Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 03:29 PM JST

PDB ID	:	6J8G
EMDB ID	:	EMD-9781
Title	:	Structure of human voltage-gated sodium channel Nav1.7 in complex with auxiliary beta subunits, huwentoxin-IV and saxitoxin (Y1755 up)
Authors	:	Shen, H.; Liu, D.; Lei, J.; Yan, N.
Deposited on	:	2019-01-19
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

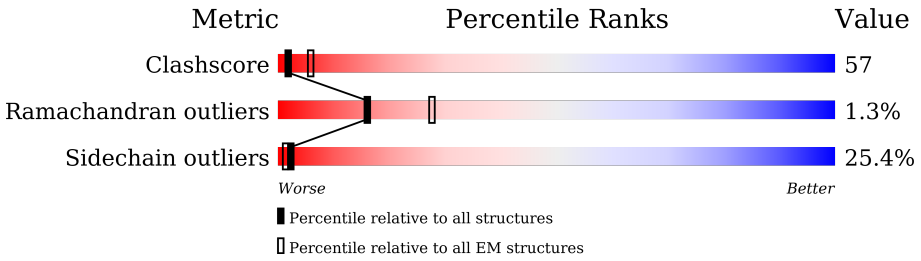
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	C	215	52% 30% 20% 5% 44%
2	A	2031	7% 20% 27% 9% 44%
3	B	218	6% 25% 38% 16% 21%
4	D	2	50% 100%
4	E	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11763 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	120	Total	C	N	O	S	0	0
			980	614	173	182	11		

- Molecule 2 is a protein called Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1140	Total	C	N	O	S	0	0
			9192	6110	1438	1568	76		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	406	LYS	GLU	variant	UNP Q15858

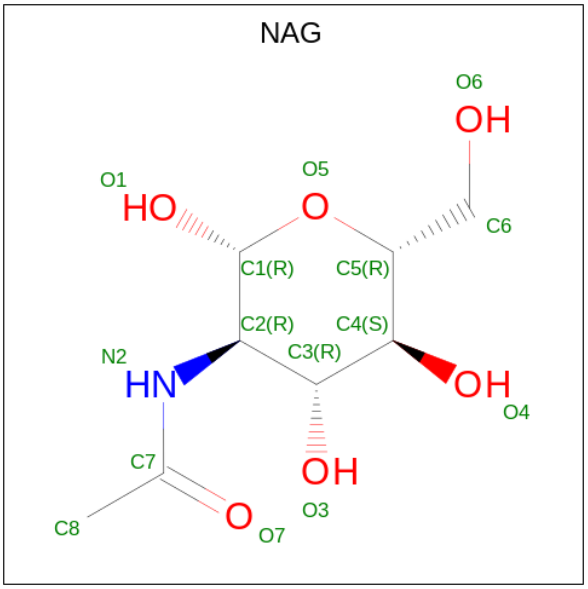
- Molecule 3 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

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

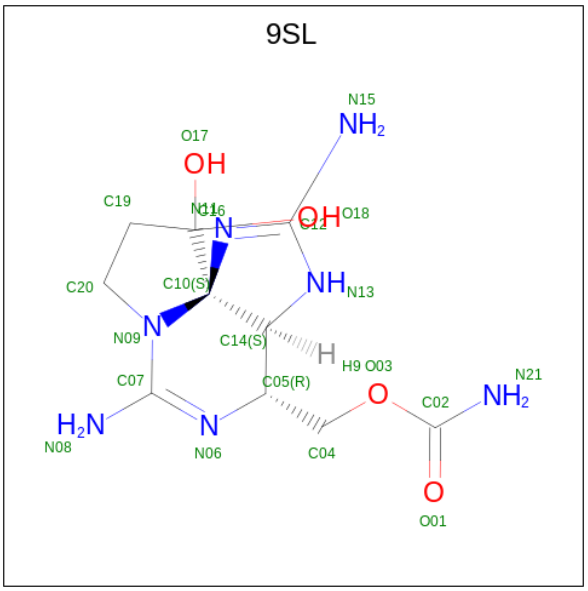
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	B	1	Total	C	N	O	0
			56	32	4	20	
5	B	1	Total	C	N	O	0
			56	32	4	20	
5	B	1	Total	C	N	O	0
			56	32	4	20	
5	B	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 6 is [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methyl carbamate (three-letter code: 9SL) (formula: $C_{10}H_{17}N_7O_4$).

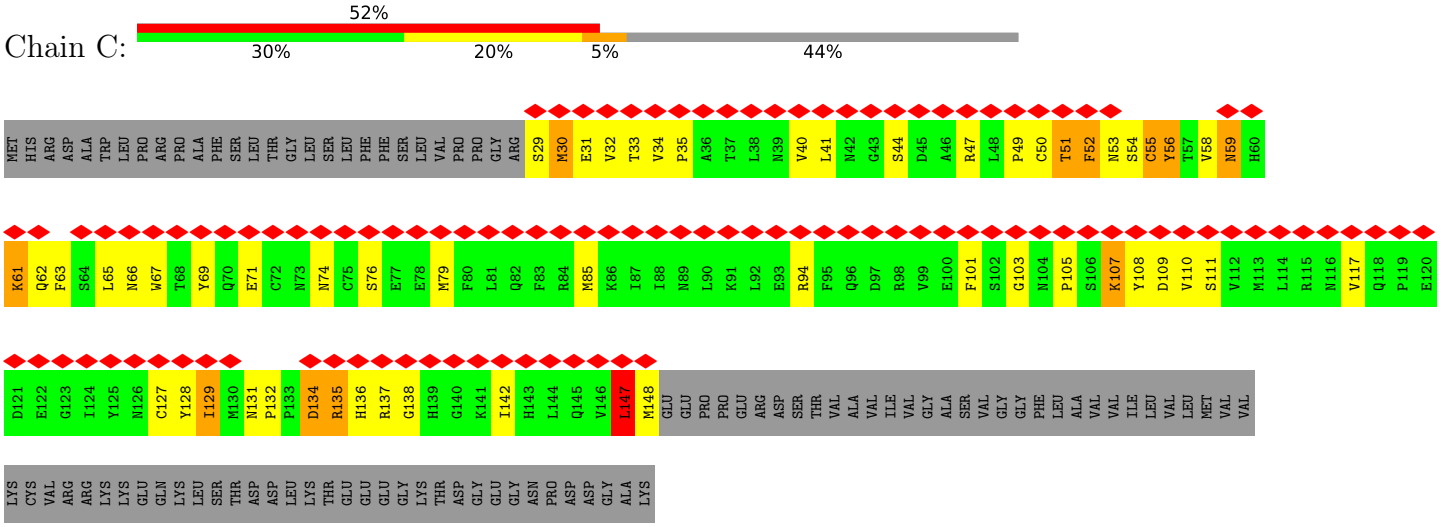


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	21	10	7	4	0

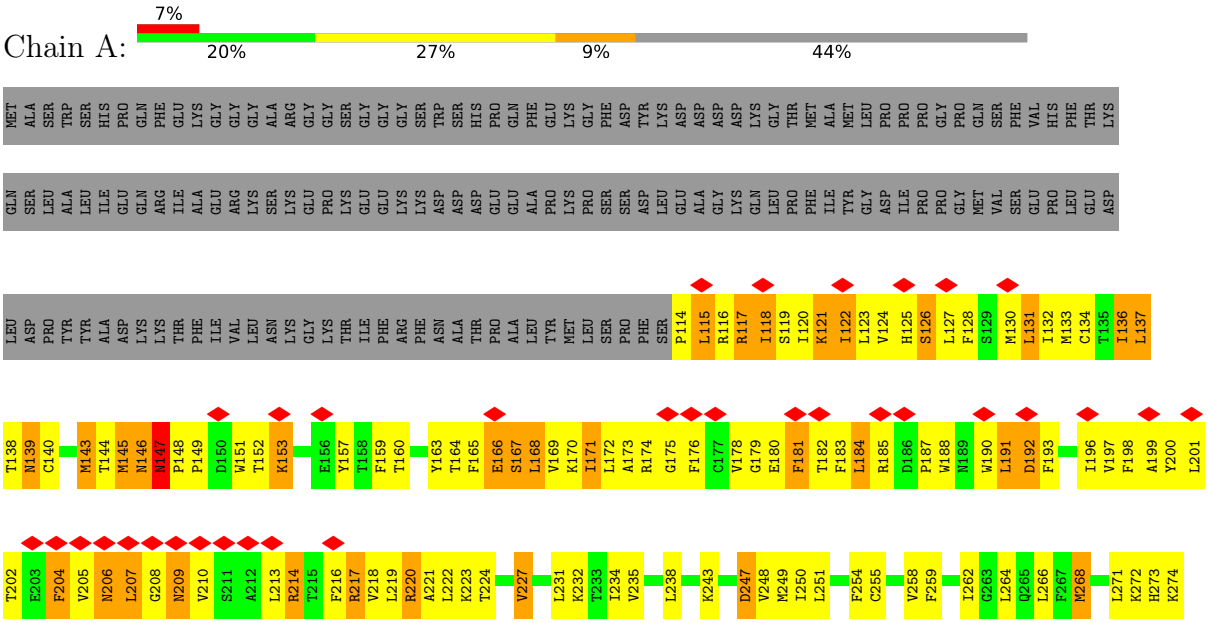
3 Residue-property plots (i)

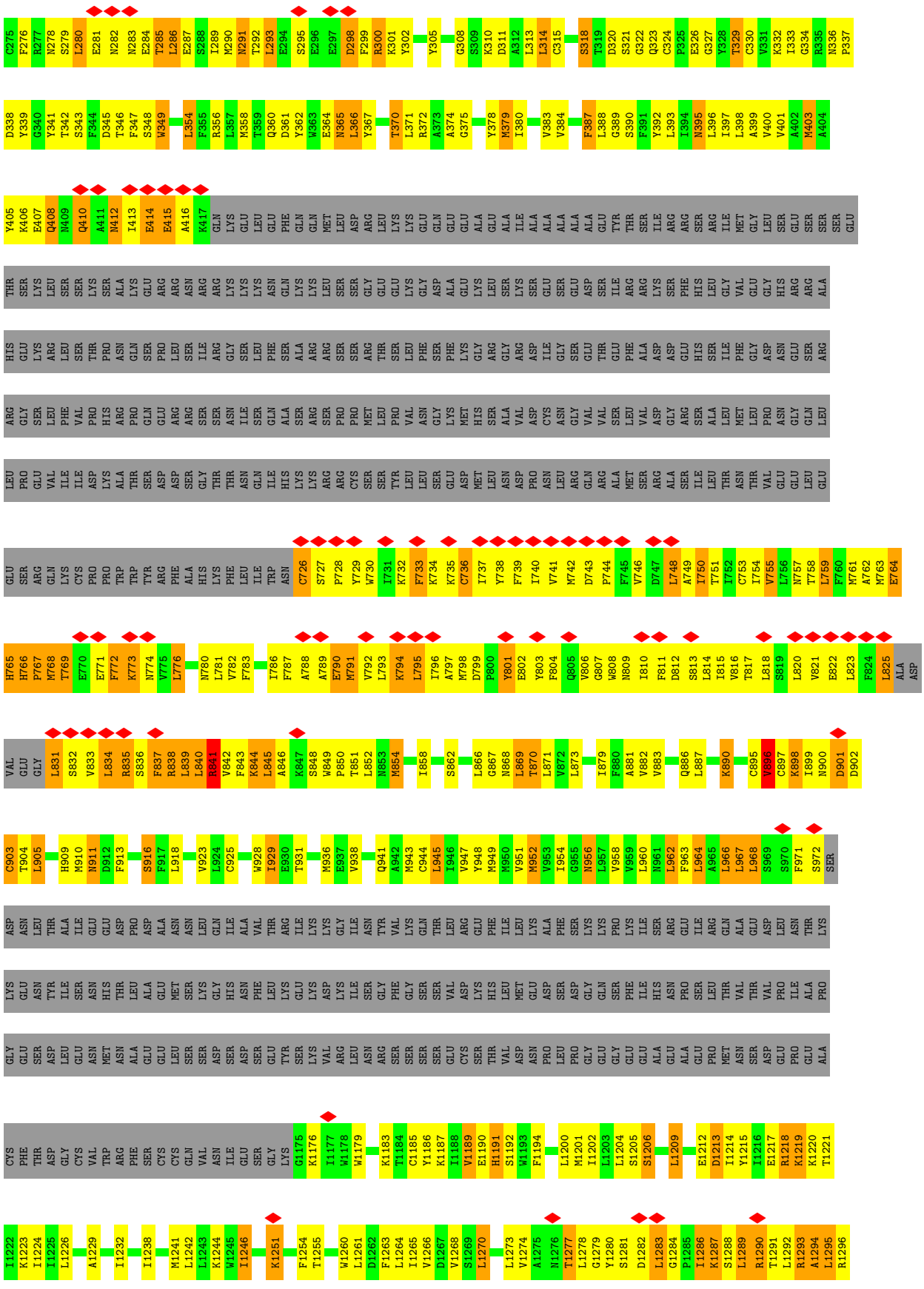
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

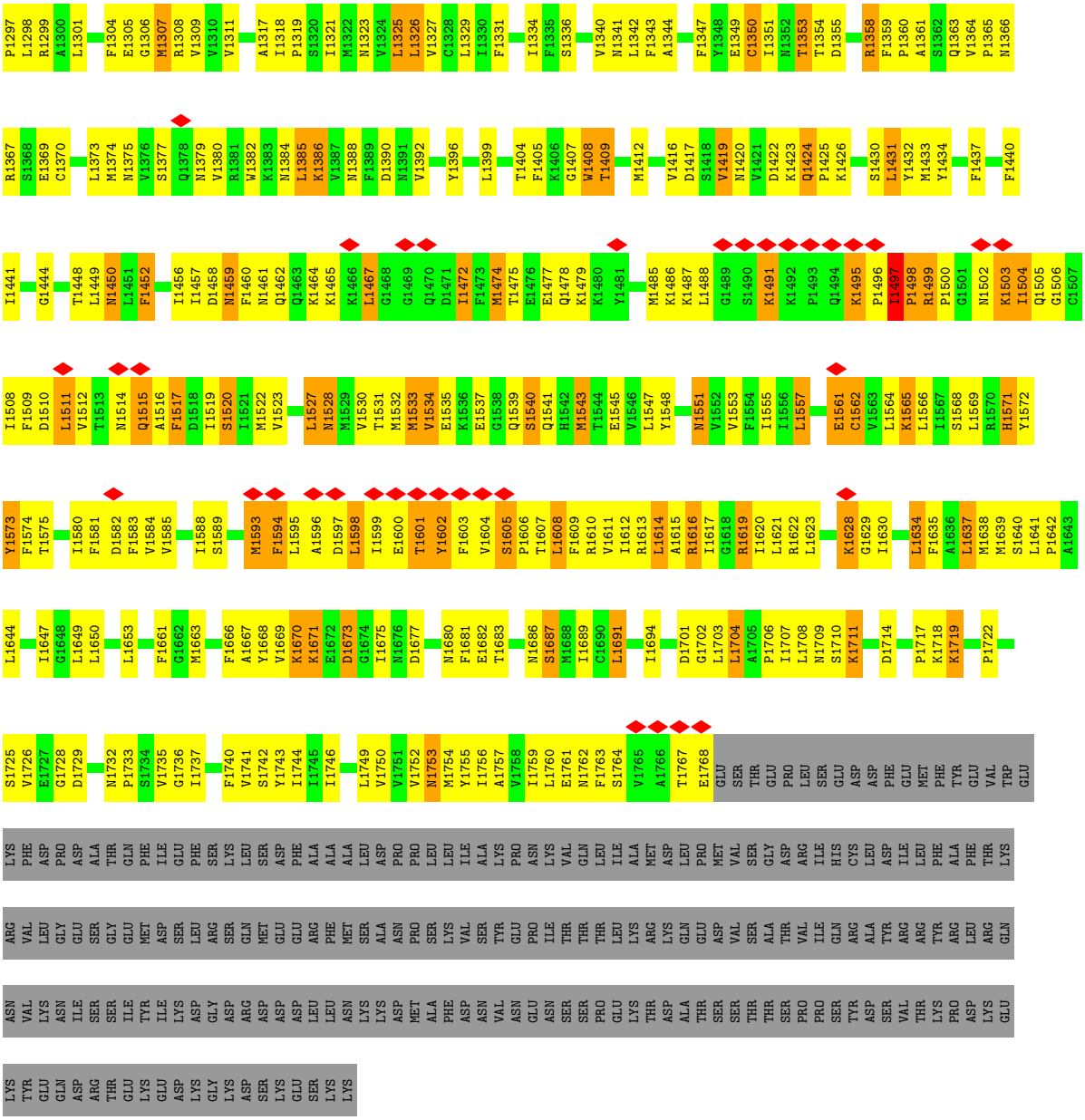
• Molecule 1: Sodium channel subunit beta-2



• Molecule 2: Sodium channel protein type 9 subunit alpha

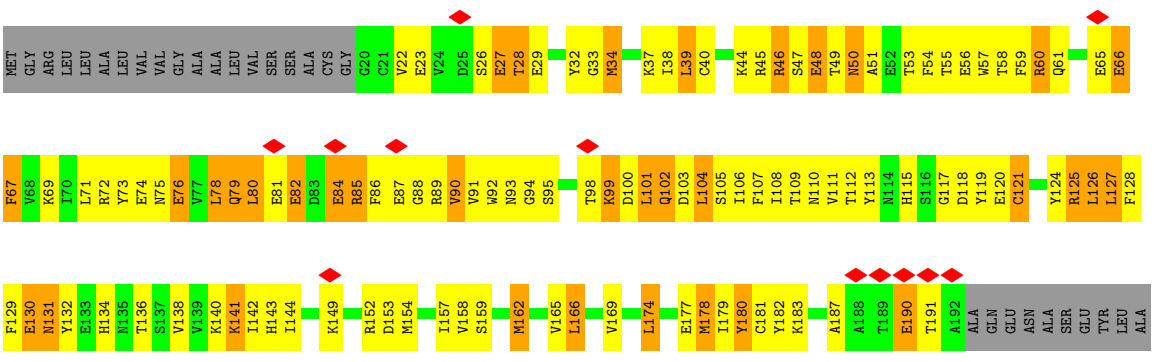



C275 F276 R277 N278 S279 L280 E281 N282 N283 E284 T285 L286 E287 S288 I289 M290 N291 T292 L293 E294 S295 E296 E297 D298 F299 R300 K301 Y302 Y305 G308 S309 K310 D311 A312 L313 L314 C315 S318 T319 D320 S321 G322 Q323 C324 P325 E326 G327 Y328 T329 C330 V331 K332 I333 G334 R335 N336 P337
D338 Y339 G340 Y341 T342 S343 F344 D345 T346 F347 S348 W349 L354 F355 R356 L357 M358 T359 Q360 D361 Y362 W363 E364 N365 L366 Y367 T370 L371 R372 A373 A374 G375 Y378 M379 I380 V383 V384 F387 L388 G389 S390 F391 Y392 L393 I394 N395 L396 I397 L398 A399 V400 V401 A402 M403 A404
Y405 K406 E407 Q408 N409 Q410 A411 N412 I413 E414 E415 A416 K417 GLN LYS GLU LEU GLU PHE GLN GLN MET LEU ASP ARG LEU LYS LYS GLU GLN GLU GLU ALA GLU ALA ILE ALA ALA ALA ALA ALA GLU GLU TYR THR SER ILE ARG ARG SER ARG ILE MET GLY LEU SER GLU SER SER GLU
THR SER LYS LEU SER SER LYS GLU ARG LYS LYS LYS LYS ASN GLN LYS LYS LEU SER SER GLY GLU GLU LYS LYS GLY ASP ALA GLU LYS LEU SER LYS SER GLU SER GLU ASP SER ILE ARG ARG LYS SER PHE HIS LEU GLY VAL GLU GLY HIS ARG ARG ALA
HIS GLU LYS ARG LEU SER THR PRO ASN GLN SER PRO LEU SER ILE ARG GLY SER LEU PHE SER ARG THR SER LEU PHE SER PHE LYS GLY ARG GLY ARG ASP ILE GLY SER GLU THR GLU PHE ALA ASP GLY HIS SER ILE PHE GLY ASP ASN GLU SER ARG
ARG GLY SER LEU PHE VAL PRO HIS ARG PRO GLN GLU GLU ARG ARG SER SER ASN ILE SER GLN ILE ALA SER ARG ARG SER PRO PRO MET LEU PRO VAL ASN GLY LYS MET HIS SER ALA VAL ASP CYS ASN GLY VAL VAL SER LEU VAL ASP GLY ARG SER ILE LEU ALA LEU MET LEU PRO ASN GLY GLN LEU
LEU PRO GLU VAL ILE ILE ASP LYS ALA THR SER ASP ASP SER GLY THR THR ASN GLN ILE HIS LYS LYS ARG ARG CYS SER SER TYR LEU LEU SER GLU ASP MET LEU ASN ASP PRO ASN LEU ARG GLN ARG ALA MET SER ARG ALA SER ILE LEU VAL GLU GLU LEU GLU
GLU SER ARG GLN LYS CYS PRO PRO TRP TRP TYR ARG PHE ALA HIS LYS PHE LEU ILE TRP ASN C726 S727 P728 Y729 W730 I731 K732 F733 K734 K735 C736 I737 Y738 F739 I740 V741 M742 D743 P744 F745 V746 D747 L748 A749 I750 T751 T752 C753 I754 V755 L756 N757 T758 L759 F760 M761 A762 M763 E764
H765 H766 P767 M768 T769 E770 E771 F772 K773 N774 V775 L776 N780 L781 V782 F783 I786 F787 A788 A789 E790 M791 V792 L793 K794 L795 I796 A797 M798 D799 P800 Y801 E802 Y803 F804 Q805 V806 G807 W808 N809 I810 F811 D812 S813 L814 I815 V816 T817 L818 S819 L820 V821 E822 L823 F824 L825 ALA ASP
VAL GLU GLY L831 S832 V833 L834 R835 S836 F837 R838 L839 L840 R841 V842 F843 K844 L845 A846 K847 S848 W849 P850 T851 L852 N853 M854 I858 S862 L866 G867 N868 L869 T870 L871 V872 L873 I879 F880 A881 V882 V883 Q886 L887 K890 C895 V896 C897 K898 I899 N900 D901 D902
C903 T904 L905 H909 M910 N911 D912 F913 S916 F917 L918 V923 L924 C925 W928 I929 E930 T931 M936 E937 V938 Q941 A942 M943 C944 L945 I946 V947 Y948 M949 M950 V951 M952 V953 I954 G955 N956 L957 V958 V959 L960 N961 L962 F963 L964 A965 L966 L967 L968 S969 S970 F971 S972 SER
ASP ASN LEU THR ALA ILE GLU GLU ASP PRO ASP ALA ASN ASN LEU GLN ILE ALA VAL THR ARG ILE LYS LYS GLY ILE ASN TYR VAL LYS GLN THR LEU ARG GLU GLU PHE ILE ILE LEU LYS ALA PHE SER LYS LYS ILE ARG GLN ALA GLU ASP LEU ASN THR LYS
LYS GLU ASN TYR ILE SER LEU HIS THR LEU ALA GLU MET SER LYS GLY HIS ASN PHE LEU LYS GLU LYS ASP LYS ILE SER GLY PHE GLY SER SER VAL ASP LYS HIS LEU MET GLU ASP SER ASP GLY GLN SER PHE ILE HIS ASN PRO SER LEU LEU THR VAL THR VAL PRO ILE ALA PRO
GLY GLU SER ASP LEU GLU GLU ASN MET ASN ALA GLU GLU LEU SER SER GLU GLY TYR SER LYS VAL ARG LEU ASN ARG SER SER SER SER GLU CYS SER THR VAL ASP ASN PRO LEU PRO GLY GLU GLY GLU GLU ALA GLU ALA GLU PRO MET ASN SER ASP GLU PRO GLU ALA
CYS PHE THR ASP GLY CYS VAL TRP ARG PHE SER CYS CYS GLN VAL ASN ILE GLU SER GLY LYS G1175 K1176 I1177 W1178 W1179 K1183 T1184 C1185 Y1186 K1187 I1188 V1189 E1190 H1191 S1192 W1193 F1194 L1200 M1201 I1202 L1203 L1204 S1205 S1206 L1209 E1212 D1213 I1214 Y1215 I1216 E1217 R1218 K1219 K1220 T1221
I1222 K1223 I1224 I1225 L1226 A1229 I1232 I1238 M1241 L1242 L1243 K1244 W1245 T1246 K1251 F1254 T1255 W1260 L1261 D1262 F1263 L1264 I1265 V1266 D1267 V1268 S1269 L1270 L1273 V1274 A1275 N1276 T1277 L1278 G1279 Y1280 S1281 D1282 L1283 G1284 P1285 I1286 K1287 S1288 L1289 R1290 T1291 L1292 R1293 A1294 L1295 R1296



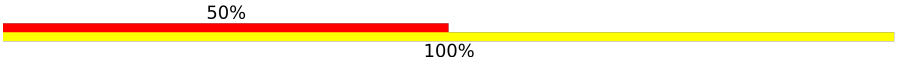
• Molecule 3: Sodium channel subunit beta-1

Chain B:



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

Chain D:



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

Chain E:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275630	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.410	Depositor
Minimum map value	-0.249	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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, 9SL

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	C	0.50	1/1002 (0.1%)	0.66	1/1354 (0.1%)
2	A	0.51	0/9417	0.65	5/12761 (0.0%)
3	B	0.45	0/1442	0.63	0/1949
All	All	0.50	1/11861 (0.0%)	0.65	6/16064 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	CYS	CB-SG	11.19	2.01	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	127	CYS	CA-CB-SG	7.87	128.16	114.00
2	A	925	CYS	N-CA-C	-6.16	94.36	111.00
2	A	766	HIS	C-N-CD	5.52	139.99	128.40
2	A	1279	GLY	N-CA-C	-5.33	99.77	113.10
2	A	1497	ILE	C-N-CD	5.14	139.20	128.40
2	A	302	TYR	N-CA-C	5.08	124.73	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	980	0	943	136	0
2	A	9192	0	9424	1049	0
3	B	1416	0	1379	173	0
4	D	28	0	25	0	0
4	E	28	0	25	6	0
5	A	28	0	26	2	0
5	B	56	0	52	0	0
5	C	14	0	13	4	0
6	A	21	0	0	2	0
All	All	11763	0	11887	1347	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 57.

All (1347) 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)
2:A:1497:ILE:HG23	2:A:1572:TYR:CD2	1.39	1.50
2:A:849:TRP:CD1	2:A:850:PRO:HD2	1.46	1.49
2:A:1694:ILE:CD1	2:A:1703:LEU:HD12	1.47	1.40
2:A:737:ILE:CG2	2:A:797:ALA:HB2	1.52	1.38
2:A:174:ARG:HD3	2:A:182:THR:CG2	1.55	1.37
1:C:65:LEU:CD1	1:C:110:VAL:HB	1.58	1.34
2:A:834:LEU:HD23	2:A:835:ARG:N	1.38	1.34
2:A:1694:ILE:HD11	2:A:1703:LEU:CD1	1.58	1.34
2:A:157:TYR:O	2:A:160:THR:HG22	1.20	1.33
2:A:1238:ILE:CD1	2:A:1270:LEU:HD23	1.59	1.32
2:A:849:TRP:HD1	2:A:850:PRO:CD	1.42	1.32
1:C:30:MET:HG3	1:C:138:GLY:CA	1.57	1.32
2:A:1497:ILE:CG2	2:A:1572:TYR:CD2	2.09	1.31
3:B:32:TYR:CD2	3:B:113:TYR:CE1	2.23	1.26
2:A:1496:PRO:O	2:A:1497:ILE:HD12	1.29	1.24
3:B:51:ALA:CB	3:B:127:LEU:HD12	1.66	1.24
2:A:179:GLY:O	2:A:180:GLU:HG2	1.31	1.24
2:A:1212:GLU:O	2:A:1663:MET:HE1	1.36	1.24
2:A:171:ILE:HG22	2:A:183:PHE:CE2	1.72	1.23
2:A:737:ILE:HB	2:A:797:ALA:CA	1.68	1.22
2:A:1238:ILE:HD11	2:A:1270:LEU:CD2	1.69	1.22
1:C:128:TYR:CD2	1:C:137:ARG:NH2	2.09	1.21
2:A:132:ILE:HD11	2:A:166:GLU:CB	1.68	1.20
2:A:839:LEU:O	2:A:842:VAL:HG23	1.41	1.20
2:A:293:LEU:HD12	2:A:298:ASP:CB	1.71	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:51:ALA:HB2	3:B:127:LEU:CD1	1.72	1.19
2:A:336:ASN:ND2	2:A:343:SER:HB3	1.56	1.19
2:A:737:ILE:CB	2:A:797:ALA:HB2	1.73	1.18
2:A:1732:ASN:HB3	2:A:1735:VAL:CG1	1.74	1.17
1:C:128:TYR:CD2	1:C:137:ARG:CZ	2.27	1.17
2:A:136:ILE:HD12	2:A:224:THR:HG22	1.22	1.17
2:A:293:LEU:CD1	2:A:298:ASP:HB3	1.72	1.17
2:A:174:ARG:HD3	2:A:182:THR:HG21	1.25	1.16
2:A:174:ARG:HB3	2:A:182:THR:HB	1.30	1.13
1:C:79:MET:HE1	5:C:301:NAG:C1	1.78	1.12
2:A:737:ILE:HB	2:A:797:ALA:HA	1.22	1.12
2:A:734:LYS:HE3	2:A:799:ASP:OD1	1.46	1.11
2:A:171:ILE:HG22	2:A:183:PHE:CD2	1.85	1.11
2:A:798:MET:HE2	2:A:803:TYR:HA	1.33	1.10
2:A:1502:ASN:HB3	2:A:1504:ILE:HD11	1.27	1.10
2:A:250:ILE:HG22	2:A:1630:ILE:HD11	1.28	1.10
2:A:149:PRO:O	2:A:152:THR:HG22	1.49	1.10
2:A:960:LEU:CD2	2:A:964:LEU:HD23	1.82	1.10
2:A:737:ILE:HB	2:A:797:ALA:CB	1.82	1.09
1:C:30:MET:SD	1:C:137:ARG:CA	2.41	1.09
2:A:794:LYS:HG2	2:A:803:TYR:CE1	1.87	1.08
2:A:1500:PRO:HG3	2:A:1505:GLN:HG2	1.13	1.08
2:A:794:LYS:HG2	2:A:803:TYR:HE1	0.97	1.08
3:B:32:TYR:CD2	3:B:113:TYR:HE1	1.64	1.08
2:A:810:ILE:O	2:A:814:LEU:HD12	1.53	1.08
3:B:60:ARG:HB3	3:B:66:GLU:O	1.53	1.08
2:A:795:LEU:HD11	2:A:803:TYR:CD2	1.89	1.08
2:A:174:ARG:CD	2:A:182:THR:HG22	1.83	1.07
2:A:822:GLU:OE2	2:A:835:ARG:HB2	1.54	1.07
2:A:960:LEU:HD23	2:A:964:LEU:HD23	1.34	1.06
2:A:1732:ASN:CB	2:A:1735:VAL:HG12	1.84	1.06
1:C:30:MET:SD	1:C:138:GLY:N	2.27	1.06
2:A:1283:LEU:HD23	2:A:1283:LEU:H	1.19	1.06
2:A:136:ILE:CD1	2:A:224:THR:HG22	1.84	1.06
2:A:1485:MET:HB3	2:A:1639:MET:HE3	1.37	1.06
3:B:51:ALA:CB	3:B:127:LEU:CD1	2.32	1.06
2:A:132:ILE:HD11	2:A:166:GLU:HB3	1.31	1.05
1:C:30:MET:HG3	1:C:138:GLY:N	1.70	1.05
2:A:174:ARG:CD	2:A:182:THR:CG2	2.33	1.05
2:A:132:ILE:HD12	2:A:166:GLU:OE2	1.55	1.05
2:A:1764:SER:O	2:A:1767:THR:HG22	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1541:GLN:OE1	2:A:1541:GLN:N	1.89	1.04
2:A:1498:PRO:CD	2:A:1572:TYR:CE2	2.40	1.04
2:A:1467:LEU:HD11	2:A:1472:ILE:HG23	1.40	1.04
2:A:1498:PRO:HD2	2:A:1572:TYR:HE2	1.21	1.04
3:B:54:PHE:CZ	3:B:124:TYR:HD2	1.76	1.04
1:C:65:LEU:HD11	1:C:110:VAL:HB	1.38	1.04
2:A:737:ILE:CG2	2:A:797:ALA:CB	2.35	1.04
1:C:101:PHE:CE2	1:C:103:GLY:O	2.11	1.03
2:A:737:ILE:HG22	2:A:797:ALA:HB2	1.05	1.03
2:A:1596:ALA:HB1	2:A:1609:PHE:CE2	1.93	1.03
2:A:1251:LYS:O	2:A:1255:THR:HG23	1.58	1.03
1:C:107:LYS:NZ	1:C:109:ASP:CB	2.20	1.03
2:A:795:LEU:CD1	2:A:803:TYR:CD2	2.41	1.03
1:C:107:LYS:HZ2	1:C:109:ASP:CB	1.70	1.03
2:A:737:ILE:HG22	2:A:797:ALA:CB	1.87	1.03
1:C:30:MET:SD	1:C:136:HIS:O	2.17	1.02
2:A:1412:MET:HE2	2:A:1434:TYR:HE1	1.22	1.02
1:C:63:PHE:HE2	1:C:105:PRO:HB3	1.21	1.02
2:A:214:ARG:O	2:A:217:ARG:CG	2.07	1.02
2:A:399:ALA:CB	2:A:1762:ASN:HD22	1.73	1.01
2:A:737:ILE:CB	2:A:797:ALA:CB	2.37	1.01
2:A:214:ARG:O	2:A:217:ARG:HG3	1.61	1.00
3:B:60:ARG:CB	3:B:66:GLU:O	2.09	1.00
3:B:39:LEU:HD23	3:B:105:SER:OG	1.60	1.00
2:A:1498:PRO:HD3	2:A:1572:TYR:CE2	1.97	1.00
3:B:54:PHE:CZ	3:B:124:TYR:CD2	2.50	0.99
2:A:336:ASN:ND2	2:A:343:SER:CB	2.26	0.99
1:C:65:LEU:CD1	1:C:110:VAL:CB	2.39	0.99
2:A:1502:ASN:HB3	2:A:1504:ILE:CD1	1.91	0.99
3:B:32:TYR:HD2	3:B:113:TYR:CE1	1.69	0.99
2:A:1496:PRO:O	2:A:1497:ILE:CD1	2.12	0.98
1:C:30:MET:CG	1:C:138:GLY:N	2.27	0.98
1:C:62:GLN:O	1:C:132:PRO:CD	2.11	0.98
3:B:34:MET:O	3:B:111:VAL:HG23	1.64	0.98
1:C:31:GLU:HB3	1:C:53:ASN:HB3	1.45	0.98
2:A:1497:ILE:CG2	2:A:1572:TYR:HD2	1.65	0.98
2:A:1374:MET:HG2	2:A:1380:VAL:HG13	1.46	0.97
2:A:1498:PRO:HD2	2:A:1572:TYR:CE2	2.00	0.97
2:A:133:MET:O	2:A:136:ILE:HG22	1.65	0.96
2:A:1498:PRO:CD	2:A:1572:TYR:HE2	1.77	0.96
2:A:157:TYR:O	2:A:160:THR:CG2	2.14	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1212:GLU:O	2:A:1663:MET:CE	2.14	0.96
1:C:52:PHE:O	1:C:108:TYR:HB3	1.63	0.96
2:A:798:MET:CE	2:A:803:TYR:HA	1.94	0.96
1:C:128:TYR:HD2	1:C:137:ARG:CZ	1.74	0.95
2:A:1694:ILE:CD1	2:A:1703:LEU:CD1	2.27	0.95
3:B:57:TRP:CZ3	3:B:142:ILE:HD12	2.00	0.95
2:A:399:ALA:HB1	2:A:1762:ASN:ND2	1.81	0.95
1:C:30:MET:SD	1:C:137:ARG:C	2.45	0.95
1:C:107:LYS:HZ2	1:C:109:ASP:HB3	1.29	0.95
2:A:399:ALA:CB	2:A:1762:ASN:ND2	2.30	0.95
2:A:1509:PHE:HB2	2:A:1568:SER:HB3	1.48	0.95
2:A:822:GLU:CD	2:A:835:ARG:NH2	2.21	0.94
3:B:32:TYR:CD2	3:B:113:TYR:CD1	2.56	0.94
2:A:1732:ASN:HB3	2:A:1735:VAL:HG12	0.95	0.94
1:C:30:MET:SD	1:C:137:ARG:HA	2.05	0.94
2:A:207:LEU:HD22	2:A:208:GLY:H	1.32	0.94
2:A:171:ILE:CG2	2:A:183:PHE:CE2	2.51	0.93
2:A:1238:ILE:CD1	2:A:1270:LEU:CD2	2.36	0.93
2:A:136:ILE:HD12	2:A:224:THR:CG2	1.97	0.93
2:A:148:PRO:HB2	2:A:152:THR:HG21	1.49	0.93
1:C:79:MET:CE	5:C:301:NAG:C1	2.45	0.93
2:A:164:THR:HG21	2:A:200:TYR:OH	1.67	0.92
1:C:52:PHE:HB2	1:C:129:ILE:HD13	1.51	0.92
2:A:132:ILE:HD11	2:A:166:GLU:HB2	1.51	0.92
2:A:1430:SER:O	2:A:1432:TYR:N	2.04	0.91
2:A:1500:PRO:CG	2:A:1505:GLN:HG2	1.99	0.91
2:A:838:ARG:HH11	2:A:838:ARG:HG3	1.35	0.91
2:A:967:LEU:CD2	2:A:968:LEU:HD13	2.01	0.91
3:B:57:TRP:CH2	3:B:142:ILE:CD1	2.54	0.91
1:C:30:MET:SD	1:C:136:HIS:C	2.49	0.91
2:A:207:LEU:HD22	2:A:208:GLY:N	1.85	0.91
2:A:1412:MET:HE2	2:A:1434:TYR:CE1	2.05	0.91
1:C:29:SER:N	1:C:136:HIS:CD2	2.39	0.90
2:A:136:ILE:CD1	2:A:224:THR:CG2	2.49	0.90
2:A:737:ILE:CB	2:A:797:ALA:CA	2.50	0.90
1:C:30:MET:HG3	1:C:138:GLY:HA2	1.53	0.90
1:C:135:ARG:HG2	1:C:135:ARG:HH21	1.36	0.90
1:C:62:GLN:O	1:C:132:PRO:HD3	1.71	0.90
2:A:813:SER:O	2:A:817:THR:HG23	1.72	0.90
2:A:834:LEU:HD23	2:A:835:ARG:H	1.00	0.90
2:A:1504:ILE:HD13	2:A:1504:ILE:H	1.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:117:ARG:HB3	2:A:117:ARG:HH11	1.35	0.89
2:A:1497:ILE:HG23	2:A:1572:TYR:CE2	2.06	0.89
3:B:60:ARG:NH2	3:B:118:ASP:OD2	2.05	0.89
2:A:360:GLN:NE2	2:A:390:SER:OG	2.05	0.89
2:A:794:LYS:CG	2:A:803:TYR:HE1	1.85	0.89
2:A:250:ILE:CG2	2:A:1630:ILE:HD11	2.03	0.88
2:A:834:LEU:CD2	2:A:835:ARG:N	2.33	0.88
1:C:59:ASN:CB	1:C:62:GLN:HB2	2.03	0.88
2:A:1284:GLY:O	2:A:1287:LYS:N	2.06	0.88
1:C:63:PHE:HE1	1:C:129:ILE:CG2	1.86	0.88
3:B:57:TRP:CZ3	3:B:142:ILE:CD1	2.55	0.88
1:C:34:VAL:HG12	1:C:50:CYS:SG	2.13	0.88
3:B:32:TYR:HD2	3:B:113:TYR:CD1	1.91	0.88
2:A:174:ARG:HD2	2:A:182:THR:HG22	1.56	0.88
2:A:378:TYR:OH	2:A:1610:ARG:NH1	2.06	0.88
2:A:321:SER:HB3	2:A:375:GLY:HA2	1.52	0.88
2:A:834:LEU:CD2	2:A:835:ARG:H	1.87	0.88
3:B:119:TYR:HB2	3:B:142:ILE:O	1.74	0.88
2:A:742:MET:HB2	2:A:746:VAL:HB	1.54	0.87
1:C:52:PHE:CB	1:C:129:ILE:HD13	2.03	0.87
2:A:822:GLU:CD	2:A:835:ARG:HH21	1.77	0.87
2:A:1581:PHE:O	2:A:1585:VAL:HG13	1.73	0.87
2:A:1639:MET:CE	2:A:1639:MET:HA	2.04	0.87
2:A:1290:ARG:HG2	2:A:1290:ARG:HH11	1.38	0.87
2:A:1596:ALA:HB1	2:A:1609:PHE:HE2	1.36	0.86
2:A:841:ARG:HG2	2:A:841:ARG:HH11	1.39	0.86
2:A:1218:ARG:O	2:A:1219:LYS:HG2	1.75	0.86
2:A:1452:PHE:O	2:A:1456:ILE:HD12	1.75	0.86
2:A:117:ARG:HH11	2:A:117:ARG:CB	1.87	0.86
2:A:895:CYS:O	2:A:897:CYS:N	2.09	0.86
1:C:69:TYR:HE2	1:C:94:ARG:NH1	1.74	0.85
2:A:862:SER:O	2:A:870:THR:HG21	1.76	0.85
2:A:168:LEU:HD23	2:A:169:VAL:N	1.92	0.85
2:A:1520:SER:O	2:A:1523:VAL:HG12	1.76	0.85
2:A:179:GLY:O	2:A:180:GLU:CG	2.22	0.85
2:A:207:LEU:HD12	2:A:213:LEU:HD23	1.59	0.85
2:A:1186:TYR:O	2:A:1190:GLU:HG2	1.75	0.85
2:A:132:ILE:HD12	2:A:166:GLU:CD	1.96	0.85
2:A:1457:ILE:HD12	2:A:1458:ASP:N	1.92	0.85
1:C:63:PHE:HE1	1:C:129:ILE:HG22	1.39	0.85
2:A:1384:ASN:OD1	2:A:1388:ASN:ND2	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1532:MET:SD	2:A:1620:ILE:HD11	2.17	0.85
1:C:29:SER:N	1:C:136:HIS:HD2	1.74	0.85
2:A:795:LEU:CD1	2:A:803:TYR:CG	2.59	0.85
2:A:1288:SER:O	2:A:1291:THR:HG22	1.75	0.84
1:C:65:LEU:HD12	1:C:110:VAL:CB	2.08	0.84
1:C:66:ASN:ND2	1:C:79:MET:CE	2.39	0.84
2:A:214:ARG:O	2:A:217:ARG:HG2	1.76	0.84
2:A:1582:ASP:O	2:A:1585:VAL:HG22	1.77	0.84
2:A:1229:ALA:O	2:A:1232:ILE:HG22	1.76	0.84
2:A:1457:ILE:HG22	2:A:1756:ILE:CD1	2.07	0.84
2:A:276:PHE:CZ	2:A:280:LEU:HD21	2.12	0.84
1:C:33:THR:O	1:C:50:CYS:HA	1.79	0.83
3:B:46:ARG:HD3	3:B:48:GLU:OE2	1.78	0.83
1:C:63:PHE:CE2	1:C:105:PRO:HB3	2.09	0.83
2:A:1613:ARG:O	2:A:1616:ARG:HG2	1.76	0.83
2:A:1295:LEU:HD12	2:A:1298:LEU:HD22	1.60	0.83
2:A:1717:PRO:O	2:A:1728:GLY:HA3	1.79	0.83
3:B:85:ARG:HG2	3:B:85:ARG:HH11	1.43	0.83
2:A:736:CYS:O	2:A:740:ILE:HG12	1.78	0.83
2:A:869:LEU:HD12	2:A:869:LEU:O	1.78	0.83
2:A:1412:MET:CE	2:A:1434:TYR:CE1	2.62	0.83
2:A:1497:ILE:HG23	2:A:1572:TYR:CG	2.14	0.83
1:C:66:ASN:ND2	1:C:79:MET:HE1	1.93	0.83
2:A:119:SER:O	2:A:122:ILE:HG22	1.79	0.82
3:B:34:MET:O	3:B:111:VAL:CG2	2.26	0.82
2:A:188:TRP:CD1	2:A:232:LYS:CE	2.61	0.82
2:A:1574:PHE:HD1	2:A:1580:ILE:HD11	1.45	0.82
2:A:1522:MET:HE1	2:A:1623:LEU:CD2	2.10	0.82
1:C:30:MET:HG3	1:C:138:GLY:HA3	1.56	0.82
2:A:179:GLY:C	2:A:180:GLU:HG2	2.00	0.82
2:A:834:LEU:O	2:A:837:PHE:HB2	1.79	0.82
3:B:72:ARG:HH22	3:B:74:GLU:CD	1.81	0.82
1:C:65:LEU:HD12	1:C:110:VAL:HB	1.61	0.82
2:A:366:LEU:O	2:A:370:THR:HG23	1.79	0.82
2:A:1457:ILE:HG22	2:A:1756:ILE:HD11	1.61	0.81
4:E:1:NAG:H3	4:E:1:NAG:H83	1.61	0.81
2:A:399:ALA:HB1	2:A:1762:ASN:HD22	1.41	0.81
2:A:300:ARG:HH22	2:A:308:GLY:H	1.28	0.81
3:B:54:PHE:CE1	3:B:124:TYR:HD2	1.97	0.81
2:A:300:ARG:HH11	2:A:300:ARG:HG2	1.45	0.81
2:A:1607:THR:HG23	2:A:1610:ARG:HH11	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:734:LYS:NZ	2:A:799:ASP:OD2	2.13	0.81
2:A:737:ILE:HG21	2:A:797:ALA:N	1.95	0.81
2:A:1460:PHE:HZ	2:A:1753:ASN:HD21	1.27	0.81
2:A:145:MET:HE2	2:A:145:MET:HA	1.60	0.81
2:A:410:GLN:O	2:A:413:ILE:HG22	1.80	0.81
4:E:2:NAG:O7	4:E:2:NAG:O3	1.98	0.81
2:A:1639:MET:HA	2:A:1639:MET:HE2	1.64	0.80
3:B:51:ALA:HB2	3:B:127:LEU:HD12	0.84	0.80
1:C:107:LYS:NZ	1:C:109:ASP:HB2	1.95	0.80
2:A:132:ILE:CD1	2:A:166:GLU:CB	2.56	0.80
2:A:327:GLY:O	3:B:132:TYR:HE2	1.64	0.80
2:A:835:ARG:HH21	2:A:835:ARG:HG3	1.46	0.80
1:C:107:LYS:NZ	1:C:109:ASP:CG	2.34	0.80
3:B:85:ARG:O	3:B:115:HIS:HE1	1.63	0.80
2:A:281:GLU:O	2:A:284:GLU:HG3	1.82	0.80
3:B:57:TRP:HZ3	3:B:142:ILE:HD12	1.44	0.80
3:B:67:PHE:CE2	3:B:120:GLU:HG3	2.16	0.80
2:A:807:GLY:O	2:A:810:ILE:HG13	1.81	0.80
2:A:1522:MET:CE	2:A:1623:LEU:CD2	2.59	0.80
1:C:128:TYR:CG	1:C:137:ARG:NH2	2.49	0.80
2:A:412:ASN:O	2:A:415:GLU:HG3	1.82	0.80
2:A:1485:MET:HB3	2:A:1639:MET:CE	2.12	0.80
3:B:39:LEU:CD2	3:B:105:SER:OG	2.29	0.80
1:C:47:ARG:O	1:C:49:PRO:HD3	1.81	0.80
2:A:293:LEU:HD12	2:A:298:ASP:HB3	0.86	0.79
2:A:163:TYR:HA	2:A:166:GLU:HG2	1.64	0.79
2:A:116:ARG:HH12	2:A:176:PHE:CB	1.95	0.79
2:A:196:ILE:HD12	2:A:197:VAL:N	1.97	0.79
2:A:1293:ARG:CB	2:A:1293:ARG:HH21	1.94	0.79
2:A:1270:LEU:HD13	2:A:1270:LEU:O	1.83	0.79
2:A:188:TRP:CD1	2:A:232:LYS:HE3	2.18	0.79
1:C:33:THR:O	1:C:51:THR:N	2.15	0.78
2:A:160:THR:O	2:A:164:THR:HG23	1.83	0.78
2:A:1467:LEU:HD11	2:A:1472:ILE:CG2	2.12	0.78
2:A:315:CYS:HB3	2:A:324:CYS:SG	2.24	0.78
2:A:199:ALA:O	2:A:202:THR:HG22	1.84	0.78
2:A:795:LEU:HD12	2:A:803:TYR:CG	2.18	0.78
1:C:33:THR:HB	1:C:51:THR:CB	2.14	0.78
2:A:879:ILE:O	2:A:883:VAL:HG23	1.84	0.78
2:A:1709:ASN:HB2	2:A:1714:ASP:HB3	1.66	0.78
1:C:59:ASN:HB2	1:C:62:GLN:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:895:CYS:CB	2:A:938:VAL:HG12	2.15	0.77
2:A:1595:LEU:O	2:A:1599:ILE:HG13	1.83	0.77
2:A:1509:PHE:CB	2:A:1568:SER:HB3	2.14	0.77
1:C:62:GLN:O	1:C:132:PRO:HD2	1.85	0.77
2:A:1755:TYR:O	2:A:1759:ILE:HG12	1.84	0.77
2:A:1637:LEU:HD22	2:A:1637:LEU:O	1.84	0.77
1:C:69:TYR:CE2	1:C:94:ARG:NH1	2.52	0.77
2:A:1677:ASP:OD2	3:B:46:ARG:NH1	2.18	0.77
2:A:136:ILE:HD13	2:A:136:ILE:O	1.84	0.77
4:E:1:NAG:H3	4:E:1:NAG:C8	2.14	0.77
2:A:765:HIS:HB2	2:A:767:PRO:HD2	1.65	0.77
3:B:51:ALA:HB1	3:B:126:LEU:O	1.85	0.77
3:B:92:TRP:CE2	3:B:94:GLY:HA3	2.20	0.77
2:A:116:ARG:HH12	2:A:176:PHE:HB2	1.48	0.77
2:A:207:LEU:HD12	2:A:213:LEU:CD2	2.14	0.76
2:A:321:SER:HB3	2:A:375:GLY:CA	2.15	0.76
1:C:52:PHE:HB2	1:C:129:ILE:CD1	2.15	0.76
1:C:107:LYS:HD2	1:C:109:ASP:HB2	1.67	0.76
2:A:336:ASN:CG	2:A:343:SER:OG	2.24	0.76
1:C:59:ASN:HB3	1:C:62:GLN:HB2	1.68	0.76
2:A:131:LEU:HD22	2:A:131:LEU:O	1.84	0.76
1:C:107:LYS:HZ3	1:C:109:ASP:CB	1.97	0.76
3:B:32:TYR:CE2	3:B:113:TYR:CD1	2.74	0.76
2:A:851:THR:HG22	2:A:1327:VAL:HG21	1.66	0.76
3:B:71:LEU:HD21	3:B:106:ILE:HD12	1.68	0.76
2:A:188:TRP:CD1	2:A:232:LYS:HE2	2.20	0.76
2:A:806:VAL:CG2	2:A:809:ASN:HB2	2.16	0.76
1:C:31:GLU:O	1:C:52:PHE:HA	1.85	0.75
2:A:395:ASN:ND2	2:A:1755:TYR:CE1	2.53	0.75
2:A:1374:MET:CG	2:A:1380:VAL:HG13	2.15	0.75
1:C:65:LEU:HD13	1:C:110:VAL:HB	1.67	0.75
2:A:1522:MET:CE	2:A:1623:LEU:HD23	2.16	0.75
3:B:76:GLU:OE2	3:B:76:GLU:HA	1.86	0.75
2:A:737:ILE:CB	2:A:797:ALA:HA	2.09	0.75
3:B:32:TYR:CE2	3:B:113:TYR:CE1	2.74	0.75
1:C:32:VAL:HA	1:C:51:THR:O	1.86	0.75
1:C:107:LYS:HZ3	1:C:109:ASP:CG	1.89	0.75
2:A:755:VAL:O	2:A:758:THR:HG22	1.87	0.75
2:A:1499:ARG:HG2	2:A:1509:PHE:CE1	2.22	0.75
3:B:72:ARG:NH2	3:B:74:GLU:OE2	2.20	0.75
1:C:135:ARG:HG2	1:C:135:ARG:NH2	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:407:GLU:HG3	2:A:408:GLN:N	2.02	0.75
2:A:909:HIS:HD2	2:A:911:ASN:H	1.34	0.75
2:A:217:ARG:HB3	2:A:217:ARG:NH1	2.00	0.75
2:A:1290:ARG:HG2	2:A:1290:ARG:NH1	1.99	0.75
3:B:126:LEU:HD13	3:B:128:PHE:CZ	2.22	0.75
1:C:63:PHE:CE1	1:C:129:ILE:CG2	2.70	0.74
1:C:103:GLY:O	1:C:105:PRO:HD3	1.87	0.74
2:A:960:LEU:HD21	2:A:964:LEU:HD23	1.68	0.74
3:B:58:THR:HG22	3:B:69:LYS:HA	1.67	0.74
2:A:395:ASN:ND2	2:A:1755:TYR:CZ	2.55	0.74
1:C:58:VAL:HG13	1:C:63:PHE:HB2	1.69	0.74
2:A:1295:LEU:HD12	2:A:1298:LEU:CD2	2.17	0.74
2:A:210:VAL:O	2:A:214:ARG:HG2	1.87	0.74
2:A:1503:LYS:CD	2:A:1503:LYS:H	2.00	0.74
2:A:1497:ILE:HG21	2:A:1572:TYR:HD2	1.53	0.74
1:C:30:MET:SD	1:C:137:ARG:N	2.61	0.74
2:A:1467:LEU:HD21	2:A:1472:ILE:CG2	2.18	0.74
2:A:1588:ILE:HG22	2:A:1615:ALA:HB1	1.70	0.74
2:A:896:VAL:O	2:A:899:ILE:HG12	1.87	0.74
2:A:838:ARG:HG3	2:A:838:ARG:NH1	2.03	0.74
2:A:1504:ILE:HG12	2:A:1505:GLN:N	2.03	0.73
2:A:118:ILE:HD13	2:A:118:ILE:N	2.04	0.73
2:A:167:SER:O	2:A:171:ILE:HG23	1.88	0.73
2:A:174:ARG:CB	2:A:182:THR:HB	2.16	0.73
2:A:116:ARG:HH12	2:A:176:PHE:CA	2.00	0.73
2:A:831:LEU:O	2:A:834:LEU:HD22	1.88	0.73
1:C:101:PHE:HE2	1:C:103:GLY:O	1.69	0.73
2:A:835:ARG:NH2	2:A:835:ARG:HG3	2.00	0.73
2:A:1283:LEU:H	2:A:1283:LEU:CD2	1.99	0.73
2:A:1504:ILE:HD13	2:A:1504:ILE:N	2.03	0.73
2:A:1430:SER:HB3	2:A:1433:MET:HG2	1.70	0.72
2:A:1531:THR:O	2:A:1534:VAL:CG2	2.37	0.72
3:B:152:ARG:HG2	3:B:157:ILE:HG13	1.71	0.72
1:C:65:LEU:HD12	1:C:110:VAL:CG1	2.19	0.72
1:C:71:GLU:HG3	1:C:94:ARG:HH12	1.53	0.72
2:A:395:ASN:OD1	2:A:1755:TYR:CD1	2.41	0.72
2:A:1598:LEU:O	2:A:1601:THR:HG23	1.88	0.72
2:A:735:LYS:HD2	2:A:735:LYS:O	1.89	0.72
2:A:410:GLN:HE21	2:A:410:GLN:C	1.92	0.72
2:A:415:GLU:OE2	2:A:416:ALA:N	2.22	0.72
2:A:1336:SER:O	2:A:1340:VAL:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:60:ARG:HB2	3:B:66:GLU:O	1.88	0.72
1:C:41:LEU:HD23	1:C:147:LEU:HB3	1.71	0.72
2:A:116:ARG:NH1	2:A:176:PHE:HB2	2.05	0.72
2:A:318:SER:HB2	2:A:320:ASP:OD1	1.89	0.72
2:A:1597:ASP:O	2:A:1601:THR:HG22	1.90	0.72
3:B:85:ARG:O	3:B:115:HIS:CE1	2.43	0.72
2:A:1304:PHE:HD2	2:A:1307:MET:CE	2.01	0.72
1:C:79:MET:HE2	5:C:301:NAG:O5	1.90	0.72
2:A:787:PHE:CD1	2:A:841:ARG:NH1	2.57	0.72
2:A:1375:ASN:OD1	5:A:2005:NAG:O5	2.03	0.72
3:B:92:TRP:CZ2	3:B:94:GLY:HA3	2.24	0.72
2:A:1474:MET:CE	2:A:1642:PRO:HB2	2.19	0.72
1:C:33:THR:HB	1:C:51:THR:OG1	1.90	0.71
3:B:54:PHE:CE2	3:B:124:TYR:HB2	2.25	0.71
3:B:104:LEU:N	3:B:104:LEU:HD22	2.05	0.71
2:A:1295:LEU:CD1	2:A:1298:LEU:HD22	2.21	0.71
2:A:1365:PRO:O	2:A:1424:GLN:HB3	1.91	0.71
2:A:841:ARG:HG2	2:A:841:ARG:NH1	2.04	0.71
2:A:399:ALA:HB3	2:A:1762:ASN:ND2	2.05	0.71
2:A:1273:LEU:HD12	2:A:1273:LEU:O	1.91	0.71
2:A:117:ARG:HA	2:A:120:ILE:HG22	1.73	0.71
2:A:822:GLU:CG	2:A:835:ARG:HH22	2.04	0.71
2:A:960:LEU:CD2	2:A:964:LEU:CD2	2.66	0.71
2:A:1504:ILE:CD1	2:A:1504:ILE:H	2.04	0.71
2:A:145:MET:HA	2:A:145:MET:CE	2.19	0.70
2:A:388:LEU:O	2:A:392:TYR:HB3	1.91	0.70
2:A:795:LEU:HD11	2:A:803:TYR:CE2	2.26	0.70
2:A:1261:LEU:O	2:A:1265:ILE:HG13	1.91	0.70
2:A:1317:ALA:O	2:A:1321:ILE:HG12	1.91	0.70
2:A:181:PHE:O	2:A:185:ARG:HG2	1.91	0.70
1:C:107:LYS:NZ	1:C:109:ASP:OD2	2.24	0.70
2:A:798:MET:HE2	2:A:803:TYR:CA	2.19	0.70
2:A:902:ASP:O	2:A:903:CYS:HB2	1.90	0.70
2:A:1485:MET:SD	2:A:1639:MET:HE1	2.31	0.70
2:A:823:LEU:HD23	2:A:823:LEU:O	1.90	0.70
2:A:726:CYS:HB2	2:A:728:PRO:HD2	1.71	0.70
2:A:790:GLU:HG3	2:A:791:MET:N	2.05	0.70
2:A:791:MET:HG2	2:A:803:TYR:OH	1.92	0.70
2:A:1574:PHE:HD1	2:A:1580:ILE:CD1	2.04	0.70
2:A:852:LEU:HD13	2:A:1327:VAL:HG13	1.72	0.70
3:B:125:ARG:NH1	3:B:125:ARG:HG3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1221:THR:O	2:A:1224:ILE:HG22	1.92	0.70
3:B:86:PHE:HZ	3:B:119:TYR:HH	1.40	0.70
2:A:166:GLU:HG3	2:A:167:SER:N	2.08	0.69
3:B:187:ALA:O	3:B:190:GLU:HG3	1.92	0.69
3:B:27:GLU:OE2	3:B:27:GLU:HA	1.92	0.69
2:A:123:LEU:HD23	2:A:123:LEU:O	1.92	0.69
1:C:71:GLU:CG	1:C:94:ARG:HH12	2.06	0.69
2:A:1238:ILE:HD11	2:A:1270:LEU:HD23	0.75	0.69
3:B:152:ARG:HG2	3:B:157:ILE:CG1	2.22	0.69
2:A:336:ASN:HD21	2:A:343:SER:HB3	1.55	0.69
3:B:71:LEU:CD2	3:B:106:ILE:HD12	2.21	0.69
1:C:33:THR:HB	1:C:51:THR:HB	1.73	0.69
3:B:71:LEU:CD2	3:B:106:ILE:CD1	2.70	0.69
2:A:1650:LEU:HD13	2:A:1650:LEU:O	1.93	0.69
1:C:33:THR:N	1:C:51:THR:O	2.26	0.68
2:A:795:LEU:CD1	2:A:803:TYR:CE2	2.76	0.68
2:A:207:LEU:C	2:A:207:LEU:HD13	2.13	0.68
2:A:207:LEU:HD21	2:A:209:ASN:OD1	1.93	0.68
2:A:822:GLU:OE2	2:A:835:ARG:CB	2.38	0.68
2:A:262:ILE:HG12	2:A:1617:ILE:HD12	1.75	0.68
2:A:840:LEU:O	2:A:842:VAL:N	2.25	0.68
2:A:1561:GLU:HG3	2:A:1562:CYS:N	2.07	0.68
3:B:125:ARG:HG3	3:B:125:ARG:HH11	1.59	0.68
2:A:207:LEU:HD11	2:A:209:ASN:OD1	1.93	0.68
2:A:1522:MET:HE1	2:A:1623:LEU:HD23	1.75	0.68
2:A:737:ILE:C	2:A:797:ALA:CB	2.61	0.68
2:A:1286:ILE:O	2:A:1289:LEU:HB2	1.93	0.68
2:A:1694:ILE:HD12	2:A:1703:LEU:CD1	2.22	0.68
2:A:1750:VAL:O	2:A:1753:ASN:HB2	1.93	0.68
1:C:61:LYS:HG3	1:C:85:MET:CE	2.24	0.68
3:B:112:THR:HG22	3:B:113:TYR:N	2.08	0.68
2:A:822:GLU:CG	2:A:835:ARG:NH2	2.57	0.68
2:A:1619:ARG:O	2:A:1622:ARG:HG3	1.94	0.68
2:A:207:LEU:CD1	2:A:213:LEU:HD23	2.23	0.67
1:C:30:MET:CG	1:C:138:GLY:CA	2.52	0.67
2:A:276:PHE:HZ	2:A:280:LEU:HD21	1.55	0.67
2:A:1304:PHE:CD2	2:A:1307:MET:CE	2.77	0.67
2:A:217:ARG:HB3	2:A:217:ARG:CZ	2.24	0.67
2:A:1412:MET:CE	2:A:1434:TYR:CD1	2.77	0.67
2:A:191:LEU:O	2:A:191:LEU:HD23	1.95	0.67
2:A:264:LEU:O	2:A:268:MET:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:50:ASN:O	3:B:50:ASN:ND2	2.28	0.67
1:C:34:VAL:HG23	1:C:142:ILE:HG12	1.76	0.67
2:A:168:LEU:HD23	2:A:168:LEU:C	2.15	0.67
2:A:812:ASP:OD2	2:A:844:LYS:NZ	2.22	0.67
1:C:65:LEU:C	1:C:65:LEU:HD23	2.15	0.67
2:A:773:LYS:HE3	2:A:773:LYS:O	1.94	0.67
2:A:967:LEU:C	2:A:967:LEU:HD23	2.14	0.67
2:A:1474:MET:HE2	2:A:1642:PRO:HB2	1.77	0.67
3:B:73:TYR:CD1	3:B:78:LEU:HB2	2.29	0.67
2:A:332:LYS:HG3	2:A:332:LYS:O	1.95	0.67
2:A:817:THR:O	2:A:821:VAL:HG23	1.95	0.67
3:B:69:LYS:NZ	3:B:81:GLU:OE2	2.28	0.67
1:C:79:MET:CE	5:C:301:NAG:O5	2.43	0.66
2:A:131:LEU:HD13	2:A:131:LEU:C	2.15	0.66
2:A:748:LEU:C	2:A:748:LEU:HD13	2.16	0.66
2:A:822:GLU:HG2	2:A:835:ARG:HH22	1.59	0.66
2:A:823:LEU:HD23	2:A:823:LEU:C	2.15	0.66
2:A:960:LEU:HD23	2:A:960:LEU:O	1.95	0.66
2:A:734:LYS:HE3	2:A:799:ASP:CG	2.15	0.66
2:A:895:CYS:HB2	2:A:938:VAL:HG12	1.76	0.66
3:B:57:TRP:CH2	3:B:142:ILE:HD11	2.29	0.66
3:B:98:THR:O	3:B:99:LYS:HB3	1.95	0.66
2:A:737:ILE:C	2:A:797:ALA:HB1	2.16	0.66
2:A:1511:LEU:C	2:A:1511:LEU:HD23	2.16	0.66
3:B:72:ARG:NH2	3:B:74:GLU:CD	2.48	0.66
2:A:881:ALA:O	2:A:916:SER:OG	2.13	0.66
2:A:116:ARG:HH12	2:A:176:PHE:HA	1.60	0.66
2:A:171:ILE:HD12	2:A:171:ILE:C	2.15	0.66
2:A:737:ILE:HG21	2:A:797:ALA:H	1.60	0.66
2:A:793:LEU:C	2:A:793:LEU:HD13	2.16	0.66
2:A:1218:ARG:HG2	2:A:1218:ARG:HH21	1.60	0.66
2:A:1286:ILE:HD12	2:A:1286:ILE:C	2.16	0.66
2:A:1363:GLN:O	2:A:1364:VAL:HG12	1.96	0.66
2:A:787:PHE:CE1	2:A:841:ARG:NH1	2.64	0.66
2:A:136:ILE:HD11	2:A:224:THR:CG2	2.25	0.66
2:A:251:LEU:HD13	2:A:1630:ILE:HG23	1.77	0.66
2:A:772:PHE:HE1	2:A:776:LEU:HD23	1.60	0.66
2:A:1202:ILE:O	2:A:1206:SER:OG	2.14	0.66
2:A:388:LEU:HD13	2:A:388:LEU:C	2.16	0.66
2:A:772:PHE:CE1	2:A:776:LEU:HD23	2.31	0.66
1:C:65:LEU:CD1	1:C:110:VAL:CG1	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:192:ASP:OD1	2:A:223:LYS:HD2	1.96	0.66
2:A:196:ILE:HD12	2:A:196:ILE:C	2.16	0.66
2:A:1318:ILE:CG1	2:A:1319:PRO:HD3	2.26	0.66
2:A:1764:SER:C	2:A:1767:THR:HG22	2.16	0.66
2:A:1304:PHE:HD2	2:A:1307:MET:HE1	1.61	0.65
2:A:1635:PHE:CD1	2:A:1638:MET:HE2	2.31	0.65
2:A:1318:ILE:HG13	2:A:1319:PRO:HD3	1.76	0.65
2:A:791:MET:HE3	2:A:795:LEU:HD22	1.79	0.65
2:A:1500:PRO:HG3	2:A:1505:GLN:CG	2.08	0.65
2:A:367:TYR:OH	2:A:1689:ILE:HG23	1.96	0.65
1:C:65:LEU:HD12	1:C:110:VAL:HG11	1.77	0.65
2:A:928:TRP:CZ3	2:A:929:ILE:HD12	2.31	0.65
2:A:220:ARG:O	2:A:223:LYS:HB2	1.97	0.65
2:A:336:ASN:CB	2:A:343:SER:OG	2.45	0.65
2:A:895:CYS:HB3	2:A:938:VAL:HG12	1.78	0.65
2:A:1457:ILE:HD12	2:A:1457:ILE:C	2.16	0.65
2:A:136:ILE:HD13	2:A:136:ILE:C	2.17	0.65
2:A:196:ILE:O	2:A:200:TYR:HD1	1.79	0.65
2:A:202:THR:OG1	2:A:214:ARG:NH1	2.30	0.64
2:A:361:ASP:OD2	2:A:929:ILE:HG22	1.97	0.64
2:A:843:PHE:O	2:A:845:LEU:N	2.31	0.64
2:A:1214:ILE:HD12	3:B:22:VAL:CG2	2.27	0.64
2:A:1602:TYR:O	2:A:1603:PHE:HB2	1.96	0.64
2:A:131:LEU:HD13	2:A:132:ILE:N	2.12	0.64
2:A:132:ILE:CD1	2:A:166:GLU:HB2	2.26	0.64
2:A:332:LYS:O	2:A:333:ILE:HG12	1.97	0.64
2:A:764:GLU:OE1	2:A:1341:ASN:ND2	2.31	0.64
2:A:851:THR:CG2	2:A:1327:VAL:HG21	2.27	0.64
2:A:1522:MET:HE1	2:A:1623:LEU:HD22	1.78	0.64
3:B:73:TYR:HD1	3:B:78:LEU:HB2	1.62	0.64
2:A:209:ASN:OD1	2:A:209:ASN:N	2.30	0.64
2:A:909:HIS:CD2	2:A:911:ASN:H	2.15	0.64
2:A:947:VAL:O	2:A:951:VAL:HG23	1.98	0.64
2:A:1460:PHE:CZ	2:A:1753:ASN:ND2	2.66	0.64
2:A:250:ILE:HG22	2:A:1630:ILE:CD1	2.18	0.64
2:A:300:ARG:NH2	2:A:308:GLY:H	1.96	0.64
2:A:945:LEU:O	2:A:949:MET:HG2	1.98	0.64
2:A:119:SER:OG	2:A:173:ALA:HB2	1.97	0.64
2:A:1431:LEU:HD12	2:A:1431:LEU:O	1.98	0.64
2:A:1732:ASN:CB	2:A:1735:VAL:CG1	2.61	0.64
2:A:866:LEU:O	2:A:870:THR:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:293:LEU:HD11	2:A:298:ASP:C	2.18	0.64
2:A:1293:ARG:HH21	2:A:1293:ARG:HB2	1.63	0.64
2:A:1385:LEU:O	2:A:1386:LYS:HB2	1.96	0.64
2:A:1467:LEU:HD21	2:A:1472:ILE:HG21	1.79	0.64
2:A:1528:ASN:HD22	2:A:1528:ASN:C	2.02	0.64
2:A:1760:LEU:HD23	2:A:1760:LEU:O	1.98	0.64
2:A:867:GLY:HA2	2:A:870:THR:CG2	2.28	0.63
2:A:1251:LYS:O	2:A:1255:THR:CG2	2.40	0.63
2:A:1491:LYS:O	2:A:1491:LYS:HD3	1.98	0.63
2:A:936:MET:CE	2:A:945:LEU:CD1	2.77	0.63
2:A:1742:SER:O	2:A:1746:ILE:HG13	1.98	0.63
3:B:46:ARG:NH2	3:B:48:GLU:OE2	2.27	0.63
2:A:117:ARG:CA	2:A:120:ILE:HG22	2.28	0.63
2:A:132:ILE:HG22	2:A:227:VAL:HG11	1.81	0.63
2:A:793:LEU:HD13	2:A:793:LEU:O	1.98	0.63
2:A:960:LEU:HD21	2:A:964:LEU:CD2	2.29	0.63
2:A:1364:VAL:HG23	2:A:1370:CYS:HA	1.80	0.63
2:A:117:ARG:HA	2:A:120:ILE:CG2	2.28	0.63
2:A:1609:PHE:CE1	2:A:1613:ARG:HD2	2.33	0.63
2:A:1671:LYS:NZ	2:A:1682:GLU:OE2	2.32	0.63
2:A:1218:ARG:O	2:A:1219:LYS:CG	2.46	0.63
2:A:1485:MET:SD	2:A:1639:MET:CE	2.87	0.63
2:A:1650:LEU:HD13	2:A:1650:LEU:C	2.18	0.63
3:B:86:PHE:HZ	3:B:119:TYR:OH	1.80	0.63
1:C:103:GLY:HA3	1:C:109:ASP:OD1	1.99	0.62
2:A:754:ILE:HG12	2:A:787:PHE:CE1	2.33	0.62
2:A:798:MET:O	2:A:802:GLU:HB2	1.99	0.62
2:A:1639:MET:HE2	2:A:1639:MET:CA	2.29	0.62
2:A:849:TRP:HD1	2:A:850:PRO:HD2	0.56	0.62
2:A:1514:ASN:HD22	2:A:1515:GLN:N	1.97	0.62
2:A:960:LEU:HD23	2:A:964:LEU:CD2	2.22	0.62
2:A:962:LEU:O	2:A:966:LEU:HB2	2.00	0.62
2:A:1294:ALA:O	2:A:1297:PRO:HD2	2.00	0.62
2:A:822:GLU:HG2	2:A:835:ARG:NH2	2.14	0.62
2:A:1353:THR:HB	2:A:1379:ASN:O	2.00	0.62
2:A:1497:ILE:CG2	2:A:1572:TYR:CE2	2.76	0.62
2:A:266:LEU:O	2:A:1610:ARG:NH2	2.33	0.62
2:A:321:SER:HB2	2:A:372:ARG:O	1.99	0.62
2:A:1504:ILE:HG12	2:A:1505:GLN:H	1.65	0.62
1:C:34:VAL:CG2	1:C:142:ILE:HG12	2.29	0.62
2:A:1287:LYS:HD3	2:A:1287:LYS:C	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1582:ASP:OD1	2:A:1622:ARG:CZ	2.47	0.62
3:B:28:THR:HG22	3:B:143:HIS:O	2.00	0.62
3:B:40:CYS:O	3:B:104:LEU:O	2.16	0.62
2:A:148:PRO:CB	2:A:152:THR:HG21	2.28	0.62
2:A:1219:LYS:HG3	2:A:1219:LYS:O	2.00	0.61
3:B:53:THR:HG22	3:B:54:PHE:N	2.15	0.61
2:A:117:ARG:HH11	2:A:117:ARG:CG	2.12	0.61
2:A:1308:ARG:CB	2:A:1308:ARG:HH21	2.13	0.61
2:A:1412:MET:CE	2:A:1434:TYR:HE1	1.99	0.61
1:C:107:LYS:HZ3	1:C:109:ASP:HB2	1.61	0.61
2:A:1531:THR:O	2:A:1534:VAL:HG23	1.99	0.61
2:A:812:ASP:O	2:A:816:VAL:HG23	2.00	0.61
2:A:862:SER:O	2:A:870:THR:CG2	2.48	0.61
3:B:153:ASP:OD1	3:B:154:MET:N	2.34	0.61
2:A:178:VAL:HG12	2:A:178:VAL:O	1.99	0.61
2:A:221:ALA:O	2:A:224:THR:HG23	2.01	0.61
2:A:1318:ILE:HG13	2:A:1319:PRO:CD	2.29	0.61
2:A:1522:MET:HE3	2:A:1623:LEU:CD2	2.30	0.61
2:A:1599:ILE:O	2:A:1603:PHE:N	2.30	0.61
3:B:51:ALA:CB	3:B:127:LEU:HD13	2.30	0.61
2:A:1367:ARG:HB2	2:A:1382:TRP:CZ2	2.36	0.61
1:C:65:LEU:HD21	1:C:67:TRP:CD1	2.35	0.61
2:A:737:ILE:CG2	2:A:797:ALA:N	2.63	0.61
2:A:967:LEU:HD23	2:A:968:LEU:N	2.16	0.61
1:C:59:ASN:O	1:C:63:PHE:N	2.30	0.61
1:C:105:PRO:HA	1:C:109:ASP:O	2.01	0.61
2:A:783:PHE:O	2:A:787:PHE:HD2	1.83	0.61
2:A:349:TRP:HA	2:A:349:TRP:CE3	2.36	0.60
2:A:849:TRP:CD1	2:A:850:PRO:CD	2.35	0.60
2:A:1304:PHE:CD2	2:A:1307:MET:HE1	2.36	0.60
2:A:1555:ILE:HD12	2:A:1593:MET:CE	2.31	0.60
2:A:1707:ILE:HG21	2:A:1736:GLY:HA3	1.84	0.60
1:C:62:GLN:C	1:C:132:PRO:HD2	2.21	0.60
2:A:132:ILE:CD1	2:A:166:GLU:OE2	2.43	0.60
2:A:738:TYR:N	2:A:797:ALA:HB1	2.17	0.60
2:A:1217:GLU:OE1	2:A:1217:GLU:HA	2.00	0.60
3:B:51:ALA:HB2	3:B:127:LEU:HA	1.83	0.60
2:A:835:ARG:HH21	2:A:835:ARG:CG	2.14	0.60
2:A:839:LEU:HD13	2:A:1334:ILE:HG23	1.84	0.60
2:A:1457:ILE:HG22	2:A:1756:ILE:HD12	1.81	0.60
3:B:38:ILE:HG22	3:B:142:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:82:GLU:OE1	3:B:82:GLU:N	2.35	0.60
2:A:1218:ARG:HG2	3:B:23:GLU:O	2.02	0.60
2:A:1498:PRO:HD3	2:A:1572:TYR:CZ	2.37	0.60
3:B:55:THR:HG22	3:B:56:GLU:N	2.16	0.60
2:A:1522:MET:HE3	2:A:1623:LEU:HD23	1.84	0.60
2:A:967:LEU:HD22	2:A:968:LEU:HD13	1.83	0.60
2:A:1179:TRP:CD1	2:A:1183:LYS:HE2	2.37	0.60
2:A:168:LEU:O	2:A:171:ILE:HG13	2.02	0.59
2:A:262:ILE:HG12	2:A:1617:ILE:CD1	2.32	0.59
2:A:337:PRO:O	2:A:338:ASP:HB2	2.02	0.59
2:A:1364:VAL:O	2:A:1364:VAL:HG13	2.00	0.59
3:B:57:TRP:HH2	3:B:142:ILE:CD1	2.09	0.59
3:B:165:VAL:O	3:B:169:VAL:HG23	2.02	0.59
1:C:66:ASN:ND2	1:C:79:MET:HE2	2.18	0.59
2:A:822:GLU:OE1	2:A:835:ARG:NH2	2.35	0.59
2:A:1218:ARG:HH21	2:A:1218:ARG:CG	2.14	0.59
2:A:157:TYR:C	2:A:160:THR:HG22	2.15	0.59
2:A:971:PHE:CE2	2:A:1458:ASP:OD2	2.56	0.59
2:A:1280:TYR:CE1	2:A:1283:LEU:HD11	2.37	0.59
2:A:1308:ARG:HH21	2:A:1308:ARG:HB2	1.67	0.59
2:A:1608:LEU:O	2:A:1612:ILE:HG12	2.03	0.59
2:A:1635:PHE:CE1	2:A:1638:MET:CE	2.86	0.59
3:B:129:PHE:HB2	3:B:132:TYR:HB3	1.84	0.59
2:A:174:ARG:HD3	2:A:182:THR:CB	2.29	0.59
2:A:1508:ILE:O	2:A:1512:VAL:HG23	2.03	0.59
2:A:1572:TYR:O	2:A:1575:THR:HG23	2.03	0.59
2:A:300:ARG:HG2	2:A:300:ARG:NH1	2.17	0.59
2:A:1509:PHE:HA	2:A:1568:SER:CB	2.32	0.59
3:B:125:ARG:HH11	3:B:125:ARG:CG	2.15	0.59
2:A:171:ILE:CG2	2:A:183:PHE:CD2	2.75	0.59
2:A:765:HIS:CD2	2:A:768:MET:HG3	2.38	0.59
3:B:32:TYR:CE2	3:B:113:TYR:HD1	2.17	0.59
2:A:1497:ILE:HG21	2:A:1572:TYR:CD2	2.24	0.59
2:A:1504:ILE:O	2:A:1508:ILE:HG13	2.03	0.58
2:A:207:LEU:CD1	2:A:209:ASN:H	2.16	0.58
2:A:389:GLY:O	2:A:393:LEU:HB2	2.03	0.58
2:A:1503:LYS:H	2:A:1503:LYS:HD2	1.66	0.58
1:C:31:GLU:O	1:C:53:ASN:N	2.37	0.58
2:A:295:SER:HB3	2:A:298:ASP:HB2	1.86	0.58
2:A:748:LEU:HD13	2:A:749:ALA:N	2.18	0.58
2:A:1318:ILE:N	2:A:1319:PRO:HD2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1408:TRP:CD1	2:A:1409:THR:HG23	2.39	0.58
2:A:1496:PRO:O	2:A:1497:ILE:CG1	2.51	0.58
1:C:65:LEU:HD23	1:C:65:LEU:O	2.04	0.58
1:C:65:LEU:HD21	1:C:67:TRP:HD1	1.67	0.58
2:A:748:LEU:HD22	2:A:748:LEU:O	2.04	0.58
2:A:1551:ASN:O	2:A:1555:ILE:HG13	2.03	0.58
2:A:742:MET:HB2	2:A:746:VAL:CB	2.30	0.58
2:A:1200:LEU:HD23	2:A:1201:MET:CE	2.34	0.58
2:A:287:GLU:HA	2:A:287:GLU:OE1	2.03	0.58
2:A:1450:ASN:HD22	2:A:1450:ASN:C	2.06	0.58
3:B:177:GLU:HA	3:B:177:GLU:OE1	2.04	0.58
2:A:1485:MET:CB	2:A:1639:MET:CE	2.81	0.58
2:A:153:LYS:HE3	2:A:157:TYR:OH	2.04	0.58
2:A:772:PHE:HE1	2:A:776:LEU:CD2	2.16	0.58
2:A:806:VAL:HG23	2:A:809:ASN:HB2	1.86	0.58
2:A:831:LEU:N	2:A:831:LEU:HD22	2.19	0.58
2:A:936:MET:CE	2:A:945:LEU:HD12	2.34	0.58
2:A:967:LEU:HD23	2:A:968:LEU:HD13	1.82	0.58
2:A:1717:PRO:O	2:A:1728:GLY:CA	2.51	0.58
2:A:810:ILE:HG13	2:A:811:PHE:N	2.18	0.57
2:A:1318:ILE:CG1	2:A:1319:PRO:CD	2.82	0.57
2:A:336:ASN:HD22	2:A:343:SER:HB3	1.61	0.57
2:A:737:ILE:CG2	2:A:797:ALA:CA	2.78	0.57
2:A:815:ILE:HD13	2:A:815:ILE:N	2.19	0.57
2:A:1179:TRP:NE1	2:A:1183:LYS:HE2	2.19	0.57
2:A:1218:ARG:HB3	2:A:1218:ARG:NH2	2.18	0.57
2:A:1539:GLN:O	2:A:1540:SER:OG	2.16	0.57
3:B:78:LEU:HD21	3:B:80:LEU:HD13	1.85	0.57
2:A:737:ILE:C	2:A:797:ALA:HB2	2.25	0.57
2:A:839:LEU:O	2:A:842:VAL:CG2	2.34	0.57
2:A:1740:PHE:O	2:A:1744:ILE:HG12	2.04	0.57
3:B:37:LYS:HB2	3:B:107:PHE:HD1	1.69	0.57
2:A:197:VAL:O	2:A:201:LEU:N	2.32	0.57
2:A:1764:SER:O	2:A:1767:THR:CG2	2.41	0.57
2:A:383:VAL:O	2:A:387:PHE:HB2	2.04	0.57
2:A:1359:PHE:HB3	2:A:1360:PRO:HD2	1.85	0.57
2:A:1440:PHE:O	2:A:1444:GLY:N	2.34	0.57
3:B:67:PHE:HE2	3:B:120:GLU:HG3	1.69	0.57
3:B:84:GLU:HA	3:B:87:GLU:HB2	1.87	0.57
2:A:1263:PHE:O	2:A:1266:VAL:HG12	2.05	0.57
2:A:1555:ILE:HD12	2:A:1593:MET:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1598:LEU:HA	2:A:1601:THR:CG2	2.34	0.57
2:A:1668:TYR:O	2:A:1729:ASP:CB	2.52	0.57
2:A:1545:GLU:OE1	2:A:1545:GLU:HA	2.03	0.57
2:A:192:ASP:O	2:A:196:ILE:HG23	2.05	0.57
2:A:790:GLU:O	2:A:794:LYS:HB2	2.04	0.57
2:A:836:SER:O	2:A:839:LEU:HG	2.04	0.57
2:A:1185:CYS:O	2:A:1189:VAL:HG22	2.04	0.57
2:A:1531:THR:O	2:A:1534:VAL:HG22	2.04	0.57
2:A:278:ASN:HD21	2:A:329:THR:CB	2.18	0.57
3:B:51:ALA:CB	3:B:126:LEU:O	2.53	0.57
2:A:193:PHE:O	2:A:196:ILE:HG13	2.04	0.56
3:B:85:ARG:HH11	3:B:85:ARG:CG	2.14	0.56
3:B:187:ALA:HA	3:B:190:GLU:OE1	2.04	0.56
2:A:414:GLU:HG3	2:A:415:GLU:N	2.19	0.56
2:A:738:TYR:O	2:A:741:VAL:HG13	2.06	0.56
2:A:789:ALA:O	2:A:792:VAL:HG12	2.05	0.56
2:A:1694:ILE:HD11	2:A:1703:LEU:HD12	0.64	0.56
2:A:1703:LEU:O	2:A:1706:PRO:HD2	2.05	0.56
2:A:163:TYR:O	2:A:167:SER:HB2	2.05	0.56
3:B:46:ARG:HB3	3:B:48:GLU:OE2	2.05	0.56
2:A:116:ARG:O	2:A:120:ILE:HG22	2.06	0.56
2:A:320:ASP:OD1	2:A:320:ASP:N	2.39	0.56
2:A:1212:GLU:O	2:A:1213:ASP:HB3	2.05	0.56
2:A:1350:CYS:HB2	2:A:1424:GLN:HE22	1.71	0.56
2:A:1704:LEU:HD22	2:A:1708:LEU:HG	1.88	0.56
2:A:843:PHE:O	2:A:846:ALA:N	2.27	0.56
2:A:1206:SER:O	2:A:1209:LEU:HB2	2.05	0.56
2:A:971:PHE:HE2	2:A:1458:ASP:OD2	1.88	0.56
2:A:737:ILE:CA	2:A:797:ALA:HB2	2.36	0.56
2:A:840:LEU:C	2:A:842:VAL:N	2.57	0.56
2:A:1325:LEU:CD1	2:A:1329:LEU:HG	2.35	0.56
2:A:184:LEU:HD11	2:A:190:TRP:CD1	2.41	0.56
1:C:101:PHE:CZ	1:C:103:GLY:O	2.56	0.56
1:C:107:LYS:O	1:C:108:TYR:HB2	2.06	0.56
2:A:327:GLY:O	3:B:132:TYR:CE2	2.52	0.56
2:A:1358:ARG:NH1	2:A:1417:ASP:OD2	2.37	0.56
2:A:336:ASN:ND2	2:A:343:SER:OG	2.38	0.55
2:A:1704:LEU:HD22	2:A:1704:LEU:O	2.06	0.55
2:A:1358:ARG:NH2	2:A:1417:ASP:OD2	2.38	0.55
2:A:1589:SER:OG	2:A:1619:ARG:NH2	2.40	0.55
1:C:44:SER:O	1:C:117:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:207:LEU:HD13	2:A:209:ASN:N	2.22	0.55
2:A:278:ASN:ND2	2:A:329:THR:HB	2.21	0.55
2:A:132:ILE:CD1	2:A:166:GLU:CD	2.71	0.55
2:A:806:VAL:HG23	2:A:809:ASN:CB	2.37	0.55
2:A:1321:ILE:HD11	2:A:1456:ILE:HG12	1.89	0.55
2:A:1635:PHE:CE1	2:A:1638:MET:HE1	2.42	0.55
3:B:74:GLU:O	3:B:75:ASN:HB3	2.05	0.55
3:B:91:VAL:HG23	3:B:107:PHE:HB3	1.88	0.55
3:B:67:PHE:CD1	3:B:67:PHE:N	2.73	0.55
2:A:832:SER:O	2:A:835:ARG:HB3	2.06	0.55
2:A:849:TRP:CH2	2:A:1326:LEU:HB3	2.42	0.55
2:A:1283:LEU:HD23	2:A:1283:LEU:N	2.03	0.55
2:A:1514:ASN:ND2	2:A:1516:ALA:H	2.05	0.55
2:A:286:LEU:HD22	2:A:286:LEU:O	2.07	0.54
2:A:806:VAL:HG23	2:A:809:ASN:H	1.72	0.54
2:A:1474:MET:HE1	2:A:1642:PRO:HB2	1.89	0.54
3:B:48:GLU:HG2	3:B:49:THR:N	2.22	0.54
2:A:116:ARG:NH1	2:A:176:PHE:CB	2.65	0.54
2:A:1512:VAL:HG11	2:A:1565:LYS:HG3	1.89	0.54
2:A:1640:SER:HB3	2:A:1761:GLU:HG3	1.89	0.54
2:A:1681:PHE:HD1	2:A:1687:SER:HG	1.53	0.54
2:A:1707:ILE:HD13	2:A:1740:PHE:CE2	2.42	0.54
1:C:59:ASN:HB3	1:C:62:GLN:CB	2.34	0.54
1:C:107:LYS:O	1:C:107:LYS:HG2	2.08	0.54
2:A:139:ASN:C	2:A:139:ASN:HD22	2.06	0.54
2:A:806:VAL:CG2	2:A:809:ASN:CB	2.85	0.54
2:A:184:LEU:CD1	2:A:190:TRP:CD1	2.91	0.54
2:A:790:GLU:O	2:A:794:LYS:N	2.38	0.54
2:A:798:MET:O	2:A:799:ASP:HB2	2.07	0.54
2:A:895:CYS:HB2	2:A:938:VAL:CG1	2.38	0.54
3:B:90:VAL:HG11	3:B:106:ILE:HD11	1.90	0.54
2:A:399:ALA:HB3	2:A:1762:ASN:HD22	1.63	0.54
2:A:803:TYR:CE1	2:A:809:ASN:ND2	2.68	0.54
2:A:1270:LEU:HD13	2:A:1270:LEU:C	2.26	0.54
2:A:217:ARG:CZ	2:A:217:ARG:CB	2.85	0.54
3:B:26:SER:HB2	3:B:39:LEU:H	1.71	0.54
1:C:33:THR:O	1:C:50:CYS:CA	2.55	0.54
2:A:145:MET:CE	2:A:145:MET:CA	2.85	0.54
2:A:196:ILE:CD1	2:A:197:VAL:N	2.70	0.54
2:A:146:ASN:O	2:A:147:ASN:HB3	2.09	0.53
2:A:1186:TYR:CZ	2:A:1190:GLU:OE2	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLN:HB3	1:C:132:PRO:HD2	1.90	0.53
2:A:810:ILE:O	2:A:814:LEU:CD1	2.43	0.53
2:A:1477:GLU:OE2	2:A:1477:GLU:HA	2.07	0.53
2:A:1535:GLU:HG2	2:A:1547:LEU:CD1	2.39	0.53
3:B:119:TYR:O	3:B:142:ILE:N	2.39	0.53
2:A:867:GLY:O	2:A:870:THR:HG23	2.09	0.53
2:A:900:ASN:OD1	2:A:902:ASP:N	2.38	0.53
3:B:71:LEU:CD2	3:B:106:ILE:HD11	2.37	0.53
4:E:2:NAG:HO3	4:E:2:NAG:C7	2.13	0.53
1:C:135:ARG:HH21	1:C:135:ARG:CG	2.14	0.53
2:A:187:PRO:HA	2:A:190:TRP:CE3	2.44	0.53
2:A:247:ASP:OD1	2:A:1629:GLY:C	2.47	0.53
2:A:741:VAL:HG23	2:A:742:MET:N	2.22	0.53
2:A:1732:ASN:OD1	2:A:1735:VAL:HB	2.08	0.53
2:A:1495:LYS:CE	2:A:1495:LYS:HA	2.38	0.53
3:B:89:ARG:NH1	3:B:110:ASN:OD1	2.42	0.53
2:A:1298:LEU:HD12	2:A:1301:LEU:HD12	1.89	0.53
2:A:1637:LEU:HD22	2:A:1637:LEU:C	2.28	0.53
2:A:772:PHE:HD1	2:A:772:PHE:O	1.92	0.53
3:B:178:MET:O	3:B:182:TYR:HB3	2.08	0.53
2:A:114:PRO:O	2:A:118:ILE:HG12	2.09	0.53
2:A:175:GLY:O	2:A:178:VAL:HB	2.09	0.53
2:A:1532:MET:CE	2:A:1616:ARG:HB2	2.39	0.52
2:A:123:LEU:HD23	2:A:123:LEU:C	2.29	0.52
2:A:176:PHE:O	2:A:178:VAL:HG23	2.08	0.52
2:A:1365:PRO:O	2:A:1424:GLN:CB	2.57	0.52
2:A:1408:TRP:CD1	2:A:1409:THR:N	2.77	0.52
2:A:165:PHE:O	2:A:169:VAL:HG13	2.09	0.52
1:C:32:VAL:CG1	1:C:50:CYS:SG	2.98	0.52
2:A:207:LEU:CD1	2:A:209:ASN:N	2.73	0.52
2:A:300:ARG:NH1	3:B:130:GLU:OE2	2.43	0.52
2:A:734:LYS:CE	2:A:799:ASP:OD2	2.58	0.52
2:A:1495:LYS:CA	2:A:1495:LYS:HE3	2.39	0.52
2:A:849:TRP:HH2	2:A:1326:LEU:HB3	1.74	0.52
2:A:1757:ALA:O	2:A:1761:GLU:HG2	2.09	0.52
3:B:57:TRP:CH2	3:B:142:ILE:HD13	2.40	0.52
2:A:114:PRO:HG2	2:A:115:LEU:H	1.74	0.52
2:A:262:ILE:CG1	2:A:1617:ILE:CD1	2.88	0.52
2:A:397:ILE:O	2:A:401:VAL:HG23	2.09	0.52
2:A:1293:ARG:O	2:A:1295:LEU:N	2.42	0.52
2:A:890:LYS:NZ	2:A:890:LYS:CB	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1512:VAL:CG1	2:A:1565:LYS:HG3	2.39	0.52
2:A:1752:VAL:O	2:A:1756:ILE:HG12	2.08	0.52
2:A:159:PHE:O	2:A:163:TYR:CD2	2.62	0.52
2:A:329:THR:CG2	2:A:330:CYS:N	2.71	0.52
2:A:338:ASP:O	2:A:339:TYR:HB2	2.10	0.52
2:A:1294:ALA:O	2:A:1297:PRO:CD	2.57	0.52
2:A:1308:ARG:CB	2:A:1308:ARG:NH2	2.73	0.52
2:A:1349:GLU:HG3	2:A:1351:ILE:CG2	2.40	0.52
2:A:1733:PRO:O	2:A:1737:ILE:HG13	2.10	0.52
3:B:75:ASN:CG	3:B:76:GLU:H	2.13	0.52
2:A:217:ARG:CG	2:A:217:ARG:HH11	2.22	0.52
2:A:224:THR:HA	2:A:227:VAL:CG2	2.40	0.51
2:A:838:ARG:NH1	2:A:838:ARG:CG	2.73	0.51
2:A:279:SER:O	2:A:280:LEU:HD12	2.10	0.51
2:A:290:MET:HG3	2:A:333:ILE:HG21	1.92	0.51
2:A:1495:LYS:CE	2:A:1495:LYS:CA	2.86	0.51
3:B:60:ARG:HD2	3:B:60:ARG:O	2.09	0.51
1:C:47:ARG:NH2	1:C:111:SER:OG	2.43	0.51
2:A:293:LEU:CD1	2:A:298:ASP:CB	2.56	0.51
2:A:300:ARG:HH11	2:A:300:ARG:CG	2.18	0.51
2:A:810:ILE:HG13	2:A:811:PHE:H	1.75	0.51
2:A:1408:TRP:NE1	2:A:1409:THR:HG22	2.25	0.51
2:A:1509:PHE:N	2:A:1568:SER:OG	2.43	0.51
3:B:85:ARG:HG2	3:B:85:ARG:NH1	2.18	0.51
2:A:1408:TRP:NE1	2:A:1409:THR:CG2	2.73	0.51
2:A:1707:ILE:HD13	2:A:1740:PHE:HE2	1.74	0.51
3:B:58:THR:HG22	3:B:69:LYS:CA	2.39	0.51
2:A:831:LEU:N	2:A:831:LEU:CD2	2.73	0.51
2:A:1281:SER:O	2:A:1282:ASP:HB2	2.10	0.51
2:A:1499:ARG:HG2	2:A:1509:PHE:CD1	2.45	0.51
2:A:1509:PHE:CA	2:A:1568:SER:HB3	2.40	0.51
2:A:144:THR:O	2:A:144:THR:HG22	2.09	0.51
2:A:207:LEU:HD12	2:A:213:LEU:CG	2.41	0.51
2:A:1680:ASN:O	2:A:1686:ASN:HB3	2.11	0.51
2:A:415:GLU:OE2	2:A:416:ALA:HB2	2.09	0.51
2:A:840:LEU:O	2:A:841:ARG:C	2.48	0.51
2:A:896:VAL:CG1	2:A:905:LEU:HD13	2.41	0.51
2:A:1190:GLU:HA	2:A:1190:GLU:OE1	2.11	0.51
2:A:1340:VAL:O	2:A:1344:ALA:HB2	2.11	0.51
2:A:117:ARG:CG	2:A:117:ARG:NH1	2.73	0.51
2:A:852:LEU:CD1	2:A:1327:VAL:HG13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1293:ARG:HH21	2:A:1293:ARG:HB3	1.75	0.51
3:B:32:TYR:CD1	3:B:32:TYR:C	2.85	0.51
2:A:843:PHE:O	2:A:844:LYS:C	2.48	0.51
2:A:278:ASN:HD21	2:A:329:THR:HB	1.76	0.50
2:A:740:ILE:O	2:A:740:ILE:HG22	2.10	0.50
2:A:1218:ARG:CG	2:A:1218:ARG:NH2	2.73	0.50
2:A:1301:LEU:HD23	2:A:1307:MET:HG2	1.93	0.50
2:A:1527:LEU:O	2:A:1530:VAL:HG12	2.11	0.50
2:A:761:MET:CE	2:A:839:LEU:HB3	2.41	0.50
2:A:803:TYR:CZ	2:A:809:ASN:ND2	2.74	0.50
2:A:901:ASP:OD1	2:A:901:ASP:N	2.44	0.50
2:A:1460:PHE:HD2	2:A:1756:ILE:HG13	1.76	0.50
2:A:1527:LEU:O	2:A:1530:VAL:CG1	2.58	0.50
2:A:1606:PRO:O	2:A:1609:PHE:HB3	2.11	0.50
1:C:128:TYR:HB3	1:C:137:ARG:HE	1.77	0.50
2:A:164:THR:O	2:A:168:LEU:N	2.35	0.50
2:A:762:ALA:O	2:A:1392:VAL:CG2	2.60	0.50
3:B:112:THR:CG2	3:B:113:TYR:N	2.74	0.50
2:A:272:LYS:NZ	2:A:345:ASP:OD2	2.44	0.50
2:A:762:ALA:O	2:A:1392:VAL:HG21	2.11	0.50
3:B:104:LEU:N	3:B:104:LEU:CD2	2.73	0.50
2:A:329:THR:HG23	2:A:330:CYS:N	2.27	0.50
2:A:1412:MET:HE3	2:A:1434:TYR:CD1	2.46	0.50
3:B:129:PHE:HB2	3:B:132:TYR:O	2.12	0.50
2:A:207:LEU:HD11	2:A:209:ASN:H	1.76	0.50
2:A:336:ASN:HB2	2:A:343:SER:OG	2.11	0.50
2:A:405:TYR:CD1	2:A:405:TYR:C	2.85	0.50
2:A:1215:TYR:HD1	2:A:1218:ARG:HD3	1.76	0.50
2:A:1573:TYR:OH	2:A:1583:PHE:HB2	2.11	0.50
3:B:46:ARG:HH21	3:B:48:GLU:CD	2.14	0.50
2:A:326:GLU:HG3	3:B:45:ARG:HG3	1.93	0.50
2:A:1514:ASN:ND2	2:A:1515:GLN:N	2.60	0.50
1:C:34:VAL:HG21	1:C:142:ILE:HG13	1.93	0.50
2:A:151:TRP:CE3	2:A:151:TRP:C	2.85	0.50
3:B:85:ARG:CG	3:B:85:ARG:NH1	2.73	0.50
2:A:321:SER:CB	2:A:375:GLY:HA2	2.34	0.50
2:A:766:HIS:CD2	2:A:766:HIS:C	2.86	0.50
2:A:1485:MET:CB	2:A:1639:MET:HE3	2.24	0.50
3:B:112:THR:HG22	3:B:113:TYR:H	1.74	0.50
2:A:117:ARG:C	2:A:120:ILE:HG22	2.32	0.49
2:A:1282:ASP:HA	2:A:1287:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1360:PRO:O	2:A:1361:ALA:HB3	2.12	0.49
2:A:1514:ASN:HD22	2:A:1515:GLN:H	1.60	0.49
2:A:207:LEU:HD11	2:A:209:ASN:CG	2.33	0.49
3:B:38:ILE:CG2	3:B:142:ILE:HD13	2.42	0.49
2:A:131:LEU:HD22	2:A:131:LEU:C	2.33	0.49
2:A:1369:GLU:OE1	2:A:1369:GLU:HA	2.12	0.49
2:A:1502:ASN:HB3	2:A:1504:ILE:HD13	1.89	0.49
2:A:1635:PHE:HE1	2:A:1638:MET:HE1	1.75	0.49
3:B:180:TYR:CD1	3:B:180:TYR:C	2.85	0.49
1:C:34:VAL:HG21	1:C:142:ILE:CG1	2.42	0.49
1:C:52:PHE:CD1	1:C:52:PHE:C	2.85	0.49
2:A:151:TRP:CE3	2:A:152:THR:HA	2.47	0.49
2:A:1509:PHE:CD1	2:A:1509:PHE:C	2.85	0.49
3:B:144:ILE:O	3:B:144:ILE:HG13	2.12	0.49
2:A:183:PHE:C	2:A:183:PHE:CD1	2.85	0.49
2:A:834:LEU:HD23	2:A:834:LEU:C	2.14	0.49
2:A:879:ILE:O	2:A:882:VAL:HG12	2.13	0.49
2:A:1287:LYS:HE3	2:A:1287:LYS:O	2.12	0.49
3:B:182:TYR:CD1	3:B:182:TYR:C	2.85	0.49
2:A:361:ASP:OD2	2:A:929:ILE:CG2	2.60	0.49
2:A:899:ILE:CG2	2:A:938:VAL:HG13	2.43	0.49
2:A:945:LEU:HD23	2:A:949:MET:HE2	1.94	0.49
2:A:1205:SER:O	2:A:1296:ARG:NH1	2.46	0.49
2:A:1640:SER:CB	2:A:1761:GLU:HG3	2.42	0.49
1:C:54:SER:HB2	1:C:134:ASP:OD2	2.13	0.49
2:A:117:ARG:O	2:A:120:ILE:HG22	2.12	0.49
2:A:758:THR:HG23	2:A:759:LEU:N	2.28	0.49
2:A:911:ASN:HD22	2:A:911:ASN:C	2.12	0.49
2:A:1220:LYS:NZ	3:B:27:GLU:OE2	2.46	0.49
1:C:128:TYR:CE2	1:C:137:ARG:NH2	2.74	0.49
2:A:125:HIS:ND1	2:A:126:SER:N	2.60	0.49
3:B:54:PHE:CE1	3:B:124:TYR:CD2	2.87	0.49
3:B:89:ARG:O	3:B:108:ILE:HA	2.13	0.49
3:B:126:LEU:HD13	3:B:128:PHE:CE1	2.46	0.49
2:A:291:ASN:ND2	2:A:292:THR:N	2.60	0.49
2:A:750:ILE:O	2:A:753:CYS:HB3	2.12	0.49
2:A:1293:ARG:CB	2:A:1293:ARG:NH2	2.73	0.49
2:A:1532:MET:HG3	2:A:1616:ARG:HH12	1.77	0.49
1:C:34:VAL:CG2	1:C:142:ILE:CG1	2.91	0.48
2:A:1573:TYR:CD1	2:A:1573:TYR:C	2.85	0.48
2:A:734:LYS:CE	2:A:799:ASP:CG	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1218:ARG:CZ	2:A:1218:ARG:CB	2.91	0.48
2:A:1509:PHE:CA	2:A:1568:SER:CB	2.92	0.48
2:A:1667:ALA:O	2:A:1668:TYR:HB2	2.13	0.48
2:A:349:TRP:HA	2:A:349:TRP:HE3	1.78	0.48
2:A:833:VAL:HG13	2:A:834:LEU:N	2.28	0.48
2:A:842:VAL:O	2:A:845:LEU:HG	2.13	0.48
2:A:890:LYS:HZ3	2:A:890:LYS:HB3	1.76	0.48
2:A:1321:ILE:CD1	2:A:1456:ILE:HG12	2.42	0.48
2:A:1574:PHE:CD1	2:A:1580:ILE:HD11	2.36	0.48
2:A:1760:LEU:HD23	2:A:1760:LEU:C	2.33	0.48
2:A:116:ARG:NH2	2:A:176:PHE:HB2	2.28	0.48
1:C:34:VAL:HG23	1:C:35:PRO:N	2.29	0.48
2:A:339:TYR:HB2	2:A:341:TYR:CD2	2.49	0.48
2:A:803:TYR:CE2	2:A:809:ASN:OD1	2.67	0.48
2:A:1318:ILE:HG13	2:A:1319:PRO:N	2.28	0.48
2:A:1407:GLY:N	6:A:2007:9SL:O01	2.47	0.48
2:A:1497:ILE:HG22	2:A:1498:PRO:CD	2.44	0.48
2:A:1517:PHE:CD1	2:A:1517:PHE:C	2.85	0.48
2:A:1254:PHE:HD1	2:A:1260:TRP:CE2	2.32	0.48
2:A:1373:LEU:O	2:A:1377:SER:HB2	2.13	0.48
2:A:1408:TRP:CD1	2:A:1409:THR:CG2	2.97	0.48
3:B:174:LEU:O	3:B:178:MET:HG2	2.13	0.48
2:A:284:GLU:HB3	2:A:289:ILE:HD11	1.95	0.48
2:A:293:LEU:CD1	2:A:298:ASP:C	2.81	0.48
1:C:61:LYS:HA	1:C:85:MET:SD	2.54	0.48
1:C:107:LYS:CD	1:C:109:ASP:HB2	2.41	0.48
2:A:286:LEU:HD11	2:A:333:ILE:HG13	1.96	0.48
2:A:327:GLY:HA3	3:B:134:HIS:CD2	2.48	0.48
2:A:733:PHE:O	2:A:737:ILE:HG12	2.14	0.48
2:A:1503:LYS:CD	2:A:1503:LYS:N	2.73	0.48
2:A:963:PHE:CD1	2:A:963:PHE:C	2.87	0.48
2:A:1191:HIS:ND1	2:A:1192:SER:N	2.61	0.48
2:A:1532:MET:SD	2:A:1620:ILE:CD1	2.98	0.48
2:A:1641:LEU:HD23	2:A:1641:LEU:HA	1.73	0.48
3:B:53:THR:CG2	3:B:54:PHE:N	2.77	0.48
2:A:322:GLY:HA3	2:A:323:GLN:HG2	1.95	0.47
2:A:1301:LEU:HD22	2:A:1311:VAL:HG21	1.95	0.47
2:A:116:ARG:HH22	2:A:176:PHE:HB2	1.79	0.47
2:A:217:ARG:NH1	2:A:217:ARG:CB	2.75	0.47
2:A:273:HIS:O	2:A:314:LEU:HD12	2.13	0.47
2:A:279:SER:C	2:A:280:LEU:HD12	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1213:ASP:HB3	2:A:1663:MET:HE3	1.96	0.47
2:A:1503:LYS:H	2:A:1503:LYS:HD3	1.78	0.47
2:A:1710:SER:O	2:A:1711:LYS:HG2	2.14	0.47
2:A:783:PHE:O	2:A:787:PHE:CD2	2.65	0.47
3:B:88:GLY:O	3:B:89:ARG:HB2	2.14	0.47
2:A:196:ILE:O	2:A:200:TYR:CD1	2.65	0.47
2:A:247:ASP:OD2	2:A:1629:GLY:HA3	2.15	0.47
2:A:1242:LEU:O	2:A:1246:ILE:HG12	2.15	0.47
2:A:1460:PHE:CE2	2:A:1753:ASN:ND2	2.82	0.47
2:A:1509:PHE:HB2	2:A:1568:SER:CB	2.31	0.47
2:A:1574:PHE:CD1	2:A:1580:ILE:CD1	2.91	0.47
2:A:116:ARG:CZ	2:A:176:PHE:HB2	2.44	0.47
2:A:248:VAL:CG2	2:A:400:VAL:HG21	2.44	0.47
2:A:1459:ASN:O	2:A:1459:ASN:ND2	2.48	0.47
2:A:1635:PHE:CD1	2:A:1638:MET:CE	2.97	0.47
2:A:1719:LYS:H	2:A:1728:GLY:N	2.13	0.47
3:B:55:THR:CG2	3:B:56:GLU:N	2.77	0.47
2:A:285:THR:O	2:A:289:ILE:HG12	2.15	0.47
2:A:1179:TRP:HE1	2:A:1183:LYS:HE2	1.80	0.47
2:A:1318:ILE:HG12	2:A:1319:PRO:HD3	1.96	0.47
3:B:101:LEU:O	3:B:103:ASP:N	2.43	0.47
4:E:1:NAG:H82	4:E:1:NAG:C1	2.44	0.47
2:A:147:ASN:HD22	2:A:147:ASN:C	2.18	0.47
2:A:361:ASP:OD2	2:A:929:ILE:CB	2.63	0.47
2:A:840:LEU:C	2:A:842:VAL:H	2.18	0.47
2:A:890:LYS:CB	2:A:890:LYS:HZ3	2.28	0.47
2:A:761:MET:HE3	2:A:839:LEU:HB3	1.97	0.47
2:A:945:LEU:HD23	2:A:949:MET:CE	2.45	0.47
2:A:259:PHE:HB2	2:A:354:LEU:HD22	1.97	0.47
2:A:1502:ASN:CB	2:A:1504:ILE:HD11	2.20	0.47
2:A:114:PRO:CG	2:A:115:LEU:H	2.27	0.46
2:A:259:PHE:HB3	2:A:354:LEU:HD21	1.97	0.46
2:A:276:PHE:CE2	2:A:280:LEU:HD21	2.47	0.46
2:A:795:LEU:HD13	2:A:803:TYR:CE2	2.49	0.46
2:A:1366:ASN:OD1	2:A:1366:ASN:N	2.46	0.46
2:A:1419:VAL:HG12	2:A:1425:PRO:HA	1.96	0.46
2:A:171:ILE:HD12	2:A:172:LEU:N	2.30	0.46
2:A:204:PHE:O	2:A:205:VAL:C	2.53	0.46
2:A:321:SER:OG	2:A:322:GLY:N	2.48	0.46
2:A:954:ILE:O	2:A:958:VAL:HG23	2.16	0.46
2:A:1420:ASN:HB3	2:A:1423:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:51:ALA:CB	3:B:127:LEU:HA	2.44	0.46
2:A:219:LEU:O	2:A:222:LEU:HB2	2.14	0.46
2:A:333:ILE:HG22	2:A:334:GLY:N	2.30	0.46
2:A:734:LYS:CE	2:A:799:ASP:OD1	2.38	0.46
2:A:1200:LEU:HD23	2:A:1201:MET:HE2	1.98	0.46
2:A:1509:PHE:HA	2:A:1568:SER:HB3	1.95	0.46
2:A:1623:LEU:HD23	2:A:1623:LEU:HA	1.75	0.46
2:A:132:ILE:CD1	2:A:166:GLU:HB3	2.23	0.46
2:A:176:PHE:HD2	2:A:178:VAL:HG21	1.80	0.46
2:A:217:ARG:HG2	2:A:217:ARG:HH11	1.80	0.46
2:A:315:CYS:CB	2:A:324:CYS:SG	3.00	0.46
2:A:399:ALA:O	2:A:403:MET:HB2	2.14	0.46
2:A:825:LEU:HD22	2:A:825:LEU:HA	1.79	0.46
2:A:1218:ARG:HB3	2:A:1218:ARG:CZ	2.45	0.46
2:A:1508:ILE:CG2	2:A:1564:LEU:CD1	2.93	0.46
2:A:1709:ASN:HB2	2:A:1714:ASP:CB	2.41	0.46
1:C:34:VAL:CG1	1:C:50:CYS:SG	2.96	0.46
3:B:66:GLU:C	3:B:67:PHE:CD1	2.88	0.46
2:A:133:MET:SD	2:A:133:MET:C	2.94	0.46
2:A:398:LEU:HD12	2:A:960:LEU:HD11	1.97	0.46
2:A:909:HIS:HD2	2:A:911:ASN:N	2.07	0.46
2:A:1349:GLU:HG3	2:A:1351:ILE:HG22	1.98	0.46
2:A:1497:ILE:HG22	2:A:1498:PRO:HD2	1.97	0.46
2:A:1571:HIS:CD2	2:A:1571:HIS:H	2.33	0.46
2:A:206:ASN:OD1	2:A:206:ASN:N	2.48	0.46
2:A:218:VAL:CG1	2:A:879:ILE:HG23	2.46	0.46
2:A:388:LEU:O	2:A:388:LEU:HD13	2.15	0.46
2:A:395:ASN:ND2	2:A:1755:TYR:CD1	2.83	0.46
2:A:214:ARG:HA	2:A:214:ARG:HD3	1.61	0.46
2:A:293:LEU:HD12	2:A:298:ASP:CG	2.30	0.46
2:A:741:VAL:CG2	2:A:742:MET:N	2.78	0.46
2:A:854:MET:O	2:A:858:ILE:HG13	2.16	0.46
2:A:931:THR:HG22	2:A:948:TYR:OH	2.16	0.46
3:B:54:PHE:CD2	3:B:124:TYR:HB2	2.51	0.46
2:A:169:VAL:HG23	2:A:170:LYS:N	2.31	0.46
2:A:964:LEU:HD13	2:A:964:LEU:HA	1.80	0.46
2:A:1308:ARG:NH2	2:A:1308:ARG:HB3	2.30	0.46
3:B:154:MET:O	3:B:158:VAL:HG23	2.16	0.46
2:A:136:ILE:HG23	2:A:137:LEU:N	2.30	0.45
2:A:902:ASP:HB3	2:A:904:THR:HG22	1.97	0.45
2:A:971:PHE:CD1	2:A:971:PHE:C	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:361:ASP:OD2	2:A:929:ILE:HB	2.15	0.45
2:A:788:ALA:HA	2:A:816:VAL:HG11	1.97	0.45
2:A:1179:TRP:CD1	2:A:1183:LYS:CE	2.99	0.45
2:A:1325:LEU:HD12	2:A:1329:LEU:HG	1.99	0.45
3:B:54:PHE:CE2	3:B:124:TYR:CB	2.96	0.45
2:A:116:ARG:NH1	2:A:176:PHE:HA	2.29	0.45
2:A:336:ASN:HD22	2:A:343:SER:CB	2.21	0.45
2:A:772:PHE:O	2:A:772:PHE:CD1	2.70	0.45
2:A:1212:GLU:O	2:A:1213:ASP:CB	2.64	0.45
2:A:1280:TYR:O	2:A:1283:LEU:HD21	2.17	0.45
3:B:67:PHE:CD2	3:B:120:GLU:HG3	2.49	0.45
2:A:132:ILE:CD1	2:A:166:GLU:CG	2.94	0.45
2:A:276:PHE:N	2:A:329:THR:O	2.46	0.45
2:A:1404:THR:O	2:A:1405:PHE:HB2	2.15	0.45
2:A:1273:LEU:HD12	2:A:1273:LEU:C	2.36	0.45
2:A:1511:LEU:C	2:A:1511:LEU:CD2	2.85	0.45
2:A:1628:LYS:CD	2:A:1628:LYS:C	2.85	0.45
2:A:248:VAL:HG21	2:A:400:VAL:HG21	1.98	0.45
2:A:314:LEU:HD12	2:A:314:LEU:HA	1.86	0.45
2:A:956:ASN:N	2:A:956:ASN:HD22	2.14	0.45
2:A:1508:ILE:HG21	2:A:1564:LEU:CD1	2.46	0.45
2:A:147:ASN:HD22	2:A:147:ASN:N	2.13	0.45
2:A:217:ARG:CG	2:A:217:ARG:NH1	2.79	0.45
2:A:846:ALA:HA	2:A:852:LEU:HD23	1.99	0.45
2:A:1273:LEU:O	2:A:1277:THR:OG1	2.34	0.45
2:A:1295:LEU:CD1	2:A:1298:LEU:CD2	2.86	0.45
2:A:1364:VAL:CG2	2:A:1370:CYS:HA	2.46	0.45
3:B:38:ILE:HB	3:B:106:ILE:HG22	1.99	0.45
3:B:128:PHE:CD1	3:B:128:PHE:N	2.84	0.45
2:A:759:LEU:HD22	2:A:759:LEU:HA	1.74	0.45
2:A:1293:ARG:C	2:A:1295:LEU:N	2.70	0.45
2:A:1405:PHE:HE1	2:A:1441:ILE:HD13	1.81	0.45
2:A:1607:THR:HG23	2:A:1610:ARG:NH1	2.25	0.45
2:A:123:LEU:C	2:A:123:LEU:CD2	2.86	0.45
2:A:147:ASN:C	2:A:147:ASN:ND2	2.70	0.45
2:A:754:ILE:HG12	2:A:787:PHE:HE1	1.77	0.45
2:A:1444:GLY:O	2:A:1448:THR:OG1	2.32	0.45
2:A:1497:ILE:HG12	2:A:1572:TYR:HB3	1.98	0.45
2:A:1681:PHE:HD1	2:A:1687:SER:OG	1.99	0.45
2:A:766:HIS:CD2	2:A:766:HIS:O	2.70	0.45
2:A:843:PHE:C	2:A:845:LEU:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:936:MET:HE2	2:A:945:LEU:HD12	1.99	0.45
2:A:1343:PHE:HB3	2:A:1347:PHE:CE1	2.51	0.45
2:A:1355:ASP:N	2:A:1355:ASP:OD1	2.50	0.45
2:A:1710:SER:O	2:A:1711:LYS:HE3	2.17	0.45
1:C:55:CYS:O	1:C:56:TYR:CD2	2.70	0.44
2:A:163:TYR:O	2:A:166:GLU:HG3	2.17	0.44
2:A:176:PHE:O	2:A:176:PHE:CG	2.70	0.44
2:A:332:LYS:C	2:A:333:ILE:HG12	2.37	0.44
2:A:371:LEU:O	2:A:375:GLY:N	2.44	0.44
2:A:1530:VAL:HA	2:A:1533:MET:HG3	1.99	0.44
2:A:1719:LYS:H	2:A:1728:GLY:H	1.65	0.44
2:A:191:LEU:C	2:A:191:LEU:CD2	2.85	0.44
2:A:279:SER:C	2:A:280:LEU:CD1	2.86	0.44
2:A:280:LEU:CD1	2:A:280:LEU:N	2.80	0.44
2:A:854:MET:HE2	2:A:854:MET:HB2	1.88	0.44
2:A:1491:LYS:C	2:A:1491:LYS:CD	2.86	0.44
2:A:1496:PRO:C	2:A:1497:ILE:CG1	2.85	0.44
1:C:131:ASN:O	1:C:134:ASP:N	2.51	0.44
2:A:300:ARG:NH1	2:A:300:ARG:CG	2.75	0.44
2:A:794:LYS:CG	2:A:803:TYR:CE1	2.75	0.44
2:A:1611:VAL:O	2:A:1614:LEU:HB2	2.17	0.44
1:C:55:CYS:O	1:C:56:TYR:CG	2.69	0.44
2:A:121:LYS:HB2	2:A:121:LYS:HE3	1.58	0.44
2:A:164:THR:HG21	2:A:200:TYR:HH	1.76	0.44
2:A:197:VAL:O	2:A:201:LEU:HB2	2.18	0.44
2:A:231:LEU:HD12	2:A:231:LEU:HA	1.73	0.44
2:A:834:LEU:O	2:A:837:PHE:CB	2.60	0.44
2:A:1270:LEU:C	2:A:1270:LEU:CD1	2.85	0.44
2:A:1298:LEU:HD12	2:A:1301:LEU:CD1	2.48	0.44
2:A:1691:LEU:HD13	2:A:1743:TYR:CE2	2.52	0.44
3:B:141:LYS:HZ2	3:B:141:LYS:HB3	1.81	0.44
2:A:743:ASP:N	2:A:744:PRO:HD2	2.32	0.44
2:A:1281:SER:OG	2:A:1282:ASP:OD1	2.32	0.44
2:A:1364:VAL:HG23	2:A:1370:CYS:CA	2.47	0.44
2:A:1569:LEU:HB2	2:A:1573:TYR:HB2	2.00	0.44
2:A:738:TYR:O	2:A:738:TYR:CD1	2.70	0.44
2:A:1280:TYR:O	2:A:1280:TYR:CD1	2.70	0.44
2:A:1280:TYR:O	2:A:1280:TYR:HD1	2.00	0.44
2:A:1292:LEU:HD12	2:A:1292:LEU:HA	1.78	0.44
3:B:119:TYR:N	3:B:142:ILE:O	2.46	0.44
1:C:41:LEU:HD21	1:C:147:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:234:ILE:HG13	2:A:868:ASN:HB3	2.00	0.44
2:A:971:PHE:HD1	2:A:972:SER:HB2	1.83	0.44
1:C:61:LYS:HG3	1:C:85:MET:SD	2.58	0.44
2:A:867:GLY:HA2	2:A:870:THR:HG22	2.00	0.44
2:A:896:VAL:HG12	2:A:905:LEU:HD13	2.00	0.44
2:A:1287:LYS:C	2:A:1287:LYS:CD	2.85	0.44
2:A:1495:LYS:HE3	2:A:1495:LYS:N	2.33	0.44
3:B:88:GLY:O	3:B:89:ARG:CB	2.65	0.44
2:A:823:LEU:C	2:A:823:LEU:CD2	2.85	0.44
2:A:1670:LYS:HB3	2:A:1670:LYS:HE3	1.71	0.44
3:B:117:GLY:O	3:B:143:HIS:HD2	2.00	0.44
2:A:139:ASN:O	2:A:139:ASN:ND2	2.39	0.43
2:A:283:ASN:HB2	5:A:2006:NAG:H2	1.99	0.43
2:A:327:GLY:CA	3:B:134:HIS:CD2	3.01	0.43
2:A:410:GLN:HA	2:A:413:ILE:HG22	1.99	0.43
2:A:757:ASN:O	2:A:757:ASN:ND2	2.51	0.43
2:A:765:HIS:HA	2:A:1390:ASP:O	2.17	0.43
2:A:789:ALA:HA	2:A:792:VAL:HG12	2.00	0.43
2:A:1213:ASP:HB3	2:A:1663:MET:CE	2.48	0.43
2:A:1407:GLY:CA	6:A:2007:9SL:O01	2.66	0.43
2:A:144:THR:HG23	2:A:913:PHE:CB	2.48	0.43
2:A:730:TRP:O	2:A:734:LYS:N	2.43	0.43
2:A:772:PHE:CD1	2:A:772:PHE:C	2.91	0.43
1:C:55:CYS:C	1:C:56:TYR:CG	2.90	0.43
2:A:118:ILE:N	2:A:118:ILE:CD1	2.73	0.43
2:A:769:THR:HG23	2:A:772:PHE:HB2	1.99	0.43
2:A:1317:ALA:CB	2:A:1459:ASN:OD1	2.66	0.43
2:A:1506:GLY:O	2:A:1510:ASP:N	2.44	0.43
3:B:101:LEU:N	3:B:101:LEU:HD13	2.33	0.43
1:C:56:TYR:HD1	2:A:898:LYS:HD2	1.83	0.43
2:A:291:ASN:HD22	2:A:291:ASN:C	2.21	0.43
2:A:782:VAL:O	2:A:786:ILE:HG12	2.17	0.43
2:A:899:ILE:HG23	2:A:938:VAL:HG13	1.99	0.43
2:A:1437:PHE:O	2:A:1441:ILE:HG13	2.17	0.43
2:A:1677:ASP:CG	3:B:46:ARG:NH1	2.72	0.43
3:B:51:ALA:HB3	3:B:127:LEU:CD1	2.41	0.43
3:B:57:TRP:HH2	3:B:142:ILE:HD13	1.78	0.43
2:A:882:VAL:O	2:A:886:GLN:HG2	2.18	0.43
1:C:61:LYS:HG3	1:C:85:MET:HE1	1.99	0.43
2:A:196:ILE:HD12	2:A:197:VAL:CA	2.48	0.43
2:A:923:VAL:HG13	2:A:928:TRP:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1675:ILE:HD12	2:A:1706:PRO:HG3	2.01	0.43
1:C:135:ARG:NH2	1:C:135:ARG:CG	2.73	0.43
2:A:140:CYS:HA	2:A:143:MET:HG3	2.00	0.43
2:A:737:ILE:O	2:A:740:ILE:HB	2.19	0.43
2:A:1189:VAL:HG11	2:A:1244:LYS:HD3	2.00	0.43
2:A:1321:ILE:CD1	2:A:1456:ILE:CG1	2.97	0.43
2:A:1760:LEU:C	2:A:1760:LEU:CD2	2.86	0.43
2:A:136:ILE:CD1	2:A:136:ILE:C	2.85	0.43
2:A:967:LEU:CD2	2:A:967:LEU:C	2.85	0.43
2:A:1232:ILE:HD11	3:B:166:LEU:HB3	2.01	0.43
2:A:1457:ILE:HD12	2:A:1458:ASP:CA	2.48	0.43
2:A:1764:SER:HA	2:A:1767:THR:HG22	2.01	0.43
1:C:108:TYR:N	1:C:108:TYR:CD1	2.86	0.43
2:A:168:LEU:HD23	2:A:169:VAL:CA	2.49	0.43
2:A:1218:ARG:NH2	2:A:1218:ARG:CB	2.82	0.43
2:A:1430:SER:HB3	2:A:1433:MET:CG	2.46	0.43
2:A:1467:LEU:HD21	2:A:1472:ILE:HG22	2.00	0.43
2:A:1650:LEU:C	2:A:1650:LEU:CD1	2.86	0.43
1:C:40:VAL:HG22	1:C:44:SER:OG	2.19	0.43
1:C:58:VAL:CG1	1:C:63:PHE:HB2	2.46	0.43
2:A:151:TRP:CE3	2:A:152:THR:N	2.87	0.43
2:A:262:ILE:HG13	2:A:1617:ILE:HD13	2.00	0.43
2:A:338:ASP:OD2	2:A:342:THR:OG1	2.29	0.43
2:A:346:THR:HG22	2:A:347:PHE:N	2.34	0.43
2:A:401:VAL:HG11	2:A:960:LEU:HD22	2.00	0.43
2:A:1675:ILE:HD12	2:A:1706:PRO:CG	2.49	0.43
2:A:1763:PHE:O	2:A:1767:THR:HB	2.18	0.43
1:C:101:PHE:CZ	1:C:105:PRO:HD3	2.54	0.42
2:A:207:LEU:HD12	2:A:213:LEU:HG	2.00	0.42
2:A:764:GLU:C	2:A:765:HIS:ND1	2.73	0.42
2:A:795:LEU:HD13	2:A:803:TYR:CZ	2.54	0.42
2:A:1408:TRP:HZ3	2:A:1441:ILE:CD1	2.32	0.42
2:A:1412:MET:CE	2:A:1434:TYR:HD1	2.29	0.42
2:A:1487:LYS:HA	2:A:1487:LYS:HD3	1.58	0.42
3:B:101:LEU:O	3:B:102:GLN:CB	2.65	0.42
3:B:178:MET:HG2	3:B:178:MET:H	1.63	0.42
1:C:34:VAL:HG23	1:C:35:PRO:O	2.18	0.42
2:A:1467:LEU:CD1	2:A:1472:ILE:CG2	2.90	0.42
3:B:67:PHE:N	3:B:67:PHE:HD1	2.17	0.42
1:C:30:MET:CG	1:C:138:GLY:HA2	2.37	0.42
1:C:59:ASN:HB3	1:C:62:GLN:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1286:ILE:HD12	2:A:1287:LYS:N	2.34	0.42
2:A:1420:ASN:CB	2:A:1423:LYS:HG3	2.50	0.42
2:A:1460:PHE:CD2	2:A:1756:ILE:HG13	2.53	0.42
2:A:1532:MET:HE2	2:A:1616:ARG:NH1	2.35	0.42
2:A:415:GLU:CD	2:A:416:ALA:N	2.73	0.42
2:A:845:LEU:HG	2:A:845:LEU:H	1.58	0.42
2:A:333:ILE:CG2	2:A:334:GLY:N	2.83	0.42
2:A:911:ASN:O	2:A:911:ASN:ND2	2.40	0.42
2:A:1369:GLU:HG2	4:E:1:NAG:H62	2.00	0.42
3:B:67:PHE:CE2	3:B:120:GLU:CG	2.94	0.42
2:A:1459:ASN:ND2	2:A:1459:ASN:C	2.73	0.42
2:A:1764:SER:HA	2:A:1767:THR:CG2	2.49	0.42
2:A:370:THR:O	2:A:374:ALA:HB3	2.19	0.42
2:A:406:LYS:HB2	2:A:406:LYS:HE2	1.78	0.42
2:A:738:TYR:CD1	2:A:738:TYR:C	2.93	0.42
2:A:1317:ALA:HA	2:A:1459:ASN:OD1	2.19	0.42
2:A:1373:LEU:O	2:A:1377:SER:N	2.52	0.42
3:B:71:LEU:HD22	3:B:106:ILE:HD11	2.00	0.42
2:A:380:ILE:O	2:A:384:VAL:HG12	2.19	0.42
2:A:1509:PHE:CA	2:A:1568:SER:OG	2.68	0.42
3:B:112:THR:CG2	3:B:113:TYR:H	2.33	0.42
2:A:128:PHE:HZ	2:A:166:GLU:HA	1.85	0.42
2:A:1325:LEU:HD13	2:A:1325:LEU:O	2.20	0.42
2:A:254:PHE:O	2:A:258:VAL:HG23	2.20	0.42
2:A:1340:VAL:O	2:A:1344:ALA:CB	2.68	0.42
2:A:1496:PRO:O	2:A:1497:ILE:CB	2.67	0.42
2:A:1613:ARG:C	2:A:1615:ALA:N	2.74	0.42
1:C:52:PHE:CB	1:C:129:ILE:CD1	2.82	0.41
2:A:202:THR:HG1	2:A:214:ARG:NH1	2.17	0.41
2:A:842:VAL:O	2:A:845:LEU:CD1	2.67	0.41
2:A:1358:ARG:CZ	2:A:1417:ASP:OD2	2.68	0.41
2:A:1539:GLN:O	2:A:1540:SER:CB	2.68	0.41
3:B:26:SER:OG	3:B:142:ILE:CG2	2.68	0.41
2:A:198:PHE:CE2	2:A:216:PHE:CD2	3.08	0.41
2:A:396:LEU:HD23	2:A:396:LEU:HA	1.76	0.41
2:A:739:PHE:O	2:A:742:MET:SD	2.78	0.41
2:A:803:TYR:HD2	2:A:804:PHE:CE1	2.39	0.41
2:A:960:LEU:HD23	2:A:960:LEU:C	2.41	0.41
2:A:1722:PRO:CB	3:B:103:ASP:HB2	2.51	0.41
2:A:1295:LEU:HD13	2:A:1295:LEU:HA	1.89	0.41
2:A:1500:PRO:HG2	2:A:1505:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1614:LEU:HD12	2:A:1614:LEU:HA	1.87	0.41
3:B:32:TYR:CE2	3:B:113:TYR:HE1	2.18	0.41
3:B:59:PHE:CZ	3:B:61:GLN:HA	2.56	0.41
2:A:301:LYS:NZ	3:B:131:ASN:OD1	2.39	0.41
2:A:801:TYR:HD1	2:A:801:TYR:HA	1.76	0.41
2:A:1408:TRP:CZ3	2:A:1441:ILE:HD11	2.55	0.41
2:A:1566:LEU:HA	2:A:1566:LEU:HD12	1.75	0.41
2:A:1600:GLU:O	2:A:1603:PHE:CD1	2.74	0.41
2:A:1668:TYR:O	2:A:1729:ASP:HB2	2.19	0.41
2:A:1673:ASP:O	2:A:1702:GLY:O	2.39	0.41
3:B:50:ASN:ND2	3:B:50:ASN:C	2.73	0.41
3:B:162:MET:O	3:B:162:MET:SD	2.79	0.41
2:A:757:ASN:ND2	2:A:757:ASN:C	2.73	0.41
2:A:1450:ASN:C	2:A:1450:ASN:ND2	2.73	0.41
2:A:1547:LEU:HD23	2:A:1547:LEU:HA	1.85	0.41
2:A:1668:TYR:CE2	2:A:1726:VAL:HG21	2.56	0.41
3:B:59:PHE:CD2	3:B:119:TYR:CE1	3.08	0.41
1:C:52:PHE:HB3	1:C:129:ILE:HD13	1.98	0.41
2:A:147:ASN:ND2	2:A:147:ASN:O	2.53	0.41
2:A:219:LEU:HA	2:A:222:LEU:HD12	2.02	0.41
2:A:291:ASN:ND2	2:A:291:ASN:C	2.74	0.41
2:A:1594:PHE:HD1	2:A:1594:PHE:HA	1.77	0.41
2:A:1707:ILE:CG2	2:A:1736:GLY:HA3	2.51	0.41
3:B:32:TYR:CD1	3:B:33:GLY:N	2.88	0.41
2:A:175:GLY:CA	2:A:180:GLU:HA	2.50	0.41
2:A:191:LEU:HD23	2:A:191:LEU:C	2.39	0.41
2:A:1218:ARG:HD2	3:B:22:VAL:HG13	2.03	0.41
2:A:1543:MET:O	2:A:1543:MET:SD	2.79	0.41
2:A:1767:THR:HG23	2:A:1768:GLU:N	2.35	0.41
3:B:23:GLU:OE1	3:B:140:LYS:NZ	2.33	0.41
3:B:46:ARG:NH2	3:B:48:GLU:CD	2.73	0.41
3:B:179:ILE:HD13	3:B:179:ILE:HA	1.86	0.41
1:C:32:VAL:HG12	1:C:50:CYS:SG	2.61	0.41
2:A:210:VAL:HG22	2:A:214:ARG:HG2	2.03	0.41
2:A:1456:ILE:HG21	2:A:1752:VAL:HG11	2.02	0.41
2:A:1508:ILE:CG2	2:A:1564:LEU:HD11	2.50	0.41
3:B:121:CYS:O	3:B:121:CYS:SG	2.79	0.41
1:C:103:GLY:C	1:C:105:PRO:HD3	2.40	0.41
2:A:174:ARG:CD	2:A:182:THR:HG21	2.16	0.41
2:A:180:GLU:HB2	2:A:183:PHE:HB3	2.02	0.41
2:A:365:ASN:HD22	2:A:365:ASN:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:379:MET:HE2	2:A:379:MET:HB3	1.88	0.41
2:A:395:ASN:OD1	2:A:1755:TYR:HA	2.20	0.41
2:A:792:VAL:CG1	2:A:793:LEU:N	2.83	0.41
2:A:1194:PHE:CD1	2:A:1194:PHE:C	2.94	0.41
2:A:1306:GLY:HA2	2:A:1475:THR:CG2	2.50	0.41
2:A:1460:PHE:HD1	2:A:1460:PHE:HA	1.78	0.41
2:A:1548:TYR:CD1	2:A:1548:TYR:C	2.94	0.41
2:A:1553:VAL:HG12	2:A:1557:LEU:HD22	2.02	0.41
2:A:1596:ALA:CB	2:A:1609:PHE:CE2	2.85	0.41
2:A:1677:ASP:OD1	2:A:1677:ASP:N	2.53	0.41
3:B:44:LYS:NZ	3:B:100:ASP:OD2	2.54	0.41
3:B:50:ASN:C	3:B:50:ASN:HD22	2.24	0.41
2:A:403:MET:O	2:A:403:MET:SD	2.79	0.41
2:A:758:THR:CG2	2:A:759:LEU:N	2.84	0.41
2:A:772:PHE:HD1	2:A:772:PHE:C	2.24	0.41
2:A:1634:LEU:HD12	2:A:1634:LEU:HA	1.86	0.41
3:B:46:ARG:NH2	3:B:48:GLU:OE1	2.53	0.41
1:C:59:ASN:CB	1:C:62:GLN:CB	2.86	0.40
2:A:196:ILE:C	2:A:196:ILE:CD1	2.85	0.40
2:A:272:LYS:O	2:A:274:LYS:HG3	2.21	0.40
2:A:851:THR:O	2:A:854:MET:HB3	2.21	0.40
2:A:1326:LEU:HD22	2:A:1326:LEU:HA	1.81	0.40
2:A:1647:ILE:HG23	2:A:1750:VAL:HG13	2.02	0.40
3:B:75:ASN:CG	3:B:76:GLU:N	2.74	0.40
2:A:146:ASN:O	2:A:147:ASN:CB	2.69	0.40
2:A:176:PHE:CD2	2:A:178:VAL:CG2	3.05	0.40
2:A:798:MET:O	2:A:799:ASP:CB	2.70	0.40
2:A:798:MET:HE3	2:A:803:TYR:HA	1.92	0.40
2:A:952:MET:O	2:A:956:ASN:HB2	2.21	0.40
2:A:1268:VAL:HG13	2:A:1289:LEU:HD13	2.02	0.40
3:B:32:TYR:HE2	3:B:113:TYR:CD1	2.30	0.40
2:A:114:PRO:CG	2:A:115:LEU:N	2.85	0.40
2:A:164:THR:O	2:A:168:LEU:HB3	2.22	0.40
2:A:1238:ILE:CD1	2:A:1270:LEU:HD21	2.40	0.40
2:A:1580:ILE:O	2:A:1584:VAL:HG23	2.21	0.40
3:B:79:GLN:HE21	3:B:79:GLN:HB2	1.55	0.40
2:A:274:LYS:NZ	2:A:333:ILE:O	2.52	0.40
2:A:971:PHE:CD1	2:A:972:SER:HB2	2.56	0.40
2:A:1241:MET:O	2:A:1244:LYS:HB2	2.22	0.40
2:A:1408:TRP:HZ3	2:A:1441:ILE:HD11	1.87	0.40
2:A:1412:MET:O	2:A:1416:VAL:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1511:LEU:HD21	2:A:1517:PHE:CD2	2.57	0.40
2:A:1545:GLU:OE1	2:A:1545:GLU:CA	2.70	0.40
2:A:1666:PHE:O	2:A:1669:VAL:HG22	2.21	0.40
2:A:1737:ILE:O	2:A:1741:VAL:HG23	2.21	0.40
2:A:251:LEU:HD13	2:A:1630:ILE:CG2	2.46	0.40
2:A:338:ASP:O	2:A:339:TYR:CB	2.70	0.40
2:A:742:MET:HB2	2:A:746:VAL:CG2	2.51	0.40
2:A:1360:PRO:O	2:A:1361:ALA:CB	2.69	0.40
2:A:1457:ILE:CD1	2:A:1458:ASP:N	2.73	0.40
3:B:37:LYS:HB2	3:B:107:PHE:CD1	2.53	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	C	118/215 (55%)	110 (93%)	5 (4%)	3 (2%)	5 32
2	A	1132/2031 (56%)	1096 (97%)	20 (2%)	16 (1%)	11 46
3	B	171/218 (78%)	167 (98%)	4 (2%)	0	100 100
All	All	1421/2464 (58%)	1373 (97%)	29 (2%)	19 (1%)	16 47

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	147	ASN
2	A	896	VAL
2	A	1431	LEU
2	A	841	ARG
2	A	844	LYS
2	A	1213	ASP
2	A	1294	ALA

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Mol	Chain	Res	Type
2	A	1540	SER
1	C	56	TYR
1	C	76	SER
2	A	305	TYR
2	A	903	CYS
2	A	1386	LYS
2	A	1497	ILE
2	A	1605	SER
1	C	147	LEU
2	A	1498	PRO
2	A	1604	VAL
2	A	767	PRO

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	C	113/193 (58%)	100 (88%)	13 (12%)	5 24
2	A	1018/1809 (56%)	752 (74%)	266 (26%)	0 2
3	B	157/190 (83%)	109 (69%)	48 (31%)	0 0
All	All	1288/2192 (59%)	961 (75%)	327 (25%)	2 2

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	MET
1	C	51	THR
1	C	52	PHE
1	C	55	CYS
1	C	59	ASN
1	C	61	LYS
1	C	74	ASN
1	C	107	LYS
1	C	129	ILE
1	C	134	ASP

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Mol	Chain	Res	Type
1	C	135	ARG
1	C	147	LEU
1	C	148	MET
2	A	115	LEU
2	A	117	ARG
2	A	118	ILE
2	A	121	LYS
2	A	122	ILE
2	A	124	VAL
2	A	126	SER
2	A	127	LEU
2	A	130	MET
2	A	131	LEU
2	A	134	CYS
2	A	136	ILE
2	A	137	LEU
2	A	138	THR
2	A	139	ASN
2	A	143	MET
2	A	145	MET
2	A	146	ASN
2	A	147	ASN
2	A	153	LYS
2	A	166	GLU
2	A	167	SER
2	A	168	LEU
2	A	171	ILE
2	A	181	PHE
2	A	184	LEU
2	A	191	LEU
2	A	192	ASP
2	A	204	PHE
2	A	206	ASN
2	A	207	LEU
2	A	209	ASN
2	A	214	ARG
2	A	217	ARG
2	A	220	ARG
2	A	227	VAL
2	A	235	VAL
2	A	238	LEU
2	A	243	LYS

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Mol	Chain	Res	Type
2	A	247	ASP
2	A	249	MET
2	A	255	CYS
2	A	268	MET
2	A	271	LEU
2	A	280	LEU
2	A	282	ASN
2	A	285	THR
2	A	286	LEU
2	A	291	ASN
2	A	293	LEU
2	A	298	ASP
2	A	299	PHE
2	A	300	ARG
2	A	310	LYS
2	A	311	ASP
2	A	313	LEU
2	A	314	LEU
2	A	318	SER
2	A	329	THR
2	A	348	SER
2	A	349	TRP
2	A	354	LEU
2	A	356	ARG
2	A	358	MET
2	A	362	TYR
2	A	364	GLU
2	A	365	ASN
2	A	366	LEU
2	A	370	THR
2	A	379	MET
2	A	387	PHE
2	A	395	ASN
2	A	403	MET
2	A	408	GLN
2	A	410	GLN
2	A	412	ASN
2	A	414	GLU
2	A	415	GLU
2	A	726	CYS
2	A	727	SER
2	A	729	TYR

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Mol	Chain	Res	Type
2	A	732	LYS
2	A	733	PHE
2	A	736	CYS
2	A	748	LEU
2	A	750	ILE
2	A	751	THR
2	A	755	VAL
2	A	759	LEU
2	A	763	MET
2	A	764	GLU
2	A	765	HIS
2	A	768	MET
2	A	769	THR
2	A	771	GLU
2	A	772	PHE
2	A	773	LYS
2	A	774	ASN
2	A	776	LEU
2	A	780	ASN
2	A	781	LEU
2	A	790	GLU
2	A	791	MET
2	A	794	LYS
2	A	795	LEU
2	A	796	ILE
2	A	801	TYR
2	A	808	TRP
2	A	818	LEU
2	A	820	LEU
2	A	825	LEU
2	A	831	LEU
2	A	834	LEU
2	A	835	ARG
2	A	837	PHE
2	A	838	ARG
2	A	839	LEU
2	A	840	LEU
2	A	841	ARG
2	A	845	LEU
2	A	848	SER
2	A	854	MET
2	A	869	LEU

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Mol	Chain	Res	Type
2	A	870	THR
2	A	871	LEU
2	A	873	LEU
2	A	887	LEU
2	A	890	LYS
2	A	896	VAL
2	A	898	LYS
2	A	901	ASP
2	A	905	LEU
2	A	910	MET
2	A	911	ASN
2	A	916	SER
2	A	918	LEU
2	A	929	ILE
2	A	941	GLN
2	A	943	MET
2	A	944	CYS
2	A	945	LEU
2	A	952	MET
2	A	956	ASN
2	A	962	LEU
2	A	964	LEU
2	A	966	LEU
2	A	967	LEU
2	A	968	LEU
2	A	1176	LYS
2	A	1187	LYS
2	A	1189	VAL
2	A	1191	HIS
2	A	1204	LEU
2	A	1206	SER
2	A	1209	LEU
2	A	1218	ARG
2	A	1219	LYS
2	A	1223	LYS
2	A	1226	LEU
2	A	1246	ILE
2	A	1251	LYS
2	A	1264	LEU
2	A	1270	LEU
2	A	1274	VAL
2	A	1277	THR

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Mol	Chain	Res	Type
2	A	1278	LEU
2	A	1283	LEU
2	A	1286	ILE
2	A	1287	LYS
2	A	1289	LEU
2	A	1290	ARG
2	A	1293	ARG
2	A	1295	LEU
2	A	1299	ARG
2	A	1305	GLU
2	A	1307	MET
2	A	1309	VAL
2	A	1323	ASN
2	A	1325	LEU
2	A	1326	LEU
2	A	1331	PHE
2	A	1342	LEU
2	A	1350	CYS
2	A	1353	THR
2	A	1354	THR
2	A	1358	ARG
2	A	1385	LEU
2	A	1396	TYR
2	A	1399	LEU
2	A	1408	TRP
2	A	1409	THR
2	A	1419	VAL
2	A	1422	ASP
2	A	1424	GLN
2	A	1426	LYS
2	A	1449	LEU
2	A	1450	ASN
2	A	1452	PHE
2	A	1459	ASN
2	A	1461	ASN
2	A	1462	GLN
2	A	1464	LYS
2	A	1465	LYS
2	A	1467	LEU
2	A	1472	ILE
2	A	1474	MET
2	A	1478	GLN

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Mol	Chain	Res	Type
2	A	1479	LYS
2	A	1486	LYS
2	A	1488	LEU
2	A	1491	LYS
2	A	1495	LYS
2	A	1499	ARG
2	A	1503	LYS
2	A	1504	ILE
2	A	1511	LEU
2	A	1515	GLN
2	A	1517	PHE
2	A	1519	ILE
2	A	1520	SER
2	A	1527	LEU
2	A	1528	ASN
2	A	1533	MET
2	A	1534	VAL
2	A	1537	GLU
2	A	1543	MET
2	A	1551	ASN
2	A	1557	LEU
2	A	1561	GLU
2	A	1562	CYS
2	A	1565	LYS
2	A	1571	HIS
2	A	1573	TYR
2	A	1593	MET
2	A	1594	PHE
2	A	1598	LEU
2	A	1601	THR
2	A	1602	TYR
2	A	1605	SER
2	A	1608	LEU
2	A	1614	LEU
2	A	1616	ARG
2	A	1619	ARG
2	A	1621	LEU
2	A	1628	LYS
2	A	1634	LEU
2	A	1637	LEU
2	A	1644	LEU
2	A	1649	LEU

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Mol	Chain	Res	Type
2	A	1653	LEU
2	A	1661	PHE
2	A	1670	LYS
2	A	1671	LYS
2	A	1673	ASP
2	A	1683	THR
2	A	1687	SER
2	A	1691	LEU
2	A	1701	ASP
2	A	1704	LEU
2	A	1711	LYS
2	A	1718	LYS
2	A	1719	LYS
2	A	1725	SER
2	A	1749	LEU
2	A	1753	ASN
2	A	1754	MET
3	B	27	GLU
3	B	28	THR
3	B	29	GLU
3	B	34	MET
3	B	39	LEU
3	B	46	ARG
3	B	47	SER
3	B	48	GLU
3	B	50	ASN
3	B	60	ARG
3	B	65	GLU
3	B	66	GLU
3	B	67	PHE
3	B	76	GLU
3	B	78	LEU
3	B	79	GLN
3	B	80	LEU
3	B	82	GLU
3	B	84	GLU
3	B	85	ARG
3	B	90	VAL
3	B	93	ASN
3	B	95	SER
3	B	99	LYS
3	B	101	LEU

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Mol	Chain	Res	Type
3	B	102	GLN
3	B	104	LEU
3	B	109	THR
3	B	121	CYS
3	B	125	ARG
3	B	126	LEU
3	B	127	LEU
3	B	130	GLU
3	B	131	ASN
3	B	136	THR
3	B	138	VAL
3	B	141	LYS
3	B	149	LYS
3	B	159	SER
3	B	162	MET
3	B	166	LEU
3	B	174	LEU
3	B	178	MET
3	B	180	TYR
3	B	181	CYS
3	B	183	LYS
3	B	190	GLU
3	B	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	118	GLN
1	C	136	HIS
2	A	147	ASN
2	A	154	ASN
2	A	278	ASN
2	A	291	ASN
2	A	360	GLN
2	A	365	ASN
2	A	410	GLN
2	A	412	ASN
2	A	766	HIS
2	A	774	ASN
2	A	909	HIS
2	A	941	GLN
2	A	956	ASN

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Mol	Chain	Res	Type
2	A	1276	ASN
2	A	1378	GLN
2	A	1424	GLN
2	A	1450	ASN
2	A	1514	ASN
2	A	1528	ASN
2	A	1551	ASN
2	A	1571	HIS
2	A	1753	ASN
2	A	1762	ASN
3	B	50	ASN
3	B	79	GLN
3	B	102	GLN
3	B	115	HIS
3	B	134	HIS
3	B	143	HIS

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

4 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	$\#\|Z\| > 2$
4	NAG	D	1	4,2	14,14,15	0.44	0	17,19,21	0.98	1 (5%)
4	NAG	D	2	4	14,14,15	0.40	0	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	1	4,2	14,14,15	0.38	0	17,19,21	1.08	2 (11%)
4	NAG	E	2	4	14,14,15	0.41	0	17,19,21	1.18	2 (11%)

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	D	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	NAG	E	1	4,2	-	6/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	O5-C1-C2	-3.09	106.40	111.29
4	E	2	NAG	C1-O5-C5	-3.04	108.07	112.19
4	D	2	NAG	C1-O5-C5	2.69	115.83	112.19
4	E	2	NAG	O5-C5-C6	2.64	111.34	107.20
4	D	2	NAG	C2-N2-C7	-2.61	119.19	122.90
4	E	1	NAG	O4-C4-C3	-2.18	105.31	110.35
4	D	1	NAG	O5-C5-C6	2.13	110.55	107.20

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7

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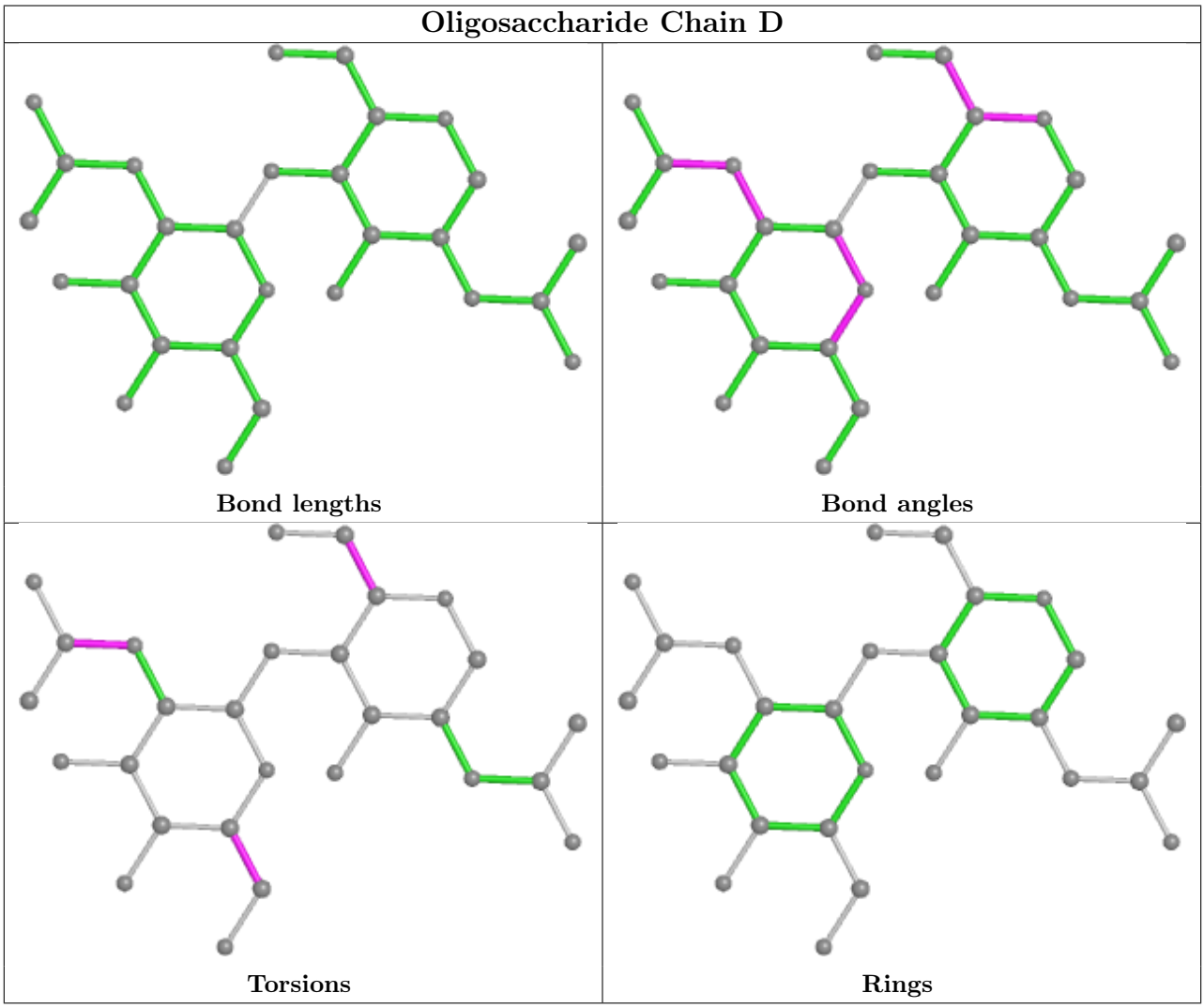
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7

There are no ring outliers.

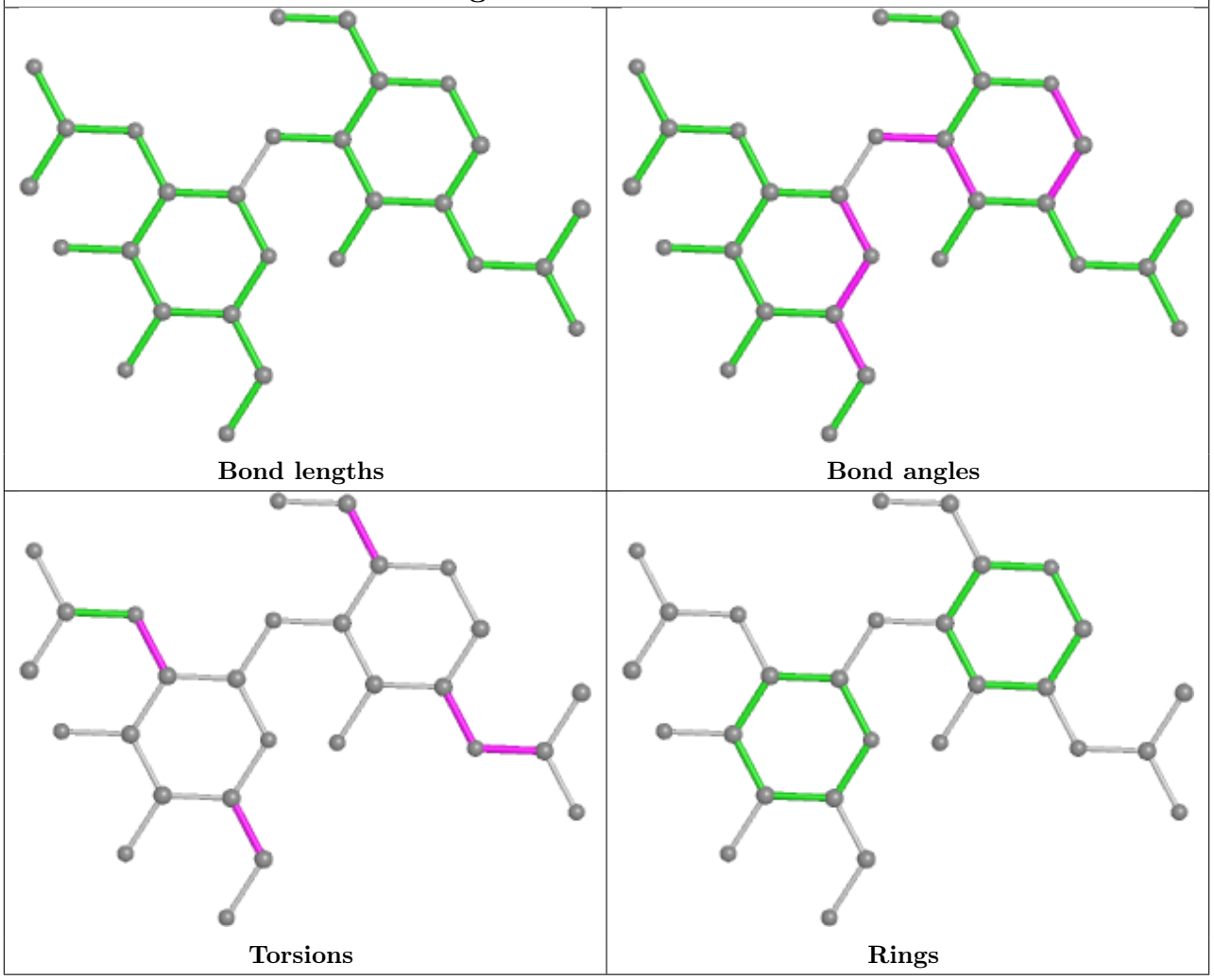
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	4	0
4	E	2	NAG	2	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 E



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
5	NAG	B	304	3	14,14,15	0.37	0	17,19,21	0.37	0
6	9SL	A	2007	-	17,23,23	3.58	8 (47%)	13,37,37	3.03	6 (46%)
5	NAG	A	2005	2	14,14,15	2.61	1 (7%)	17,19,21	2.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	2006	2	14,14,15	0.35	0	17,19,21	0.36	0
5	NAG	C	301	1	14,14,15	0.34	0	17,19,21	0.37	0
5	NAG	B	301	3	14,14,15	0.44	0	17,19,21	1.10	0
5	NAG	B	302	3	14,14,15	0.35	0	17,19,21	0.46	0
5	NAG	B	303	3	14,14,15	0.34	0	17,19,21	0.49	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
5	NAG	B	304	3	-	2/6/23/26	0/1/1/1
6	9SL	A	2007	-	-	4/5/53/53	0/3/3/3
5	NAG	A	2005	2	-	2/6/23/26	0/1/1/1
5	NAG	A	2006	2	-	2/6/23/26	0/1/1/1
5	NAG	C	301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	301	3	-	6/6/23/26	0/1/1/1
5	NAG	B	302	3	-	2/6/23/26	0/1/1/1
5	NAG	B	303	3	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2005	NAG	C1-C2	9.63	1.66	1.52
6	A	2007	9SL	C12-N13	8.73	1.49	1.35
6	A	2007	9SL	C07-N08	6.03	1.45	1.34
6	A	2007	9SL	C02-N21	5.89	1.44	1.33
6	A	2007	9SL	C12-N15	4.53	1.45	1.34
6	A	2007	9SL	C05-C14	3.63	1.60	1.52
6	A	2007	9SL	O01-C02	-3.45	1.17	1.21
6	A	2007	9SL	O03-C02	3.01	1.39	1.35
6	A	2007	9SL	C05-N06	-2.52	1.43	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2005	NAG	C1-O5-C5	-8.24	101.03	112.19
6	A	2007	9SL	O03-C02-N21	7.83	120.80	111.08
5	A	2005	NAG	O5-C1-C2	-4.59	104.05	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2007	9SL	O01-C02-N21	-4.22	118.55	125.51
6	A	2007	9SL	N09-C07-N06	-3.32	120.80	125.42
6	A	2007	9SL	N13-C12-N11	-3.08	107.65	115.45
6	A	2007	9SL	O03-C02-O01	-2.56	120.64	123.07
6	A	2007	9SL	O03-C04-C05	2.31	112.96	108.40

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	NAG	C8-C7-N2-C2
5	B	301	NAG	O7-C7-N2-C2
6	A	2007	9SL	O01-C02-O03-C04
6	A	2007	9SL	N21-C02-O03-C04
6	A	2007	9SL	O03-C04-C05-N06
6	A	2007	9SL	O03-C04-C05-C14
5	C	301	NAG	O5-C5-C6-O6
5	A	2005	NAG	O5-C5-C6-O6
5	A	2006	NAG	O5-C5-C6-O6
5	B	303	NAG	O5-C5-C6-O6
5	B	304	NAG	O5-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
5	C	301	NAG	C4-C5-C6-O6
5	A	2005	NAG	C4-C5-C6-O6
5	A	2006	NAG	C4-C5-C6-O6
5	B	304	NAG	C4-C5-C6-O6
5	B	301	NAG	C1-C2-N2-C7
5	B	303	NAG	C4-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	B	302	NAG	C4-C5-C6-O6
5	B	302	NAG	O5-C5-C6-O6
5	B	301	NAG	C3-C2-N2-C7

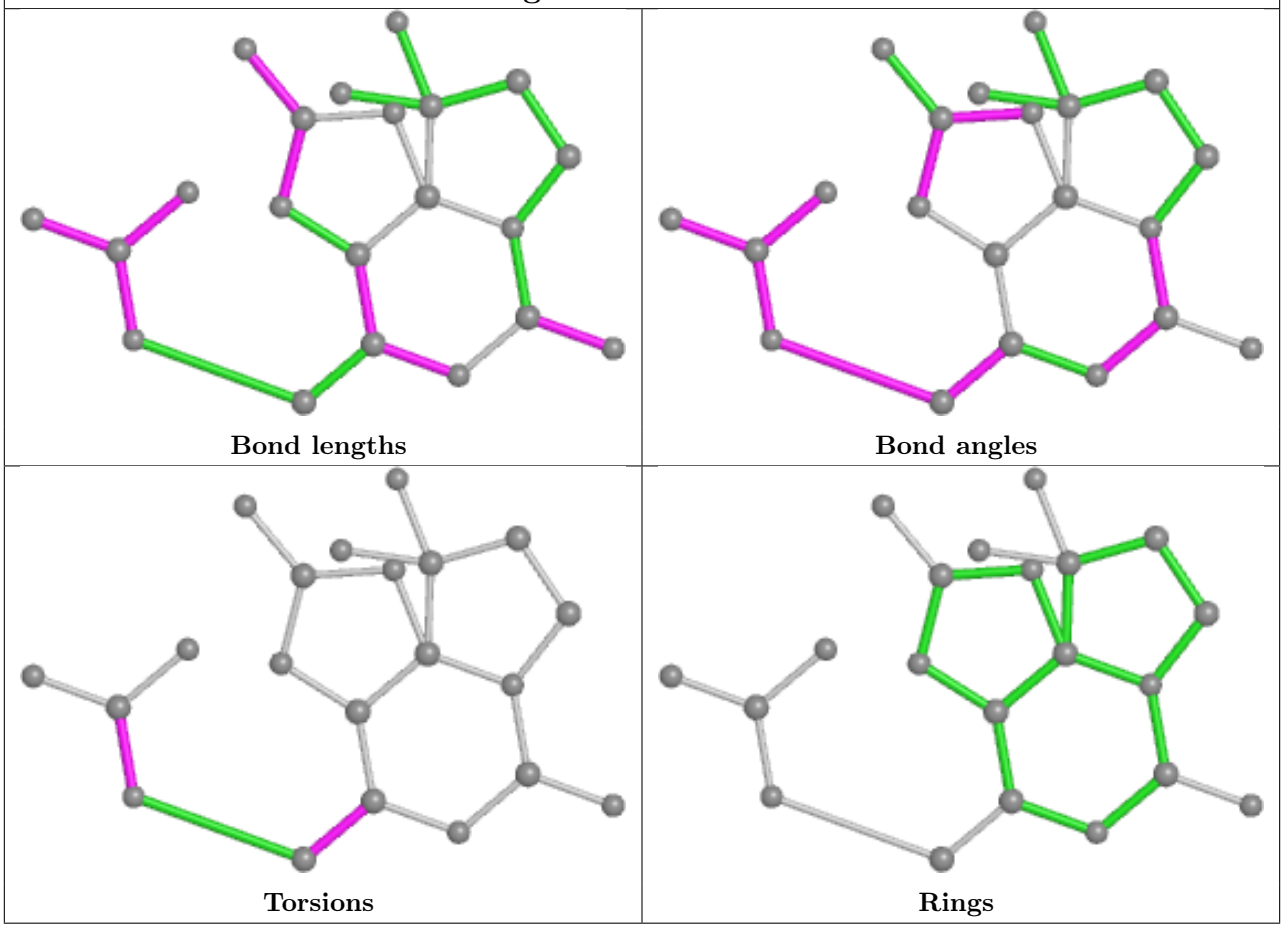
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2007	9SL	2	0
5	A	2005	NAG	1	0
5	A	2006	NAG	1	0
5	C	301	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 9SL A 2007



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

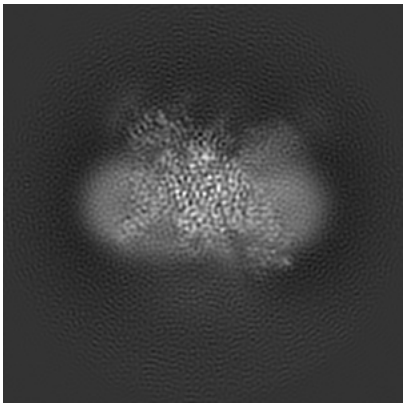
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9781. These allow visual inspection of the internal detail of the map and identification of artifacts.

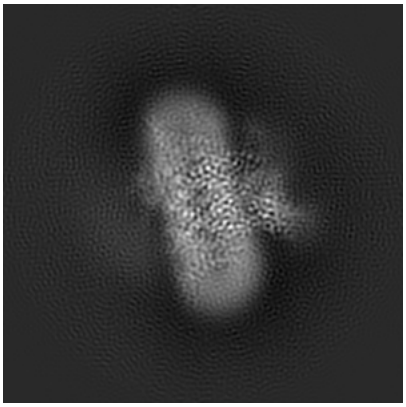
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

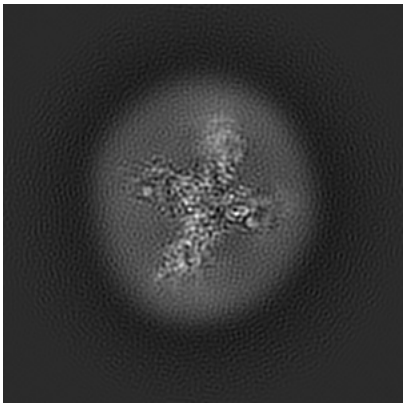
6.1.1 Primary map



X



Y

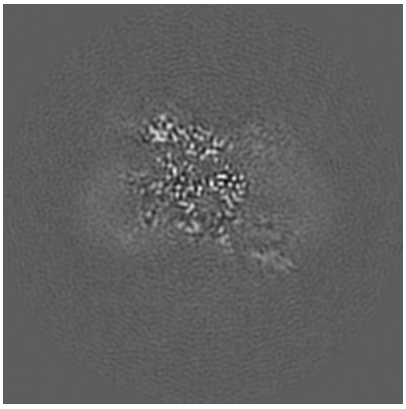


Z

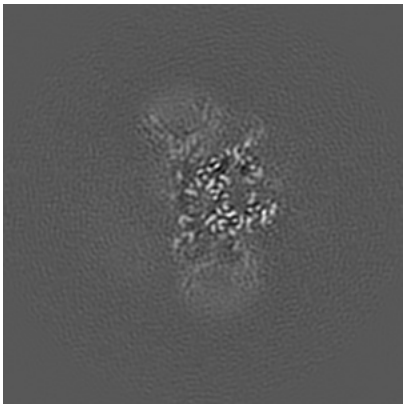
The images above show the map projected in three orthogonal directions.

6.2 Central slices

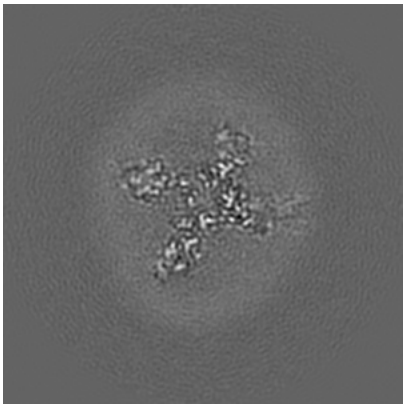
6.2.1 Primary map



X Index: 120



Y Index: 120

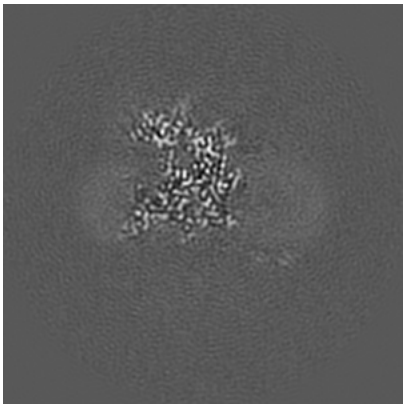


Z Index: 120

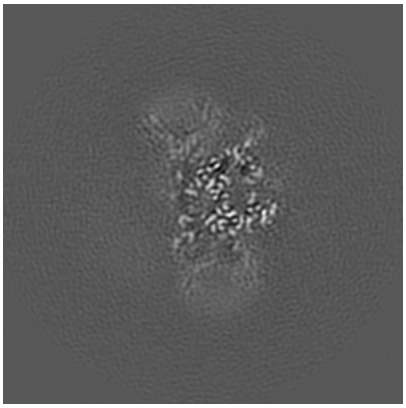
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

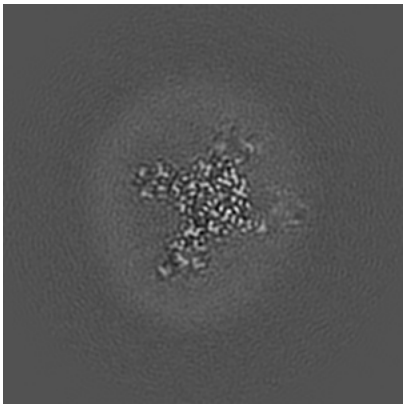
6.3.1 Primary map



X Index: 112



Y Index: 120



Z Index: 127

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

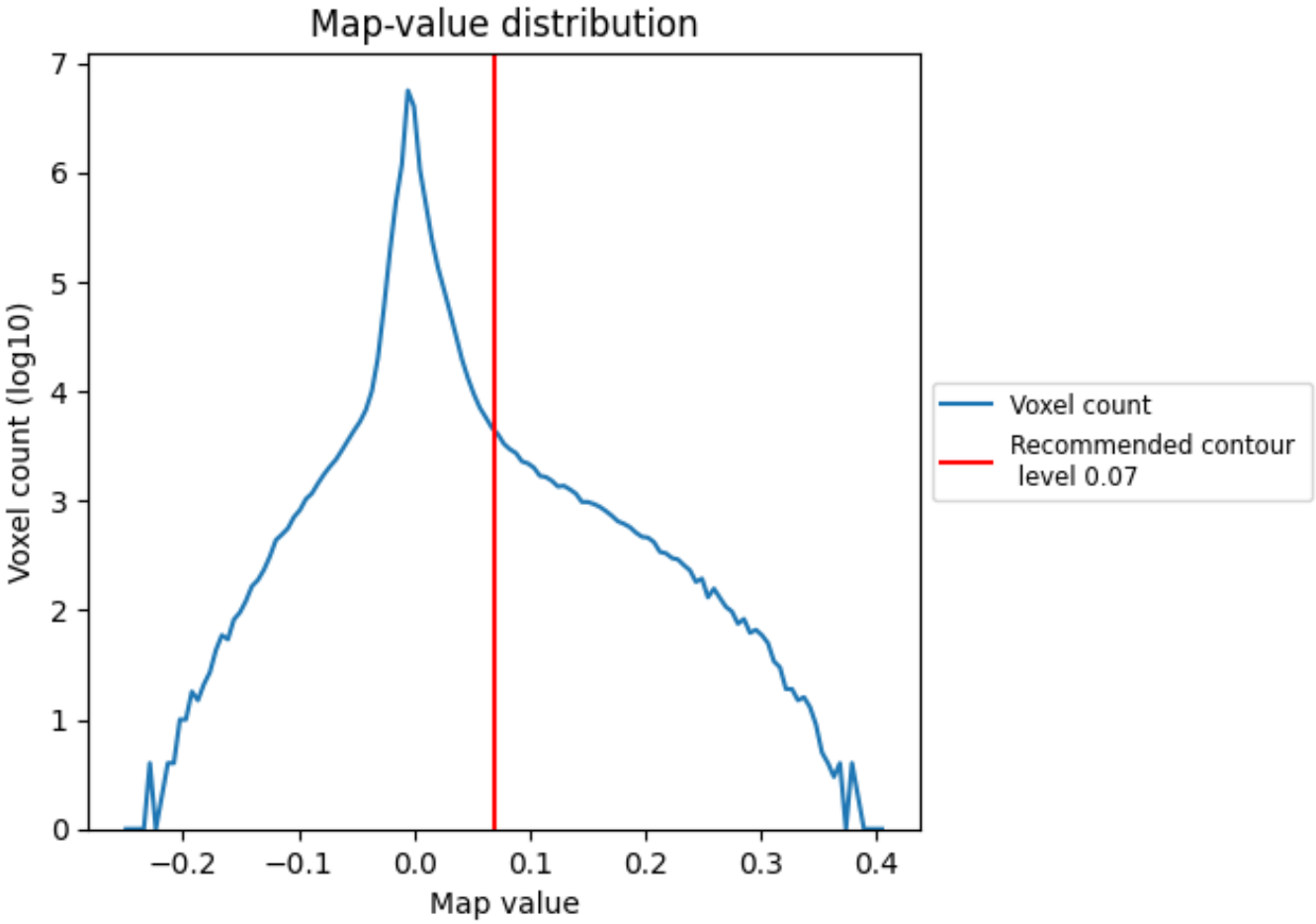
6.5 Mask visualisation (i)

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

7 Map analysis

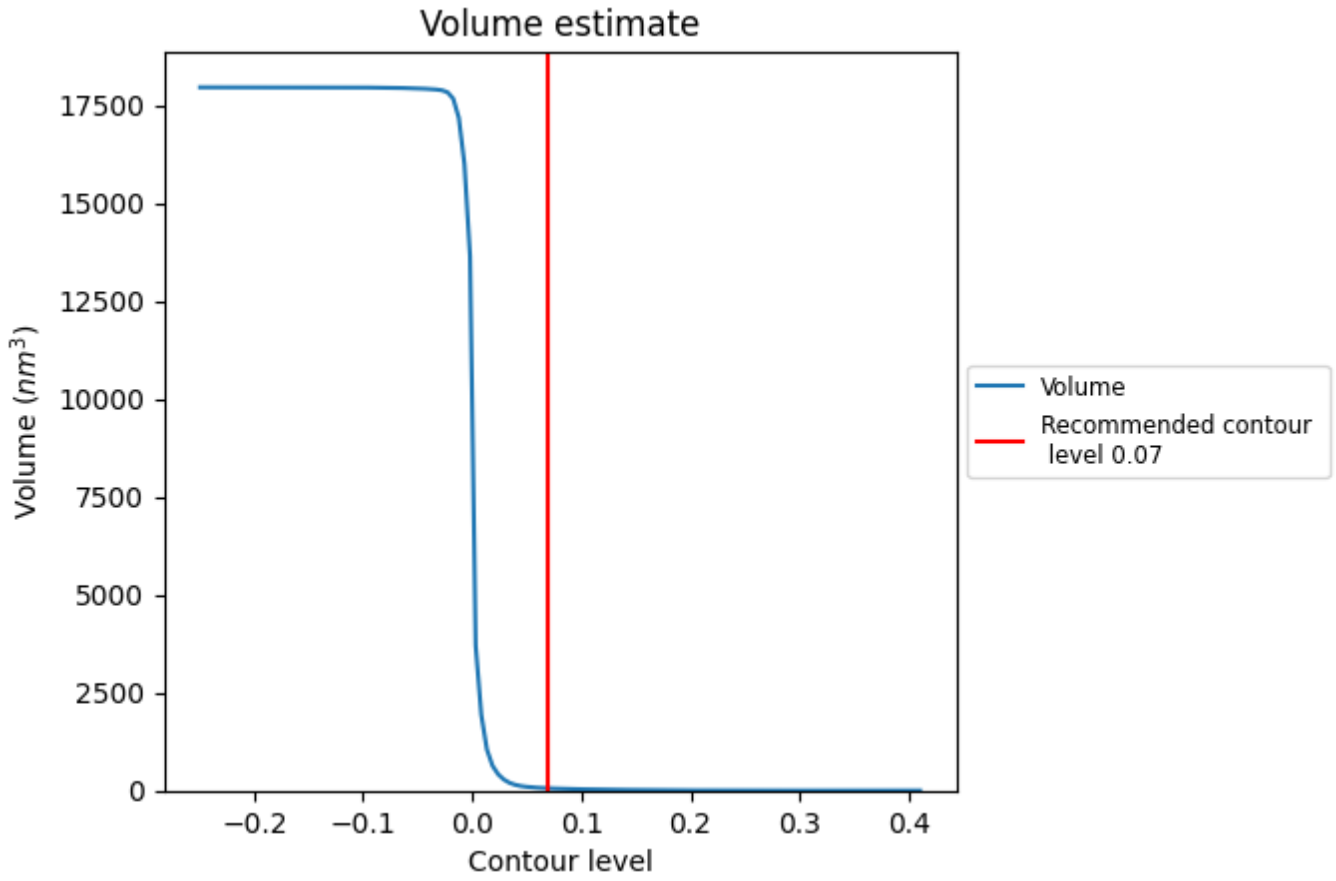
This section contains the results of statistical analysis of the map.

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.

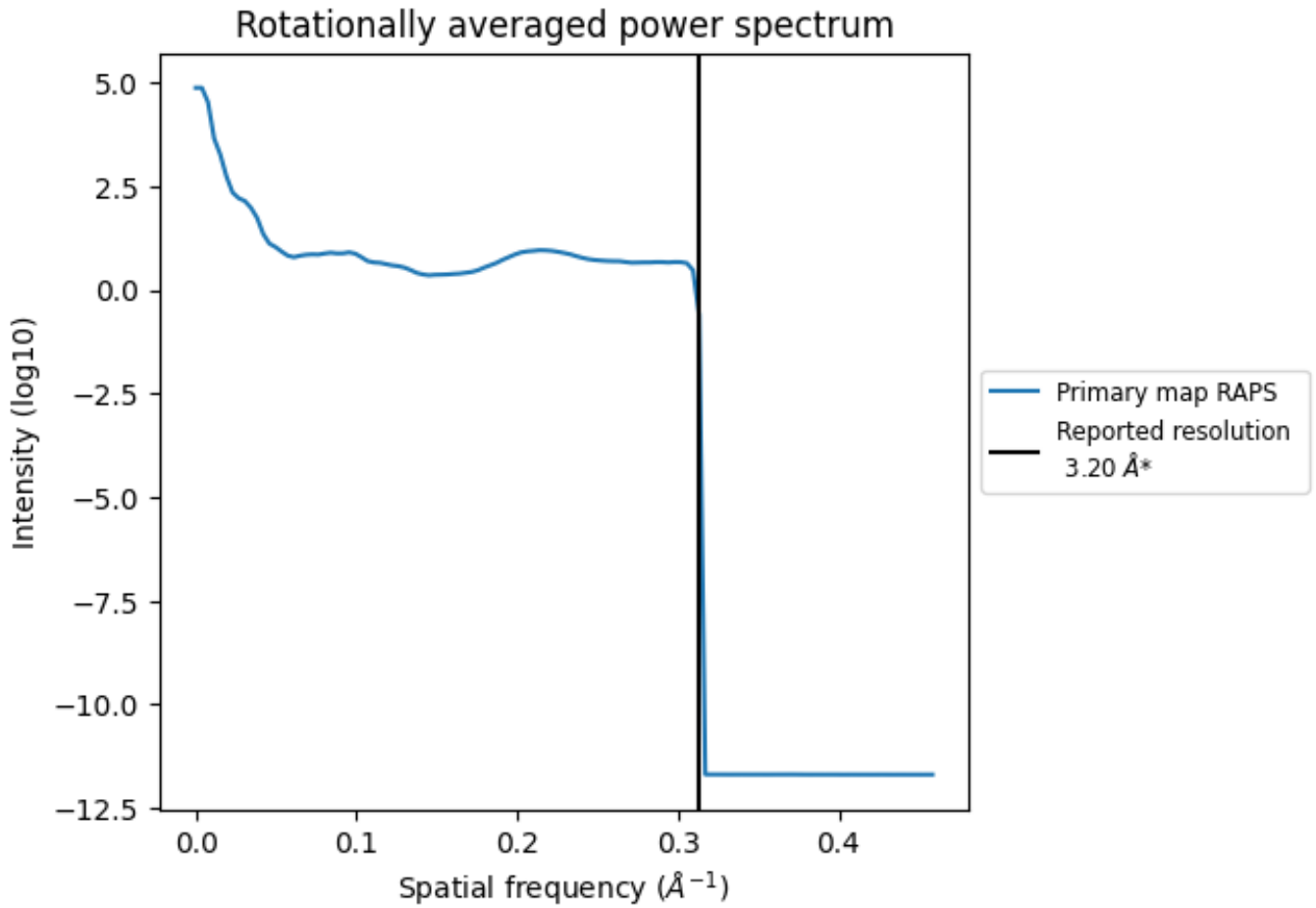
7.2 Volume estimate



The volume at the recommended contour level is 57 nm^3; this corresponds to an approximate mass of 52 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 0.312 $Å^{-1}$

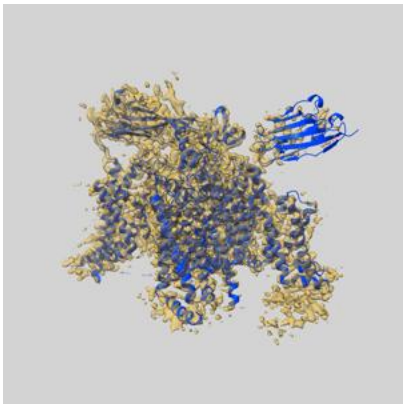
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

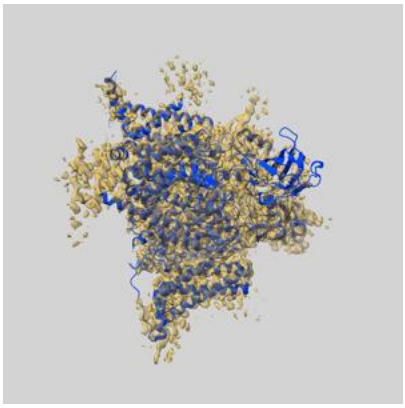
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9781 and PDB model 6J8G. Per-residue inclusion information can be found in section 3 on page 7.

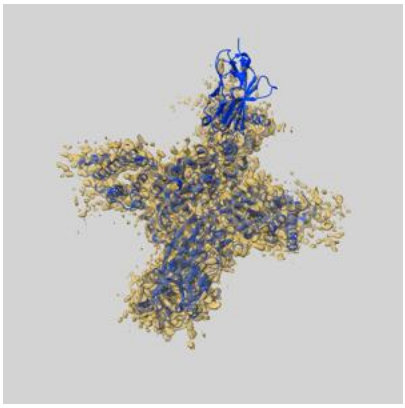
9.1 Map-model overlay



X



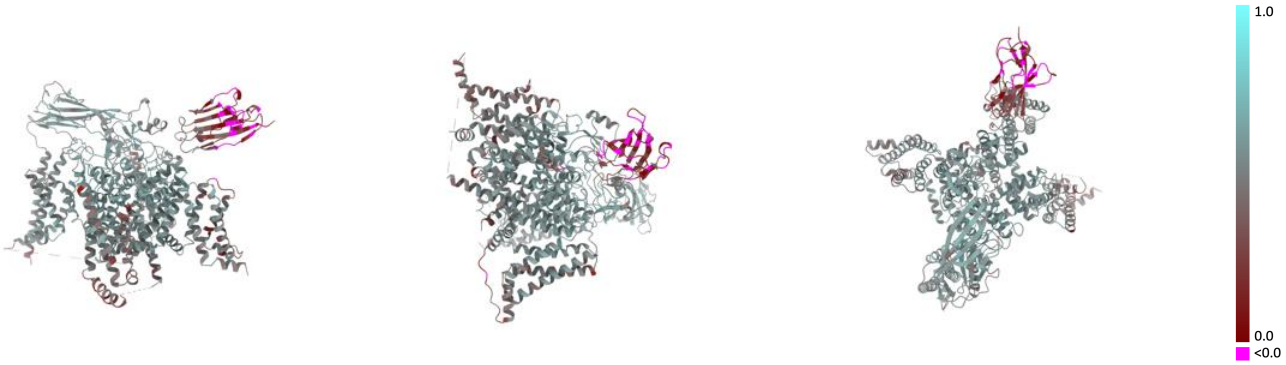
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



X Y Z

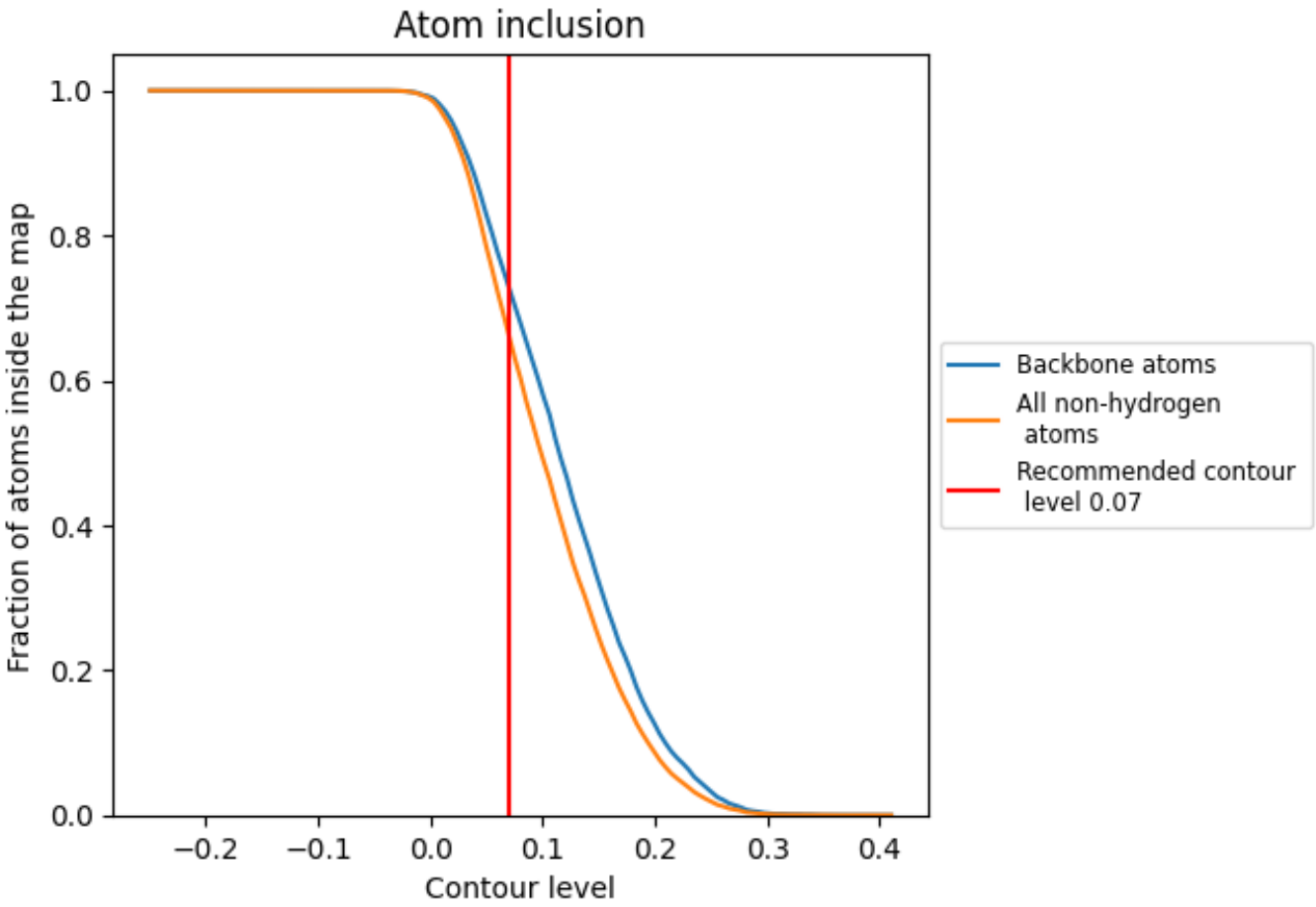
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6614	0.4950
A	0.7092	0.5250
B	0.7399	0.5180
C	0.1068	0.1800
D	0.3929	0.3450
E	0.6429	0.4580