Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:30 PM EST

PDB ID	:	7M7F
EMDB ID	:	EMD-23711
Title	:	6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 1
Authors	:	Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.
Deposited on	:	2021-03-28
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:

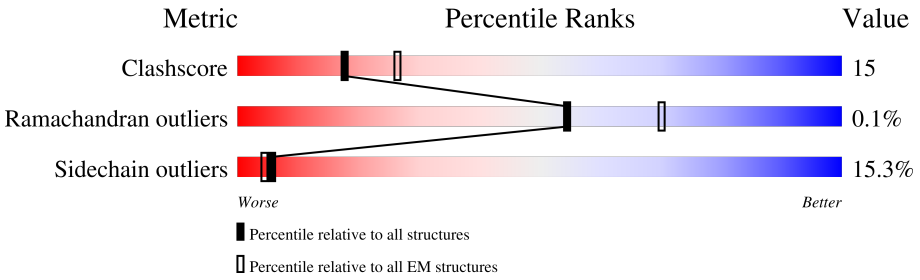
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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	A	1784	11% 47% 27% • 22%
1	B	1784	6% 34% 19% • 44%
2	C	249	• 44% 31% 6% • 18%
2	E	249	• 44% 32% 6% 18%
3	D	236	• 44% 39% • 13%
3	F	236	• 44% 40% • 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23971 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 EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	999	Total 7417	C 4613	N 1363	O 1414	S 27	0	0
1	A	1390	Total 10319	C 6413	N 1899	O 1972	S 35	0	0

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ARG	-	expression tag	UNP Q5UNP6
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1486	THR	-	linker	UNP Q5UNP6
B	1487	SER	-	linker	UNP Q5UNP6
B	1488	GLU	-	linker	UNP Q5UNP6
B	1489	LEU	-	linker	UNP Q5UNP6
B	1490	GLY	-	linker	UNP Q5UNP6
B	1768	SER	-	expression tag	UNP Q03133
B	1769	SER	-	expression tag	UNP Q03133
B	1770	VAL	-	expression tag	UNP Q03133
B	1771	ASP	-	expression tag	UNP Q03133
B	1772	LYS	-	expression tag	UNP Q03133
B	1773	LEU	-	expression tag	UNP Q03133
B	1774	ALA	-	expression tag	UNP Q03133
B	1775	ALA	-	expression tag	UNP Q03133
B	1776	ALA	-	expression tag	UNP Q03133
B	1777	LEU	-	expression tag	UNP Q03133
B	1778	GLU	-	expression tag	UNP Q03133
B	1779	HIS	-	expression tag	UNP Q03133
B	1780	HIS	-	expression tag	UNP Q03133
B	1781	HIS	-	expression tag	UNP Q03133
B	1782	HIS	-	expression tag	UNP Q03133
B	1783	HIS	-	expression tag	UNP Q03133
B	1784	HIS	-	expression tag	UNP Q03133
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1486	THR	-	linker	UNP Q5UNP6
A	1487	SER	-	linker	UNP Q5UNP6
A	1488	GLU	-	linker	UNP Q5UNP6
A	1489	LEU	-	linker	UNP Q5UNP6
A	1490	GLY	-	linker	UNP Q5UNP6
A	1768	SER	-	expression tag	UNP Q03133
A	1769	SER	-	expression tag	UNP Q03133
A	1770	VAL	-	expression tag	UNP Q03133
A	1771	ASP	-	expression tag	UNP Q03133
A	1772	LYS	-	expression tag	UNP Q03133
A	1773	LEU	-	expression tag	UNP Q03133
A	1774	ALA	-	expression tag	UNP Q03133
A	1775	ALA	-	expression tag	UNP Q03133
A	1776	ALA	-	expression tag	UNP Q03133
A	1777	LEU	-	expression tag	UNP Q03133
A	1778	GLU	-	expression tag	UNP Q03133
A	1779	HIS	-	expression tag	UNP Q03133
A	1780	HIS	-	expression tag	UNP Q03133
A	1781	HIS	-	expression tag	UNP Q03133
A	1782	HIS	-	expression tag	UNP Q03133
A	1783	HIS	-	expression tag	UNP Q03133
A	1784	HIS	-	expression tag	UNP Q03133

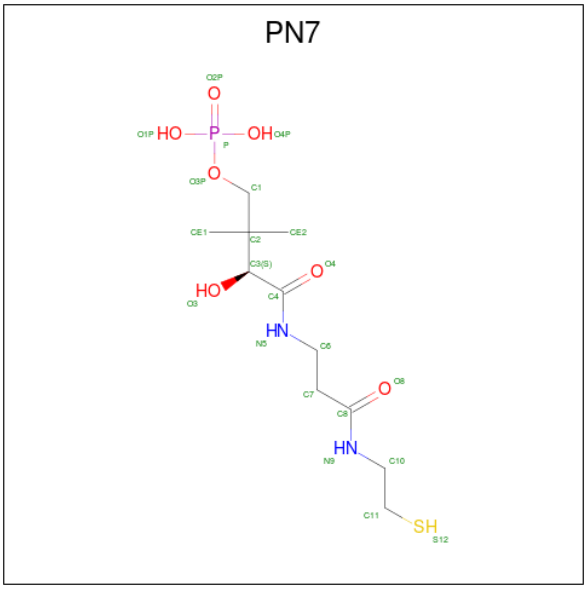
- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

- Molecule 3 is a protein called 1B2 (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

- Molecule 4 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanylethyl)-beta-alaninamide (three-letter code: PN7) (formula: $C_{11}H_{23}N_2O_7PS$).



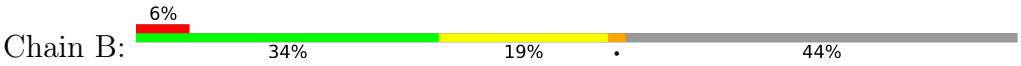
Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

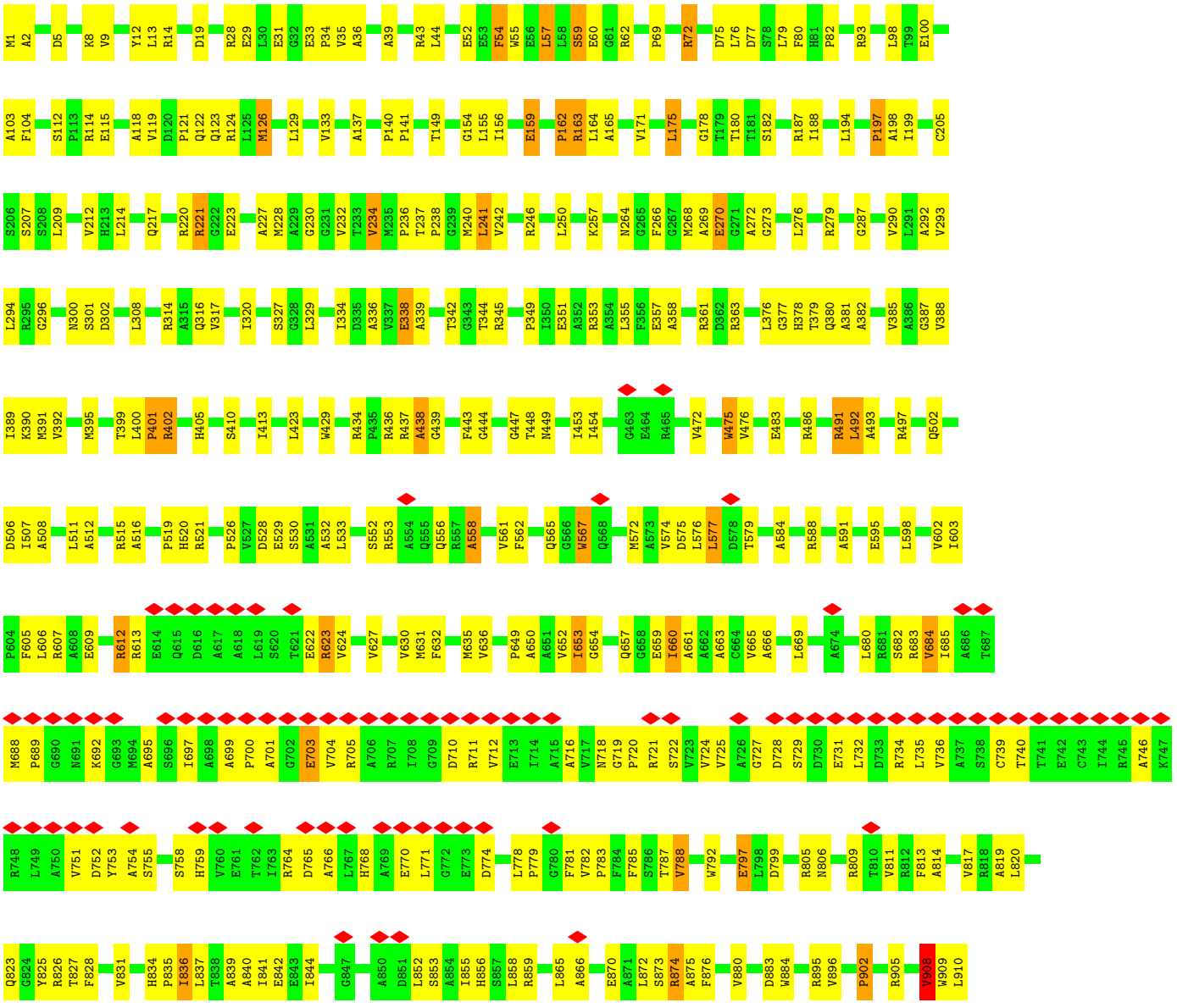
3 Residue-property plots (i)

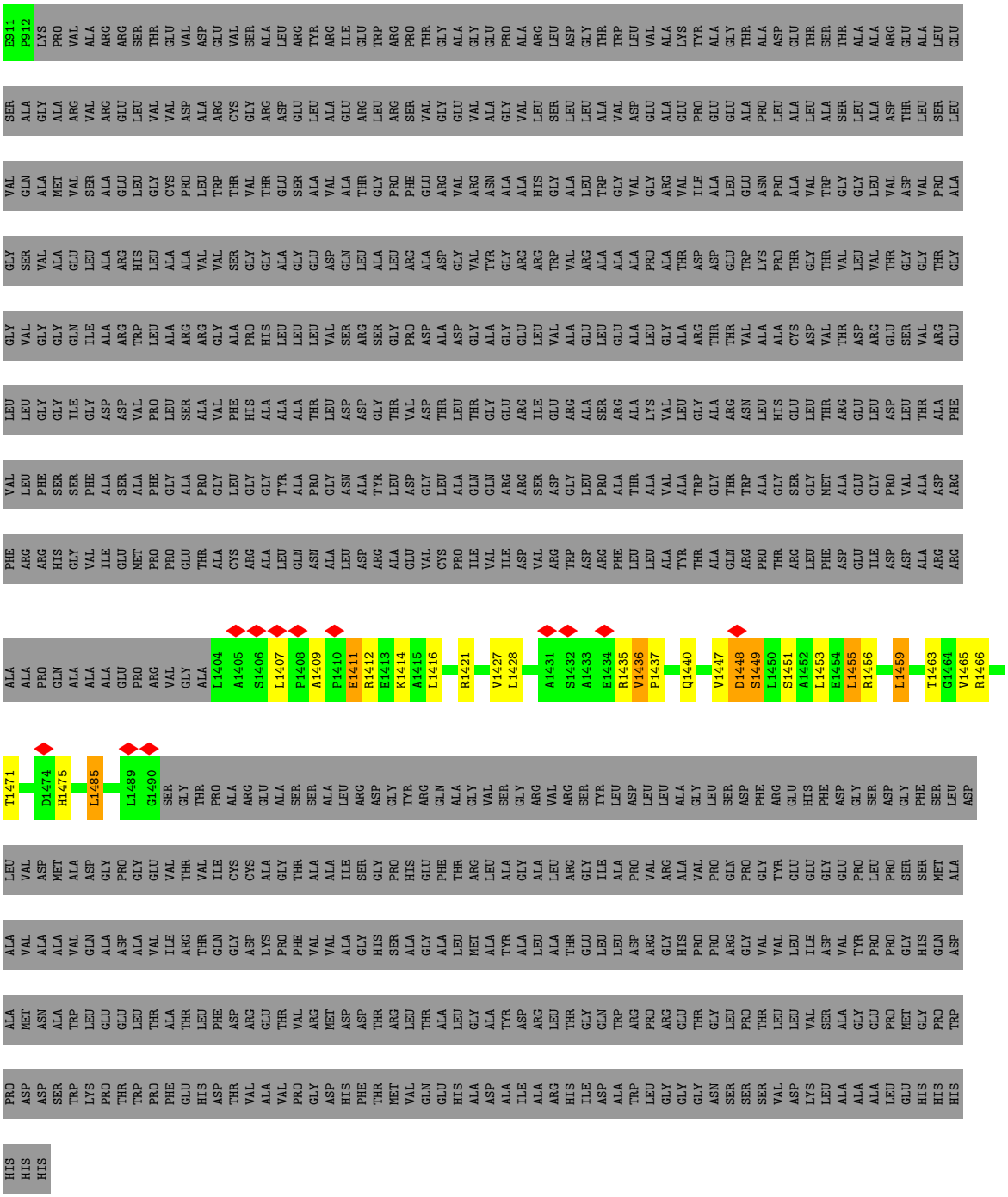
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

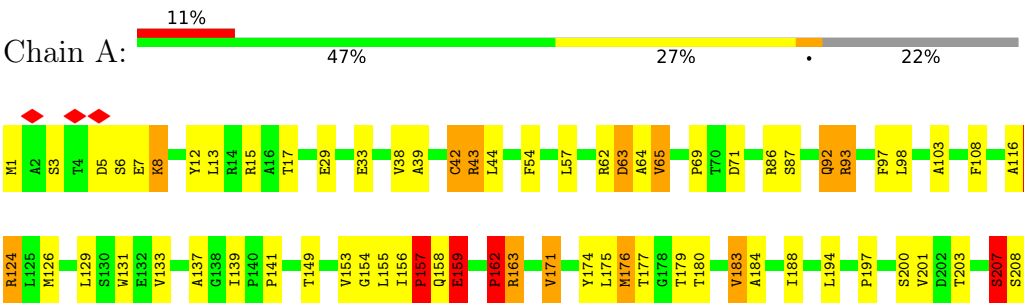
Chain B:

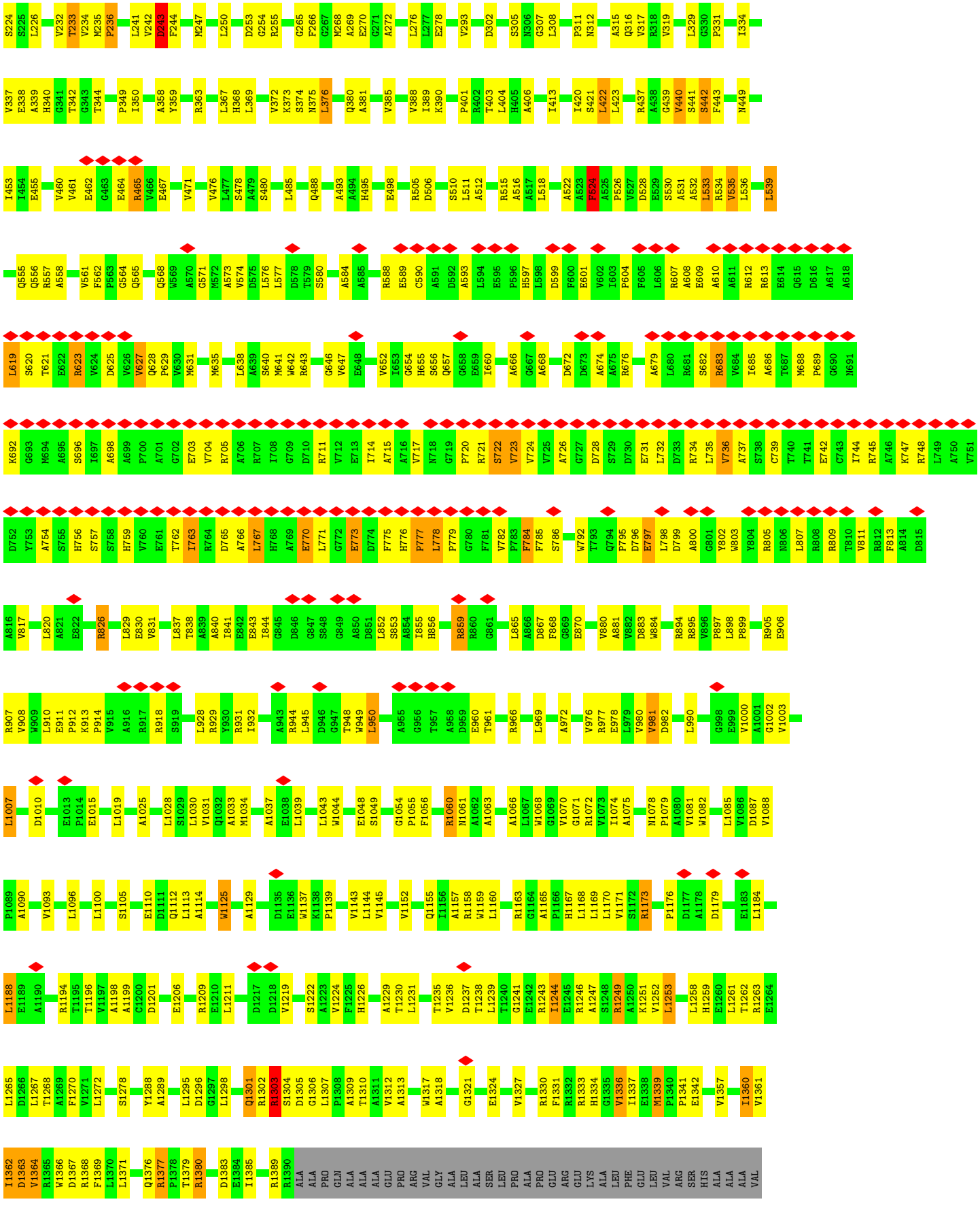


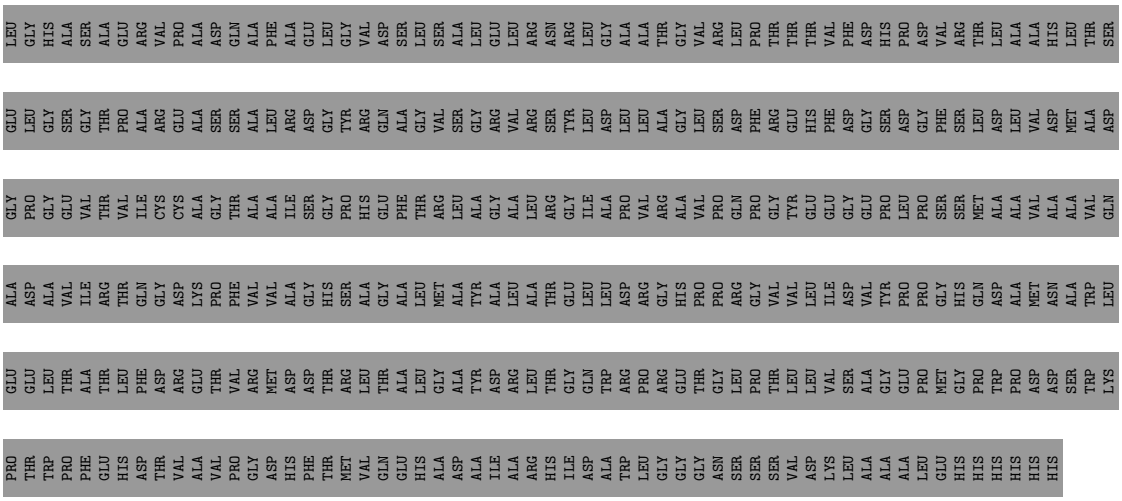




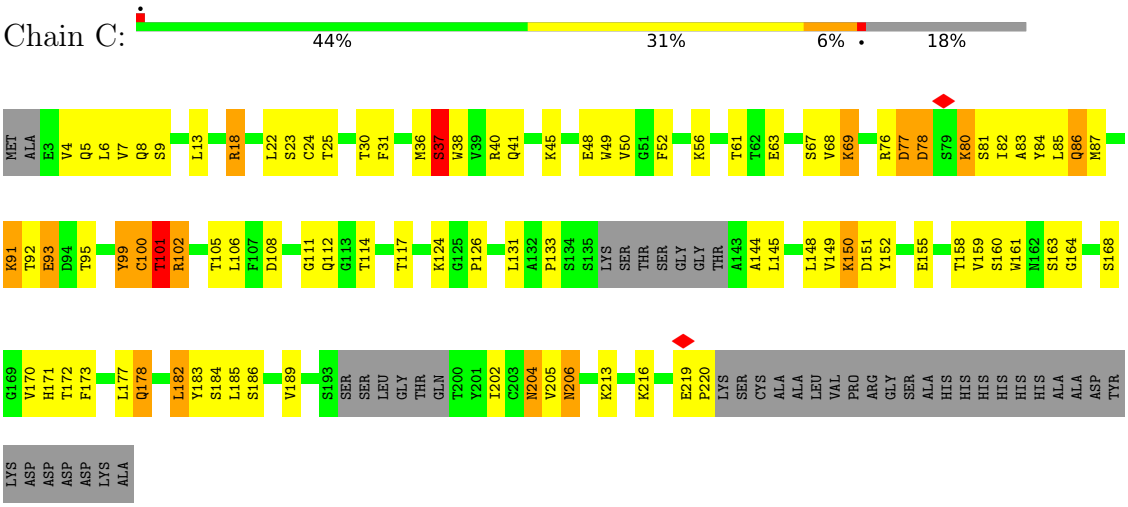
• Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera



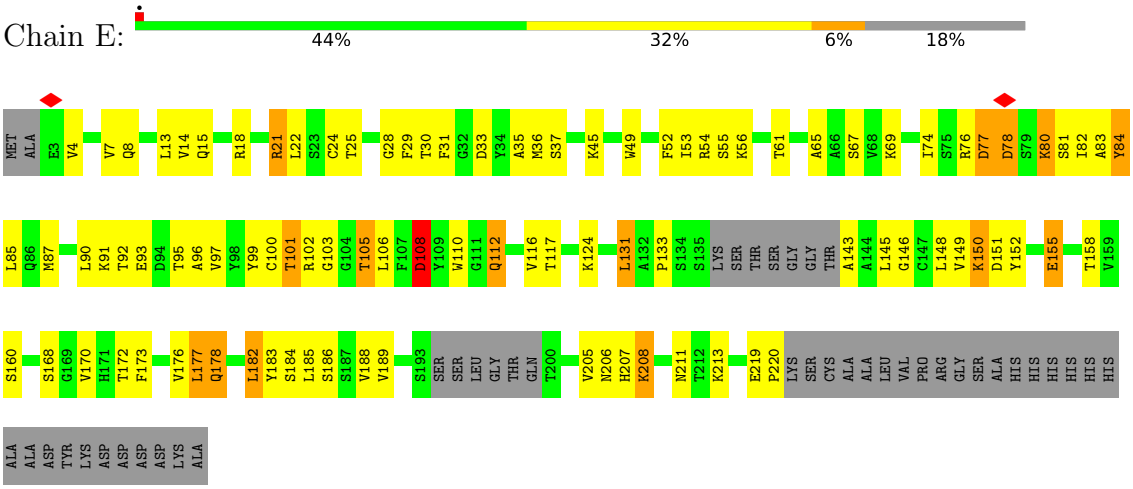

S224 S225 L226 V232 T233 V234 M235 P236 L241 V242 D243 F244 M247 L250 D253 G254 R255 G265 F266 G267 M268 A269 E270 G271 A272 L276 L277 E278 V293 D302 S305 N306 G307 L308 P311 M312 A315 Q316 V317 R318 V319 L329 G330 P331 I334
V337 E338 A339 H340 G341 T342 G343 T344 P349 I350 A358 Y359 R363 L367 H368 L369 V372 K373 S374 N375 L376 Q380 A381 V385 V388 I389 K390 P401 R402 T403 L404 H405 A406 I413 I420 S421 L422 L423 R437 A438 G439 V440 S441 S442 F443 N449
I453 I454 E455 V460 V461 E462 G463 E464 R465 V466 E467 V471 V476 L477 S478 A479 S480 L485 Q488 A493 A494 H495 E498 R505 D506 S510 L511 A512 R515 A516 A517 L518 A522 A523 F524 A525 P526 V527 D528 E529 S530 A531 A532 L533 R534 V535 L536 L539
Q555 Q556 R557 A558 V561 F562 P563 G564 Q565 Q568 W569 A570 G571 M572 A573 V574 D575 L576 L577 D578 T579 S580 A584 A585 R588 E589 C590 A591 D592 A593 L594 E595 P596 H597 L598 D599 F600 E601 V602 I603 P604 F605 L606 R607 A608 E609 A610 A611 R612 R613 E614 Q615 D616 A617 A618
L619 S620 T621 E622 R623 V624 D625 V626 V627 Q628 P629 V630 M631 M635 L638 A639 S640 M641 W642 R643 G646 V647 E648 V652 I653 G654 H655 S656 Q657 G658 E659 I660 A666 G667 A668 D672 D673 A674 A675 R676 A679 L680 R681 S682 R683 V684 I685 A686 T687 M688 P689 G690 N691
K692 G693 M694 A695 S696 I697 A698 A699 P700 A701 G702 E703 V704 R705 A706 R707 I708 G709 D710 R711 V712 E713 I714 A715 A716 V717 N718 G719 P720 R721 S722 V723 V724 V725 A726 G727 D728 S729 D730 E731 L732 D733 R734 L735 V736 A737 S738 C739 T740 T741 E742 C743 I744 R745 A746 K747 R748 L749 A750 V751
D752 Y753 A754 S755 H756 S757 S758 H759 V760 E761 T762 I763 R764 D765 A766 L767 H768 A769 E770 L771 G772 E773 D774 F775 H776 P777 L778 P779 G780 F781 V782 P783 F784 F785 S786 W792 T793 Q794 P795 D796 E797 L798 D799 A800 G801 Y802 W803 Y804 R805 N806 L807 R808 R809 T810 V811 R812 F813 A814 D815
A816 V817 L820 A821 E822 R826 L829 E830 V831 L837 T838 A839 A840 I841 E842 E843 I844 G845 D846 G847 S848 G849 A850 D851 L852 S853 A854 I855 H856 R859 R860 G861 L865 A866 D867 F868 G869 E870 V880 A881 V882 D883 W884 R894 R895 V896 P897 L898 P899 R905 E906
R907 V908 W909 L910 E911 P912 K913 P914 V915 A916 R917 R918 S919 L928 R929 Y930 R931 I932 A943 R944 L945 D946 G947 T948 W949 L960 A955 G956 T957 A958 D959 E960 T961 R966 L969 A972 V976 R977 E978 L979 V980 V981 D982 L990 G998 E999 V1000 A1001 G1002 V1003
L1007 D1010 E1013 P1014 E1015 L1019 A1025 L1028 S1029 L1030 V1031 Q1032 A1033 M1034 A1037 E1038 L1039 L1043 W1044 E1048 S1049 G1054 P1055 F1056 R1060 N1061 A1062 A1063 A1066 L1067 W1068 G1069 V1070 G1071 R1072 V1073 I1074 A1075 N1078 P1079 A1080 V1081 W1082 L1085 V1086 D1087 V1088
P1089 A1090 V1093 L1096 L1100 S1105 E1110 D1111 Q1112 L1113 A1114 W1125 A1129 D1135 E1136 W1137 K1138 P1139 V1143 L1144 V1145 V1152 Q1155 I1156 A1157 R1158 W1159 L1160 R1163 G1164 A1165 P1166 H1167 L1168 L1169 L1170 V1171 S1172 R1173 P1176 D1177 A1178 D1179 E1183 L1184
L1188 E1189 A1190 R1194 T1195 T1196 Y1197 A1198 A1199 C1200 D1201 E1206 R1209 E1210 L1211 D1217 D1218 V1219 S1222 A1223 V1224 F1225 H1226 A1229 T1230 L1231 T1235 V1236 D1237 T1238 L1239 T1240 G1241 E1242 R1243 I1244 E1245 R1246 A1247 S1248 R1249 A1250 K1251 V1252 L1253 L1258 H1259 E1260 L1261 T1262 R1263 E1264
L1265 D1266 L1267 T1268 A1269 F1270 V1271 L1272 S1278 Y1288 A1289 L1295 D1296 G1297 L1298 Q1301 R1302 R1303 S1304 D1305 G1306 L1307 P1308 A1309 T1310 A1311 V1312 A1313 W1317 A1318 G1321 E1324 V1327 R1330 F1331 R1332 R1333 H1334 G1335 V1336 I1337 E1338 M1339 P1340 E1342 V1357 I1360 V1361
I1362 D1363 V1364 R1365 W1366 D1367 R1368 F1369 L1370 L1371 Q1376 R1377 P1378 T1379 R1380 D1383 E1384 I1385 R1389 R1390 ALA ALA PRO GLN ALA ALA ALA GLU PRO ARG VAL GLY ALA LEU ALA SER LEU PRO ALA PRO GLU ARG GLU LYS ALA LEU PHE GLU LEU VAL ARG SER HIS ALA ALA ALA VAL



• Molecule 2: 1B2 (heavy chain)

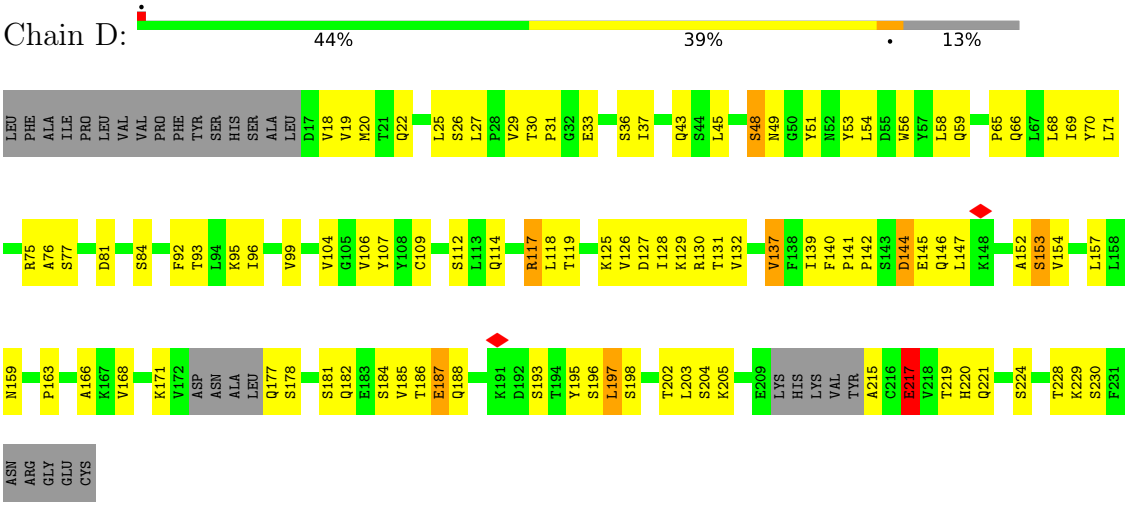


• Molecule 2: 1B2 (heavy chain)



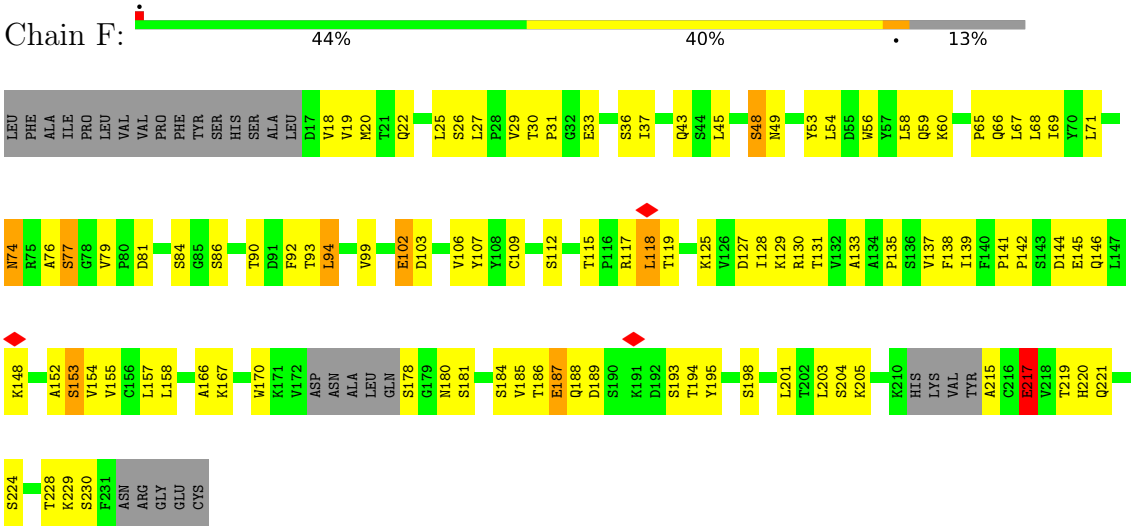
• Molecule 3: 1B2 (light chain)

Chain D:



• Molecule 3: 1B2 (light chain)

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	172352	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.734	Depositor
Minimum map value	-4.602	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PN7

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	24/10522 (0.2%)	0.85	27/14323 (0.2%)
1	B	0.66	21/7566 (0.3%)	0.86	28/10293 (0.3%)
2	C	0.62	3/1575 (0.2%)	0.86	5/2141 (0.2%)
2	E	0.59	1/1575 (0.1%)	0.87	4/2141 (0.2%)
3	D	0.46	1/1601 (0.1%)	0.68	1/2175 (0.0%)
3	F	0.54	3/1601 (0.2%)	0.76	5/2174 (0.2%)
All	All	0.64	53/24440 (0.2%)	0.84	70/33247 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
2	E	0	3
3	F	0	1
All	All	0	6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	SER	CA-CB	-16.15	1.28	1.52
1	A	442	SER	CA-CB	-14.72	1.30	1.52
1	A	441	SER	CA-CB	-10.75	1.36	1.52
1	A	374	SER	CA-CB	-9.77	1.38	1.52
1	B	230	GLY	C-O	-8.63	1.09	1.23
1	B	59	SER	CA-CB	-8.29	1.40	1.52
1	B	197	PRO	C-O	-8.29	1.06	1.23
1	A	43	ARG	C-O	-8.23	1.07	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	908	VAL	C-O	-8.02	1.08	1.23
1	B	399	THR	C-O	-7.66	1.08	1.23
1	A	120	ASP	C-O	-7.28	1.09	1.23
1	A	442	SER	C-O	-7.11	1.09	1.23
1	B	439	GLY	C-O	-7.04	1.12	1.23
1	B	54	PHE	C-O	-6.99	1.10	1.23
1	B	388	VAL	C-O	-6.94	1.10	1.23
1	A	440	VAL	C-O	-6.82	1.10	1.23
1	B	43	ARG	C-O	-6.37	1.11	1.23
2	C	37	SER	CA-CB	-6.32	1.43	1.52
1	A	183	VAL	C-O	-6.21	1.11	1.23
1	B	57	LEU	C-O	-6.15	1.11	1.23
1	B	338	GLU	C-O	-6.04	1.11	1.23
1	A	524	PHE	C-O	-6.00	1.11	1.23
1	B	338	GLU	CD-OE2	-5.87	1.19	1.25
1	A	118	ALA	CA-CB	-5.82	1.40	1.52
3	F	198	SER	CA-CB	-5.78	1.44	1.52
1	A	270	GLU	CD-OE1	-5.77	1.19	1.25
1	A	243	ASP	C-O	-5.68	1.12	1.23
1	B	475	TRP	C-O	-5.68	1.12	1.23
2	E	103	GLY	C-O	-5.68	1.14	1.23
1	B	234	VAL	C-O	-5.64	1.12	1.23
1	A	116	ALA	C-O	-5.63	1.12	1.23
1	B	266	PHE	C-N	-5.46	1.23	1.33
1	A	270	GLU	C-O	-5.46	1.12	1.23
3	F	48	SER	CA-CB	-5.45	1.44	1.52
1	A	233	THR	C-O	-5.32	1.13	1.23
1	A	162	PRO	C-O	-5.23	1.12	1.23
2	C	99	TYR	C-O	-5.23	1.13	1.23
1	B	493	ALA	CA-CB	-5.23	1.41	1.52
3	F	74	ASN	C-O	-5.21	1.13	1.23
1	A	162	PRO	N-CA	-5.19	1.38	1.47
1	A	236	PRO	C-O	-5.18	1.12	1.23
1	A	157	PRO	N-CA	-5.18	1.38	1.47
3	D	48	SER	CA-CB	-5.17	1.45	1.52
1	B	454	ILE	C-O	-5.13	1.13	1.23
2	C	101	THR	C-O	-5.13	1.13	1.23
1	A	234	VAL	C-O	-5.13	1.13	1.23
1	B	266	PHE	C-O	-5.08	1.13	1.23
1	A	116	ALA	CA-CB	-5.06	1.41	1.52
1	A	207	SER	C-O	-5.05	1.13	1.23
1	B	198	ALA	CA-CB	-5.05	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	LEU	C-O	-5.04	1.13	1.23
1	B	438	ALA	C-N	-5.03	1.24	1.33
1	B	492	LEU	C-O	-5.00	1.13	1.23

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	PRO	N-CA-CB	-16.54	83.45	103.30
1	A	159	GLU	CB-CA-C	-16.14	78.12	110.40
1	B	883	ASP	CB-CA-C	-15.95	78.51	110.40
1	A	43	ARG	CB-CA-C	-13.60	83.20	110.40
1	A	157	PRO	N-CA-CB	-12.39	88.43	103.30
2	C	102	ARG	CB-CA-C	-10.26	89.87	110.40
2	E	102	ARG	CB-CA-C	-10.23	89.93	110.40
1	A	233	THR	CA-CB-OG1	-10.22	87.54	109.00
1	B	902	PRO	CB-CA-C	-10.16	86.60	112.00
1	B	401	PRO	N-CA-CB	-9.51	91.89	103.30
1	A	236	PRO	N-CA-CB	-9.43	91.98	103.30
1	B	401	PRO	N-CD-CG	-9.34	89.19	103.20
1	A	43	ARG	N-CA-CB	-9.19	94.06	110.60
1	A	63	ASP	CB-CA-C	-8.59	93.22	110.40
1	B	72	ARG	CB-CG-CD	-8.57	89.33	111.60
1	A	914	PRO	N-CA-C	8.49	134.18	112.10
1	A	243	ASP	CB-CA-C	-8.31	93.78	110.40
1	B	266	PHE	CB-CA-C	-8.09	94.22	110.40
1	A	233	THR	CB-CA-C	-7.80	90.54	111.60
2	C	101	THR	N-CA-CB	-7.79	95.50	110.30
1	B	198	ALA	N-CA-CB	-7.60	99.45	110.10
1	B	197	PRO	CB-CA-C	-7.49	93.27	112.00
1	A	403	THR	N-CA-C	-7.49	90.79	111.00
1	A	270	GLU	CB-CG-CD	-7.39	94.24	114.20
1	B	266	PHE	CA-CB-CG	7.35	131.55	113.90
1	B	54	PHE	CB-CA-C	-7.30	95.79	110.40
1	A	162	PRO	CB-CA-C	-7.22	93.95	112.00
1	A	174	TYR	CB-CA-C	-7.19	96.01	110.40
1	B	491	ARG	CG-CD-NE	-7.11	96.88	111.80
3	F	180	ASN	CB-CA-C	-6.91	96.58	110.40
1	B	5	ASP	CB-CA-C	6.82	124.05	110.40
1	A	162	PRO	CA-N-CD	-6.78	102.01	111.50
1	A	234	VAL	N-CA-C	-6.71	92.88	111.00
2	E	100	CYS	CB-CA-C	-6.44	97.53	110.40
1	A	62	ARG	CB-CA-C	-6.43	97.54	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1303	ARG	CB-CA-C	6.37	123.15	110.40
1	A	236	PRO	N-CD-CG	-6.37	93.65	103.20
1	B	266	PHE	N-CA-CB	6.36	122.05	110.60
2	E	101	THR	N-CA-CB	-6.32	98.29	110.30
1	B	390	LYS	CB-CA-C	-6.24	97.92	110.40
1	B	198	ALA	CB-CA-C	-6.20	100.80	110.10
1	A	441	SER	CB-CA-C	-6.17	98.37	110.10
2	E	108	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	B	72	ARG	N-CA-CB	-5.86	100.05	110.60
1	B	57	LEU	CB-CA-C	-5.86	99.07	110.20
2	C	100	CYS	CB-CA-C	-5.84	98.72	110.40
1	B	197	PRO	N-CA-CB	-5.75	96.27	102.60
1	B	401	PRO	CA-N-CD	5.74	119.73	111.70
3	F	217	GLU	CA-CB-CG	5.70	125.94	113.40
3	D	217	GLU	CA-CB-CG	5.69	125.92	113.40
1	A	124	ARG	N-CA-CB	-5.61	100.50	110.60
1	A	176	MET	CB-CG-SD	-5.55	95.76	112.40
1	B	902	PRO	CA-N-CD	-5.50	103.81	111.50
1	B	43	ARG	N-CA-C	-5.46	96.26	111.00
1	A	1380	ARG	CB-CA-C	5.46	121.32	110.40
1	B	402	ARG	CB-CA-C	-5.45	99.51	110.40
3	F	166	ALA	N-CA-CB	-5.45	102.47	110.10
1	B	558	ALA	CB-CA-C	-5.44	101.93	110.10
1	A	524	PHE	CB-CA-C	-5.43	99.53	110.40
1	A	43	ARG	CA-C-O	-5.42	108.72	120.10
2	C	41	GLN	CB-CA-C	-5.41	99.58	110.40
1	B	902	PRO	N-CD-CG	-5.34	95.19	103.20
1	B	234	VAL	N-CA-C	-5.33	96.61	111.00
1	B	389	ILE	O-C-N	-5.31	114.20	122.70
1	A	92	GLN	CB-CG-CD	-5.29	97.84	111.60
2	C	101	THR	CA-CB-OG1	-5.25	97.98	109.00
3	F	48	SER	N-CA-CB	-5.17	102.75	110.50
1	B	387	GLY	O-C-N	-5.09	114.55	122.70
3	F	76	ALA	N-CA-CB	-5.04	103.05	110.10
1	B	399	THR	CB-CA-C	-5.03	98.01	111.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1301	GLN	Mainchain
2	C	155	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	E	155	GLU	Peptide
2	E	21	ARG	Sidechain
2	E	96	ALA	Mainchain
3	F	115	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10319	0	10164	311	0
1	B	7417	0	7306	208	0
2	C	1539	0	1511	59	0
2	E	1539	0	1511	61	0
3	D	1568	0	1528	54	0
3	F	1568	0	1533	62	0
4	B	21	0	22	2	0
All	All	23971	0	23575	714	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 15.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PRO:HB3	1:A:796:ASP:HA	1.54	0.88
2:C:86:GLN:HA	2:C:86:GLN:HE21	1.38	0.87
1:B:567:TRP:HB3	1:B:834:HIS:HB3	1.68	0.74
1:A:1019:LEU:HD13	1:A:1244:ILE:HG22	1.70	0.73
2:E:108:ASP:CG	3:F:67:LEU:CD2	2.60	0.70
2:E:108:ASP:CG	3:F:67:LEU:HD23	2.11	0.70
1:A:1249:ARG:HB2	1:A:1253:LEU:HD13	1.74	0.69
1:A:526:PRO:HG3	1:A:532:ALA:HB2	1.74	0.69
1:B:528:ASP:OD1	1:B:530:SER:N	2.24	0.69
1:A:43:ARG:HG2	1:A:129:LEU:HD11	1.75	0.69
2:E:108:ASP:OD1	3:F:67:LEU:HD23	1.93	0.69
1:A:1157:ALA:HA	1:A:1160:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:HB3	1:A:123:GLN:HG3	1.76	0.67
2:E:87:MET:HE1	2:E:116:VAL:HG11	1.75	0.67
1:A:739:CYS:HB3	1:A:744:ILE:HG22	1.77	0.66
1:A:54:PHE:HE1	1:A:376:LEU:HD21	1.61	0.66
1:A:981:VAL:HB	1:A:990:LEU:HD21	1.78	0.66
1:A:734:ARG:HA	1:A:737:ALA:HB3	1.77	0.65
1:A:126:MET:HB3	1:A:188:ILE:HD11	1.79	0.65
1:A:1171:VAL:HG21	1:A:1211:LEU:HD21	1.77	0.65
2:C:86:GLN:HA	2:C:86:GLN:NE2	2.10	0.65
2:E:8:GLN:HE22	2:E:99:TYR:HA	1.62	0.65
1:B:14:ARG:HG2	3:D:51:TYR:HE2	1.62	0.64
2:C:144:ALA:HB3	3:D:140:PHE:HZ	1.63	0.64
1:A:1000:VAL:HB	1:A:1039:LEU:HD21	1.81	0.63
1:B:561:VAL:HG13	1:B:828:PHE:HB2	1.81	0.62
1:A:817:VAL:HA	1:A:820:LEU:HD12	1.81	0.62
2:E:87:MET:HB3	2:E:90:LEU:HD21	1.81	0.62
1:B:122:GLN:HB3	1:B:155:LEU:HD23	1.81	0.62
1:A:117:LEU:HA	1:A:908:VAL:CG1	2.29	0.62
1:B:1416:LEU:HD21	1:B:1485:LEU:HB3	1.79	0.62
2:E:146:GLY:HA3	2:E:188:VAL:HG22	1.81	0.62
1:A:1239:LEU:HD23	1:A:1243:ARG:HD3	1.81	0.62
3:F:99:VAL:HG13	3:F:103:ASP:HB2	1.82	0.62
2:C:163:SER:HA	2:C:204:ASN:HD21	1.65	0.61
1:A:704:VAL:HG11	1:A:723:VAL:HG21	1.81	0.61
1:B:1428:LEU:HD21	1:B:1447:VAL:HG22	1.82	0.61
1:A:721:ARG:HB2	1:A:843:GLU:HB3	1.82	0.61
1:A:562:PHE:HB2	1:A:654:GLY:HA2	1.82	0.61
1:B:76:LEU:H	1:B:79:LEU:HD13	1.65	0.61
1:A:13:LEU:HD21	3:F:71:LEU:HD11	1.81	0.61
1:A:1075:ALA:HB2	1:A:1082:TRP:HD1	1.66	0.61
1:A:1231:LEU:HD13	1:A:1288:TYR:HB2	1.83	0.61
3:D:188:GLN:NE2	3:D:193:SER:HB2	2.16	0.61
3:F:188:GLN:NE2	3:F:193:SER:HB2	2.16	0.61
1:A:149:THR:HB	1:A:194:LEU:HD22	1.83	0.60
1:A:155:LEU:HD11	1:A:184:ALA:HB3	1.83	0.60
1:A:766:ALA:HA	1:A:770:GLU:HB3	1.83	0.60
1:A:642:TRP:HB3	1:A:647:VAL:HB	1.83	0.60
3:D:203:LEU:HG	3:D:204:SER:H	1.66	0.60
3:F:68:LEU:HA	3:F:79:VAL:HG21	1.83	0.60
2:E:4:VAL:HA	2:E:28:GLY:HA3	1.83	0.60
3:F:69:ILE:HD12	3:F:94:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:HB2	1:A:171:VAL:HG12	1.84	0.60
1:B:205:CYS:HB2	1:B:444:GLY:HA2	1.84	0.60
1:A:117:LEU:HA	1:A:908:VAL:HG13	1.84	0.60
3:F:203:LEU:HG	3:F:204:SER:H	1.66	0.60
1:B:624:VAL:HA	1:B:627:VAL:HG12	1.84	0.60
1:B:855:ILE:HG23	1:B:874:ARG:HG3	1.83	0.60
1:B:1427:VAL:HG22	1:B:1451:SER:HA	1.84	0.60
1:A:830:GLU:HB2	1:A:838:THR:HG23	1.83	0.60
3:F:152:ALA:HB3	3:F:203:LEU:HB3	1.84	0.60
1:B:35:VAL:HA	1:B:279:ARG:HA	1.84	0.60
1:B:609:GLU:H	1:B:612:ARG:HG3	1.66	0.60
1:B:577:LEU:HD12	1:B:584:ALA:HA	1.84	0.59
1:B:783:PRO:HB3	1:B:792:TRP:HE1	1.67	0.59
1:A:629:PRO:HG3	1:A:679:ALA:HA	1.84	0.59
1:B:82:PRO:HB3	1:A:1306:GLY:HA2	1.83	0.59
2:C:9:SER:HG	2:C:23:SER:HG	1.50	0.59
3:D:29:VAL:O	3:D:129:LYS:N	2.36	0.59
2:E:149:VAL:O	2:E:152:TYR:HD1	1.85	0.59
3:F:135:PRO:HB2	3:F:158:LEU:HD12	1.85	0.59
3:F:137:VAL:HG22	3:F:158:LEU:HD11	1.84	0.59
1:B:1:MET:O	2:E:54:ARG:NH2	2.35	0.59
1:B:692:LYS:HB3	1:B:754:ALA:HB2	1.84	0.59
1:A:493:ALA:HB2	1:A:536:LEU:HB3	1.83	0.59
1:B:13:LEU:HD21	3:D:71:LEU:HD11	1.84	0.59
1:B:700:PRO:HB2	1:B:703:GLU:HB3	1.85	0.59
1:A:1230:THR:OG1	1:A:1247:ALA:O	2.16	0.59
1:B:395:MET:O	1:B:436:ARG:NH2	2.35	0.59
1:A:610:ALA:HB2	1:A:613:ARG:HH21	1.68	0.59
1:B:296:GLY:HA3	1:B:327:SER:HB3	1.84	0.58
1:B:692:LYS:HE2	1:B:728:ASP:HB3	1.85	0.58
1:B:162:PRO:HG2	1:B:175:LEU:HD11	1.86	0.58
1:A:1070:VAL:O	1:A:1074:ILE:HG13	2.01	0.58
3:D:152:ALA:HB3	3:D:203:LEU:HB3	1.84	0.58
1:B:835:PRO:HD3	1:B:858:LEU:O	2.03	0.58
1:A:928:LEU:HB3	1:A:1361:VAL:HG13	1.85	0.58
2:E:4:VAL:HG23	2:E:29:PHE:HD1	1.68	0.58
1:A:720:PRO:HB2	1:A:721:ARG:HH11	1.69	0.58
1:A:1222:SER:HA	1:A:1267:LEU:HA	1.86	0.58
2:E:65:ALA:HB1	3:F:118:LEU:HD11	1.85	0.58
3:F:29:VAL:O	3:F:129:LYS:N	2.36	0.58
1:A:1025:ALA:HB2	1:A:1241:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ARG:NH1	1:B:758:SER:OG	2.37	0.57
1:B:787:THR:HB	1:B:811:VAL:HG13	1.84	0.57
1:A:966:ARG:HA	1:A:969:LEU:HB2	1.86	0.57
1:B:828:PHE:CZ	1:B:841:ILE:HB	2.40	0.57
1:A:316:GLN:HA	1:A:319:VAL:HG12	1.86	0.57
1:A:331:PRO:O	1:A:363:ARG:NH1	2.38	0.57
1:A:929:ARG:NH2	1:A:1129:ALA:O	2.38	0.57
1:A:1125:TRP:HH2	1:A:1362:ILE:HG13	1.70	0.57
1:A:608:ALA:HB1	1:A:612:ARG:HG3	1.86	0.57
1:B:29:GLU:HA	1:B:33:GLU:HB2	1.86	0.57
1:B:316:GLN:O	1:B:320:ILE:HG13	2.05	0.57
1:A:580:SER:HB3	1:A:865:LEU:HD22	1.87	0.57
1:A:561:VAL:HG23	1:A:813:PHE:HZ	1.69	0.56
1:A:966:ARG:HB2	1:A:976:VAL:HG21	1.86	0.56
3:D:188:GLN:HE21	3:D:193:SER:HB2	1.71	0.56
3:F:188:GLN:HE21	3:F:193:SER:HB2	1.70	0.56
1:A:1060:ARG:HG3	1:A:1061:ASN:N	2.21	0.56
1:B:55:TRP:CH2	1:B:401:PRO:HG3	2.41	0.56
1:A:302:ASP:OD1	1:A:449:ASN:ND2	2.34	0.56
2:C:149:VAL:O	2:C:152:TYR:HD1	1.89	0.56
1:A:945:LEU:N	1:A:972:ALA:O	2.37	0.56
2:C:6:LEU:O	2:C:111:GLY:HA2	2.04	0.56
2:E:95:THR:HG23	2:E:117:THR:HG23	1.86	0.56
2:E:155:GLU:HG2	2:E:183:TYR:CE2	2.41	0.56
1:A:334:ILE:HD13	1:A:359:TYR:HE1	1.70	0.56
1:A:737:ALA:C	1:A:739:CYS:H	2.09	0.56
1:B:649:PRO:HB2	1:B:782:VAL:HG11	1.87	0.56
1:B:729:SER:HA	1:B:732:LEU:HB2	1.88	0.56
1:A:1226:HIS:HD2	1:A:1258:LEU:HD12	1.71	0.56
1:A:715:ALA:HB3	1:A:724:VAL:HG12	1.88	0.55
1:A:1031:VAL:HG13	1:A:1078:ASN:HD21	1.71	0.55
1:B:476:VAL:HG11	1:B:884:TRP:CZ2	2.41	0.55
1:B:624:VAL:HG11	1:B:685:ILE:HG22	1.89	0.55
1:A:1063:ALA:O	1:A:1066:ALA:HB3	2.07	0.55
1:A:565:GLN:OE1	1:A:657:GLN:NE2	2.40	0.55
1:A:1048:GLU:HG3	1:A:1090:ALA:HA	1.87	0.55
1:A:1236:VAL:HA	1:A:1239:LEU:HB2	1.89	0.55
2:E:150:LYS:NZ	3:F:146:GLN:OE1	2.35	0.55
1:B:241:LEU:HA	1:B:250:LEU:HD11	1.88	0.55
3:D:58:LEU:HB2	3:D:68:LEU:HD11	1.89	0.55
2:E:15:GLN:HB2	2:E:18:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:54:LEU:HD11	3:F:109:CYS:SG	2.47	0.55
1:B:232:VAL:HG23	1:B:272:ALA:HB2	1.89	0.55
1:A:1222:SER:HB3	1:A:1268:THR:HG22	1.88	0.55
1:A:209:LEU:HD12	1:A:442:SER:OG	2.06	0.55
1:B:60:GLU:HG3	1:B:62:ARG:HG3	1.89	0.54
3:D:54:LEU:HD11	3:D:109:CYS:SG	2.47	0.54
1:A:8:LYS:HB2	2:C:105:THR:HG21	1.88	0.54
3:F:58:LEU:HB2	3:F:68:LEU:HD11	1.89	0.54
1:A:562:PHE:HB3	1:A:635:MET:HE1	1.89	0.54
1:A:65:VAL:HG21	1:A:255:ARG:HG3	1.89	0.54
2:C:22:LEU:HB2	2:C:85:LEU:HB3	1.90	0.54
1:B:126:MET:HB3	1:B:188:ILE:HD11	1.88	0.54
1:B:199:ILE:HG23	1:A:201:VAL:HG23	1.88	0.54
1:B:301:SER:HA	1:B:448:THR:HA	1.89	0.54
2:E:22:LEU:HB2	2:E:85:LEU:HB3	1.90	0.54
1:B:716:ALA:HB3	1:B:724:VAL:HB	1.90	0.54
1:B:104:PHE:HB3	1:B:908:VAL:HG21	1.90	0.54
1:B:778:LEU:HD12	1:B:779:PRO:HD2	1.89	0.53
1:A:1262:THR:HA	1:A:1265:LEU:HD13	1.88	0.53
2:E:77:ASP:O	2:E:81:SER:HA	2.08	0.53
3:F:130:ARG:NH1	3:F:133:ALA:HB2	2.23	0.53
3:D:171:LYS:HD3	3:D:177:GLN:HB3	1.90	0.53
1:A:340:HIS:CD2	1:A:442:SER:HA	2.44	0.53
2:E:149:VAL:HG13	2:E:205:VAL:HG11	1.89	0.53
1:A:945:LEU:HD21	1:A:1105:SER:HB3	1.90	0.53
2:C:40:ARG:HH22	2:C:68:VAL:HG11	1.73	0.53
3:F:30:THR:HB	3:F:129:LYS:HB3	1.91	0.53
1:B:287:GLY:O	1:B:895:ARG:NH1	2.42	0.53
1:A:646:GLY:HA3	1:A:883:ASP:HB3	1.90	0.53
3:F:19:VAL:HG11	3:F:45:LEU:HD21	1.90	0.53
3:F:56:TRP:HB2	3:F:69:ILE:HB	1.90	0.53
1:B:528:ASP:OD1	1:B:529:GLU:N	2.42	0.53
2:C:173:PHE:CZ	3:D:196:SER:HB3	2.43	0.53
1:A:162:PRO:HB2	1:A:175:LEU:HD21	1.90	0.53
1:A:1272:LEU:HD23	1:A:1295:LEU:HD22	1.91	0.53
1:B:187:ARG:HA	1:A:308:LEU:HD11	1.90	0.53
1:B:712:VAL:HA	1:B:727:GLY:HA3	1.90	0.53
1:A:233:THR:HG21	1:A:380:GLN:NE2	2.23	0.53
1:A:368:HIS:HB3	1:A:423:LEU:HD21	1.90	0.53
1:A:642:TRP:HZ3	1:A:831:VAL:HG13	1.72	0.53
1:A:1072:ARG:HG2	1:A:1112:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:HB1	1:B:905:ARG:HB3	1.90	0.53
1:A:613:ARG:NH2	1:A:620:SER:OG	2.42	0.53
1:A:692:LYS:HG3	1:A:728:ASP:HA	1.91	0.53
1:A:1028:LEU:HD11	1:A:1244:ILE:HD11	1.91	0.53
2:C:8:GLN:HE22	2:C:99:TYR:HA	1.74	0.53
3:F:142:PRO:HD3	3:F:154:VAL:HB	1.91	0.53
3:D:56:TRP:HB2	3:D:69:ILE:HB	1.90	0.53
1:B:591:ALA:HB2	1:B:602:VAL:HG22	1.91	0.52
1:B:680:LEU:HA	1:B:683:ARG:HE	1.73	0.52
3:D:142:PRO:HD3	3:D:154:VAL:HB	1.91	0.52
3:F:19:VAL:HG22	3:F:43:GLN:HB2	1.91	0.52
1:B:14:ARG:HG2	3:D:51:TYR:CE2	2.42	0.52
1:A:86:ARG:HG3	1:A:87:SER:H	1.73	0.52
1:A:950:LEU:HB2	1:A:1003:VAL:HG22	1.91	0.52
1:A:1313:ALA:HB3	1:A:1360:ILE:HG23	1.91	0.52
3:D:19:VAL:HG11	3:D:45:LEU:HD21	1.90	0.52
2:C:77:ASP:O	2:C:81:SER:HA	2.08	0.52
3:D:19:VAL:HG22	3:D:43:GLN:HB2	1.91	0.52
3:D:30:THR:HB	3:D:129:LYS:HB3	1.91	0.52
1:B:339:ALA:HB1	1:B:351:GLU:OE2	2.10	0.52
1:A:1074:ILE:HG22	1:A:1082:TRP:HB2	1.91	0.52
3:D:27:LEU:HD13	3:D:37:ILE:HG13	1.92	0.52
2:E:206:ASN:HB3	2:E:213:LYS:HG3	1.89	0.52
1:A:1259:HIS:CE1	1:A:1302:ARG:HG3	2.44	0.52
1:B:609:GLU:O	1:B:613:ARG:HB2	2.10	0.52
1:A:153:VAL:HG12	1:A:155:LEU:HG	1.92	0.52
1:A:906:GLU:HG2	1:A:907:ARG:H	1.75	0.52
2:C:177:LEU:HD13	2:C:183:TYR:CE1	2.44	0.52
3:D:127:ASP:OD1	3:D:195:TYR:OH	2.28	0.52
1:A:208:SER:HB2	1:A:385:VAL:HB	1.92	0.52
1:A:1170:LEU:H	1:A:1170:LEU:HD12	1.74	0.52
3:D:130:ARG:HG3	3:D:131:THR:O	2.11	0.52
1:B:817:VAL:O	1:B:820:LEU:HB3	2.09	0.51
1:A:154:GLY:HA3	1:A:207:SER:HB3	1.91	0.51
1:B:133:VAL:HG22	1:B:276:LEU:HB2	1.91	0.51
1:B:519:PRO:O	1:B:520:HIS:ND1	2.44	0.51
1:A:43:ARG:HB2	1:A:272:ALA:HB3	1.92	0.51
1:B:558:ALA:HB2	1:B:880:VAL:HG13	1.91	0.51
2:C:171:HIS:CE1	3:D:159:ASN:HD21	2.28	0.51
1:B:788:VAL:HB	1:B:806:ASN:HA	1.93	0.51
3:F:27:LEU:HD13	3:F:37:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:TRP:HZ2	1:A:1087:ASP:HB2	1.76	0.51
1:B:8:LYS:HG2	2:E:105:THR:HG21	1.92	0.51
1:B:605:PHE:CD2	1:B:630:VAL:HG11	2.46	0.51
1:B:605:PHE:HD2	1:B:630:VAL:HG11	1.74	0.51
1:A:511:LEU:HD13	1:A:898:LEU:HD13	1.93	0.51
1:A:571:GLY:O	1:A:574:VAL:HG13	2.10	0.51
2:E:101:THR:HG22	2:E:110:TRP:CD2	2.46	0.51
3:F:130:ARG:HG3	3:F:131:THR:O	2.10	0.51
1:B:1427:VAL:HG11	1:B:1455:LEU:HB2	1.93	0.51
1:A:293:VAL:HG23	1:A:455:GLU:HB3	1.93	0.51
1:A:619:LEU:HB2	1:A:623:ARG:HG3	1.91	0.51
1:A:1278:SER:OG	1:A:1289:ALA:O	2.29	0.51
2:C:150:LYS:NZ	3:D:146:GLN:OE1	2.39	0.51
1:B:149:THR:HB	1:B:194:LEU:HD22	1.92	0.51
1:A:38:VAL:N	1:A:276:LEU:O	2.40	0.51
1:A:155:LEU:HD23	1:A:232:VAL:HG13	1.92	0.51
1:B:602:VAL:HG12	1:B:630:VAL:HG12	1.93	0.51
1:A:92:GLN:HE21	1:A:254:GLY:HA2	1.75	0.51
1:A:269:ALA:O	1:A:380:GLN:NE2	2.44	0.51
1:A:390:LYS:HE3	1:A:401:PRO:HG2	1.92	0.51
1:A:1087:ASP:HB3	1:A:1114:ALA:HA	1.93	0.51
3:F:127:ASP:OD1	3:F:195:TYR:OH	2.28	0.51
1:A:558:ALA:HB2	1:A:880:VAL:HG13	1.92	0.51
1:A:1209:ARG:HA	1:A:1261:LEU:HD21	1.92	0.51
1:A:1301:GLN:C	1:A:1304:SER:H	2.15	0.51
2:E:24:CYS:HB3	2:E:83:ALA:HB3	1.92	0.51
1:B:828:PHE:HE1	1:B:852:LEU:HB3	1.76	0.50
1:A:367:LEU:HB3	1:A:420:ILE:HG12	1.92	0.50
1:A:471:VAL:HG11	1:A:865:LEU:HD23	1.93	0.50
1:A:577:LEU:HB2	1:A:584:ALA:HB2	1.93	0.50
1:A:692:LYS:HE3	1:A:754:ALA:HA	1.91	0.50
1:A:797:GLU:HB2	1:A:805:ARG:HH22	1.76	0.50
2:C:24:CYS:HB3	2:C:83:ALA:HB3	1.92	0.50
1:B:623:ARG:O	1:B:627:VAL:N	2.33	0.50
1:B:683:ARG:HD2	1:B:770:GLU:HG2	1.92	0.50
2:C:105:THR:HA	3:D:117:ARG:HH22	1.75	0.50
1:B:576:LEU:HD22	1:B:858:LEU:HD11	1.94	0.50
1:A:54:PHE:HZ	1:A:372:VAL:HG21	1.77	0.50
1:A:171:VAL:HG21	1:A:910:LEU:HD11	1.94	0.50
1:A:339:ALA:HB2	1:A:369:LEU:HD11	1.93	0.50
3:F:130:ARG:HD2	3:F:193:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:ARG:HA	1:A:1305:ASP:OD2	2.12	0.50
3:F:170:TRP:CD2	3:F:201:LEU:HD13	2.47	0.50
1:A:1337:ILE:HG22	1:A:1363:ASP:HB3	1.94	0.50
3:F:69:ILE:HG23	3:F:74:ASN:O	2.11	0.50
1:B:141:PRO:HD2	1:B:516:ALA:HB2	1.93	0.50
1:A:329:LEU:HD13	1:A:437:ARG:HD3	1.93	0.50
1:A:627:VAL:O	1:A:631:MET:HG2	2.12	0.50
2:C:91:LYS:HE3	2:C:93:GLU:HB3	1.94	0.50
2:C:178:GLN:OE1	2:C:184:SER:OG	2.15	0.50
2:E:178:GLN:OE1	2:E:184:SER:OG	2.15	0.50
1:B:292:ALA:HB3	1:B:392:VAL:HG22	1.94	0.50
1:B:666:ALA:O	1:B:781:PHE:N	2.29	0.50
1:B:701:ALA:HA	1:B:704:VAL:HG22	1.94	0.50
1:A:1302:ARG:HD3	1:A:1309:ALA:HB2	1.94	0.50
2:E:170:VAL:HG22	2:E:189:VAL:HG12	1.94	0.50
2:C:170:VAL:HG22	2:C:189:VAL:HG12	1.94	0.50
2:E:177:LEU:HB2	2:E:183:TYR:HE1	1.77	0.50
1:B:93:ARG:NH2	1:A:1055:PRO:O	2.27	0.49
1:B:595:GLU:HA	1:B:598:LEU:O	2.12	0.49
1:A:597:HIS:CE1	1:A:676:ARG:HB2	2.47	0.49
1:A:776:HIS:HB2	2:C:213:LYS:NZ	2.27	0.49
1:B:736:VAL:HG22	1:B:746:ALA:HB3	1.94	0.49
1:A:698:ALA:HA	1:A:722:SER:HA	1.94	0.49
1:A:837:LEU:O	1:A:841:ILE:N	2.45	0.49
1:A:800:ALA:HA	1:A:803:TRP:CD1	2.48	0.49
3:D:130:ARG:HD2	3:D:193:SER:OG	2.11	0.49
1:A:38:VAL:HG12	1:A:137:ALA:HB1	1.93	0.49
1:A:108:PHE:HZ	1:A:131:TRP:CE2	2.30	0.49
1:A:642:TRP:CD1	1:A:829:LEU:HD21	2.47	0.49
2:C:133:PRO:HG2	2:C:220:PRO:HB3	1.94	0.49
3:D:217:GLU:HB3	3:D:228:THR:HA	1.95	0.49
1:B:300:ASN:O	1:B:449:ASN:N	2.45	0.49
1:A:840:ALA:HA	1:A:843:GLU:OE1	2.13	0.49
1:B:77:ASP:OD2	1:A:931:ARG:NE	2.46	0.49
1:A:932:ILE:HD11	1:A:1125:TRP:CD1	2.47	0.49
2:E:177:LEU:HB2	2:E:183:TYR:CE1	2.47	0.49
1:A:103:ALA:HB1	1:A:905:ARG:HB3	1.95	0.49
1:A:841:ILE:O	1:A:844:ILE:HB	2.13	0.49
1:A:1068:TRP:CZ2	1:A:1087:ASP:HB2	2.48	0.49
1:B:162:PRO:HD2	1:B:175:LEU:HD21	1.94	0.49
1:A:1019:LEU:HG	1:A:1252:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:O	1:A:157:PRO:C	2.51	0.49
1:A:1383:ASP:OD1	1:A:1389:ARG:NH2	2.46	0.49
1:A:305:SER:OG	1:A:307:GLY:O	2.29	0.48
2:C:160:SER:HB3	2:C:164:GLY:H	1.78	0.48
2:C:177:LEU:HD13	2:C:183:TYR:HE1	1.76	0.48
3:D:25:LEU:O	3:D:125:LYS:N	2.41	0.48
2:E:133:PRO:HG2	2:E:220:PRO:HB3	1.95	0.48
1:A:704:VAL:HG22	1:A:714:ILE:HD11	1.95	0.48
1:A:1270:PHE:O	1:A:1272:LEU:HD12	2.13	0.48
2:C:6:LEU:HD11	2:C:102:ARG:HG3	1.95	0.48
1:A:838:THR:HA	1:A:841:ILE:HB	1.96	0.48
2:C:151:ASP:HA	2:C:182:LEU:HB3	1.95	0.48
1:B:98:LEU:HD12	1:B:234:VAL:HG22	1.96	0.48
1:B:688:MET:N	1:B:689:PRO:HD3	2.28	0.48
1:B:712:VAL:HG12	1:B:725:VAL:HG22	1.95	0.48
1:B:718:ASN:O	1:B:840:ALA:HB1	2.13	0.48
3:F:217:GLU:HB3	3:F:228:THR:HA	1.95	0.48
1:B:622:GLU:OE1	1:B:623:ARG:NH1	2.46	0.48
1:A:162:PRO:HD2	1:A:910:LEU:HG	1.95	0.48
1:A:1096:LEU:HA	1:A:1100:LEU:HG	1.94	0.48
2:C:131:LEU:HD11	2:C:148:LEU:HG	1.94	0.48
2:C:177:LEU:O	3:D:182:GLN:NE2	2.24	0.48
3:D:187:GLU:OE1	3:D:187:GLU:N	2.47	0.48
1:B:302:ASP:N	1:B:447:GLY:O	2.46	0.48
1:B:764:ARG:HE	1:B:768:HIS:CD2	2.32	0.48
1:A:71:ASP:O	1:A:907:ARG:NH2	2.46	0.48
1:A:156:ILE:HG13	1:A:381:ALA:HB2	1.95	0.48
1:A:385:VAL:O	1:A:389:ILE:HG13	2.13	0.48
1:A:1143:VAL:HG11	1:A:1160:LEU:HD13	1.94	0.48
3:F:187:GLU:N	3:F:187:GLU:OE1	2.47	0.48
1:B:257:LYS:HG3	1:B:405:HIS:HB3	1.96	0.48
1:B:491:ARG:HD3	1:B:902:PRO:HD3	1.96	0.48
2:C:149:VAL:CG1	2:C:205:VAL:HG11	2.43	0.48
1:B:562:PHE:HB2	1:B:654:GLY:HA2	1.96	0.48
1:B:663:ALA:HB1	1:B:669:LEU:HB2	1.96	0.48
1:B:680:LEU:HD23	1:B:771:LEU:HA	1.95	0.48
1:B:814:ALA:HB1	1:B:844:ILE:HD11	1.96	0.48
1:A:15:ARG:HH21	3:D:76:ALA:HB1	1.79	0.48
2:C:95:THR:HG23	2:C:117:THR:HG23	1.95	0.48
3:D:58:LEU:HD13	3:D:107:TYR:CZ	2.49	0.48
1:B:475:TRP:CD1	1:B:508:ALA:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:VAL:HA	1:A:739:CYS:HB2	1.96	0.48
1:A:784:PHE:O	1:A:792:TRP:HD1	1.96	0.47
1:B:19:ASP:OD1	3:F:77:SER:HB3	2.13	0.47
1:A:568:GLN:OE1	1:A:568:GLN:N	2.36	0.47
1:A:1171:VAL:HG22	1:A:1198:ALA:HB3	1.96	0.47
1:B:429:TRP:HH2	1:B:438:ALA:HB2	1.79	0.47
1:B:783:PRO:HB3	1:B:792:TRP:NE1	2.28	0.47
1:B:819:ALA:O	1:B:823:GLN:HB2	2.15	0.47
1:A:197:PRO:HD2	1:A:224:SER:HB3	1.96	0.47
1:A:1158:ARG:HG2	1:A:1188:LEU:HD23	1.96	0.47
1:A:1313:ALA:HB3	1:A:1360:ILE:HA	1.95	0.47
2:E:155:GLU:HG2	2:E:183:TYR:CD2	2.49	0.47
2:E:185:LEU:HD23	2:E:186:SER:N	2.29	0.47
1:B:273:GLY:HA3	1:B:385:VAL:HG13	1.97	0.47
1:B:329:LEU:HD13	1:B:437:ARG:HD3	1.97	0.47
2:E:151:ASP:HA	2:E:182:LEU:HB3	1.95	0.47
1:B:12:TYR:CD1	2:E:106:LEU:HD22	2.49	0.47
1:B:159:GLU:HG2	1:A:163:ARG:HE	1.79	0.47
3:D:184:SER:HB3	3:D:198:SER:HB3	1.96	0.47
3:F:58:LEU:HD13	3:F:107:TYR:CZ	2.49	0.47
1:B:502:GLN:HB2	1:B:507:ILE:HD11	1.96	0.47
1:A:652:VAL:HG21	1:A:666:ALA:HB2	1.96	0.47
1:B:242:VAL:O	1:B:246:ARG:HG2	2.14	0.47
1:B:308:LEU:HD21	1:A:183:VAL:HB	1.97	0.47
1:B:391:MET:O	1:B:395:MET:HG3	2.14	0.47
1:B:753:TYR:HE2	1:B:755:SER:HB2	1.79	0.47
4:B:1801:PN7:O2P	4:B:1801:PN7:O3	2.32	0.47
1:A:683:ARG:HA	1:A:683:ARG:HD3	1.69	0.47
1:A:688:MET:N	1:A:689:PRO:HD2	2.30	0.47
1:A:802:TYR:HA	1:A:805:ARG:HE	1.80	0.47
1:A:1152:VAL:HG22	1:A:1317:TRP:CD1	2.49	0.47
1:A:226:LEU:HD12	1:A:278:GLU:HB2	1.96	0.47
1:A:1000:VAL:HG12	1:A:1002:GLY:H	1.78	0.47
1:B:28:ARG:HH21	3:D:75:ARG:HH21	1.63	0.47
1:B:118:ALA:O	1:B:178:GLY:HA3	2.15	0.47
1:B:154:GLY:HA3	1:B:207:SER:HB3	1.97	0.47
1:A:312:ASN:HD22	1:A:315:ALA:HB2	1.80	0.47
1:A:340:HIS:HD2	1:A:442:SER:HA	1.80	0.47
1:A:478:SER:O	1:A:488:GLN:NE2	2.48	0.47
1:A:524:PHE:HE2	1:A:532:ALA:HB1	1.80	0.47
3:D:163:PRO:O	3:D:220:HIS:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:VAL:HG21	1:B:866:ALA:HA	1.97	0.47
1:A:555:GLN:O	1:A:557:ARG:HG2	2.15	0.47
1:B:835:PRO:HB3	1:B:856:HIS:HB2	1.96	0.46
1:A:856:HIS:CE1	1:A:859:ARG:HG2	2.50	0.46
1:B:680:LEU:HG	1:B:770:GLU:HG3	1.98	0.46
1:B:476:VAL:HB	1:B:876:PHE:CE2	2.51	0.46
2:E:7:VAL:HG23	2:E:25:THR:HB	1.98	0.46
1:B:680:LEU:O	1:B:684:VAL:HG13	2.16	0.46
1:B:855:ILE:HG12	1:B:875:ALA:HA	1.97	0.46
1:A:638:LEU:HB3	1:A:642:TRP:CZ3	2.51	0.46
1:A:1079:PRO:HB3	1:A:1377:ARG:HG2	1.98	0.46
1:B:69:PRO:CG	1:B:72:ARG:HD2	2.45	0.46
1:A:485:LEU:HD21	1:A:522:ALA:HB2	1.95	0.46
1:A:495:HIS:NE2	1:A:897:PRO:O	2.47	0.46
1:A:756:HIS:H	1:A:807:LEU:HA	1.81	0.46
3:D:166:ALA:HB2	3:D:220:HIS:HB2	1.97	0.46
2:E:208:LYS:HA	2:E:208:LYS:HD2	1.70	0.46
1:B:562:PHE:CE1	1:B:652:VAL:HG13	2.51	0.46
1:B:632:PHE:CE1	1:B:660:ILE:HB	2.50	0.46
1:A:317:VAL:HG13	1:A:358:ALA:HB2	1.98	0.46
1:A:660:ILE:HG22	1:A:674:ALA:HB1	1.96	0.46
2:E:152:TYR:HB2	2:E:207:HIS:CD2	2.50	0.46
1:B:121:PRO:HG2	1:B:236:PRO:HB3	1.97	0.46
1:B:400:LEU:HD22	1:B:423:LEU:HD11	1.98	0.46
1:A:476:VAL:O	1:A:511:LEU:HG	2.16	0.46
1:A:1137:TRP:HE1	1:A:1268:THR:HG23	1.81	0.46
1:A:1176:PRO:HD2	1:A:1199:ALA:HB2	1.97	0.46
1:A:1272:LEU:HD23	1:A:1295:LEU:CD2	2.46	0.46
1:B:121:PRO:HG3	1:B:909:TRP:CZ3	2.51	0.46
1:B:336:ALA:HB2	1:B:400:LEU:HD11	1.98	0.46
1:B:1421:ARG:NH1	1:B:1436:VAL:H	2.14	0.46
2:E:13:LEU:HD13	2:E:117:THR:HB	1.98	0.46
2:E:31:PHE:HB3	2:E:78:ASP:OD1	2.16	0.46
1:B:207:SER:HB2	1:B:381:ALA:HB1	1.98	0.46
1:B:521:ARG:HD3	1:B:876:PHE:O	2.16	0.46
1:B:526:PRO:HB3	1:B:532:ALA:HB2	1.97	0.46
1:B:731:GLU:O	1:B:735:LEU:HG	2.16	0.46
1:A:349:PRO:HA	1:A:413:ILE:HG12	1.98	0.46
1:A:1209:ARG:HD2	1:A:1261:LEU:HD11	1.98	0.46
3:D:144:ASP:HA	3:D:147:LEU:HD12	1.98	0.46
2:E:31:PHE:CE2	2:E:76:ARG:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH1	1:B:552:SER:OG	2.49	0.45
1:A:241:LEU:HB3	1:A:268:MET:CE	2.47	0.45
1:A:584:ALA:O	1:A:588:ARG:HG2	2.15	0.45
1:A:692:LYS:NZ	1:A:726:ALA:HB1	2.31	0.45
2:E:143:ALA:HA	3:F:138:PHE:HE2	1.81	0.45
2:E:188:VAL:HG21	3:F:157:LEU:HD12	1.99	0.45
1:B:339:ALA:HB2	1:B:355:LEU:HD11	1.99	0.45
1:A:510:SER:HB3	1:A:895:ARG:HB2	1.98	0.45
2:E:37:SER:HB2	2:E:101:THR:OG1	2.15	0.45
3:F:58:LEU:O	3:F:66:GLN:N	2.40	0.45
1:B:205:CYS:HB3	1:B:378:HIS:NE2	2.32	0.45
1:B:165:ALA:O	1:A:242:VAL:HG11	2.15	0.45
1:B:351:GLU:HG3	1:B:443:PHE:HE2	1.81	0.45
1:B:443:PHE:CD1	1:B:449:ASN:HB3	2.50	0.45
1:B:632:PHE:HE1	1:B:661:ALA:N	2.14	0.45
1:A:340:HIS:HA	1:A:373:LYS:HZ3	1.81	0.45
1:A:388:VAL:HG22	1:A:440:VAL:HG21	1.99	0.45
2:C:31:PHE:HB3	2:C:78:ASP:OD1	2.16	0.45
1:B:2:ALA:HA	2:E:54:ARG:HH21	1.81	0.45
1:B:765:ASP:OD1	1:B:766:ALA:N	2.49	0.45
1:A:1229:ALA:HB1	1:A:1288:TYR:HE1	1.82	0.45
1:A:1377:ARG:HA	1:A:1377:ARG:HD2	1.77	0.45
2:C:31:PHE:CE2	2:C:76:ARG:HB2	2.51	0.45
1:A:17:THR:HG23	3:F:74:ASN:HD21	1.81	0.45
2:E:77:ASP:O	2:E:81:SER:CA	2.64	0.45
3:F:137:VAL:HB	3:F:229:LYS:NZ	2.32	0.45
1:A:805:ARG:HD2	1:A:809:ARG:NH2	2.32	0.45
2:C:77:ASP:O	2:C:81:SER:CA	2.64	0.45
1:B:797:GLU:H	1:B:797:GLU:HG3	1.66	0.45
1:A:539:LEU:HD22	1:A:539:LEU:HA	1.70	0.45
1:A:826:ARG:HG3	1:A:852:LEU:HA	1.99	0.45
2:C:7:VAL:HG23	2:C:25:THR:HB	1.98	0.45
1:A:696:SER:HB2	1:A:747:LYS:HE2	1.99	0.45
3:D:58:LEU:HD13	3:D:107:TYR:CE2	2.52	0.45
2:E:176:VAL:CG2	3:F:184:SER:HB2	2.47	0.45
1:B:561:VAL:CG1	1:B:828:PHE:HB2	2.47	0.45
1:B:565:GLN:HG2	1:B:657:GLN:HE22	1.82	0.45
1:B:782:VAL:HG12	1:B:783:PRO:O	2.17	0.45
1:A:103:ALA:HA	1:A:906:GLU:O	2.17	0.45
1:A:1034:MET:SD	1:A:1081:VAL:HG13	2.57	0.45
3:F:137:VAL:HG22	3:F:158:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD21	1:B:238:PRO:HB3	1.99	0.44
2:E:131:LEU:HD12	2:E:131:LEU:HA	1.81	0.44
1:B:661:ALA:O	1:B:665:VAL:HG22	2.18	0.44
1:A:243:ASP:O	1:A:244:PHE:C	2.52	0.44
1:A:1043:LEU:N	1:A:1081:VAL:O	2.48	0.44
1:A:1139:PRO:HB2	1:A:1165:ALA:HA	1.99	0.44
1:A:1310:THR:HG22	1:A:1312:VAL:HG13	1.98	0.44
1:A:1362:ILE:HB	1:A:1364:VAL:HG12	2.00	0.44
2:E:148:LEU:HD21	3:F:155:VAL:HG21	2.00	0.44
3:F:58:LEU:HD13	3:F:107:TYR:CE2	2.52	0.44
1:A:763:ILE:HB	1:A:767:LEU:HB2	1.99	0.44
1:A:784:PHE:CE2	1:A:798:LEU:HD11	2.52	0.44
1:A:1068:TRP:O	1:A:1072:ARG:HG3	2.16	0.44
1:A:1188:LEU:H	1:A:1188:LEU:HG	1.50	0.44
2:E:207:HIS:O	2:E:211:ASN:N	2.49	0.44
1:B:483:GLU:OE1	1:B:486:ARG:NH2	2.49	0.44
1:B:813:PHE:CE2	1:B:841:ILE:HD11	2.52	0.44
1:A:329:LEU:HD12	1:A:453:ILE:HG21	1.99	0.44
1:A:528:ASP:H	1:A:531:ALA:HB3	1.83	0.44
2:C:52:PHE:CE1	2:C:63:GLU:HB3	2.53	0.44
3:D:58:LEU:O	3:D:66:GLN:N	2.40	0.44
1:B:349:PRO:HA	1:B:413:ILE:HG12	1.99	0.44
1:A:480:SER:HB2	1:A:518:LEU:HD22	2.00	0.44
1:A:619:LEU:HD12	1:A:619:LEU:HA	1.71	0.44
1:A:720:PRO:HB2	1:A:721:ARG:HD2	1.99	0.44
3:F:158:LEU:HD13	3:F:158:LEU:HA	1.82	0.44
1:B:44:LEU:HD22	1:B:376:LEU:HD13	2.00	0.44
1:B:1459:LEU:HD12	1:B:1459:LEU:HA	1.82	0.44
1:A:302:ASP:HB3	1:A:312:ASN:HB2	2.00	0.44
1:A:568:GLN:HE21	1:A:621:THR:HG21	1.82	0.44
1:A:655:HIS:NE2	1:A:724:VAL:HG21	2.33	0.44
1:B:317:VAL:HG13	1:B:358:ALA:HB2	1.99	0.44
1:B:529:GLU:O	1:B:533:LEU:HD13	2.16	0.44
1:B:710:ASP:HB2	1:B:731:GLU:HG3	1.98	0.44
2:E:35:ALA:CB	2:E:54:ARG:HA	2.48	0.44
1:B:234:VAL:HA	1:B:270:GLU:HG3	2.00	0.44
1:A:682:SER:HA	1:A:685:ILE:HG22	2.00	0.44
1:A:1093:VAL:HB	1:A:1096:LEU:HD12	1.98	0.44
1:A:1143:VAL:HG21	1:A:1160:LEU:HD22	2.00	0.44
1:A:1224:VAL:HB	1:A:1270:PHE:HD1	1.83	0.44
2:C:37:SER:O	2:C:101:THR:OG1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:25:LEU:O	3:F:125:LYS:N	2.41	0.44
1:B:512:ALA:HB1	1:B:884:TRP:HB3	2.00	0.43
1:B:588:ARG:HD2	1:B:603:ILE:HG13	2.00	0.43
1:A:69:PRO:HG3	1:A:97:PHE:HB3	2.00	0.43
1:A:778:LEU:HD22	1:A:778:LEU:HA	1.81	0.43
1:B:34:PRO:HB2	1:B:293:VAL:HG11	1.99	0.43
1:A:1028:LEU:HD21	1:A:1070:VAL:HG21	1.99	0.43
1:A:1096:LEU:HD22	1:A:1100:LEU:HD11	2.00	0.43
1:A:1110:GLU:HB2	1:A:1113:LEU:HD21	1.99	0.43
1:A:1298:LEU:O	1:A:1302:ARG:HB2	2.18	0.43
3:F:22:GLN:N	3:F:22:GLN:OE1	2.51	0.43
1:B:171:VAL:HG21	1:B:910:LEU:HD21	1.99	0.43
1:B:379:THR:HB	1:B:382:ALA:HB3	2.00	0.43
1:A:573:ALA:HB1	1:A:576:LEU:HB3	2.00	0.43
1:A:1071:GLY:HA3	1:A:1085:LEU:HD11	2.00	0.43
1:A:1167:HIS:CD2	1:A:1219:VAL:HG11	2.53	0.43
3:D:128:ILE:HB	3:D:188:GLN:NE2	2.34	0.43
1:A:177:THR:O	1:A:183:VAL:HG21	2.19	0.43
1:A:703:GLU:HG2	1:A:704:VAL:N	2.34	0.43
1:B:492:LEU:HD21	1:B:511:LEU:HD11	2.01	0.43
1:A:149:THR:HA	1:A:226:LEU:O	2.19	0.43
1:A:705:ARG:HG2	1:A:714:ILE:HG13	2.00	0.43
1:A:949:TRP:HZ3	1:A:1044:TRP:HD1	1.65	0.43
3:F:31:PRO:HA	3:F:99:VAL:O	2.19	0.43
1:B:80:PHE:CE1	1:B:93:ARG:HD2	2.53	0.43
1:B:338:GLU:O	1:B:338:GLU:HG3	2.18	0.43
1:A:641:MET:HG2	1:A:868:PHE:CZ	2.53	0.43
3:D:22:GLN:OE1	3:D:22:GLN:N	2.51	0.43
1:B:697:ILE:HG12	1:B:699:ALA:H	1.84	0.43
2:C:8:GLN:HE21	2:C:100:CYS:HB2	1.83	0.43
1:A:155:LEU:HD12	1:A:200:SER:OG	2.19	0.43
1:A:610:ALA:HA	1:A:613:ARG:HE	1.83	0.43
1:A:1088:VAL:HG11	1:A:1096:LEU:HD23	2.00	0.43
3:D:31:PRO:HA	3:D:99:VAL:O	2.19	0.43
3:D:137:VAL:HB	3:D:229:LYS:NZ	2.34	0.43
2:E:80:LYS:O	2:E:82:ILE:HG12	2.18	0.43
2:E:205:VAL:O	2:E:213:LYS:HA	2.19	0.43
1:B:632:PHE:O	1:B:636:VAL:HG12	2.19	0.43
1:A:39:ALA:HB2	1:A:137:ALA:HB2	2.00	0.43
1:A:593:ALA:HB1	1:A:672:ASP:HA	2.00	0.43
2:E:53:ILE:HB	2:E:74:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:ASP:CG	3:F:67:LEU:HD22	2.37	0.43
2:E:112:GLN:H	2:E:112:GLN:HG3	1.17	0.43
3:F:29:VAL:HB	3:F:99:VAL:HG11	2.00	0.43
3:F:106:VAL:HG22	3:F:125:LYS:HD2	2.01	0.43
1:B:739:CYS:SG	1:B:740:THR:N	2.91	0.43
1:B:836:ILE:H	1:B:836:ILE:HG13	1.36	0.43
1:A:406:ALA:HB1	1:A:422:LEU:HD13	2.01	0.43
1:A:512:ALA:HB1	1:A:884:TRP:CG	2.54	0.43
1:A:1155:GLN:HG3	1:A:1158:ARG:NH1	2.34	0.43
1:A:1173:ARG:HD2	1:A:1201:ASP:HA	2.00	0.43
3:F:58:LEU:HD21	3:F:60:LYS:HG3	2.01	0.43
1:A:64:ALA:N	1:A:375:ASN:O	2.45	0.42
1:A:235:MET:HA	1:A:236:PRO:HD2	1.83	0.42
1:A:367:LEU:O	1:A:421:SER:N	2.39	0.42
1:A:1033:ALA:O	1:A:1037:ALA:N	2.50	0.42
1:A:1143:VAL:HG11	1:A:1160:LEU:CD1	2.49	0.42
1:B:349:PRO:O	1:B:353:ARG:HG3	2.18	0.42
1:B:805:ARG:HG2	1:B:809:ARG:HH12	1.84	0.42
1:A:29:GLU:HA	1:A:33:GLU:HB2	2.01	0.42
1:A:532:ALA:HA	1:A:535:VAL:HG23	2.01	0.42
1:A:608:ALA:HA	1:A:612:ARG:HE	1.85	0.42
2:C:49:TRP:HZ2	2:C:52:PHE:HD1	1.66	0.42
2:C:80:LYS:O	2:C:82:ILE:HG12	2.19	0.42
2:C:185:LEU:HD23	2:C:186:SER:N	2.34	0.42
3:D:141:PRO:HA	3:D:154:VAL:HG23	2.01	0.42
3:F:215:ALA:HA	3:F:230:SER:HA	2.01	0.42
1:B:334:ILE:O	1:B:363:ARG:NH1	2.33	0.42
1:B:719:GLY:H	1:B:814:ALA:HB2	1.83	0.42
1:B:35:VAL:HG23	1:B:294:LEU:HB2	2.01	0.42
1:B:36:ALA:HB1	1:B:290:VAL:HG13	2.02	0.42
1:B:731:GLU:HA	1:B:734:ARG:HG2	2.00	0.42
4:B:1801:PN7:H15	1:A:311:PRO:HD3	2.01	0.42
1:A:337:VAL:HG23	1:A:367:LEU:HD11	2.02	0.42
1:A:668:ALA:HB2	1:A:795:PRO:HB2	2.01	0.42
1:A:1159:TRP:HE1	1:A:1163:ARG:CZ	2.32	0.42
1:B:774:ASP:OD1	1:B:774:ASP:N	2.52	0.42
1:A:495:HIS:CG	1:A:899:PRO:HD3	2.55	0.42
1:A:739:CYS:HA	1:A:742:GLU:HG2	2.02	0.42
1:A:1007:LEU:H	1:A:1007:LEU:HG	1.42	0.42
1:A:1301:GLN:C	1:A:1303:ARG:N	2.70	0.42
1:A:1339:MET:H	1:A:1339:MET:HG3	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:29:VAL:HB	3:D:99:VAL:HG11	2.00	0.42
3:D:54:LEU:HD13	3:D:92:PHE:CG	2.54	0.42
1:B:228:MET:HG2	1:B:276:LEU:HD13	2.02	0.42
1:B:410:SER:HB3	1:B:413:ILE:HD12	2.02	0.42
1:B:731:GLU:HG2	1:B:734:ARG:HH11	1.84	0.42
1:A:241:LEU:HB3	1:A:268:MET:HE2	2.01	0.42
1:A:944:ARG:HD3	1:A:944:ARG:HA	1.92	0.42
2:C:69:LYS:HA	2:C:69:LYS:HD3	1.84	0.42
2:C:206:ASN:HD22	2:C:213:LYS:HG3	1.85	0.42
1:B:269:ALA:HB2	1:B:377:GLY:HA3	2.01	0.42
1:B:434:ARG:HE	1:B:434:ARG:HB3	1.61	0.42
1:B:1465:VAL:HG21	1:B:1485:LEU:HD11	2.02	0.42
1:A:1049:SER:N	1:A:1088:VAL:O	2.50	0.42
1:A:1331:PHE:HB3	1:A:1336:VAL:HG13	2.02	0.42
3:F:128:ILE:HB	3:F:188:GLN:NE2	2.34	0.42
1:B:378:HIS:CD2	1:B:380:GLN:H	2.38	0.42
1:A:265:GLY:HA2	1:A:344:THR:HA	2.02	0.42
1:A:338:GLU:N	1:A:439:GLY:O	2.46	0.42
1:A:556:GLN:HG3	1:A:881:ALA:HB2	2.02	0.42
1:A:628:GLN:HB2	1:A:682:SER:HB2	2.02	0.42
1:A:737:ALA:C	1:A:739:CYS:N	2.70	0.42
3:F:102:GLU:H	3:F:102:GLU:HG2	1.66	0.42
1:B:652:VAL:C	1:B:653:ILE:HG12	2.40	0.42
1:A:506:ASP:OD2	1:A:894:ARG:NH1	2.53	0.42
1:A:577:LEU:HD23	1:A:577:LEU:H	1.85	0.42
1:A:589:GLU:HG2	1:A:590:CYS:N	2.35	0.42
1:A:1222:SER:HB3	1:A:1268:THR:H	1.85	0.42
3:D:168:VAL:HG21	3:D:197:LEU:HD22	2.02	0.42
1:A:465:ARG:HD2	1:A:465:ARG:HA	1.39	0.42
2:C:149:VAL:HG13	2:C:205:VAL:HG11	2.01	0.42
3:F:118:LEU:HD13	3:F:118:LEU:HA	1.83	0.42
1:B:400:LEU:HA	1:B:401:PRO:HD3	1.88	0.41
1:B:695:ALA:O	1:B:725:VAL:HG12	2.20	0.41
1:A:311:PRO:HG2	1:A:350:ILE:HD12	2.01	0.41
2:C:18:ARG:HA	2:C:18:ARG:HD3	1.74	0.41
2:C:38:TRP:O	2:C:50:VAL:HB	2.19	0.41
1:A:253:ASP:OD2	1:A:255:ARG:HD3	2.20	0.41
1:A:811:VAL:HG12	1:A:813:PHE:HB2	2.01	0.41
2:C:171:HIS:CE1	3:D:159:ASN:ND2	2.88	0.41
3:D:215:ALA:HA	3:D:230:SER:HA	2.01	0.41
2:E:49:TRP:HZ2	2:E:52:PHE:HD1	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PRO:HB2	1:B:293:VAL:CG1	2.50	0.41
1:B:39:ALA:HB2	1:B:137:ALA:HB2	2.01	0.41
1:B:221:ARG:HD2	1:B:223:GLU:HB2	2.03	0.41
1:A:12:TYR:CE1	3:D:70:TYR:HB2	2.55	0.41
1:A:802:TYR:HD1	1:A:805:ARG:HH21	1.68	0.41
3:D:106:VAL:HG22	3:D:125:LYS:HD2	2.01	0.41
1:B:55:TRP:O	1:B:59:SER:HB3	2.20	0.41
1:B:650:ALA:HB1	1:B:825:TYR:CZ	2.56	0.41
1:B:1437:PRO:HB2	1:B:1440:GLN:HB2	2.02	0.41
1:A:604:PRO:HB3	1:A:607:ARG:HH21	1.86	0.41
2:E:21:ARG:NH1	2:E:84:TYR:CD2	2.88	0.41
2:E:53:ILE:HG23	2:E:76:ARG:HH11	1.84	0.41
2:E:80:LYS:NZ	2:E:82:ILE:HG13	2.36	0.41
1:B:227:ALA:O	1:B:276:LEU:HD12	2.21	0.41
1:B:1409:ALA:HB3	1:B:1411:GLU:CG	2.51	0.41
1:A:139:ILE:HD12	1:A:139:ILE:H	1.85	0.41
1:A:171:VAL:HG21	1:A:910:LEU:CD1	2.50	0.41
1:A:625:ASP:HB3	1:A:686:ALA:HB2	2.01	0.41
2:C:6:LEU:HD22	2:C:24:CYS:SG	2.61	0.41
3:D:146:GLN:OE1	3:D:153:SER:HB2	2.20	0.41
2:E:131:LEU:HB2	2:E:146:GLY:C	2.40	0.41
3:F:59:GLN:OE1	3:F:65:PRO:HG3	2.20	0.41
1:B:140:PRO:HA	1:B:141:PRO:HD3	1.96	0.41
1:B:1471:THR:HG23	1:B:1475:HIS:HD2	1.85	0.41
1:A:1030:LEU:O	1:A:1034:MET:HG3	2.21	0.41
2:E:77:ASP:O	2:E:81:SER:N	2.54	0.41
3:F:141:PRO:HA	3:F:154:VAL:HG23	2.01	0.41
3:F:146:GLN:OE1	3:F:153:SER:HB2	2.20	0.41
1:B:329:LEU:HD12	1:B:453:ILE:HG21	2.03	0.41
1:B:512:ALA:HB1	1:B:884:TRP:CG	2.56	0.41
1:B:562:PHE:HD2	1:B:635:MET:HE2	1.85	0.41
2:C:80:LYS:NZ	2:C:82:ILE:HG13	2.36	0.41
1:A:92:GLN:HB2	1:A:250:LEU:HD23	2.01	0.41
1:A:865:LEU:HD12	1:A:865:LEU:HA	1.86	0.41
2:C:126:PRO:HB3	2:C:149:VAL:CG1	2.51	0.41
3:D:59:GLN:OE1	3:D:65:PRO:HG3	2.20	0.41
3:F:189:ASP:OD1	3:F:194:THR:N	2.49	0.41
1:B:115:GLU:O	1:B:119:VAL:HG23	2.21	0.41
1:B:357:GLU:HA	1:B:361:ARG:HG2	2.02	0.41
1:A:141:PRO:HG2	1:A:516:ALA:HB2	2.03	0.41
1:A:1054:GLY:HA3	1:A:1056:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:PHE:HE2	2:C:76:ARG:HB2	1.86	0.41
2:C:37:SER:HB3	2:C:52:PHE:HB3	2.03	0.41
2:C:149:VAL:HG12	2:C:152:TYR:CD1	2.55	0.41
2:C:161:TRP:HD1	2:C:170:VAL:HG13	1.85	0.41
1:B:511:LEU:O	1:B:515:ARG:HB2	2.20	0.41
1:B:839:ALA:HA	1:B:842:GLU:HB2	2.03	0.41
1:A:564:GLY:HA3	1:A:656:SER:HG	1.85	0.41
1:A:773:GLU:H	1:A:773:GLU:HG3	1.47	0.41
1:A:911:GLU:HA	1:A:912:PRO:HD2	1.86	0.41
1:A:1206:GLU:HA	1:A:1209:ARG:HB3	2.03	0.41
1:A:1318:ALA:HB3	1:A:1341:PRO:HD3	2.03	0.41
3:F:53:TYR:O	3:F:112:SER:N	2.54	0.41
3:F:130:ARG:HH12	3:F:133:ALA:HB2	1.85	0.41
1:B:689:PRO:HG3	1:B:753:TYR:HB3	2.02	0.40
1:B:692:LYS:HG3	1:B:759:HIS:CD2	2.56	0.40
1:B:712:VAL:HG22	1:B:727:GLY:HA3	2.02	0.40
1:A:692:LYS:HE2	1:A:757:SER:OG	2.20	0.40
1:A:1334:HIS:HA	1:A:1368:ARG:HB3	2.03	0.40
2:C:77:ASP:O	2:C:81:SER:N	2.54	0.40
2:C:159:VAL:HG22	2:C:205:VAL:HG13	2.03	0.40
1:A:533:LEU:HD13	1:A:533:LEU:HA	1.75	0.40
1:A:805:ARG:HD2	1:A:809:ARG:HH21	1.85	0.40
2:C:13:LEU:HD13	2:C:117:THR:HB	2.03	0.40
3:D:104:VAL:HG23	3:D:126:VAL:HG12	2.03	0.40
2:E:173:PHE:O	2:E:185:LEU:HG	2.21	0.40
3:F:135:PRO:HG3	3:F:220:HIS:HB3	2.04	0.40
1:B:506:ASP:HB3	1:B:896:VAL:HG21	2.03	0.40
1:B:1448:ASP:O	1:B:1449:SER:C	2.59	0.40
1:A:443:PHE:HA	1:A:449:ASN:HA	2.04	0.40
1:A:1239:LEU:HD23	1:A:1239:LEU:HA	1.95	0.40
2:E:31:PHE:O	2:E:76:ARG:NH2	2.54	0.40
1:A:133:VAL:HG22	1:A:276:LEU:HB2	2.04	0.40
1:A:609:GLU:O	1:A:613:ARG:N	2.54	0.40
1:A:1321:GLY:HA2	1:A:1324:GLU:HB3	2.04	0.40
1:A:1366:TRP:HA	1:A:1369:PHE:HB3	2.02	0.40
3:D:53:TYR:O	3:D:112:SER:N	2.54	0.40
1:B:163:ARG:HE	1:A:159:GLU:HG2	1.86	0.40
1:B:217:GLN:HG3	1:A:221:ARG:NH1	2.37	0.40
1:B:659:GLU:HG3	1:B:806:ASN:ND2	2.37	0.40
1:B:680:LEU:HD12	1:B:683:ARG:NH2	2.36	0.40
1:A:42:CYS:O	1:A:42:CYS:SG	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:HE	1:A:93:ARG:HB3	1.42	0.40
1:A:640:SER:HA	1:A:643:ARG:HD3	2.04	0.40
1:A:682:SER:O	1:A:685:ILE:HG22	2.21	0.40
2:C:6:LEU:HD23	2:C:6:LEU:HA	1.93	0.40
2:C:40:ARG:N	2:C:48:GLU:O	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1388/1784 (78%)	1264 (91%)	123 (9%)	1 (0%)	51 83
1	B	995/1784 (56%)	915 (92%)	78 (8%)	2 (0%)	47 79
2	C	199/249 (80%)	179 (90%)	20 (10%)	0	100 100
2	E	199/249 (80%)	176 (88%)	23 (12%)	0	100 100
3	D	200/236 (85%)	184 (92%)	16 (8%)	0	100 100
3	F	200/236 (85%)	187 (94%)	13 (6%)	0	100 100
All	All	3181/4538 (70%)	2905 (91%)	273 (9%)	3 (0%)	54 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1449	SER
1	B	720	PRO
1	A	779	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	A	1028/1325 (78%)	884 (86%)	144 (14%)	3 16
1	B	746/1325 (56%)	653 (88%)	93 (12%)	4 21
2	C	170/203 (84%)	132 (78%)	38 (22%)	1 4
2	E	170/203 (84%)	136 (80%)	34 (20%)	1 6
3	D	182/208 (88%)	146 (80%)	36 (20%)	1 7
3	F	182/208 (88%)	147 (81%)	35 (19%)	1 8
All	All	2478/3472 (71%)	2098 (85%)	380 (15%)	6 13

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	VAL
1	B	31	GLU
1	B	52	GLU
1	B	54	PHE
1	B	57	LEU
1	B	75	ASP
1	B	100	GLU
1	B	112	SER
1	B	114	ARG
1	B	123	GLN
1	B	124	ARG
1	B	126	MET
1	B	129	LEU
1	B	156	ILE
1	B	159	GLU
1	B	162	PRO
1	B	163	ARG
1	B	164	LEU
1	B	175	LEU
1	B	180	THR
1	B	182	SER
1	B	197	PRO

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Mol	Chain	Res	Type
1	B	209	LEU
1	B	212	VAL
1	B	214	LEU
1	B	220	ARG
1	B	221	ARG
1	B	237	THR
1	B	240	MET
1	B	241	LEU
1	B	264	ASN
1	B	268	MET
1	B	270	GLU
1	B	314	ARG
1	B	342	THR
1	B	344	THR
1	B	345	ARG
1	B	402	ARG
1	B	497	ARG
1	B	553	ARG
1	B	556	GLN
1	B	567	TRP
1	B	572	MET
1	B	574	VAL
1	B	575	ASP
1	B	577	LEU
1	B	579	THR
1	B	606	LEU
1	B	607	ARG
1	B	612	ARG
1	B	623	ARG
1	B	631	MET
1	B	653	ILE
1	B	660	ILE
1	B	682	SER
1	B	684	VAL
1	B	703	GLU
1	B	705	ARG
1	B	721	ARG
1	B	722	SER
1	B	751	VAL
1	B	752	ASP
1	B	785	PHE
1	B	788	VAL

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Mol	Chain	Res	Type
1	B	797	GLU
1	B	799	ASP
1	B	826	ARG
1	B	827	THR
1	B	831	VAL
1	B	836	ILE
1	B	837	LEU
1	B	853	SER
1	B	859	ARG
1	B	865	LEU
1	B	870	GLU
1	B	872	LEU
1	B	873	SER
1	B	874	ARG
1	B	908	VAL
1	B	1407	LEU
1	B	1411	GLU
1	B	1412	ARG
1	B	1414	LYS
1	B	1435	ARG
1	B	1436	VAL
1	B	1448	ASP
1	B	1453	LEU
1	B	1455	LEU
1	B	1456	ARG
1	B	1459	LEU
1	B	1463	THR
1	B	1466	ARG
1	B	1485	LEU
1	A	1	MET
1	A	3	SER
1	A	5	ASP
1	A	6	SER
1	A	7	GLU
1	A	8	LYS
1	A	42	CYS
1	A	44	LEU
1	A	57	LEU
1	A	63	ASP
1	A	65	VAL
1	A	93	ARG
1	A	98	LEU

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Mol	Chain	Res	Type
1	A	117	LEU
1	A	124	ARG
1	A	157	PRO
1	A	158	GLN
1	A	159	GLU
1	A	162	PRO
1	A	163	ARG
1	A	171	VAL
1	A	176	MET
1	A	179	THR
1	A	180	THR
1	A	203	THR
1	A	207	SER
1	A	220	ARG
1	A	243	ASP
1	A	247	MET
1	A	266	PHE
1	A	342	THR
1	A	376	LEU
1	A	404	LEU
1	A	422	LEU
1	A	460	VAL
1	A	461	VAL
1	A	462	GLU
1	A	464	GLU
1	A	465	ARG
1	A	467	GLU
1	A	498	GLU
1	A	505	ARG
1	A	515	ARG
1	A	524	PHE
1	A	530	SER
1	A	533	LEU
1	A	534	ARG
1	A	535	VAL
1	A	539	LEU
1	A	599	ASP
1	A	601	GLU
1	A	619	LEU
1	A	623	ARG
1	A	627	VAL
1	A	683	ARG

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Mol	Chain	Res	Type
1	A	711	ARG
1	A	717	VAL
1	A	722	SER
1	A	723	VAL
1	A	731	GLU
1	A	732	LEU
1	A	735	LEU
1	A	736	VAL
1	A	745	ARG
1	A	748	ARG
1	A	759	HIS
1	A	762	THR
1	A	763	ILE
1	A	765	ASP
1	A	767	LEU
1	A	770	GLU
1	A	771	LEU
1	A	773	GLU
1	A	775	PHE
1	A	777	PRO
1	A	778	LEU
1	A	782	VAL
1	A	784	PHE
1	A	785	PHE
1	A	786	SER
1	A	797	GLU
1	A	799	ASP
1	A	826	ARG
1	A	853	SER
1	A	855	ILE
1	A	859	ARG
1	A	867	ASP
1	A	870	GLU
1	A	913	LYS
1	A	918	ARG
1	A	948	THR
1	A	950	LEU
1	A	960	GLU
1	A	961	THR
1	A	977	ARG
1	A	978	GLU
1	A	980	VAL

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Mol	Chain	Res	Type
1	A	981	VAL
1	A	982	ASP
1	A	1007	LEU
1	A	1010	ASP
1	A	1015	GLU
1	A	1060	ARG
1	A	1125	TRP
1	A	1144	LEU
1	A	1145	VAL
1	A	1168	LEU
1	A	1169	LEU
1	A	1173	ARG
1	A	1179	ASP
1	A	1184	LEU
1	A	1188	LEU
1	A	1194	ARG
1	A	1196	THR
1	A	1235	THR
1	A	1237	ASP
1	A	1238	THR
1	A	1244	ILE
1	A	1246	ARG
1	A	1249	ARG
1	A	1251	LYS
1	A	1253	LEU
1	A	1263	ARG
1	A	1296	ASP
1	A	1303	ARG
1	A	1307	LEU
1	A	1327	VAL
1	A	1330	ARG
1	A	1333	ARG
1	A	1336	VAL
1	A	1339	MET
1	A	1342	GLU
1	A	1357	VAL
1	A	1360	ILE
1	A	1362	ILE
1	A	1363	ASP
1	A	1364	VAL
1	A	1367	ASP
1	A	1371	LEU

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Mol	Chain	Res	Type
1	A	1376	GLN
1	A	1377	ARG
1	A	1379	THR
1	A	1380	ARG
1	A	1385	ILE
2	C	4	VAL
2	C	5	GLN
2	C	18	ARG
2	C	30	THR
2	C	36	MET
2	C	37	SER
2	C	45	LYS
2	C	56	LYS
2	C	61	THR
2	C	67	SER
2	C	69	LYS
2	C	77	ASP
2	C	78	ASP
2	C	80	LYS
2	C	84	TYR
2	C	86	GLN
2	C	87	MET
2	C	91	LYS
2	C	92	THR
2	C	93	GLU
2	C	101	THR
2	C	106	LEU
2	C	108	ASP
2	C	112	GLN
2	C	114	THR
2	C	124	LYS
2	C	145	LEU
2	C	150	LYS
2	C	158	THR
2	C	168	SER
2	C	172	THR
2	C	178	GLN
2	C	182	LEU
2	C	202	ILE
2	C	204	ASN
2	C	206	ASN
2	C	216	LYS

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Mol	Chain	Res	Type
2	C	219	GLU
3	D	18	VAL
3	D	20	MET
3	D	26	SER
3	D	33	GLU
3	D	36	SER
3	D	48	SER
3	D	49	ASN
3	D	77	SER
3	D	81	ASP
3	D	84	SER
3	D	93	THR
3	D	95	LYS
3	D	96	ILE
3	D	114	GLN
3	D	117	ARG
3	D	118	LEU
3	D	119	THR
3	D	132	VAL
3	D	137	VAL
3	D	139	ILE
3	D	144	ASP
3	D	145	GLU
3	D	153	SER
3	D	157	LEU
3	D	178	SER
3	D	181	SER
3	D	185	VAL
3	D	186	THR
3	D	187	GLU
3	D	197	LEU
3	D	202	THR
3	D	205	LYS
3	D	217	GLU
3	D	219	THR
3	D	221	GLN
3	D	224	SER
2	E	14	VAL
2	E	30	THR
2	E	33	ASP
2	E	36	MET
2	E	45	LYS

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Mol	Chain	Res	Type
2	E	55	SER
2	E	56	LYS
2	E	61	THR
2	E	67	SER
2	E	69	LYS
2	E	77	ASP
2	E	78	ASP
2	E	80	LYS
2	E	84	TYR
2	E	91	LYS
2	E	92	THR
2	E	93	GLU
2	E	97	VAL
2	E	105	THR
2	E	108	ASP
2	E	112	GLN
2	E	124	LYS
2	E	131	LEU
2	E	145	LEU
2	E	150	LYS
2	E	158	THR
2	E	160	SER
2	E	168	SER
2	E	172	THR
2	E	177	LEU
2	E	178	GLN
2	E	182	LEU
2	E	208	LYS
2	E	219	GLU
3	F	18	VAL
3	F	20	MET
3	F	26	SER
3	F	33	GLU
3	F	36	SER
3	F	48	SER
3	F	49	ASN
3	F	77	SER
3	F	81	ASP
3	F	84	SER
3	F	86	SER
3	F	90	THR
3	F	92	PHE

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Mol	Chain	Res	Type
3	F	93	THR
3	F	94	LEU
3	F	102	GLU
3	F	117	ARG
3	F	118	LEU
3	F	119	THR
3	F	139	ILE
3	F	144	ASP
3	F	145	GLU
3	F	148	LYS
3	F	153	SER
3	F	167	LYS
3	F	178	SER
3	F	181	SER
3	F	185	VAL
3	F	186	THR
3	F	187	GLU
3	F	205	LYS
3	F	217	GLU
3	F	219	THR
3	F	221	GLN
3	F	224	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	ASN
1	A	340	HIS
1	A	378	HIS
1	A	776	HIS
1	A	1226	HIS
2	C	8	GLN
2	C	41	GLN
2	C	86	GLN
2	C	112	GLN
2	C	171	HIS
2	C	204	ASN
2	C	206	ASN
3	D	188	GLN
3	F	188	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	PN7	B	1801	1	13,20,21	2.33	4 (30%)	18,26,29	1.41	4 (22%)

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	PN7	B	1801	1	-	10/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1801	PN7	C4-N5	5.34	1.45	1.33
4	B	1801	PN7	C8-N9	5.21	1.45	1.33
4	B	1801	PN7	O4-C4	-2.28	1.18	1.23

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1801	PN7	O8-C8	-2.10	1.19	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1801	PN7	C6-C7-C8	2.45	116.44	112.36
4	B	1801	PN7	C6-N5-C4	-2.29	118.50	122.59
4	B	1801	PN7	CE2-C2-C3	2.14	112.52	108.82
4	B	1801	PN7	C11-C10-N9	-2.02	107.68	112.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1801	PN7	C1-C2-C3-O3
4	B	1801	PN7	C1-C2-C3-C4
4	B	1801	PN7	CE1-C2-C3-O3
4	B	1801	PN7	CE1-C2-C3-C4
4	B	1801	PN7	CE2-C2-C3-O3
4	B	1801	PN7	CE2-C2-C3-C4
4	B	1801	PN7	N9-C10-C11-S12
4	B	1801	PN7	N5-C6-C7-C8
4	B	1801	PN7	O3P-C1-C2-CE1
4	B	1801	PN7	O3P-C1-C2-CE2

There are no ring outliers.

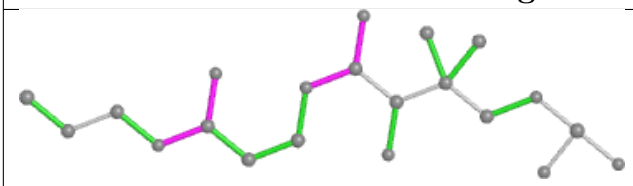
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1801	PN7	2	0

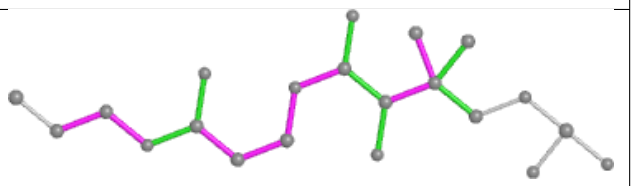
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

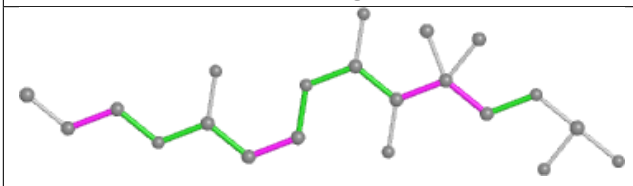
Ligand PN7 B 1801



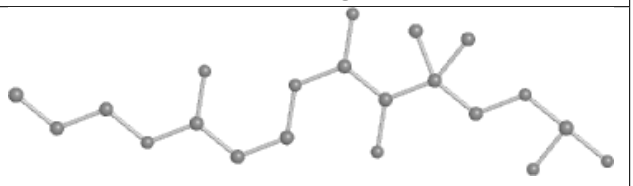
Bond lengths



Bond angles



Torsions



Rings

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.

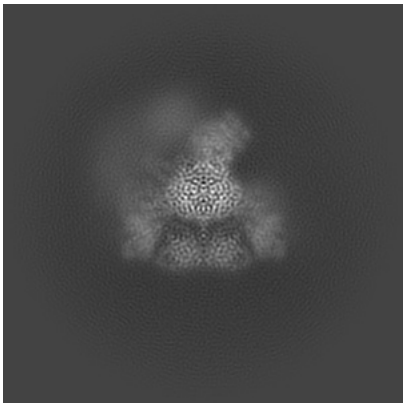
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23711. These allow visual inspection of the internal detail of the map and identification of artifacts.

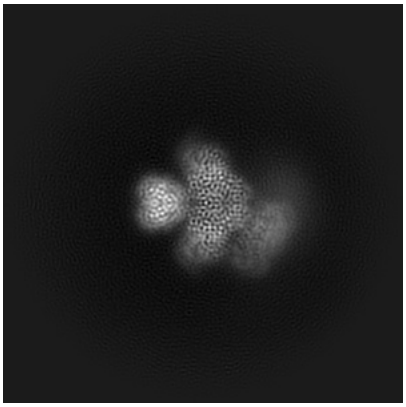
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

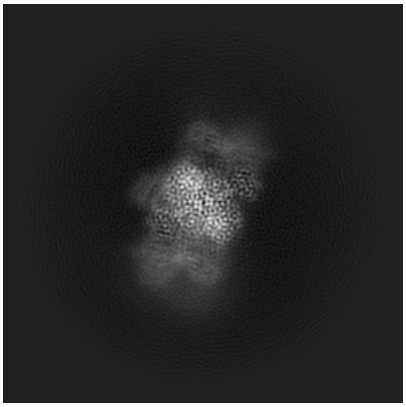
6.1.1 Primary map



X



Y

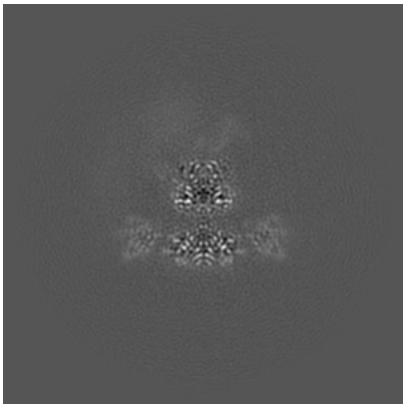


Z

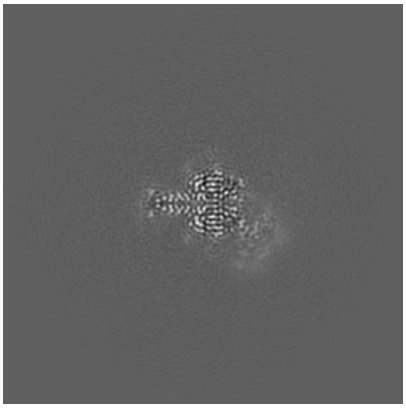
The images above show the map projected in three orthogonal directions.

6.2 Central slices

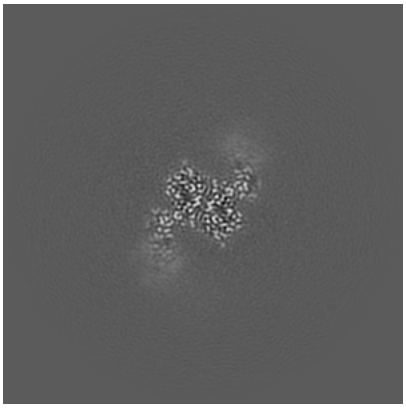
6.2.1 Primary map



X Index: 168



Y Index: 168

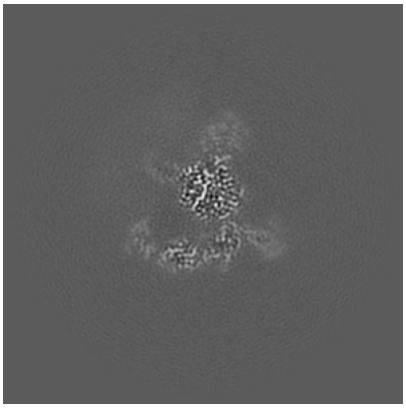


Z Index: 168

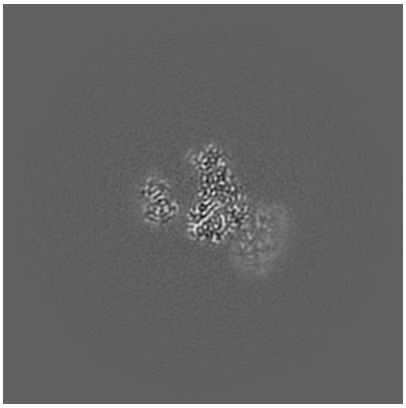
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

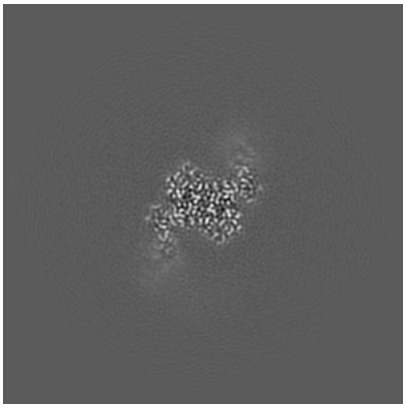
6.3.1 Primary map



X Index: 157



Y Index: 181



Z Index: 173

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

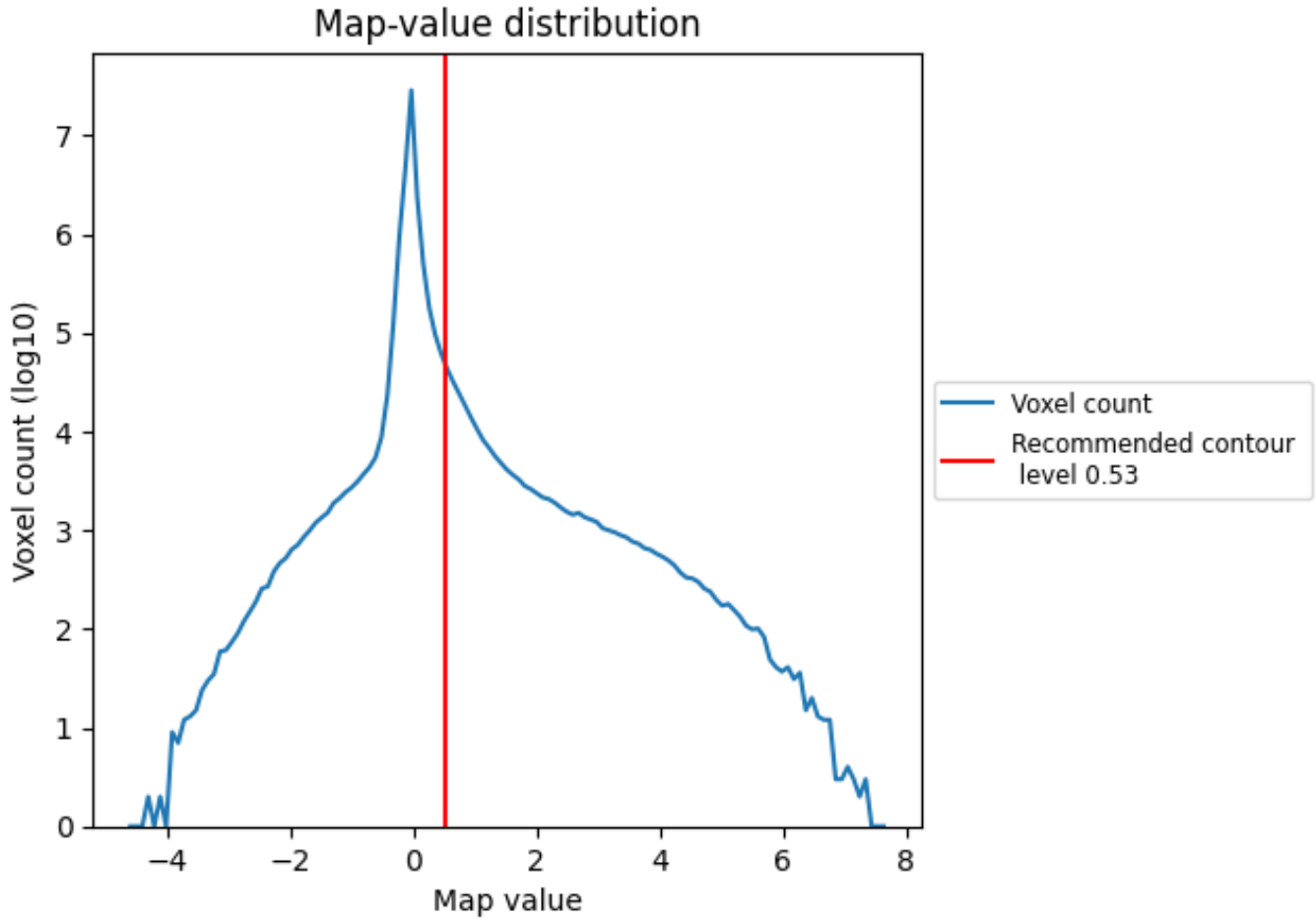
6.5 Mask visualisation (i)

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

7 Map analysis

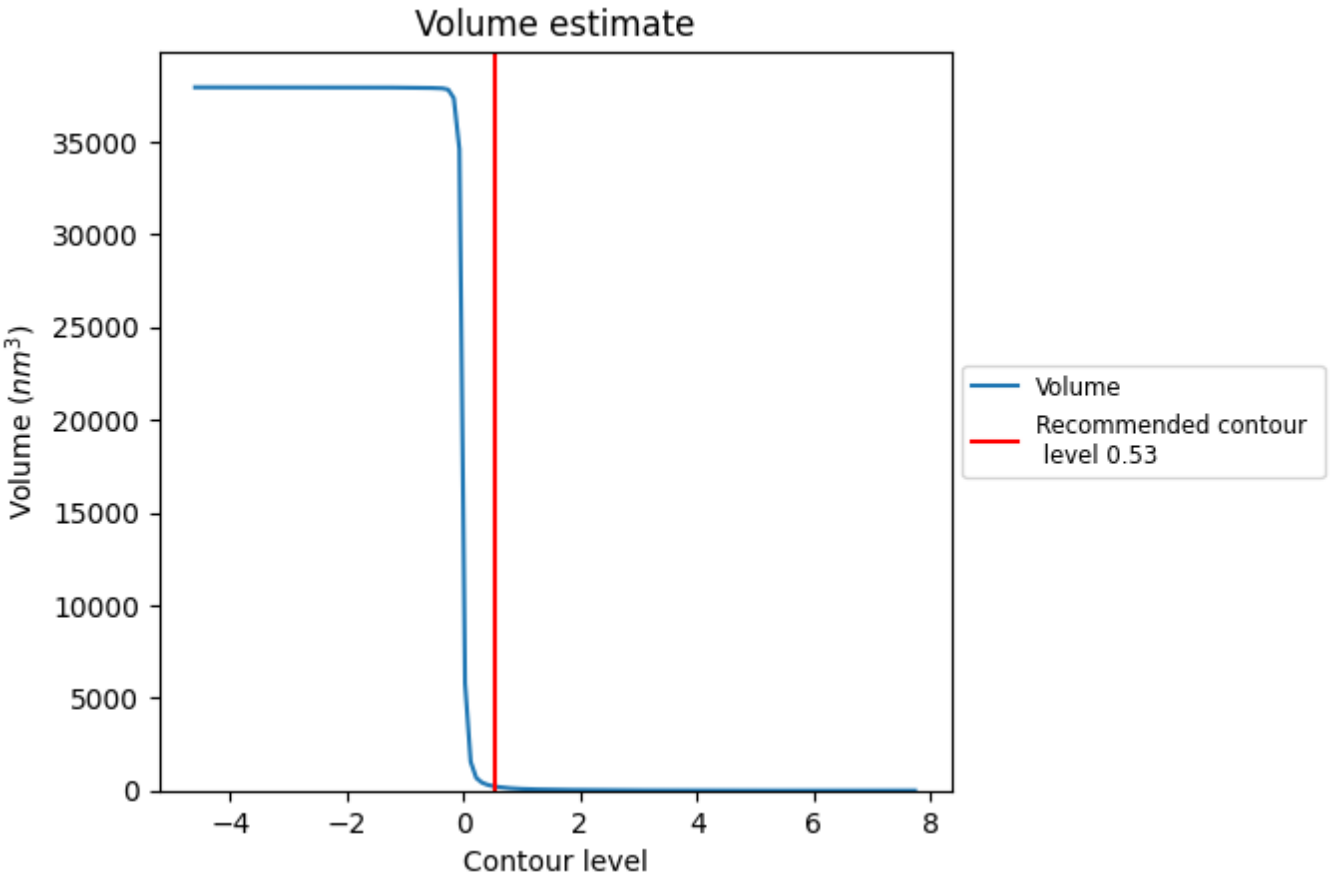
This section contains the results of statistical analysis of the map.

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.

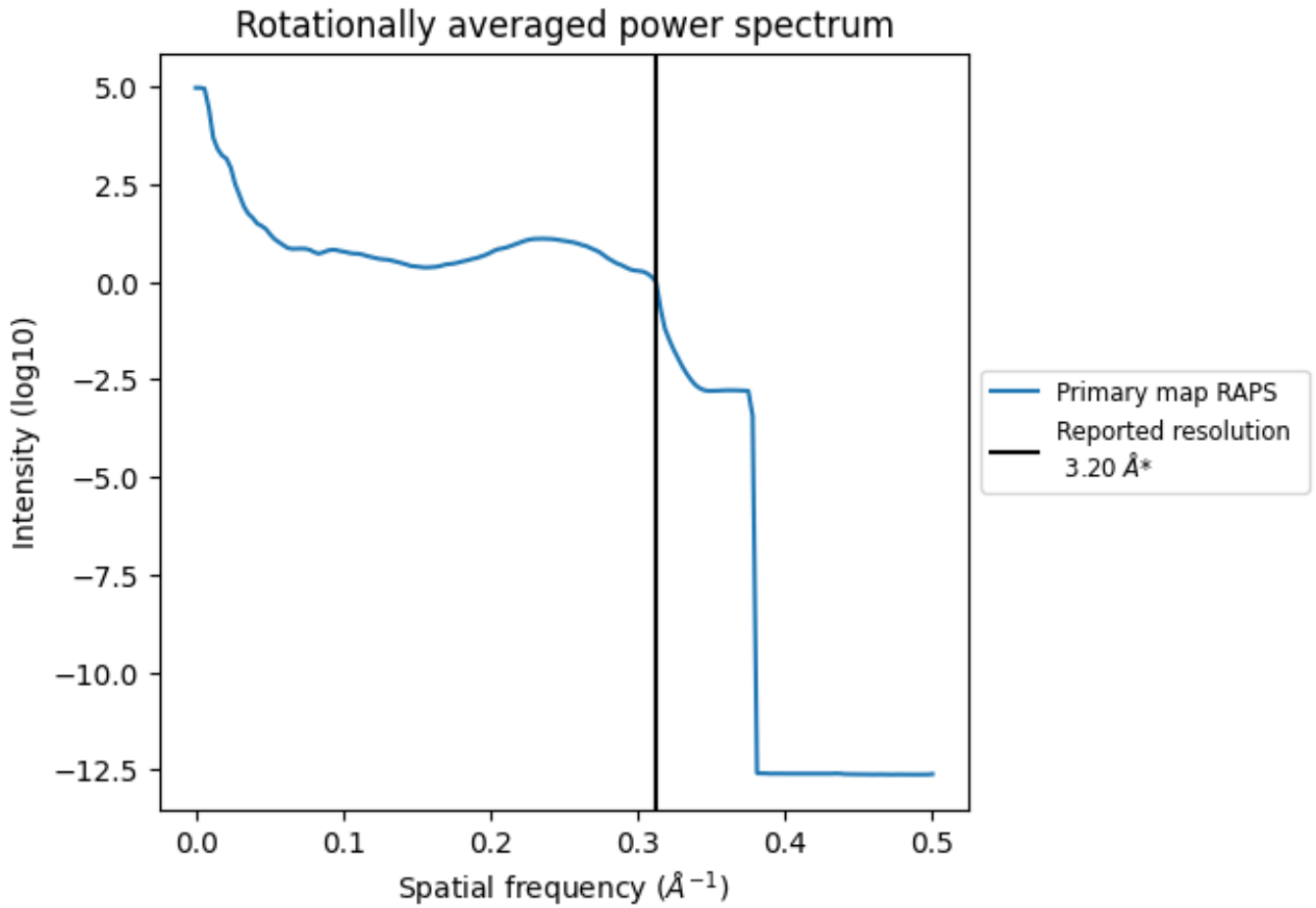
7.2 Volume estimate



The volume at the recommended contour level is 226 nm^3; this corresponds to an approximate mass of 204 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 $Å^{-1}$

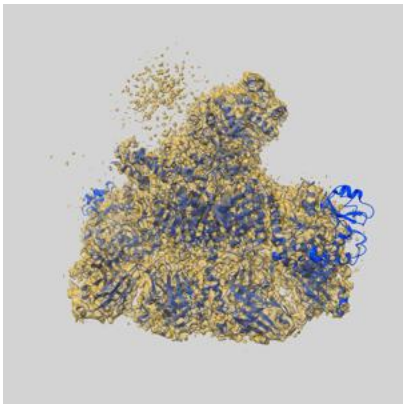
8 Fourier-Shell correlation (i)

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

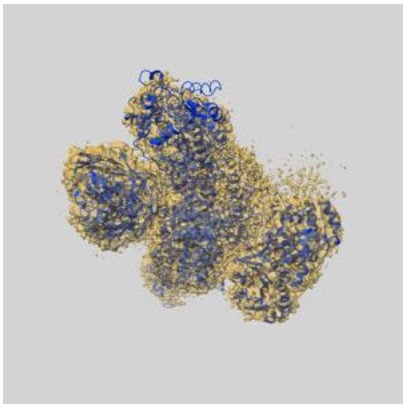
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23711 and PDB model 7M7F. Per-residue inclusion information can be found in section 3 on page 7.

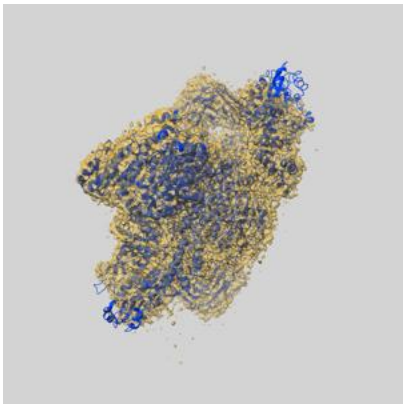
9.1 Map-model overlay



X



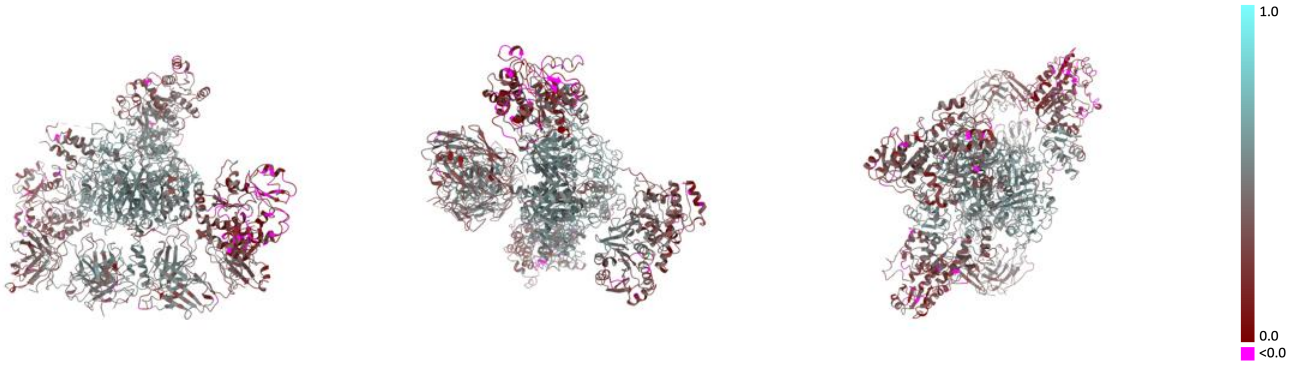
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.53 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.

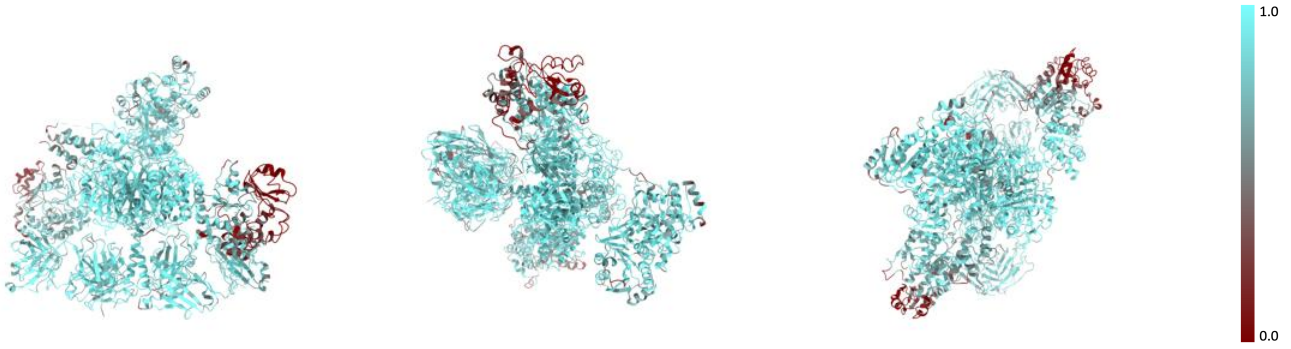
9.2 Q-score mapped to coordinate model (i)



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.

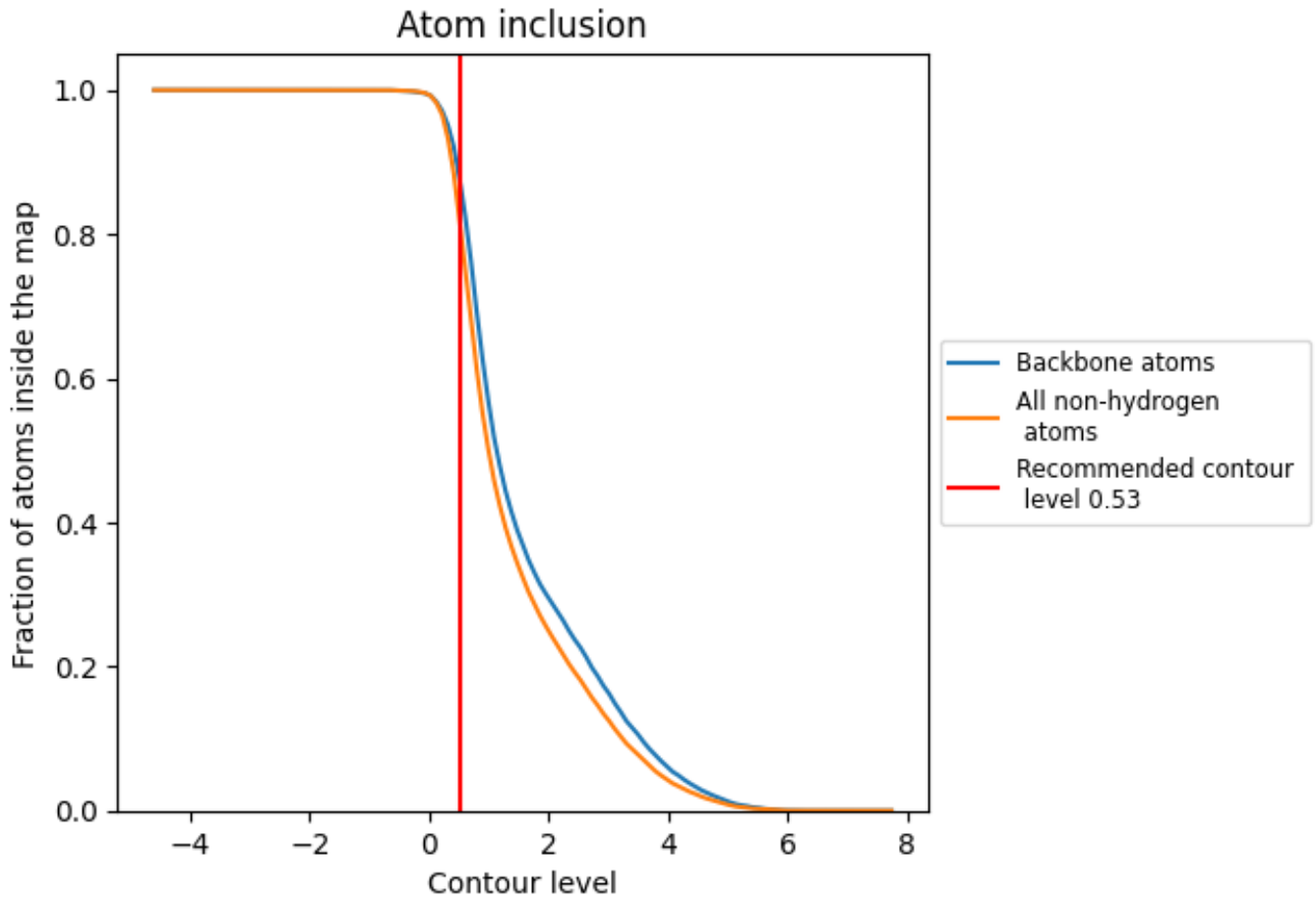
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.53).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8035	0.4030
A	0.7706	0.3800
B	0.8075	0.4320
C	0.8312	0.3850
D	0.8633	0.4110
E	0.8637	0.4200
F	0.8522	0.4070