Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:59 AM EST

PDB ID	:	7M7H
EMDB ID	:	EMD-23713
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	:	4.10 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:

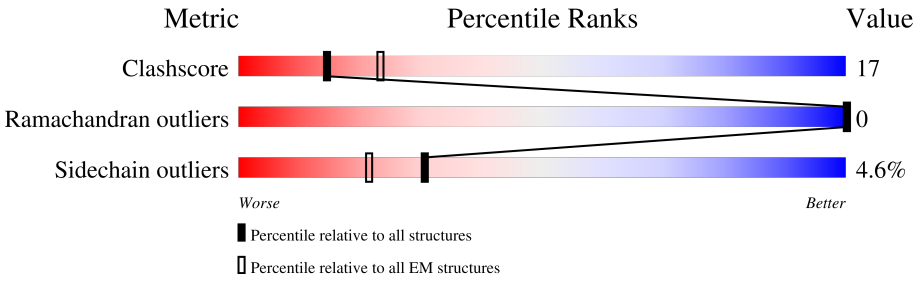
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	19% 48% 29% · 22%
1	B	1784	17% 52% 27% · 20%
2	C	249	54% 27% · 18%
2	E	249	53% 29% · 18%
3	D	236	51% 33% · 13%
3	F	236	49% 34% · 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27046 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	1425	Total	C	N	O	S	0	0
			10513	6533	1929	2016	35		
1	A	1390	Total	C	N	O	S	0	0
			10319	6413	1899	1972	35		

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).

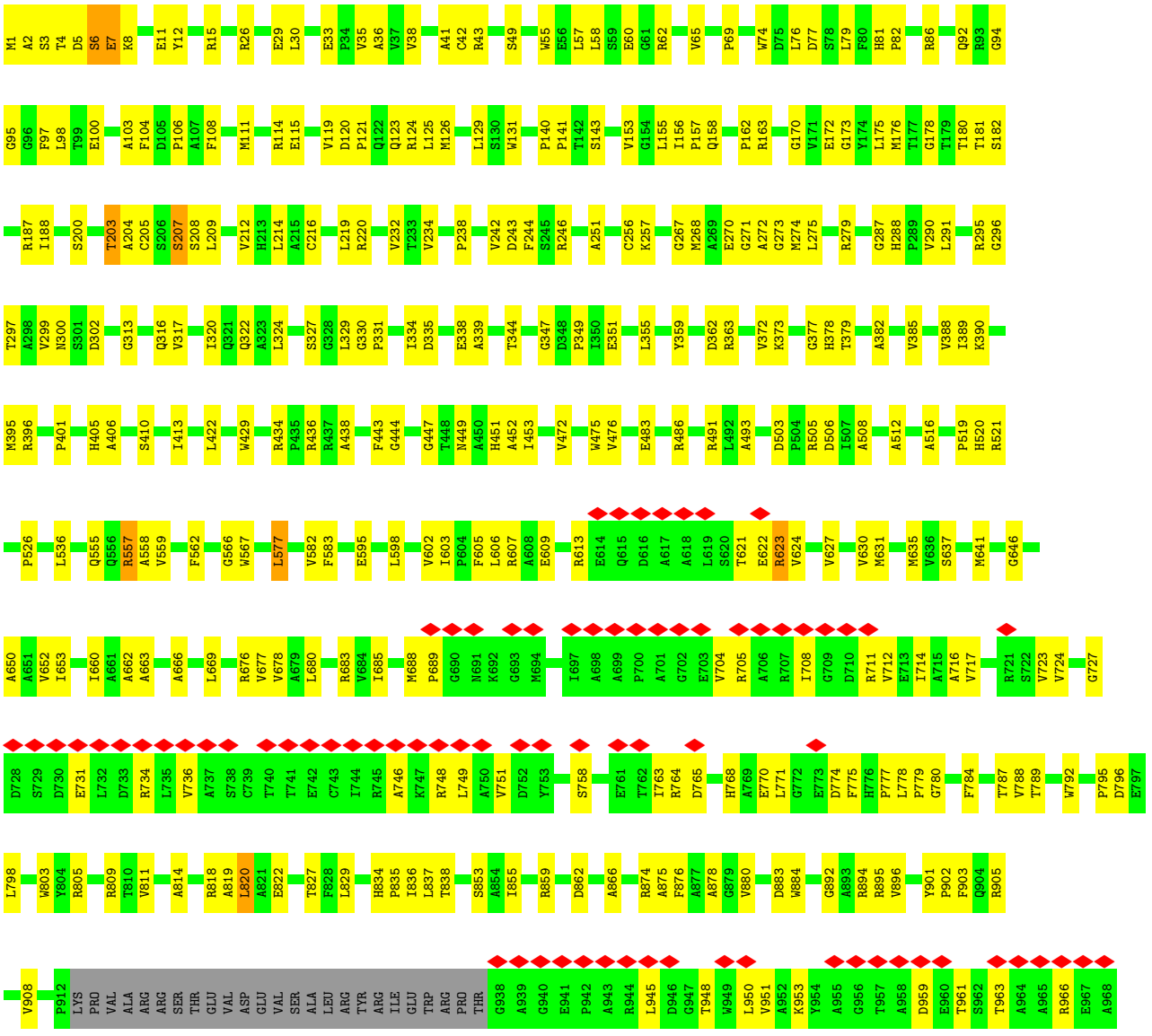
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

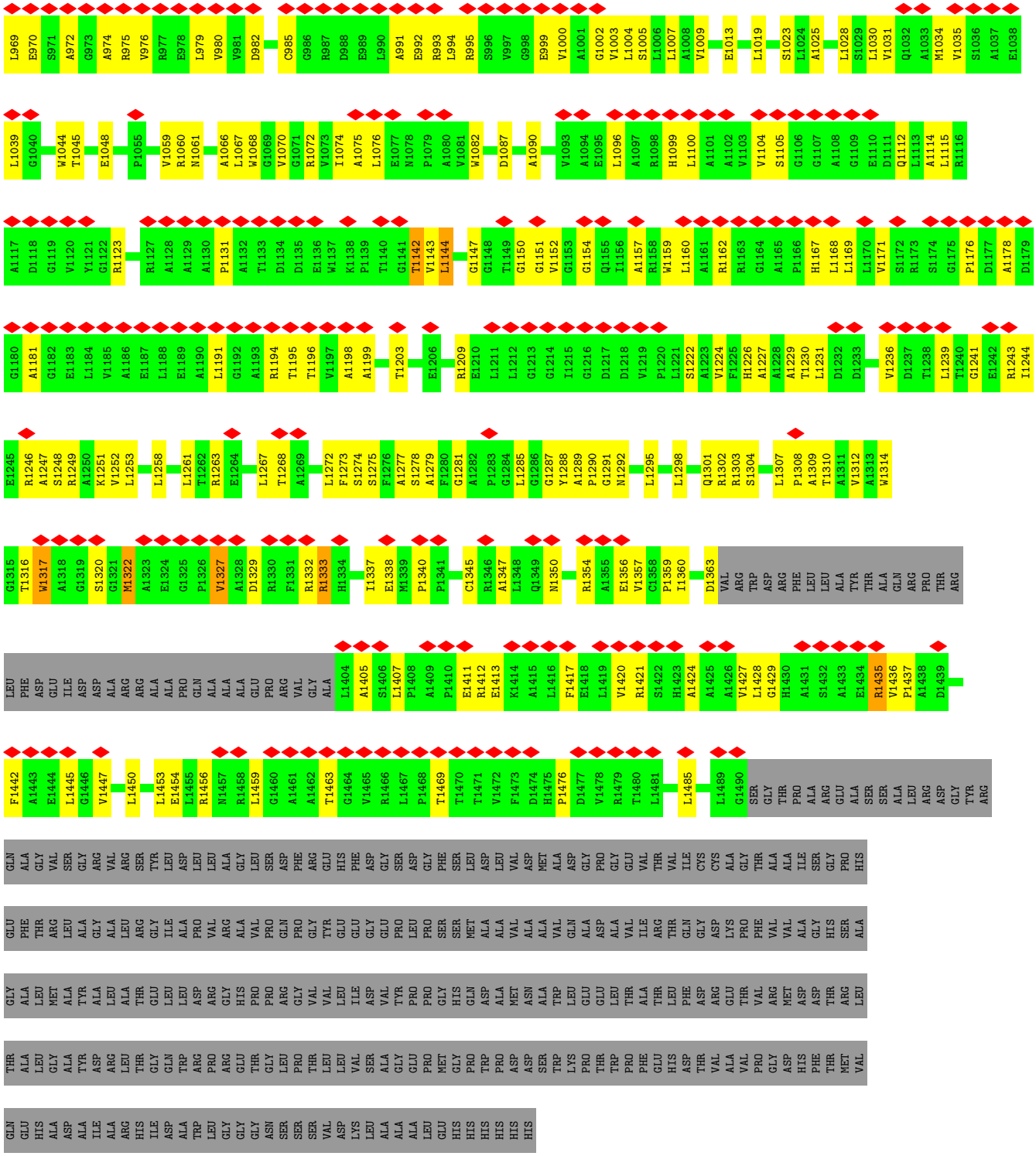
3 Residue-property plots (i)

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.

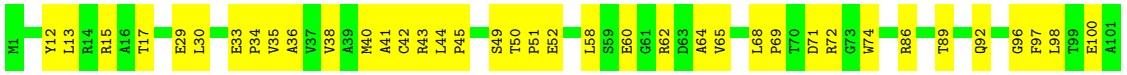
- Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

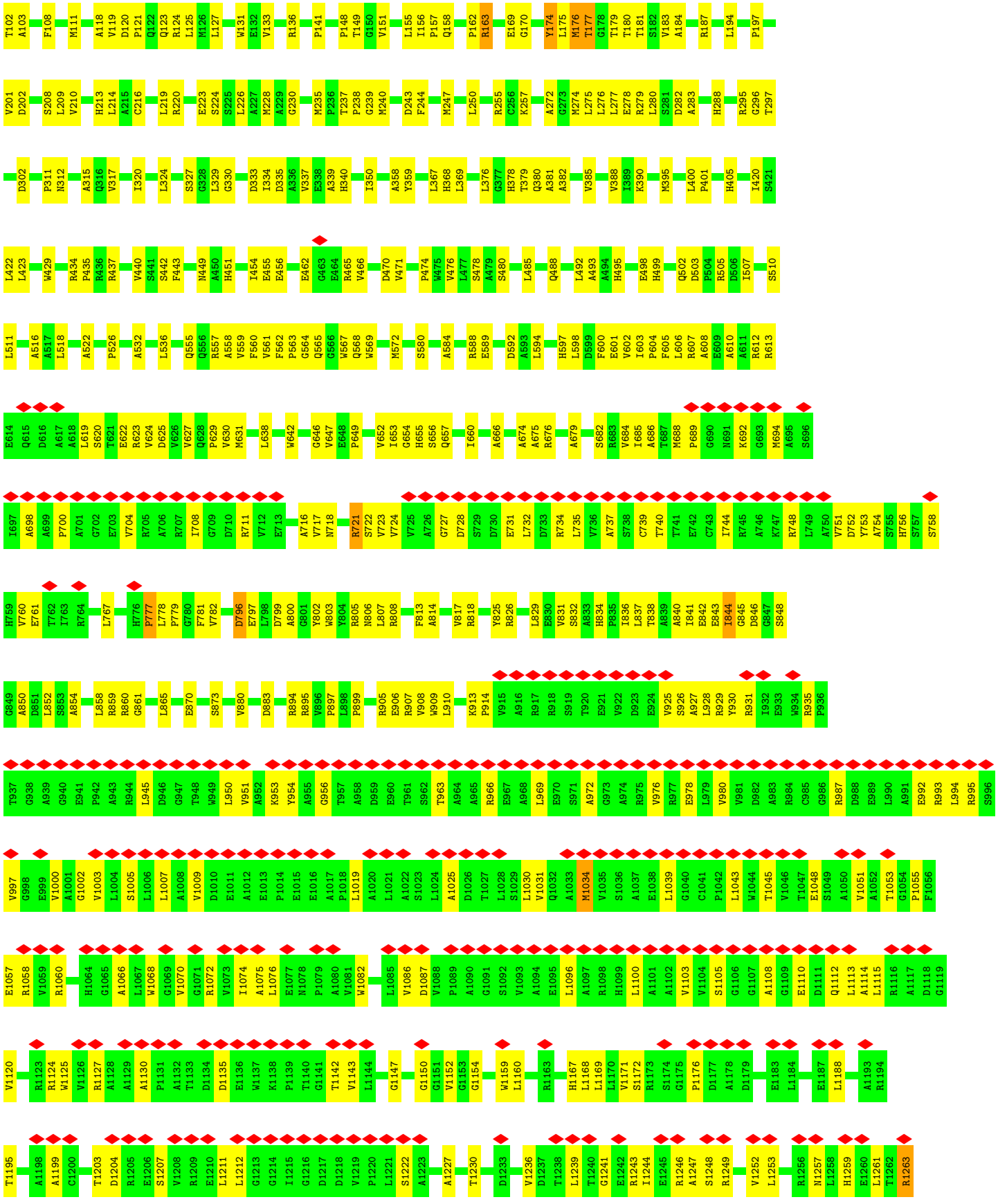
Chain B:

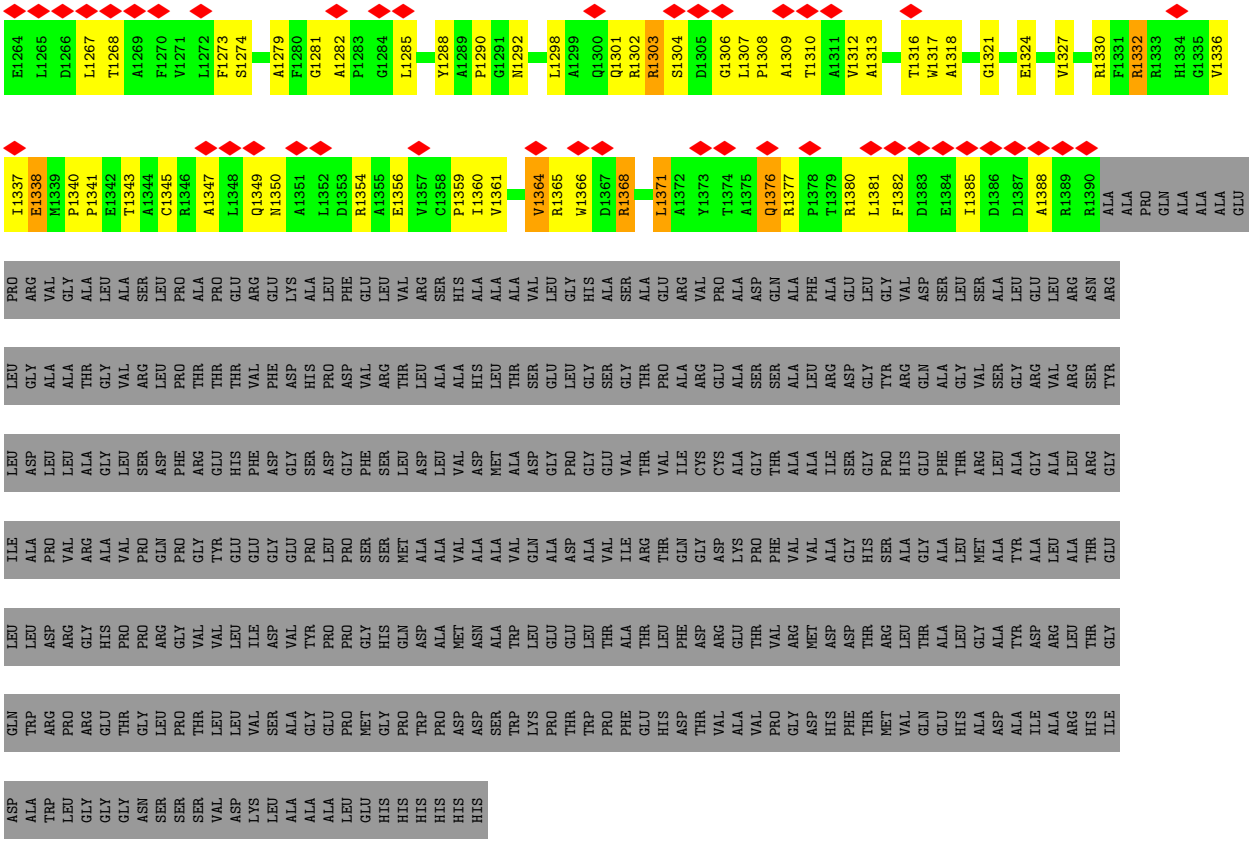




• Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

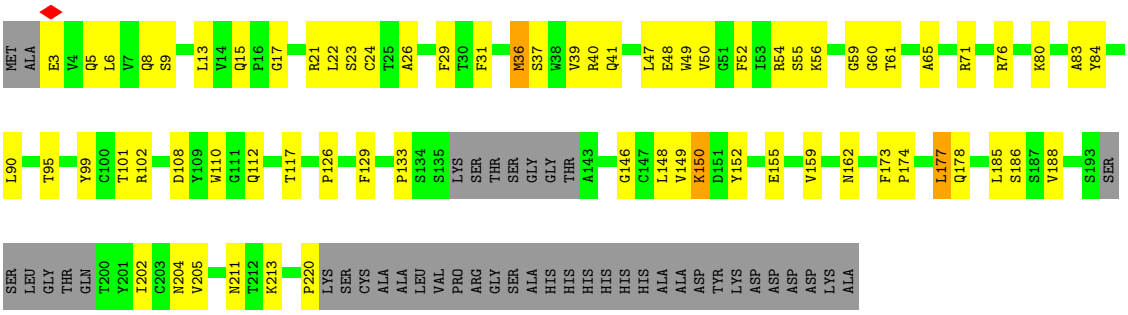



T102 A103 F108 M111 A118 V119 D120 P121 Q122 Q123 R124 L125 M126 L127 W131 E132 V133 R136 P141 P148 T149 G150 V151 L155 I156 P157 Q158 P162 R163 E169 G170 Y174 L175 M176 T177 G178 T179 T180 T181 S182 V183 A184 R187 L194 P197
V201 D202 S208 L209 V210 H213 L214 A215 C216 L219 R220 E223 S224 S225 L226 A227 M228 A229 G230 M235 P236 T237 P238 G239 M240 D243 F244 M247 L250 R255 C256 K257 A272 G273 M274 L275 L276 L277 E278 R279 L280 S281 D282 A283 H288 R295 G296 T297
D302 P311 N312 A315 Q316 V317 I320 L324 S327 G328 L329 G330 D333 I334 D335 A336 V337 E338 A339 H340 I350 A358 Y359 L367 H368 L369 L376 G377 H378 T379 Q380 A381 A382 V385 V388 I389 K390 M395 L400 P401 H405 I420 S421
L422 L423 W429 R434 P435 R436 R437 V440 S441 S442 F443 N449 A450 H451 I454 E455 E456 E462 G463 E464 R465 V466 D470 V471 P474 W475 V476 L477 S478 A479 S480 L485 Q488 L492 A493 A494 H495 E498 H499 Q502 D503 P504 R505 D506 I507 S510
L511 A516 A517 L518 A522 P526 A532 L536 Q555 Q556 R557 A558 V559 F560 V561 F562 P563 G564 Q565 G566 W567 Q568 W569 M572 S580 A584 R588 E589 D592 A593 L594 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 L638 W642 G646 V647 E648 P649 V652 I653 G654 H655 S656 Q657 I660 A666 A674 A675 R676 A679 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 A716 V717 N718 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 L767 H776 P777 L778 P779 G780 F781 V782 D796 E797 L798 D799 A800 G801 Y802 W803 Y804 R805 N806 L807 R808 F813 A814 V817 R818 Y825 R826 L829 E830 V831 S832 A833 H834 P835 I836 L837 T838 A839 A840 I841 E842 E843 I844 G845 D846 G847 S848
G849 A850 D851 L852 S853 A854 L858 R859 R860 G861 L865 E870 S873 V880 D883 R894 R895 V896 P897 L898 P899 R905 E906 R907 V908 W909 L910 K913 P914 V915 A916 R917 R918 S919 T920 E921 V922 D923 E924 V925 S926 A927 L928 R929 Y930 R931 I932 E933 W934 R935 P936
T937 G938 A939 G940 E941 P942 A943 R944 L945 D946 G947 T948 W949 L950 V951 A952 K953 Y954 A955 G956 T957 A958 D959 E960 T961 S962 T963 A964 A965 R966 E967 A968 L969 E970 S971 A972 G973 A974 R975 V976 R977 E978 L979 V980 V981 D982 A983 R984 C985 G986 R987 D988 E989 L990 A991 E992 R993 L994 R995 S996
V997 G998 E999 V1000 A1001 G1002 V1003 L1004 S1005 L1006 L1007 A1008 V1009 D1010 E1011 A1012 E1013 P1014 E1015 E1016 A1017 P1018 L1019 A1020 L1021 A1022 S1023 L1024 A1025 D1026 T1027 L1028 S1029 L1030 V1031 Q1032 A1033 M1034 V1035 S1036 A1037 E1038 L1039 G1040 C1041 P1042 L1043 W1044 T1045 V1046 T1047 E1048 S1049 A1050 V1051 A1052 T1053 G1054 P1055 F1056
E1057 R1058 V1059 R1060 H1064 G1065 A1066 L1067 W1068 G1069 V1070 G1071 R1072 V1073 I1074 A1075 L1076 E1077 N1078 P1079 A1080 V1081 W1082 L1085 V1086 D1087 V1088 P1089 A1090 G1091 S1092 V1093 A1094 E1095 L1096 A1097 R1098 H1099 L1100 A1101 A1102 V1103 V1104 S1105 G1106 G1107 A1108 G1109 E1110 D1111 Q1112 L1113 A1114 L1115 R1116 A1117 D1118 G1119
V1120 R1123 R1124 W1125 V1126 R1127 A1128 A1129 A1130 P1131 A1132 T1133 D1134 D1135 E1136 W1137 K1138 P1139 T1140 G1141 T1142 V1143 L1144 G1147 G1150 G1151 V1152 G1153 G1154 W1159 L1160 R1163 H1167 L1168 L1169 L1170 V1171 S1172 R1173 S1174 G1175 P1176 D1177 A1178 D1179 E1183 L1184 E1187 L1188 A1193 R1194
T1196 A1198 A1199 C1200 T1203 D1204 R1205 E1206 S1207 V1208 R1209 E1210 L1211 L1212 G1213 G1214 I1215 G1216 D1217 D1218 V1219 P1220 L1221 S1222 A1223 A1227 T1230 D1233 V1236 D1237 T1238 L1239 T1240 G1241 E1242 R1243 I1244 E1245 R1246 A1247 S1248 R1249 V1252 L1253 R1256 N1257 L1258 H1259 E1260 L1261 T1262 R1263



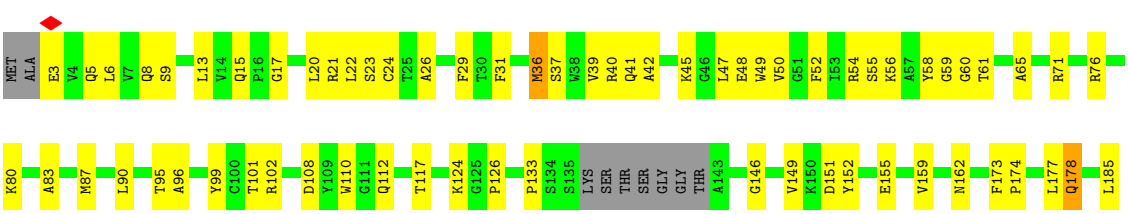
• Molecule 2: 1B2 (heavy chain)

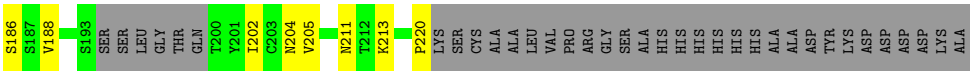
Chain C:



• Molecule 2: 1B2 (heavy chain)

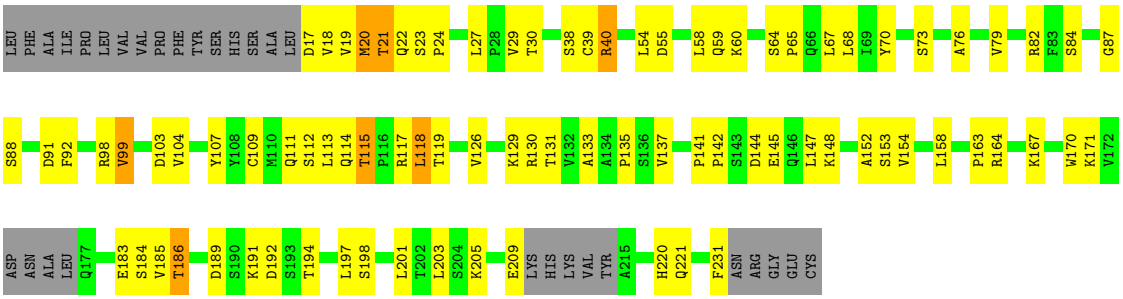
Chain E:





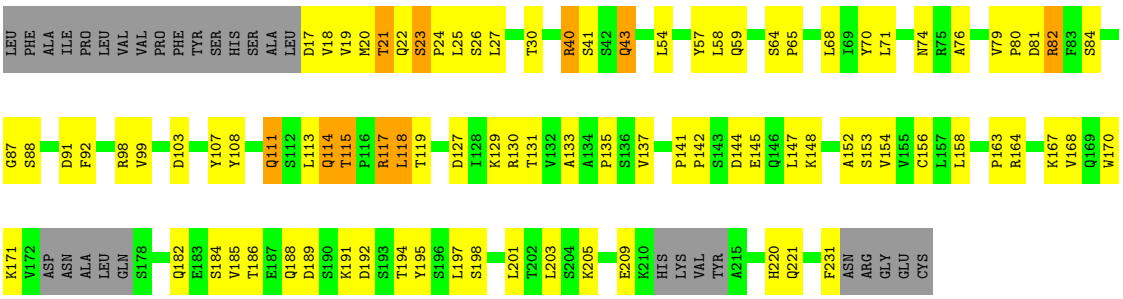
• Molecule 3: 1B2 (light chain)

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	58206	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	1.525	Depositor
Minimum map value	-0.358	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.28	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

5.1 Standard geometry

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	0.29	0/10522	0.57	0/14323
1	B	0.29	0/10715	0.57	0/14587
2	C	0.29	0/1575	0.58	0/2141
2	E	0.28	0/1575	0.58	0/2141
3	D	0.40	0/1601	0.60	1/2175 (0.0%)
3	F	0.39	0/1601	0.57	0/2174
All	All	0.30	0/27589	0.57	1/37541 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	E	0	1
3	D	0	1
3	F	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	24	PRO	N-CA-C	-5.91	96.72	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	155	GLU	Peptide
3	D	115	THR	Peptide

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Mol	Chain	Res	Type	Group
2	E	155	GLU	Peptide
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	385	0
1	B	10513	0	10362	374	0
2	C	1539	0	1511	51	0
2	E	1539	0	1511	52	0
3	D	1568	0	1528	51	0
3	F	1568	0	1533	57	0
All	All	27046	0	26609	918	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 17.

All (918) 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:B:1333:ARG:HD3	1:A:927:ALA:HB1	1.63	0.81
1:B:1144:LEU:HD13	1:B:1169:LEU:HD23	1.62	0.81
3:D:184:SER:HB3	3:D:198:SER:HB3	1.64	0.79
1:A:158:GLN:NE2	1:A:235:MET:SD	2.60	0.74
1:A:1019:LEU:HD13	1:A:1244:ILE:HG22	1.67	0.74
2:C:41:GLN:HB2	2:C:47:LEU:HD23	1.70	0.71
3:F:164:ARG:HE	3:F:185:VAL:HG11	1.55	0.71
1:B:123:GLN:NE2	1:B:180:THR:O	2.25	0.70
1:B:157:PRO:HB3	1:A:157:PRO:HB3	1.73	0.70
2:E:41:GLN:NE2	2:E:42:ALA:O	2.23	0.70
1:A:148:PRO:HB2	1:A:224:SER:HA	1.74	0.70
1:B:162:PRO:HA	1:A:163:ARG:HH22	1.55	0.70
1:B:559:VAL:HG11	1:B:820:LEU:HD11	1.74	0.70
1:B:1244:ILE:HD13	1:B:1290:PRO:HG2	1.74	0.69
1:A:208:SER:HB2	1:A:385:VAL:HB	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:VAL:HG23	1:A:1253:LEU:HD12	1.74	0.69
1:A:685:ILE:HG12	1:A:753:TYR:HD2	1.57	0.69
3:F:18:VAL:HA	3:F:114:GLN:HE22	1.56	0.69
3:F:19:VAL:HG22	3:F:43:GLN:HB2	1.73	0.69
1:A:213:HIS:HD2	1:A:214:LEU:HD22	1.57	0.69
2:C:24:CYS:HB3	2:C:83:ALA:HB3	1.75	0.69
1:B:2:ALA:HB1	1:B:8:LYS:H	1.56	0.69
1:B:120:ASP:HB3	1:B:123:GLN:HG3	1.73	0.69
1:B:275:LEU:HD11	1:B:388:VAL:HG11	1.74	0.69
1:B:491:ARG:HD3	1:B:902:PRO:HG3	1.74	0.69
1:B:646:GLY:HA3	1:B:883:ASP:HB2	1.75	0.69
2:E:174:PRO:HD3	3:F:186:THR:HG22	1.75	0.68
1:A:704:VAL:HG21	1:A:723:VAL:HG21	1.75	0.68
1:A:777:PRO:HB3	1:A:796:ASP:HA	1.76	0.68
2:E:24:CYS:HB3	2:E:83:ALA:HB3	1.75	0.68
1:A:629:PRO:HG3	1:A:679:ALA:HA	1.76	0.67
1:B:124:ARG:NH1	1:B:908:VAL:O	2.24	0.67
1:A:844:ILE:HG22	1:A:852:LEU:HD21	1.76	0.67
1:A:120:ASP:HB2	1:A:179:THR:HA	1.76	0.67
1:B:58:LEU:HB3	1:B:401:PRO:HB3	1.77	0.67
1:A:120:ASP:HB3	1:A:123:GLN:HG3	1.77	0.67
1:B:660:ILE:HG21	1:B:678:VAL:HB	1.77	0.67
3:D:40:ARG:HA	3:D:40:ARG:NE	2.10	0.66
1:B:1428:LEU:HD21	1:B:1447:VAL:HG22	1.77	0.66
1:B:1194:ARG:NH1	1:B:1196:THR:OG1	2.29	0.66
1:B:111:MET:SD	1:B:187:ARG:NH1	2.69	0.66
1:B:1143:VAL:HG11	1:B:1160:LEU:HD13	1.77	0.66
1:B:344:THR:HG23	1:B:347:GLY:H	1.60	0.66
2:C:146:GLY:HA3	2:C:188:VAL:HG22	1.78	0.66
3:D:158:LEU:HB2	3:D:197:LEU:HB3	1.77	0.66
1:B:205:CYS:HB3	1:B:378:HIS:HE2	1.60	0.66
3:D:21:THR:HA	3:D:40:ARG:O	1.95	0.66
1:B:1066:ALA:HB1	1:B:1290:PRO:HB3	1.78	0.65
1:A:565:GLN:OE1	1:A:657:GLN:NE2	2.29	0.65
1:B:558:ALA:HB2	1:B:880:VAL:HG13	1.78	0.65
1:B:603:ILE:HG22	1:B:607:ARG:HH21	1.62	0.65
1:B:980:VAL:O	1:B:993:ARG:NH1	2.30	0.65
1:B:1252:VAL:HG23	1:B:1253:LEU:HD12	1.79	0.65
1:A:466:VAL:HG23	1:A:505:ARG:HH22	1.61	0.64
1:A:1337:ILE:HG12	1:A:1338:GLU:HG2	1.79	0.64
1:B:680:LEU:HA	1:B:683:ARG:HE	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1275:SER:HA	1:B:1314:TRP:H	1.62	0.64
1:A:478:SER:H	1:A:488:GLN:HE22	1.45	0.64
2:E:146:GLY:HA3	2:E:188:VAL:HG22	1.78	0.64
3:F:158:LEU:HB2	3:F:197:LEU:HB3	1.77	0.64
1:A:228:MET:HE3	1:A:274:MET:HG3	1.79	0.64
1:B:1000:VAL:HG12	1:B:1002:GLY:H	1.62	0.64
1:A:219:LEU:O	1:A:279:ARG:NH1	2.28	0.64
1:B:503:ASP:OD2	1:B:505:ARG:NH1	2.30	0.64
1:B:1450:LEU:HD13	1:A:247:MET:HA	1.78	0.64
1:A:485:LEU:HD21	1:A:522:ALA:HB2	1.80	0.64
1:A:1000:VAL:HG12	1:A:1002:GLY:H	1.63	0.64
1:A:980:VAL:O	1:A:993:ARG:NH1	2.31	0.64
1:B:1005:SER:HB2	1:B:1045:THR:HA	1.80	0.63
1:B:663:ALA:HB1	1:B:669:LEU:HB2	1.80	0.63
1:B:244:PHE:HD2	1:B:268:MET:HE1	1.62	0.63
1:A:610:ALA:HB2	1:A:613:ARG:HH21	1.63	0.63
1:B:15:ARG:HH21	3:F:76:ALA:HB1	1.63	0.63
2:C:3:GLU:HG3	2:C:5:GLN:HE22	1.63	0.63
1:A:565:GLN:HE21	1:A:751:VAL:HG11	1.63	0.63
1:B:1302:ARG:HH11	1:B:1309:ALA:HB2	1.64	0.63
1:A:1087:ASP:HB3	1:A:1114:ALA:HA	1.80	0.63
1:A:330:GLY:N	3:F:98:ARG:HH12	1.96	0.63
3:D:144:ASP:HA	3:D:147:LEU:HD12	1.81	0.63
2:E:3:GLU:HG3	2:E:5:GLN:HE22	1.63	0.62
1:B:748:ARG:NH1	1:B:749:LEU:O	2.32	0.62
1:B:969:LEU:HD11	1:B:1004:LEU:HD12	1.81	0.62
1:B:959:ASP:HB3	1:B:961:THR:HG22	1.82	0.62
3:D:145:GLU:HA	3:D:148:LYS:HG2	1.81	0.62
3:F:144:ASP:HA	3:F:147:LEU:HD12	1.81	0.62
1:A:29:GLU:HA	1:A:33:GLU:HB2	1.82	0.62
1:A:1176:PRO:HD2	1:A:1199:ALA:HB2	1.81	0.61
1:A:40:MET:HG3	1:A:275:LEU:HD22	1.81	0.61
1:B:330:GLY:N	3:D:98:ARG:HH12	1.98	0.61
1:A:17:THR:HG23	3:F:74:ASN:HD21	1.64	0.61
1:A:1076:LEU:HD13	1:A:1281:GLY:HA3	1.83	0.61
3:F:145:GLU:HA	3:F:148:LYS:HG2	1.81	0.61
1:B:121:PRO:HB2	1:B:234:VAL:HG11	1.83	0.61
1:A:613:ARG:NH2	1:A:620:SER:OG	2.33	0.61
3:D:163:PRO:HD2	3:D:221:GLN:HE21	1.64	0.61
1:B:555:GLN:NE2	1:B:878:ALA:O	2.34	0.61
1:A:388:VAL:HG12	1:A:454:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:VAL:O	1:A:814:ALA:N	2.34	0.61
1:B:156:ILE:HD11	1:B:204:ALA:HA	1.83	0.61
1:A:35:VAL:HG12	1:A:277:LEU:HD12	1.82	0.61
3:F:163:PRO:HD2	3:F:221:GLN:HE21	1.64	0.60
1:A:734:ARG:HA	1:A:737:ALA:HB3	1.83	0.60
3:F:130:ARG:HH12	3:F:133:ALA:HB2	1.66	0.60
1:A:1072:ARG:HG2	1:A:1112:GLN:HE21	1.66	0.60
3:D:147:LEU:O	3:D:205:LYS:NZ	2.28	0.60
3:F:99:VAL:HG13	3:F:103:ASP:HB2	1.82	0.60
1:A:642:TRP:HB3	1:A:647:VAL:HB	1.82	0.60
2:E:162:ASN:N	2:E:202:ILE:O	2.32	0.60
1:B:121:PRO:HA	1:B:124:ARG:HG2	1.82	0.60
1:A:684:VAL:HB	1:A:767:LEU:HD21	1.83	0.60
1:B:705:ARG:HH11	1:B:708:ILE:HD11	1.66	0.60
1:A:36:ALA:N	1:A:278:GLU:O	2.35	0.60
1:B:1087:ASP:HB3	1:B:1114:ALA:HA	1.84	0.59
1:A:1354:ARG:HB2	1:A:1356:GLU:HG2	1.84	0.59
1:B:1048:GLU:HG3	1:B:1090:ALA:HA	1.84	0.59
1:A:567:TRP:HB3	1:A:836:ILE:HG12	1.84	0.59
1:B:602:VAL:HG12	1:B:630:VAL:HG12	1.83	0.59
1:B:777:PRO:HB3	1:B:798:LEU:H	1.68	0.59
1:B:835:PRO:O	1:B:838:THR:OG1	2.21	0.59
2:C:162:ASN:N	2:C:202:ILE:O	2.32	0.59
1:B:1072:ARG:HG2	1:B:1112:GLN:HE21	1.67	0.59
1:B:1000:VAL:HB	1:B:1039:LEU:HD21	1.84	0.59
1:A:505:ARG:HH21	1:A:894:ARG:HH22	1.51	0.59
2:C:149:VAL:HG11	2:C:205:VAL:HG11	1.83	0.59
1:B:1301:GLN:O	1:B:1304:SER:OG	2.21	0.59
1:B:60:GLU:HG3	1:B:62:ARG:HG3	1.85	0.58
1:B:97:PHE:HA	1:B:270:GLU:HG2	1.85	0.58
1:A:121:PRO:HA	1:A:124:ARG:HG2	1.83	0.58
1:A:1239:LEU:HD23	1:A:1243:ARG:HD3	1.85	0.58
1:A:1302:ARG:HH11	1:A:1309:ALA:HB2	1.67	0.58
1:B:334:ILE:O	1:B:363:ARG:NH1	2.32	0.58
1:B:1151:GLY:HA3	1:B:1320:SER:HB2	1.84	0.58
1:B:1176:PRO:HD2	1:B:1199:ALA:HB2	1.84	0.58
1:A:379:THR:HB	1:A:382:ALA:HB3	1.86	0.58
1:A:945:LEU:HD21	1:A:1105:SER:HB3	1.84	0.58
1:A:395:MET:SD	1:A:456:GLU:HA	2.43	0.58
3:D:130:ARG:HH12	3:D:133:ALA:HB2	1.66	0.58
1:B:1236:VAL:HA	1:B:1239:LEU:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ARG:HD2	2:E:60:GLY:HA3	1.86	0.58
1:B:1150:GLY:O	1:B:1154:GLY:N	2.35	0.58
1:A:564:GLY:HA3	1:A:656:SER:HG	1.69	0.58
1:A:727:GLY:H	1:A:732:LEU:HD22	1.69	0.58
2:C:40:ARG:NH1	2:C:48:GLU:OE1	2.36	0.58
3:D:54:LEU:HD13	3:D:92:PHE:CD2	2.38	0.58
2:E:40:ARG:NH1	2:E:48:GLU:OE1	2.36	0.58
1:A:1168:LEU:HD13	1:A:1195:THR:HG22	1.86	0.58
1:A:1259:HIS:O	1:A:1263:ARG:HD3	2.04	0.58
1:A:493:ALA:HB2	1:A:536:LEU:HB3	1.85	0.57
1:A:1337:ILE:HG12	1:A:1338:GLU:H	1.68	0.57
1:B:1076:LEU:HD13	1:B:1281:GLY:HA3	1.85	0.57
1:A:45:PRO:HD2	1:A:376:LEU:HD23	1.86	0.57
1:A:560:PHE:HB2	1:A:652:VAL:HG12	1.85	0.57
1:A:602:VAL:HG13	1:A:630:VAL:HG22	1.85	0.57
2:E:133:PRO:HG2	2:E:220:PRO:HB3	1.87	0.57
1:B:12:TYR:HE1	3:F:70:TYR:HB2	1.68	0.57
1:B:1068:TRP:HZ2	1:B:1087:ASP:HB2	1.69	0.57
1:A:69:PRO:HG2	1:A:72:ARG:HH21	1.69	0.57
1:B:1437:PRO:HG2	1:B:1445:LEU:HD21	1.87	0.57
1:A:694:MET:O	1:A:748:ARG:NH2	2.37	0.57
1:A:685:ILE:HD11	1:A:754:ALA:HB3	1.86	0.57
1:B:1332:ARG:HA	1:A:1365:ARG:CZ	2.35	0.57
1:A:213:HIS:CD2	1:A:214:LEU:HD22	2.39	0.57
1:A:1171:VAL:HG21	1:A:1211:LEU:HD21	1.86	0.57
2:C:49:TRP:HB3	3:D:118:LEU:HA	1.85	0.57
3:D:54:LEU:HD13	3:D:92:PHE:HD2	1.68	0.57
1:B:1167:HIS:CD2	1:B:1194:ARG:HG2	2.39	0.57
1:A:158:GLN:HE22	1:A:240:MET:HG2	1.68	0.57
1:A:118:ALA:HB3	1:A:174:TYR:HB2	1.86	0.57
1:A:1005:SER:HB2	1:A:1045:THR:HA	1.85	0.57
1:A:1222:SER:HB3	1:A:1268:THR:H	1.69	0.57
2:C:54:ARG:HD2	2:C:60:GLY:HA3	1.86	0.57
2:E:36:MET:H	2:E:76:ARG:HH12	1.52	0.57
1:A:567:TRP:CD2	1:A:832:SER:HB2	2.39	0.57
2:C:133:PRO:HG2	2:C:220:PRO:HB3	1.87	0.57
1:B:624:VAL:HA	1:B:627:VAL:HG12	1.87	0.56
1:B:1251:LYS:HE3	1:B:1291:GLY:HA3	1.86	0.56
1:B:1347:ALA:HA	1:B:1350:ASN:HD21	1.69	0.56
1:B:1337:ILE:HG22	1:B:1363:ASP:HB2	1.86	0.56
1:A:718:ASN:HA	1:A:813:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:PHE:CD2	3:D:198:SER:HB2	2.40	0.56
1:B:621:THR:HB	1:B:627:VAL:HG23	1.88	0.56
1:B:1159:TRP:CD1	1:B:1345:CYS:HB2	2.40	0.56
1:A:700:PRO:HA	1:A:721:ARG:HA	1.87	0.56
3:F:130:ARG:HH21	3:F:194:THR:HG22	1.69	0.56
1:B:244:PHE:CD2	1:B:268:MET:HE1	2.40	0.56
1:A:1068:TRP:HZ2	1:A:1087:ASP:HB2	1.70	0.56
1:B:296:GLY:HA3	1:B:327:SER:HB3	1.87	0.56
1:B:566:GLY:HA3	1:B:836:ILE:HG12	1.88	0.56
1:A:608:ALA:HB1	1:A:612:ARG:HG3	1.86	0.56
3:F:30:THR:HB	3:F:129:LYS:HB3	1.88	0.56
1:B:287:GLY:O	1:B:895:ARG:NH1	2.38	0.56
1:A:127:LEU:HD21	1:A:187:ARG:HB3	1.88	0.56
1:A:1212:LEU:HD13	1:A:1261:LEU:HG	1.88	0.56
3:D:130:ARG:HH21	3:D:194:THR:HG22	1.69	0.56
2:E:49:TRP:HB3	3:F:118:LEU:HA	1.87	0.56
1:B:5:ASP:HA	1:B:8:LYS:HB2	1.88	0.56
1:B:637:SER:O	1:B:641:MET:HG2	2.05	0.56
2:C:36:MET:H	2:C:76:ARG:HH12	1.52	0.56
1:A:64:ALA:HB3	1:A:376:LEU:HA	1.88	0.56
1:A:330:GLY:CA	3:F:98:ARG:HH12	2.19	0.56
1:B:999:GLU:HB2	1:B:1405:ALA:HA	1.88	0.56
1:A:1000:VAL:HB	1:A:1039:LEU:HD21	1.88	0.56
1:A:1236:VAL:HA	1:A:1239:LEU:HB2	1.87	0.56
1:A:1263:ARG:HA	1:A:1307:LEU:HD11	1.88	0.56
3:D:17:ASP:OD1	3:D:18:VAL:N	2.35	0.56
3:D:30:THR:HB	3:D:129:LYS:HB3	1.88	0.55
1:B:1356:GLU:HB3	1:B:1359:PRO:HG3	1.87	0.55
1:A:162:PRO:HD2	1:A:910:LEU:HG	1.88	0.55
1:A:320:ILE:O	1:A:324:LEU:HB2	2.06	0.55
1:A:928:LEU:HB3	1:A:1361:VAL:HG13	1.88	0.55
1:A:474:PRO:HB3	1:A:873:SER:HB2	1.88	0.55
1:A:558:ALA:HB2	1:A:880:VAL:HG13	1.89	0.55
1:A:562:PHE:HB2	1:A:654:GLY:HA2	1.89	0.55
1:B:1310:THR:HG22	1:B:1312:VAL:HG13	1.89	0.55
1:B:1420:VAL:HG22	1:B:1459:LEU:HD11	1.89	0.55
1:B:1272:LEU:HD21	1:B:1298:LEU:HD23	1.88	0.55
1:B:950:LEU:HB2	1:B:1003:VAL:HG22	1.88	0.55
1:A:1142:THR:HA	1:A:1167:HIS:HB2	1.88	0.55
1:A:930:TYR:O	1:A:1360:ILE:N	2.39	0.55
2:C:110:TRP:HB3	3:D:64:SER:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:CYS:HB2	1:A:44:LEU:HD23	1.89	0.55
1:A:646:GLY:HA3	1:A:883:ASP:HB3	1.89	0.55
1:B:712:VAL:HG22	1:B:727:GLY:HA3	1.89	0.55
1:A:43:ARG:HG2	1:A:125:LEU:HD22	1.88	0.55
1:A:124:ARG:NH1	1:A:908:VAL:O	2.40	0.55
1:A:698:ALA:HA	1:A:722:SER:HA	1.89	0.55
1:B:1230:THR:OG1	1:B:1247:ALA:O	2.22	0.55
2:E:55:SER:O	2:E:59:GLY:N	2.37	0.55
2:E:21:ARG:HE	2:E:22:LEU:H	1.54	0.54
1:B:205:CYS:HB2	1:B:444:GLY:HA2	1.90	0.54
1:B:1360:ILE:HG13	1:B:1360:ILE:O	2.07	0.54
1:B:788:VAL:HG13	1:B:789:THR:HG23	1.88	0.54
1:A:12:TYR:HE1	3:D:70:TYR:HB2	1.71	0.54
1:A:1150:GLY:O	1:A:1154:GLY:N	2.40	0.54
1:A:50:THR:HG1	1:A:136:ARG:HH12	1.48	0.54
1:A:526:PRO:HG3	1:A:532:ALA:HB2	1.88	0.54
1:A:1321:GLY:HA2	1:A:1324:GLU:HB3	1.90	0.54
2:C:49:TRP:CZ2	2:C:52:PHE:HD1	2.25	0.54
2:E:49:TRP:CZ2	2:E:52:PHE:HD1	2.25	0.54
1:A:1031:VAL:HG21	1:A:1074:ILE:HD13	1.90	0.54
1:B:82:PRO:HB3	1:A:1306:GLY:HA2	1.89	0.54
1:B:685:ILE:HD13	1:B:688:MET:HE1	1.90	0.54
2:E:41:GLN:HB2	2:E:47:LEU:HD23	1.90	0.54
1:B:41:ALA:O	1:B:274:MET:N	2.39	0.54
1:B:155:LEU:HB2	1:B:181:THR:HG23	1.90	0.54
1:B:291:LEU:HA	1:B:396:ARG:HH22	1.71	0.54
1:A:756:HIS:ND1	1:A:806:ASN:O	2.41	0.54
2:C:21:ARG:HE	2:C:22:LEU:H	1.55	0.54
3:F:184:SER:HB3	3:F:198:SER:HB3	1.90	0.54
1:A:797:GLU:HB2	1:A:805:ARG:HH22	1.72	0.54
2:C:55:SER:O	2:C:59:GLY:N	2.38	0.54
1:B:379:THR:HB	1:B:382:ALA:HB3	1.90	0.54
1:A:642:TRP:HZ3	1:A:831:VAL:HG13	1.73	0.54
1:A:1188:LEU:HB3	1:A:1195:THR:HG21	1.90	0.54
1:A:1055:PRO:HB3	1:A:1303:ARG:HH22	1.72	0.53
1:A:368:HIS:HB3	1:A:423:LEU:HD21	1.89	0.53
1:A:1336:VAL:HG12	1:A:1364:VAL:HA	1.90	0.53
1:B:680:LEU:HD23	1:B:771:LEU:HA	1.89	0.53
1:A:1125:TRP:CH2	1:A:1279:ALA:HB1	2.44	0.53
1:B:945:LEU:N	1:B:972:ALA:O	2.41	0.53
1:B:1456:ARG:NH1	1:B:1469:THR:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ALA:HB1	1:B:7:GLU:HB2	1.91	0.53
1:B:1144:LEU:HB3	1:B:1224:VAL:HA	1.91	0.53
1:B:948:THR:HG22	1:B:975:ARG:HE	1.74	0.53
1:A:98:LEU:HD13	1:A:100:GLU:HB2	1.91	0.53
1:A:385:VAL:HA	1:A:388:VAL:HG22	1.91	0.53
1:A:950:LEU:HB2	1:A:1003:VAL:HG22	1.91	0.53
1:A:43:ARG:NH1	1:A:49:SER:OG	2.42	0.53
1:A:752:ASP:OD1	1:A:752:ASP:N	2.42	0.53
1:B:3:SER:HB3	1:B:6:SER:HB2	1.91	0.53
1:A:945:LEU:N	1:A:972:ALA:O	2.42	0.53
2:C:31:PHE:O	2:C:76:ARG:NH2	2.41	0.53
2:E:31:PHE:O	2:E:76:ARG:NH2	2.41	0.53
1:B:1226:HIS:HD2	1:B:1258:LEU:HD12	1.74	0.52
1:B:1004:LEU:HD23	1:B:1044:TRP:HB2	1.92	0.52
1:A:367:LEU:HB3	1:A:420:ILE:HG12	1.92	0.52
1:A:1108:ALA:O	1:A:1380:ARG:NH1	2.42	0.52
1:B:717:VAL:O	1:B:814:ALA:N	2.39	0.52
1:B:1463:THR:HG21	1:B:1485:LEU:HD21	1.90	0.52
1:A:43:ARG:O	1:A:272:ALA:N	2.39	0.52
1:B:76:LEU:H	1:B:79:LEU:HD13	1.74	0.52
1:B:961:THR:HG21	1:B:1009:VAL:HG21	1.92	0.52
1:A:180:THR:O	1:A:183:VAL:HG22	2.09	0.52
1:A:279:ARG:NE	1:A:282:ASP:OD2	2.41	0.52
1:B:351:GLU:HG3	1:B:443:PHE:HE2	1.72	0.52
1:B:390:LYS:HE2	1:B:401:PRO:HB2	1.91	0.52
1:A:625:ASP:HB3	1:A:686:ALA:HB2	1.92	0.52
1:A:826:ARG:HH22	1:A:850:ALA:HB1	1.75	0.52
1:B:49:SER:OG	1:B:100:GLU:OE2	2.25	0.52
1:B:320:ILE:HG22	1:B:451:HIS:CG	2.44	0.52
1:B:1068:TRP:CZ2	1:B:1087:ASP:HB2	2.45	0.52
1:A:228:MET:CE	1:A:274:MET:HG3	2.38	0.52
2:C:54:ARG:HH11	2:C:61:THR:H	1.56	0.52
1:A:330:GLY:HA3	3:F:98:ARG:HH12	1.74	0.52
1:A:778:LEU:HG	1:A:779:PRO:HD2	1.91	0.52
1:B:295:ARG:HD3	1:B:329:LEU:HD11	1.90	0.52
1:B:798:LEU:HD11	1:B:803:TRP:CH2	2.44	0.52
1:B:1278:SER:OG	1:B:1289:ALA:O	2.28	0.52
1:B:1248:SER:O	1:B:1252:VAL:HG22	2.10	0.52
1:A:65:VAL:HG12	1:A:96:GLY:N	2.25	0.52
1:A:156:ILE:HG13	1:A:381:ALA:HB2	1.92	0.52
1:A:302:ASP:OD1	1:A:449:ASN:ND2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:HB2	1:B:1429:GLY:HA3	1.93	0.52
1:A:817:VAL:HG11	1:A:844:ILE:HG21	1.92	0.52
2:C:126:PRO:HB3	2:C:152:TYR:HB3	1.91	0.52
2:E:126:PRO:HB3	2:E:152:TYR:HB3	1.91	0.52
1:B:156:ILE:HG21	1:B:158:GLN:HE21	1.75	0.51
1:A:50:THR:OG1	1:A:136:ARG:NH1	2.28	0.51
1:A:133:VAL:HG11	1:A:228:MET:CE	2.40	0.51
1:A:502:GLN:HB3	1:A:507:ILE:HD11	1.92	0.51
1:A:638:LEU:HB3	1:A:642:TRP:CZ3	2.46	0.51
1:B:892:GLY:O	1:B:894:ARG:NH1	2.44	0.51
1:B:1168:LEU:HD12	1:B:1195:THR:HG22	1.91	0.51
1:A:492:LEU:HD23	1:A:536:LEU:HD21	1.92	0.51
1:A:1159:TRP:CG	1:A:1345:CYS:HB2	2.46	0.51
2:E:54:ARG:HH11	2:E:61:THR:H	1.56	0.51
1:B:1354:ARG:HB2	1:B:1356:GLU:HG2	1.91	0.51
1:B:1421:ARG:NH2	1:B:1436:VAL:H	2.08	0.51
1:B:77:ASP:OD2	1:A:931:ARG:NE	2.31	0.51
1:B:622:GLU:OE1	1:B:623:ARG:NH1	2.44	0.51
1:B:829:LEU:HD11	1:B:880:VAL:HG21	1.92	0.51
1:A:209:LEU:HD11	1:A:440:VAL:HG12	1.93	0.51
1:A:758:SER:HA	1:A:761:GLU:HB2	1.92	0.51
1:A:1068:TRP:CZ2	1:A:1087:ASP:HB2	2.46	0.51
3:D:58:LEU:HB2	3:D:68:LEU:HD11	1.93	0.51
1:B:43:ARG:O	1:B:272:ALA:N	2.42	0.51
1:B:291:LEU:O	1:B:396:ARG:NH2	2.44	0.51
3:F:147:LEU:O	3:F:205:LYS:NZ	2.28	0.51
1:B:36:ALA:HB1	1:B:290:VAL:HG13	1.92	0.51
1:A:71:ASP:O	1:A:907:ARG:NH2	2.44	0.51
1:A:711:ARG:NH2	1:A:758:SER:H	2.08	0.51
1:B:395:MET:O	1:B:436:ARG:NH2	2.43	0.51
3:F:70:TYR:N	3:F:74:ASN:O	2.42	0.51
1:B:30:LEU:HD13	1:A:30:LEU:HD22	1.92	0.51
1:B:1450:LEU:O	1:B:1454:GLU:HG2	2.10	0.51
1:B:1459:LEU:O	1:B:1463:THR:OG1	2.24	0.51
1:A:1066:ALA:HB1	1:A:1290:PRO:HB3	1.92	0.51
1:B:1239:LEU:HD23	1:B:1243:ARG:HD3	1.93	0.50
1:A:244:PHE:HB3	1:A:250:LEU:CD2	2.41	0.50
2:E:31:PHE:CE2	2:E:76:ARG:HB2	2.46	0.50
1:A:711:ARG:HH22	1:A:758:SER:H	1.59	0.50
1:B:338:GLU:OE2	1:B:372:VAL:N	2.39	0.50
1:B:1142:THR:HA	1:B:1167:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1203:THR:HG21	1:B:1249:ARG:HE	1.75	0.50
1:A:966:ARG:HB2	1:A:976:VAL:HG21	1.93	0.50
2:E:8:GLN:H	2:E:112:GLN:HE22	1.59	0.50
3:F:58:LEU:HB2	3:F:68:LEU:HD11	1.93	0.50
1:B:716:ALA:HB3	1:B:724:VAL:HB	1.93	0.50
1:B:216:CYS:HB3	1:B:220:ARG:HE	1.76	0.50
1:A:480:SER:HB2	1:A:518:LEU:HD22	1.93	0.50
1:A:826:ARG:HG3	1:A:852:LEU:HA	1.93	0.50
1:B:7:GLU:HG3	2:E:58:TYR:CE2	2.47	0.50
1:B:704:VAL:HG23	1:B:714:ILE:HD11	1.92	0.50
1:B:1347:ALA:HA	1:B:1350:ASN:ND2	2.27	0.50
2:E:21:ARG:HE	2:E:22:LEU:N	2.10	0.50
1:B:982:ASP:HB3	1:B:985:CYS:HB3	1.93	0.50
1:B:1025:ALA:HB2	1:B:1241:GLY:HA3	1.94	0.50
1:A:1301:GLN:O	1:A:1304:SER:OG	2.25	0.50
2:C:31:PHE:CE2	2:C:76:ARG:HB2	2.47	0.50
3:F:127:ASP:HB3	3:F:188:GLN:NE2	2.27	0.50
1:B:76:LEU:HD23	1:B:79:LEU:HD22	1.94	0.50
1:B:410:SER:HB3	1:B:413:ILE:HD12	1.94	0.50
1:B:1453:LEU:O	1:B:1456:ARG:HG2	2.11	0.50
1:A:682:SER:HA	1:A:685:ILE:HG22	1.92	0.50
2:C:8:GLN:H	2:C:112:GLN:HE22	1.59	0.50
3:D:22:GLN:HG2	3:D:40:ARG:HB2	1.93	0.50
1:A:716:ALA:HB3	1:A:724:VAL:HB	1.94	0.49
1:A:800:ALA:HA	1:A:803:TRP:CD1	2.47	0.49
3:D:142:PRO:HD3	3:D:154:VAL:HB	1.94	0.49
1:B:519:PRO:O	1:B:520:HIS:ND1	2.45	0.49
1:B:567:TRP:HB3	1:B:834:HIS:HB3	1.94	0.49
1:B:582:VAL:HG12	1:B:641:MET:HE1	1.93	0.49
1:B:602:VAL:O	1:B:606:LEU:N	2.40	0.49
1:B:652:VAL:HB	1:B:784:PHE:HD1	1.76	0.49
1:A:1248:SER:O	1:A:1252:VAL:HG22	2.11	0.49
1:B:963:THR:HA	1:B:966:ARG:HG2	1.94	0.49
1:A:466:VAL:HG23	1:A:505:ARG:NH2	2.26	0.49
1:A:692:LYS:HB2	1:A:728:ASP:HA	1.93	0.49
1:A:1143:VAL:HG11	1:A:1160:LEU:HD13	1.93	0.49
1:A:1340:PRO:HB2	1:A:1343:THR:HG22	1.94	0.49
2:C:21:ARG:HE	2:C:22:LEU:N	2.10	0.49
1:B:339:ALA:HB2	1:B:355:LEU:HD11	1.93	0.49
1:B:512:ALA:HB1	1:B:884:TRP:HB3	1.95	0.49
1:B:627:VAL:O	1:B:631:MET:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:VAL:HG21	1:B:1074:ILE:HD13	1.95	0.49
1:B:1152:VAL:HG21	1:B:1322:MET:HB3	1.94	0.49
1:B:74:TRP:CD1	1:B:238:PRO:HD3	2.48	0.49
1:A:966:ARG:HA	1:A:969:LEU:HB2	1.94	0.49
1:B:300:ASN:O	1:B:449:ASN:N	2.41	0.49
1:B:1332:ARG:HG3	1:A:1365:ARG:NH2	2.28	0.49
3:F:88:SER:N	3:F:91:ASP:O	2.43	0.49
1:A:339:ALA:HB2	1:A:369:LEU:HD11	1.95	0.49
2:C:49:TRP:HZ2	2:C:52:PHE:HD1	1.61	0.49
3:F:142:PRO:HD3	3:F:154:VAL:HB	1.94	0.49
1:B:945:LEU:HD21	1:B:1105:SER:HB3	1.93	0.49
1:B:1209:ARG:HA	1:B:1261:LEU:HD21	1.94	0.49
1:B:1249:ARG:HB2	1:B:1253:LEU:HD13	1.93	0.49
1:B:1316:THR:O	1:B:1338:GLU:HA	2.12	0.49
1:B:1337:ILE:HA	1:A:1365:ARG:NH2	2.28	0.49
1:A:601:GLU:HG3	1:A:603:ILE:H	1.78	0.49
3:F:114:GLN:H	3:F:117:ARG:HH22	1.60	0.49
1:A:15:ARG:HH21	3:D:76:ALA:HB1	1.78	0.49
1:A:390:LYS:HE3	1:A:401:PRO:HG2	1.95	0.49
1:A:624:VAL:HA	1:A:627:VAL:HG22	1.94	0.49
1:A:369:LEU:HB3	1:A:422:LEU:HD23	1.95	0.49
1:A:1310:THR:HG22	1:A:1312:VAL:HG13	1.95	0.49
1:B:562:PHE:CE1	1:B:652:VAL:HG13	2.48	0.48
1:A:859:ARG:HH12	1:A:870:GLU:CD	2.16	0.48
1:A:1025:ALA:HB2	1:A:1241:GLY:HA3	1.95	0.48
1:A:1159:TRP:CZ2	1:A:1349:GLN:HB2	2.48	0.48
1:A:1368:ARG:HE	1:A:1368:ARG:HB2	1.45	0.48
3:D:29:VAL:HG23	3:D:99:VAL:HG11	1.95	0.48
1:B:43:ARG:CG	1:B:129:LEU:HD21	2.43	0.48
1:A:330:GLY:HA3	3:F:98:ARG:NH1	2.28	0.48
1:A:627:VAL:O	1:A:631:MET:N	2.40	0.48
1:A:660:ILE:HG22	1:A:674:ALA:HB1	1.94	0.48
1:A:1230:THR:OG1	1:A:1247:ALA:O	2.23	0.48
1:B:251:ALA:H	1:B:267:GLY:H	1.60	0.48
1:B:557:ARG:HG3	1:B:650:ALA:HB2	1.95	0.48
1:B:1251:LYS:HD2	1:B:1295:LEU:HD11	1.94	0.48
1:B:1274:SER:HB2	1:B:1292:ASN:HB3	1.94	0.48
1:A:1316:THR:O	1:A:1338:GLU:HA	2.13	0.48
3:F:185:VAL:HG22	3:F:197:LEU:HA	1.96	0.48
1:B:331:PRO:HB3	1:B:359:TYR:HA	1.95	0.48
1:B:792:TRP:HZ3	1:B:819:ALA:HB1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1171:VAL:HG12	1:B:1198:ALA:HB3	1.94	0.48
1:B:1004:LEU:HD21	1:B:1104:VAL:HG11	1.94	0.48
1:A:235:MET:SD	1:A:240:MET:HG2	2.53	0.48
1:A:717:VAL:HG23	1:A:723:VAL:HG12	1.96	0.48
3:F:127:ASP:HB3	3:F:188:GLN:HE22	1.78	0.48
1:B:953:LYS:HA	1:B:1007:LEU:HB3	1.94	0.48
1:B:1074:ILE:HG22	1:B:1082:TRP:HB2	1.94	0.48
1:B:1442:PHE:N	1:B:1476:PRO:O	2.44	0.48
1:A:17:THR:HG23	3:F:74:ASN:ND2	2.29	0.48
1:A:761:GLU:HG3	1:A:808:ARG:HD2	1.94	0.48
3:F:130:ARG:NH1	3:F:131:THR:O	2.47	0.48
1:B:316:GLN:O	1:B:320:ILE:HG12	2.13	0.48
1:B:114:ARG:NE	1:B:170:GLY:O	2.47	0.48
1:B:176:MET:HE3	1:A:243:ASP:HB3	1.95	0.48
1:B:558:ALA:HA	1:B:827:THR:HG23	1.95	0.48
1:B:1152:VAL:HA	1:B:1317:TRP:HZ2	1.78	0.48
3:D:189:ASP:OD1	3:D:189:ASP:N	2.42	0.48
1:B:855:ILE:HG12	1:B:875:ALA:HA	1.96	0.48
1:B:1285:LEU:HG	1:B:1327:VAL:HG11	1.96	0.48
1:A:244:PHE:HB3	1:A:250:LEU:HD21	1.95	0.48
1:B:558:ALA:HB1	1:B:829:LEU:HD13	1.96	0.48
1:A:133:VAL:HG11	1:A:228:MET:HE1	1.96	0.47
1:A:963:THR:HA	1:A:966:ARG:HG2	1.96	0.47
2:C:31:PHE:HE2	2:C:76:ARG:HB2	1.79	0.47
3:D:29:VAL:HG21	3:D:99:VAL:HG21	1.96	0.47
3:D:130:ARG:NH1	3:D:131:THR:O	2.47	0.47
1:A:1074:ILE:HG22	1:A:1082:TRP:HB2	1.95	0.47
3:D:163:PRO:O	3:D:220:HIS:NE2	2.47	0.47
2:E:31:PHE:HE2	2:E:76:ARG:HB2	1.79	0.47
1:B:69:PRO:HD3	1:B:97:PHE:CG	2.50	0.47
1:B:677:VAL:HG11	1:B:803:TRP:CE2	2.49	0.47
1:A:568:GLN:O	1:A:860:ARG:NH1	2.47	0.47
1:A:600:PHE:HE2	1:A:605:PHE:HB2	1.79	0.47
2:C:9:SER:OG	2:C:23:SER:OG	2.32	0.47
3:F:59:GLN:HA	3:F:65:PRO:HA	1.96	0.47
1:B:104:PHE:HB2	1:B:124:ARG:HD3	1.96	0.47
1:B:1123:ARG:HH22	1:B:1279:ALA:HA	1.78	0.47
1:A:149:THR:HB	1:A:194:LEU:HD22	1.95	0.47
1:A:471:VAL:HG11	1:A:865:LEU:HD23	1.96	0.47
1:A:1222:SER:HB3	1:A:1268:THR:HG22	1.96	0.47
3:D:54:LEU:HD11	3:D:109:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:118:LEU:H	3:D:118:LEU:HG	1.44	0.47
1:B:736:VAL:HG22	1:B:746:ALA:HB3	1.97	0.47
1:B:1007:LEU:HD23	1:B:1007:LEU:H	1.80	0.47
1:B:1048:GLU:O	1:B:1060:ARG:NE	2.44	0.47
1:B:1417:PHE:CZ	1:B:1421:ARG:HD2	2.49	0.47
1:A:1356:GLU:HB3	1:A:1359:PRO:HG3	1.95	0.47
2:E:49:TRP:HZ2	2:E:52:PHE:HD1	1.61	0.47
3:F:130:ARG:HD2	3:F:131:THR:N	2.29	0.47
1:B:521:ARG:HD3	1:B:876:PHE:O	2.14	0.47
1:A:69:PRO:HG3	1:A:97:PHE:HB3	1.96	0.47
3:F:40:ARG:HD2	3:F:40:ARG:HA	1.38	0.47
1:B:778:LEU:HD12	1:B:779:PRO:HD2	1.96	0.47
1:B:1068:TRP:O	1:B:1072:ARG:HG3	2.13	0.47
1:A:35:VAL:HG23	1:A:220:ARG:HE	1.79	0.47
1:A:174:TYR:HA	1:A:177:THR:HG22	1.96	0.47
1:A:295:ARG:HG3	1:A:329:LEU:HD11	1.97	0.47
1:A:605:PHE:CZ	1:A:627:VAL:HG12	2.50	0.47
2:E:173:PHE:CD2	3:F:198:SER:HB2	2.50	0.47
3:F:163:PRO:O	3:F:220:HIS:NE2	2.47	0.47
1:B:966:ARG:HB2	1:B:976:VAL:HG21	1.95	0.47
1:A:51:PRO:HD2	1:A:136:ARG:CZ	2.44	0.47
1:A:739:CYS:HB3	1:A:744:ILE:HG22	1.97	0.47
1:A:954:TYR:HD2	1:A:956:GLY:H	1.63	0.47
1:A:1068:TRP:O	1:A:1072:ARG:HG3	2.15	0.47
3:D:59:GLN:HA	3:D:65:PRO:HA	1.96	0.47
1:B:777:PRO:HB2	1:B:796:ASP:OD1	2.15	0.47
1:B:1427:VAL:HG23	1:B:1454:GLU:HG3	1.96	0.47
1:A:50:THR:HG23	1:A:52:GLU:HG3	1.97	0.47
1:A:842:GLU:HG3	1:A:854:ALA:HB3	1.97	0.47
1:B:140:PRO:HB2	1:B:143:SER:HB3	1.95	0.47
1:B:859:ARG:HB3	1:B:862:ASP:HB2	1.96	0.47
2:C:71:ARG:HH21	2:C:90:LEU:HA	1.80	0.47
2:C:112:GLN:OE1	2:C:112:GLN:N	2.43	0.47
2:C:150:LYS:HB3	2:C:150:LYS:HE2	1.50	0.47
1:B:1048:GLU:HB3	1:B:1060:ARG:HE	1.80	0.46
1:B:1226:HIS:HE1	1:B:1251:LYS:HA	1.80	0.46
3:F:17:ASP:OD1	3:F:18:VAL:N	2.47	0.46
1:B:624:VAL:HG11	1:B:685:ILE:HG22	1.96	0.46
1:B:1009:VAL:HA	1:B:1048:GLU:HB2	1.97	0.46
1:B:1178:ALA:HB3	1:B:1181:ALA:HB2	1.97	0.46
1:A:257:LYS:HE3	1:A:257:LYS:HB3	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:ARG:HG3	1:A:1359:PRO:HB3	1.97	0.46
2:C:50:VAL:O	2:C:65:ALA:N	2.46	0.46
3:D:130:ARG:HD2	3:D:131:THR:N	2.29	0.46
2:E:112:GLN:OE1	2:E:112:GLN:N	2.43	0.46
1:B:331:PRO:O	1:B:363:ARG:NH1	2.47	0.46
1:B:577:LEU:HA	1:B:583:PHE:HB3	1.97	0.46
1:A:201:VAL:HG21	1:A:210:VAL:HG12	1.97	0.46
1:A:838:THR:HA	1:A:841:ILE:HB	1.98	0.46
1:A:1312:VAL:HG12	1:A:1359:PRO:HB2	1.97	0.46
3:D:38:SER:OG	3:D:39:CYS:N	2.47	0.46
3:D:88:SER:N	3:D:91:ASP:O	2.43	0.46
2:E:50:VAL:O	2:E:65:ALA:N	2.46	0.46
1:B:176:MET:HE1	1:A:244:PHE:CD2	2.51	0.46
1:B:373:LYS:O	1:B:377:GLY:N	2.46	0.46
1:B:1028:LEU:HD11	1:B:1244:ILE:HD12	1.96	0.46
2:C:39:VAL:O	2:C:99:TYR:N	2.38	0.46
1:B:623:ARG:O	1:B:627:VAL:N	2.37	0.46
1:A:13:LEU:HD21	3:F:71:LEU:HD11	1.96	0.46
1:A:584:ALA:O	1:A:588:ARG:HG2	2.15	0.46
1:A:619:LEU:H	1:A:623:ARG:HG3	1.79	0.46
2:E:9:SER:OG	2:E:23:SER:OG	2.32	0.46
1:B:951:VAL:HG13	1:B:951:VAL:O	2.16	0.46
1:B:1222:SER:HB3	1:B:1268:THR:H	1.81	0.46
1:B:1291:GLY:O	1:B:1295:LEU:HG	2.16	0.46
1:B:660:ILE:HD13	1:B:803:TRP:CZ3	2.51	0.46
1:B:1453:LEU:HA	1:B:1456:ARG:NE	2.31	0.46
2:C:95:THR:HG23	2:C:117:THR:HG23	1.98	0.46
1:B:631:MET:O	1:B:635:MET:HB2	2.16	0.46
1:A:43:ARG:HB3	1:A:272:ALA:HB3	1.97	0.46
1:A:841:ILE:HG22	1:A:854:ALA:HB2	1.98	0.46
1:A:845:GLY:HA2	1:A:848:SER:HB2	1.98	0.46
1:A:1147:GLY:N	1:A:1171:VAL:O	2.42	0.46
2:C:102:ARG:HB3	2:C:108:ASP:OD1	2.16	0.46
1:B:652:VAL:HG21	1:B:666:ALA:HB2	1.97	0.46
1:B:1435:ARG:NH1	1:B:1437:PRO:HA	2.31	0.46
1:A:1318:ALA:HB3	1:A:1341:PRO:HD3	1.97	0.46
2:E:71:ARG:HH21	2:E:90:LEU:HA	1.80	0.46
2:E:110:TRP:HB3	3:F:64:SER:HB2	1.97	0.46
3:F:57:TYR:HB2	3:F:108:TYR:HB2	1.98	0.46
1:A:40:MET:HB2	1:A:51:PRO:HG2	1.98	0.46
1:A:141:PRO:HG2	1:A:516:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:ARG:NH2	1:A:846:ASP:H	2.14	0.46
3:F:58:LEU:HD13	3:F:107:TYR:CE1	2.51	0.46
1:B:43:ARG:HG3	1:B:129:LEU:HD21	1.98	0.45
1:B:1244:ILE:HG12	1:B:1287:GLY:HA2	1.97	0.45
1:A:111:MET:HE2	1:A:119:VAL:HG21	1.98	0.45
1:A:340:HIS:HD2	1:A:442:SER:HA	1.81	0.45
1:A:594:LEU:HG	1:A:675:ALA:HB1	1.98	0.45
1:A:1285:LEU:HD22	1:A:1288:TYR:CD2	2.52	0.45
1:B:141:PRO:HD2	1:B:516:ALA:HB2	1.97	0.45
1:A:1203:THR:OG1	1:A:1249:ARG:NH1	2.41	0.45
1:B:38:VAL:HG13	1:B:288:HIS:HB3	1.99	0.45
1:B:329:LEU:HD12	1:B:453:ILE:HG21	1.98	0.45
1:B:676:ARG:HH21	1:B:775:PHE:HB3	1.81	0.45
1:B:712:VAL:HG21	1:B:731:GLU:HB2	1.98	0.45
1:A:208:SER:HB3	1:A:381:ALA:O	2.17	0.45
1:B:103:ALA:HB1	1:B:905:ARG:HB3	1.99	0.45
1:B:688:MET:N	1:B:689:PRO:HD3	2.31	0.45
1:A:92:GLN:HE21	1:A:250:LEU:HD12	1.81	0.45
1:A:760:VAL:HG21	1:A:807:LEU:HD22	1.98	0.45
1:B:493:ALA:HB2	1:B:536:LEU:HB3	1.98	0.45
1:B:583:PHE:CA	1:B:641:MET:HE3	2.47	0.45
1:B:1303:ARG:HG2	1:B:1357:VAL:HG22	1.99	0.45
1:B:1424:ALA:HA	1:B:1427:VAL:HG12	1.98	0.45
1:A:149:THR:HA	1:A:226:LEU:O	2.16	0.45
2:E:95:THR:HG23	2:E:117:THR:HG23	1.98	0.45
1:B:731:GLU:HA	1:B:734:ARG:HG2	1.99	0.45
1:B:805:ARG:HG2	1:B:809:ARG:HH12	1.80	0.45
1:A:235:MET:HG3	1:A:237:THR:O	2.16	0.45
1:A:756:HIS:H	1:A:807:LEU:HA	1.82	0.45
1:A:951:VAL:HG13	1:A:951:VAL:O	2.16	0.45
3:F:188:GLN:HG3	3:F:195:TYR:CZ	2.51	0.45
1:B:330:GLY:CA	3:D:98:ARG:HH12	2.30	0.45
1:B:555:GLN:HE21	1:B:827:THR:HB	1.81	0.45
1:B:749:LEU:HG	1:B:751:VAL:HG23	1.99	0.45
1:B:1019:LEU:HG	1:B:1252:VAL:HG21	1.98	0.45
1:B:1226:HIS:CE1	1:B:1251:LYS:HA	2.52	0.45
1:A:12:TYR:CE1	3:D:70:TYR:HB2	2.51	0.45
1:A:108:PHE:HZ	1:A:131:TRP:CE2	2.34	0.45
2:E:41:GLN:NE2	2:E:45:LYS:O	2.41	0.45
2:E:124:LYS:NZ	2:E:151:ASP:HB3	2.32	0.45
2:E:185:LEU:HD23	2:E:186:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:135:PRO:HB2	3:F:158:LEU:HD12	1.99	0.45
1:B:1157:ALA:HA	1:B:1160:LEU:HD12	1.99	0.44
1:B:1277:ALA:HB2	1:B:1285:LEU:HD13	1.99	0.44
1:A:560:PHE:CE1	1:A:829:LEU:HD23	2.51	0.44
1:A:1110:GLU:HB2	1:A:1113:LEU:HD21	2.00	0.44
3:D:135:PRO:HB2	3:D:158:LEU:HD12	1.99	0.44
3:F:80:PRO:HB2	3:F:82:ARG:HG3	1.98	0.44
1:A:33:GLU:O	1:A:220:ARG:NE	2.50	0.44
1:A:334:ILE:HD13	1:A:359:TYR:HE1	1.82	0.44
3:D:87:GLY:HA3	3:D:92:PHE:HD1	1.82	0.44
1:B:42:CYS:HB3	1:B:389:ILE:HD13	2.00	0.44
1:B:966:ARG:HA	1:B:969:LEU:HB2	1.99	0.44
1:B:1411:GLU:C	1:B:1413:GLU:N	2.70	0.44
1:B:114:ARG:HH12	1:B:173:GLY:H	1.66	0.44
1:A:688:MET:N	1:A:689:PRO:HD2	2.32	0.44
1:A:987:ARG:NH1	1:A:1239:LEU:O	2.51	0.44
2:C:185:LEU:HD23	2:C:186:SER:N	2.32	0.44
1:B:81:HIS:CD2	1:B:82:PRO:HD2	2.52	0.44
1:B:243:ASP:HB3	1:A:176:MET:SD	2.57	0.44
1:B:1075:ALA:HB2	1:B:1082:TRP:HD1	1.82	0.44
1:A:1034:MET:HE2	1:A:1034:MET:HB2	1.70	0.44
1:A:1159:TRP:CD1	1:A:1345:CYS:HB2	2.52	0.44
2:E:102:ARG:HB3	2:E:108:ASP:OD1	2.16	0.44
3:F:87:GLY:HA3	3:F:92:PHE:HD1	1.82	0.44
1:B:555:GLN:NE2	1:B:827:THR:HB	2.33	0.44
1:B:780:GLY:H	1:B:795:PRO:HB2	1.82	0.44
1:B:1263:ARG:HA	1:B:1307:LEU:HD11	1.99	0.44
1:B:1298:LEU:O	1:B:1302:ARG:HG3	2.17	0.44
1:B:1337:ILE:HG13	1:A:1365:ARG:CZ	2.47	0.44
1:A:103:ALA:HB1	1:A:905:ARG:HB3	1.99	0.44
1:A:992:GLU:HA	1:A:995:ARG:HE	1.83	0.44
2:E:13:LEU:HD13	2:E:117:THR:HB	1.99	0.44
1:B:92:GLN:NE2	1:B:94:GLY:O	2.51	0.44
1:B:324:LEU:HB3	1:B:329:LEU:O	2.17	0.44
1:B:362:ASP:OD1	1:B:362:ASP:N	2.50	0.44
1:A:216:CYS:O	1:A:220:ARG:HG2	2.18	0.44
1:A:296:GLY:HA3	1:A:327:SER:HB3	2.00	0.44
1:A:1076:LEU:HG	1:A:1376:GLN:HE22	1.83	0.44
3:D:189:ASP:OD2	3:D:192:ASP:HB3	2.17	0.44
1:B:108:PHE:HZ	1:B:131:TRP:CE2	2.35	0.44
1:B:115:GLU:O	1:B:119:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:HG12	1:A:197:PRO:HA	2.00	0.44
1:B:322:GLN:HE22	1:A:223:GLU:HG3	1.83	0.44
1:B:731:GLU:HG2	1:B:734:ARG:HH11	1.83	0.44
1:A:41:ALA:HB2	1:A:133:VAL:HB	1.98	0.44
1:A:103:ALA:HB1	1:A:905:ARG:HD3	2.00	0.44
1:A:329:LEU:C	3:F:98:ARG:HH12	2.21	0.44
1:A:1222:SER:HA	1:A:1267:LEU:HA	1.98	0.44
1:A:1302:ARG:NH2	1:A:1307:LEU:HB3	2.33	0.44
2:E:3:GLU:HG3	2:E:5:GLN:NE2	2.33	0.44
1:B:35:VAL:HA	1:B:279:ARG:HA	2.00	0.44
1:B:834:HIS:HD2	1:B:836:ILE:HG13	1.83	0.44
1:A:58:LEU:HD13	1:A:390:LYS:HG3	2.00	0.44
1:A:103:ALA:HA	1:A:906:GLU:O	2.18	0.44
1:A:748:ARG:NH2	1:A:752:ASP:HB3	2.32	0.44
1:A:802:TYR:HA	1:A:805:ARG:HE	1.82	0.44
1:A:834:HIS:HA	1:A:858:LEU:O	2.18	0.44
1:A:841:ILE:HA	1:A:844:ILE:HB	1.99	0.44
1:A:906:GLU:HG2	1:A:907:ARG:H	1.83	0.44
2:C:110:TRP:CE2	3:D:65:PRO:HB2	2.53	0.44
3:F:189:ASP:OD2	3:F:192:ASP:HB3	2.17	0.44
1:B:175:LEU:HB2	1:A:243:ASP:OD2	2.17	0.43
1:B:475:TRP:CE2	1:B:526:PRO:HG3	2.53	0.43
1:B:787:THR:HB	1:B:811:VAL:HG13	2.00	0.43
1:B:1333:ARG:HG2	1:A:1127:ARG:HH12	1.82	0.43
1:A:337:VAL:HG23	1:A:367:LEU:HD11	2.00	0.43
1:A:1005:SER:OG	1:A:1043:LEU:HD11	2.18	0.43
3:D:20:MET:HB3	3:D:22:GLN:HE22	1.83	0.43
1:B:120:ASP:HB2	1:B:178:GLY:O	2.17	0.43
1:B:627:VAL:HG22	1:B:631:MET:HG2	2.00	0.43
1:A:60:GLU:OE2	1:A:62:ARG:NH2	2.51	0.43
1:A:317:VAL:HG13	1:A:358:ALA:HB2	1.99	0.43
1:A:559:VAL:HG21	1:A:825:TYR:HB3	2.00	0.43
1:A:1086:VAL:HA	1:A:1113:LEU:HB2	1.99	0.43
1:A:1096:LEU:HD22	1:A:1100:LEU:HD11	1.99	0.43
1:A:1147:GLY:HA2	1:A:1172:SER:HB3	2.00	0.43
1:B:2:ALA:HB3	1:B:8:LYS:HE2	2.00	0.43
1:B:55:TRP:CZ3	1:B:401:PRO:HG3	2.53	0.43
1:B:157:PRO:HG3	1:A:181:THR:H	1.83	0.43
1:B:182:SER:HB2	1:A:202:ASP:OD1	2.18	0.43
1:B:434:ARG:HE	1:B:434:ARG:HB3	1.61	0.43
1:B:705:ARG:CZ	1:B:714:ILE:HD12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:HIS:O	1:B:836:ILE:HD12	2.17	0.43
1:B:1272:LEU:HD23	1:B:1295:LEU:HD22	2.00	0.43
1:A:42:CYS:HB2	1:A:44:LEU:CD2	2.48	0.43
2:C:149:VAL:CG1	2:C:205:VAL:HG11	2.48	0.43
1:B:1229:ALA:HB1	1:B:1288:TYR:HE1	1.83	0.43
1:A:569:TRP:CZ3	1:A:861:GLY:HA2	2.54	0.43
1:A:1302:ARG:NH1	1:A:1308:PRO:O	2.39	0.43
2:E:8:GLN:HB2	2:E:112:GLN:HE22	1.84	0.43
1:B:7:GLU:O	1:B:11:GLU:N	2.47	0.43
1:A:589:GLU:HA	1:A:592:ASP:OD2	2.19	0.43
1:B:12:TYR:CE1	3:F:70:TYR:HB2	2.52	0.43
1:B:663:ALA:HB2	1:B:798:LEU:HD21	2.00	0.43
1:A:283:ALA:HB1	1:A:288:HIS:HB2	1.99	0.43
1:A:320:ILE:HA	1:A:451:HIS:CD2	2.54	0.43
1:A:462:GLU:O	1:A:465:ARG:HG2	2.19	0.43
1:A:652:VAL:HG21	1:A:666:ALA:HB2	2.00	0.43
1:A:1227:ALA:HB2	1:A:1273:PHE:HD2	1.83	0.43
3:D:152:ALA:HB3	3:D:203:LEU:HB3	2.01	0.43
1:A:155:LEU:HD11	1:A:184:ALA:HB3	2.00	0.43
1:A:563:PRO:HB2	1:A:567:TRP:CD1	2.54	0.43
1:A:619:LEU:HD23	1:A:622:GLU:HB2	2.00	0.43
1:A:781:PHE:CD2	1:A:782:VAL:HG12	2.53	0.43
1:B:98:LEU:HD11	1:B:271:GLY:HA2	2.00	0.43
1:B:472:VAL:HG21	1:B:866:ALA:HA	2.01	0.43
1:B:652:VAL:HG11	1:B:662:ALA:HA	1.99	0.43
1:B:1227:ALA:HB2	1:B:1273:PHE:HD2	1.84	0.43
1:A:470:ASP:OD2	1:A:471:VAL:HG12	2.18	0.43
1:A:498:GLU:HG3	1:A:499:HIS:CE1	2.54	0.43
1:A:560:PHE:CG	1:A:649:PRO:HB3	2.54	0.43
1:A:1274:SER:HB2	1:A:1292:ASN:HB3	2.00	0.43
1:B:205:CYS:HB3	1:B:378:HIS:NE2	2.29	0.43
1:A:34:PRO:HB2	1:A:280:LEU:HB2	2.01	0.43
1:B:1031:VAL:O	1:B:1035:VAL:HG23	2.19	0.43
1:B:1147:GLY:N	1:B:1171:VAL:O	2.51	0.43
1:B:1152:VAL:HA	1:B:1317:TRP:CZ2	2.53	0.43
1:A:169:GLU:HG2	1:A:170:GLY:N	2.34	0.43
2:C:3:GLU:HG3	2:C:5:GLN:NE2	2.33	0.43
2:C:8:GLN:HB2	2:C:112:GLN:HE22	1.83	0.43
2:C:13:LEU:HD13	2:C:117:THR:HB	2.00	0.43
3:F:152:ALA:HB3	3:F:203:LEU:HB3	2.01	0.43
1:B:2:ALA:CA	1:B:7:GLU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:CYS:HA	1:B:273:GLY:HA2	2.00	0.42
1:B:57:LEU:HD12	1:B:62:ARG:HB2	2.00	0.42
1:B:188:ILE:HD12	1:B:188:ILE:H	1.84	0.42
1:B:429:TRP:HH2	1:B:438:ALA:HB2	1.83	0.42
1:B:1302:ARG:NH1	1:B:1308:PRO:O	2.44	0.42
1:A:1203:THR:O	1:A:1257:ASN:ND2	2.52	0.42
1:A:1327:VAL:HA	1:A:1330:ARG:HD2	2.01	0.42
2:C:108:ASP:HA	3:D:67:LEU:HB2	2.01	0.42
1:B:950:LEU:HD13	1:B:979:LEU:HD22	2.01	0.42
1:B:1030:LEU:HD23	1:B:1034:MET:SD	2.59	0.42
1:A:255:ARG:HG2	1:A:405:HIS:NE2	2.34	0.42
1:A:1125:TRP:N	1:A:1381:LEU:O	2.47	0.42
2:C:211:ASN:HA	2:C:213:LYS:HE3	2.01	0.42
2:E:211:ASN:HA	2:E:213:LYS:HE3	2.01	0.42
1:B:104:PHE:O	1:B:106:PRO:HD3	2.20	0.42
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.84	0.42
1:B:1028:LEU:HD21	1:B:1070:VAL:HG21	2.00	0.42
1:A:68:LEU:HD22	1:A:74:TRP:HZ3	1.84	0.42
1:A:333:ASP:O	1:A:434:ARG:NH1	2.52	0.42
1:A:564:GLY:N	1:A:655:HIS:HB3	2.35	0.42
1:B:29:GLU:HA	1:B:33:GLU:HB2	2.02	0.42
1:B:257:LYS:HG3	1:B:405:HIS:HB3	2.02	0.42
1:B:483:GLU:OE1	1:B:486:ARG:NH2	2.50	0.42
1:B:711:ARG:NH1	1:B:758:SER:OG	2.52	0.42
1:B:765:ASP:OD1	1:B:765:ASP:N	2.52	0.42
1:A:1075:ALA:HB1	1:A:1377:ARG:HD3	2.01	0.42
1:A:1096:LEU:HA	1:A:1100:LEU:HG	2.01	0.42
1:A:1282:ALA:HB1	1:A:1285:LEU:HD12	2.01	0.42
2:E:6:LEU:HD23	2:E:6:LEU:HA	1.95	0.42
2:E:20:LEU:HB3	2:E:87:MET:HE2	2.02	0.42
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.93	0.42
1:B:764:ARG:HE	1:B:768:HIS:CD2	2.37	0.42
1:A:226:LEU:HD21	1:A:276:LEU:HD11	2.00	0.42
1:A:608:ALA:HA	1:A:612:ARG:HE	1.85	0.42
1:B:126:MET:HG3	1:B:153:VAL:HG11	2.00	0.42
1:B:1131:PRO:N	1:B:1354:ARG:HH22	2.18	0.42
1:B:1239:LEU:HD22	1:B:1244:ILE:HG13	2.01	0.42
1:A:335:ASP:OD2	1:A:434:ARG:NH2	2.52	0.42
3:D:107:TYR:CD1	3:D:126:VAL:HG21	2.55	0.42
1:B:331:PRO:HA	1:B:359:TYR:HD1	1.84	0.42
1:B:970:GLU:HA	1:B:974:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:HD2	1:A:405:HIS:HB3	2.01	0.42
1:A:476:VAL:O	1:A:511:LEU:HG	2.19	0.42
1:A:704:VAL:O	1:A:708:ILE:HG23	2.18	0.42
1:A:721:ARG:HH22	1:A:846:ASP:H	1.68	0.42
1:A:1298:LEU:O	1:A:1302:ARG:HG3	2.19	0.42
2:C:174:PRO:HD3	3:D:186:THR:HG23	2.01	0.42
2:E:204:ASN:N	2:E:204:ASN:OD1	2.53	0.42
1:B:297:THR:HG23	1:B:452:ALA:HB2	2.01	0.42
1:B:705:ARG:HA	1:B:705:ARG:HD3	1.83	0.42
1:A:69:PRO:HG2	1:A:72:ARG:NH2	2.33	0.42
1:A:151:VAL:HA	1:A:228:MET:HB3	2.02	0.42
1:A:580:SER:HB3	1:A:865:LEU:HD22	2.00	0.42
1:A:913:LYS:N	1:A:914:PRO:HD3	2.34	0.42
1:A:1103:VAL:HG13	1:A:1113:LEU:HG	2.02	0.42
2:C:129:PHE:O	2:C:148:LEU:N	2.52	0.42
3:F:171:LYS:HA	3:F:171:LYS:HD3	1.92	0.42
1:B:232:VAL:HG23	1:B:272:ALA:HB2	2.02	0.42
1:B:1143:VAL:HG11	1:B:1160:LEU:CD1	2.48	0.42
1:A:86:ARG:HB3	1:A:89:THR:OG1	2.20	0.42
1:A:235:MET:HE2	1:A:240:MET:H	1.84	0.42
1:A:555:GLN:O	1:A:557:ARG:HG2	2.19	0.42
1:A:605:PHE:CD2	1:A:630:VAL:HG11	2.55	0.42
1:A:978:GLU:OE1	1:A:978:GLU:N	2.52	0.42
3:F:137:VAL:HG22	3:F:158:LEU:HD11	2.01	0.42
1:B:1096:LEU:HD22	1:B:1100:LEU:HD11	2.02	0.42
1:A:302:ASP:O	1:A:312:ASN:ND2	2.53	0.42
1:A:378:HIS:CD2	1:A:380:GLN:H	2.38	0.42
1:A:619:LEU:HB3	1:A:623:ARG:HG2	2.00	0.42
1:A:1009:VAL:HA	1:A:1048:GLU:OE1	2.19	0.42
1:B:834:HIS:CD2	1:B:836:ILE:HG13	2.55	0.41
1:B:1162:ARG:HG2	1:B:1191:LEU:HD22	2.02	0.41
1:A:935:ARG:HB2	1:A:1124:ARG:HG3	2.02	0.41
1:A:1366:TRP:HE1	1:A:1382:PHE:HD1	1.66	0.41
1:B:131:TRP:HE1	1:B:901:TYR:HB2	1.85	0.41
1:B:385:VAL:HA	1:B:388:VAL:HG12	2.01	0.41
1:B:512:ALA:HB1	1:B:884:TRP:CG	2.55	0.41
1:B:1222:SER:HB3	1:B:1268:THR:HG22	2.01	0.41
1:A:38:VAL:HB	1:A:276:LEU:HD23	2.01	0.41
1:A:435:PRO:HA	1:A:456:GLU:OE2	2.20	0.41
1:A:731:GLU:O	1:A:735:LEU:N	2.53	0.41
1:A:925:VAL:HG13	1:A:1347:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:GLY:N	2:C:90:LEU:O	2.53	0.41
2:E:41:GLN:O	2:E:96:ALA:HB1	2.21	0.41
1:B:114:ARG:CZ	1:B:172:GLU:H	2.33	0.41
1:B:156:ILE:HG22	1:B:158:GLN:HG2	2.02	0.41
1:B:475:TRP:CD1	1:B:508:ALA:HB2	2.54	0.41
1:B:853:SER:HB3	1:B:878:ALA:HB1	2.02	0.41
1:B:1096:LEU:HA	1:B:1100:LEU:HG	2.00	0.41
1:A:43:ARG:HD2	1:A:100:GLU:HG3	2.02	0.41
1:A:311:PRO:HG2	1:A:350:ILE:HD12	2.01	0.41
1:A:572:MET:O	1:A:606:LEU:HB2	2.21	0.41
1:A:953:LYS:HA	1:A:1007:LEU:HB3	2.02	0.41
3:D:164:ARG:HE	3:D:185:VAL:HG11	1.85	0.41
2:E:39:VAL:O	2:E:99:TYR:N	2.37	0.41
1:B:82:PRO:HG2	1:A:1308:PRO:HG3	2.02	0.41
1:B:131:TRP:HB3	1:B:903:PHE:HZ	1.86	0.41
1:B:242:VAL:O	1:B:246:ARG:NH1	2.54	0.41
1:A:74:TRP:CD1	1:A:238:PRO:HD3	2.56	0.41
1:A:503:ASP:O	1:A:507:ILE:HG12	2.20	0.41
1:A:604:PRO:HB3	1:A:607:ARG:HH21	1.85	0.41
2:C:159:VAL:HG13	2:C:205:VAL:HG22	2.02	0.41
3:F:23:SER:HA	3:F:24:PRO:HD2	1.93	0.41
1:B:125:LEU:O	1:B:129:LEU:HD23	2.20	0.41
1:B:506:ASP:HB3	1:B:896:VAL:HG21	2.02	0.41
1:B:605:PHE:CD2	1:B:630:VAL:HG11	2.55	0.41
1:B:763:ILE:O	1:B:763:ILE:HG22	2.20	0.41
1:B:992:GLU:HA	1:B:995:ARG:HE	1.85	0.41
1:B:1013:GLU:HB2	1:B:1061:ASN:HD21	1.86	0.41
1:B:1059:VAL:O	1:B:1301:GLN:NE2	2.54	0.41
1:A:176:MET:SD	1:A:176:MET:N	2.94	0.41
1:A:235:MET:HE2	1:A:239:GLY:H	1.85	0.41
1:A:340:HIS:CD2	1:A:443:PHE:H	2.39	0.41
1:A:470:ASP:CG	1:A:471:VAL:H	2.24	0.41
1:A:597:HIS:CE1	1:A:676:ARG:HB2	2.56	0.41
1:A:610:ALA:HA	1:A:613:ARG:HE	1.84	0.41
1:A:737:ALA:HA	1:A:740:THR:HG22	2.02	0.41
2:E:17:GLY:N	2:E:90:LEU:O	2.53	0.41
1:B:43:ARG:HH21	1:B:905:ARG:NH2	2.18	0.41
1:B:219:LEU:O	1:B:279:ARG:NH1	2.53	0.41
1:B:302:ASP:N	1:B:447:GLY:O	2.49	0.41
1:B:603:ILE:HD13	1:B:606:LEU:HD12	2.03	0.41
1:B:609:GLU:O	1:B:613:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:LEU:HD13	1:B:1288:TYR:HB2	2.03	0.41
1:A:102:THR:HG22	1:A:909:TRP:CD2	2.56	0.41
1:A:994:LEU:HA	1:A:997:VAL:HG12	2.01	0.41
3:D:137:VAL:HG22	3:D:158:LEU:HD11	2.02	0.41
2:E:159:VAL:HG13	2:E:205:VAL:HG22	2.02	0.41
3:F:141:PRO:HB3	3:F:231:PHE:HB2	2.02	0.41
1:B:335:ASP:HB2	1:B:429:TRP:CZ2	2.56	0.41
1:B:406:ALA:HB1	1:B:422:LEU:HD21	2.02	0.41
1:B:683:ARG:HD2	1:B:770:GLU:HG2	2.03	0.41
1:B:704:VAL:HG21	1:B:723:VAL:HG11	2.03	0.41
1:A:30:LEU:O	1:A:220:ARG:HB3	2.21	0.41
1:A:312:ASN:HD22	1:A:315:ALA:HB2	1.85	0.41
1:A:400:LEU:HG	1:A:429:TRP:HB2	2.02	0.41
1:A:602:VAL:HG12	1:A:606:LEU:HD23	2.03	0.41
1:A:1125:TRP:HH2	1:A:1279:ALA:HB1	1.85	0.41
1:A:1313:ALA:HB3	1:A:1360:ILE:HG23	2.03	0.41
2:C:177:LEU:HD13	2:C:177:LEU:HA	1.93	0.41
3:F:156:CYS:HB3	3:F:168:VAL:HG11	2.02	0.41
1:B:313:GLY:O	1:B:317:VAL:HG23	2.21	0.41
1:B:476:VAL:HG11	1:B:884:TRP:CZ2	2.55	0.41
1:B:836:ILE:HG22	1:B:837:LEU:CD2	2.51	0.41
1:A:156:ILE:HD12	1:A:380:GLN:OE1	2.20	0.41
1:A:495:HIS:NE2	1:A:897:PRO:O	2.53	0.41
1:A:561:VAL:HA	1:A:653:ILE:HG23	2.02	0.41
2:C:26:ALA:HB1	2:C:29:PHE:CE1	2.56	0.41
3:F:21:THR:HG21	3:F:111:GLN:HB3	2.03	0.41
1:B:2:ALA:CB	1:B:7:GLU:HB2	2.51	0.41
1:B:256:CYS:SG	1:B:378:HIS:N	2.94	0.41
1:B:349:PRO:HA	1:B:413:ILE:HG12	2.03	0.41
1:B:605:PHE:HD2	1:B:630:VAL:HG11	1.86	0.41
1:B:1222:SER:HA	1:B:1267:LEU:HA	2.03	0.41
1:B:1340:PRO:HG2	1:A:1332:ARG:HH21	1.86	0.41
1:A:213:HIS:HB2	1:A:297:THR:HB	2.03	0.41
1:A:437:ARG:HG2	1:A:455:GLU:HG3	2.03	0.41
1:A:1048:GLU:O	1:A:1060:ARG:NE	2.54	0.41
2:C:21:ARG:HH22	2:C:84:TYR:HB3	1.86	0.41
3:D:141:PRO:HB3	3:D:231:PHE:HB2	2.02	0.41
2:E:37:SER:HB2	2:E:101:THR:OG1	2.20	0.41
1:B:330:GLY:HA3	3:D:98:ARG:HH12	1.86	0.41
1:A:929:ARG:HH22	1:A:1354:ARG:NH1	2.19	0.41
1:A:1169:LEU:O	1:A:1171:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:ASP:HB3	1:A:1207:SER:HB3	2.02	0.41
1:A:1385:ILE:HB	1:A:1388:ALA:HB2	2.02	0.41
3:D:170:TRP:CE3	3:D:201:LEU:HD22	2.56	0.41
1:B:121:PRO:HB2	1:B:234:VAL:CG1	2.50	0.40
1:A:568:GLN:HA	1:A:572:MET:CE	2.49	0.40
1:A:926:SER:HB3	1:A:1130:ALA:HB3	2.04	0.40
1:A:1337:ILE:HG23	1:A:1338:GLU:N	2.36	0.40
2:E:26:ALA:HB1	2:E:29:PHE:CE1	2.56	0.40
2:E:149:VAL:HG13	2:E:205:VAL:HG11	2.02	0.40
1:B:26:ARG:HA	1:B:29:GLU:HG2	2.03	0.40
1:B:86:ARG:NH1	1:A:1135:ASP:OD2	2.47	0.40
1:B:595:GLU:HA	1:B:598:LEU:O	2.21	0.40
1:A:230:GLY:HA3	1:A:274:MET:HA	2.02	0.40
1:A:510:SER:HB3	1:A:895:ARG:HA	2.03	0.40
1:A:594:LEU:O	1:A:598:LEU:N	2.54	0.40
1:A:1110:GLU:OE2	1:A:1380:ARG:HD2	2.20	0.40
1:A:1115:LEU:HD22	1:A:1120:VAL:HG12	2.04	0.40
2:C:6:LEU:HD23	2:C:6:LEU:HA	1.95	0.40
2:C:37:SER:HB2	2:C:101:THR:OG1	2.21	0.40
2:C:204:ASN:OD1	2:C:204:ASN:N	2.53	0.40
2:E:36:MET:H	2:E:76:ARG:NH1	2.17	0.40
2:E:178:GLN:HE21	2:E:178:GLN:HB2	1.70	0.40
3:F:170:TRP:CE3	3:F:201:LEU:HD22	2.56	0.40
1:B:65:VAL:HG13	1:B:95:GLY:H	1.86	0.40
1:B:203:THR:OG1	1:B:207:SER:HA	2.21	0.40
1:B:1099:HIS:HB2	1:B:1115:LEU:HD13	2.03	0.40
1:A:312:ASN:HB3	1:A:315:ALA:HB3	2.02	0.40
1:A:495:HIS:CG	1:A:899:PRO:HD3	2.57	0.40
1:A:564:GLY:HA3	1:A:656:SER:OG	2.20	0.40
1:A:837:LEU:HD12	1:A:840:ALA:HB3	2.04	0.40
2:C:36:MET:H	2:C:76:ARG:NH1	2.18	0.40
1:B:157:PRO:HD2	1:A:180:THR:HG23	2.04	0.40
1:B:324:LEU:HD13	1:B:331:PRO:HD3	2.04	0.40
1:B:991:ALA:HA	1:B:994:LEU:HD12	2.04	0.40
1:B:1023:SER:HB2	1:B:1067:LEU:HD21	2.03	0.40
1:B:1227:ALA:HB2	1:B:1273:PHE:CD2	2.56	0.40
1:A:1019:LEU:HD23	1:A:1019:LEU:HA	1.93	0.40
1:A:1152:VAL:HG22	1:A:1317:TRP:CD1	2.57	0.40
3:D:171:LYS:HA	3:D:171:LYS:HD3	1.91	0.40
1:B:359:TYR:O	1:B:363:ARG:HG2	2.20	0.40
1:B:855:ILE:HG23	1:B:874:ARG:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:LEU:HD12	1:A:1371:LEU:HA	1.83	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%)	1303 (94%)	85 (6%)	0	100	100
1	B	1419/1784 (80%)	1353 (95%)	66 (5%)	0	100	100
2	C	199/249 (80%)	186 (94%)	13 (6%)	0	100	100
2	E	199/249 (80%)	187 (94%)	12 (6%)	0	100	100
3	D	200/236 (85%)	182 (91%)	18 (9%)	0	100	100
3	F	200/236 (85%)	183 (92%)	17 (8%)	0	100	100
All	All	3605/4538 (79%)	3394 (94%)	211 (6%)	0	100	100

There are no Ramachandran outliers to report.

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%)	999 (97%)	29 (3%)	43	65
1	B	1047/1325 (79%)	1017 (97%)	30 (3%)	42	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	170/203 (84%)	163 (96%)	7 (4%)	30 57
2	E	170/203 (84%)	164 (96%)	6 (4%)	36 61
3	D	182/208 (88%)	153 (84%)	29 (16%)	2 15
3	F	182/208 (88%)	155 (85%)	27 (15%)	3 17
All	All	2779/3472 (80%)	2651 (95%)	128 (5%)	31 54

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	4	THR
1	B	6	SER
1	B	7	GLU
1	B	163	ARG
1	B	200	SER
1	B	203	THR
1	B	207	SER
1	B	208	SER
1	B	212	VAL
1	B	214	LEU
1	B	557	ARG
1	B	577	LEU
1	B	623	ARG
1	B	653	ILE
1	B	774	ASP
1	B	818	ARG
1	B	820	LEU
1	B	822	GLU
1	B	1142	THR
1	B	1144	LEU
1	B	1246	ARG
1	B	1317	TRP
1	B	1322	MET
1	B	1327	VAL
1	B	1329	ASP
1	B	1333	ARG
1	B	1407	LEU
1	B	1412	ARG
1	B	1435	ARG
1	A	163	ARG
1	A	174	TYR

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Mol	Chain	Res	Type
1	A	175	LEU
1	A	176	MET
1	A	177	THR
1	A	721	ARG
1	A	777	PRO
1	A	796	ASP
1	A	799	ASP
1	A	818	ARG
1	A	843	GLU
1	A	844	ILE
1	A	1030	LEU
1	A	1034	MET
1	A	1051	VAL
1	A	1053	THR
1	A	1057	GLU
1	A	1058	ARG
1	A	1070	VAL
1	A	1246	ARG
1	A	1263	ARG
1	A	1303	ARG
1	A	1332	ARG
1	A	1338	GLU
1	A	1350	ASN
1	A	1364	VAL
1	A	1368	ARG
1	A	1371	LEU
1	A	1376	GLN
2	C	15	GLN
2	C	36	MET
2	C	56	LYS
2	C	80	LYS
2	C	150	LYS
2	C	177	LEU
2	C	178	GLN
3	D	19	VAL
3	D	20	MET
3	D	21	THR
3	D	23	SER
3	D	27	LEU
3	D	40	ARG
3	D	55	ASP
3	D	60	LYS

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Mol	Chain	Res	Type
3	D	73	SER
3	D	79	VAL
3	D	82	ARG
3	D	84	SER
3	D	99	VAL
3	D	103	ASP
3	D	104	VAL
3	D	111	GLN
3	D	112	SER
3	D	113	LEU
3	D	114	GLN
3	D	115	THR
3	D	117	ARG
3	D	118	LEU
3	D	119	THR
3	D	153	SER
3	D	167	LYS
3	D	183	GLU
3	D	186	THR
3	D	191	LYS
3	D	209	GLU
2	E	15	GLN
2	E	36	MET
2	E	56	LYS
2	E	80	LYS
2	E	177	LEU
2	E	178	GLN
3	F	20	MET
3	F	21	THR
3	F	22	GLN
3	F	23	SER
3	F	25	LEU
3	F	26	SER
3	F	27	LEU
3	F	40	ARG
3	F	41	SER
3	F	43	GLN
3	F	54	LEU
3	F	79	VAL
3	F	81	ASP
3	F	82	ARG
3	F	84	SER

Continued on next page...

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Mol	Chain	Res	Type
3	F	111	GLN
3	F	113	LEU
3	F	114	GLN
3	F	115	THR
3	F	117	ARG
3	F	118	LEU
3	F	119	THR
3	F	153	SER
3	F	167	LYS
3	F	182	GLN
3	F	191	LYS
3	F	209	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	555	GLN
1	B	1112	GLN
1	B	1226	HIS
1	B	1350	ASN
1	A	158	GLN
1	A	312	ASN
1	A	340	HIS
1	A	565	GLN
1	A	657	GLN
1	A	856	HIS
1	A	1112	GLN
2	C	5	GLN
3	F	74	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

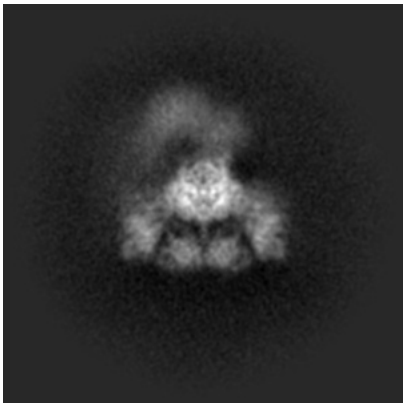
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23713. These allow visual inspection of the internal detail of the map and identification of artifacts.

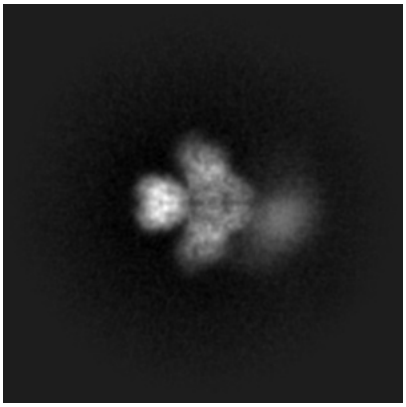
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

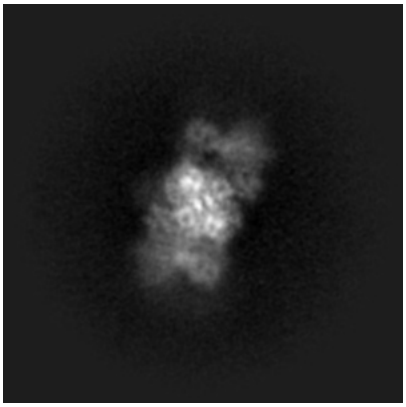
6.1.1 Primary map



X



Y

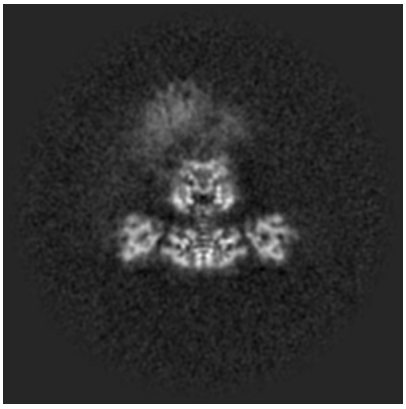


Z

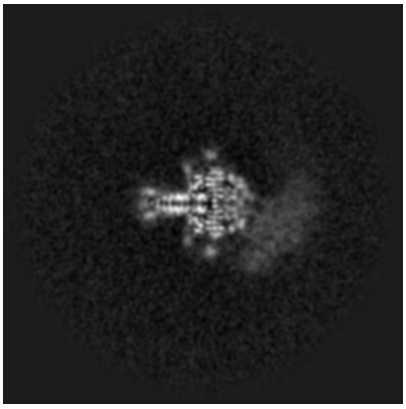
The images above show the map projected in three orthogonal directions.

6.2 Central slices

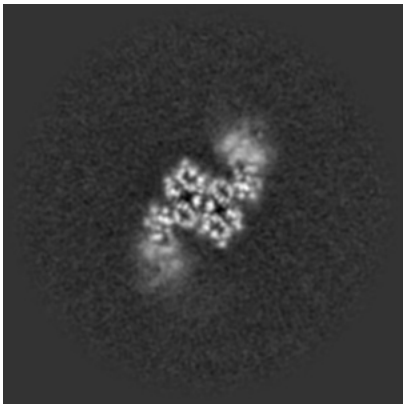
6.2.1 Primary map



X Index: 168



Y Index: 168

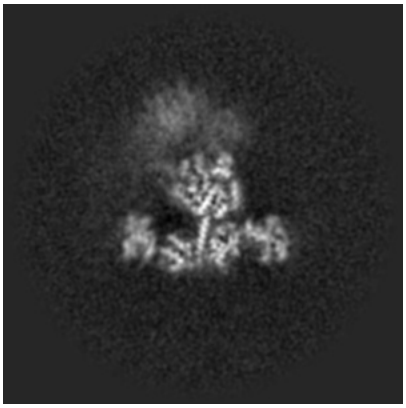


Z Index: 168

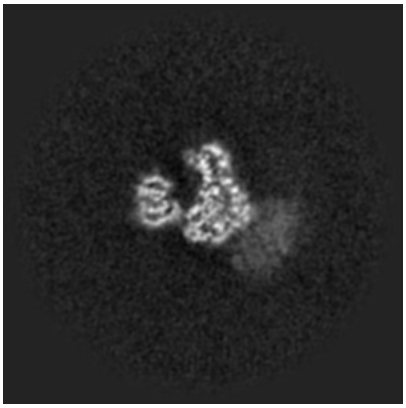
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

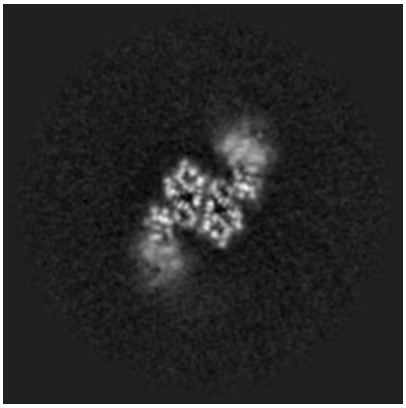
6.3.1 Primary map



X Index: 162



Y Index: 183

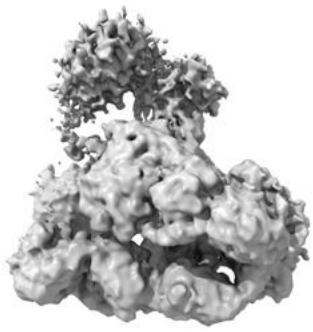


Z Index: 167

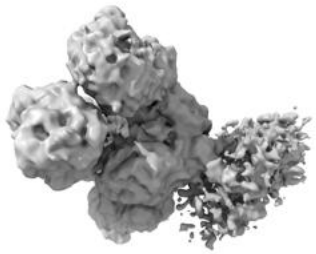
The images above show the largest variance slices of the map in three orthogonal directions.

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

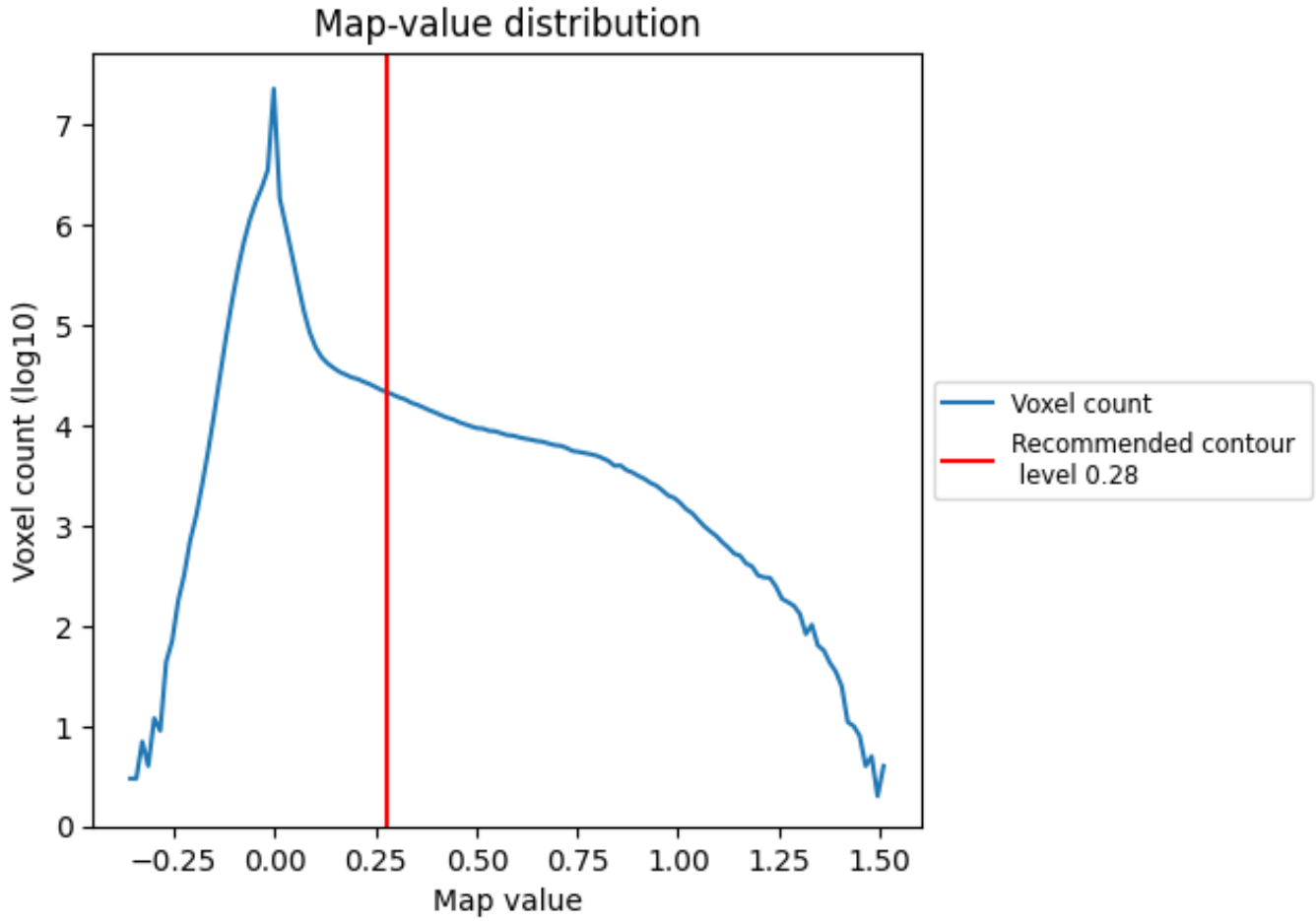
6.5 Mask visualisation (i)

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

7 Map analysis

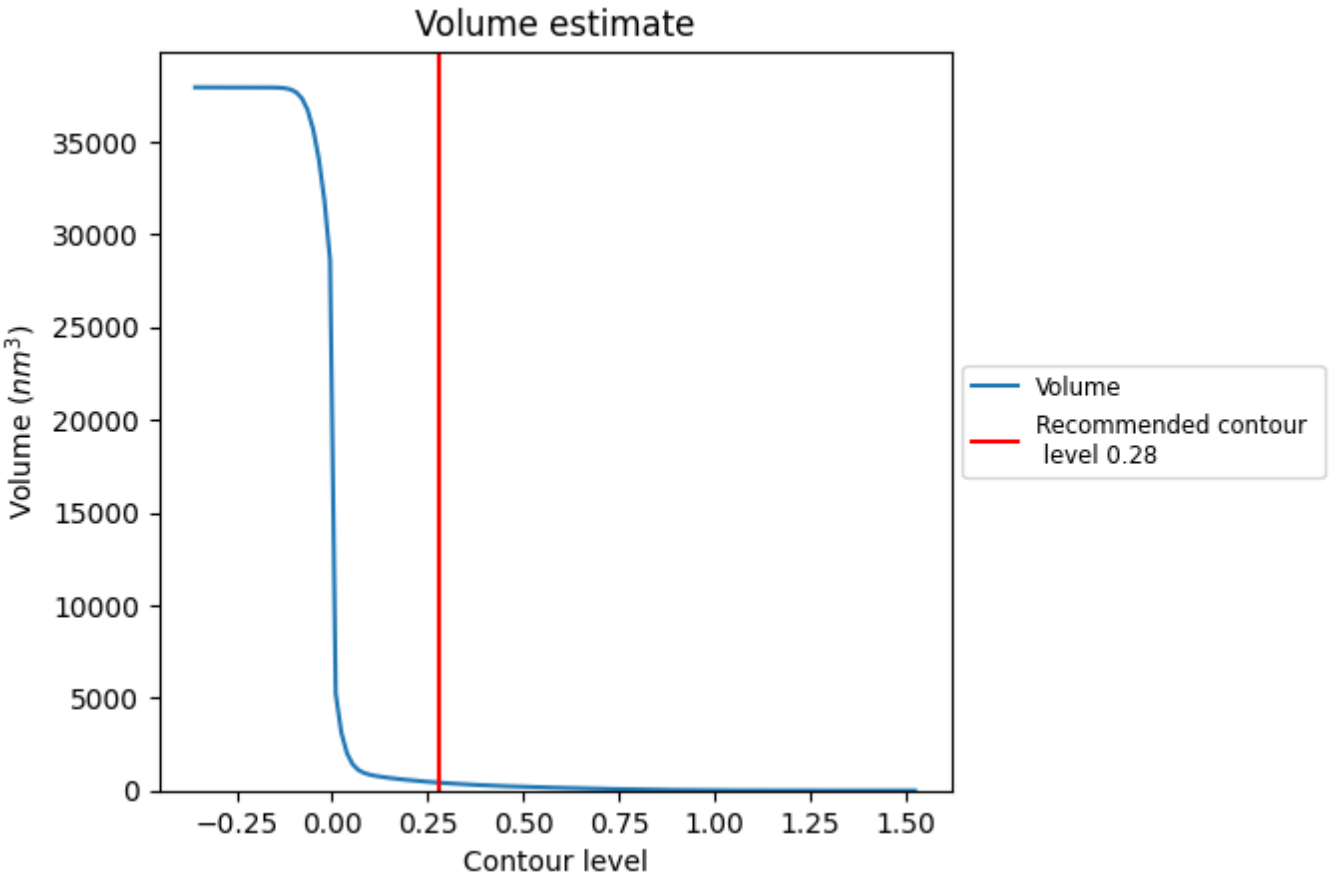
This section contains the results of statistical analysis of the map.

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.

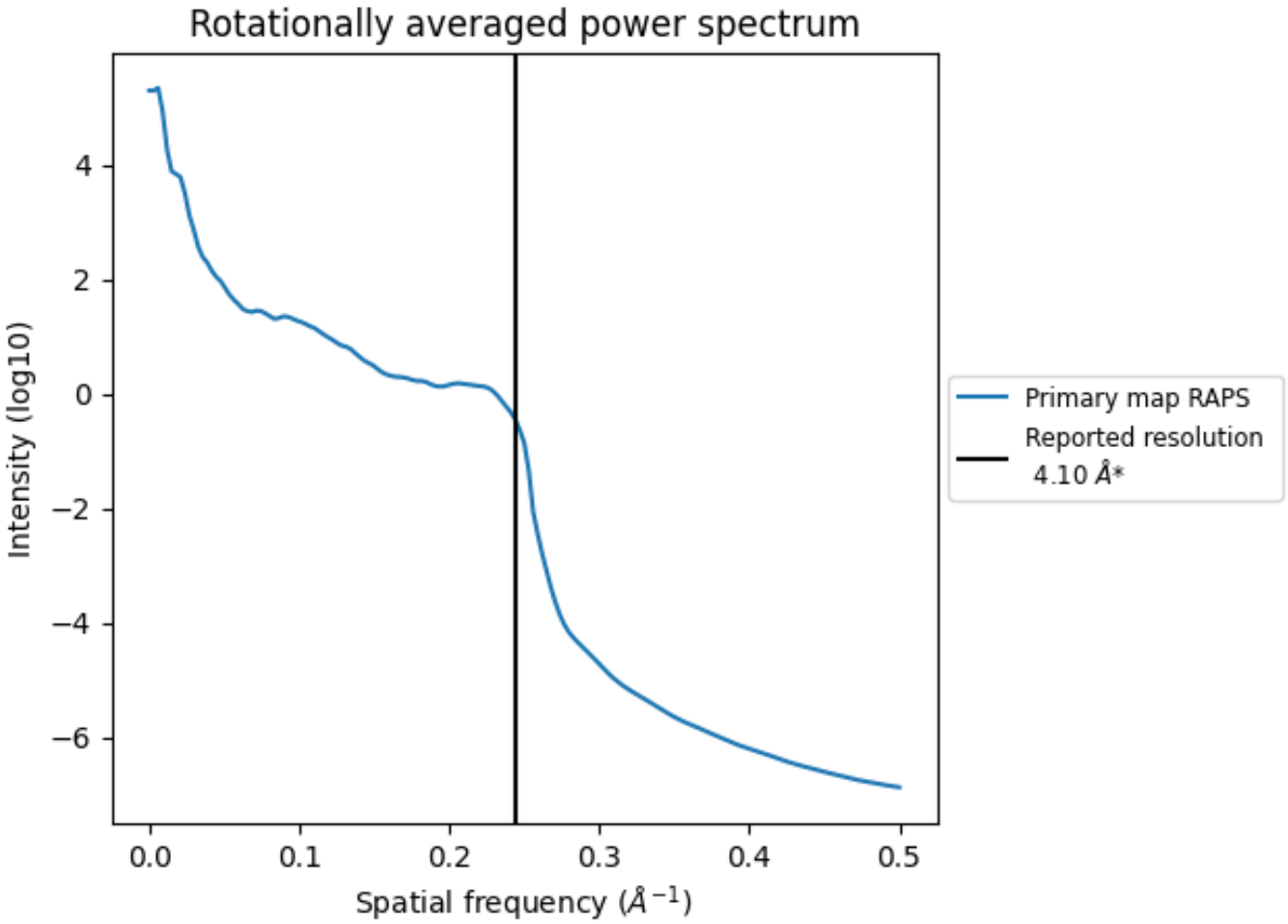
7.2 Volume estimate



The volume at the recommended contour level is 425 nm^3; this corresponds to an approximate mass of 384 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 0.244 Å^{-1}

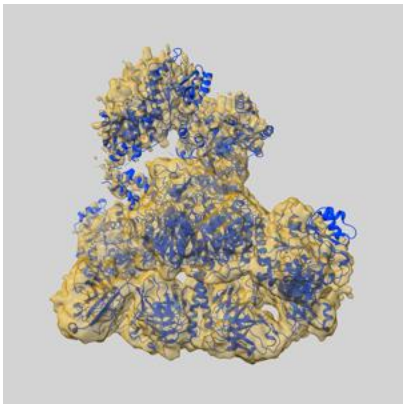
8 Fourier-Shell correlation (i)

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

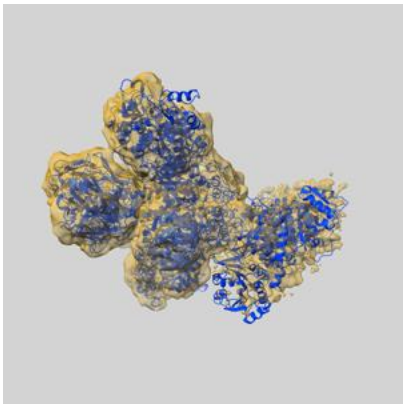
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23713 and PDB model 7M7H. Per-residue inclusion information can be found in section 3 on page 7.

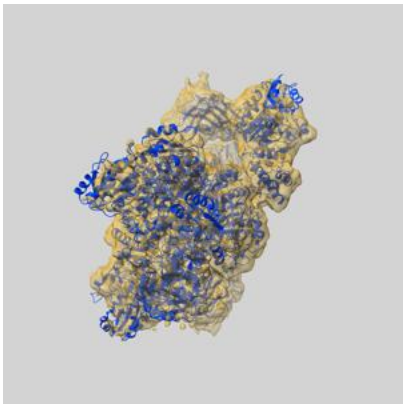
9.1 Map-model overlay



X



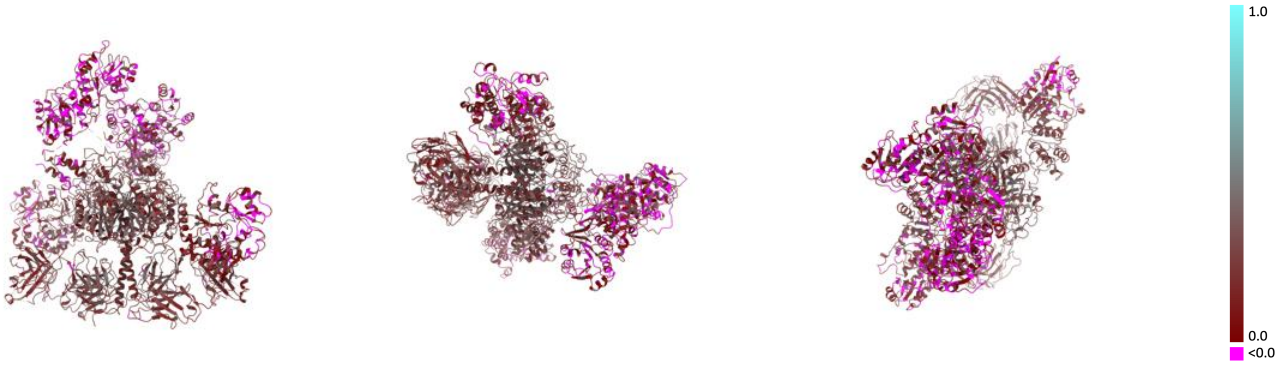
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 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.

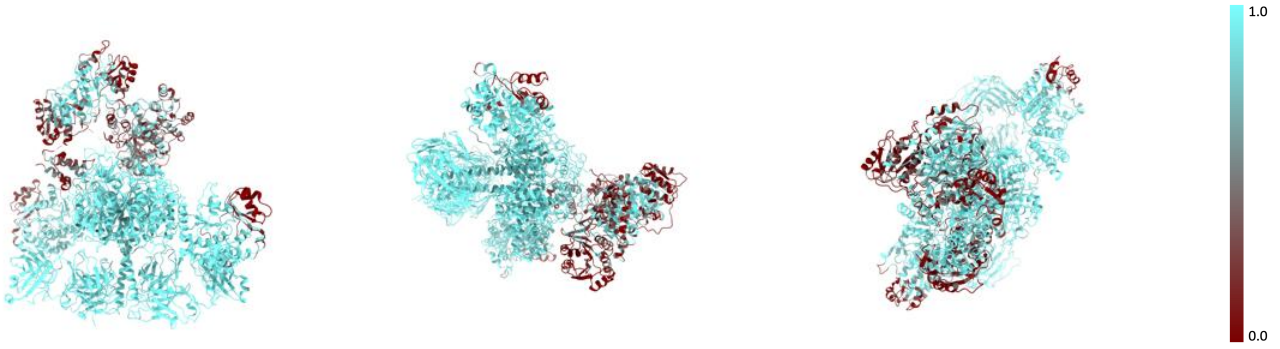
9.2 Q-score mapped to coordinate model (i)



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.

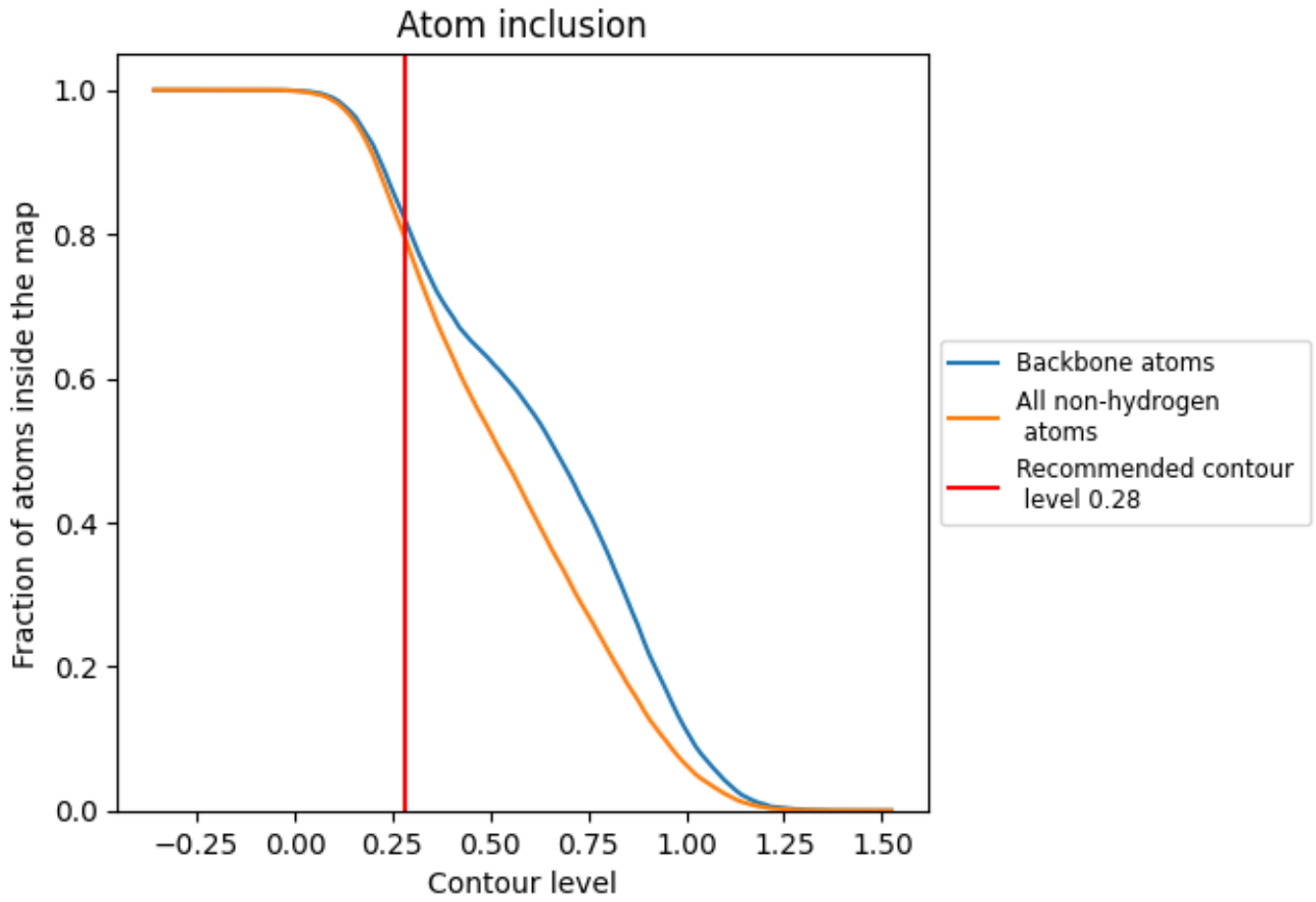
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 82% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7979	0.1900
A	0.7314	0.1780
B	0.7574	0.1670
C	0.9715	0.2360
D	0.9754	0.2620
E	0.9815	0.2410
F	0.9715	0.2610