	901	GLN	CD-NE2	-6.39	1.16	1.32
1	A	18	LEU	CG-CD1	-6.38	1.28	1.51
1	C	18	LEU	CG-CD1	-6.37	1.28	1.51
1	A	905	ARG	CG-CD	6.37	1.67	1.51
1	B	18	LEU	CG-CD1	-6.36	1.28	1.51
1	C	160	TYR	CG-CD1	-6.35	1.30	1.39
1	C	905	ARG	CG-CD	6.35	1.67	1.51
1	B	905	ARG	CG-CD	6.33	1.67	1.51
1	A	160	TYR	CG-CD1	-6.32	1.30	1.39
1	C	170	TYR	CE1-CZ	-6.32	1.30	1.38
1	B	170	TYR	CE1-CZ	-6.26	1.30	1.38
1	A	170	TYR	CE1-CZ	-6.24	1.30	1.38
1	C	1106	GLN	CD-NE2	-6.20	1.17	1.32
1	B	1106	GLN	CD-NE2	-6.17	1.17	1.32
1	A	1106	GLN	CD-NE2	-6.16	1.17	1.32
1	A	610	VAL	CB-CG1	-6.12	1.40	1.52
1	C	802	PHE	CE1-CZ	-6.12	1.25	1.37
1	A	802	PHE	CE1-CZ	-6.11	1.25	1.37
1	B	610	VAL	CB-CG1	-6.09	1.40	1.52
1	B	802	PHE	CE1-CZ	-6.08	1.25	1.37
1	C	610	VAL	CB-CG1	-6.06	1.40	1.52
1	B	821	LEU	CG-CD2	6.01	1.74	1.51
1	A	28	TYR	CD2-CE2	-5.99	1.30	1.39
1	C	776	LYS	CG-CD	5.99	1.72	1.52
1	A	821	LEU	CG-CD2	5.98	1.74	1.51
1	B	776	LYS	CG-CD	5.98	1.72	1.52
1	C	821	LEU	CG-CD2	5.98	1.74	1.51
1	A	776	LYS	CG-CD	5.97	1.72	1.52
1	B	28	TYR	CD2-CE2	-5.96	1.30	1.39
1	C	28	TYR	CD2-CE2	-5.96	1.30	1.39
1	A	18	LEU	CG-CD2	-5.92	1.29	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	LEU	CG-CD2	-5.90	1.30	1.51
1	B	18	LEU	CG-CD2	-5.90	1.30	1.51
1	A	901	GLN	CG-CD	5.76	1.64	1.51
1	B	997	ILE	CB-CG1	-5.76	1.38	1.54
1	B	901	GLN	CG-CD	5.76	1.64	1.51
1	C	997	ILE	CB-CG1	-5.75	1.38	1.54
1	C	901	GLN	CG-CD	5.75	1.64	1.51
1	A	997	ILE	CB-CG1	-5.75	1.38	1.54
1	B	168	PHE	CD2-CE2	-5.55	1.28	1.39
1	A	168	PHE	CD2-CE2	-5.53	1.28	1.39
1	C	168	PHE	CD2-CE2	-5.52	1.28	1.39
1	B	1013	ILE	CB-CG2	-5.48	1.35	1.52
1	B	170	TYR	CD1-CE1	-5.48	1.31	1.39
1	C	1013	ILE	CB-CG2	-5.47	1.35	1.52
1	A	1013	ILE	CB-CG2	-5.44	1.35	1.52
1	C	135	PHE	CD1-CE1	-5.44	1.28	1.39
1	C	170	TYR	CD1-CE1	-5.43	1.31	1.39
1	A	135	PHE	CD1-CE1	-5.42	1.28	1.39
1	A	170	TYR	CD1-CE1	-5.41	1.31	1.39
1	B	135	PHE	CD1-CE1	-5.41	1.28	1.39
1	B	299	THR	CB-CG2	-5.31	1.34	1.52
1	A	299	THR	CB-CG2	-5.31	1.34	1.52
1	C	299	THR	CB-CG2	-5.31	1.34	1.52
1	C	991	VAL	CB-CG1	-5.31	1.41	1.52
1	A	991	VAL	CB-CG1	-5.27	1.41	1.52
1	B	991	VAL	CB-CG1	-5.24	1.41	1.52
1	B	160	TYR	CE2-CZ	-5.23	1.31	1.38
1	C	719	THR	CB-CG2	-5.20	1.35	1.52
1	A	719	THR	CB-CG2	-5.19	1.35	1.52
1	B	877	LEU	CG-CD2	-5.19	1.32	1.51
1	B	1089	PHE	CG-CD1	-5.19	1.30	1.38
1	C	802	PHE	CE2-CZ	-5.19	1.27	1.37
1	B	719	THR	CB-CG2	-5.18	1.35	1.52
1	C	877	LEU	CG-CD2	-5.18	1.32	1.51
1	B	802	PHE	CE2-CZ	-5.17	1.27	1.37
1	A	877	LEU	CG-CD2	-5.17	1.32	1.51
1	C	160	TYR	CD2-CE2	-5.17	1.31	1.39
1	A	160	TYR	CD2-CE2	-5.16	1.31	1.39
1	B	160	TYR	CD2-CE2	-5.16	1.31	1.39
1	A	802	PHE	CE2-CZ	-5.14	1.27	1.37
1	A	160	TYR	CE2-CZ	-5.13	1.31	1.38
1	C	1089	PHE	CG-CD1	-5.13	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	TYR	CE2-CZ	-5.12	1.31	1.38
1	C	160	TYR	CE2-CZ	-5.11	1.31	1.38
1	B	141	LEU	CB-CG	5.11	1.67	1.52
1	A	1089	PHE	CG-CD1	-5.11	1.31	1.38
1	C	141	LEU	CB-CG	5.10	1.67	1.52
1	B	269	TYR	CE2-CZ	-5.09	1.31	1.38
1	A	141	LEU	CB-CG	5.09	1.67	1.52
1	C	133	PHE	CD1-CE1	-5.09	1.29	1.39
1	C	741	TYR	CZ-OH	-5.09	1.29	1.37
1	B	741	TYR	CZ-OH	-5.08	1.29	1.37
1	B	133	PHE	CD1-CE1	-5.07	1.29	1.39
1	A	741	TYR	CZ-OH	-5.06	1.29	1.37
1	C	269	TYR	CE2-CZ	-5.05	1.31	1.38
1	B	230	PRO	N-CD	5.05	1.54	1.47
1	A	1065	VAL	CB-CG2	5.04	1.63	1.52
1	C	1065	VAL	CB-CG2	5.03	1.63	1.52
1	C	230	PRO	N-CD	5.03	1.54	1.47
1	A	135	PHE	CD2-CE2	-5.01	1.29	1.39
1	B	1065	VAL	CB-CG2	5.00	1.63	1.52

All (717) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	PHE	CB-CG-CD1	56.88	160.62	120.80
1	C	192	PHE	CB-CG-CD1	56.85	160.60	120.80
1	A	192	PHE	CB-CG-CD1	56.80	160.56	120.80
1	B	192	PHE	CB-CG-CD2	-51.66	84.64	120.80
1	A	192	PHE	CB-CG-CD2	-51.65	84.65	120.80
1	C	192	PHE	CB-CG-CD2	-51.61	84.67	120.80
1	B	741	TYR	CB-CG-CD1	48.82	150.29	121.00
1	A	741	TYR	CB-CG-CD1	48.78	150.27	121.00
1	C	741	TYR	CB-CG-CD1	48.71	150.23	121.00
1	B	741	TYR	CB-CG-CD2	-42.21	95.67	121.00
1	C	741	TYR	CB-CG-CD2	-42.21	95.67	121.00
1	A	741	TYR	CB-CG-CD2	-42.18	95.69	121.00
1	A	741	TYR	CD1-CG-CD2	-38.91	75.09	117.90
1	C	741	TYR	CD1-CG-CD2	-38.91	75.10	117.90
1	B	741	TYR	CD1-CG-CD2	-38.87	75.14	117.90
1	A	802	PHE	CB-CG-CD2	-34.93	96.35	120.80
1	C	802	PHE	CB-CG-CD2	-34.89	96.38	120.80
1	B	802	PHE	CB-CG-CD2	-34.87	96.39	120.80
1	B	1106	GLN	CA-CB-CG	30.26	179.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1106	GLN	CA-CB-CG	30.25	179.96	113.40
1	C	1106	GLN	CA-CB-CG	30.24	179.93	113.40
1	B	959	LEU	CB-CG-CD1	28.16	158.87	111.00
1	C	959	LEU	CB-CG-CD1	28.14	158.84	111.00
1	A	959	LEU	CB-CG-CD1	28.13	158.83	111.00
1	A	1012	LEU	CB-CG-CD1	27.59	157.91	111.00
1	B	1012	LEU	CB-CG-CD1	27.57	157.86	111.00
1	C	1012	LEU	CB-CG-CD1	27.55	157.83	111.00
1	B	911	VAL	CG1-CB-CG2	-26.16	69.05	110.90
1	C	911	VAL	CG1-CB-CG2	-26.14	69.07	110.90
1	A	911	VAL	CG1-CB-CG2	-26.14	69.08	110.90
1	C	909	ILE	CG1-CB-CG2	-25.02	56.34	111.40
1	A	909	ILE	CG1-CB-CG2	-25.02	56.36	111.40
1	B	909	ILE	CG1-CB-CG2	-25.02	56.36	111.40
1	B	802	PHE	CB-CG-CD1	23.88	137.51	120.80
1	A	192	PHE	CD1-CG-CD2	-23.85	87.29	118.30
1	B	192	PHE	CD1-CG-CD2	-23.84	87.31	118.30
1	C	192	PHE	CD1-CG-CD2	-23.84	87.31	118.30
1	C	802	PHE	CB-CG-CD1	23.82	137.47	120.80
1	A	802	PHE	CB-CG-CD1	23.80	137.46	120.80
1	A	43	PHE	CB-CG-CD2	-22.98	104.71	120.80
1	C	43	PHE	CB-CG-CD2	-22.98	104.72	120.80
1	B	43	PHE	CB-CG-CD2	-22.97	104.72	120.80
1	A	1065	VAL	CG1-CB-CG2	-22.78	74.45	110.90
1	B	595	VAL	CG1-CB-CG2	-22.78	74.46	110.90
1	C	1065	VAL	CG1-CB-CG2	-22.77	74.47	110.90
1	B	1065	VAL	CG1-CB-CG2	-22.76	74.48	110.90
1	A	595	VAL	CG1-CB-CG2	-22.75	74.50	110.90
1	C	595	VAL	CG1-CB-CG2	-22.74	74.51	110.90
1	C	927	PHE	CB-CG-CD2	-21.31	105.88	120.80
1	A	927	PHE	CB-CG-CD2	-21.30	105.89	120.80
1	B	927	PHE	CB-CG-CD2	-21.30	105.89	120.80
1	C	160	TYR	CB-CG-CD2	-20.82	108.51	121.00
1	A	160	TYR	CB-CG-CD2	-20.81	108.52	121.00
1	B	160	TYR	CB-CG-CD2	-20.80	108.52	121.00
1	C	959	LEU	CB-CG-CD2	-19.97	77.05	111.00
1	A	959	LEU	CB-CG-CD2	-19.95	77.09	111.00
1	B	959	LEU	CB-CG-CD2	-19.93	77.11	111.00
1	A	770	ILE	CG1-CB-CG2	-19.82	67.80	111.40
1	B	770	ILE	CG1-CB-CG2	-19.82	67.80	111.40
1	C	770	ILE	CG1-CB-CG2	-19.82	67.81	111.40
1	A	962	LEU	CB-CG-CD1	-19.74	77.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	962	LEU	CB-CG-CD1	-19.74	77.45	111.00
1	C	962	LEU	CB-CG-CD1	-19.74	77.45	111.00
1	B	192	PHE	CG-CD1-CE1	19.60	142.36	120.80
1	A	192	PHE	CG-CD1-CE1	19.58	142.34	120.80
1	C	192	PHE	CG-CD1-CE1	19.57	142.33	120.80
1	A	802	PHE	CD1-CG-CD2	-19.55	92.88	118.30
1	C	802	PHE	CD1-CG-CD2	-19.55	92.89	118.30
1	B	802	PHE	CD1-CG-CD2	-19.53	92.92	118.30
1	C	1012	LEU	CB-CG-CD2	-18.38	79.76	111.00
1	B	1012	LEU	CB-CG-CD2	-18.37	79.78	111.00
1	A	1012	LEU	CB-CG-CD2	-18.36	79.80	111.00
1	A	776	LYS	CD-CE-NZ	18.35	153.91	111.70
1	C	776	LYS	CD-CE-NZ	18.33	153.86	111.70
1	B	776	LYS	CD-CE-NZ	18.33	153.85	111.70
1	C	610	VAL	CG1-CB-CG2	-18.28	81.65	110.90
1	B	610	VAL	CG1-CB-CG2	-18.26	81.68	110.90
1	A	610	VAL	CG1-CB-CG2	-18.25	81.70	110.90
1	B	308	VAL	CG1-CB-CG2	-17.91	82.24	110.90
1	A	308	VAL	CG1-CB-CG2	-17.91	82.24	110.90
1	C	308	VAL	CG1-CB-CG2	-17.91	82.25	110.90
1	B	765	ARG	CD-NE-CZ	16.86	147.20	123.60
1	C	765	ARG	CD-NE-CZ	16.85	147.19	123.60
1	A	765	ARG	CD-NE-CZ	16.82	147.15	123.60
1	C	905	ARG	NE-CZ-NH2	-16.42	112.09	120.30
1	A	905	ARG	NE-CZ-NH2	-16.38	112.11	120.30
1	B	905	ARG	NE-CZ-NH2	-16.35	112.12	120.30
1	B	741	TYR	CG-CD1-CE1	16.05	134.14	121.30
1	A	741	TYR	CG-CD1-CE1	16.00	134.10	121.30
1	C	741	TYR	CG-CD1-CE1	15.97	134.08	121.30
1	A	905	ARG	CG-CD-NE	15.84	145.06	111.80
1	B	905	ARG	CG-CD-NE	15.83	145.04	111.80
1	C	905	ARG	CG-CD-NE	15.82	145.02	111.80
1	B	1116	THR	OG1-CB-CG2	-15.16	75.12	110.00
1	A	1116	THR	OG1-CB-CG2	-15.16	75.13	110.00
1	C	1116	THR	OG1-CB-CG2	-15.14	75.18	110.00
1	C	814	LYS	CD-CE-NZ	15.02	146.25	111.70
1	A	814	LYS	CD-CE-NZ	15.02	146.25	111.70
1	B	814	LYS	CD-CE-NZ	15.02	146.24	111.70
1	B	43	PHE	CB-CG-CD1	14.47	130.93	120.80
1	A	821	LEU	CB-CG-CD1	14.46	135.59	111.00
1	A	43	PHE	CB-CG-CD1	14.46	130.92	120.80
1	C	821	LEU	CB-CG-CD1	14.45	135.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	821	LEU	CB-CG-CD1	14.44	135.54	111.00
1	C	43	PHE	CB-CG-CD1	14.37	130.86	120.80
1	A	1012	LEU	CA-CB-CG	14.29	148.16	115.30
1	B	1012	LEU	CA-CB-CG	14.29	148.16	115.30
1	C	1012	LEU	CA-CB-CG	14.28	148.15	115.30
1	A	962	LEU	CB-CG-CD2	14.28	135.28	111.00
1	C	962	LEU	CB-CG-CD2	14.28	135.28	111.00
1	B	962	LEU	CB-CG-CD2	14.25	135.22	111.00
1	C	741	TYR	CD1-CE1-CZ	-14.23	106.99	119.80
1	A	741	TYR	CD1-CE1-CZ	-14.23	107.00	119.80
1	B	741	TYR	CD1-CE1-CZ	-14.18	107.04	119.80
1	C	927	PHE	CB-CG-CD1	13.97	130.58	120.80
1	A	927	PHE	CB-CG-CD1	13.95	130.56	120.80
1	B	927	PHE	CB-CG-CD1	13.94	130.56	120.80
1	A	230	PRO	CA-N-CD	-13.94	91.99	111.50
1	B	230	PRO	CA-N-CD	-13.92	92.01	111.50
1	C	230	PRO	CA-N-CD	-13.92	92.01	111.50
1	C	1141	LEU	CB-CG-CD2	13.75	134.37	111.00
1	B	1141	LEU	CB-CG-CD2	13.73	134.35	111.00
1	A	1141	LEU	CB-CG-CD2	13.73	134.34	111.00
1	B	141	LEU	CA-CB-CG	-13.33	84.64	115.30
1	C	141	LEU	CA-CB-CG	-13.32	84.67	115.30
1	A	141	LEU	CA-CB-CG	-13.32	84.67	115.30
1	B	699	LEU	CD1-CG-CD2	-12.91	71.76	110.50
1	C	699	LEU	CD1-CG-CD2	-12.91	71.78	110.50
1	A	699	LEU	CD1-CG-CD2	-12.90	71.78	110.50
1	C	821	LEU	CB-CG-CD2	-12.71	89.39	111.00
1	B	821	LEU	CB-CG-CD2	-12.71	89.39	111.00
1	A	821	LEU	CB-CG-CD2	-12.68	89.44	111.00
1	A	991	VAL	CG1-CB-CG2	-12.65	90.66	110.90
1	C	991	VAL	CG1-CB-CG2	-12.64	90.68	110.90
1	B	991	VAL	CG1-CB-CG2	-12.63	90.69	110.90
1	A	911	VAL	CA-CB-CG1	12.62	129.83	110.90
1	B	911	VAL	CA-CB-CG1	12.60	129.80	110.90
1	C	911	VAL	CA-CB-CG1	12.60	129.79	110.90
1	B	997	ILE	CA-CB-CG1	12.51	134.77	111.00
1	A	821	LEU	CD1-CG-CD2	-12.50	73.00	110.50
1	B	821	LEU	CD1-CG-CD2	-12.50	73.00	110.50
1	C	821	LEU	CD1-CG-CD2	-12.50	73.01	110.50
1	C	997	ILE	CA-CB-CG1	12.50	134.74	111.00
1	A	997	ILE	CA-CB-CG1	12.49	134.72	111.00
1	A	909	ILE	CA-CB-CG2	-12.44	86.03	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	909	ILE	CA-CB-CG2	-12.43	86.05	110.90
1	C	909	ILE	CA-CB-CG2	-12.42	86.07	110.90
1	B	909	ILE	CA-CB-CG1	12.37	134.51	111.00
1	C	909	ILE	CA-CB-CG1	12.37	134.51	111.00
1	A	909	ILE	CA-CB-CG1	12.36	134.48	111.00
1	A	216	LEU	CA-CB-CG	12.21	143.38	115.30
1	C	216	LEU	CA-CB-CG	12.19	143.33	115.30
1	B	216	LEU	CA-CB-CG	12.18	143.32	115.30
1	B	902	MET	CB-CG-SD	12.09	148.66	112.40
1	C	902	MET	CB-CG-SD	12.07	148.62	112.40
1	A	902	MET	CB-CG-SD	12.07	148.61	112.40
1	C	1079	PRO	CA-N-CD	-11.98	94.73	111.50
1	B	1079	PRO	CA-N-CD	-11.95	94.78	111.50
1	A	1079	PRO	CA-N-CD	-11.93	94.80	111.50
1	C	1141	LEU	CA-CB-CG	11.87	142.60	115.30
1	B	1141	LEU	CA-CB-CG	11.86	142.58	115.30
1	A	1141	LEU	CA-CB-CG	11.84	142.54	115.30
1	A	1116	THR	CA-CB-OG1	11.62	133.39	109.00
1	C	1116	THR	CA-CB-OG1	11.61	133.38	109.00
1	A	278	LYS	CD-CE-NZ	11.61	138.40	111.70
1	B	1116	THR	CA-CB-OG1	11.59	133.35	109.00
1	C	278	LYS	CD-CE-NZ	11.59	138.35	111.70
1	A	43	PHE	CD1-CG-CD2	-11.57	103.25	118.30
1	B	278	LYS	CD-CE-NZ	11.57	138.32	111.70
1	C	43	PHE	CD1-CG-CD2	-11.54	103.29	118.30
1	B	43	PHE	CD1-CG-CD2	-11.53	103.31	118.30
1	B	927	PHE	CD1-CG-CD2	-11.52	103.32	118.30
1	A	927	PHE	CD1-CG-CD2	-11.51	103.33	118.30
1	C	927	PHE	CD1-CG-CD2	-11.51	103.34	118.30
1	B	1091	ARG	CA-CB-CG	11.45	138.58	113.40
1	C	1091	ARG	CA-CB-CG	11.42	138.52	113.40
1	A	1091	ARG	CA-CB-CG	11.41	138.51	113.40
1	B	762	GLN	CG-CD-OE1	11.40	144.39	121.60
1	C	762	GLN	CG-CD-OE1	11.38	144.36	121.60
1	A	762	GLN	CG-CD-OE1	11.37	144.34	121.60
1	B	1005	GLN	CA-CB-CG	11.36	138.39	113.40
1	C	1005	GLN	CA-CB-CG	11.36	138.38	113.40
1	A	1005	GLN	CA-CB-CG	11.35	138.37	113.40
1	A	762	GLN	CG-CD-NE2	-11.27	89.64	116.70
1	B	762	GLN	CG-CD-NE2	-11.27	89.66	116.70
1	C	762	GLN	CG-CD-NE2	-11.26	89.68	116.70
1	B	817	PHE	CD1-CG-CD2	-10.97	104.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	817	PHE	CD1-CG-CD2	-10.94	104.08	118.30
1	A	1013	ILE	CA-CB-CG1	10.93	131.76	111.00
1	A	817	PHE	CD1-CG-CD2	-10.92	104.10	118.30
1	C	901	GLN	CG-CD-OE1	10.91	143.41	121.60
1	C	1013	ILE	CA-CB-CG1	10.90	131.72	111.00
1	A	901	GLN	CG-CD-OE1	10.90	143.40	121.60
1	B	1013	ILE	CA-CB-CG1	10.90	131.70	111.00
1	A	170	TYR	CD1-CE1-CZ	-10.89	110.00	119.80
1	B	901	GLN	CG-CD-OE1	10.88	143.37	121.60
1	C	911	VAL	CA-CB-CG2	-10.87	94.59	110.90
1	B	911	VAL	CA-CB-CG2	-10.86	94.61	110.90
1	A	911	VAL	CA-CB-CG2	-10.84	94.64	110.90
1	A	666	ILE	CB-CG1-CD1	10.83	144.23	113.90
1	C	170	TYR	CD1-CE1-CZ	-10.83	110.05	119.80
1	B	170	TYR	CD1-CE1-CZ	-10.81	110.07	119.80
1	B	666	ILE	CB-CG1-CD1	10.81	144.16	113.90
1	C	666	ILE	CB-CG1-CD1	10.80	144.15	113.90
1	C	1012	LEU	CD1-CG-CD2	-10.80	78.10	110.50
1	B	1012	LEU	CD1-CG-CD2	-10.79	78.12	110.50
1	A	1012	LEU	CD1-CG-CD2	-10.79	78.14	110.50
1	C	241	LEU	CA-CB-CG	10.71	139.92	115.30
1	A	241	LEU	CA-CB-CG	10.69	139.88	115.30
1	B	241	LEU	CA-CB-CG	10.68	139.85	115.30
1	C	1029	MET	CA-CB-CG	10.62	131.35	113.30
1	A	1029	MET	CA-CB-CG	10.61	131.33	113.30
1	B	1029	MET	CA-CB-CG	10.61	131.33	113.30
1	A	301	CYS	CA-CB-SG	10.60	133.08	114.00
1	C	301	CYS	CA-CB-SG	10.60	133.07	114.00
1	B	301	CYS	CA-CB-SG	10.58	133.05	114.00
1	C	977	LEU	CA-CB-CG	10.51	139.48	115.30
1	A	977	LEU	CA-CB-CG	10.50	139.46	115.30
1	B	977	LEU	CA-CB-CG	10.49	139.42	115.30
1	C	821	LEU	CA-CB-CG	10.27	138.92	115.30
1	B	821	LEU	CA-CB-CG	10.26	138.89	115.30
1	A	821	LEU	CA-CB-CG	10.24	138.86	115.30
1	A	729	VAL	CG1-CB-CG2	-10.19	94.60	110.90
1	B	729	VAL	CG1-CB-CG2	-10.18	94.62	110.90
1	C	729	VAL	CG1-CB-CG2	-10.17	94.63	110.90
1	B	756	TYR	CB-CG-CD2	-10.16	114.91	121.00
1	A	756	TYR	CB-CG-CD2	-10.14	114.92	121.00
1	C	756	TYR	CB-CG-CD2	-10.13	114.92	121.00
1	B	1089	PHE	N-CA-CB	-10.12	92.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1089	PHE	N-CA-CB	-10.11	92.40	110.60
1	C	1089	PHE	N-CA-CB	-10.10	92.43	110.60
1	B	206	LYS	CD-CE-NZ	10.06	134.84	111.70
1	C	206	LYS	CD-CE-NZ	10.06	134.84	111.70
1	A	206	LYS	CD-CE-NZ	10.05	134.81	111.70
1	B	900	MET	CG-SD-CE	9.98	116.17	100.20
1	A	900	MET	CG-SD-CE	9.97	116.15	100.20
1	C	900	MET	CG-SD-CE	9.95	116.13	100.20
1	C	699	LEU	CB-CG-CD1	9.93	127.88	111.00
1	A	859	THR	OG1-CB-CG2	-9.91	87.20	110.00
1	B	699	LEU	CB-CG-CD1	9.91	127.85	111.00
1	C	859	THR	OG1-CB-CG2	-9.91	87.20	110.00
1	A	118	LEU	CA-CB-CG	9.91	138.09	115.30
1	B	859	THR	OG1-CB-CG2	-9.91	87.21	110.00
1	C	118	LEU	CA-CB-CG	9.90	138.08	115.30
1	A	699	LEU	CB-CG-CD1	9.90	127.83	111.00
1	B	118	LEU	CA-CB-CG	9.90	138.06	115.30
1	A	160	TYR	CD1-CG-CD2	-9.80	107.12	117.90
1	C	160	TYR	CD1-CG-CD2	-9.80	107.12	117.90
1	B	160	TYR	CD1-CG-CD2	-9.73	107.20	117.90
1	B	1116	THR	CA-CB-CG2	-9.73	98.78	112.40
1	C	1116	THR	CA-CB-CG2	-9.71	98.81	112.40
1	C	160	TYR	CB-CG-CD1	9.69	126.81	121.00
1	A	1116	THR	CA-CB-CG2	-9.68	98.85	112.40
1	A	160	TYR	CB-CG-CD1	9.60	126.76	121.00
1	A	877	LEU	CB-CG-CD2	-9.60	94.69	111.00
1	C	877	LEU	CB-CG-CD2	-9.59	94.70	111.00
1	B	160	TYR	CB-CG-CD1	9.58	126.75	121.00
1	C	1065	VAL	CA-CB-CG1	9.57	125.25	110.90
1	B	877	LEU	CB-CG-CD2	-9.56	94.74	111.00
1	B	1065	VAL	CA-CB-CG1	9.54	125.22	110.90
1	A	997	ILE	CG1-CB-CG2	-9.52	90.45	111.40
1	A	1065	VAL	CA-CB-CG1	9.52	125.19	110.90
1	C	997	ILE	CG1-CB-CG2	-9.52	90.45	111.40
1	A	963	VAL	CG1-CB-CG2	-9.52	95.67	110.90
1	C	963	VAL	CG1-CB-CG2	-9.51	95.68	110.90
1	B	997	ILE	CG1-CB-CG2	-9.50	90.49	111.40
1	B	963	VAL	CG1-CB-CG2	-9.50	95.70	110.90
1	B	756	TYR	CB-CG-CD1	9.40	126.64	121.00
1	A	756	TYR	CB-CG-CD1	9.36	126.62	121.00
1	C	756	TYR	CB-CG-CD1	9.32	126.59	121.00
1	C	230	PRO	N-CD-CG	-9.31	89.23	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	230	PRO	N-CD-CG	-9.29	89.26	103.20
1	A	814	LYS	CB-CG-CD	9.26	135.67	111.60
1	B	814	LYS	CB-CG-CD	9.26	135.67	111.60
1	C	814	LYS	CB-CG-CD	9.26	135.67	111.60
1	A	230	PRO	N-CD-CG	-9.25	89.32	103.20
1	A	977	LEU	CB-CG-CD1	-9.08	95.57	111.00
1	C	977	LEU	CB-CG-CD1	-9.06	95.60	111.00
1	B	977	LEU	CB-CG-CD1	-9.04	95.63	111.00
1	A	670	ILE	CB-CG1-CD1	8.90	138.81	113.90
1	B	670	ILE	CB-CG1-CD1	8.90	138.81	113.90
1	C	670	ILE	CB-CG1-CD1	8.90	138.81	113.90
1	A	905	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	B	1029	MET	CB-CG-SD	8.88	139.03	112.40
1	A	1029	MET	CB-CG-SD	8.86	138.97	112.40
1	C	1029	MET	CB-CG-SD	8.86	138.97	112.40
1	C	905	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	595	VAL	CA-CB-CG2	-8.75	97.77	110.90
1	B	905	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	C	595	VAL	CA-CB-CG2	-8.74	97.79	110.90
1	A	595	VAL	CA-CB-CG2	-8.73	97.80	110.90
1	C	762	GLN	CA-CB-CG	8.68	132.49	113.40
1	A	762	GLN	CA-CB-CG	8.65	132.44	113.40
1	C	207	HIS	N-CA-CB	-8.64	95.05	110.60
1	B	762	GLN	CA-CB-CG	8.64	132.40	113.40
1	A	207	HIS	N-CA-CB	-8.64	95.06	110.60
1	B	207	HIS	N-CA-CB	-8.64	95.06	110.60
1	C	170	TYR	CB-CG-CD2	-8.60	115.84	121.00
1	A	170	TYR	CB-CG-CD2	-8.52	115.89	121.00
1	B	66	HIS	N-CA-CB	8.52	125.93	110.60
1	B	170	TYR	CB-CG-CD2	-8.51	115.90	121.00
1	C	66	HIS	N-CA-CB	8.50	125.90	110.60
1	A	66	HIS	N-CA-CB	8.49	125.89	110.60
1	A	670	ILE	CA-CB-CG1	8.39	126.94	111.00
1	C	670	ILE	CA-CB-CG1	8.38	126.93	111.00
1	B	901	GLN	CG-CD-NE2	-8.35	96.65	116.70
1	B	670	ILE	CA-CB-CG1	8.35	126.87	111.00
1	C	901	GLN	CG-CD-NE2	-8.34	96.67	116.70
1	A	901	GLN	CG-CD-NE2	-8.34	96.69	116.70
1	B	207	HIS	CB-CA-C	8.28	126.97	110.40
1	A	241	LEU	CB-CG-CD1	8.28	125.07	111.00
1	A	877	LEU	CA-CB-CG	8.28	134.33	115.30
1	C	207	HIS	CB-CA-C	8.28	126.95	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	877	LEU	CA-CB-CG	8.27	134.33	115.30
1	B	877	LEU	CA-CB-CG	8.27	134.32	115.30
1	A	207	HIS	CB-CA-C	8.27	126.93	110.40
1	C	241	LEU	CB-CG-CD1	8.25	125.03	111.00
1	B	241	LEU	CB-CG-CD1	8.24	125.01	111.00
1	A	942	PRO	CA-N-CD	-8.23	99.97	111.50
1	C	942	PRO	CA-N-CD	-8.23	99.98	111.50
1	B	942	PRO	CA-N-CD	-8.19	100.03	111.50
1	C	811	LYS	CB-CG-CD	8.12	132.71	111.60
1	A	811	LYS	CB-CG-CD	8.11	132.69	111.60
1	B	811	LYS	CB-CG-CD	8.11	132.68	111.60
1	A	959	LEU	CD1-CG-CD2	-8.09	86.22	110.50
1	B	959	LEU	CD1-CG-CD2	-8.08	86.26	110.50
1	C	959	LEU	CD1-CG-CD2	-8.07	86.28	110.50
1	A	869	MET	CA-CB-CG	8.06	127.00	113.30
1	C	962	LEU	CA-CB-CG	8.06	133.83	115.30
1	A	962	LEU	CA-CB-CG	8.05	133.82	115.30
1	B	962	LEU	CA-CB-CG	8.04	133.79	115.30
1	B	869	MET	CA-CB-CG	8.03	126.96	113.30
1	C	869	MET	CA-CB-CG	8.03	126.95	113.30
1	B	767	LEU	CB-CG-CD2	-8.02	97.38	111.00
1	A	1088	HIS	C-N-CA	8.01	141.74	121.70
1	A	767	LEU	CB-CG-CD2	-8.01	97.38	111.00
1	B	1088	HIS	C-N-CA	8.01	141.72	121.70
1	C	767	LEU	CB-CG-CD2	-8.01	97.39	111.00
1	C	1088	HIS	C-N-CA	8.00	141.69	121.70
1	B	729	VAL	CA-CB-CG1	7.98	122.87	110.90
1	A	729	VAL	CA-CB-CG1	7.96	122.84	110.90
1	C	729	VAL	CA-CB-CG1	7.96	122.84	110.90
1	C	1038	LYS	CB-CG-CD	7.95	132.27	111.60
1	B	1038	LYS	CB-CG-CD	7.94	132.25	111.60
1	A	1038	LYS	CB-CG-CD	7.92	132.21	111.60
1	B	1008	VAL	CG1-CB-CG2	7.91	123.56	110.90
1	C	1040	VAL	CG1-CB-CG2	7.91	123.56	110.90
1	C	1008	VAL	CG1-CB-CG2	7.91	123.55	110.90
1	A	1040	VAL	CG1-CB-CG2	7.89	123.53	110.90
1	B	1040	VAL	CG1-CB-CG2	7.89	123.53	110.90
1	A	1008	VAL	CG1-CB-CG2	7.89	123.52	110.90
1	C	752	LEU	CB-CG-CD1	7.88	124.40	111.00
1	A	595	VAL	CA-CB-CG1	7.88	122.71	110.90
1	A	752	LEU	CB-CG-CD1	7.88	124.39	111.00
1	B	595	VAL	CA-CB-CG1	7.87	122.71	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	752	LEU	CB-CG-CD1	7.86	124.36	111.00
1	C	595	VAL	CA-CB-CG1	7.85	122.68	110.90
1	A	699	LEU	N-CA-CB	-7.84	94.72	110.40
1	A	269	TYR	CB-CG-CD2	-7.84	116.30	121.00
1	B	269	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	B	699	LEU	N-CA-CB	-7.83	94.75	110.40
1	B	792	PRO	CA-N-CD	-7.83	100.54	111.50
1	C	699	LEU	N-CA-CB	-7.82	94.77	110.40
1	A	792	PRO	CA-N-CD	-7.79	100.59	111.50
1	C	792	PRO	CA-N-CD	-7.79	100.60	111.50
1	B	781	VAL	CG1-CB-CG2	7.79	123.36	110.90
1	C	269	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	C	802	PHE	CG-CD1-CE1	7.75	129.32	120.80
1	B	141	LEU	CB-CA-C	-7.74	95.50	110.20
1	A	781	VAL	CG1-CB-CG2	7.74	123.28	110.90
1	C	781	VAL	CG1-CB-CG2	7.74	123.28	110.90
1	A	802	PHE	CG-CD1-CE1	7.72	129.29	120.80
1	A	909	ILE	CB-CA-C	-7.72	96.16	111.60
1	B	909	ILE	CB-CA-C	-7.72	96.16	111.60
1	C	141	LEU	CB-CG-CD2	7.72	124.12	111.00
1	A	141	LEU	CB-CA-C	-7.72	95.54	110.20
1	B	802	PHE	CG-CD1-CE1	7.71	129.28	120.80
1	C	909	ILE	CB-CA-C	-7.71	96.17	111.60
1	C	141	LEU	CB-CA-C	-7.71	95.56	110.20
1	A	141	LEU	CB-CG-CD2	7.70	124.09	111.00
1	B	141	LEU	CB-CG-CD2	7.70	124.09	111.00
1	C	216	LEU	CB-CG-CD1	7.68	124.05	111.00
1	B	216	LEU	CB-CG-CD1	7.67	124.05	111.00
1	A	216	LEU	CB-CG-CD1	7.65	124.01	111.00
1	B	242	LEU	CA-CB-CG	7.60	132.78	115.30
1	C	242	LEU	CA-CB-CG	7.60	132.78	115.30
1	A	242	LEU	CA-CB-CG	7.59	132.76	115.30
1	B	230	PRO	CA-CB-CG	-7.51	89.73	104.00
1	C	230	PRO	CA-CB-CG	-7.50	89.74	104.00
1	A	997	ILE	CB-CG1-CD1	7.48	134.85	113.90
1	C	997	ILE	CB-CG1-CD1	7.48	134.85	113.90
1	B	699	LEU	CA-CB-CG	7.47	132.49	115.30
1	A	699	LEU	CA-CB-CG	7.47	132.48	115.30
1	A	230	PRO	CA-CB-CG	-7.47	89.81	104.00
1	B	192	PHE	CG-CD2-CE2	7.47	129.01	120.80
1	B	997	ILE	CB-CG1-CD1	7.46	134.80	113.90
1	C	699	LEU	CA-CB-CG	7.46	132.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	192	PHE	CG-CD2-CE2	7.46	129.01	120.80
1	A	192	PHE	CG-CD2-CE2	7.46	129.00	120.80
1	C	18	LEU	CB-CG-CD1	7.44	123.65	111.00
1	B	18	LEU	CB-CG-CD1	7.43	123.64	111.00
1	A	18	LEU	CB-CG-CD1	7.42	123.62	111.00
1	A	1065	VAL	CA-CB-CG2	-7.40	99.80	110.90
1	B	1065	VAL	CA-CB-CG2	-7.37	99.85	110.90
1	C	754	LEU	CA-CB-CG	7.37	132.24	115.30
1	B	269	TYR	CD1-CG-CD2	-7.36	109.81	117.90
1	C	1065	VAL	CA-CB-CG2	-7.36	99.86	110.90
1	B	754	LEU	CA-CB-CG	7.35	132.21	115.30
1	A	754	LEU	CA-CB-CG	7.35	132.20	115.30
1	C	269	TYR	CD1-CG-CD2	-7.34	109.83	117.90
1	C	65	PHE	C-N-CA	-7.32	103.40	121.70
1	A	65	PHE	C-N-CA	-7.31	103.42	121.70
1	B	65	PHE	C-N-CA	-7.31	103.43	121.70
1	A	269	TYR	CD1-CG-CD2	-7.30	109.87	117.90
1	C	767	LEU	CD1-CG-CD2	-7.27	88.68	110.50
1	B	767	LEU	CD1-CG-CD2	-7.27	88.70	110.50
1	A	767	LEU	CD1-CG-CD2	-7.26	88.71	110.50
1	B	791	THR	OG1-CB-CG2	-7.21	93.42	110.00
1	C	726	ILE	CA-CB-CG1	7.20	124.69	111.00
1	A	726	ILE	CA-CB-CG1	7.20	124.67	111.00
1	B	726	ILE	CA-CB-CG1	7.20	124.67	111.00
1	A	791	THR	OG1-CB-CG2	-7.19	93.47	110.00
1	C	791	THR	OG1-CB-CG2	-7.18	93.50	110.00
1	C	666	ILE	CA-CB-CG1	7.16	124.60	111.00
1	C	1141	LEU	CB-CA-C	-7.16	96.60	110.20
1	A	666	ILE	CA-CB-CG1	7.16	124.59	111.00
1	A	1141	LEU	CB-CA-C	-7.15	96.61	110.20
1	B	1141	LEU	CB-CA-C	-7.14	96.63	110.20
1	C	814	LYS	CA-CB-CG	7.13	129.09	113.40
1	A	814	LYS	CA-CB-CG	7.13	129.09	113.40
1	B	666	ILE	CA-CB-CG1	7.13	124.55	111.00
1	B	814	LYS	CA-CB-CG	7.12	129.06	113.40
1	C	878	LEU	CB-CG-CD2	7.03	122.94	111.00
1	B	878	LEU	CB-CG-CD2	7.02	122.94	111.00
1	B	765	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	A	878	LEU	CB-CG-CD2	7.01	122.91	111.00
1	A	308	VAL	CA-CB-CG2	-7.00	100.40	110.90
1	C	308	VAL	CA-CB-CG2	-7.00	100.41	110.90
1	A	765	ARG	NE-CZ-NH1	-6.98	116.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1005	GLN	CB-CG-CD	6.98	129.74	111.60
1	B	308	VAL	CA-CB-CG2	-6.97	100.44	110.90
1	C	1005	GLN	CB-CG-CD	6.97	129.74	111.60
1	C	741	TYR	CB-CA-C	-6.97	96.46	110.40
1	B	1005	GLN	CB-CG-CD	6.96	129.71	111.60
1	C	765	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	A	741	TYR	CB-CA-C	-6.96	96.48	110.40
1	B	741	TYR	CB-CA-C	-6.95	96.49	110.40
1	C	1014	ARG	CG-CD-NE	-6.94	97.23	111.80
1	C	772	VAL	CA-CB-CG2	6.93	121.30	110.90
1	A	1014	ARG	CG-CD-NE	-6.93	97.25	111.80
1	A	772	VAL	CA-CB-CG2	6.92	121.28	110.90
1	B	772	VAL	CA-CB-CG2	6.92	121.28	110.90
1	B	770	ILE	CA-CB-CG1	6.91	124.13	111.00
1	B	1014	ARG	CG-CD-NE	-6.91	97.29	111.80
1	C	770	ILE	CA-CB-CG1	6.91	124.13	111.00
1	C	1089	PHE	CB-CG-CD2	-6.89	115.97	120.80
1	B	1089	PHE	CB-CG-CD2	-6.88	115.98	120.80
1	A	770	ILE	CA-CB-CG1	6.88	124.07	111.00
1	C	229	LEU	C-N-CD	-6.87	105.48	120.60
1	B	229	LEU	C-N-CD	-6.87	105.48	120.60
1	C	860	VAL	CG1-CB-CG2	-6.87	99.91	110.90
1	A	229	LEU	C-N-CD	-6.86	105.50	120.60
1	A	860	VAL	CG1-CB-CG2	-6.85	99.94	110.90
1	B	860	VAL	CG1-CB-CG2	-6.85	99.94	110.90
1	A	1089	PHE	CB-CG-CD2	-6.83	116.02	120.80
1	C	43	PHE	CB-CA-C	-6.83	96.73	110.40
1	A	43	PHE	CB-CA-C	-6.83	96.73	110.40
1	B	43	PHE	CB-CA-C	-6.82	96.76	110.40
1	A	752	LEU	CB-CG-CD2	-6.81	99.42	111.00
1	C	752	LEU	CB-CG-CD2	-6.79	99.46	111.00
1	B	752	LEU	CB-CG-CD2	-6.78	99.48	111.00
1	C	729	VAL	CA-CB-CG2	-6.74	100.80	110.90
1	A	729	VAL	CA-CB-CG2	-6.74	100.80	110.90
1	B	729	VAL	CA-CB-CG2	-6.73	100.81	110.90
1	C	66	HIS	CB-CA-C	-6.72	96.96	110.40
1	C	66	HIS	N-CA-C	-6.71	92.89	111.00
1	B	66	HIS	CB-CA-C	-6.70	97.00	110.40
1	A	66	HIS	N-CA-C	-6.70	92.92	111.00
1	B	66	HIS	N-CA-C	-6.70	92.91	111.00
1	A	66	HIS	CB-CA-C	-6.69	97.02	110.40
1	B	869	MET	N-CA-CB	6.69	122.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	869	MET	N-CA-CB	6.69	122.64	110.60
1	C	869	MET	N-CA-CB	6.68	122.63	110.60
1	C	1038	LYS	CG-CD-CE	6.65	131.85	111.90
1	B	1038	LYS	CG-CD-CE	6.65	131.84	111.90
1	A	767	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	1038	LYS	CG-CD-CE	6.64	131.82	111.90
1	C	767	LEU	CA-CB-CG	6.64	130.57	115.30
1	B	767	LEU	CA-CB-CG	6.62	130.53	115.30
1	C	1018	ILE	CG1-CB-CG2	-6.59	96.89	111.40
1	A	1018	ILE	CG1-CB-CG2	-6.59	96.90	111.40
1	B	269	TYR	N-CA-CB	-6.59	98.74	110.60
1	C	269	TYR	N-CA-CB	-6.59	98.74	110.60
1	B	1018	ILE	CG1-CB-CG2	-6.57	96.94	111.40
1	A	269	TYR	N-CA-CB	-6.56	98.80	110.60
1	C	18	LEU	CA-CB-CG	6.53	130.32	115.30
1	B	18	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	18	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	1009	THR	CA-CB-OG1	6.50	122.64	109.00
1	C	1009	THR	CA-CB-OG1	6.50	122.64	109.00
1	B	1009	THR	CA-CB-OG1	6.48	122.61	109.00
1	A	954	GLN	CA-CB-CG	6.48	127.65	113.40
1	C	954	GLN	CA-CB-CG	6.46	127.61	113.40
1	B	905	ARG	CB-CG-CD	-6.45	94.82	111.60
1	A	905	ARG	CB-CG-CD	-6.45	94.83	111.60
1	C	905	ARG	CB-CG-CD	-6.45	94.83	111.60
1	B	954	GLN	CA-CB-CG	6.44	127.58	113.40
1	A	817	PHE	CB-CG-CD2	-6.39	116.33	120.80
1	C	141	LEU	N-CA-C	-6.37	93.79	111.00
1	B	1106	GLN	CB-CA-C	-6.37	97.66	110.40
1	B	141	LEU	N-CA-C	-6.37	93.80	111.00
1	A	141	LEU	N-CA-C	-6.37	93.80	111.00
1	B	1079	PRO	N-CD-CG	-6.37	93.65	103.20
1	A	1079	PRO	N-CD-CG	-6.36	93.66	103.20
1	A	1106	GLN	CB-CA-C	-6.36	97.68	110.40
1	C	1106	GLN	CB-CA-C	-6.36	97.69	110.40
1	B	762	GLN	OE1-CD-NE2	-6.35	107.28	121.90
1	C	811	LYS	CG-CD-CE	6.35	130.96	111.90
1	A	811	LYS	CG-CD-CE	6.35	130.94	111.90
1	B	811	LYS	CG-CD-CE	6.35	130.94	111.90
1	C	762	GLN	OE1-CD-NE2	-6.34	107.31	121.90
1	C	1079	PRO	N-CD-CG	-6.33	93.70	103.20
1	C	817	PHE	CB-CG-CD2	-6.33	116.37	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	762	GLN	OE1-CD-NE2	-6.32	107.36	121.90
1	B	817	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	A	1089	PHE	CD1-CG-CD2	-6.30	110.10	118.30
1	B	811	LYS	CD-CE-NZ	-6.28	97.26	111.70
1	C	811	LYS	CD-CE-NZ	-6.28	97.26	111.70
1	C	1089	PHE	CD1-CG-CD2	-6.28	110.14	118.30
1	B	57	PRO	CA-N-CD	-6.27	102.72	111.50
1	A	57	PRO	CA-N-CD	-6.27	102.72	111.50
1	A	811	LYS	CD-CE-NZ	-6.27	97.28	111.70
1	C	57	PRO	CA-N-CD	-6.26	102.74	111.50
1	B	1089	PHE	CD1-CG-CD2	-6.26	110.17	118.30
1	C	610	VAL	CA-CB-CG2	-6.24	101.54	110.90
1	B	610	VAL	CA-CB-CG2	-6.23	101.55	110.90
1	A	610	VAL	CA-CB-CG2	-6.23	101.56	110.90
1	C	1028	LYS	CD-CE-NZ	6.21	125.99	111.70
1	B	1028	LYS	CD-CE-NZ	6.21	125.97	111.70
1	A	1028	LYS	CD-CE-NZ	6.19	125.94	111.70
1	B	207	HIS	CA-CB-CG	6.18	124.11	113.60
1	C	781	VAL	CA-CB-CG2	6.18	120.17	110.90
1	A	781	VAL	CA-CB-CG2	6.17	120.16	110.90
1	C	991	VAL	CA-CB-CG2	-6.17	101.64	110.90
1	A	991	VAL	CA-CB-CG2	-6.17	101.65	110.90
1	B	991	VAL	CA-CB-CG2	-6.17	101.65	110.90
1	A	207	HIS	CA-CB-CG	6.17	124.08	113.60
1	C	207	HIS	CA-CB-CG	6.16	124.06	113.60
1	B	781	VAL	CA-CB-CG2	6.13	120.09	110.90
1	A	477[A]	SER	C-N-CA	6.00	136.71	121.70
1	A	477[B]	SER	C-N-CA	6.00	136.71	121.70
1	B	191	GLU	C-N-CA	-5.97	106.78	121.70
1	C	191	GLU	C-N-CA	-5.96	106.79	121.70
1	A	997	ILE	CB-CA-C	5.96	123.52	111.60
1	A	191	GLU	C-N-CA	-5.96	106.81	121.70
1	B	997	ILE	CB-CA-C	5.95	123.51	111.60
1	C	997	ILE	CB-CA-C	5.95	123.50	111.60
1	C	218	GLN	CB-CG-CD	5.94	127.05	111.60
1	C	216	LEU	N-CA-C	-5.93	94.97	111.00
1	A	218	GLN	CB-CG-CD	5.92	127.00	111.60
1	A	216	LEU	N-CA-C	-5.92	95.01	111.00
1	B	216	LEU	N-CA-C	-5.91	95.03	111.00
1	B	218	GLN	CB-CG-CD	5.91	126.97	111.60
1	B	741	TYR	CE1-CZ-CE2	-5.90	110.36	119.80
1	C	741	TYR	CE1-CZ-CE2	-5.89	110.38	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	741	TYR	CE1-CZ-CE2	-5.89	110.38	119.80
1	B	817	PHE	CB-CA-C	5.85	122.10	110.40
1	A	308	VAL	CA-CB-CG1	5.84	119.66	110.90
1	B	318	PHE	CD1-CG-CD2	-5.84	110.71	118.30
1	A	817	PHE	CB-CA-C	5.84	122.08	110.40
1	C	726	ILE	CG1-CB-CG2	-5.84	98.55	111.40
1	B	308	VAL	CA-CB-CG1	5.84	119.66	110.90
1	B	726	ILE	CG1-CB-CG2	-5.84	98.56	111.40
1	C	308	VAL	CA-CB-CG1	5.84	119.65	110.90
1	A	726	ILE	CG1-CB-CG2	-5.83	98.57	111.40
1	A	318	PHE	CD1-CG-CD2	-5.83	110.72	118.30
1	C	817	PHE	CB-CA-C	5.83	122.05	110.40
1	B	768	THR	OG1-CB-CG2	5.82	123.38	110.00
1	C	318	PHE	CD1-CG-CD2	-5.82	110.74	118.30
1	C	768	THR	OG1-CB-CG2	5.82	123.38	110.00
1	A	768	THR	OG1-CB-CG2	5.82	123.38	110.00
1	B	770	ILE	CA-CB-CG2	-5.81	99.28	110.90
1	A	770	ILE	CA-CB-CG2	-5.80	99.30	110.90
1	C	770	ILE	CA-CB-CG2	-5.79	99.31	110.90
1	C	735	SER	CA-CB-OG	5.77	126.78	111.20
1	A	735	SER	CA-CB-OG	5.77	126.77	111.20
1	B	735	SER	CA-CB-OG	5.76	126.76	111.20
1	B	274	THR	CA-CB-CG2	5.76	120.46	112.40
1	C	274	THR	CA-CB-CG2	5.75	120.45	112.40
1	A	274	THR	CA-CB-CG2	5.72	120.40	112.40
1	A	229	LEU	CA-CB-CG	5.67	128.33	115.30
1	B	229	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	1091	ARG	CB-CG-CD	5.66	126.33	111.60
1	A	1091	ARG	CB-CG-CD	5.66	126.32	111.60
1	C	1091	ARG	CB-CG-CD	5.66	126.32	111.60
1	C	229	LEU	CA-CB-CG	5.65	128.29	115.30
1	C	655	HIS	ND1-CG-CD2	-5.61	98.14	106.00
1	A	655	HIS	ND1-CG-CD2	-5.61	98.14	106.00
1	B	655	HIS	ND1-CG-CD2	-5.61	98.15	106.00
1	B	869	MET	CB-CG-SD	5.60	129.21	112.40
1	A	869	MET	CB-CG-SD	5.60	129.19	112.40
1	C	883	THR	OG1-CB-CG2	5.60	122.87	110.00
1	C	869	MET	CB-CG-SD	5.59	129.18	112.40
1	A	883	THR	OG1-CB-CG2	5.59	122.86	110.00
1	B	883	THR	OG1-CB-CG2	5.59	122.85	110.00
1	C	141	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	A	141	LEU	CB-CG-CD1	-5.55	101.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	140	PHE	C-N-CA	-5.55	107.84	121.70
1	A	140	PHE	C-N-CA	-5.54	107.86	121.70
1	B	141	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	B	140	PHE	C-N-CA	-5.53	107.88	121.70
1	C	859	THR	N-CA-C	-5.52	96.09	111.00
1	A	859	THR	N-CA-C	-5.52	96.10	111.00
1	B	859	THR	N-CA-C	-5.52	96.10	111.00
1	B	980	ILE	CG1-CB-CG2	5.51	123.53	111.40
1	A	980	ILE	CG1-CB-CG2	5.49	123.48	111.40
1	C	478	THR	CA-CB-CG2	5.49	120.08	112.40
1	B	821	LEU	N-CA-CB	-5.48	99.44	110.40
1	C	821	LEU	N-CA-CB	-5.48	99.44	110.40
1	C	980	ILE	CG1-CB-CG2	5.48	123.45	111.40
1	A	821	LEU	N-CA-CB	-5.46	99.48	110.40
1	B	818	ILE	CG1-CB-CG2	-5.46	99.39	111.40
1	A	818	ILE	CG1-CB-CG2	-5.45	99.41	111.40
1	C	818	ILE	CG1-CB-CG2	-5.45	99.41	111.40
1	B	794	ILE	CG1-CB-CG2	5.43	123.36	111.40
1	C	756	TYR	CZ-CE2-CD2	-5.43	114.91	119.80
1	C	794	ILE	CG1-CB-CG2	5.43	123.35	111.40
1	B	1039	ARG	CG-CD-NE	5.43	123.20	111.80
1	C	1039	ARG	CG-CD-NE	5.43	123.20	111.80
1	C	1008	VAL	CA-CB-CG1	5.42	119.03	110.90
1	A	794	ILE	CG1-CB-CG2	5.41	123.30	111.40
1	A	1039	ARG	CG-CD-NE	5.41	123.15	111.80
1	C	276	LEU	CB-CG-CD2	5.41	120.19	111.00
1	B	1008	VAL	CA-CB-CG1	5.40	119.00	110.90
1	A	1008	VAL	CA-CB-CG1	5.40	118.99	110.90
1	B	756	TYR	CZ-CE2-CD2	-5.40	114.94	119.80
1	A	756	TYR	CZ-CE2-CD2	-5.39	114.95	119.80
1	A	276	LEU	CB-CG-CD2	5.38	120.15	111.00
1	A	699	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	B	1113	GLN	CA-CB-CG	5.38	125.23	113.40
1	B	276	LEU	CB-CG-CD2	5.37	120.13	111.00
1	B	699	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	C	1113	GLN	CA-CB-CG	5.37	125.21	113.40
1	C	699	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	A	1113	GLN	CA-CB-CG	5.36	125.19	113.40
1	B	192	PHE	CA-CB-CG	-5.36	101.05	113.90
1	C	192	PHE	CA-CB-CG	-5.35	101.07	113.90
1	A	192	PHE	CA-CB-CG	-5.34	101.07	113.90
1	C	269	TYR	CB-CA-C	5.34	121.08	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	TYR	CB-CA-C	5.33	121.05	110.40
1	B	286	THR	CA-CB-CG2	5.32	119.85	112.40
1	B	269	TYR	CB-CA-C	5.31	121.03	110.40
1	A	286	THR	CA-CB-CG2	5.30	119.82	112.40
1	C	286	THR	CA-CB-CG2	5.30	119.81	112.40
1	A	1091	ARG	CD-NE-CZ	5.29	131.01	123.60
1	B	1091	ARG	CD-NE-CZ	5.28	130.99	123.60
1	B	1006	THR	OG1-CB-CG2	5.27	122.13	110.00
1	C	1091	ARG	CD-NE-CZ	5.26	130.97	123.60
1	C	1006	THR	OG1-CB-CG2	5.26	122.10	110.00
1	A	655	HIS	CB-CG-CD2	-5.26	114.50	130.80
1	C	655	HIS	CB-CG-CD2	-5.26	114.50	130.80
1	A	170	TYR	CG-CD1-CE1	5.25	125.50	121.30
1	A	1006	THR	OG1-CB-CG2	5.25	122.08	110.00
1	B	655	HIS	CB-CG-CD2	-5.25	114.54	130.80
1	A	699	LEU	N-CA-C	5.24	125.14	111.00
1	A	1058	HIS	N-CA-CB	5.24	120.03	110.60
1	C	170	TYR	CG-CD1-CE1	5.23	125.48	121.30
1	B	170	TYR	CG-CD1-CE1	5.23	125.48	121.30
1	B	1058	HIS	N-CA-CB	5.23	120.01	110.60
1	B	699	LEU	N-CA-C	5.23	125.11	111.00
1	C	1001	LEU	CB-CG-CD2	5.23	119.89	111.00
1	B	1122	VAL	CG1-CB-CG2	5.22	119.26	110.90
1	A	1018	ILE	CB-CG1-CD1	5.22	128.52	113.90
1	C	699	LEU	N-CA-C	5.22	125.10	111.00
1	C	1018	ILE	CB-CG1-CD1	5.22	128.52	113.90
1	A	1001	LEU	CB-CG-CD2	5.22	119.87	111.00
1	C	1058	HIS	N-CA-CB	5.21	119.99	110.60
1	B	1018	ILE	CB-CG1-CD1	5.21	128.50	113.90
1	B	1001	LEU	CB-CG-CD2	5.20	119.83	111.00
1	C	1122	VAL	CG1-CB-CG2	5.19	119.21	110.90
1	A	1122	VAL	CG1-CB-CG2	5.18	119.19	110.90
1	C	741	TYR	OH-CZ-CE2	5.17	134.06	120.10
1	A	977	LEU	CB-CG-CD2	5.17	119.79	111.00
1	B	741	TYR	OH-CZ-CE2	5.17	134.05	120.10
1	A	802	PHE	N-CA-CB	5.17	119.90	110.60
1	A	1006	THR	CA-CB-OG1	5.16	119.84	109.00
1	C	1006	THR	CA-CB-OG1	5.16	119.84	109.00
1	A	741	TYR	OH-CZ-CE2	5.16	134.03	120.10
1	B	1006	THR	CA-CB-OG1	5.16	119.84	109.00
1	C	802	PHE	N-CA-CB	5.16	119.88	110.60
1	C	977	LEU	CB-CG-CD2	5.16	119.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	977	LEU	CB-CG-CD2	5.15	119.76	111.00
1	B	764	ASN	C-N-CA	-5.14	108.84	121.70
1	B	802	PHE	N-CA-CB	5.13	119.83	110.60
1	C	764	ASN	C-N-CA	-5.12	108.90	121.70
1	B	160	TYR	N-CA-CB	-5.12	101.39	110.60
1	A	764	ASN	C-N-CA	-5.11	108.92	121.70
1	A	17	ASN	CB-CA-C	-5.11	100.19	110.40
1	A	160	TYR	N-CA-CB	-5.11	101.41	110.60
1	C	160	TYR	N-CA-CB	-5.10	101.42	110.60
1	B	17	ASN	CB-CA-C	-5.09	100.21	110.40
1	C	909	ILE	N-CA-CB	5.09	122.50	110.80
1	C	17	ASN	CB-CA-C	-5.08	100.23	110.40
1	C	909	ILE	CB-CG1-CD1	5.08	128.12	113.90
1	A	909	ILE	CB-CG1-CD1	5.07	128.11	113.90
1	B	964	LYS	CA-CB-CG	5.07	124.56	113.40
1	A	964	LYS	CA-CB-CG	5.07	124.55	113.40
1	B	909	ILE	N-CA-CB	5.07	122.45	110.80
1	A	909	ILE	N-CA-CB	5.06	122.45	110.80
1	C	964	LYS	CA-CB-CG	5.06	124.54	113.40
1	B	909	ILE	CB-CG1-CD1	5.06	128.06	113.90
1	C	726	ILE	CB-CG1-CD1	5.06	128.06	113.90
1	B	726	ILE	CB-CG1-CD1	5.05	128.05	113.90
1	A	43	PHE	N-CA-CB	5.05	119.69	110.60
1	A	726	ILE	CB-CG1-CD1	5.04	128.02	113.90
1	B	43	PHE	N-CA-CB	5.03	119.65	110.60
1	C	43	PHE	N-CA-CB	5.02	119.64	110.60

All (33) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	274	THR	CB
1	A	286	THR	CB
1	A	299	THR	CB
1	A	719	THR	CB
1	A	761	THR	CB
1	A	980	ILE	CB
1	A	997	ILE	CB
1	A	1006	THR	CB
1	A	1009	THR	CB
1	A	1013	ILE	CB
1	A	1116	THR	CB
1	B	274	THR	CB

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Mol	Chain	Res	Type	Atom
1	B	286	THR	CB
1	B	299	THR	CB
1	B	719	THR	CB
1	B	761	THR	CB
1	B	980	ILE	CB
1	B	997	ILE	CB
1	B	1006	THR	CB
1	B	1009	THR	CB
1	B	1013	ILE	CB
1	B	1116	THR	CB
1	C	274	THR	CB
1	C	286	THR	CB
1	C	299	THR	CB
1	C	719	THR	CB
1	C	761	THR	CB
1	C	980	ILE	CB
1	C	997	ILE	CB
1	C	1006	THR	CB
1	C	1009	THR	CB
1	C	1013	ILE	CB
1	C	1116	THR	CB

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	ARG	Sidechain
1	A	1039	ARG	Sidechain,Peptide
1	A	1058	HIS	Sidechain
1	A	1064	HIS	Sidechain,Peptide
1	A	1089	PHE	Sidechain
1	A	1091	ARG	Sidechain
1	A	158	ARG	Sidechain
1	A	159	VAL	Peptide
1	A	160	TYR	Sidechain
1	A	170	TYR	Sidechain
1	A	192	PHE	Sidechain
1	A	206	LYS	Peptide
1	A	207	HIS	Sidechain,Peptide
1	A	25	PRO	Peptide
1	A	266	TYR	Sidechain
1	A	269	TYR	Sidechain
1	A	318	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	43	PHE	Sidechain
1	A	476	GLY	Peptide
1	A	477[A]	SER	Peptide
1	A	477[B]	SER	Peptide
1	A	655	HIS	Sidechain
1	A	66	HIS	Sidechain
1	A	741	TYR	Sidechain
1	A	762	GLN	Sidechain
1	A	764	ASN	Peptide
1	A	765	ARG	Sidechain
1	A	802	PHE	Sidechain
1	A	817	PHE	Sidechain
1	A	872	GLN	Sidechain
1	A	901	GLN	Sidechain
1	A	905	ARG	Sidechain
1	A	926	GLN	Sidechain
1	A	927	PHE	Sidechain
1	A	961	THR	Peptide
1	A	969	ASN	Sidechain
1	B	1014	ARG	Sidechain
1	B	1039	ARG	Sidechain,Peptide
1	B	1058	HIS	Sidechain
1	B	1064	HIS	Sidechain,Peptide
1	B	1089	PHE	Sidechain
1	B	1091	ARG	Sidechain
1	B	158	ARG	Sidechain
1	B	159	VAL	Peptide
1	B	160	TYR	Sidechain
1	B	170	TYR	Sidechain
1	B	192	PHE	Sidechain
1	B	206	LYS	Peptide
1	B	207	HIS	Sidechain,Peptide
1	B	25	PRO	Peptide
1	B	266	TYR	Sidechain
1	B	269	TYR	Sidechain
1	B	318	PHE	Sidechain
1	B	43	PHE	Sidechain
1	B	488	CYS	Peptide
1	B	489	TYR	Peptide
1	B	655	HIS	Sidechain
1	B	66	HIS	Sidechain
1	B	741	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	762	GLN	Sidechain
1	B	764	ASN	Peptide
1	B	765	ARG	Sidechain
1	B	802	PHE	Sidechain
1	B	817	PHE	Sidechain
1	B	872	GLN	Sidechain
1	B	901	GLN	Sidechain
1	B	905	ARG	Sidechain
1	B	926	GLN	Sidechain
1	B	927	PHE	Sidechain
1	B	961	THR	Peptide
1	B	969	ASN	Sidechain
1	C	1014	ARG	Sidechain
1	C	1039	ARG	Sidechain,Peptide
1	C	1058	HIS	Sidechain
1	C	1064	HIS	Sidechain,Peptide
1	C	1089	PHE	Sidechain
1	C	1091	ARG	Sidechain
1	C	158	ARG	Sidechain
1	C	159	VAL	Peptide
1	C	160	TYR	Sidechain
1	C	170	TYR	Sidechain
1	C	192	PHE	Sidechain
1	C	206	LYS	Peptide
1	C	207	HIS	Sidechain,Peptide
1	C	25	PRO	Peptide
1	C	266	TYR	Sidechain
1	C	269	TYR	Sidechain
1	C	318	PHE	Sidechain
1	C	43	PHE	Sidechain
1	C	459	SER	Peptide
1	C	476	GLY	Peptide
1	C	655	HIS	Sidechain
1	C	66	HIS	Sidechain
1	C	741	TYR	Sidechain
1	C	762	GLN	Sidechain
1	C	764	ASN	Peptide
1	C	765	ARG	Sidechain
1	C	802	PHE	Sidechain
1	C	817	PHE	Sidechain
1	C	872	GLN	Sidechain
1	C	901	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	C	905	ARG	Sidechain
1	C	926	GLN	Sidechain
1	C	927	PHE	Sidechain
1	C	961	THR	Peptide
1	C	969	ASN	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8301	8079	8081	468	0
1	B	8253	8034	8043	502	0
1	C	8292	8069	8072	473	0
2	D	895	0	839	124	0
2	E	895	0	839	146	0
3	F	28	25	25	2	0
3	G	28	25	25	0	0
3	H	28	25	25	0	0
3	I	28	25	25	1	0
3	J	28	25	25	2	0
4	A	196	181	182	15	0
4	B	182	167	169	26	0
4	C	84	64	78	8	0
All	All	27238	24719	26428	1551	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 29.

All (1551) 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)
1:A:770:ILE:CB	1:A:770:ILE:CG2	1.76	1.63
1:C:699:LEU:CD2	1:C:699:LEU:CG	1.76	1.63
1:C:959:LEU:CG	1:C:959:LEU:CD2	1.77	1.62
1:B:911:VAL:CG2	1:B:911:VAL:HG13	1.28	1.61
1:C:911:VAL:CG1	1:C:911:VAL:CG2	1.78	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:VAL:CG2	1:A:911:VAL:CB	1.78	1.60
1:B:770:ILE:CG2	1:B:770:ILE:CB	1.76	1.59
1:C:911:VAL:CG2	1:C:911:VAL:HG13	1.28	1.58
1:C:770:ILE:CG1	1:C:770:ILE:CG2	1.82	1.58
1:A:911:VAL:CG2	1:A:911:VAL:HG13	1.28	1.57
1:B:911:VAL:CG2	1:B:911:VAL:CB	1.78	1.57
1:C:770:ILE:CG2	1:C:770:ILE:CB	1.76	1.57
1:A:699:LEU:CD1	1:A:699:LEU:CD2	1.82	1.57
1:A:959:LEU:CG	1:A:959:LEU:CD2	1.77	1.55
1:B:959:LEU:CD2	1:B:959:LEU:CG	1.77	1.55
1:B:699:LEU:CD1	1:B:699:LEU:CD2	1.82	1.55
1:C:911:VAL:CG2	1:C:911:VAL:CB	1.78	1.55
1:A:911:VAL:CG2	1:A:911:VAL:CG1	1.78	1.54
1:B:911:VAL:CG2	1:B:911:VAL:CG1	1.78	1.54
1:B:699:LEU:CD2	1:B:699:LEU:CG	1.76	1.53
1:A:699:LEU:CD2	1:A:699:LEU:CG	1.76	1.53
1:B:770:ILE:CG2	1:B:770:ILE:CG1	1.82	1.53
1:A:770:ILE:CG2	1:A:770:ILE:CG1	1.82	1.52
1:C:699:LEU:CD2	1:C:699:LEU:CD1	1.82	1.51
1:A:770:ILE:CG2	1:A:770:ILE:HG12	1.38	1.44
1:B:770:ILE:CG2	1:B:770:ILE:HG12	1.38	1.43
1:A:699:LEU:CD2	1:A:699:LEU:HD13	1.45	1.38
1:B:699:LEU:CD2	1:B:699:LEU:HD13	1.45	1.36
1:C:770:ILE:CG2	1:C:770:ILE:HG12	1.38	1.35
1:A:959:LEU:CD2	1:A:959:LEU:CB	2.06	1.33
1:C:959:LEU:CD2	1:C:959:LEU:CB	2.06	1.31
1:C:699:LEU:CD2	1:C:699:LEU:HD13	1.45	1.31
1:B:959:LEU:CD2	1:B:959:LEU:CB	2.06	1.31
1:A:192:PHE:CE1	1:A:192:PHE:CE2	1.96	1.22
1:C:192:PHE:CZ	1:C:192:PHE:CD1	1.95	1.21
1:B:959:LEU:CD2	1:B:959:LEU:CD1	2.25	1.15
1:A:192:PHE:CZ	1:A:192:PHE:CD1	1.95	1.14
1:B:959:LEU:CD2	1:B:959:LEU:HB3	1.78	1.14
1:C:192:PHE:CE1	1:C:192:PHE:CE2	1.96	1.14
1:A:959:LEU:CD2	1:A:959:LEU:CD1	2.25	1.13
1:C:699:LEU:HD13	1:C:699:LEU:HD22	1.29	1.13
1:C:959:LEU:CD2	1:C:959:LEU:CD1	2.25	1.13
1:A:770:ILE:HG12	1:A:770:ILE:HG23	1.22	1.12
1:C:911:VAL:HG13	1:C:911:VAL:HG22	1.28	1.12
1:C:959:LEU:CD2	1:C:959:LEU:HB3	1.78	1.12
1:B:192:PHE:CZ	1:B:192:PHE:CD1	1.96	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:LEU:HG	1:C:872:GLN:OE1	1.46	1.11
1:B:192:PHE:CE1	1:B:192:PHE:CE2	1.96	1.10
1:B:911:VAL:HG13	1:B:911:VAL:HG22	1.28	1.10
1:A:699:LEU:HD13	1:A:699:LEU:HD22	1.29	1.09
1:C:770:ILE:HG12	1:C:770:ILE:HG23	1.22	1.09
1:A:911:VAL:HG13	1:A:911:VAL:HG22	1.28	1.08
1:B:770:ILE:HG12	1:B:770:ILE:HG23	1.22	1.08
1:B:699:LEU:HD13	1:B:699:LEU:HD22	1.29	1.08
1:B:480:CYS:O	1:B:482:GLY:N	1.87	1.07
1:A:1005:GLN:HE22	1:C:1006:THR:CG2	1.67	1.06
1:A:959:LEU:CD2	1:A:959:LEU:HB3	1.78	1.05
1:A:911:VAL:HG13	1:A:911:VAL:HG21	1.34	1.05
1:B:911:VAL:HG13	1:B:911:VAL:HG21	1.34	1.05
2:D:31:THR:HG21	2:D:98:SER:HB3	1.07	1.05
1:C:911:VAL:HG13	1:C:911:VAL:HG21	1.34	1.05
2:E:69:THR:HG22	2:E:82:GLN:HB3	1.40	1.04
2:E:31:THR:HG21	2:E:98:SER:HB3	1.06	1.04
1:B:378:LYS:HD2	2:E:106:TYR:HD2	1.22	1.04
1:A:282:ASN:ND2	4:A:1303:NAG:O5	1.89	1.04
2:D:69:THR:HG22	2:D:82:GLN:HB3	1.40	1.02
1:B:378:LYS:HD2	2:E:106:TYR:CD2	1.95	1.01
1:B:376:THR:HG23	2:E:106:TYR:HB2	1.43	1.00
1:B:770:ILE:CG1	1:B:770:ILE:HG21	1.91	1.00
1:A:911:VAL:CG1	1:A:911:VAL:HG21	1.88	1.00
1:C:959:LEU:HD13	1:C:959:LEU:HD21	1.44	0.99
2:D:22:CYS:HB3	2:D:79:VAL:HG12	1.45	0.99
1:A:759:PHE:HA	1:A:762:GLN:OE1	1.64	0.98
1:B:759:PHE:HA	1:B:762:GLN:OE1	1.64	0.98
1:B:357:ARG:NH2	1:B:396:TYR:OH	1.97	0.98
1:C:759:PHE:HA	1:C:762:GLN:OE1	1.63	0.98
1:A:959:LEU:HD13	1:A:959:LEU:HD21	1.44	0.97
1:B:959:LEU:HD21	1:B:959:LEU:HD13	1.44	0.97
1:C:770:ILE:CG1	1:C:770:ILE:HG21	1.91	0.97
1:B:911:VAL:CG1	1:B:911:VAL:HG21	1.88	0.97
1:A:1005:GLN:HE22	1:C:1006:THR:HG23	1.30	0.96
1:B:699:LEU:CD1	1:B:699:LEU:HD21	1.96	0.96
1:B:770:ILE:HG12	1:B:770:ILE:HG21	1.46	0.95
2:E:64:VAL:HA	2:E:67:ARG:HE	1.30	0.95
1:A:699:LEU:CD1	1:A:699:LEU:HD21	1.96	0.95
1:A:770:ILE:CG1	1:A:770:ILE:HG21	1.91	0.94
2:D:64:VAL:HA	2:D:67:ARG:HE	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:VAL:CG2	1:B:911:VAL:CA	2.46	0.94
1:C:699:LEU:CD1	1:C:699:LEU:HD21	1.96	0.94
2:E:22:CYS:HB3	2:E:79:VAL:HG12	1.45	0.94
1:A:911:VAL:CG2	1:A:911:VAL:CA	2.46	0.94
1:C:911:VAL:CG2	1:C:911:VAL:CA	2.46	0.94
2:D:101:TYR:HE1	2:D:103:ALA:HB3	1.33	0.93
1:B:376:THR:OG1	2:E:106:TYR:CD1	2.18	0.93
1:B:669:GLY:CA	1:C:869:MET:CE	2.47	0.93
2:E:101:TYR:HE1	2:E:103:ALA:HB3	1.33	0.93
1:A:149:ASN:HD21	4:A:1301:NAG:C1	1.82	0.92
1:B:669:GLY:HA2	1:C:869:MET:CE	1.99	0.92
2:E:31:THR:CG2	2:E:98:SER:HB3	1.98	0.92
1:A:959:LEU:HB3	1:A:959:LEU:HD23	1.52	0.91
1:C:911:VAL:CG1	1:C:911:VAL:HG21	1.88	0.91
1:B:192:PHE:CZ	1:B:192:PHE:CE1	0.91	0.91
1:C:192:PHE:CZ	1:C:192:PHE:CE1	0.91	0.91
2:D:31:THR:CG2	2:D:98:SER:HB3	1.99	0.91
1:A:192:PHE:CE1	1:A:192:PHE:CZ	0.91	0.91
1:B:596:SER:OG	1:B:613:GLN:OE1	1.89	0.91
1:C:130:VAL:HG21	1:C:231:ILE:HG21	1.53	0.90
1:C:959:LEU:HB3	1:C:959:LEU:HD23	1.52	0.90
1:A:596:SER:OG	1:A:613:GLN:OE1	1.89	0.90
1:A:282:ASN:ND2	4:A:1303:NAG:C1	2.34	0.89
1:A:959:LEU:CD2	1:A:959:LEU:HD13	1.98	0.89
1:C:596:SER:OG	1:C:613:GLN:OE1	1.89	0.89
1:B:959:LEU:HB3	1:B:959:LEU:HD23	1.52	0.89
1:A:192:PHE:CZ	1:A:192:PHE:HE1	1.60	0.89
1:B:192:PHE:CE1	1:B:192:PHE:HZ	1.63	0.89
1:B:130:VAL:HG21	1:B:231:ILE:HG21	1.53	0.89
1:B:708:SER:HB3	1:B:711:SER:HB3	1.52	0.89
1:B:770:ILE:CG2	1:B:770:ILE:CA	2.51	0.89
1:C:192:PHE:CE1	1:C:192:PHE:HZ	1.63	0.88
1:A:770:ILE:CG2	1:A:770:ILE:CA	2.51	0.88
1:B:959:LEU:CD2	1:B:959:LEU:HD13	1.98	0.88
1:C:280:ASN:OD1	1:C:281:GLU:N	2.07	0.88
1:B:376:THR:OG1	2:E:106:TYR:HD1	1.56	0.88
1:B:699:LEU:CG	1:C:872:GLN:OE1	2.21	0.88
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.07	0.88
1:B:280:ASN:OD1	1:B:281:GLU:N	2.07	0.88
1:C:280:ASN:OD1	1:C:282:ASN:N	2.07	0.88
1:A:130:VAL:HG21	1:A:231:ILE:HG21	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CE1	1:A:192:PHE:HZ	1.63	0.88
1:B:699:LEU:CD2	1:B:699:LEU:CB	2.52	0.87
1:A:280:ASN:OD1	1:A:282:ASN:N	2.07	0.87
1:C:699:LEU:CD2	1:C:699:LEU:CB	2.52	0.87
1:C:770:ILE:CG2	1:C:770:ILE:CA	2.51	0.87
4:B:1304:NAG:H83	4:B:1304:NAG:H3	1.54	0.87
1:B:901:GLN:O	1:B:905:ARG:HG2	1.75	0.87
1:C:192:PHE:CZ	1:C:192:PHE:HE1	1.60	0.87
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.07	0.87
1:A:699:LEU:CD2	1:A:699:LEU:CB	2.52	0.87
1:A:280:ASN:OD1	1:A:281:GLU:N	2.07	0.86
1:A:901:GLN:O	1:A:905:ARG:HG2	1.75	0.86
1:B:192:PHE:CZ	1:B:192:PHE:HE1	1.60	0.86
1:B:376:THR:HG1	2:E:106:TYR:HD1	0.93	0.86
1:C:770:ILE:HG12	1:C:770:ILE:HG21	1.46	0.86
1:B:280:ASN:OD1	1:B:282:ASN:N	2.07	0.86
1:B:669:GLY:CA	1:C:869:MET:HE1	2.05	0.86
1:C:901:GLN:O	1:C:905:ARG:HG2	1.75	0.86
2:E:105:GLY:HA2	2:E:108:PHE:CE1	2.11	0.86
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.07	0.86
2:D:105:GLY:HA2	2:D:108:PHE:CE1	2.11	0.85
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.59	0.85
1:B:699:LEU:HB3	1:C:788:ILE:HG13	1.58	0.85
1:B:349:SER:OG	1:B:452:LEU:O	1.93	0.85
1:A:282:ASN:HD21	4:A:1303:NAG:C1	1.88	0.84
1:B:770:ILE:CG2	1:B:770:ILE:C	2.46	0.84
2:D:101:TYR:CE1	2:D:103:ALA:HB3	2.13	0.84
1:C:770:ILE:CG2	1:C:770:ILE:C	2.46	0.84
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.59	0.84
1:C:905:ARG:NH1	1:C:1050:MET:HB3	1.93	0.83
2:E:101:TYR:CE1	2:E:103:ALA:HB3	2.13	0.83
1:A:770:ILE:CG2	1:A:770:ILE:C	2.46	0.83
1:A:17:ASN:OD1	3:F:1:NAG:C1	2.27	0.83
1:A:1005:GLN:NE2	1:C:1006:THR:HG23	1.93	0.83
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.11	0.83
1:B:14:GLN:NE2	1:B:15:CYS:O	2.11	0.83
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.11	0.83
1:A:14:GLN:NE2	1:A:15:CYS:O	2.11	0.83
1:B:376:THR:HG23	2:E:106:TYR:CB	2.08	0.83
1:A:770:ILE:HG12	1:A:770:ILE:HG21	1.46	0.83
1:C:14:GLN:NE2	1:C:15:CYS:O	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:ARG:NH1	1:B:1050:MET:HB3	1.94	0.82
1:A:905:ARG:NH1	1:A:1050:MET:HB3	1.93	0.82
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.11	0.82
2:D:12:VAL:HG21	2:D:86:LEU:HD12	1.62	0.82
1:B:705:VAL:HG12	1:C:895:GLN:HB3	1.62	0.81
2:E:109:ASN:HA	2:E:111:TRP:CZ3	2.14	0.81
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.63	0.81
2:E:12:VAL:HG21	2:E:86:LEU:HD12	1.62	0.81
2:E:67:ARG:HG3	2:E:68:PHE:HD1	1.45	0.81
1:C:959:LEU:CD2	1:C:959:LEU:HD13	1.98	0.81
2:D:109:ASN:HA	2:D:111:TRP:CZ3	2.14	0.81
1:B:949:GLN:O	1:B:953:ASN:OD1	2.00	0.80
1:B:669:GLY:CA	1:C:869:MET:HE3	2.09	0.80
1:A:894:LEU:HD13	1:C:713:ALA:O	1.80	0.80
1:A:1080:ALA:HB2	1:A:1089:PHE:CE2	2.17	0.80
1:A:949:GLN:O	1:A:953:ASN:OD1	1.99	0.80
1:B:1080:ALA:HB2	1:B:1089:PHE:CE2	2.17	0.80
1:B:669:GLY:HA2	1:C:869:MET:HE3	1.64	0.80
1:A:886:TRP:HZ3	1:A:905:ARG:HD3	1.47	0.79
2:D:67:ARG:HG3	2:D:68:PHE:HD1	1.45	0.79
1:B:378:LYS:CD	2:E:106:TYR:HD2	1.95	0.79
1:B:820:ASP:O	1:B:824:ASN:OD1	2.01	0.79
1:C:1080:ALA:HB2	1:C:1089:PHE:CE2	2.17	0.79
1:C:820:ASP:O	1:C:824:ASN:OD1	2.01	0.79
1:C:886:TRP:HZ3	1:C:905:ARG:HD3	1.47	0.79
1:A:917:TYR:CZ	1:C:1079:PRO:HB3	2.17	0.79
1:B:669:GLY:HA3	1:C:869:MET:CE	2.12	0.79
1:B:376:THR:CG2	2:E:106:TYR:HB2	2.12	0.79
1:A:589:PRO:HG2	1:B:855:PHE:HD1	1.48	0.79
1:C:919:ASN:OD1	1:C:923:ILE:HG13	1.84	0.78
1:C:949:GLN:O	1:C:953:ASN:OD1	2.00	0.78
1:B:886:TRP:HZ3	1:B:905:ARG:HD3	1.47	0.78
1:A:762:GLN:HE21	1:C:961:THR:HG21	1.48	0.78
2:E:81:LEU:HG	2:E:83:MET:SD	2.23	0.78
1:A:892:ALA:CB	1:C:1072:GLU:OE2	2.32	0.78
1:B:378:LYS:CD	2:E:106:TYR:CD2	2.67	0.78
1:A:820:ASP:O	1:A:824:ASN:OD1	2.01	0.78
2:D:81:LEU:HG	2:D:83:MET:SD	2.23	0.78
1:B:393:THR:O	1:B:523:THR:OG1	2.01	0.77
1:C:130:VAL:HG21	1:C:231:ILE:CG2	2.14	0.77
2:D:38:ARG:CG	2:D:92:ALA:HB3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:ARG:CG	2:E:92:ALA:HB3	2.14	0.77
1:B:919:ASN:OD1	1:B:923:ILE:HG13	1.84	0.77
1:A:802:PHE:O	1:A:806:LEU:HB2	1.85	0.77
1:B:658:ASN:OD1	1:B:660:TYR:CE1	2.38	0.77
2:E:67:ARG:HG3	2:E:68:PHE:CD1	2.20	0.77
1:C:973:ILE:HD11	1:C:980:ILE:HG23	1.67	0.77
1:A:658:ASN:OD1	1:A:660:TYR:CE1	2.38	0.77
1:A:130:VAL:HG21	1:A:231:ILE:CG2	2.14	0.76
1:A:802:PHE:N	1:A:802:PHE:CD2	2.53	0.76
1:C:658:ASN:OD1	1:C:660:TYR:CE1	2.38	0.76
1:C:802:PHE:O	1:C:806:LEU:HB2	1.85	0.76
1:B:802:PHE:N	1:B:802:PHE:CD2	2.53	0.76
1:A:332:ILE:CD1	1:A:527:PRO:HA	2.15	0.76
1:A:919:ASN:OD1	1:A:923:ILE:HG13	1.83	0.76
1:B:802:PHE:O	1:B:806:LEU:HB2	1.85	0.76
1:A:897:PRO:HB3	1:C:709:ASN:O	1.86	0.76
1:B:130:VAL:HG21	1:B:231:ILE:CG2	2.14	0.76
1:B:707:TYR:OH	1:C:897:PRO:O	2.03	0.75
1:C:802:PHE:N	1:C:802:PHE:CD2	2.53	0.75
2:D:67:ARG:HG3	2:D:68:PHE:CD1	2.20	0.75
1:A:1005:GLN:HE22	1:C:1006:THR:HG21	1.49	0.75
1:B:922:LEU:HD11	4:B:1310:NAG:C6	2.15	0.75
1:C:661:GLU:O	1:C:695:TYR:OH	2.05	0.75
1:B:667:GLY:HA2	1:C:864:LEU:HA	1.68	0.75
1:B:661:GLU:O	1:B:695:TYR:OH	2.04	0.75
1:B:774:GLN:HA	1:B:777:ASN:OD1	1.87	0.75
1:B:973:ILE:HD11	1:B:980:ILE:HG23	1.67	0.74
1:A:973:ILE:HD11	1:A:980:ILE:HG23	1.67	0.74
2:E:105:GLY:HA2	2:E:108:PHE:HE1	1.51	0.74
1:A:1030:SER:O	1:C:1040:VAL:HG11	1.87	0.74
1:A:661:GLU:O	1:A:695:TYR:OH	2.05	0.74
1:A:918:GLU:HA	1:C:1128:VAL:HG22	1.69	0.73
1:B:407:VAL:O	2:E:106:TYR:OH	2.06	0.73
1:C:774:GLN:HA	1:C:777:ASN:OD1	1.87	0.73
1:A:774:GLN:HA	1:A:777:ASN:OD1	1.87	0.73
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.71	0.73
1:A:1005:GLN:NE2	1:C:1006:THR:CG2	2.47	0.73
2:D:105:GLY:HA2	2:D:108:PHE:HE1	1.51	0.73
1:A:914:ASN:HB3	1:C:1089:PHE:HE1	1.53	0.73
1:B:454:ARG:NH1	1:B:467:ASP:OD2	2.21	0.73
1:B:669:GLY:HA3	1:C:869:MET:HE1	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:933:LYS:O	1:C:936:ASP:OD2	2.07	0.73
1:C:762:GLN:HA	1:C:765:ARG:NH1	2.04	0.73
1:B:959:LEU:CB	1:B:959:LEU:HD22	2.18	0.73
1:A:748:GLU:O	1:A:752:LEU:HG	1.89	0.73
1:B:933:LYS:O	1:B:936:ASP:OD2	2.07	0.73
1:B:748:GLU:O	1:B:752:LEU:HG	1.89	0.72
2:E:98:SER:O	2:E:108:PHE:HA	1.89	0.72
1:C:318:PHE:HD2	1:C:319:ARG:N	1.87	0.72
1:A:762:GLN:HA	1:A:765:ARG:NH1	2.04	0.72
2:D:98:SER:O	2:D:108:PHE:HA	1.89	0.72
1:B:117:LEU:HD13	1:B:130:VAL:HG22	1.71	0.72
1:C:748:GLU:O	1:C:752:LEU:HG	1.89	0.72
1:C:959:LEU:CB	1:C:959:LEU:HD22	2.18	0.72
1:B:372:ALA:HA	2:E:47:ARG:HH12	1.54	0.72
1:B:762:GLN:HA	1:B:765:ARG:NH1	2.04	0.72
2:D:20:LEU:HD12	2:D:21:SER:N	2.05	0.72
1:B:318:PHE:HD2	1:B:319:ARG:N	1.87	0.72
4:B:1302:NAG:O7	4:B:1302:NAG:O3	2.07	0.72
1:C:476:GLY:O	1:C:487:ASN:ND2	2.23	0.72
2:E:20:LEU:HD12	2:E:21:SER:N	2.05	0.72
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.71	0.71
1:A:933:LYS:O	1:A:936:ASP:OD2	2.07	0.71
1:A:318:PHE:HD2	1:A:319:ARG:N	1.88	0.71
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.71	0.71
1:A:762:GLN:NE2	1:C:961:THR:HG21	2.05	0.71
2:D:60:TYR:HD2	2:D:64:VAL:HG23	1.55	0.71
2:E:95:TYR:HD2	2:E:114:GLY:HA3	1.55	0.71
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.71	0.71
1:B:707:TYR:CE2	1:C:897:PRO:HA	2.26	0.71
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.71	0.71
1:C:802:PHE:N	1:C:802:PHE:HD2	1.88	0.71
1:C:974:SER:OG	1:C:979:ASP:OD2	2.09	0.71
2:E:60:TYR:HD2	2:E:64:VAL:HG23	1.55	0.71
1:A:43:PHE:HD1	1:A:44:ARG:N	1.89	0.71
1:B:43:PHE:HD1	1:B:44:ARG:N	1.89	0.71
1:B:708:SER:HB3	1:B:711:SER:CB	2.21	0.71
1:C:962:LEU:C	1:C:962:LEU:HD12	2.11	0.70
1:A:703:ASN:OD1	1:B:787:GLN:OE1	2.09	0.70
1:A:962:LEU:C	1:A:962:LEU:HD12	2.11	0.70
1:C:1062:PHE:HB2	1:C:1064:HIS:HE2	1.56	0.70
1:C:43:PHE:HD1	1:C:44:ARG:N	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:PRO:HG2	1:B:855:PHE:CD1	2.26	0.70
1:B:922:LEU:HD11	4:B:1310:NAG:H62	1.72	0.70
1:A:974:SER:OG	1:A:979:ASP:OD2	2.09	0.70
1:B:407:VAL:C	2:E:106:TYR:OH	2.30	0.70
1:B:802:PHE:N	1:B:802:PHE:HD2	1.88	0.70
2:E:19:ARG:CD	2:E:80:TYR:CE1	2.75	0.70
1:A:1062:PHE:HB2	1:A:1064:HIS:HE2	1.56	0.70
1:B:974:SER:OG	1:B:979:ASP:OD2	2.09	0.70
2:D:95:TYR:HD2	2:D:114:GLY:HA3	1.55	0.70
1:A:149:ASN:ND2	4:A:1301:NAG:C1	2.53	0.69
1:B:962:LEU:HD12	1:B:962:LEU:C	2.11	0.69
1:C:806:LEU:HD23	1:C:878:LEU:HD22	1.75	0.69
1:A:802:PHE:N	1:A:802:PHE:HD2	1.88	0.69
1:A:914:ASN:HB3	1:C:1089:PHE:CE1	2.27	0.69
1:B:1062:PHE:HB2	1:B:1064:HIS:HE2	1.56	0.69
1:B:911:VAL:CG2	1:B:911:VAL:N	2.56	0.69
2:D:19:ARG:HD3	2:D:80:TYR:CD1	2.28	0.69
1:A:806:LEU:HD23	1:A:878:LEU:HD22	1.75	0.69
1:C:699:LEU:CD2	1:C:699:LEU:HD11	2.16	0.69
1:A:911:VAL:CG2	1:A:911:VAL:N	2.56	0.69
1:A:959:LEU:CB	1:A:959:LEU:HD22	2.18	0.69
2:D:19:ARG:CD	2:D:80:TYR:CE1	2.75	0.69
1:A:1094:VAL:N	1:A:1105:THR:O	2.25	0.69
1:C:911:VAL:CG2	1:C:911:VAL:N	2.56	0.69
2:D:30:ASN:HB3	2:D:100:TYR:CE2	2.28	0.69
2:D:93:LEU:HB3	2:D:95:TYR:CZ	2.28	0.68
1:A:699:LEU:CD2	1:A:699:LEU:HD11	2.16	0.68
1:B:376:THR:HB	1:B:435:ALA:H	1.58	0.68
1:C:17:ASN:OD1	3:I:1:NAG:C1	2.42	0.68
2:E:30:ASN:HB3	2:E:100:TYR:CE2	2.28	0.68
2:E:109:ASN:HA	2:E:111:TRP:HZ3	1.58	0.68
2:E:67:ARG:NH1	2:E:87:LYS:HD3	2.09	0.68
1:B:404:GLY:O	1:B:407:VAL:HG22	1.94	0.68
2:E:19:ARG:HD3	2:E:80:TYR:CD1	2.28	0.68
1:B:472:ILE:HG23	1:B:489:TYR:O	1.94	0.67
2:D:20:LEU:HD12	2:D:21:SER:H	1.59	0.67
2:E:38:ARG:HG3	2:E:92:ALA:HB3	1.76	0.67
1:B:806:LEU:HD23	1:B:878:LEU:HD22	1.75	0.67
1:B:669:GLY:HA2	1:C:869:MET:HE1	1.68	0.67
2:D:67:ARG:NH1	2:D:87:LYS:HD3	2.09	0.67
2:E:93:LEU:HB3	2:E:95:TYR:CZ	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1072:GLU:HG2	1:C:894:LEU:CD2	2.24	0.67
1:A:707:TYR:CD1	1:B:883:THR:HG22	2.30	0.67
1:B:354:ASN:OD1	1:B:399:SER:OG	2.13	0.67
2:E:65:LYS:HE2	2:E:65:LYS:HA	1.76	0.67
2:E:68:PHE:CD2	2:E:81:LEU:HD11	2.30	0.67
1:A:703:ASN:CG	1:B:787:GLN:OE1	2.34	0.66
1:C:1094:VAL:N	1:C:1105:THR:O	2.25	0.66
4:A:1301:NAG:O7	4:A:1301:NAG:O3	2.12	0.66
2:E:70:ILE:HD12	2:E:80:TYR:O	1.96	0.66
1:A:869:MET:HB2	1:C:699:LEU:HD11	1.78	0.66
2:D:68:PHE:CD2	2:D:81:LEU:HD11	2.30	0.66
2:D:70:ILE:HD12	2:D:80:TYR:O	1.96	0.66
2:D:67:ARG:HB2	2:D:84:ASN:O	1.96	0.66
1:A:894:LEU:CB	1:C:713:ALA:HB3	2.26	0.66
2:D:65:LYS:HA	2:D:65:LYS:HE2	1.76	0.66
1:A:670:ILE:HG23	1:A:695:TYR:O	1.96	0.66
2:D:38:ARG:HG3	2:D:92:ALA:HB3	1.76	0.66
2:E:20:LEU:HD12	2:E:21:SER:H	1.59	0.66
1:B:670:ILE:HG23	1:B:695:TYR:O	1.96	0.66
2:E:67:ARG:HB2	2:E:84:ASN:O	1.96	0.66
1:A:765:ARG:NE	1:C:957:GLN:NE2	2.44	0.65
2:D:109:ASN:HA	2:D:111:TRP:HZ3	1.58	0.65
1:B:1094:VAL:N	1:B:1105:THR:O	2.25	0.65
1:A:897:PRO:HD2	1:A:900:MET:HG3	1.79	0.65
1:B:376:THR:HG23	2:E:106:TYR:CG	2.32	0.65
1:B:309:GLU:O	1:B:313:TYR:OH	2.11	0.65
1:B:475:ALA:HB2	1:B:489:TYR:HE2	1.62	0.65
2:D:95:TYR:CD2	2:D:114:GLY:HA3	2.31	0.65
1:B:390:LEU:HD11	1:C:983:ARG:HG2	1.78	0.64
1:C:699:LEU:HD13	1:C:699:LEU:HD21	1.64	0.64
2:D:37:PHE:CZ	2:D:95:TYR:HD1	2.15	0.64
2:E:37:PHE:CZ	2:E:95:TYR:HD1	2.15	0.64
2:E:95:TYR:CD2	2:E:114:GLY:HA3	2.31	0.64
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.78	0.64
1:A:703:ASN:OD1	1:B:787:GLN:HB3	1.97	0.64
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.08	0.64
1:C:670:ILE:HG23	1:C:695:TYR:O	1.96	0.64
1:C:578:ASP:OD1	1:C:583:GLU:N	2.31	0.64
1:A:377:PHE:CD1	1:A:434:ILE:HD12	2.32	0.64
1:B:61:ASN:HD21	4:B:1307:NAG:C1	2.11	0.64
1:B:699:LEU:CD2	1:B:699:LEU:HD11	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:HG3	1:A:179:LEU:HD12	1.79	0.64
1:A:1119:ASN:OD1	1:A:1119:ASN:O	2.16	0.64
1:B:177:MET:HG3	1:B:179:LEU:HD12	1.79	0.64
1:C:177:MET:HG3	1:C:179:LEU:HD12	1.78	0.64
1:C:1119:ASN:OD1	1:C:1119:ASN:O	2.16	0.64
1:A:309:GLU:O	1:A:313:TYR:OH	2.11	0.64
1:A:578:ASP:OD1	1:A:583:GLU:N	2.30	0.64
1:B:1010:GLN:OE1	1:C:1012:LEU:HD11	1.98	0.64
1:C:377:PHE:CD1	1:C:434:ILE:HD12	2.32	0.64
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	1.80	0.64
1:B:61:ASN:HD22	4:B:1307:NAG:C7	2.10	0.63
2:D:101:TYR:HD1	2:D:103:ALA:H	1.47	0.63
1:B:897:PRO:HD2	1:B:900:MET:HG3	1.79	0.63
1:C:478:THR:HG23	1:C:479:PRO:HD2	1.81	0.63
2:E:65:LYS:HD3	2:E:66:GLY:N	2.13	0.63
2:D:22:CYS:HB2	2:D:36:TRP:CZ2	2.34	0.63
2:E:109:ASN:HA	2:E:111:TRP:CE3	2.33	0.63
2:D:35:ALA:HB2	2:D:50:VAL:HG13	1.80	0.63
1:A:76:THR:OG1	1:A:77:LYS:N	2.32	0.63
1:C:897:PRO:HD2	1:C:900:MET:HG3	1.79	0.63
2:D:109:ASN:HA	2:D:111:TRP:CE3	2.33	0.63
1:B:22:THR:OG1	1:B:76:THR:HA	1.99	0.63
1:C:46:SER:N	1:C:280:ASN:O	2.32	0.63
1:A:611:LEU:HD22	1:A:666:ILE:HG23	1.81	0.62
1:B:61:ASN:ND2	4:B:1307:NAG:C7	2.62	0.62
1:B:699:LEU:HB3	1:C:788:ILE:CG1	2.28	0.62
1:B:1119:ASN:OD1	1:B:1119:ASN:O	2.16	0.62
2:D:65:LYS:HD3	2:D:66:GLY:N	2.14	0.62
2:E:60:TYR:HE2	2:E:68:PHE:CB	2.12	0.62
2:E:101:TYR:HD1	2:E:103:ALA:H	1.47	0.62
2:D:60:TYR:HE2	2:D:68:PHE:CB	2.12	0.62
2:E:35:ALA:HB2	2:E:50:VAL:HG13	1.80	0.62
1:A:22:THR:OG1	1:A:76:THR:HA	1.99	0.62
1:B:46:SER:N	1:B:280:ASN:O	2.32	0.62
1:B:699:LEU:HD13	1:B:699:LEU:HD21	1.65	0.62
1:B:472:ILE:HG23	1:B:489:TYR:C	2.21	0.61
1:B:886:TRP:HZ3	1:B:905:ARG:CD	2.13	0.61
1:C:280:ASN:OD1	1:C:282:ASN:OD1	2.18	0.61
1:C:309:GLU:O	1:C:313:TYR:OH	2.11	0.61
2:E:83:MET:CB	2:E:86:LEU:HD21	2.29	0.61
1:A:280:ASN:OD1	1:A:282:ASN:OD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:N	1:A:280:ASN:O	2.32	0.61
1:A:917:TYR:CE1	1:C:1079:PRO:HB3	2.36	0.61
1:B:770:ILE:HG21	1:B:770:ILE:CD1	2.30	0.61
4:B:1304:NAG:H3	4:B:1304:NAG:C8	2.29	0.61
1:C:924:ALA:O	1:C:928:ASN:OD1	2.18	0.61
2:E:22:CYS:HB2	2:E:36:TRP:CZ2	2.34	0.61
1:A:770:ILE:HG21	1:A:770:ILE:CD1	2.30	0.61
1:C:22:THR:OG1	1:C:76:THR:HA	1.99	0.61
2:D:83:MET:CB	2:D:86:LEU:HD21	2.29	0.61
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.83	0.61
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.81	0.61
1:C:611:LEU:HD22	1:C:666:ILE:HG23	1.81	0.61
1:C:886:TRP:HE3	1:C:905:ARG:HH21	1.49	0.61
2:E:40:ALA:HB1	2:E:41:PRO:HD2	1.83	0.60
1:A:886:TRP:HZ3	1:A:905:ARG:CD	2.14	0.60
1:A:924:ALA:O	1:A:928:ASN:OD1	2.18	0.60
1:A:1030:SER:O	1:C:1040:VAL:CG1	2.49	0.60
1:B:280:ASN:OD1	1:B:282:ASN:OD1	2.18	0.60
1:B:1017:GLU:OE1	1:C:1019:ARG:NH2	2.34	0.60
2:E:93:LEU:HB3	2:E:95:TYR:OH	2.02	0.60
1:B:76:THR:OG1	1:B:77:LYS:N	2.32	0.60
1:B:924:ALA:O	1:B:928:ASN:OD1	2.18	0.60
2:D:93:LEU:HB3	2:D:95:TYR:OH	2.02	0.60
2:E:4:LEU:HD21	2:E:98:SER:OG	2.02	0.60
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.37	0.60
1:A:886:TRP:HE3	1:A:905:ARG:HH21	1.49	0.60
1:B:1126:CYS:CB	1:B:1132:ILE:HD13	2.31	0.60
1:B:376:THR:CB	2:E:106:TYR:HB2	2.32	0.60
1:B:740:MET:O	1:B:744:GLY:N	2.35	0.60
1:B:886:TRP:HE3	1:B:905:ARG:HH21	1.49	0.60
1:C:616:ASN:HD21	4:C:1304:NAG:H2	1.66	0.60
1:A:658:ASN:OD1	1:A:660:TYR:CD1	2.55	0.59
1:A:740:MET:O	1:A:744:GLY:N	2.35	0.59
1:C:770:ILE:HG21	1:C:770:ILE:CD1	2.30	0.59
2:D:4:LEU:HD21	2:D:98:SER:OG	2.02	0.59
2:D:19:ARG:CD	2:D:80:TYR:CD1	2.86	0.59
1:A:872:GLN:OE1	1:C:699:LEU:HG	2.02	0.59
1:B:190:ARG:HH11	1:B:207:HIS:CE1	2.20	0.59
1:C:76:THR:OG1	1:C:77:LYS:N	2.32	0.59
1:C:740:MET:O	1:C:744:GLY:N	2.35	0.59
1:A:914:ASN:ND2	1:C:1123:SER:OG	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:PRO:HB2	1:C:864:LEU:HD22	1.84	0.59
1:B:1089:PHE:CE1	1:C:914:ASN:HB3	2.37	0.59
1:C:86:PHE:N	1:C:236:THR:O	2.36	0.59
1:C:1126:CYS:CB	1:C:1132:ILE:HD13	2.31	0.59
4:C:1306:NAG:C1	4:C:1306:NAG:O7	2.49	0.59
2:D:58:THR:HG21	2:D:70:ILE:HG22	1.84	0.59
2:E:21:SER:HB2	2:E:80:TYR:CE1	2.37	0.59
1:A:855:PHE:HD1	1:C:589:PRO:HG2	1.68	0.59
1:A:110:LEU:O	1:A:135:PHE:HB2	2.02	0.59
1:A:895:GLN:O	1:C:712:ILE:HA	2.02	0.59
1:C:190:ARG:HH11	1:C:207:HIS:CE1	2.20	0.59
1:C:658:ASN:OD1	1:C:660:TYR:CD1	2.55	0.59
2:D:38:ARG:NH2	2:D:46:GLU:HB3	2.18	0.59
1:B:658:ASN:OD1	1:B:660:TYR:CD1	2.55	0.59
2:D:2:VAL:HG23	2:D:110:ASN:ND2	2.18	0.59
1:A:1126:CYS:CB	1:A:1132:ILE:HD13	2.32	0.59
1:B:922:LEU:CD2	4:B:1310:NAG:H5	2.32	0.59
2:D:12:VAL:HG21	2:D:86:LEU:CD1	2.33	0.59
2:D:18:LEU:HB2	2:D:83:MET:HE2	1.84	0.59
2:D:21:SER:HB2	2:D:80:TYR:CE1	2.37	0.59
2:E:12:VAL:HG21	2:E:86:LEU:CD1	2.33	0.59
2:E:19:ARG:CD	2:E:80:TYR:CD1	2.86	0.59
1:C:110:LEU:O	1:C:135:PHE:HB2	2.02	0.59
1:C:868:GLU:N	1:C:868:GLU:OE1	2.36	0.59
2:E:38:ARG:HG3	2:E:94:TYR:CE2	2.38	0.59
2:E:64:VAL:HA	2:E:67:ARG:NE	2.12	0.59
1:B:318:PHE:C	1:B:318:PHE:CD2	2.77	0.58
1:C:709:ASN:ND2	4:C:1306:NAG:O7	2.35	0.58
2:D:20:LEU:O	2:D:80:TYR:HD1	1.86	0.58
1:A:603:ASN:ND2	4:A:1306:NAG:C1	2.66	0.58
1:B:110:LEU:O	1:B:135:PHE:HB2	2.02	0.58
1:B:1106:GLN:OE1	1:B:1109:PHE:HB3	2.04	0.58
2:E:58:THR:HG21	2:E:70:ILE:HG22	1.84	0.58
1:A:190:ARG:HH11	1:A:207:HIS:CE1	2.20	0.58
1:A:868:GLU:N	1:A:868:GLU:OE1	2.36	0.58
1:C:318:PHE:C	1:C:318:PHE:CD2	2.77	0.58
2:D:19:ARG:HD2	2:D:80:TYR:CE1	2.38	0.58
2:E:37:PHE:CZ	2:E:95:TYR:CD1	2.91	0.58
1:A:64:TRP:CE2	1:A:66:HIS:CE1	2.92	0.58
1:A:817:PHE:C	1:A:817:PHE:CD2	2.77	0.58
1:A:133:PHE:CD1	1:A:160:TYR:CD2	2.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ILE:CG2	1:A:770:ILE:CD1	2.76	0.58
2:D:38:ARG:HG3	2:D:94:TYR:CE2	2.38	0.58
2:E:20:LEU:O	2:E:80:TYR:HD1	1.86	0.58
1:A:269:TYR:O	1:A:271:GLN:OE1	2.22	0.58
1:A:318:PHE:C	1:A:318:PHE:CD2	2.77	0.58
1:B:376:THR:HB	1:B:435:ALA:N	2.17	0.58
1:C:43:PHE:HE1	1:C:283:GLY:HA2	1.69	0.58
1:B:43:PHE:HE1	1:B:283:GLY:HA2	1.68	0.58
1:B:589:PRO:HG2	1:C:855:PHE:HD1	1.69	0.58
1:C:817:PHE:HA	1:C:820:ASP:OD2	2.04	0.58
1:A:589:PRO:CG	1:B:855:PHE:HD1	2.16	0.58
1:A:997:ILE:O	1:A:1001:LEU:HB2	2.04	0.58
1:B:64:TRP:CE2	1:B:66:HIS:CE1	2.92	0.58
1:B:868:GLU:N	1:B:868:GLU:OE1	2.36	0.58
1:C:133:PHE:CD1	1:C:160:TYR:CD2	2.92	0.58
1:C:314:GLN:OE1	1:C:595:VAL:O	2.22	0.58
2:D:65:LYS:HD3	2:D:66:GLY:H	1.69	0.58
1:A:86:PHE:N	1:A:236:THR:O	2.36	0.58
1:B:269:TYR:O	1:B:271:GLN:OE1	2.22	0.58
1:B:668:ALA:C	1:C:866:THR:HG23	2.24	0.58
1:B:997:ILE:O	1:B:1001:LEU:HB2	2.04	0.58
1:C:817:PHE:C	1:C:817:PHE:CD2	2.77	0.58
1:C:886:TRP:HZ3	1:C:905:ARG:CD	2.13	0.58
1:B:725:GLU:OE1	1:B:1028:LYS:HE3	2.04	0.58
1:B:817:PHE:C	1:B:817:PHE:CD2	2.77	0.58
2:E:2:VAL:HG23	2:E:110:ASN:ND2	2.18	0.58
1:C:269:TYR:O	1:C:271:GLN:OE1	2.22	0.57
1:C:997:ILE:O	1:C:1001:LEU:HB2	2.04	0.57
2:D:20:LEU:HG	2:D:36:TRP:CH2	2.39	0.57
2:E:38:ARG:NH2	2:E:46:GLU:HB3	2.18	0.57
1:A:314:GLN:OE1	1:A:595:VAL:O	2.22	0.57
1:A:705:VAL:HG23	1:B:789:TYR:HD1	1.68	0.57
1:A:817:PHE:HA	1:A:820:ASP:OD2	2.04	0.57
1:B:133:PHE:CD1	1:B:160:TYR:CD2	2.92	0.57
1:C:64:TRP:CE2	1:C:66:HIS:CE1	2.92	0.57
2:E:65:LYS:HD3	2:E:66:GLY:H	1.69	0.57
1:A:748:GLU:HA	1:A:751:ASN:OD1	2.04	0.57
1:C:568:ASP:OD1	1:C:569:ILE:N	2.35	0.57
2:D:64:VAL:HA	2:D:67:ARG:NE	2.12	0.57
2:E:20:LEU:HG	2:E:36:TRP:CH2	2.39	0.57
1:A:725:GLU:OE1	1:A:1028:LYS:HE3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:N	1:B:236:THR:O	2.36	0.57
2:D:37:PHE:CZ	2:D:95:TYR:CD1	2.91	0.57
1:A:568:ASP:OD1	1:A:569:ILE:N	2.34	0.57
1:A:883:THR:HG22	1:C:707:TYR:HB2	1.86	0.57
1:B:206:LYS:HD2	1:B:223:LEU:HA	1.87	0.57
1:A:43:PHE:HE1	1:A:283:GLY:CA	2.18	0.57
1:B:817:PHE:HA	1:B:820:ASP:OD2	2.04	0.57
1:B:915:VAL:O	1:B:919:ASN:HB3	2.05	0.57
1:C:748:GLU:HA	1:C:751:ASN:OD1	2.04	0.57
1:C:725:GLU:OE1	1:C:1028:LYS:HE3	2.04	0.57
1:A:43:PHE:HE1	1:A:283:GLY:HA2	1.68	0.57
1:B:748:GLU:HA	1:B:751:ASN:OD1	2.04	0.57
1:B:1104:VAL:CG1	1:B:1119:ASN:HD21	2.18	0.57
1:C:1106:GLN:OE1	1:C:1109:PHE:HB3	2.03	0.57
1:B:43:PHE:HE1	1:B:283:GLY:CA	2.18	0.57
1:B:314:GLN:OE1	1:B:595:VAL:O	2.22	0.57
1:C:332:ILE:O	1:C:332:ILE:HG23	2.05	0.57
1:C:1104:VAL:CG1	1:C:1119:ASN:HD21	2.18	0.57
2:E:19:ARG:HD2	2:E:80:TYR:CE1	2.38	0.57
1:A:406:GLU:N	1:A:406:GLU:OE1	2.39	0.56
1:A:1104:VAL:CG1	1:A:1119:ASN:HD21	2.18	0.56
1:B:378:LYS:HE2	1:B:380:TYR:CE2	2.40	0.56
4:B:1307:NAG:O7	4:B:1307:NAG:H3	2.03	0.56
1:C:43:PHE:HE1	1:C:283:GLY:CA	2.18	0.56
1:C:310:LYS:HG2	1:C:600:PRO:HA	1.87	0.56
1:C:527:PRO:O	1:C:528:LYS:HG3	2.05	0.56
1:A:206:LYS:HD2	1:A:223:LEU:HA	1.87	0.56
1:A:597:VAL:HG13	1:A:608:VAL:CG1	2.36	0.56
1:A:915:VAL:O	1:A:919:ASN:HB3	2.05	0.56
1:A:1106:GLN:OE1	1:A:1109:PHE:HB3	2.03	0.56
1:B:141:LEU:HD23	1:B:157:PHE:HA	1.88	0.56
1:B:1094:VAL:HG11	1:C:904:TYR:OH	2.05	0.56
1:C:736:VAL:HG22	1:C:858:LEU:HD23	1.88	0.56
2:E:38:ARG:HG2	2:E:39:GLN:N	2.21	0.56
1:A:332:ILE:HD12	1:A:527:PRO:HA	1.88	0.56
1:B:43:PHE:CD1	1:B:44:ARG:N	2.73	0.56
1:C:802:PHE:HB3	1:C:805:ILE:CG1	2.36	0.56
2:E:58:THR:HG21	2:E:70:ILE:CG2	2.36	0.56
1:A:318:PHE:HD2	1:A:318:PHE:C	2.09	0.56
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.87	0.56
2:D:58:THR:HG21	2:D:70:ILE:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:PHE:HB3	1:B:805:ILE:CG1	2.36	0.56
2:D:38:ARG:HG2	2:D:39:GLN:N	2.21	0.56
2:E:18:LEU:HB2	2:E:83:MET:HE2	1.86	0.56
1:A:966:LEU:HD12	1:A:1000:ARG:NE	2.21	0.56
1:B:87:ASN:OD1	1:B:269:TYR:CE2	2.59	0.56
1:B:200:TYR:CD2	1:B:228:ASP:OD2	2.59	0.56
1:C:206:LYS:HD2	1:C:223:LEU:HA	1.87	0.56
1:B:210:ILE:HG21	1:B:212:LEU:HD23	1.88	0.56
1:C:87:ASN:OD1	1:C:269:TYR:CE2	2.59	0.56
1:C:802:PHE:HB3	1:C:805:ILE:HG12	1.88	0.56
1:A:457:ARG:NH1	1:A:459[A]:SER:O	2.39	0.56
1:B:318:PHE:HD2	1:B:318:PHE:C	2.09	0.56
1:B:331:ASN:HB2	4:B:1305:NAG:C1	2.36	0.56
1:B:372:ALA:CA	2:E:47:ARG:HH12	2.18	0.56
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.87	0.56
1:B:524:VAL:O	1:B:524:VAL:HG13	2.06	0.56
1:C:597:VAL:HG13	1:C:608:VAL:CG1	2.36	0.56
1:C:915:VAL:O	1:C:919:ASN:HB3	2.05	0.56
2:D:83:MET:SD	2:D:83:MET:N	2.79	0.56
1:A:802:PHE:HB3	1:A:805:ILE:CG1	2.36	0.56
1:C:43:PHE:CD1	1:C:44:ARG:N	2.73	0.56
1:C:318:PHE:HD2	1:C:318:PHE:C	2.09	0.56
1:C:966:LEU:HD12	1:C:1000:ARG:NE	2.21	0.56
1:A:87:ASN:OD1	1:A:269:TYR:CE2	2.59	0.55
1:B:597:VAL:HG13	1:B:608:VAL:CG1	2.36	0.55
1:C:141:LEU:HD23	1:C:157:PHE:HA	1.87	0.55
1:C:200:TYR:CD2	1:C:228:ASP:OD2	2.59	0.55
1:C:406:GLU:OE1	1:C:406:GLU:N	2.38	0.55
1:C:484:GLU:N	1:C:484:GLU:OE1	2.38	0.55
1:A:200:TYR:CD2	1:A:228:ASP:OD2	2.59	0.55
1:A:699:LEU:HD13	1:A:699:LEU:HD21	1.65	0.55
1:A:802:PHE:HB3	1:A:805:ILE:HG12	1.88	0.55
1:A:865:LEU:HD22	1:A:869:MET:HG3	1.89	0.55
1:B:802:PHE:HB3	1:B:805:ILE:HG12	1.88	0.55
1:C:210:ILE:HG21	1:C:212:LEU:HD23	1.88	0.55
1:A:43:PHE:CD1	1:A:44:ARG:N	2.73	0.55
1:A:457:ARG:NH1	1:A:459[B]:SER:O	2.39	0.55
1:B:310:LYS:HG2	1:B:600:PRO:HA	1.87	0.55
1:A:141:LEU:HD23	1:A:157:PHE:HA	1.88	0.55
1:A:711:SER:OG	1:B:895:GLN:NE2	2.31	0.55
1:B:966:LEU:HD12	1:B:1000:ARG:NE	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:ALA:HB2	1:B:1089:PHE:HE2	1.70	0.55
1:B:736:VAL:HG22	1:B:858:LEU:HD23	1.87	0.55
1:C:29:THR:HG21	1:C:216:LEU:HD12	1.88	0.55
2:E:83:MET:SD	2:E:83:MET:N	2.79	0.55
1:A:118:LEU:HD13	1:A:120:VAL:HG23	1.89	0.55
1:B:376:THR:CA	2:E:106:TYR:HB2	2.37	0.55
1:B:665:PRO:HB3	1:C:864:LEU:HD21	1.89	0.55
1:C:327:VAL:HG12	1:C:542:ASN:HB3	1.88	0.55
1:A:1141:LEU:O	1:A:1144:GLU:N	2.39	0.55
1:B:357:ARG:CZ	1:B:396:TYR:OH	2.55	0.55
1:C:865:LEU:HD22	1:C:869:MET:HG3	1.89	0.55
1:C:1141:LEU:O	1:C:1144:GLU:OE2	2.25	0.55
1:A:310:LYS:HG2	1:A:600:PRO:HA	1.87	0.55
1:B:29:THR:HG21	1:B:216:LEU:HD12	1.88	0.55
1:B:378:LYS:HD2	2:E:106:TYR:CE2	2.40	0.55
1:C:190:ARG:HD3	1:C:207:HIS:CE1	2.42	0.55
1:A:193:VAL:HG23	1:A:223:LEU:HD12	1.89	0.55
1:A:894:LEU:HD22	1:C:713:ALA:CB	2.37	0.55
1:B:61:ASN:ND2	4:B:1307:NAG:C1	2.69	0.55
1:B:865:LEU:HD22	1:B:869:MET:HG3	1.89	0.54
1:A:855:PHE:CD1	1:C:589:PRO:HG2	2.41	0.54
1:A:1141:LEU:C	1:A:1144:GLU:OE2	2.46	0.54
1:C:925:ASN:HA	1:C:928:ASN:OD1	2.08	0.54
1:A:280:ASN:HB2	1:A:286:THR:HG21	1.89	0.54
1:A:1141:LEU:O	1:A:1144:GLU:OE2	2.25	0.54
1:B:1141:LEU:C	1:B:1144:GLU:OE2	2.46	0.54
1:B:1141:LEU:O	1:B:1144:GLU:OE2	2.25	0.54
1:C:117:LEU:CD1	1:C:130:VAL:HG22	2.36	0.54
1:C:193:VAL:HG23	1:C:223:LEU:HD12	1.90	0.54
1:C:1141:LEU:C	1:C:1144:GLU:OE2	2.46	0.54
1:A:29:THR:HG21	1:A:216:LEU:HD12	1.88	0.54
1:C:1141:LEU:O	1:C:1144:GLU:N	2.39	0.54
1:B:922:LEU:CD1	4:B:1310:NAG:H5	2.38	0.54
1:C:118:LEU:HD13	1:C:120:VAL:HG23	1.89	0.54
1:A:190:ARG:HD3	1:A:207:HIS:CE1	2.42	0.54
1:A:274:THR:OG1	1:A:291:CYS:HB2	2.08	0.54
1:B:118:LEU:HD13	1:B:120:VAL:HG23	1.89	0.54
1:B:274:THR:OG1	1:B:291:CYS:HB2	2.08	0.54
1:B:770:ILE:CG1	1:B:770:ILE:HG23	1.97	0.54
1:A:958:ALA:O	1:A:961:THR:OG1	2.22	0.54
1:B:756:TYR:O	1:B:756:TYR:CD1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ILE:CG2	1:B:770:ILE:CD1	2.76	0.54
1:B:280:ASN:HB2	1:B:286:THR:HG21	1.89	0.54
1:B:925:ASN:HA	1:B:928:ASN:OD1	2.08	0.54
1:C:756:TYR:O	1:C:756:TYR:CD1	2.61	0.54
1:A:210:ILE:HG21	1:A:212:LEU:HD23	1.88	0.54
1:A:925:ASN:HA	1:A:928:ASN:OD1	2.08	0.53
1:B:190:ARG:HD3	1:B:207:HIS:CE1	2.42	0.53
1:B:1111:GLU:O	1:B:1111:GLU:HG2	2.08	0.53
1:C:280:ASN:HB2	1:C:286:THR:HG21	1.89	0.53
1:A:657:ASN:CB	4:A:1309:NAG:O5	2.56	0.53
1:B:376:THR:CG2	2:E:106:TYR:CG	2.91	0.53
1:B:748:GLU:OE2	1:B:748:GLU:N	2.29	0.53
1:B:979:ASP:OD2	1:B:980:ILE:N	2.42	0.53
1:A:705:VAL:CG2	1:B:789:TYR:CD1	2.91	0.53
1:A:979:ASP:OD2	1:A:980:ILE:N	2.42	0.53
1:B:193:VAL:HG23	1:B:223:LEU:HD12	1.89	0.53
1:B:465:GLU:OE1	3:J:1:NAG:C8	2.56	0.53
1:C:616:ASN:HD21	4:C:1304:NAG:C1	2.22	0.53
2:E:60:TYR:OH	2:E:70:ILE:N	2.41	0.53
1:A:756:TYR:CD1	1:A:756:TYR:O	2.61	0.53
1:C:979:ASP:OD2	1:C:980:ILE:N	2.42	0.53
2:D:60:TYR:OH	2:D:70:ILE:N	2.42	0.53
1:A:153:MET:HA	1:A:179:LEU:HD22	1.91	0.53
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.90	0.53
1:A:954:GLN:HG2	1:A:1014:ARG:CZ	2.39	0.53
1:A:1111:GLU:O	1:A:1111:GLU:HG2	2.08	0.53
1:C:274:THR:OG1	1:C:291:CYS:HB2	2.08	0.53
1:B:190:ARG:NH1	1:B:207:HIS:HE1	2.07	0.53
1:B:452:LEU:HD12	1:B:493:GLN:O	2.08	0.53
1:B:922:LEU:HD21	4:B:1310:NAG:H5	1.91	0.53
1:C:331:ASN:ND2	1:C:580:GLN:O	2.42	0.53
2:E:60:TYR:HE2	2:E:68:PHE:HB2	1.73	0.53
1:A:117:LEU:CD1	1:A:130:VAL:HG22	2.36	0.53
1:A:159:VAL:HG23	1:A:160:TYR:HB3	1.91	0.53
1:B:1062:PHE:CB	1:B:1064:HIS:HE2	2.21	0.53
1:C:905:ARG:HH12	1:C:1050:MET:HB3	1.72	0.53
1:A:892:ALA:HB3	1:C:1072:GLU:OE2	2.06	0.53
1:C:1074:ASN:O	1:C:1075:PHE:CG	2.62	0.53
1:A:892:ALA:HB1	1:C:1072:GLU:OE2	2.08	0.53
1:C:159:VAL:HG23	1:C:160:TYR:HB3	1.91	0.53
1:C:1097:SER:HA	1:C:1101:HIS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:LYS:HA	2:D:65:LYS:CE	2.38	0.53
1:A:770:ILE:HG23	1:A:770:ILE:C	2.29	0.53
1:A:1097:SER:HA	1:A:1101:HIS:O	2.09	0.53
1:B:954:GLN:HG2	1:B:1014:ARG:CZ	2.39	0.53
2:D:36:TRP:O	2:D:48:VAL:HG22	2.10	0.53
1:A:190:ARG:NH1	1:A:207:HIS:HE1	2.07	0.52
1:A:224:GLU:N	1:A:224:GLU:OE1	2.42	0.52
1:A:765:ARG:CZ	1:C:957:GLN:HE21	2.22	0.52
1:A:897:PRO:HD2	1:A:900:MET:SD	2.50	0.52
1:B:1141:LEU:O	1:B:1144:GLU:N	2.39	0.52
1:A:708:SER:HB3	1:A:711:SER:HB3	1.91	0.52
1:A:817:PHE:O	1:A:821:LEU:HB2	2.10	0.52
1:A:897:PRO:HD2	1:A:900:MET:CG	2.38	0.52
1:B:117:LEU:CD1	1:B:130:VAL:HG22	2.36	0.52
1:B:117:LEU:HD12	1:B:129:LYS:O	2.09	0.52
1:B:224:GLU:N	1:B:224:GLU:OE1	2.42	0.52
1:B:391:CYS:CB	1:B:525:CYS:HA	2.39	0.52
1:B:817:PHE:O	1:B:821:LEU:HB2	2.10	0.52
1:B:897:PRO:HD2	1:B:900:MET:CG	2.38	0.52
1:B:969:ASN:OD1	1:B:972:ALA:O	2.27	0.52
1:A:918:GLU:HA	1:C:1128:VAL:CG2	2.40	0.52
1:B:294:ASP:OD2	1:B:294:ASP:C	2.48	0.52
1:B:699:LEU:HD21	1:B:699:LEU:HD11	1.85	0.52
1:B:1097:SER:HA	1:B:1101:HIS:O	2.09	0.52
1:C:190:ARG:NH1	1:C:207:HIS:HE1	2.07	0.52
1:A:770:ILE:HG22	1:A:771:ALA:N	2.24	0.52
1:A:787:GLN:HB3	1:C:703:ASN:OD1	2.10	0.52
1:A:869:MET:CB	1:C:699:LEU:HD11	2.40	0.52
1:A:895:GLN:HE21	1:C:711:SER:HG	1.58	0.52
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.44	0.52
1:C:897:PRO:HD2	1:C:900:MET:CG	2.38	0.52
2:D:60:TYR:HE2	2:D:68:PHE:HB2	1.74	0.52
2:E:36:TRP:O	2:E:48:VAL:HG22	2.10	0.52
1:A:117:LEU:HD12	1:A:129:LYS:O	2.10	0.52
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.40	0.52
1:A:905:ARG:HH12	1:A:1050:MET:HB3	1.72	0.52
1:A:1074:ASN:O	1:A:1075:PHE:CG	2.62	0.52
1:B:159:VAL:HG23	1:B:160:TYR:HB3	1.91	0.52
1:B:470:THR:HG22	1:B:470:THR:O	2.09	0.52
1:B:1074:ASN:O	1:B:1075:PHE:CG	2.62	0.52
1:C:117:LEU:HD12	1:C:129:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:ILE:HG22	1:C:771:ALA:N	2.25	0.52
1:C:1111:GLU:O	1:C:1111:GLU:HG2	2.08	0.52
1:B:736:VAL:HG22	1:B:858:LEU:CD2	2.40	0.52
1:C:224:GLU:N	1:C:224:GLU:OE1	2.42	0.52
1:C:468:ILE:HG22	1:C:468:ILE:O	2.10	0.52
1:C:616:ASN:ND2	4:C:1304:NAG:H2	2.24	0.52
1:C:736:VAL:HG22	1:C:858:LEU:CD2	2.40	0.52
1:A:165:ASN:HD21	4:A:1302:NAG:C7	2.23	0.52
1:B:314:GLN:OE1	1:B:314:GLN:HA	2.09	0.52
1:C:954:GLN:HG2	1:C:1014:ARG:CZ	2.39	0.52
2:E:83:MET:HB3	2:E:86:LEU:CD2	2.37	0.52
1:B:897:PRO:HD2	1:B:900:MET:SD	2.50	0.52
1:C:817:PHE:O	1:C:821:LEU:HB2	2.10	0.52
1:A:298:GLU:OE2	1:A:315:THR:OG1	2.26	0.52
1:A:314:GLN:OE1	1:A:314:GLN:HA	2.10	0.52
1:A:327:VAL:HG12	1:A:542:ASN:HB3	1.92	0.52
1:A:897:PRO:CB	1:C:709:ASN:O	2.58	0.52
1:A:1062:PHE:CB	1:A:1064:HIS:HE2	2.21	0.52
1:B:770:ILE:HG22	1:B:771:ALA:N	2.24	0.52
1:C:619:GLU:N	1:C:619:GLU:OE1	2.43	0.52
1:C:718:PHE:CZ	1:C:919:ASN:ND2	2.78	0.52
1:C:897:PRO:HD2	1:C:900:MET:SD	2.50	0.52
2:D:83:MET:HB3	2:D:86:LEU:CD2	2.37	0.52
1:C:153:MET:HA	1:C:179:LEU:HD22	1.91	0.51
1:C:314:GLN:OE1	1:C:314:GLN:HA	2.09	0.51
1:A:718:PHE:CZ	1:A:919:ASN:ND2	2.78	0.51
1:B:378:LYS:CD	2:E:106:TYR:CE2	2.93	0.51
1:B:392:PHE:CE1	1:B:517:LEU:HD11	2.45	0.51
1:C:1062:PHE:CB	1:C:1064:HIS:HE2	2.21	0.51
1:A:294:ASP:C	1:A:294:ASP:OD2	2.48	0.51
1:C:969:ASN:OD1	1:C:972:ALA:O	2.27	0.51
1:C:1080:ALA:HB2	1:C:1089:PHE:HE2	1.70	0.51
1:B:619:GLU:N	1:B:619:GLU:OE1	2.43	0.51
1:A:619:GLU:OE1	1:A:619:GLU:N	2.43	0.51
1:A:817:PHE:C	1:A:817:PHE:HD2	2.14	0.51
1:B:153:MET:HA	1:B:179:LEU:HD22	1.91	0.51
1:B:1072:GLU:HG2	1:C:894:LEU:HD21	1.93	0.51
2:E:39:GLN:HG2	2:E:95:TYR:HE1	1.75	0.51
1:A:193:VAL:HG23	1:A:223:LEU:CD1	2.41	0.51
1:A:1013:ILE:CD1	1:C:1013:ILE:HD12	2.39	0.51
1:B:718:PHE:CZ	1:B:919:ASN:ND2	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:817:PHE:C	1:C:817:PHE:HD2	2.14	0.51
2:E:65:LYS:HA	2:E:65:LYS:CE	2.38	0.51
1:A:43:PHE:HB3	1:C:566:GLY:HA2	1.92	0.51
2:D:30:ASN:HB3	2:D:100:TYR:CD2	2.46	0.51
2:D:82:GLN:OE1	2:D:83:MET:N	2.43	0.51
2:E:82:GLN:OE1	2:E:83:MET:N	2.43	0.51
1:A:468:ILE:HG22	1:A:468:ILE:O	2.10	0.51
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.43	0.51
1:B:663:ASP:C	1:B:663:ASP:OD1	2.49	0.51
1:C:294:ASP:OD2	1:C:294:ASP:C	2.48	0.51
1:C:617:CYS:O	1:C:620:VAL:HG22	2.11	0.51
2:D:39:GLN:HG2	2:D:95:TYR:HE1	1.75	0.51
1:A:762:GLN:NE2	1:C:961:THR:CG2	2.74	0.51
1:A:813:SER:O	1:A:814:LYS:HB2	2.10	0.51
1:B:386:LYS:NZ	1:C:982:SER:HA	2.26	0.51
1:B:905:ARG:NH1	1:B:1050:MET:CB	2.72	0.51
1:C:193:VAL:HG23	1:C:223:LEU:CD1	2.41	0.51
1:C:658:ASN:CG	1:C:659:SER:N	2.65	0.51
2:E:39:GLN:HG2	2:E:95:TYR:CE1	2.46	0.51
1:A:53:ASP:OD2	1:A:53:ASP:C	2.48	0.51
1:B:53:ASP:OD2	1:B:53:ASP:C	2.48	0.51
1:B:193:VAL:HG23	1:B:223:LEU:CD1	2.41	0.51
1:B:206:LYS:HD2	1:B:222:ALA:O	2.11	0.51
1:A:206:LYS:HD2	1:A:222:ALA:O	2.12	0.50
1:A:663:ASP:OD1	1:A:663:ASP:C	2.49	0.50
1:A:969:ASN:OD1	1:A:972:ALA:O	2.27	0.50
1:B:53:ASP:OD2	1:B:55:PHE:CE2	2.64	0.50
1:B:190:ARG:HH11	1:B:207:HIS:HE1	1.58	0.50
1:B:390:LEU:HD11	1:C:983:ARG:CG	2.40	0.50
1:B:503:VAL:HG11	2:E:111:TRP:CD1	2.46	0.50
1:B:702:GLU:HA	1:C:788:ILE:O	2.10	0.50
1:C:53:ASP:OD2	1:C:53:ASP:C	2.49	0.50
1:A:560:LEU:O	1:A:577:ARG:NH2	2.44	0.50
1:A:658:ASN:CG	1:A:659:SER:N	2.65	0.50
1:A:707:TYR:CG	1:B:883:THR:HG22	2.46	0.50
1:B:813:SER:O	1:B:814:LYS:HB2	2.10	0.50
1:C:53:ASP:OD2	1:C:55:PHE:CE2	2.64	0.50
1:C:958:ALA:O	1:C:961:THR:OG1	2.22	0.50
2:D:39:GLN:HG2	2:D:95:TYR:CE1	2.46	0.50
2:E:31:THR:HG23	2:E:99:GLY:N	2.25	0.50
1:A:1080:ALA:HB2	1:A:1089:PHE:HE2	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LYS:HE2	1:B:380:TYR:CZ	2.46	0.50
2:D:60:TYR:HE2	2:D:68:PHE:HB3	1.77	0.50
1:B:1002:GLN:HE21	1:B:1002:GLN:C	2.15	0.50
2:D:91:THR:HG23	2:D:118:THR:HA	1.94	0.50
2:E:30:ASN:HB3	2:E:100:TYR:CD2	2.46	0.50
2:E:60:TYR:HE2	2:E:68:PHE:HB3	1.77	0.50
1:A:317:ASN:OD1	1:A:317:ASN:N	2.43	0.50
1:A:1005:GLN:CD	1:C:1006:THR:HG23	2.31	0.50
1:C:190:ARG:HH11	1:C:207:HIS:HE1	1.57	0.50
2:E:58:THR:HG23	2:E:70:ILE:HG21	1.94	0.50
1:A:190:ARG:HH11	1:A:207:HIS:HE1	1.58	0.50
1:A:332:ILE:HD11	1:A:527:PRO:HA	1.94	0.50
1:A:372:ALA:HB1	2:D:63:SER:OG	2.11	0.50
1:A:1002:GLN:HE21	1:A:1002:GLN:C	2.15	0.50
1:B:192:PHE:HB2	1:B:194:PHE:CZ	2.47	0.50
1:B:317:ASN:OD1	1:B:317:ASN:N	2.43	0.50
1:B:357:ARG:NH2	1:C:200:TYR:CE1	2.79	0.50
1:B:617:CYS:O	1:B:620:VAL:HG22	2.11	0.50
1:B:658:ASN:CG	1:B:659:SER:N	2.65	0.50
1:B:817:PHE:C	1:B:817:PHE:HD2	2.14	0.50
1:C:97:LYS:HD2	1:C:182:LYS:HB2	1.93	0.50
1:C:658:ASN:OD1	1:C:660:TYR:CZ	2.65	0.50
2:D:31:THR:HG23	2:D:99:GLY:N	2.25	0.50
1:B:608:VAL:HG12	1:B:609:ALA:N	2.27	0.50
1:C:524:VAL:O	1:C:524:VAL:HG13	2.12	0.50
1:C:813:SER:O	1:C:814:LYS:HB2	2.10	0.50
1:A:608:VAL:HG12	1:A:609:ALA:N	2.27	0.50
1:B:97:LYS:HD2	1:B:182:LYS:HB2	1.93	0.50
1:B:767:LEU:HD21	1:B:1008:VAL:HG22	1.94	0.50
1:B:770:ILE:HG23	1:B:770:ILE:C	2.29	0.50
1:C:560:LEU:O	1:C:577:ARG:NH2	2.44	0.50
2:D:93:LEU:HD22	2:D:95:TYR:HE2	1.76	0.50
2:E:93:LEU:HD22	2:E:95:TYR:HE2	1.76	0.50
1:A:53:ASP:OD2	1:A:55:PHE:CE2	2.64	0.50
1:A:617:CYS:O	1:A:620:VAL:HG22	2.11	0.50
1:A:1017:GLU:OE1	1:B:1019:ARG:NH2	2.45	0.50
1:B:647:ALA:HA	1:C:862:PRO:HG3	1.94	0.50
1:C:317:ASN:N	1:C:317:ASN:OD1	2.43	0.50
2:D:1:GLN:O	2:D:26:GLY:HA3	2.12	0.50
2:E:95:TYR:HD2	2:E:114:GLY:CA	2.22	0.50
1:A:768:THR:O	1:A:769:GLY:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:THR:O	1:A:770:ILE:N	2.45	0.49
1:C:768:THR:O	1:C:770:ILE:N	2.45	0.49
1:A:97:LYS:HD2	1:A:182:LYS:HB2	1.93	0.49
1:A:658:ASN:OD1	1:A:660:TYR:CZ	2.65	0.49
1:B:905:ARG:HH12	1:B:1050:MET:HB3	1.72	0.49
1:C:884:SER:C	1:C:901:GLN:OE1	2.51	0.49
2:E:1:GLN:O	2:E:26:GLY:HA3	2.12	0.49
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.94	0.49
1:C:192:PHE:HB2	1:C:194:PHE:CZ	2.47	0.49
1:B:214:ARG:HG2	1:B:214:ARG:O	2.12	0.49
1:B:386:LYS:HZ1	1:C:982:SER:HA	1.77	0.49
1:B:487:ASN:HA	1:B:489:TYR:CZ	2.47	0.49
1:C:608:VAL:HG12	1:C:609:ALA:N	2.27	0.49
1:C:725:GLU:CD	1:C:1028:LYS:HE3	2.33	0.49
2:D:4:LEU:HD23	2:D:22:CYS:SG	2.53	0.49
2:E:4:LEU:HD23	2:E:22:CYS:SG	2.53	0.49
1:A:192:PHE:HB2	1:A:194:PHE:CZ	2.47	0.49
4:B:1302:NAG:HO3	4:B:1302:NAG:C7	2.18	0.49
2:E:68:PHE:HA	2:E:82:GLN:O	2.13	0.49
1:B:282:ASN:OD1	4:B:1304:NAG:N2	2.45	0.49
1:B:671:CYS:SG	1:B:697:MET:SD	3.11	0.49
1:B:768:THR:O	1:B:769:GLY:C	2.50	0.49
1:C:726:ILE:HG23	1:C:1061:VAL:HG22	1.95	0.49
1:A:131:CYS:HA	1:A:166:CYS:HB3	1.95	0.49
1:B:658:ASN:OD1	1:B:660:TYR:CZ	2.65	0.49
1:C:206:LYS:HD2	1:C:222:ALA:O	2.12	0.49
1:C:768:THR:O	1:C:769:GLY:C	2.50	0.49
2:D:58:THR:CG2	2:D:70:ILE:CG2	2.91	0.49
2:D:68:PHE:HA	2:D:82:GLN:O	2.13	0.49
1:A:324:GLU:O	1:A:539:VAL:HG13	2.12	0.49
1:A:767:LEU:HD21	1:A:1008:VAL:HG22	1.94	0.49
1:B:487:ASN:HA	1:B:489:TYR:OH	2.13	0.49
1:C:452:LEU:HD12	1:C:492:LEU:HD13	1.95	0.49
1:C:663:ASP:OD1	1:C:663:ASP:C	2.49	0.49
2:E:91:THR:HG23	2:E:118:THR:HA	1.94	0.49
1:A:273:ARG:NH2	1:A:290:ASP:OD2	2.45	0.49
1:A:726:ILE:HG23	1:A:1061:VAL:HG22	1.95	0.49
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.74	0.49
1:B:665:PRO:HB2	1:C:864:LEU:CD2	2.42	0.49
1:C:273:ARG:NH2	1:C:290:ASP:OD2	2.45	0.49
1:A:671:CYS:SG	1:A:697:MET:SD	3.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LEU:HB2	1:B:608:VAL:HG21	1.94	0.49
1:B:377:PHE:C	2:E:104:SER:OG	2.51	0.49
1:B:725:GLU:CD	1:B:1028:LYS:HE3	2.33	0.49
1:B:726:ILE:HG23	1:B:1061:VAL:HG22	1.95	0.49
1:C:296:LEU:HB2	1:C:608:VAL:HG21	1.94	0.49
1:C:671:CYS:SG	1:C:697:MET:SD	3.11	0.49
1:A:712:ILE:O	1:A:1074:ASN:HA	2.13	0.48
1:A:767:LEU:CD2	1:A:1008:VAL:HG22	2.43	0.48
1:A:894:LEU:HB3	1:C:713:ALA:O	2.12	0.48
1:B:273:ARG:NH2	1:B:290:ASP:OD2	2.45	0.48
1:B:718:PHE:HZ	1:B:919:ASN:CG	2.17	0.48
1:C:30:ASN:OD1	4:C:1303:NAG:H81	2.12	0.48
1:C:767:LEU:HD21	1:C:1008:VAL:HG22	1.94	0.48
1:A:214:ARG:O	1:A:214:ARG:HG2	2.12	0.48
1:A:537:LYS:N	1:A:551:VAL:HG23	2.28	0.48
1:B:768:THR:O	1:B:770:ILE:N	2.45	0.48
1:C:214:ARG:O	1:C:214:ARG:HG2	2.12	0.48
1:C:770:ILE:CG1	1:C:770:ILE:HG23	1.97	0.48
1:A:177:MET:CG	1:A:179:LEU:HD12	2.44	0.48
1:A:884:SER:C	1:A:901:GLN:OE1	2.51	0.48
1:B:331:ASN:CB	4:B:1305:NAG:C1	2.91	0.48
1:C:712:ILE:O	1:C:1074:ASN:HA	2.14	0.48
1:C:770:ILE:HG23	1:C:770:ILE:C	2.29	0.48
2:D:2:VAL:HG23	2:D:110:ASN:CG	2.33	0.48
2:D:58:THR:CG2	2:D:70:ILE:HG21	2.43	0.48
1:A:524:VAL:O	1:A:524:VAL:HG13	2.12	0.48
1:A:725:GLU:CD	1:A:1028:LYS:HE3	2.33	0.48
1:B:767:LEU:CD2	1:B:1008:VAL:HG22	2.43	0.48
1:B:884:SER:C	1:B:901:GLN:OE1	2.51	0.48
1:C:452:LEU:HD12	1:C:492:LEU:CD1	2.44	0.48
2:D:4:LEU:HD13	2:D:110:ASN:CB	2.43	0.48
1:B:665:PRO:CB	1:C:864:LEU:CD2	2.91	0.48
1:B:770:ILE:HG21	1:B:770:ILE:HD13	1.96	0.48
1:A:283:GLY:HA3	1:C:563:GLN:HE22	1.77	0.48
1:A:452:LEU:HD12	1:A:492:LEU:HD13	1.94	0.48
1:A:452:LEU:HD12	1:A:492:LEU:CD1	2.44	0.48
1:A:603:ASN:HD21	4:A:1306:NAG:C1	2.27	0.48
1:A:748:GLU:OE2	1:A:748:GLU:N	2.29	0.48
1:C:767:LEU:CD2	1:C:1008:VAL:HG22	2.43	0.48
2:D:58:THR:HG23	2:D:70:ILE:HG21	1.94	0.48
1:A:770:ILE:HG21	1:A:770:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:THR:HB	1:B:435:ALA:HB3	1.95	0.48
1:C:177:MET:CG	1:C:179:LEU:HD12	2.44	0.48
1:C:770:ILE:C	1:C:770:ILE:HG22	2.32	0.48
2:D:4:LEU:HB2	2:D:110:ASN:O	2.14	0.48
2:E:6:GLU:HG2	2:E:95:TYR:HA	1.96	0.48
1:A:280:ASN:CG	1:A:281:GLU:N	2.67	0.48
1:A:963:VAL:O	1:A:966:LEU:HB3	2.14	0.48
1:B:280:ASN:CG	1:B:281:GLU:N	2.67	0.48
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.95	0.48
1:C:537:LYS:N	1:C:551:VAL:HG23	2.29	0.48
2:E:4:LEU:HD13	2:E:110:ASN:CB	2.43	0.48
2:E:12:VAL:HG11	2:E:18:LEU:HG	1.96	0.48
2:E:58:THR:CG2	2:E:70:ILE:HG21	2.43	0.48
2:E:58:THR:CG2	2:E:70:ILE:CG2	2.91	0.48
1:A:765:ARG:NE	1:C:957:GLN:HE21	2.11	0.48
1:B:712:ILE:O	1:B:1074:ASN:HA	2.13	0.48
1:B:977:LEU:HA	1:B:980:ILE:HD11	1.96	0.48
2:E:2:VAL:HG23	2:E:110:ASN:CG	2.33	0.48
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.95	0.47
1:C:616:ASN:HD21	4:C:1304:NAG:C2	2.27	0.47
1:C:963:VAL:O	1:C:966:LEU:HB3	2.14	0.47
2:E:94:TYR:CE2	2:E:117:VAL:CG1	2.97	0.47
1:A:765:ARG:CD	1:C:957:GLN:HE22	2.27	0.47
1:A:905:ARG:NH1	1:A:1050:MET:CB	2.72	0.47
1:B:61:ASN:ND2	4:B:1307:NAG:N2	2.62	0.47
1:C:718:PHE:HZ	1:C:919:ASN:CG	2.17	0.47
1:C:905:ARG:NH1	1:C:1050:MET:CB	2.72	0.47
2:D:6:GLU:HG2	2:D:95:TYR:HA	1.96	0.47
2:D:39:GLN:C	2:D:92:ALA:HB1	2.34	0.47
2:E:39:GLN:C	2:E:92:ALA:HB1	2.34	0.47
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.50	0.47
1:A:571:ASP:OD1	1:B:44:ARG:NH1	2.47	0.47
1:B:963:VAL:O	1:B:966:LEU:HB3	2.14	0.47
1:C:974:SER:HG	1:C:979:ASP:CG	2.13	0.47
1:C:994:ASP:C	1:C:994:ASP:OD2	2.53	0.47
2:D:73:ASP:CG	2:D:76:LYS:HG2	2.35	0.47
2:D:95:TYR:HD2	2:D:114:GLY:CA	2.22	0.47
2:E:4:LEU:HB2	2:E:110:ASN:O	2.14	0.47
2:E:73:ASP:CG	2:E:76:LYS:HG2	2.35	0.47
1:A:64:TRP:NE1	1:A:66:HIS:CE1	2.82	0.47
1:A:749:CYS:HA	1:A:752:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ARG:HD2	1:C:957:GLN:HE22	1.80	0.47
1:A:904:TYR:OH	1:C:1094:VAL:HG12	2.13	0.47
1:B:475:ALA:CB	1:B:489:TYR:HE2	2.27	0.47
1:C:334:ASN:O	1:C:362:VAL:HG12	2.14	0.47
1:A:455:LEU:HD11	1:A:493:GLN:HB2	1.96	0.47
1:A:770:ILE:C	1:A:770:ILE:HG22	2.32	0.47
1:B:618:THR:OG1	1:B:619:GLU:OE1	2.24	0.47
1:B:911:VAL:N	1:B:911:VAL:HG23	2.30	0.47
1:B:994:ASP:OD2	1:B:994:ASP:C	2.53	0.47
1:A:569:ILE:HD12	1:A:569:ILE:H	1.79	0.47
1:A:1029:MET:HE2	1:A:1062:PHE:CE1	2.49	0.47
1:B:190:ARG:HB2	1:B:192:PHE:CE1	2.50	0.47
1:B:658:ASN:O	1:B:659:SER:OG	2.27	0.47
1:B:922:LEU:HD11	4:B:1310:NAG:C5	2.45	0.47
1:B:1080:ALA:HB2	1:B:1089:PHE:CD2	2.49	0.47
1:C:770:ILE:HG21	1:C:770:ILE:HD13	1.96	0.47
1:A:568:ASP:OD1	1:A:569:ILE:HD12	2.14	0.47
1:A:611:LEU:HD12	1:A:649:CYS:O	2.15	0.47
1:A:718:PHE:HZ	1:A:919:ASN:CG	2.17	0.47
1:B:922:LEU:HD11	4:B:1310:NAG:H5	1.96	0.47
1:B:1039:ARG:NH2	1:B:1042:PHE:CD1	2.83	0.47
1:C:314:GLN:OE1	1:C:314:GLN:CA	2.63	0.47
1:C:737:ASP:OD2	1:C:740:MET:HB3	2.15	0.47
1:C:749:CYS:HA	1:C:752:LEU:HD12	1.97	0.47
2:D:94:TYR:CE2	2:D:117:VAL:CG1	2.97	0.47
1:A:190:ARG:HB2	1:A:192:PHE:CE1	2.50	0.47
1:A:618:THR:OG1	1:A:619:GLU:OE1	2.24	0.47
1:A:1002:GLN:O	1:A:1002:GLN:NE2	2.40	0.47
1:B:131:CYS:HA	1:B:166:CYS:HB3	1.95	0.47
1:B:1064:HIS:N	1:B:1064:HIS:CD2	2.83	0.47
1:B:1107:ARG:NH2	1:C:913:GLN:NE2	2.63	0.47
2:E:20:LEU:O	2:E:80:TYR:CD1	2.67	0.47
1:A:699:LEU:HD21	1:A:699:LEU:HD11	1.85	0.47
1:A:705:VAL:CG2	1:B:789:TYR:HD1	2.28	0.47
1:A:1030:SER:OG	1:C:1041:ASP:HB2	2.14	0.47
1:B:472:ILE:CG2	1:B:489:TYR:O	2.63	0.47
1:B:487:ASN:HA	1:B:489:TYR:CE1	2.49	0.47
1:C:64:TRP:NE1	1:C:66:HIS:CE1	2.82	0.47
2:E:69:THR:CG2	2:E:82:GLN:HB3	2.29	0.47
1:A:146:HIS:O	1:A:150:LYS:HA	2.15	0.47
1:A:314:GLN:OE1	1:A:314:GLN:CA	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:O	1:A:362:VAL:HG12	2.15	0.47
1:A:408:ARG:HE	2:D:103:ALA:HB1	1.79	0.47
1:A:551:VAL:HG12	1:A:588:THR:O	2.15	0.47
1:A:737:ASP:OD2	1:A:740:MET:HB3	2.15	0.47
1:A:781:VAL:HG23	1:A:782:PHE:CD2	2.50	0.47
1:A:1050:MET:SD	1:A:1052:PHE:CZ	3.08	0.47
1:B:177:MET:CG	1:B:179:LEU:HD12	2.44	0.47
1:A:1039:ARG:NH2	1:A:1042:PHE:CD1	2.83	0.46
1:A:1062:PHE:CB	1:A:1064:HIS:NE2	2.79	0.46
1:A:1064:HIS:N	1:A:1064:HIS:CD2	2.83	0.46
1:B:146:HIS:O	1:B:150:LYS:HA	2.15	0.46
1:C:190:ARG:HB2	1:C:192:PHE:CE1	2.50	0.46
1:C:611:LEU:HD12	1:C:649:CYS:O	2.15	0.46
1:C:781:VAL:HG23	1:C:782:PHE:CD2	2.50	0.46
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.30	0.46
1:A:403:ARG:NH1	1:A:406:GLU:OE2	2.48	0.46
1:A:1031:GLU:OE1	1:C:1039:ARG:HG2	2.14	0.46
1:A:1080:ALA:HB2	1:A:1089:PHE:CD2	2.49	0.46
1:B:64:TRP:NE1	1:B:66:HIS:CE1	2.82	0.46
1:B:737:ASP:OD2	1:B:740:MET:HB3	2.15	0.46
1:B:1050:MET:SD	1:B:1052:PHE:CZ	3.08	0.46
1:B:1062:PHE:CB	1:B:1064:HIS:NE2	2.79	0.46
1:C:403:ARG:NH1	1:C:406:GLU:OE2	2.48	0.46
1:C:618:THR:OG1	1:C:619:GLU:OE1	2.24	0.46
2:D:12:VAL:HG11	2:D:18:LEU:HG	1.96	0.46
2:D:36:TRP:HD1	2:D:70:ILE:HD13	1.80	0.46
1:A:894:LEU:HA	1:C:713:ALA:HB3	1.96	0.46
1:A:1019:ARG:NH2	1:C:1017:GLU:OE1	2.48	0.46
1:B:364:ASP:OD1	1:B:367:VAL:HG22	2.15	0.46
4:B:1310:NAG:O7	4:B:1310:NAG:H3	2.14	0.46
1:C:404:GLY:O	1:C:407:VAL:HG22	2.15	0.46
1:C:734:THR:HG21	1:C:959:LEU:CD1	2.45	0.46
1:A:314:GLN:OE1	1:A:595:VAL:C	2.54	0.46
1:A:734:THR:HG21	1:A:959:LEU:CD1	2.45	0.46
1:A:965:GLN:OE1	1:A:1003:SER:HB3	2.16	0.46
1:B:314:GLN:OE1	1:B:595:VAL:C	2.54	0.46
1:B:465:GLU:OE1	3:J:1:NAG:H81	2.16	0.46
1:C:146:HIS:O	1:C:150:LYS:HA	2.15	0.46
1:C:770:ILE:CG2	1:C:770:ILE:CD1	2.76	0.46
2:D:93:LEU:HB3	2:D:95:TYR:CE2	2.50	0.46
2:E:93:LEU:HB3	2:E:95:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:ASP:OD2	1:A:994:ASP:C	2.53	0.46
1:A:1005:GLN:OE1	1:C:1006:THR:HG23	2.16	0.46
1:B:423:TYR:HE2	1:B:512:VAL:HG21	1.79	0.46
1:B:452:LEU:HD12	1:B:493:GLN:C	2.36	0.46
1:B:611:LEU:HD12	1:B:649:CYS:O	2.15	0.46
1:B:734:THR:HG21	1:B:959:LEU:CD1	2.45	0.46
1:C:280:ASN:CG	1:C:281:GLU:N	2.67	0.46
1:C:569:ILE:H	1:C:569:ILE:HD12	1.80	0.46
1:C:1039:ARG:NH2	1:C:1042:PHE:CD1	2.83	0.46
1:C:1050:MET:SD	1:C:1052:PHE:CZ	3.08	0.46
1:A:1005:GLN:NE2	1:C:1006:THR:HG21	2.23	0.46
1:B:357:ARG:HH21	1:C:200:TYR:HE1	1.63	0.46
1:B:749:CYS:HA	1:B:752:LEU:HD12	1.97	0.46
1:B:1107:ARG:HH21	1:C:913:GLN:NE2	2.13	0.46
1:C:87:ASN:OD1	1:C:269:TYR:HE2	1.98	0.46
1:C:314:GLN:OE1	1:C:595:VAL:C	2.54	0.46
1:C:1062:PHE:CB	1:C:1064:HIS:NE2	2.79	0.46
1:C:1080:ALA:HB2	1:C:1089:PHE:CD2	2.49	0.46
1:C:1116:THR:OG1	1:C:1118:ASP:OD2	2.32	0.46
1:A:96:GLU:OE2	1:A:263:ALA:HB1	2.16	0.46
1:A:377:PHE:HD1	1:A:434:ILE:HD12	1.81	0.46
1:A:661:GLU:OE1	1:A:661:GLU:HA	2.16	0.46
1:A:904:TYR:OH	1:C:1094:VAL:CG1	2.64	0.46
1:B:139:PRO:HB3	1:B:159:VAL:HG12	1.98	0.46
1:B:457:ARG:NH1	1:B:459[A]:SER:O	2.41	0.46
1:B:457:ARG:NH1	1:B:459[B]:SER:O	2.41	0.46
1:B:473:TYR:HB3	1:B:489:TYR:HB2	1.97	0.46
1:B:781:VAL:HG23	1:B:782:PHE:CD2	2.50	0.46
1:C:139:PRO:HB3	1:C:159:VAL:HG12	1.97	0.46
1:C:568:ASP:OD1	1:C:569:ILE:HD12	2.16	0.46
1:C:977:LEU:HA	1:C:980:ILE:HD11	1.96	0.46
1:A:977:LEU:HA	1:A:980:ILE:HD11	1.96	0.46
1:B:958:ALA:O	1:B:961:THR:OG1	2.22	0.46
1:C:661:GLU:OE1	1:C:661:GLU:HA	2.16	0.46
1:B:87:ASN:OD1	1:B:269:TYR:HE2	1.98	0.46
1:B:96:GLU:OE2	1:B:96:GLU:HA	2.16	0.46
1:C:658:ASN:O	1:C:659:SER:OG	2.27	0.46
1:B:707:TYR:HE2	1:C:896:ILE:O	1.99	0.46
1:A:404:GLY:O	1:A:407:VAL:HG22	2.15	0.45
1:B:1104:VAL:O	1:B:1104:VAL:HG13	2.16	0.45
1:C:96:GLU:OE2	1:C:96:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:HIS:N	1:C:1064:HIS:CD2	2.83	0.45
1:C:1104:VAL:O	1:C:1104:VAL:HG13	2.16	0.45
1:B:332:ILE:HG13	1:B:362:VAL:CG1	2.46	0.45
1:B:702:GLU:HG2	1:C:788:ILE:HB	1.98	0.45
1:A:17:ASN:OD1	3:F:1:NAG:C2	2.64	0.45
1:A:405:ASP:N	1:A:504:GLY:O	2.48	0.45
1:B:661:GLU:HA	1:B:661:GLU:OE1	2.16	0.45
1:C:911:VAL:N	1:C:911:VAL:HG23	2.30	0.45
1:C:965:GLN:OE1	1:C:1003:SER:HB3	2.16	0.45
1:A:139:PRO:HB3	1:A:159:VAL:HG12	1.97	0.45
1:A:1030:SER:C	1:C:1040:VAL:HG12	2.36	0.45
1:B:326:ILE:HD11	1:B:552:LEU:HD11	1.98	0.45
1:B:919:ASN:OD1	1:B:923:ILE:CG1	2.61	0.45
1:C:751:ASN:HA	1:C:754:LEU:HG	1.99	0.45
2:D:24:ALA:HB1	2:D:28:THR:HG21	1.97	0.45
1:A:894:LEU:HD22	1:C:713:ALA:HB1	1.97	0.45
1:B:699:LEU:HG	1:C:872:GLN:CD	2.27	0.45
1:C:718:PHE:HZ	1:C:919:ASN:ND2	2.15	0.45
2:D:68:PHE:HD2	2:D:81:LEU:HD11	1.81	0.45
2:E:24:ALA:HB1	2:E:28:THR:HG21	1.97	0.45
2:E:87:LYS:HB3	2:E:88:PRO:HD2	1.98	0.45
1:A:165:ASN:OD1	4:A:1302:NAG:H83	2.16	0.45
1:A:894:LEU:CA	1:C:713:ALA:HB3	2.47	0.45
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.31	0.45
1:B:965:GLN:OE1	1:B:1003:SER:HB3	2.15	0.45
1:B:984:LEU:HD13	1:B:988:GLU:HG2	1.99	0.45
1:C:96:GLU:OE2	1:C:263:ALA:HB1	2.16	0.45
1:C:826:VAL:HG23	1:C:945:LEU:HD22	1.99	0.45
1:A:1116:THR:OG1	1:A:1118:ASP:OD2	2.32	0.45
1:B:96:GLU:OE2	1:B:263:ALA:HB1	2.16	0.45
1:B:314:GLN:OE1	1:B:314:GLN:CA	2.63	0.45
1:B:1116:THR:OG1	1:B:1118:ASP:OD2	2.32	0.45
2:D:87:LYS:HB3	2:D:88:PRO:HD2	1.98	0.45
1:B:43:PHE:CE1	1:B:283:GLY:CA	3.00	0.45
1:B:158:ARG:HG3	1:B:158:ARG:HH11	1.82	0.45
2:D:6:GLU:HB3	2:D:115:THR:HG23	1.99	0.45
1:A:645:THR:HB	1:A:670:ILE:HD13	1.99	0.45
1:A:765:ARG:O	1:A:768:THR:OG1	2.30	0.45
1:B:1029:MET:HE2	1:B:1062:PHE:CE1	2.52	0.45
1:C:158:ARG:HG3	1:C:158:ARG:HH11	1.82	0.45
1:C:377:PHE:HD1	1:C:434:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:HD11	1:C:493:GLN:HB2	1.98	0.45
1:C:748:GLU:OE2	1:C:748:GLU:N	2.29	0.45
1:A:96:GLU:OE2	1:A:96:GLU:HA	2.16	0.45
1:A:718:PHE:HZ	1:A:919:ASN:ND2	2.15	0.45
1:A:984:LEU:HD13	1:A:988:GLU:HG2	1.99	0.45
1:A:1104:VAL:HG13	1:A:1104:VAL:O	2.16	0.45
1:B:131:CYS:SG	1:B:163:ALA:HB1	2.57	0.45
1:B:376:THR:HG22	1:B:434:ILE:HA	1.98	0.45
1:B:751:ASN:HA	1:B:754:LEU:HG	1.99	0.45
1:B:921:LYS:O	1:B:922:LEU:C	2.55	0.45
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.31	0.45
2:D:20:LEU:O	2:D:80:TYR:CD1	2.67	0.45
2:D:45:ASP:OD1	2:D:46:GLU:N	2.50	0.45
1:A:43:PHE:CD1	1:A:43:PHE:C	2.91	0.44
1:B:376:THR:HA	2:E:106:TYR:HB2	1.98	0.44
1:B:457:ARG:CZ	1:B:461:LEU:HD23	2.47	0.44
1:C:131:CYS:SG	1:C:163:ALA:HB1	2.58	0.44
1:C:1029:MET:HE2	1:C:1062:PHE:CE1	2.52	0.44
2:E:34:VAL:HG11	2:E:79:VAL:HG11	1.99	0.44
2:E:45:ASP:OD1	2:E:46:GLU:N	2.50	0.44
1:A:21:ARG:HD3	1:A:79:PHE:HB3	2.00	0.44
1:A:131:CYS:SG	1:A:163:ALA:HB1	2.57	0.44
1:B:705:VAL:CG1	1:C:895:GLN:HB3	2.40	0.44
1:B:933:LYS:HA	1:B:936:ASP:OD2	2.18	0.44
4:B:1307:NAG:O7	4:B:1307:NAG:C3	2.65	0.44
1:C:699:LEU:HD21	1:C:699:LEU:HD11	1.85	0.44
1:C:1062:PHE:HB3	1:C:1064:HIS:CD2	2.53	0.44
2:E:36:TRP:HD1	2:E:70:ILE:HD13	1.80	0.44
1:B:665:PRO:CB	1:C:864:LEU:HD22	2.47	0.44
1:B:1062:PHE:HB3	1:B:1064:HIS:CD2	2.53	0.44
1:C:858:LEU:CD2	1:C:962:LEU:HD21	2.48	0.44
1:C:984:LEU:HD13	1:C:988:GLU:HG2	1.99	0.44
1:A:826:VAL:HG23	1:A:945:LEU:HD22	1.99	0.44
1:A:1013:ILE:HD12	1:B:1013:ILE:HD12	1.98	0.44
1:B:709:ASN:HB3	1:C:796:ASP:OD2	2.17	0.44
1:C:645:THR:HB	1:C:670:ILE:HD13	1.99	0.44
1:A:87:ASN:OD1	1:A:269:TYR:HE2	1.98	0.44
1:A:1019:ARG:NH2	1:C:1017:GLU:CD	2.70	0.44
1:C:43:PHE:CD1	1:C:43:PHE:C	2.91	0.44
1:C:997:ILE:HD12	1:C:997:ILE:HG21	1.82	0.44
1:A:610:VAL:O	1:A:650:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:THR:O	1:A:1102:TRP:CH2	2.71	0.44
1:B:668:ALA:HA	1:C:866:THR:HG23	2.00	0.44
1:B:826:VAL:HG23	1:B:945:LEU:HD22	1.99	0.44
1:A:21:ARG:HD2	1:A:79:PHE:O	2.18	0.44
1:A:962:LEU:HD12	1:A:962:LEU:O	2.18	0.44
1:B:200:TYR:HD2	1:B:228:ASP:OD2	2.01	0.44
1:B:645:THR:HB	1:B:670:ILE:HD13	1.99	0.44
1:B:921:LYS:O	1:B:925:ASN:OD1	2.36	0.44
1:C:610:VAL:O	1:C:650:LEU:HD12	2.17	0.44
2:D:19:ARG:HD3	2:D:80:TYR:CE1	2.48	0.44
2:D:81:LEU:HD12	2:D:82:GLN:N	2.32	0.44
1:A:44:ARG:NH1	1:C:571:ASP:OD1	2.51	0.44
1:A:158:ARG:HG3	1:A:158:ARG:HH11	1.82	0.44
1:A:787:GLN:OE1	1:C:703:ASN:OD1	2.35	0.44
1:B:503:VAL:HG11	2:E:111:TRP:NE1	2.33	0.44
1:B:718:PHE:HZ	1:B:919:ASN:ND2	2.15	0.44
1:B:1002:GLN:O	1:B:1002:GLN:NE2	2.40	0.44
2:E:81:LEU:HD12	2:E:82:GLN:N	2.32	0.44
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.75	0.44
1:A:474:GLN:HG2	1:A:476:GLY:H	1.83	0.44
1:A:751:ASN:HA	1:A:754:LEU:HG	1.99	0.44
1:A:919:ASN:OD1	1:A:923:ILE:CG1	2.61	0.44
1:B:770:ILE:C	1:B:770:ILE:HG22	2.32	0.44
1:B:858:LEU:CD2	1:B:962:LEU:HD21	2.48	0.44
1:B:962:LEU:HD12	1:B:962:LEU:O	2.18	0.44
1:B:1076:THR:O	1:B:1102:TRP:CH2	2.71	0.44
2:D:64:VAL:O	2:D:67:ARG:HG2	2.18	0.44
2:E:6:GLU:HB3	2:E:115:THR:HG23	1.98	0.44
1:A:883:THR:CG2	1:C:707:TYR:HB2	2.47	0.43
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.45	0.43
1:A:911:VAL:N	1:A:911:VAL:HG23	2.30	0.43
1:A:919:ASN:OD1	1:A:919:ASN:O	2.36	0.43
1:B:21:ARG:HD2	1:B:79:PHE:O	2.18	0.43
1:B:569:ILE:HD12	1:B:569:ILE:H	1.83	0.43
1:B:610:VAL:O	1:B:650:LEU:HD12	2.17	0.43
1:B:800:PHE:HB3	1:B:802:PHE:CZ	2.53	0.43
1:C:569:ILE:O	1:C:570:ALA:HB3	2.18	0.43
1:C:1076:THR:O	1:C:1102:TRP:CH2	2.71	0.43
2:D:37:PHE:HB2	2:D:46:GLU:O	2.19	0.43
2:E:68:PHE:CE2	2:E:83:MET:HG3	2.53	0.43
1:B:280:ASN:OD1	1:B:281:GLU:CA	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLU:OE2	1:B:315:THR:OG1	2.26	0.43
1:C:405:ASP:N	1:C:504:GLY:O	2.49	0.43
1:C:800:PHE:HB3	1:C:802:PHE:CZ	2.53	0.43
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.45	0.43
1:A:280:ASN:OD1	1:A:281:GLU:CA	2.66	0.43
1:A:294:ASP:OD2	1:A:296:LEU:N	2.52	0.43
1:A:824:ASN:OD1	1:A:824:ASN:N	2.43	0.43
1:B:376:THR:CB	1:B:435:ALA:HB3	2.48	0.43
1:B:743:CYS:SG	1:B:753:LEU:HD23	2.59	0.43
1:B:919:ASN:OD1	1:B:919:ASN:O	2.36	0.43
1:C:21:ARG:HD2	1:C:79:PHE:O	2.18	0.43
1:C:100:ILE:O	1:C:243:ALA:N	2.45	0.43
1:C:921:LYS:O	1:C:925:ASN:OD1	2.36	0.43
1:A:921:LYS:O	1:A:925:ASN:OD1	2.36	0.43
1:B:21:ARG:HD3	1:B:79:PHE:HB3	2.00	0.43
1:B:131:CYS:HA	1:B:166:CYS:CB	2.49	0.43
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.53	0.43
1:B:922:LEU:HA	1:B:925:ASN:OD1	2.19	0.43
4:B:1304:NAG:H83	4:B:1304:NAG:C3	2.37	0.43
1:C:21:ARG:HD3	1:C:79:PHE:HB3	2.00	0.43
1:C:131:CYS:HA	1:C:166:CYS:CB	2.49	0.43
1:C:280:ASN:OD1	1:C:281:GLU:CA	2.66	0.43
1:C:323:THR:O	1:C:539:VAL:HG22	2.19	0.43
1:C:743:CYS:SG	1:C:753:LEU:HD23	2.59	0.43
1:C:878:LEU:O	1:C:882:ILE:HG13	2.19	0.43
2:E:37:PHE:HB2	2:E:46:GLU:O	2.18	0.43
1:A:711:SER:O	1:B:895:GLN:CG	2.67	0.43
1:A:755:GLN:NE2	1:C:969:ASN:HB3	2.33	0.43
1:A:800:PHE:HB3	1:A:802:PHE:CZ	2.53	0.43
1:A:921:LYS:O	1:A:922:LEU:C	2.55	0.43
1:A:974:SER:HG	1:A:979:ASP:CG	2.19	0.43
1:A:997:ILE:HD12	1:A:997:ILE:HG21	1.82	0.43
1:B:294:ASP:OD2	1:B:296:LEU:N	2.52	0.43
1:B:936:ASP:OD2	1:B:936:ASP:N	2.50	0.43
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.19	0.43
1:C:984:LEU:HD13	1:C:988:GLU:CG	2.49	0.43
2:D:6:GLU:CB	2:D:115:THR:HG23	2.49	0.43
2:E:4:LEU:HD13	2:E:110:ASN:HB3	2.01	0.43
2:E:19:ARG:HD3	2:E:80:TYR:CE1	2.49	0.43
1:A:858:LEU:CD2	1:A:962:LEU:HD21	2.48	0.43
1:A:933:LYS:HA	1:A:936:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:ASP:OD2	1:A:936:ASP:N	2.50	0.43
1:C:919:ASN:OD1	1:C:919:ASN:O	2.36	0.43
1:C:936:ASP:OD2	1:C:936:ASP:N	2.50	0.43
2:D:34:VAL:HG11	2:D:79:VAL:HG11	1.99	0.43
1:A:131:CYS:HB3	1:A:133:PHE:CE2	2.54	0.43
1:B:43:PHE:CD1	1:B:43:PHE:C	2.91	0.43
1:B:376:THR:HB	1:B:435:ALA:O	2.18	0.43
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.45	0.43
1:C:131:CYS:HB3	1:C:133:PHE:CE2	2.54	0.43
1:C:663:ASP:OD1	1:C:664:ILE:HG13	2.19	0.43
1:C:921:LYS:O	1:C:922:LEU:C	2.55	0.43
2:E:6:GLU:CB	2:E:115:THR:HG23	2.49	0.43
1:A:743:CYS:SG	1:A:753:LEU:HD23	2.59	0.43
1:A:984:LEU:HD13	1:A:988:GLU:CG	2.49	0.43
1:A:1062:PHE:HB3	1:A:1064:HIS:CD2	2.53	0.43
1:B:239:GLN:HG2	1:B:240:THR:O	2.19	0.43
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	2.01	0.43
1:C:96:GLU:OE1	1:C:264:ALA:O	2.37	0.43
1:C:294:ASP:OD2	1:C:296:LEU:N	2.52	0.43
1:C:1056:ALA:HB1	1:C:1057:PRO:HD2	2.01	0.43
2:D:4:LEU:HD23	2:D:96:CYS:SG	2.59	0.43
2:D:68:PHE:CE2	2:D:83:MET:HG3	2.53	0.43
1:A:43:PHE:CE1	1:A:283:GLY:CA	3.00	0.43
1:A:503:VAL:HG23	2:D:45:ASP:HB3	2.01	0.43
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.19	0.43
1:B:376:THR:HB	1:B:435:ALA:CA	2.48	0.43
2:E:4:LEU:HD23	2:E:96:CYS:SG	2.59	0.43
2:E:60:TYR:HD2	2:E:64:VAL:CG2	2.29	0.43
1:A:216:LEU:O	1:A:217:PRO:O	2.37	0.43
1:A:372:ALA:CB	2:D:63:SER:OG	2.67	0.43
1:A:569:ILE:O	1:A:570:ALA:HB3	2.18	0.43
1:A:878:LEU:O	1:A:882:ILE:HG13	2.19	0.43
1:A:922:LEU:HA	1:A:925:ASN:OD1	2.18	0.43
1:B:128:ILE:HG21	1:B:229:LEU:HD11	2.01	0.43
1:B:765:ARG:O	1:B:768:THR:OG1	2.30	0.43
1:C:878:LEU:HD23	1:C:882:ILE:HD11	2.01	0.43
1:C:933:LYS:HA	1:C:936:ASP:OD2	2.18	0.43
1:A:883:THR:HG22	1:C:707:TYR:CD1	2.54	0.42
1:A:1056:ALA:HB1	1:A:1057:PRO:HD2	2.01	0.42
1:B:96:GLU:OE1	1:B:264:ALA:O	2.37	0.42
1:B:974:SER:HG	1:B:979:ASP:CG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:LEU:HD13	1:B:988:GLU:CG	2.49	0.42
1:C:324:GLU:O	1:C:539:VAL:HG13	2.19	0.42
1:A:1075:PHE:HB3	1:A:1096:VAL:HB	2.01	0.42
1:B:171:VAL:HG21	4:B:1301:NAG:H62	2.01	0.42
1:C:239:GLN:HG2	1:C:240:THR:O	2.19	0.42
2:D:7:SER:O	2:D:20:LEU:HD12	2.19	0.42
1:A:96:GLU:OE1	1:A:264:ALA:O	2.37	0.42
1:A:131:CYS:HA	1:A:166:CYS:CB	2.48	0.42
1:A:239:GLN:HG2	1:A:240:THR:O	2.19	0.42
1:A:455:LEU:HD11	1:A:493:GLN:CB	2.49	0.42
1:A:1101:HIS:ND1	4:A:1313:NAG:H5	2.34	0.42
1:B:228:ASP:O	1:B:230:PRO:HD2	2.19	0.42
2:E:7:SER:O	2:E:20:LEU:HD12	2.19	0.42
2:E:64:VAL:O	2:E:67:ARG:HG2	2.18	0.42
1:A:103:GLY:HA3	1:A:119:ILE:O	2.20	0.42
1:A:855:PHE:HD1	1:C:589:PRO:CG	2.31	0.42
1:A:897:PRO:CG	1:C:709:ASN:O	2.67	0.42
1:A:964:LYS:HD3	1:A:964:LYS:O	2.20	0.42
1:B:466:ARG:O	1:B:466:ARG:CG	2.68	0.42
1:C:922:LEU:HA	1:C:925:ASN:OD1	2.18	0.42
2:E:98:SER:C	2:E:108:PHE:HA	2.40	0.42
1:A:592:PHE:HE2	1:B:857:GLY:HA2	1.84	0.42
1:A:878:LEU:HD23	1:A:882:ILE:HD11	2.01	0.42
1:A:885:GLY:HA3	1:A:901:GLN:OE1	2.20	0.42
1:A:979:ASP:O	1:A:983:ARG:HG3	2.20	0.42
1:B:216:LEU:O	1:B:217:PRO:O	2.37	0.42
1:B:390:LEU:CD1	1:C:983:ARG:HG2	2.48	0.42
1:B:878:LEU:O	1:B:882:ILE:HG13	2.19	0.42
1:B:898:PHE:HA	1:B:901:GLN:HB3	2.01	0.42
1:C:43:PHE:CE1	1:C:283:GLY:CA	3.00	0.42
1:C:898:PHE:HA	1:C:901:GLN:HB3	2.01	0.42
1:C:1043:CYS:C	1:C:1064:HIS:ND1	2.73	0.42
1:A:128:ILE:HG21	1:A:229:LEU:HD11	2.01	0.42
1:B:171:VAL:CG2	4:B:1301:NAG:H62	2.50	0.42
1:B:361:CYS:O	1:B:524:VAL:HG23	2.19	0.42
1:B:465:GLU:OE2	1:B:466:ARG:O	2.37	0.42
1:B:743:CYS:HA	1:B:977:LEU:HD21	2.02	0.42
1:C:765:ARG:O	1:C:768:THR:OG1	2.30	0.42
1:A:743:CYS:HA	1:A:977:LEU:HD21	2.02	0.42
1:A:898:PHE:HA	1:A:901:GLN:HB3	2.01	0.42
1:A:1103:PHE:HB3	1:A:1113:GLN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PHE:CE1	1:B:160:TYR:CE2	3.08	0.42
1:B:663:ASP:OD1	1:B:664:ILE:HG13	2.19	0.42
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	2.02	0.42
1:B:985:ASP:O	1:B:986:PRO:C	2.58	0.42
1:C:985:ASP:O	1:C:986:PRO:C	2.58	0.42
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.19	0.42
2:D:60:TYR:HD2	2:D:64:VAL:CG2	2.29	0.42
1:A:133:PHE:CE1	1:A:160:TYR:CE2	3.08	0.42
1:A:711:SER:O	1:B:895:GLN:HG2	2.19	0.42
1:A:869:MET:HB2	1:C:699:LEU:CD1	2.48	0.42
1:A:1141:LEU:O	1:A:1144:GLU:HB2	2.20	0.42
1:B:193:VAL:CG2	1:B:223:LEU:HD12	2.50	0.42
1:B:280:ASN:HB2	1:B:286:THR:CG2	2.50	0.42
1:B:392:PHE:HE1	1:B:517:LEU:HD11	1.84	0.42
1:B:772:VAL:HA	1:B:775:ASP:OD2	2.20	0.42
1:B:1103:PHE:HB3	1:B:1113:GLN:H	1.84	0.42
1:C:200:TYR:HD2	1:C:228:ASP:OD2	2.01	0.42
1:C:964:LYS:O	1:C:964:LYS:HD3	2.20	0.42
2:D:3:GLN:C	2:D:4:LEU:HD12	2.40	0.42
2:D:20:LEU:HD21	2:D:36:TRP:CZ3	2.55	0.42
2:D:69:THR:CG2	2:D:82:GLN:HB3	2.29	0.42
2:E:3:GLN:C	2:E:4:LEU:HD12	2.40	0.42
2:E:99:GLY:HA3	2:E:107:ASP:OD1	2.20	0.42
1:A:666:ILE:CD1	1:A:672:ALA:HB2	2.50	0.42
1:A:1043:CYS:C	1:A:1064:HIS:ND1	2.73	0.42
4:A:1301:NAG:HO3	4:A:1301:NAG:C7	2.25	0.42
1:B:103:GLY:HA3	1:B:119:ILE:O	2.20	0.42
1:B:473:TYR:HD2	1:B:489:TYR:CD2	2.38	0.42
1:B:885:GLY:HA3	1:B:901:GLN:OE1	2.20	0.42
1:B:964:LYS:O	1:B:964:LYS:HD3	2.20	0.42
2:E:60:TYR:CE2	2:E:68:PHE:HB2	2.55	0.42
1:A:282:ASN:HD22	4:A:1303:NAG:C1	2.23	0.42
1:A:308:VAL:HB	1:A:602:THR:HG23	2.02	0.42
1:A:592:PHE:CE2	1:B:857:GLY:HA2	2.55	0.42
1:A:663:ASP:OD1	1:A:664:ILE:HG13	2.19	0.42
1:A:985:ASP:O	1:A:986:PRO:C	2.58	0.42
1:B:555:SER:OG	1:B:586:ASP:OD1	2.35	0.42
1:B:878:LEU:HD23	1:B:882:ILE:HD11	2.01	0.42
1:B:1043:CYS:C	1:B:1064:HIS:ND1	2.73	0.42
1:C:103:GLY:HA3	1:C:119:ILE:O	2.20	0.42
1:C:359:SER:OG	1:C:394:ASN:OD1	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:962:LEU:HD12	1:C:962:LEU:O	2.18	0.42
1:C:1075:PHE:HB3	1:C:1096:VAL:HB	2.01	0.42
1:A:139:PRO:HD2	1:A:239:GLN:OE1	2.20	0.41
1:A:752:LEU:HG	1:A:752:LEU:H	1.75	0.41
1:C:228:ASP:O	1:C:230:PRO:HD2	2.19	0.41
2:D:99:GLY:HA3	2:D:107:ASP:OD1	2.20	0.41
1:A:597:VAL:HG13	1:A:608:VAL:HG11	2.02	0.41
1:A:770:ILE:CG1	1:A:770:ILE:HG23	1.97	0.41
1:B:378:LYS:HD3	2:E:106:TYR:CE2	2.56	0.41
1:B:907:ASN:HA	1:B:911:VAL:O	2.21	0.41
1:C:411:ALA:HB3	1:C:414:GLN:NE2	2.35	0.41
1:C:885:GLY:HA3	1:C:901:GLN:OE1	2.20	0.41
1:C:905:ARG:HG2	1:C:905:ARG:H	1.52	0.41
1:C:1103:PHE:HB3	1:C:1113:GLN:H	1.84	0.41
1:A:228:ASP:O	1:A:230:PRO:HD2	2.19	0.41
1:A:713:ALA:O	1:B:894:LEU:HD13	2.20	0.41
1:B:385:THR:O	1:B:385:THR:HG23	2.20	0.41
1:B:979:ASP:O	1:B:983:ARG:HG3	2.20	0.41
1:B:993:ILE:O	1:B:997:ILE:HG12	2.21	0.41
1:B:997:ILE:HD12	1:B:997:ILE:HG21	1.82	0.41
1:C:216:LEU:O	1:C:217:PRO:O	2.37	0.41
2:E:93:LEU:HD22	2:E:95:TYR:CE2	2.54	0.41
1:A:61:ASN:OD1	1:A:61:ASN:N	2.51	0.41
1:A:141:LEU:CD2	1:A:157:PHE:HD2	2.33	0.41
1:A:727:LEU:HD11	1:A:1028:LYS:HD2	2.02	0.41
1:B:391:CYS:HB2	1:B:524:VAL:O	2.20	0.41
1:B:517:LEU:N	1:B:517:LEU:HD12	2.35	0.41
1:B:558:LYS:NZ	4:C:1301:NAG:H82	2.34	0.41
1:C:81:ASN:N	1:C:82:PRO:HD3	2.36	0.41
1:C:128:ILE:HG21	1:C:229:LEU:HD11	2.01	0.41
1:C:979:ASP:O	1:C:983:ARG:HG3	2.20	0.41
1:A:737:ASP:OD1	1:A:739:THR:OG1	2.32	0.41
1:B:707:TYR:CE2	1:C:896:ILE:O	2.74	0.41
2:D:91:THR:O	2:D:92:ALA:HB2	2.21	0.41
1:A:53:ASP:OD2	1:A:55:PHE:CD2	2.74	0.41
1:A:411:ALA:HB3	1:A:414:GLN:NE2	2.35	0.41
1:B:1028:LYS:O	1:B:1029:MET:C	2.59	0.41
1:B:1075:PHE:HB3	1:B:1096:VAL:HB	2.01	0.41
1:C:149:ASN:OD1	1:C:149:ASN:O	2.39	0.41
1:C:280:ASN:HB2	1:C:286:THR:CG2	2.50	0.41
1:C:410:ILE:O	1:C:410:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:PHE:C	1:B:376:THR:N	2.73	0.41
1:C:133:PHE:CE1	1:C:160:TYR:CE2	3.08	0.41
1:C:139:PRO:HD2	1:C:239:GLN:OE1	2.20	0.41
1:C:410:ILE:HD13	1:C:510:VAL:HG11	2.03	0.41
1:C:666:ILE:CD1	1:C:672:ALA:HB2	2.50	0.41
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	2.02	0.41
1:C:812:PRO:O	1:C:813:SER:HB3	2.21	0.41
1:C:993:ILE:O	1:C:997:ILE:HG12	2.21	0.41
2:D:4:LEU:HD13	2:D:110:ASN:HB3	2.01	0.41
2:E:68:PHE:HD2	2:E:81:LEU:HD11	1.81	0.41
1:A:96:GLU:OE2	1:A:263:ALA:CB	2.69	0.41
1:A:280:ASN:HB2	1:A:286:THR:CG2	2.50	0.41
1:B:81:ASN:N	1:B:82:PRO:HD3	2.36	0.41
1:B:139:PRO:HD2	1:B:239:GLN:OE1	2.20	0.41
1:B:812:PRO:O	1:B:813:SER:HB3	2.21	0.41
1:C:43:PHE:CZ	1:C:45:SER:HB2	2.56	0.41
1:C:658:ASN:CG	1:C:659:SER:H	2.24	0.41
1:C:743:CYS:HA	1:C:977:LEU:HD21	2.02	0.41
1:C:1096:VAL:CA	1:C:1102:TRP:HZ3	2.34	0.41
2:D:37:PHE:CE2	2:D:95:TYR:HD1	2.38	0.41
1:A:388:ASN:CB	1:A:527:PRO:HD2	2.51	0.41
1:A:410:ILE:HD13	1:A:510:VAL:HG11	2.03	0.41
1:A:565:PHE:CE2	1:B:42:VAL:HG22	2.56	0.41
1:A:657:ASN:HB2	4:A:1309:NAG:H2	2.02	0.41
1:A:712:ILE:HG13	1:B:895:GLN:O	2.21	0.41
1:A:746:SER:CB	1:A:977:LEU:HD11	2.51	0.41
1:A:767:LEU:HD21	1:A:1008:VAL:CG2	2.51	0.41
1:A:781:VAL:CG2	1:A:782:PHE:CD2	3.04	0.41
1:A:812:PRO:O	1:A:813:SER:HB3	2.21	0.41
1:A:986:PRO:O	1:A:990:GLU:HG3	2.21	0.41
1:A:1040:VAL:CG1	1:B:1030:SER:O	2.69	0.41
1:A:1088:HIS:CE1	1:A:1122:VAL:HG23	2.56	0.41
1:B:53:ASP:OD2	1:B:55:PHE:CD2	2.74	0.41
1:B:308:VAL:HB	1:B:602:THR:HG23	2.02	0.41
1:B:378:LYS:CE	1:B:380:TYR:OH	2.69	0.41
1:B:666:ILE:CD1	1:B:672:ALA:HB2	2.50	0.41
1:B:747:THR:O	1:B:751:ASN:OD1	2.39	0.41
1:B:1088:HIS:CE1	1:B:1122:VAL:HG23	2.56	0.41
1:C:53:ASP:OD2	1:C:55:PHE:CD2	2.74	0.41
1:C:97:LYS:O	1:C:97:LYS:HD3	2.21	0.41
1:C:781:VAL:CG2	1:C:782:PHE:CD2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1028:LYS:O	1:C:1029:MET:C	2.59	0.41
1:C:1088:HIS:CE1	1:C:1122:VAL:HG23	2.56	0.41
2:D:38:ARG:CD	2:D:92:ALA:HB3	2.51	0.41
2:E:1:GLN:O	2:E:1:GLN:HG2	2.20	0.41
2:E:20:LEU:HD21	2:E:36:TRP:CZ3	2.55	0.41
2:E:106:TYR:O	2:E:108:PHE:O	2.38	0.41
1:A:918:GLU:HG2	1:C:1128:VAL:HG11	2.03	0.41
1:A:993:ILE:O	1:A:997:ILE:HG12	2.21	0.41
1:A:1074:ASN:O	1:A:1075:PHE:CD1	2.74	0.41
1:B:531:THR:HG22	1:B:532:ASN:N	2.35	0.41
1:B:569:ILE:O	1:B:570:ALA:HB3	2.21	0.41
1:B:746:SER:CB	1:B:977:LEU:HD11	2.51	0.41
1:B:781:VAL:CG2	1:B:782:PHE:CD2	3.04	0.41
1:B:824:ASN:OD1	1:B:824:ASN:N	2.43	0.41
1:B:1141:LEU:O	1:B:1144:GLU:HB2	2.20	0.41
1:C:986:PRO:O	1:C:990:GLU:HG3	2.21	0.41
2:D:1:GLN:O	2:D:1:GLN:HG2	2.20	0.41
2:E:91:THR:O	2:E:92:ALA:HB2	2.21	0.41
1:A:410:ILE:O	1:A:410:ILE:HG22	2.20	0.40
1:A:658:ASN:CG	1:A:659:SER:H	2.24	0.40
1:A:907:ASN:HA	1:A:911:VAL:O	2.20	0.40
1:A:911:VAL:HG12	1:A:1106:GLN:HE22	1.86	0.40
1:A:1094:VAL:HG12	1:B:904:TYR:OH	2.21	0.40
1:B:376:THR:N	1:B:435:ALA:O	2.54	0.40
1:B:784:GLN:OE1	1:B:1034:LEU:HD11	2.21	0.40
1:B:922:LEU:CD1	4:B:1310:NAG:H62	2.44	0.40
1:B:954:GLN:OE1	1:B:1014:ARG:CD	2.69	0.40
1:C:308:VAL:HB	1:C:602:THR:HG23	2.02	0.40
1:C:455:LEU:HD11	1:C:493:GLN:CB	2.51	0.40
1:C:907:ASN:HA	1:C:911:VAL:O	2.21	0.40
1:C:954:GLN:OE1	1:C:1014:ARG:CD	2.69	0.40
2:E:93:LEU:HD23	2:E:115:THR:C	2.41	0.40
1:A:43:PHE:CZ	1:A:45:SER:HB2	2.56	0.40
1:A:97:LYS:O	1:A:97:LYS:HD3	2.21	0.40
1:A:1074:ASN:C	1:A:1075:PHE:CG	2.95	0.40
1:A:1096:VAL:CA	1:A:1102:TRP:HZ3	2.34	0.40
1:B:141:LEU:CD2	1:B:157:PHE:HD2	2.33	0.40
1:B:262:ALA:O	1:B:263:ALA:HB2	2.22	0.40
1:B:986:PRO:O	1:B:990:GLU:HG3	2.21	0.40
1:C:767:LEU:HD21	1:C:1008:VAL:CG2	2.51	0.40
1:C:772:VAL:HA	1:C:775:ASP:OD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLU:HG2	1:A:485:GLY:N	2.37	0.40
1:A:733:LYS:NZ	1:A:775:ASP:OD1	2.48	0.40
1:A:772:VAL:HA	1:A:775:ASP:OD2	2.20	0.40
1:B:407:VAL:CG2	2:E:106:TYR:HE1	2.34	0.40
1:C:746:SER:CB	1:C:977:LEU:HD11	2.51	0.40
2:D:93:LEU:HD22	2:D:95:TYR:CE2	2.54	0.40
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.57	0.40
1:A:705:VAL:HG23	1:B:789:TYR:CD1	2.50	0.40
1:A:747:THR:O	1:A:751:ASN:OD1	2.39	0.40
1:B:97:LYS:O	1:B:97:LYS:HD3	2.21	0.40
1:B:149:ASN:O	1:B:149:ASN:OD1	2.39	0.40
1:B:695:TYR:HE1	1:B:697:MET:HA	1.87	0.40
1:B:777:ASN:HB3	1:B:1022:ALA:CB	2.52	0.40
1:B:1040:VAL:O	1:B:1041:ASP:HB2	2.22	0.40
1:B:1062:PHE:HB3	1:B:1064:HIS:NE2	2.37	0.40
1:C:141:LEU:CD2	1:C:157:PHE:HD2	2.33	0.40
1:C:330:PRO:HA	1:C:579:PRO:HB2	2.03	0.40
1:C:747:THR:O	1:C:751:ASN:OD1	2.39	0.40
1:C:1141:LEU:O	1:C:1144:GLU:HB2	2.20	0.40
2:D:39:GLN:O	2:D:92:ALA:HB1	2.21	0.40
2:D:60:TYR:OH	2:D:69:THR:C	2.60	0.40
2:D:106:TYR:O	2:D:108:PHE:O	2.38	0.40
2:E:39:GLN:O	2:E:92:ALA:HB1	2.21	0.40
1:B:96:GLU:OE2	1:B:263:ALA:CB	2.69	0.40
1:B:1089:PHE:CD1	1:C:914:ASN:HB3	2.56	0.40
1:C:310:LYS:C	1:C:310:LYS:HD2	2.42	0.40
1:C:502:GLY:O	1:C:506:GLN:N	2.55	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	1044/1264 (83%)	948 (91%)	94 (9%)	2 (0%)	47 79
1	B	1039/1264 (82%)	938 (90%)	99 (10%)	2 (0%)	47 79
1	C	1042/1264 (82%)	946 (91%)	92 (9%)	4 (0%)	34 71
2	D	118/126 (94%)	114 (97%)	4 (3%)	0	100 100
2	E	118/126 (94%)	114 (97%)	4 (3%)	0	100 100
All	All	3361/4044 (83%)	3060 (91%)	293 (9%)	8 (0%)	50 79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	459	SER
1	A	25	PRO
1	A	699	LEU
1	B	25	PRO
1	B	699	LEU
1	C	25	PRO
1	C	699	LEU
1	C	709	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	931/1100 (85%)	891 (96%)	40 (4%)	29 63
1	B	925/1100 (84%)	887 (96%)	38 (4%)	30 64
1	C	929/1100 (84%)	892 (96%)	37 (4%)	31 65
2	D	92/97 (95%)	86 (94%)	6 (6%)	17 51
2	E	92/97 (95%)	86 (94%)	6 (6%)	17 51
All	All	2969/3494 (85%)	2842 (96%)	127 (4%)	33 63

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	53	ASP
1	A	160	TYR
1	A	192	PHE
1	A	206	LYS
1	A	216	LEU
1	A	241	LEU
1	A	269	TYR
1	A	286	THR
1	A	294	ASP
1	A	329	PHE
1	A	477[A]	SER
1	A	477[B]	SER
1	A	643	PHE
1	A	730	SER
1	A	741	TYR
1	A	751	ASN
1	A	761	THR
1	A	767	LEU
1	A	777	ASN
1	A	781	VAL
1	A	791	THR
1	A	802	PHE
1	A	817	PHE
1	A	869	MET
1	A	873	TYR
1	A	886	TRP
1	A	887	THR
1	A	926	GLN
1	A	928	ASN
1	A	961	THR
1	A	1002	GLN
1	A	1005	GLN
1	A	1014	ARG
1	A	1040	VAL
1	A	1091	ARG
1	A	1102	TRP
1	A	1106	GLN
1	A	1118	ASP
1	A	1122	VAL
1	B	43	PHE
1	B	53	ASP
1	B	160	TYR

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Mol	Chain	Res	Type
1	B	192	PHE
1	B	206	LYS
1	B	216	LEU
1	B	241	LEU
1	B	269	TYR
1	B	286	THR
1	B	294	ASP
1	B	444	LYS
1	B	643	PHE
1	B	730	SER
1	B	741	TYR
1	B	751	ASN
1	B	761	THR
1	B	767	LEU
1	B	777	ASN
1	B	781	VAL
1	B	791	THR
1	B	802	PHE
1	B	817	PHE
1	B	869	MET
1	B	873	TYR
1	B	886	TRP
1	B	887	THR
1	B	926	GLN
1	B	928	ASN
1	B	961	THR
1	B	1002	GLN
1	B	1005	GLN
1	B	1014	ARG
1	B	1040	VAL
1	B	1091	ARG
1	B	1102	TRP
1	B	1106	GLN
1	B	1118	ASP
1	B	1122	VAL
1	C	43	PHE
1	C	53	ASP
1	C	160	TYR
1	C	192	PHE
1	C	206	LYS
1	C	216	LEU
1	C	241	LEU

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Mol	Chain	Res	Type
1	C	269	TYR
1	C	286	THR
1	C	294	ASP
1	C	643	PHE
1	C	730	SER
1	C	741	TYR
1	C	751	ASN
1	C	761	THR
1	C	767	LEU
1	C	777	ASN
1	C	781	VAL
1	C	791	THR
1	C	802	PHE
1	C	817	PHE
1	C	869	MET
1	C	873	TYR
1	C	886	TRP
1	C	887	THR
1	C	926	GLN
1	C	928	ASN
1	C	961	THR
1	C	1002	GLN
1	C	1005	GLN
1	C	1014	ARG
1	C	1040	VAL
1	C	1091	ARG
1	C	1102	TRP
1	C	1106	GLN
1	C	1118	ASP
1	C	1122	VAL
2	D	37	PHE
2	D	52	TYR
2	D	59	ASN
2	D	80	TYR
2	D	95	TYR
2	D	108	PHE
2	E	37	PHE
2	E	52	TYR
2	E	59	ASN
2	E	80	TYR
2	E	95	TYR
2	E	108	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	99	ASN
1	A	165	ASN
1	A	207	HIS
1	A	603	ASN
1	A	1002	GLN
1	A	1005	GLN
1	A	1119	ASN
1	B	66	HIS
1	B	99	ASN
1	B	207	HIS
1	B	1002	GLN
1	B	1119	ASN
1	C	66	HIS
1	C	99	ASN
1	C	207	HIS
1	C	616	ASN
1	C	957	GLN
1	C	1119	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	1	3	14,14,15	1.19	1 (7%)	17,19,21	0.87	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.32	0
3	NAG	G	1	3	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	H	1	3	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	I	1	3	14,14,15	0.70	1 (7%)	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.18	0	17,19,21	0.38	0
3	NAG	J	1	1,3	14,14,15	0.44	0	17,19,21	0.70	1 (5%)
3	NAG	J	2	3	14,14,15	0.24	0	17,19,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C1-C2	4.21	1.58	1.52
3	I	1	NAG	O5-C1	-2.59	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

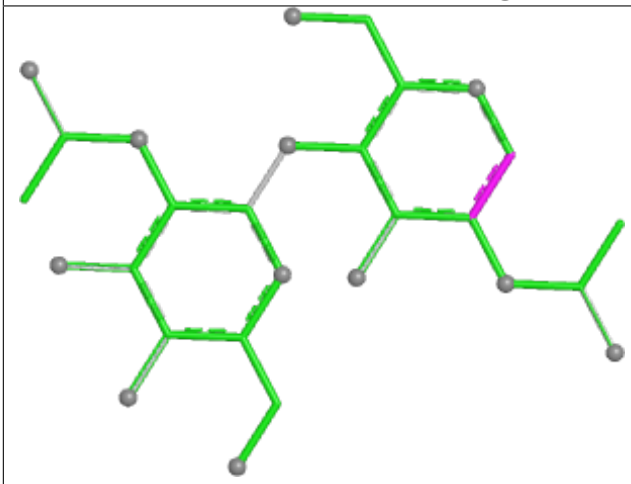
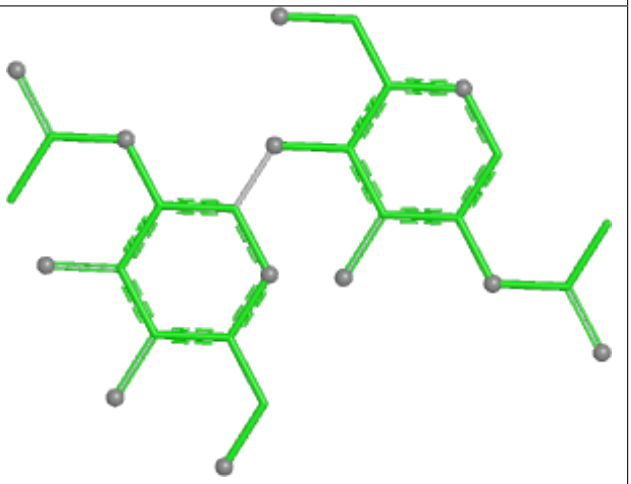
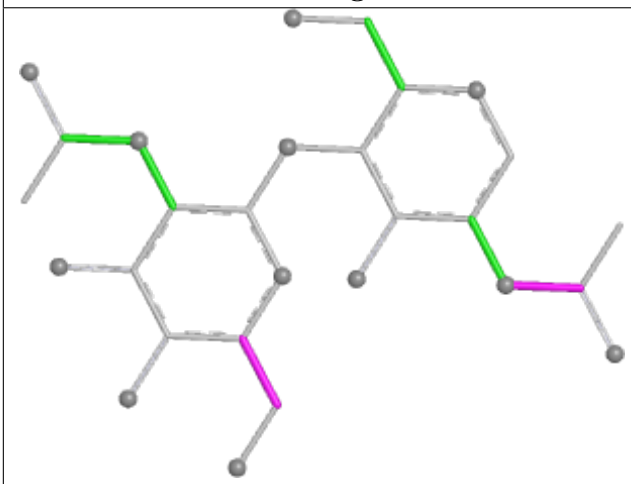
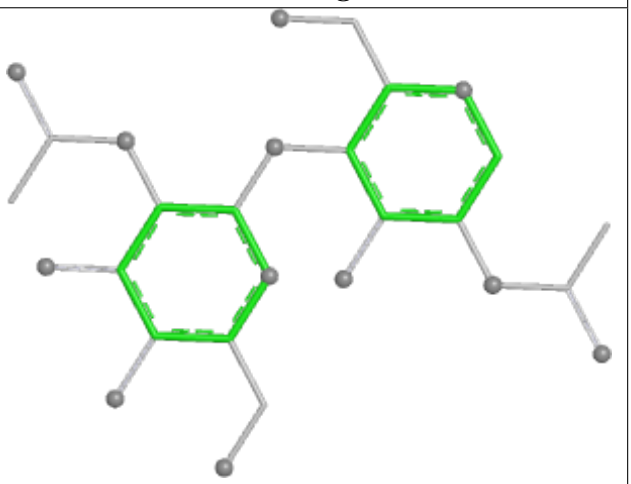
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

There are no ring outliers.

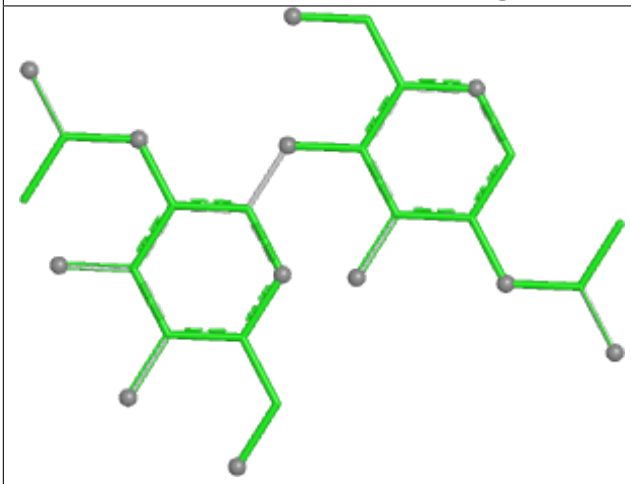
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	2	0
3	F	1	NAG	2	0
3	I	1	NAG	1	0

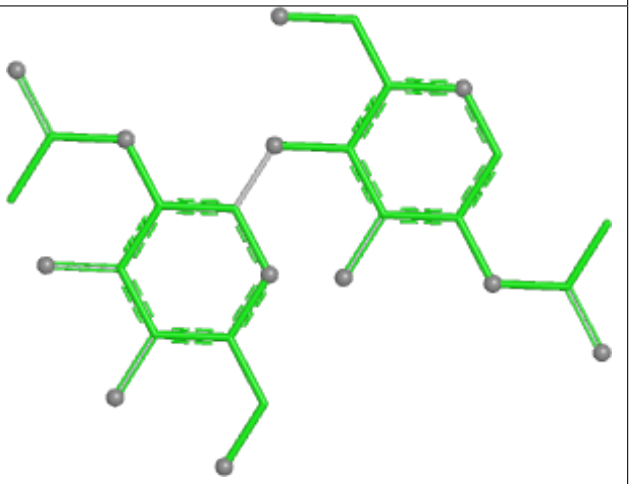
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain F	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

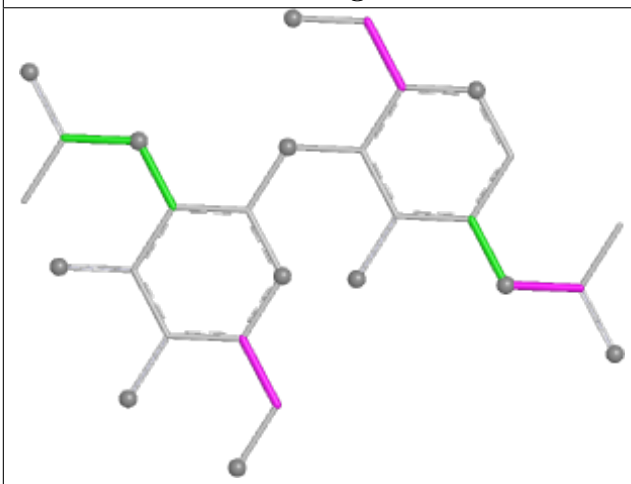
Oligosaccharide Chain G



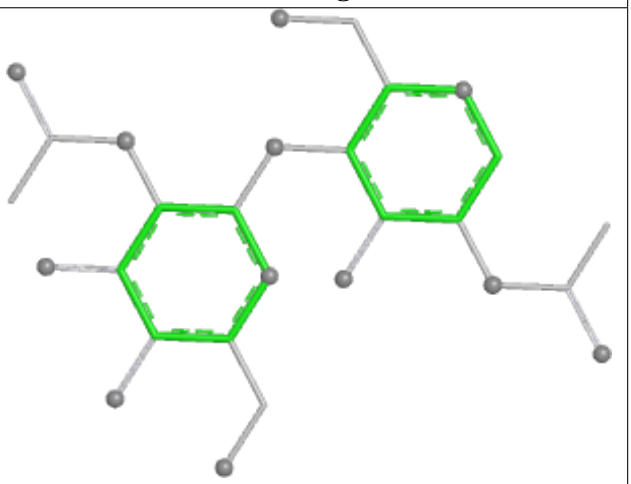
Bond lengths



Bond angles

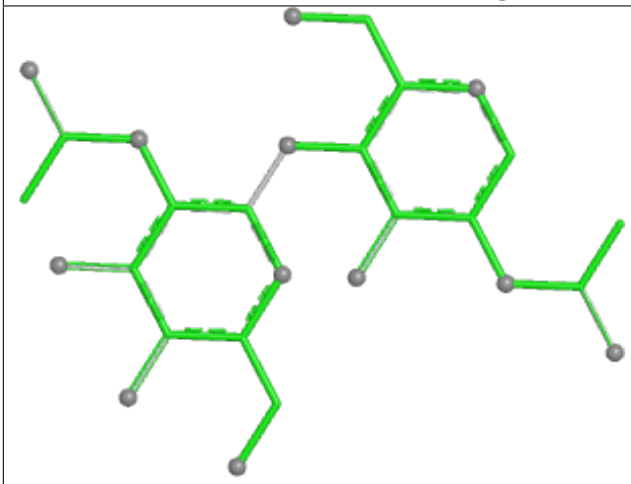


Torsions

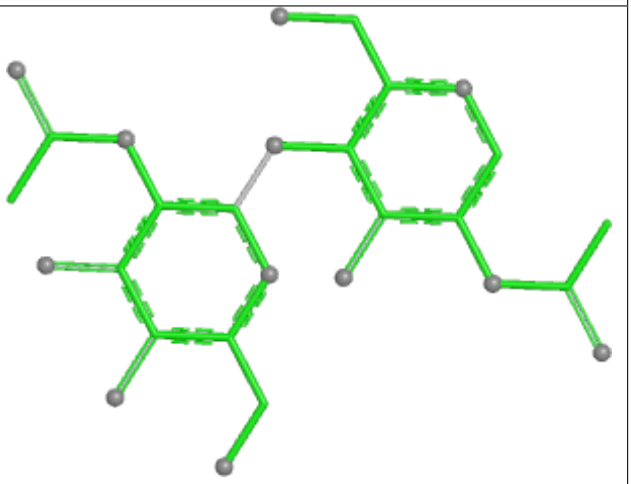


Rings

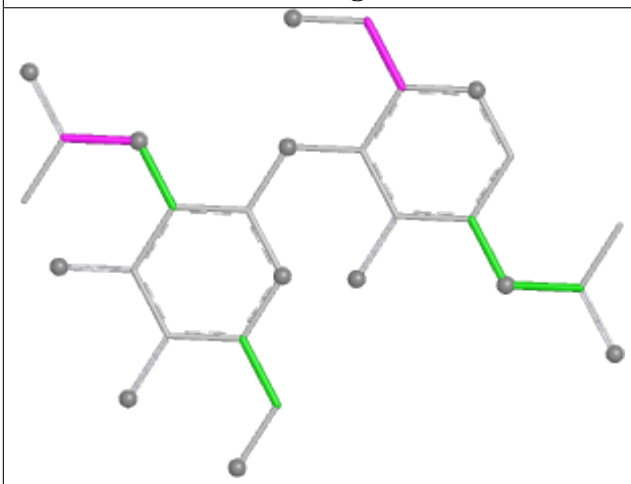
Oligosaccharide Chain H



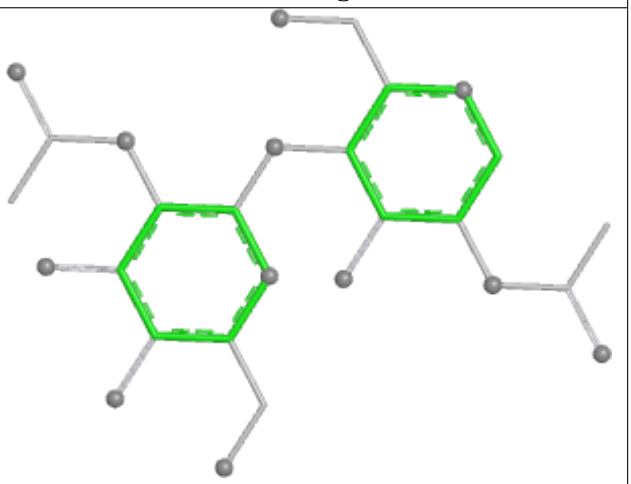
Bond lengths



Bond angles

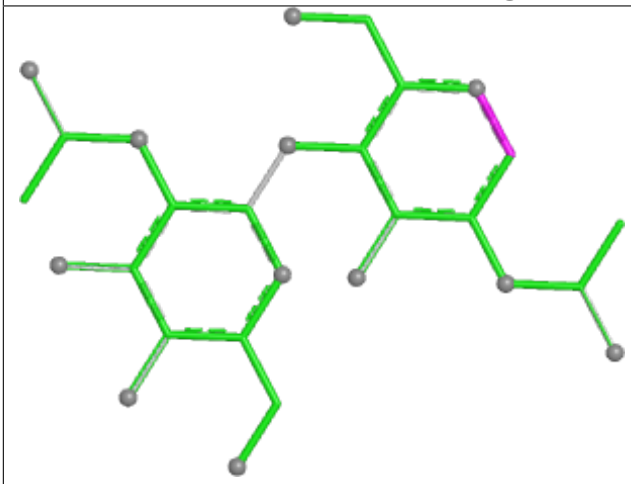


Torsions

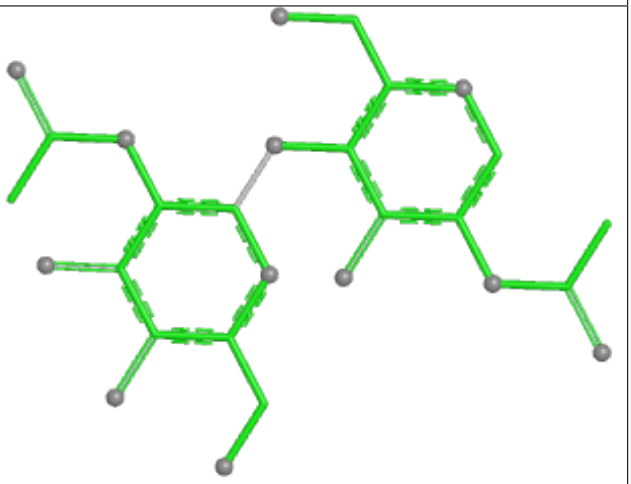


Rings

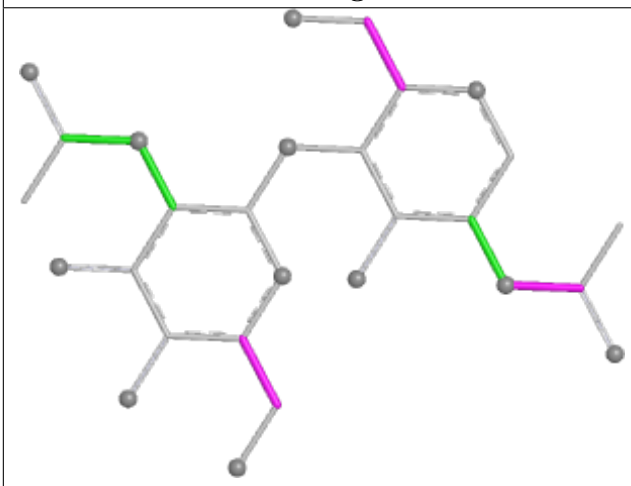
Oligosaccharide Chain I



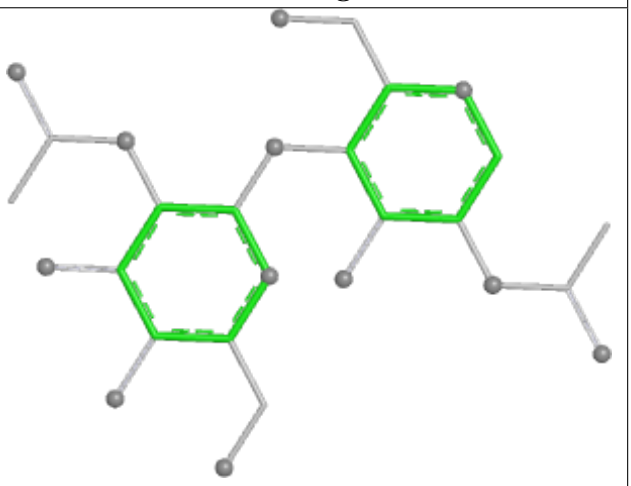
Bond lengths



Bond angles

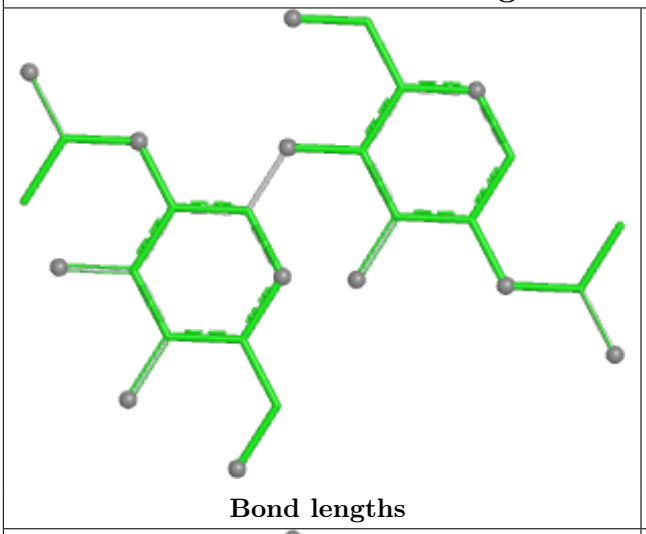


Torsions

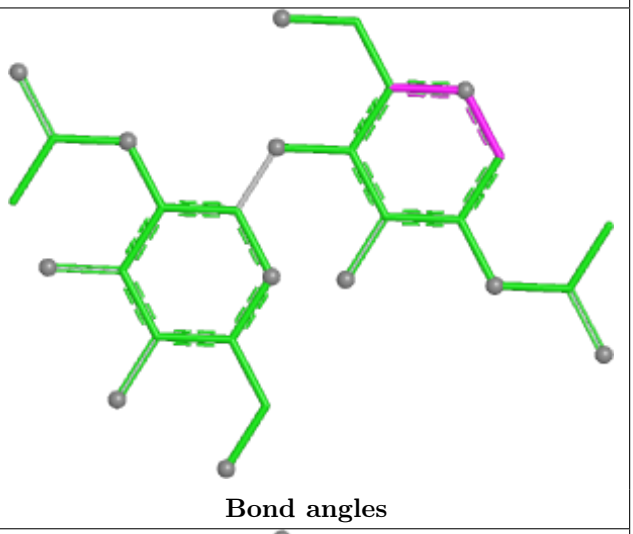


Rings

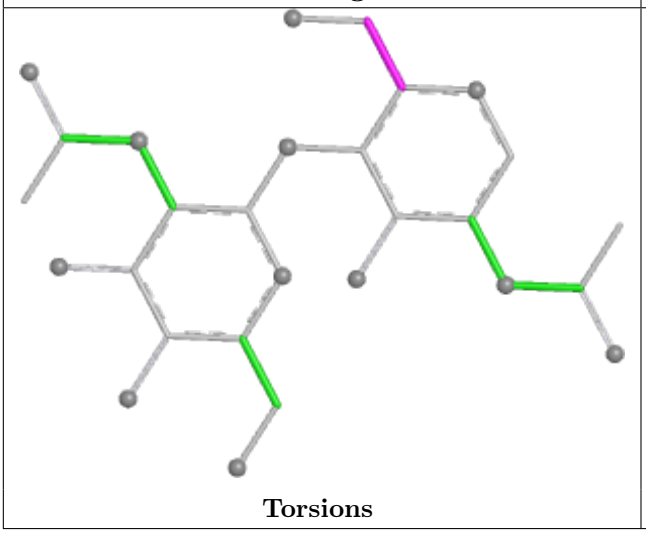
Oligosaccharide Chain J



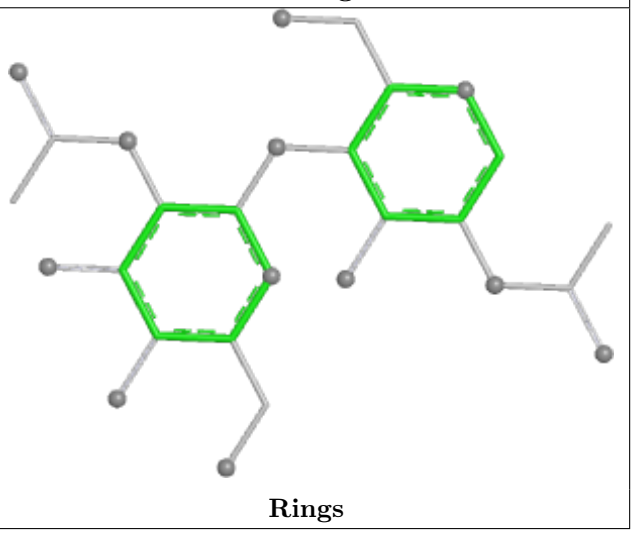
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1310	1	14,14,15	3.30	2 (14%)	17,19,21	2.13	1 (5%)
4	NAG	A	1312	-	14,14,15	0.65	1 (7%)	17,19,21	0.77	1 (5%)
4	NAG	B	1306	-	14,14,15	0.30	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1314	1	14,14,15	0.36	0	17,19,21	0.46	0
4	NAG	C	1303	1	14,14,15	0.87	1 (7%)	17,19,21	0.66	1 (5%)
4	NAG	B	1311	1	14,14,15	1.66	2 (14%)	17,19,21	1.35	2 (11%)
4	NAG	A	1311	1	14,14,15	1.76	2 (14%)	17,19,21	1.44	1 (5%)
4	NAG	B	1312	-	14,14,15	2.78	2 (14%)	17,19,21	1.04	1 (5%)
4	NAG	A	1308	1	14,14,15	0.47	0	17,19,21	1.37	1 (5%)
4	NAG	B	1313	1	14,14,15	0.98	1 (7%)	17,19,21	0.69	1 (5%)
4	NAG	A	1305	1	14,14,15	1.74	2 (14%)	17,19,21	0.66	0
4	NAG	A	1304	1	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	B	1309	1	14,14,15	1.06	1 (7%)	17,19,21	0.69	0
4	NAG	B	1301	-	14,14,15	0.35	0	17,19,21	0.46	0
4	NAG	B	1308	1	14,14,15	1.17	2 (14%)	17,19,21	0.94	1 (5%)
4	NAG	A	1302	-	14,14,15	0.16	0	17,19,21	0.61	0
4	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.35	0
4	NAG	A	1303	-	14,14,15	1.41	2 (14%)	17,19,21	1.02	2 (11%)
4	NAG	A	1301	-	14,14,15	0.89	1 (7%)	17,19,21	0.66	0
4	NAG	C	1301	1	14,14,15	0.92	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	B	1307	-	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
4	NAG	B	1302	-	14,14,15	0.56	0	17,19,21	0.44	0
4	NAG	B	1305	-	14,14,15	0.69	1 (7%)	17,19,21	0.51	0
4	NAG	B	1304	1	14,14,15	1.81	2 (14%)	17,19,21	1.12	2 (11%)
4	NAG	A	1306	-	14,14,15	0.63	0	17,19,21	0.45	0
4	NAG	A	1307	1	14,14,15	1.66	2 (14%)	17,19,21	2.00	1 (5%)
4	NAG	C	1305	1	14,14,15	2.18	1 (7%)	17,19,21	2.18	1 (5%)
4	NAG	C	1302	1	14,14,15	0.51	0	17,19,21	1.10	2 (11%)
4	NAG	A	1313	1	14,14,15	0.74	1 (7%)	17,19,21	0.41	0
4	NAG	B	1303	-	14,14,15	0.20	0	17,19,21	0.52	0
4	NAG	C	1306	1	14,14,15	2.34	2 (14%)	17,19,21	1.28	1 (5%)
4	NAG	C	1304	-	14,14,15	1.00	2 (14%)	17,19,21	1.45	3 (17%)
4	NAG	A	1309	1	14,14,15	1.29	1 (7%)	17,19,21	1.02	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1310	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1312	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1310	NAG	O5-C1	11.92	1.62	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1312	NAG	O5-C1	9.95	1.59	1.43
4	C	1306	NAG	O5-C1	8.02	1.56	1.43
4	C	1305	NAG	O5-C1	7.93	1.56	1.43
4	B	1304	NAG	C1-C2	6.29	1.61	1.52
4	A	1311	NAG	O5-C1	5.92	1.53	1.43
4	A	1305	NAG	O5-C1	5.72	1.52	1.43
4	A	1307	NAG	O5-C1	5.68	1.52	1.43
4	B	1311	NAG	O5-C1	-4.89	1.35	1.43
4	A	1309	NAG	O5-C1	4.73	1.51	1.43
4	A	1303	NAG	C1-C2	-3.68	1.46	1.52
4	A	1303	NAG	O5-C1	-3.67	1.37	1.43
4	B	1311	NAG	C1-C2	-3.48	1.47	1.52
4	B	1309	NAG	C1-C2	3.44	1.57	1.52
4	C	1301	NAG	O5-C1	-3.39	1.38	1.43
4	C	1306	NAG	C1-C2	3.32	1.57	1.52
4	B	1308	NAG	O5-C1	3.29	1.49	1.43
4	B	1313	NAG	C1-C2	-3.23	1.47	1.52
4	C	1303	NAG	O5-C1	-2.89	1.39	1.43
4	A	1305	NAG	C1-C2	2.88	1.56	1.52
4	B	1308	NAG	C1-C2	2.82	1.56	1.52
4	A	1301	NAG	O5-C1	-2.71	1.39	1.43
4	B	1310	NAG	C1-C2	2.59	1.56	1.52
4	C	1304	NAG	O5-C1	-2.57	1.39	1.43
4	A	1311	NAG	C1-C2	2.57	1.56	1.52
4	A	1313	NAG	O5-C1	-2.53	1.39	1.43
4	B	1304	NAG	O5-C1	2.37	1.47	1.43
4	B	1305	NAG	O5-C1	-2.34	1.40	1.43
4	A	1307	NAG	C1-C2	2.20	1.55	1.52
4	A	1312	NAG	O5-C1	-2.11	1.40	1.43
4	C	1304	NAG	C1-C2	-2.10	1.49	1.52
4	B	1312	NAG	C1-C2	2.06	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1305	NAG	C1-O5-C5	8.40	123.57	112.19
4	B	1310	NAG	C1-O5-C5	8.22	123.33	112.19
4	A	1307	NAG	C1-O5-C5	7.87	122.86	112.19
4	A	1311	NAG	C1-O5-C5	5.35	119.44	112.19
4	A	1308	NAG	C1-O5-C5	5.23	119.28	112.19
4	C	1306	NAG	C1-O5-C5	4.32	118.05	112.19
4	C	1304	NAG	C1-O5-C5	3.86	117.42	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1309	NAG	C1-O5-C5	3.83	117.38	112.19
4	B	1311	NAG	O5-C5-C4	-3.27	102.88	110.83
4	B	1304	NAG	C2-N2-C7	3.08	127.28	122.90
4	B	1308	NAG	C1-O5-C5	3.06	116.33	112.19
4	C	1301	NAG	C1-O5-C5	2.96	116.20	112.19
4	B	1311	NAG	C1-O5-C5	-2.88	108.29	112.19
4	C	1302	NAG	O5-C5-C4	-2.73	104.18	110.83
4	B	1312	NAG	C1-O5-C5	2.67	115.81	112.19
4	B	1304	NAG	C1-C2-N2	2.61	114.95	110.49
4	A	1303	NAG	C2-N2-C7	2.59	126.59	122.90
4	C	1304	NAG	C3-C4-C5	2.39	114.51	110.24
4	C	1304	NAG	C4-C3-C2	-2.37	107.54	111.02
4	A	1303	NAG	C1-C2-N2	-2.22	106.69	110.49
4	B	1307	NAG	C2-N2-C7	2.20	126.04	122.90
4	C	1302	NAG	C3-C4-C5	-2.17	106.37	110.24
4	A	1312	NAG	C1-O5-C5	2.15	115.10	112.19
4	B	1313	NAG	C1-O5-C5	-2.03	109.44	112.19
4	C	1303	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1307	NAG	C3-C2-N2-C7
4	C	1306	NAG	C1-C2-N2-C7
4	A	1304	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	A	1314	NAG	O5-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	A	1301	NAG	C1-C2-N2-C7
4	C	1306	NAG	C4-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1305	NAG	O5-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	A	1313	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	A	1314	NAG	C4-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1313	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	B	1302	NAG	C1-C2-N2-C7
4	A	1303	NAG	C1-C2-N2-C7
4	A	1312	NAG	C1-C2-N2-C7
4	B	1308	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	B	1302	NAG	C3-C2-N2-C7
4	B	1304	NAG	C3-C2-N2-C7
4	B	1310	NAG	C3-C2-N2-C7
4	A	1307	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	B	1312	NAG	C1-C2-N2-C7
4	B	1301	NAG	O5-C5-C6-O6
4	A	1301	NAG	C3-C2-N2-C7
4	A	1307	NAG	C3-C2-N2-C7
4	B	1311	NAG	O5-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	C	1303	NAG	C1-C2-N2-C7
4	C	1301	NAG	C4-C5-C6-O6
4	A	1312	NAG	C3-C2-N2-C7
4	B	1312	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	C	1303	NAG	C3-C2-N2-C7

There are no ring outliers.

16 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1310	NAG	9	0
4	C	1303	NAG	1	0
4	B	1301	NAG	2	0
4	A	1302	NAG	2	0
4	A	1303	NAG	4	0
4	A	1301	NAG	4	0
4	C	1301	NAG	1	0
4	B	1307	NAG	7	0
4	B	1302	NAG	2	0
4	B	1305	NAG	2	0
4	B	1304	NAG	4	0
4	A	1306	NAG	2	0
4	A	1313	NAG	1	0
4	C	1306	NAG	2	0
4	C	1304	NAG	4	0
4	A	1309	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	A	3
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	332:ILE	C	333:THR	N	6.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	527:PRO	C	528:LYS	N	4.26
1	B	481:ASN	C	482:GLY	N	3.38
1	C	528:LYS	C	529:LYS	N	3.28
1	A	527:PRO	C	528:LYS	N	3.23
1	A	458:LYS	C	459[A]:SER	N	3.12
1	A	458:LYS	C	459[B]:SER	N	3.07

6 Map visualisation

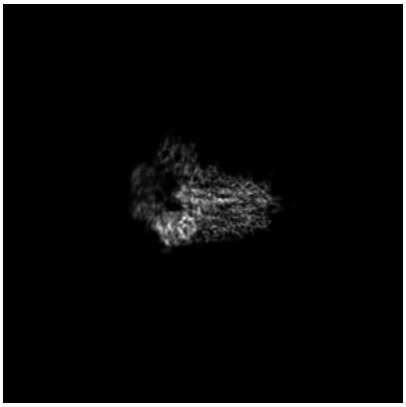
This section contains visualisations of the EMDB entry EMD-14314. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

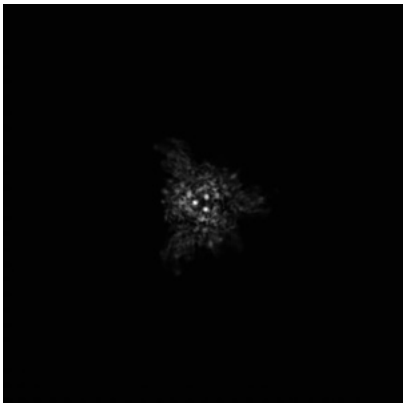
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



Z

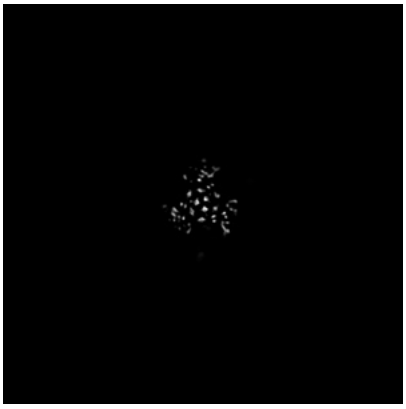
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 246

Y Index: 246



Z Index: 246

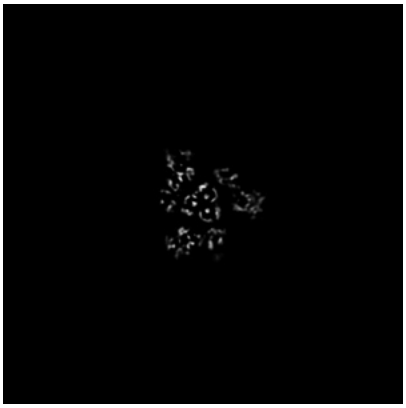
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 249

Y Index: 238



Z Index: 222

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

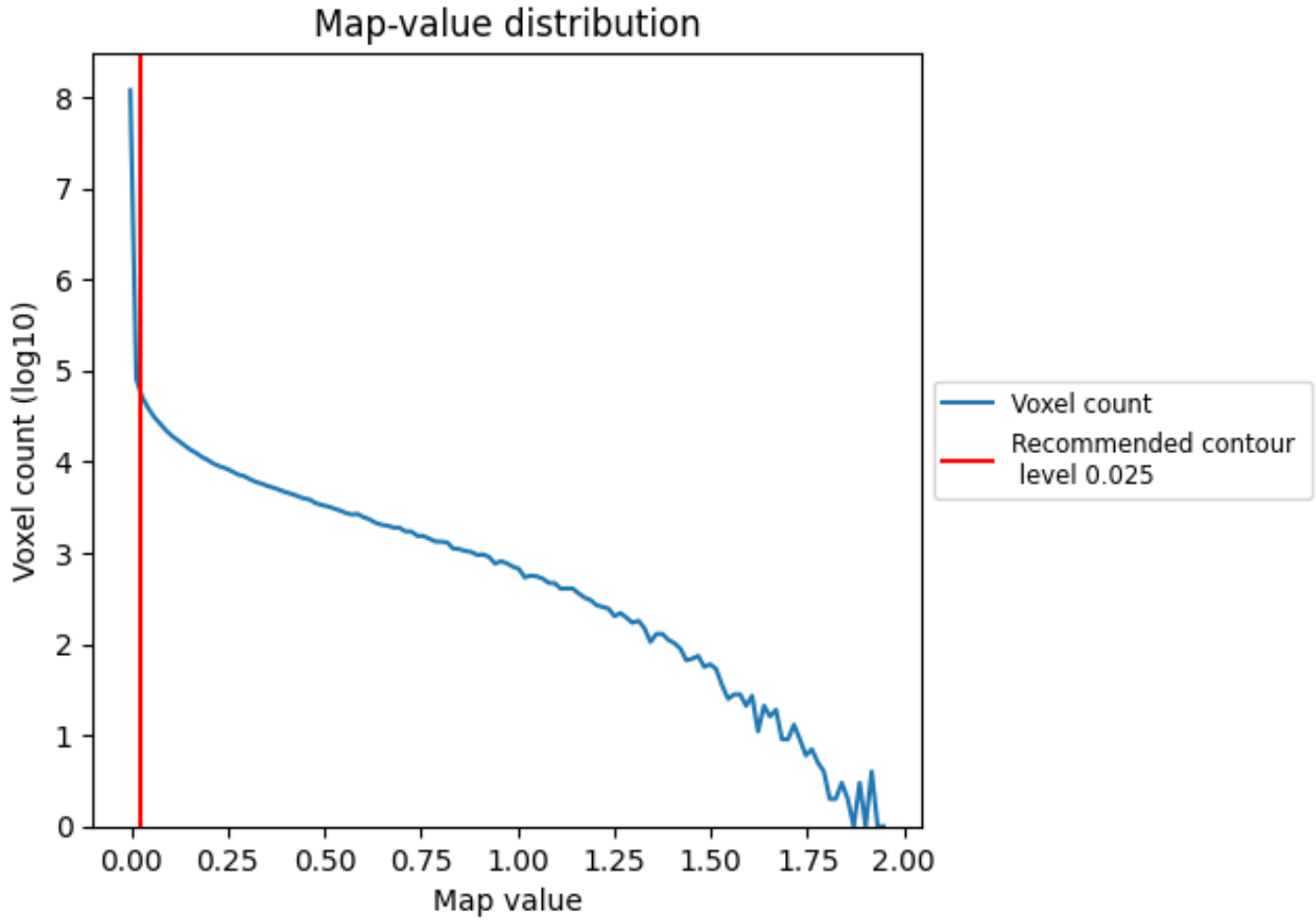
6.5 Mask visualisation (i)

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

7 Map analysis

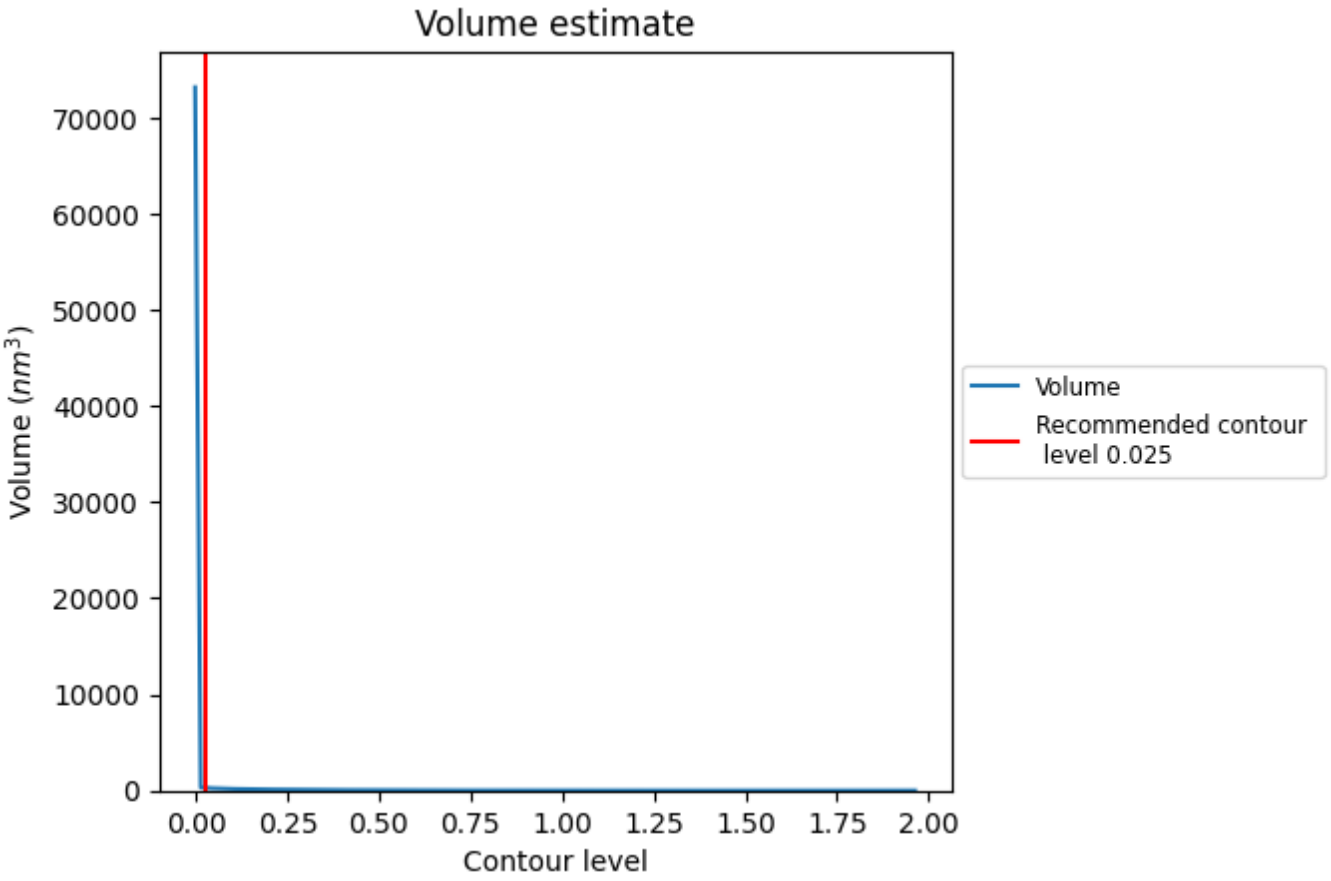
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

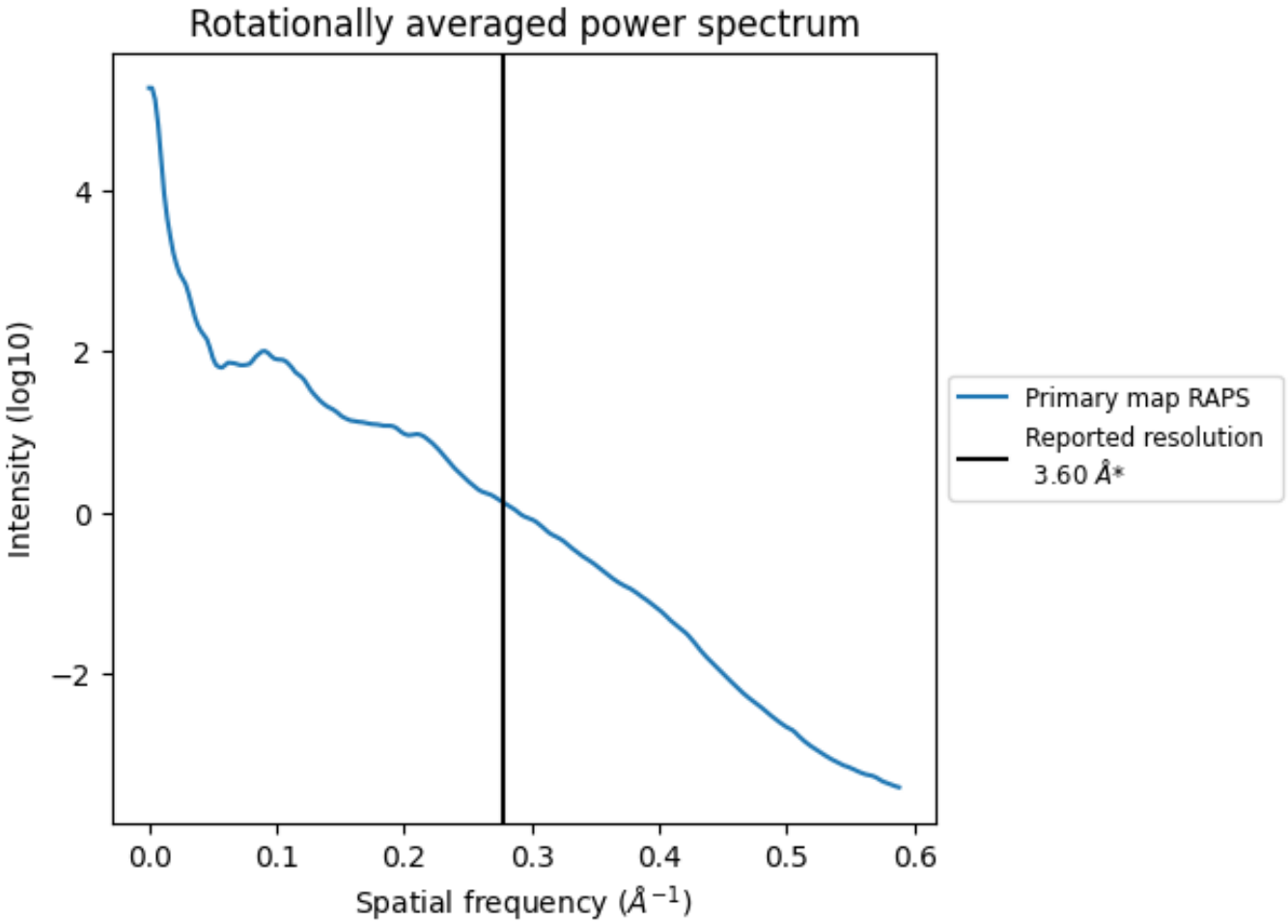
7.2 Volume estimate (i)



The volume at the recommended contour level is 284 nm^3; this corresponds to an approximate mass of 256 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)

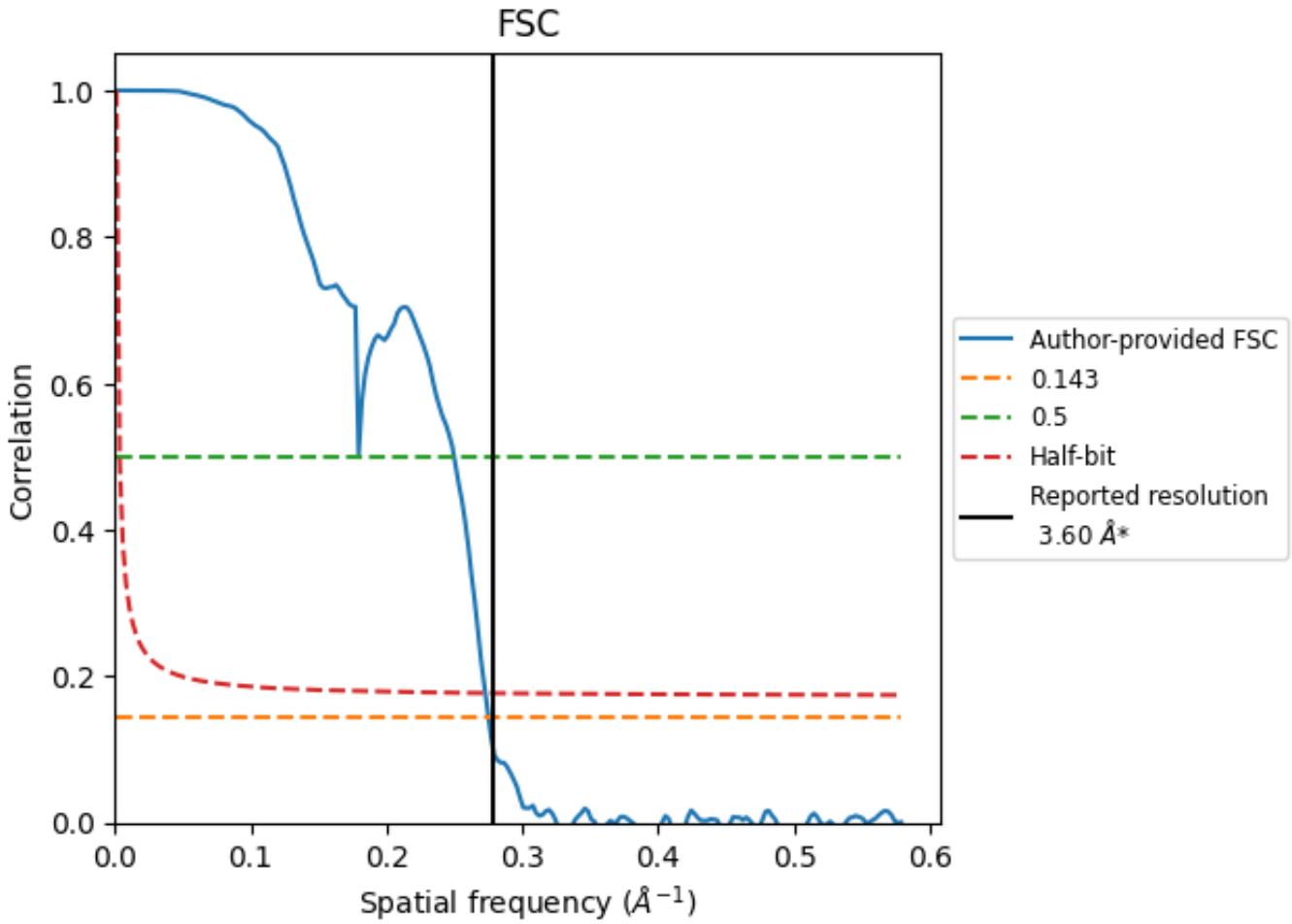


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

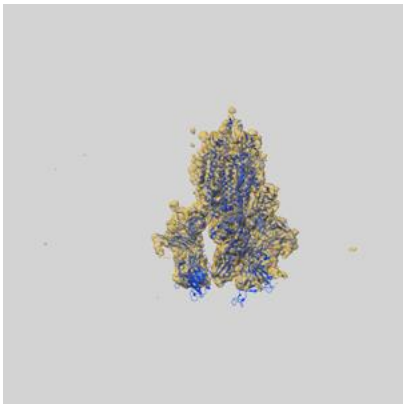
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.64	4.00	3.67
Unmasked-calculated*	-	-	-

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

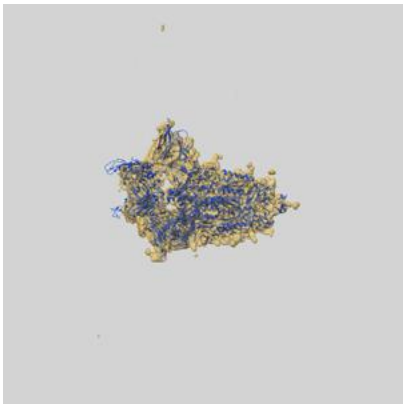
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14314 and PDB model 7R4Q. Per-residue inclusion information can be found in section 3 on page 12.

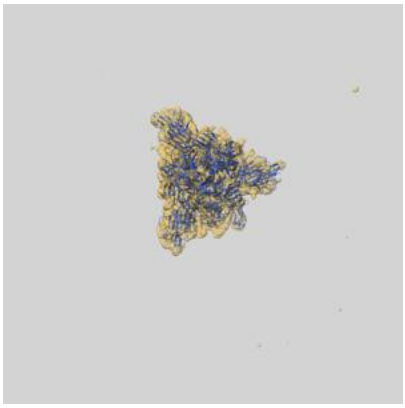
9.1 Map-model overlay



X



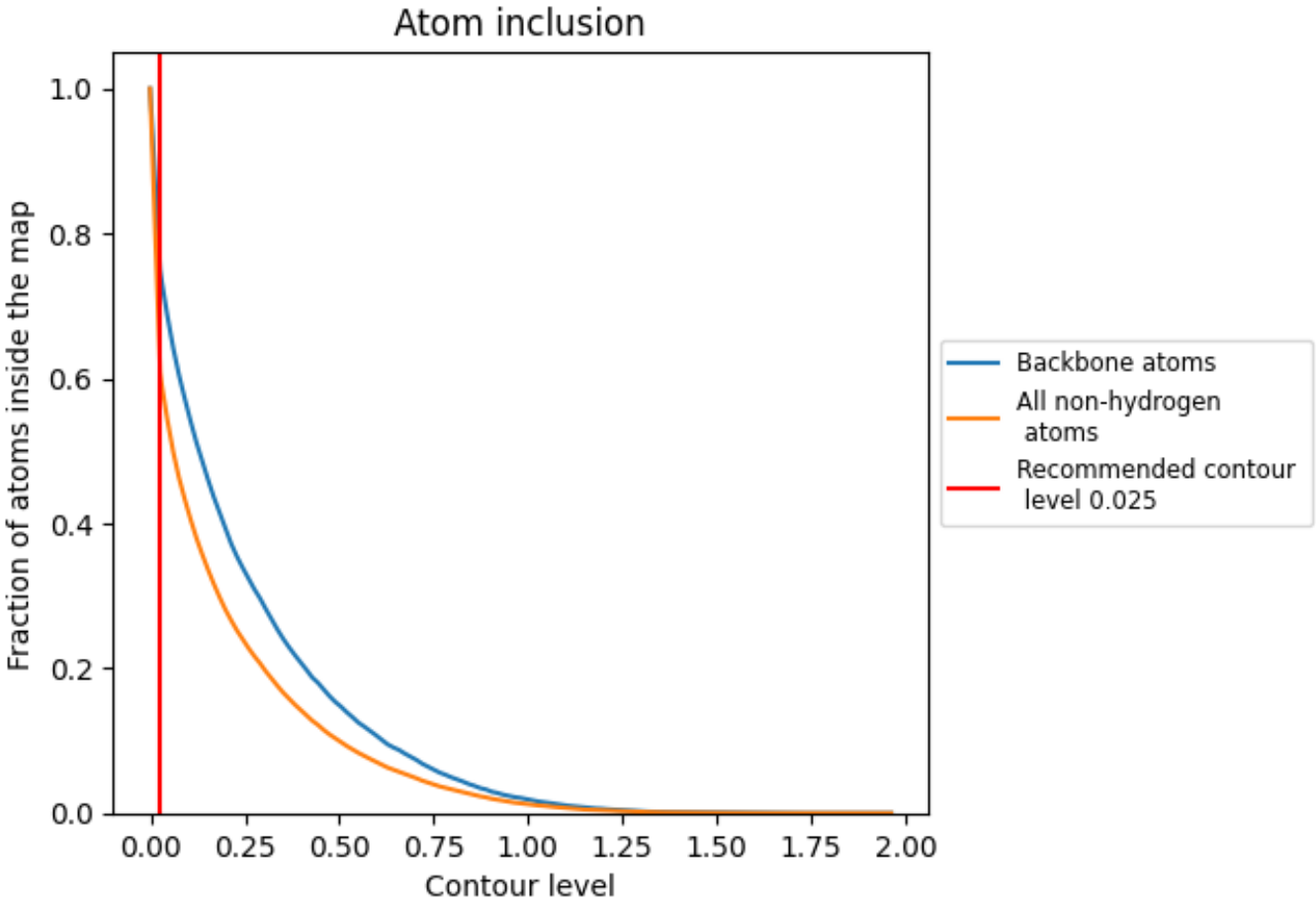
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.