WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Sep 3, 2023 – 04:23 AM EDT

PDB ID	:	8STA
EMDB ID	:	EMD-40758
Title	:	Isobutyryl-CoA mutase fused in the presence of GMPPCP
Authors	:	Vaccaro, F.A.; Drennan, C.L.
Deposited on	:	2023-05-09
Resolution	:	7.30 Å(reported)
Based on initial model	:	4XC6

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

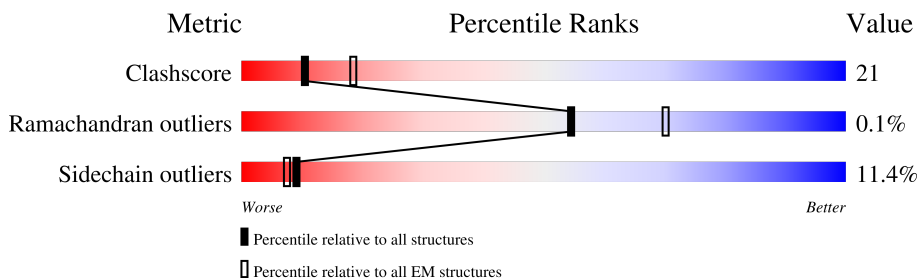|		
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 7.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		21
Ramachandran outliers		0.1%
Sidechain outliers		11.4%

Worse | *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	1113	5% / 51% 39% 5% 5%
1	B	1113	12% / 56% 34% 5% 5%
1	C	1113	27% / 60% 31% · 5%
1	D	1113	10% / 51% 39% 6% 5%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 32458 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 Isobutyryl-CoA mutase fused.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			8116	5061	1469	1549	37		
1	B	1061	Total	C	N	O	S	0	0
			8116	5061	1469	1549	37		
1	C	1061	Total	C	N	O	S	0	0
			8116	5061	1469	1549	37		
1	D	1061	Total	C	N	O	S	0	0
			8110	5059	1468	1546	37		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression tag	UNP Q1LRY0
A	-12	HIS	-	expression tag	UNP Q1LRY0
A	-11	HIS	-	expression tag	UNP Q1LRY0
A	-10	HIS	-	expression tag	UNP Q1LRY0
A	-9	SER	-	expression tag	UNP Q1LRY0
A	-8	SER	-	expression tag	UNP Q1LRY0
A	-7	GLY	-	expression tag	UNP Q1LRY0
A	-6	LEU	-	expression tag	UNP Q1LRY0
A	-5	VAL	-	expression tag	UNP Q1LRY0
A	-4	PRO	-	expression tag	UNP Q1LRY0
A	-3	ARG	-	expression tag	UNP Q1LRY0
A	-2	GLY	-	expression tag	UNP Q1LRY0
A	-1	SER	-	expression tag	UNP Q1LRY0
A	0	HIS	-	expression tag	UNP Q1LRY0
B	-19	MET	-	initiating methionine	UNP Q1LRY0
B	-18	GLY	-	expression tag	UNP Q1LRY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q1LRY0
B	-16	SER	-	expression tag	UNP Q1LRY0
B	-15	HIS	-	expression tag	UNP Q1LRY0
B	-14	HIS	-	expression tag	UNP Q1LRY0
B	-13	HIS	-	expression tag	UNP Q1LRY0
B	-12	HIS	-	expression tag	UNP Q1LRY0
B	-11	HIS	-	expression tag	UNP Q1LRY0
B	-10	HIS	-	expression tag	UNP Q1LRY0
B	-9	SER	-	expression tag	UNP Q1LRY0
B	-8	SER	-	expression tag	UNP Q1LRY0
B	-7	GLY	-	expression tag	UNP Q1LRY0
B	-6	LEU	-	expression tag	UNP Q1LRY0
B	-5	VAL	-	expression tag	UNP Q1LRY0
B	-4	PRO	-	expression tag	UNP Q1LRY0
B	-3	ARG	-	expression tag	UNP Q1LRY0
B	-2	GLY	-	expression tag	UNP Q1LRY0
B	-1	SER	-	expression tag	UNP Q1LRY0
B	0	HIS	-	expression tag	UNP Q1LRY0
C	-19	MET	-	initiating methionine	UNP Q1LRY0
C	-18	GLY	-	expression tag	UNP Q1LRY0
C	-17	SER	-	expression tag	UNP Q1LRY0
C	-16	SER	-	expression tag	UNP Q1LRY0
C	-15	HIS	-	expression tag	UNP Q1LRY0
C	-14	HIS	-	expression tag	UNP Q1LRY0
C	-13	HIS	-	expression tag	UNP Q1LRY0
C	-12	HIS	-	expression tag	UNP Q1LRY0
C	-11	HIS	-	expression tag	UNP Q1LRY0
C	-10	HIS	-	expression tag	UNP Q1LRY0
C	-9	SER	-	expression tag	UNP Q1LRY0
C	-8	SER	-	expression tag	UNP Q1LRY0
C	-7	GLY	-	expression tag	UNP Q1LRY0
C	-6	LEU	-	expression tag	UNP Q1LRY0
C	-5	VAL	-	expression tag	UNP Q1LRY0
C	-4	PRO	-	expression tag	UNP Q1LRY0
C	-3	ARG	-	expression tag	UNP Q1LRY0
C	-2	GLY	-	expression tag	UNP Q1LRY0
C	-1	SER	-	expression tag	UNP Q1LRY0
C	0	HIS	-	expression tag	UNP Q1LRY0
D	-19	MET	-	initiating methionine	UNP Q1LRY0
D	-18	GLY	-	expression tag	UNP Q1LRY0
D	-17	SER	-	expression tag	UNP Q1LRY0
D	-16	SER	-	expression tag	UNP Q1LRY0

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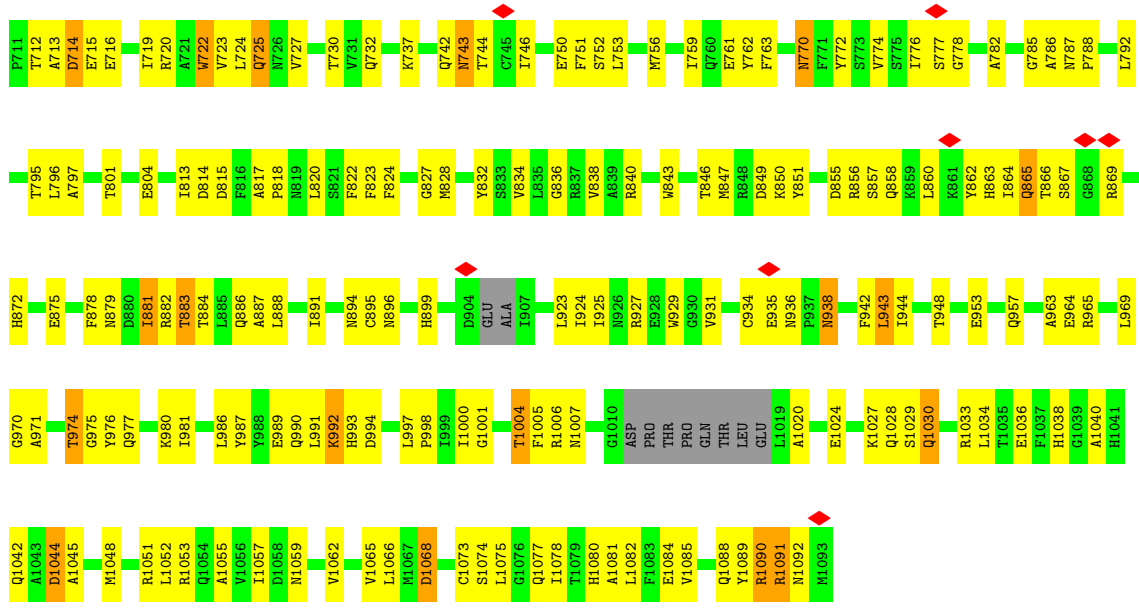
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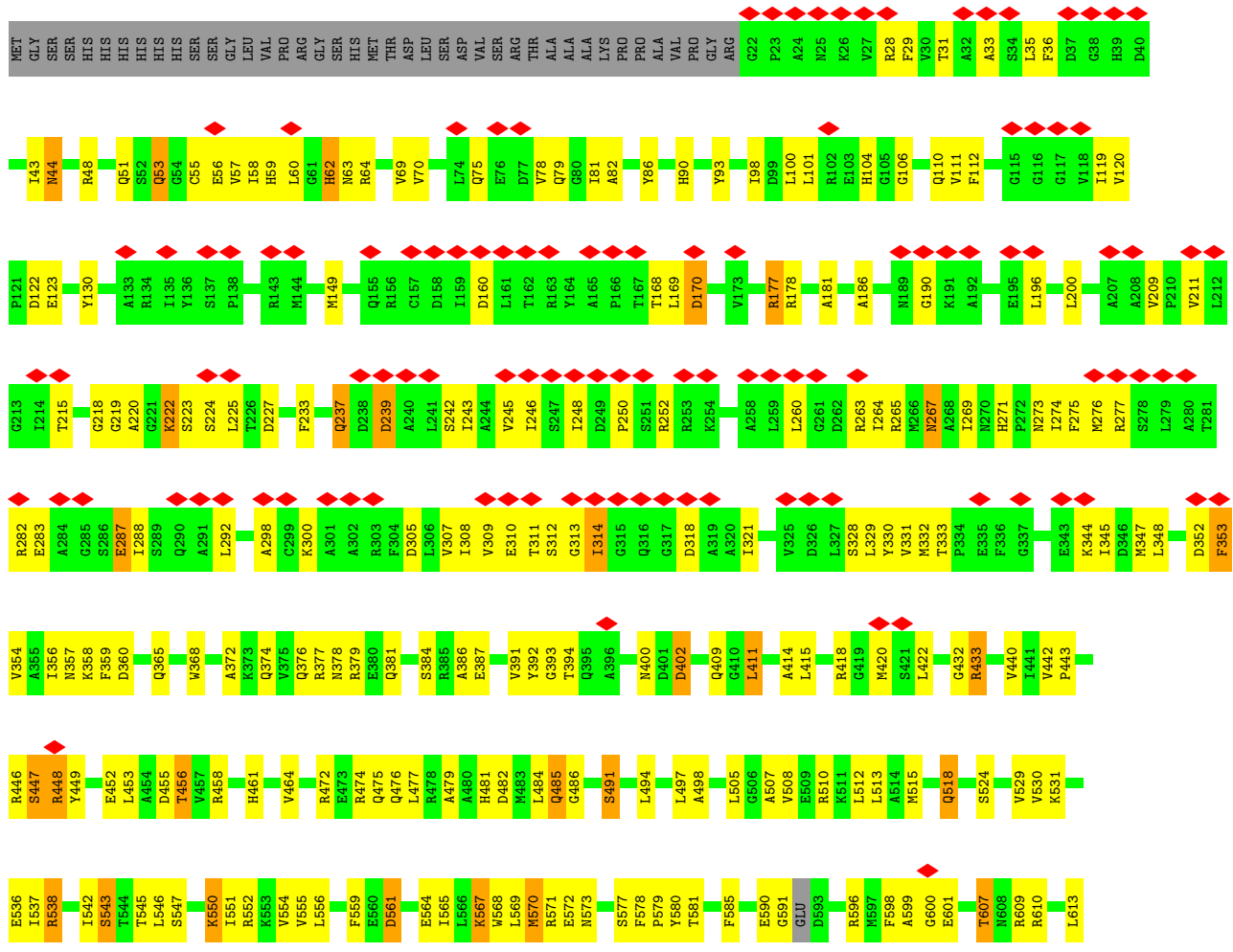| Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP Q1LRY0
D	-14	HIS	-	expression tag	UNP Q1LRY0
D	-13	HIS	-	expression tag	UNP Q1LRY0
D	-12	HIS	-	expression tag	UNP Q1LRY0
D	-11	HIS	-	expression tag	UNP Q1LRY0
D	-10	HIS	-	expression tag	UNP Q1LRY0
D	-9	SER	-	expression tag	UNP Q1LRY0
D	-8	SER	-	expression tag	UNP Q1LRY0
D	-7	GLY	-	expression tag	UNP Q1LRY0
D	-6	LEU	-	expression tag	UNP Q1LRY0
D	-5	VAL	-	expression tag	UNP Q1LRY0
D	-4	PRO	-	expression tag	UNP Q1LRY0
D	-3	ARG	-	expression tag	UNP Q1LRY0
D	-2	GLY	-	expression tag	UNP Q1LRY0
D	-1	SER	-	expression tag	UNP Q1LRY0
D	0	HIS	-	expression tag	UNP Q1LRY0

3   Residue-property plots ⓘ

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.
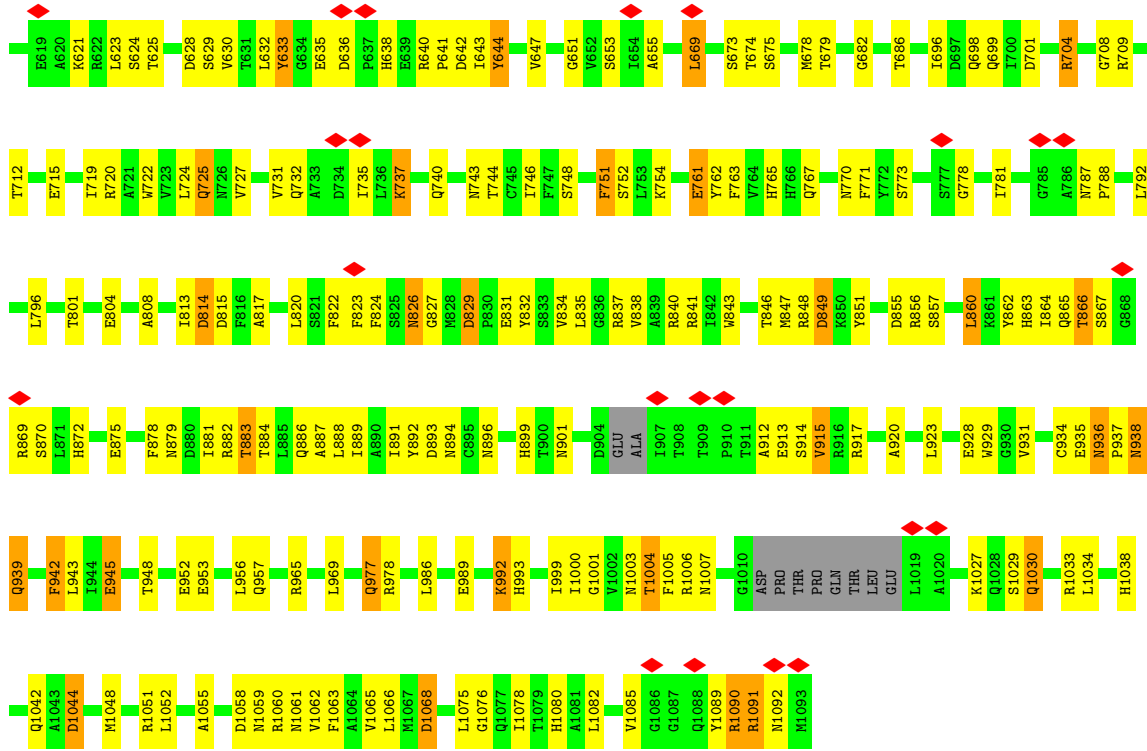
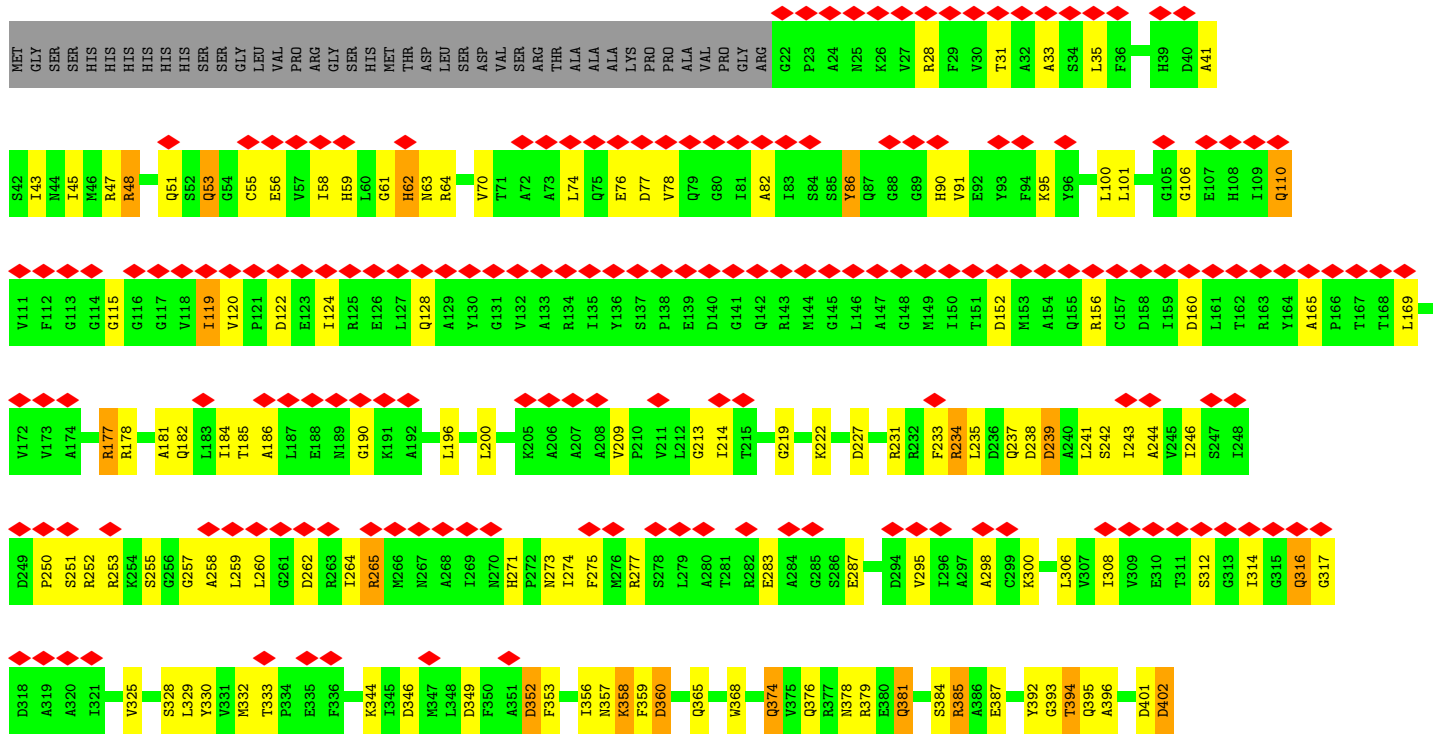• Molecule 1: Isobutyryl-CoA mutase fused

P711 T712 A713 D714 E715 E716 I719 R720 A721 W722 V723 L724 Q725 N726 V727 T730 T731 Q732 K737 Q742 N743 T744 C745 I746 E750 F751 S752 L753 M756 I759 Q760 E761 Y762 F763 N770 F771 Y772 S773 V774 S775 I776 S777 G778 A782 G785 A786 N787 P788 L792

T795 L796 A797 T801 E804 I813 D814 D815 F816 A817 P818 N819 L820 S821 F822 F823 F824 G827 M828 Y832 S833 V834 L835 G836 H837 V838 A839 R840 W843 T846 M847 H848 K850 Y851 D855 R856 S857 Q858 K859 L860 K861 Y862 H863 I864 Q865 T866 S867 G868 R869

H872 E875 F878 N879 D880 I881 R882 T883 T884 L885 Q886 A887 L888 I891 N894 C895 N896 H899 D904 GLU ALA I907 L923 I924 I925 N926 R927 E928 W929 G930 V931 C934 E935 N936 P937 N938 F942 L943 I944 T948 E953 Q957 A963 E964 R965 L969

G970 A971 T974 G975 Y976 Q977 K980 I981 L986 Y987 V988 E989 Q990 L991 K992 H993 D994 L997 P998 I999 I1000 G1001 T1004 F1005 R1006 N1007 G1010 ASP PRO THR PRO GLN THR LEU GLU L1019 A1020 E1024 K1027 Q1028 S1029 Q1030 R1033 L1034 T1035 E1036 F1037 H1038 G1039 A1040 H1041

Q1042 A1043 D1044 A1045 M1048 R1051 L1052 R1053 Q1054 A1055 V1056 I1057 D1058 N1059 V1062 V1065 L1066 M1067 D1068 C1073 S1074 L1075 G1076 Q1077 I1078 T1079 H1080 A1081 L1082 F1083 E1084 V1085 Q1088 Y1089 R1090 R1091 N1092 M1093

• Molecule 1: Isobutyryl-CoA mutase fused

Chain B:

12%
56%　　　34%　　　5% 5%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR ASP LEU SER ASP VAL SER ARG THR ALA ALA ALA LYS PRO PRO ALA VAL PRO GLY ARG G22 P23 A24 N25 K26 V27 R28 F29 V30 T31 A32 A33 S34 L35 F36 D37 G38 H39 D40

I43 N44 R48 Q51 S52 Q53 G54 C55 E56 V57 I58 H59 L60 G61 H62 N63 R64 V69 V70 L74 Q75 E76 D77 V78 Q79 G80 I81 A82 Y86 H90 Y93 I98 D99 L100 L101 R102 E103 H104 G105 G106 Q110 V111 F112 G115 G116 G117 V118 I119 V120

P121 D122 E123 Y130 A133 R134 I135 Y136 S137 P138 R143 M144 M149 Q155 R156 C157 D158 I159 D160 L161 T162 R163 Y164 A165 P166 T167 T168 L169 D170 V173 R177 R178 A181 A186 N189 G190 K191 A192 E195 L196 L200 A207 A208 V209 P210 V211 L212

G213 I214 T215 G218 G219 A220 G221 K222 S223 S224 L225 T226 D227 F233 Q237 D238 D239 A240 L241 S242 I243 A244 V245 I246 S247 I248 D249 P250 S251 R252 R253 K254 A258 L259 L260 G261 D262 R263 I264 R265 M266 N267 A268 I269 N270 H271 P272 N273 I274 F275 M276 R277 S278 L279 A280 T281

R282 E283 A284 G285 S286 E287 I288 S289 Q290 A291 L292 A298 C299 K300 A301 A302 R303 F304 D305 L306 V307 I308 V309 E310 T311 S312 G313 I314 Q315 Q316 G317 D318 A319 A320 I321 V325 D326 L327 S328 L329 Y330 V331 M332 T333 P334 E335 F336 G337 E343 K344 I345 D346 M347 L348 D352 F353

V354 A355 I356 N357 K358 F359 D360 Q365 W368 A372 K373 Q374 V375 Q376 R377 N378 R379 E380 Q381 S384 R385 A386 E387 V391 Y392 G393 T394 Q395 A396 N400 D401 D402 Q409 G410 L411 A414 L415 R418 G419 M420 S421 L422 G432 R433 V440 I441 V442 P443

R446 S447 R448 Y449 E452 L453 A454 D455 T456 V457 R458 H461 V464 R472 E473 R474 Q475 Q476 L477 D478 A479 A480 H481 D482 M483 L484 G486 S491 L494 L497 A498 L505 G506 A507 V508 E509 R510 K511 L512 L513 A514 M515 Q518 S524 V529 V530 K531

E536 I537 R538 I542 S543 T544 T545 L546 S547 K550 I551 R552 K553 V554 V555 L556 F559 E560 D561 E564 I565 L566 K567 W568 L569 M570 R571 E572 N573 S577 F578 Y580 P579 T581 F585 E590 G591 GLU D593 R596 M597 F598 A599 G600 E601 T607 N608 R609 R610 L613

• Molecule 1: Isobutyryl-CoA mutase fused

Chain C:

• Molecule 1: Isobutyryl-CoA mutase fused

Chain D:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	42.81	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	11.211	Depositor
Minimum map value	0.000	Depositor
Average map value	0.273	Depositor
Map value standard deviation	0.956	Depositor
Recommended contour level	2.36	Depositor
Map size (Å)	257.8304, 257.8304, 257.8304	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0143, 2.0143, 2.0143	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.27	0/8254	0.49	0/11168
1	B	0.26	0/8254	0.49	0/11168
1	C	0.25	0/8254	0.49	0/11168
1	D	0.28	0/8248	0.52	0/11160
All	All	0.27	0/33010	0.50	0/44664

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8116	0	7885	388	0
1	B	8116	0	7885	315	0
1	C	8116	0	7885	297	0
1	D	8110	0	7879	414	0
All	All	32458	0	31534	1353	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 21.

All (1353) 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:C:796:LEU:HD12	1:C:800:PHE:CZ	1.44	1.51
1:C:796:LEU:HD12	1:C:800:PHE:CE1	1.57	1.39
1:B:344:LYS:NZ	1:C:258:ALA:HB1	1.38	1.38
1:A:441:ILE:HD11	1:A:750:GLU:CB	1.53	1.38
1:D:442:VAL:HG22	1:D:443:PRO:CD	1.57	1.31
1:D:800:PHE:HZ	1:D:843:TRP:CE3	1.47	1.31
1:D:442:VAL:CG2	1:D:443:PRO:HD2	1.60	1.31
1:D:800:PHE:CZ	1:D:843:TRP:CZ3	2.20	1.30
1:D:800:PHE:CZ	1:D:843:TRP:CE3	2.32	1.17
1:A:442:VAL:HG22	1:A:443:PRO:CD	1.75	1.16
1:A:441:ILE:HD11	1:A:750:GLU:CA	1.73	1.15
1:C:796:LEU:HG	1:C:959:PHE:HZ	1.11	1.15
1:A:442:VAL:HG22	1:A:443:PRO:HD2	1.22	1.11
1:A:445:ALA:HA	1:D:448:ARG:NH1	1.66	1.11
1:C:796:LEU:CD1	1:C:800:PHE:CZ	2.35	1.09
1:A:441:ILE:HG21	1:A:969:LEU:HD21	1.34	1.08
1:B:443:PRO:HG2	1:B:446:ARG:HE	1.09	1.08
1:C:796:LEU:HG	1:C:959:PHE:CZ	1.88	1.07
1:D:798:ASN:O	1:D:801:THR:HG22	1.54	1.07
1:A:441:ILE:HD11	1:A:750:GLU:HB3	1.35	1.06
1:D:797:ALA:HB2	1:D:959:PHE:HE1	1.20	1.05
1:C:796:LEU:CD1	1:C:800:PHE:CE1	2.40	1.05
1:D:800:PHE:HZ	1:D:843:TRP:CZ3	1.67	1.04
1:C:796:LEU:CG	1:C:959:PHE:HZ	1.70	1.04
1:A:441:ILE:HD11	1:A:750:GLU:HA	1.41	1.00
1:B:344:LYS:HZ3	1:C:258:ALA:HB1	1.19	0.99
1:D:449:TYR:OH	1:D:801:THR:HB	1.61	0.99
1:A:441:ILE:CD1	1:A:750:GLU:CB	2.44	0.96
1:D:800:PHE:CZ	1:D:843:TRP:HZ3	1.84	0.95
1:A:446:ARG:HA	1:A:446:ARG:NH1	1.83	0.93
1:D:792:LEU:HD23	1:D:835:LEU:HD21	1.46	0.93
1:B:447:SER:O	1:B:449:TYR:HD1	1.50	0.93
1:B:440:VAL:HG13	1:B:440:VAL:O	1.67	0.93
1:A:441:ILE:CD1	1:A:750:GLU:HA	1.99	0.92
1:D:603:ASP:OD2	1:D:605:PHE:HB2	1.69	0.92
1:D:797:ALA:HB2	1:D:959:PHE:CE1	2.05	0.91
1:A:441:ILE:CD1	1:A:750:GLU:HB3	1.99	0.91
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.34	0.90
1:A:445:ALA:HA	1:D:448:ARG:HH12	1.36	0.90
1:C:801:THR:HG21	1:C:968:VAL:HG21	1.54	0.90
1:B:443:PRO:HG2	1:B:446:ARG:NE	1.88	0.89
1:D:555:VAL:H	1:D:936:ASN:HD21	1.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:787:ASN:CB	1:D:789:ILE:CD1	2.52	0.87
1:B:447:SER:O	1:B:449:TYR:CD1	2.26	0.87
1:C:801:THR:CG2	1:C:968:VAL:HG21	2.06	0.85
1:D:630:VAL:HG13	1:D:635:GLU:HB2	1.59	0.85
1:C:449:TYR:OH	1:C:801:THR:CG2	2.25	0.84
1:A:242:SER:HB2	1:A:305:ASP:H	1.43	0.83
1:D:444:PRO:O	1:D:447:SER:HB3	1.79	0.82
1:B:344:LYS:HZ2	1:C:258:ALA:HB1	1.41	0.82
1:C:449:TYR:HE2	1:C:800:PHE:CB	1.93	0.81
1:C:449:TYR:OH	1:C:801:THR:HG23	1.80	0.81
1:A:35:LEU:HA	1:A:63:ASN:HA	1.63	0.81
1:D:603:ASP:OD2	1:D:605:PHE:CB	2.29	0.81
1:D:792:LEU:CD2	1:D:835:LEU:HD11	2.12	0.80
1:D:35:LEU:HA	1:D:63:ASN:HA	1.64	0.80
1:D:61:GLY:HA3	1:D:1091:ARG:HE	1.46	0.80
1:A:476:GLN:HG3	1:B:476:GLN:HG3	1.63	0.79
1:A:543:SER:HB2	1:A:551:ILE:HB	1.62	0.79
1:A:441:ILE:CG1	1:A:750:GLU:HB3	2.13	0.78
1:A:477:LEU:HD11	1:A:497:LEU:HB3	1.64	0.78
1:A:402:ASP:OD1	1:A:402:ASP:N	2.17	0.78
1:A:441:ILE:CG2	1:A:969:LEU:HD21	2.13	0.78
1:B:242:SER:HB2	1:B:305:ASP:H	1.46	0.78
1:B:250:PRO:HD3	1:B:312:SER:HB2	1.65	0.77
1:D:792:LEU:HD21	1:D:835:LEU:HD11	1.64	0.77
1:A:445:ALA:CA	1:D:448:ARG:NH1	2.46	0.77
1:B:446:ARG:HD3	1:B:804:GLU:HB2	1.66	0.77
1:D:636:ASP:HB2	1:D:1076:GLY:HA3	1.64	0.77
1:A:442:VAL:CG2	1:A:443:PRO:CD	2.60	0.77
1:C:251:SER:HA	1:C:258:ALA:HB2	1.64	0.77
1:B:817:ALA:HB3	1:B:857:SER:HB3	1.66	0.77
1:A:446:ARG:HA	1:A:446:ARG:CZ	2.15	0.76
1:A:61:GLY:HA3	1:A:1091:ARG:HE	1.50	0.75
1:B:35:LEU:HA	1:B:63:ASN:HA	1.67	0.75
1:C:449:TYR:CE2	1:C:800:PHE:CB	2.69	0.75
1:D:366:ASP:OD1	1:D:366:ASP:N	2.18	0.74
1:B:477:LEU:HD11	1:B:497:LEU:HB3	1.69	0.74
1:C:329:LEU:HD23	1:C:353:PHE:HB3	1.70	0.74
1:C:794:PHE:O	1:C:797:ALA:HB3	1.88	0.74
1:D:629:SER:HB2	1:D:633:TYR:CE2	2.22	0.74
1:D:991:LEU:HB3	1:D:997:LEU:HB2	1.70	0.74
1:A:564:GLU:O	1:A:567:LYS:NZ	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:VAL:O	1:B:440:VAL:CG1	2.36	0.73
1:C:597:MET:HB2	1:C:623:LEU:HA	1.70	0.73
1:C:633:TYR:HB3	1:C:635:GLU:HG2	1.71	0.73
1:D:200:LEU:HD11	1:D:298:ALA:HA	1.71	0.73
1:A:442:VAL:HG22	1:A:443:PRO:HD3	1.68	0.73
1:C:991:LEU:HB3	1:C:997:LEU:HB2	1.71	0.73
1:A:1090:ARG:O	1:A:1092:ASN:ND2	2.21	0.73
1:D:398:ARG:HH22	1:D:441:ILE:HG12	1.54	0.73
1:A:441:ILE:HD11	1:A:750:GLU:HB2	1.64	0.73
1:B:448:ARG:NH1	1:C:444:PRO:O	2.21	0.73
1:C:837:ARG:HH11	1:C:938:ASN:HD22	1.36	0.72
1:D:792:LEU:CD2	1:D:835:LEU:HD21	2.18	0.72
1:C:796:LEU:CB	1:C:959:PHE:HZ	2.01	0.72
1:C:699:GLN:HE21	1:C:719:ILE:HG13	1.54	0.72
1:D:720:ARG:HH12	1:D:724:LEU:HG	1.54	0.72
1:A:218:GLY:HA2	1:A:222:LYS:HZ3	1.52	0.72
1:A:598:PHE:HA	1:A:624:SER:HB2	1.70	0.72
1:A:398:ARG:NH2	1:A:441:ILE:H	1.87	0.72
1:C:449:TYR:HE2	1:C:800:PHE:HB2	1.54	0.72
1:A:633:TYR:HB3	1:A:635:GLU:HG2	1.70	0.72
1:C:824:PHE:N	1:C:863:HIS:O	2.23	0.72
1:D:794:PHE:HZ	1:D:980:LYS:HE2	1.55	0.72
1:A:746:ILE:O	1:A:1089:TYR:N	2.23	0.71
1:B:555:VAL:H	1:B:936:ASN:HD21	1.36	0.71
1:B:581:THR:O	1:B:840:ARG:NH2	2.23	0.71
1:B:621:LYS:HB2	1:B:674:THR:HA	1.72	0.71
1:C:449:TYR:CE2	1:C:800:PHE:HB2	2.25	0.71
1:D:263:ARG:HH12	1:D:269:ILE:HG21	1.54	0.71
1:D:441:ILE:N	1:D:441:ILE:HD13	2.05	0.71
1:A:365:GLN:HB3	1:D:965:ARG:HH22	1.55	0.71
1:A:824:PHE:N	1:A:863:HIS:O	2.23	0.71
1:D:62:HIS:O	1:D:1091:ARG:NH2	2.24	0.71
1:C:450:LEU:HB2	1:C:963:ALA:HB2	1.72	0.71
1:B:344:LYS:HZ1	1:C:258:ALA:HB1	1.52	0.70
1:C:796:LEU:HD12	1:C:800:PHE:HZ	1.43	0.70
1:D:444:PRO:O	1:D:447:SER:CB	2.40	0.70
1:A:62:HIS:O	1:A:1091:ARG:NH2	2.24	0.70
1:A:872:HIS:O	1:A:879:ASN:ND2	2.24	0.70
1:A:398:ARG:HH22	1:A:441:ILE:HG12	1.56	0.70
1:B:365:GLN:HB3	1:C:965:ARG:HH22	1.57	0.70
1:D:863:HIS:HA	1:D:897:SER:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ILE:HG22	1:C:277:ARG:HB3	1.73	0.69
1:D:637:PRO:HG2	1:D:1034:LEU:HD22	1.74	0.69
1:D:543:SER:HB2	1:D:551:ILE:HB	1.75	0.69
1:B:53:GLN:NE2	1:B:55:CYS:SG	2.66	0.69
1:B:376:GLN:NE2	1:B:381:GLN:O	2.25	0.69
1:B:1006:ARG:NH1	1:B:1007:ASN:OD1	2.25	0.69
1:D:629:SER:HB2	1:D:633:TYR:HE2	1.56	0.69
1:C:449:TYR:OH	1:C:801:THR:HG22	1.93	0.69
1:D:570:MET:SD	1:D:570:MET:N	2.66	0.69
1:B:104:HIS:HB3	1:B:178:ARG:HH22	1.58	0.68
1:A:686:THR:HG21	1:A:1075:LEU:HD13	1.75	0.68
1:A:505:LEU:O	1:A:510:ARG:NH2	2.26	0.68
1:C:61:GLY:HA3	1:C:1091:ARG:HE	1.58	0.68
1:D:628:ASP:OD1	1:D:628:ASP:N	2.18	0.68
1:D:785:GLY:HA2	1:D:869:ARG:HD3	1.74	0.68
1:A:630:VAL:HG13	1:A:635:GLU:HB2	1.76	0.68
1:D:402:ASP:OD1	1:D:402:ASP:N	2.25	0.68
1:D:709:ARG:NH2	1:D:715:GLU:OE2	2.27	0.68
1:D:787:ASN:CB	1:D:789:ILE:HD13	2.24	0.68
1:D:1049:LEU:HA	1:D:1052:LEU:HD23	1.76	0.68
1:A:234:ARG:HH21	1:A:271:HIS:HB2	1.59	0.67
1:B:505:LEU:O	1:B:510:ARG:NH2	2.27	0.67
1:B:344:LYS:NZ	1:C:258:ALA:CB	2.35	0.67
1:C:446:ARG:NH2	1:C:452:GLU:OE1	2.26	0.67
1:D:789:ILE:HD12	1:D:789:ILE:H	1.59	0.67
1:A:709:ARG:NH2	1:A:715:GLU:OE2	2.27	0.67
1:B:62:HIS:O	1:B:1091:ARG:NH2	2.27	0.67
1:A:177:ARG:HA	1:A:180:LEU:HB2	1.75	0.67
1:D:903:TYR:H	1:D:910:PRO:HB3	1.59	0.67
1:C:796:LEU:CG	1:C:959:PHE:CZ	2.60	0.67
1:A:443:PRO:HB2	1:A:446:ARG:HB2	1.75	0.67
1:A:264:ILE:HG23	1:A:265:ARG:HD3	1.77	0.67
1:A:445:ALA:O	1:D:448:ARG:NH1	2.28	0.67
1:A:862:TYR:O	1:A:896:ASN:ND2	2.26	0.66
1:C:379:ARG:O	1:C:381:GLN:NE2	2.28	0.66
1:A:463:ARG:NH1	1:A:509:GLU:OE2	2.26	0.66
1:B:209:VAL:HG22	1:B:300:LYS:HG2	1.77	0.66
1:B:252:ARG:HH21	1:C:349:ASP:HB2	1.59	0.66
1:A:376:GLN:NE2	1:A:384:SER:O	2.28	0.66
1:A:445:ALA:HA	1:D:448:ARG:HH11	1.58	0.66
1:C:801:THR:HG21	1:C:968:VAL:CG2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ALA:CA	1:D:448:ARG:HH12	2.06	0.66
1:B:543:SER:O	1:B:551:ILE:N	2.22	0.66
1:B:838:VAL:HG22	1:B:948:THR:HG23	1.77	0.66
1:A:570:MET:SD	1:A:570:MET:N	2.68	0.66
1:D:529:VAL:HA	1:D:538:ARG:HA	1.77	0.66
1:A:458:ARG:HH12	1:A:462:ARG:HH11	1.42	0.66
1:D:1058:ASP:O	1:D:1060:ARG:NH1	2.29	0.66
1:C:169:LEU:HD21	1:C:196:LEU:HD11	1.78	0.66
1:C:543:SER:HB2	1:C:551:ILE:HB	1.77	0.66
1:D:747:PHE:HB3	1:D:751:PHE:HE1	1.60	0.66
1:C:356:ILE:HB	1:C:393:GLY:HA2	1.77	0.65
1:D:330:TYR:HB3	1:D:354:VAL:HG22	1.78	0.65
1:D:746:ILE:O	1:D:1089:TYR:N	2.28	0.65
1:C:450:LEU:CD2	1:C:800:PHE:CD2	2.79	0.65
1:D:213:GLY:O	1:D:329:LEU:N	2.29	0.65
1:D:242:SER:OG	1:D:273:ASN:ND2	2.30	0.65
1:D:356:ILE:HB	1:D:393:GLY:HA2	1.77	0.65
1:D:1036:GLU:O	1:D:1040:ALA:N	2.29	0.65
1:A:186:ALA:O	1:A:190:GLY:N	2.29	0.65
1:A:372:ALA:HB1	1:A:386:ALA:HB1	1.79	0.65
1:B:1058:ASP:O	1:B:1060:ARG:NH1	2.30	0.65
1:D:1001:GLY:O	1:D:1006:ARG:NH2	2.30	0.65
1:A:555:VAL:H	1:A:936:ASN:HD21	1.44	0.65
1:B:329:LEU:HD23	1:B:353:PHE:HB3	1.79	0.65
1:B:647:VAL:O	1:B:1027:LYS:NZ	2.29	0.65
1:C:647:VAL:O	1:C:1027:LYS:NZ	2.30	0.65
1:B:378:ASN:OD1	1:C:48:ARG:NH2	2.30	0.65
1:B:554:VAL:HG22	1:B:935:GLU:HB2	1.78	0.65
1:C:328:SER:HB3	1:C:352:ASP:H	1.62	0.65
1:A:545:THR:HG22	1:A:549:THR:H	1.63	0.64
1:A:1024:GLU:OE2	1:A:1028:GLN:NE2	2.30	0.64
1:B:344:LYS:HZ3	1:C:258:ALA:CB	2.02	0.64
1:A:378:ASN:OD1	1:D:48:ARG:NH2	2.30	0.64
1:A:649:ASN:ND2	1:A:1020:ALA:O	2.30	0.64
1:C:449:TYR:CE2	1:C:800:PHE:HB3	2.31	0.64
1:D:305:ASP:N	1:D:305:ASP:OD1	2.29	0.64
1:B:33:ALA:HB3	1:B:62:HIS:HA	1.78	0.64
1:D:31:THR:HG22	1:D:82:ALA:HB3	1.78	0.64
1:A:263:ARG:HD2	1:A:276:MET:HG3	1.80	0.64
1:B:264:ILE:HG23	1:B:265:ARG:HD3	1.78	0.64
1:B:530:VAL:O	1:B:537:ILE:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLN:NE2	1:C:384:SER:O	2.29	0.64
1:D:794:PHE:CZ	1:D:980:LYS:HE2	2.31	0.64
1:C:838:VAL:HG22	1:C:948:THR:HG23	1.80	0.64
1:C:869:ARG:O	1:C:872:HIS:NE2	2.30	0.64
1:D:914:SER:HA	1:D:917:ARG:HD2	1.78	0.64
1:D:40:ASP:OD1	1:D:40:ASP:N	2.31	0.64
1:A:252:ARG:NH1	1:D:343:GLU:O	2.30	0.64
1:B:633:TYR:HB3	1:B:635:GLU:HG2	1.79	0.64
1:B:862:TYR:O	1:B:896:ASN:ND2	2.25	0.64
1:A:720:ARG:HH22	1:A:724:LEU:HD21	1.62	0.63
1:B:936:ASN:OD1	1:B:936:ASN:N	2.30	0.63
1:C:579:PRO:HG2	1:C:581:THR:HG23	1.80	0.63
1:D:722:TRP:O	1:D:725:GLN:NE2	2.31	0.63
1:D:826:ASN:HD22	1:D:832:TYR:HB3	1.63	0.63
1:A:344:LYS:HD3	1:D:250:PRO:HD2	1.79	0.63
1:A:398:ARG:NH2	1:A:441:ILE:HG12	2.13	0.63
1:B:579:PRO:HG2	1:B:581:THR:HG23	1.80	0.63
1:A:450:LEU:HB2	1:A:963:ALA:HB2	1.80	0.63
1:A:543:SER:O	1:A:551:ILE:N	2.29	0.63
1:D:699:GLN:HE21	1:D:719:ILE:HG13	1.63	0.63
1:D:827:GLY:HA2	1:D:867:SER:HB2	1.81	0.63
1:A:398:ARG:HH22	1:A:441:ILE:N	1.96	0.63
1:B:814:ASP:OD1	1:B:814:ASP:N	2.30	0.63
1:C:48:ARG:HG2	1:C:51:GLN:HE21	1.64	0.63
1:D:640:ARG:HA	1:D:640:ARG:HH11	1.63	0.63
1:D:826:ASN:HB3	1:D:889:ILE:HD11	1.79	0.63
1:A:497:LEU:HD21	1:B:484:LEU:HD13	1.80	0.62
1:C:814:ASP:OD1	1:C:814:ASP:N	2.31	0.62
1:A:786:ALA:O	1:A:869:ARG:NH2	2.32	0.62
1:C:863:HIS:HA	1:C:897:SER:HB2	1.80	0.62
1:D:800:PHE:CZ	1:D:843:TRP:HE3	2.09	0.62
1:A:1090:ARG:HG2	1:A:1092:ASN:HD22	1.65	0.62
1:B:242:SER:OG	1:B:273:ASN:ND2	2.32	0.62
1:B:328:SER:HB3	1:B:352:ASP:H	1.63	0.62
1:D:186:ALA:O	1:D:190:GLY:N	2.32	0.62
1:D:379:ARG:O	1:D:381:GLN:NE2	2.33	0.62
1:D:649:ASN:ND2	1:D:1020:ALA:O	2.27	0.62
1:B:484:LEU:HD23	1:B:494:LEU:HD11	1.80	0.62
1:A:446:ARG:HB3	1:A:804:GLU:OE2	2.00	0.62
1:C:530:VAL:O	1:C:537:ILE:N	2.29	0.62
1:D:58:ILE:HG12	1:D:260:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ARG:NH1	1:D:439:ASN:O	2.33	0.62
1:A:104:HIS:HB3	1:A:178:ARG:HH22	1.64	0.62
1:D:598:PHE:HA	1:D:624:SER:HB2	1.81	0.62
1:D:789:ILE:HD12	1:D:789:ILE:N	2.15	0.62
1:D:264:ILE:HD11	1:D:1091:ARG:HG2	1.82	0.62
1:B:869:ARG:O	1:B:872:HIS:NE2	2.33	0.62
1:C:62:HIS:O	1:C:1091:ARG:NH2	2.32	0.62
1:D:542:ILE:HD11	1:D:550:LYS:HG2	1.81	0.62
1:C:529:VAL:HA	1:C:538:ARG:HA	1.82	0.61
1:C:953:GLU:OE2	1:C:957:GLN:NE2	2.33	0.61
1:D:1055:ALA:HB2	1:D:1065:VAL:HG21	1.81	0.61
1:B:953:GLU:OE2	1:B:957:GLN:NE2	2.33	0.61
1:C:531:LYS:HA	1:C:536:GLU:HA	1.82	0.61
1:C:569:LEU:O	1:C:573:ASN:ND2	2.32	0.61
1:D:442:VAL:CG2	1:D:443:PRO:CD	2.44	0.61
1:D:219:GLY:HA2	1:D:265:ARG:HH22	1.66	0.61
1:A:814:ASP:N	1:A:814:ASP:OD1	2.29	0.61
1:A:722:TRP:O	1:A:725:GLN:NE2	2.33	0.61
1:C:63:ASN:ND2	1:C:633:TYR:OH	2.32	0.61
1:A:356:ILE:HB	1:A:393:GLY:HA2	1.82	0.61
1:A:401:ASP:OD2	1:A:404:VAL:N	2.33	0.61
1:A:1068:ASP:OD1	1:A:1068:ASP:N	2.32	0.61
1:B:31:THR:HG22	1:B:82:ALA:HB3	1.83	0.61
1:B:464:VAL:HG21	1:B:571:ARG:HH12	1.66	0.61
1:D:395:GLN:HE22	1:D:397:SER:HB3	1.66	0.61
1:D:862:TYR:O	1:D:896:ASN:ND2	2.32	0.61
1:A:209:VAL:HG22	1:A:300:LYS:HG2	1.82	0.61
1:B:447:SER:O	1:B:449:TYR:N	2.33	0.61
1:D:193:ASP:HB3	1:D:196:LEU:HB3	1.83	0.61
1:A:215:THR:HG22	1:A:311:THR:HG21	1.82	0.61
1:C:526:ASP:HB2	1:C:542:ILE:HB	1.82	0.61
1:A:65:SER:HB3	1:A:68:GLU:HB2	1.83	0.60
1:C:796:LEU:CB	1:C:959:PHE:CZ	2.83	0.60
1:D:962:ILE:CD1	1:D:976:TYR:CE2	2.84	0.60
1:B:529:VAL:HA	1:B:538:ARG:HA	1.82	0.60
1:A:62:HIS:NE2	1:A:743:ASN:O	2.35	0.60
1:A:242:SER:OG	1:A:273:ASN:ND2	2.34	0.60
1:D:1082:LEU:O	1:D:1085:VAL:HG12	2.02	0.60
1:A:369:ARG:HH22	1:D:979:GLY:HA3	1.66	0.60
1:B:211:VAL:HG22	1:B:307:VAL:HB	1.83	0.60
1:C:358:LYS:HE3	1:C:396:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ILE:O	1:B:1089:TYR:N	2.34	0.60
1:D:359:PHE:N	1:D:394:THR:O	2.34	0.60
1:D:477:LEU:HD11	1:D:497:LEU:HB3	1.83	0.60
1:A:329:LEU:HD23	1:A:353:PHE:HB3	1.84	0.60
1:A:647:VAL:O	1:A:1027:LYS:NZ	2.34	0.60
1:B:81:ILE:HB	1:B:111:VAL:HA	1.82	0.60
1:C:638:HIS:H	1:C:643:ILE:HD11	1.66	0.60
1:D:647:VAL:O	1:D:1027:LYS:NZ	2.34	0.60
1:A:603:ASP:O	1:A:607:THR:OG1	2.20	0.60
1:C:450:LEU:HD21	1:C:800:PHE:CD2	2.37	0.60
1:D:1044:ASP:OD1	1:D:1044:ASP:N	2.35	0.60
1:A:53:GLN:NE2	1:A:55:CYS:SG	2.75	0.60
1:A:464:VAL:HG21	1:A:571:ARG:HH12	1.66	0.60
1:A:602:GLY:HA3	1:A:606:ARG:HD3	1.82	0.60
1:D:211:VAL:HG22	1:D:307:VAL:HB	1.84	0.60
1:D:442:VAL:CB	1:D:443:PRO:HD2	2.31	0.60
1:A:640:ARG:HA	1:A:640:ARG:HH11	1.65	0.60
1:B:564:GLU:O	1:B:567:LYS:NZ	2.35	0.60
1:B:679:THR:HA	1:B:732:GLN:HB2	1.82	0.60
1:C:250:PRO:HD3	1:C:312:SER:HB2	1.82	0.60
1:D:62:HIS:NE2	1:D:743:ASN:O	2.30	0.60
1:A:452:GLU:O	1:A:456:THR:OG1	2.20	0.59
1:A:229:LEU:HD22	1:A:408:TYR:HB2	1.83	0.59
1:D:569:LEU:O	1:D:573:ASN:ND2	2.35	0.59
1:B:524:SER:O	1:B:552:ARG:NH2	2.35	0.59
1:C:186:ALA:O	1:C:190:GLY:N	2.29	0.59
1:B:712:THR:HG22	1:B:715:GLU:HG3	1.83	0.59
1:C:796:LEU:CD1	1:C:800:PHE:HE1	2.14	0.59
1:D:642:ASP:OD1	1:D:643:ILE:N	2.34	0.59
1:A:200:LEU:HD11	1:A:298:ALA:HA	1.83	0.59
1:C:262:ASP:OD1	1:C:265:ARG:NH2	2.36	0.59
1:C:598:PHE:HA	1:C:624:SER:HB2	1.84	0.59
1:D:681:ASN:ND2	1:D:738:GLU:OE2	2.35	0.59
1:A:567:LYS:HZ2	1:A:567:LYS:HB3	1.67	0.59
1:A:1044:ASP:OD1	1:A:1044:ASP:N	2.33	0.59
1:B:822:PHE:HD2	1:B:860:LEU:HD21	1.66	0.59
1:C:209:VAL:HG22	1:C:300:LYS:HG2	1.84	0.59
1:D:244:ALA:O	1:D:308:ILE:N	2.32	0.59
1:B:250:PRO:HG2	1:C:344:LYS:HG3	1.83	0.59
1:C:101:LEU:O	1:C:106:GLY:N	2.25	0.59
1:D:795:THR:HG23	1:D:796:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG13	1:A:101:LEU:HD21	1.85	0.59
1:D:696:ILE:HG23	1:D:719:ILE:HG21	1.84	0.59
1:B:737:LYS:HA	1:B:740:GLN:HG2	1.85	0.59
1:B:804:GLU:O	1:B:808:ALA:N	2.27	0.59
1:D:329:LEU:HD23	1:D:353:PHE:HB3	1.84	0.59
1:D:962:ILE:HD11	1:D:976:TYR:CE2	2.37	0.59
1:A:797:ALA:O	1:A:801:THR:OG1	2.20	0.58
1:C:31:THR:HG22	1:C:82:ALA:HB3	1.85	0.58
1:A:56:GLU:OE1	1:A:56:GLU:N	2.36	0.58
1:B:929:TRP:NE1	1:B:931:VAL:HB	2.18	0.58
1:C:242:SER:OG	1:C:273:ASN:ND2	2.35	0.58
1:C:253:ARG:NH1	1:C:283:GLU:O	2.36	0.58
1:A:288:ILE:HD12	1:A:321:ILE:HD11	1.85	0.58
1:B:792:LEU:HD22	1:B:835:LEU:HD11	1.83	0.58
1:A:31:THR:O	1:A:59:HIS:ND1	2.34	0.58
1:C:376:GLN:NE2	1:C:381:GLN:O	2.35	0.58
1:D:245:VAL:HG22	1:D:308:ILE:HB	1.84	0.58
1:C:832:TYR:OH	1:C:869:ARG:NH2	2.35	0.58
1:A:81:ILE:O	1:A:112:PHE:N	2.34	0.58
1:A:838:VAL:HG22	1:A:948:THR:HG23	1.86	0.58
1:A:1055:ALA:HB2	1:A:1065:VAL:HG21	1.85	0.58
1:A:476:GLN:HE21	1:B:476:GLN:HA	1.67	0.58
1:B:442:VAL:HG21	1:B:969:LEU:HD21	1.84	0.58
1:B:870:SER:O	1:B:882:ARG:NH2	2.36	0.58
1:C:543:SER:O	1:C:551:ILE:N	2.32	0.58
1:C:924:ILE:HG23	1:C:928:GLU:HB2	1.85	0.58
1:A:175:GLY:O	1:A:177:ARG:NE	2.37	0.58
1:B:636:ASP:HB2	1:B:1076:GLY:HA3	1.86	0.58
1:A:346:ASP:OD2	1:D:253:ARG:N	2.36	0.58
1:C:543:SER:N	1:C:551:ILE:O	2.37	0.58
1:D:234:ARG:HH21	1:D:271:HIS:HB2	1.68	0.58
1:D:821:SER:HA	1:D:861:LYS:HG3	1.85	0.58
1:A:252:ARG:HH21	1:D:349:ASP:HB2	1.68	0.57
1:A:879:ASN:O	1:A:883:THR:OG1	2.22	0.57
1:C:770:ASN:O	1:C:770:ASN:ND2	2.36	0.57
1:A:398:ARG:HH22	1:A:441:ILE:H	1.52	0.57
1:B:200:LEU:HD11	1:B:298:ALA:HA	1.85	0.57
1:D:629:SER:O	1:D:633:TYR:HD2	1.87	0.57
1:A:568:TRP:O	1:A:572:GLU:N	2.23	0.57
1:A:929:TRP:NE1	1:A:931:VAL:HB	2.19	0.57
1:C:1053:ARG:HA	1:C:1056:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:PRO:O	1:D:447:SER:N	2.37	0.57
1:A:218:GLY:HA2	1:A:222:LYS:NZ	2.20	0.57
1:A:442:VAL:CG2	1:A:443:PRO:HD3	2.30	0.57
1:B:832:TYR:OH	1:B:869:ARG:NH2	2.38	0.57
1:B:1044:ASP:OD1	1:B:1044:ASP:N	2.38	0.57
1:A:817:ALA:HB3	1:A:857:SER:HB3	1.86	0.57
1:A:953:GLU:OE2	1:A:957:GLN:NE2	2.38	0.57
1:C:200:LEU:HD11	1:C:298:ALA:HA	1.87	0.57
1:D:481:HIS:HA	1:D:494:LEU:HD13	1.87	0.57
1:A:398:ARG:NH2	1:A:441:ILE:N	2.52	0.57
1:A:638:HIS:H	1:A:643:ILE:HD11	1.69	0.57
1:B:682:GLY:HA2	1:B:735:ILE:HD11	1.86	0.57
1:C:1063:PHE:HA	1:C:1066:LEU:HB2	1.85	0.57
1:A:543:SER:N	1:A:551:ILE:O	2.35	0.57
1:B:914:SER:HA	1:B:917:ARG:HD2	1.86	0.57
1:C:77:ASP:OD2	1:C:182:GLN:NE2	2.38	0.57
1:D:442:VAL:HG22	1:D:443:PRO:HD2	0.70	0.57
1:A:224:SER:HB3	1:A:396:ALA:HB1	1.87	0.56
1:A:414:ALA:O	1:A:418:ARG:N	2.36	0.56
1:A:884:THR:O	1:A:888:LEU:HG	2.04	0.56
1:C:450:LEU:HD21	1:C:800:PHE:HD2	1.69	0.56
1:D:477:LEU:HD21	1:D:497:LEU:HB3	1.86	0.56
1:C:219:GLY:HA2	1:C:265:ARG:HH22	1.70	0.56
1:B:224:SER:OG	1:B:1090:ARG:NH1	2.39	0.56
1:C:477:LEU:HD21	1:C:497:LEU:HB3	1.88	0.56
1:D:814:ASP:N	1:D:814:ASP:OD1	2.38	0.56
1:A:788:PRO:HB3	1:A:832:TYR:CE1	2.40	0.56
1:B:28:ARG:H	1:B:79:GLN:HG2	1.71	0.56
1:C:165:ALA:HA	1:C:182:GLN:HB3	1.88	0.56
1:D:603:ASP:OD1	1:D:606:ARG:N	2.24	0.56
1:B:120:VAL:HG12	1:B:122:ASP:H	1.70	0.56
1:C:941:SER:HB3	1:C:944:ILE:HG12	1.86	0.56
1:D:1002:VAL:HA	1:D:1006:ARG:HH21	1.70	0.56
1:A:262:ASP:OD1	1:A:265:ARG:NH2	2.39	0.56
1:B:219:GLY:HA2	1:B:265:ARG:HH22	1.70	0.56
1:C:700:ILE:HG23	1:C:711:PRO:HG2	1.87	0.56
1:A:526:ASP:HB2	1:A:542:ILE:HB	1.88	0.56
1:B:449:TYR:OH	1:B:801:THR:OG1	2.23	0.56
1:C:801:THR:CG2	1:C:968:VAL:CG2	2.82	0.56
1:D:763:PHE:O	1:D:767:GLN:N	2.39	0.56
1:D:800:PHE:CE1	1:D:843:TRP:CZ3	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:GLY:HA2	1:B:433:ARG:HH21	1.71	0.56
1:B:568:TRP:O	1:B:572:GLU:N	2.28	0.56
1:D:214:ILE:HG23	1:D:329:LEU:HD12	1.87	0.56
1:D:660:MET:HB3	1:D:664:TYR:CE2	2.41	0.56
1:D:219:GLY:HA2	1:D:265:ARG:NH2	2.20	0.56
1:D:603:ASP:OD2	1:D:605:PHE:CG	2.59	0.56
1:A:864:ILE:O	1:A:899:HIS:N	2.37	0.55
1:B:621:LYS:O	1:B:675:SER:N	2.28	0.55
1:D:962:ILE:HD11	1:D:976:TYR:HE2	1.71	0.55
1:C:524:SER:O	1:C:552:ARG:NH2	2.40	0.55
1:D:215:THR:HG22	1:D:311:THR:HG21	1.88	0.55
1:A:1001:GLY:N	1:A:1004:THR:O	2.37	0.55
1:B:177:ARG:CZ	1:B:177:ARG:H	2.19	0.55
1:B:376:GLN:NE2	1:B:384:SER:O	2.39	0.55
1:B:556:LEU:HD23	1:B:556:LEU:H	1.70	0.55
1:A:330:TYR:HD2	1:A:354:VAL:HG13	1.70	0.55
1:B:641:PRO:HA	1:B:644:TYR:HB2	1.88	0.55
1:C:679:THR:HA	1:C:732:GLN:HB2	1.89	0.55
1:D:1063:PHE:O	1:D:1067:MET:N	2.33	0.55
1:B:227:ASP:OD1	1:B:267:ASN:ND2	2.40	0.55
1:D:70:VAL:HG11	1:D:100:LEU:HD23	1.87	0.55
1:B:75:GLN:NE2	1:B:276:MET:O	2.40	0.55
1:D:264:ILE:HG23	1:D:265:ARG:HD3	1.87	0.55
1:B:287:GLU:HB3	1:C:316:GLN:HE22	1.71	0.55
1:B:372:ALA:HB1	1:B:386:ALA:HB1	1.89	0.55
1:B:433:ARG:H	1:B:433:ARG:HE	1.55	0.55
1:B:629:SER:HA	1:B:632:LEU:HB2	1.88	0.55
1:C:720:ARG:HH22	1:C:724:LEU:HD21	1.72	0.55
1:D:79:GLN:HA	1:D:109:ILE:HD12	1.88	0.55
1:D:177:ARG:CZ	1:D:177:ARG:H	2.20	0.55
1:A:409:GLN:HE22	1:A:429:ASN:HA	1.72	0.55
1:B:727:VAL:HG22	1:B:771:PHE:HB2	1.89	0.55
1:C:177:ARG:H	1:C:177:ARG:CZ	2.20	0.55
1:C:317:GLY:HA2	1:C:346:ASP:HB3	1.89	0.55
1:C:800:PHE:HZ	1:C:959:PHE:CZ	2.25	0.55
1:A:936:ASN:N	1:A:936:ASN:OD1	2.40	0.54
1:A:965:ARG:HH22	1:D:365:GLN:HB3	1.72	0.54
1:A:1048:MET:SD	1:A:1048:MET:N	2.80	0.54
1:B:505:LEU:HD22	1:B:510:ARG:HB2	1.88	0.54
1:B:638:HIS:H	1:B:643:ILE:HD11	1.71	0.54
1:B:999:ILE:H	1:B:1003:ASN:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:THR:HG22	1:D:715:GLU:HG3	1.89	0.54
1:A:28:ARG:HB2	1:A:78:VAL:HA	1.89	0.54
1:A:346:ASP:HA	1:D:252:ARG:HE	1.72	0.54
1:C:555:VAL:HB	1:C:936:ASN:HD21	1.73	0.54
1:D:169:LEU:O	1:D:173:VAL:N	2.29	0.54
1:D:800:PHE:HE2	1:D:847:MET:SD	2.30	0.54
1:D:871:LEU:HA	1:D:882:ARG:HH22	1.71	0.54
1:A:374:GLN:OE1	1:D:48:ARG:NH2	2.41	0.54
1:B:36:PHE:HZ	1:B:635:GLU:HG3	1.71	0.54
1:C:683:PRO:HB3	1:C:1075:LEU:HD11	1.90	0.54
1:C:796:LEU:HB3	1:C:959:PHE:CZ	2.42	0.54
1:B:181:ALA:HA	1:B:277:ARG:HH12	1.72	0.54
1:C:28:ARG:HH22	1:C:185:THR:HG22	1.71	0.54
1:C:374:GLN:NE2	1:C:378:ASN:OD1	2.39	0.54
1:D:372:ALA:HB1	1:D:386:ALA:HB1	1.89	0.54
1:A:446:ARG:NH1	1:A:446:ARG:HG3	2.13	0.54
1:A:1006:ARG:NH1	1:A:1007:ASN:OD1	2.40	0.54
1:A:878:PHE:O	1:A:882:ARG:HG3	2.07	0.54
1:B:447:SER:C	1:B:449:TYR:H	2.11	0.54
1:B:477:LEU:HD22	1:B:498:ALA:HB2	1.89	0.54
1:C:642:ASP:OD1	1:C:643:ILE:N	2.41	0.54
1:B:356:ILE:HB	1:B:393:GLY:HA2	1.90	0.54
1:A:234:ARG:NH1	1:A:239:ASP:OD2	2.41	0.54
1:B:452:GLU:O	1:B:456:THR:OG1	2.26	0.54
1:C:115:GLY:H	1:C:119:ILE:HD11	1.72	0.54
1:C:264:ILE:HG23	1:C:265:ARG:HD3	1.89	0.54
1:C:603:ASP:O	1:C:607:THR:OG1	2.26	0.54
1:C:1082:LEU:O	1:C:1085:VAL:HG12	2.08	0.54
1:A:28:ARG:H	1:A:79:GLN:HG2	1.73	0.53
1:A:834:VAL:HG11	1:A:944:ILE:HG23	1.89	0.53
1:B:531:LYS:HA	1:B:536:GLU:HA	1.90	0.53
1:C:332:MET:O	1:C:357:ASN:N	2.41	0.53
1:C:1051:ARG:HE	1:C:1065:VAL:HG13	1.73	0.53
1:D:218:GLY:HA2	1:D:222:LYS:HZ3	1.72	0.53
1:A:379:ARG:O	1:A:381:GLN:NE2	2.40	0.53
1:A:621:LYS:O	1:A:675:SER:N	2.32	0.53
1:A:997:LEU:HD12	1:A:998:PRO:HD2	1.90	0.53
1:B:570:MET:SD	1:B:570:MET:N	2.81	0.53
1:C:56:GLU:OE1	1:C:56:GLU:N	2.41	0.53
1:C:796:LEU:CD1	1:C:800:PHE:HZ	2.05	0.53
1:D:621:LYS:HB2	1:D:674:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLY:HA3	1:C:325:VAL:HG21	1.90	0.53
1:C:578:PHE:CZ	1:C:848:ARG:HD2	2.42	0.53
1:D:961:ARG:HH21	1:D:965:ARG:HE	1.55	0.53
1:B:598:PHE:HA	1:B:624:SER:HB2	1.89	0.53
1:C:213:GLY:O	1:C:329:LEU:N	2.40	0.53
1:A:46:MET:O	1:A:50:LEU:HG	2.08	0.53
1:A:446:ARG:CZ	1:A:446:ARG:CA	2.84	0.53
1:B:866:THR:OG1	1:B:867:SER:N	2.42	0.53
1:A:448:ARG:CZ	1:D:448:ARG:HE	2.22	0.53
1:B:448:ARG:HE	1:C:448:ARG:HH21	1.57	0.53
1:D:433:ARG:H	1:D:433:ARG:HE	1.56	0.53
1:A:177:ARG:CZ	1:A:177:ARG:H	2.22	0.53
1:C:1041:HIS:ND1	1:C:1044:ASP:OD2	2.42	0.53
1:D:524:SER:O	1:D:552:ARG:NH2	2.42	0.53
1:C:676:VAL:O	1:C:730:THR:N	2.37	0.53
1:D:608:ASN:ND2	1:D:662:VAL:O	2.37	0.53
1:D:64:ARG:HA	1:D:64:ARG:NH1	2.23	0.53
1:D:737:LYS:HZ1	1:D:780:HIS:HB2	1.74	0.53
1:C:401:ASP:OD1	1:C:435:SER:OG	2.25	0.53
1:D:239:ASP:OD1	1:D:239:ASP:N	2.41	0.53
1:A:62:HIS:HE2	1:A:744:THR:HA	1.73	0.52
1:D:886:GLN:O	1:D:889:ILE:HG12	2.09	0.52
1:B:332:MET:HG3	1:B:356:ILE:HA	1.91	0.52
1:D:193:ASP:OD2	1:D:196:LEU:N	2.39	0.52
1:D:505:LEU:O	1:D:510:ARG:NH2	2.42	0.52
1:D:1027:LYS:O	1:D:1030:GLN:NE2	2.42	0.52
1:A:177:ARG:HG2	1:A:275:PHE:CG	2.43	0.52
1:B:218:GLY:HA2	1:B:222:LYS:NZ	2.25	0.52
1:B:243:ILE:HB	1:B:274:ILE:HG23	1.91	0.52
1:B:345:ILE:HG22	1:B:348:LEU:H	1.74	0.52
1:C:359:PHE:N	1:C:394:THR:O	2.42	0.52
1:C:360:ASP:OD2	1:C:395:GLN:NE2	2.42	0.52
1:C:1055:ALA:HB2	1:C:1065:VAL:HG21	1.91	0.52
1:C:1068:ASP:OD1	1:C:1068:ASP:N	2.41	0.52
1:D:770:ASN:O	1:D:770:ASN:ND2	2.32	0.52
1:D:849:ASP:OD1	1:D:849:ASP:N	2.42	0.52
1:A:234:ARG:NH2	1:A:270:ASN:O	2.42	0.52
1:B:414:ALA:O	1:B:418:ARG:N	2.42	0.52
1:B:1082:LEU:O	1:B:1085:VAL:HG12	2.09	0.52
1:C:607:THR:HB	1:C:663:LEU:HD11	1.90	0.52
1:C:737:LYS:HA	1:C:740:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLN:HB3	1:A:275:PHE:CE1	2.45	0.52
1:A:671:ASN:HD21	1:A:673:SER:HB2	1.75	0.52
1:A:1001:GLY:O	1:A:1006:ARG:NH2	2.31	0.52
1:B:220:ALA:O	1:B:357:ASN:ND2	2.43	0.52
1:C:70:VAL:HG11	1:C:100:LEU:HD23	1.90	0.52
1:D:330:TYR:N	1:D:353:PHE:O	2.32	0.52
1:B:647:VAL:HB	1:B:1027:LYS:HD3	1.92	0.52
1:C:620:ALA:HA	1:C:673:SER:HB3	1.91	0.52
1:C:1044:ASP:OD1	1:C:1044:ASP:N	2.41	0.52
1:D:801:THR:O	1:D:804:GLU:HB3	2.10	0.52
1:A:112:PHE:HB3	1:A:136:TYR:HE2	1.74	0.52
1:A:601:GLU:OE1	1:A:651:GLY:N	2.43	0.52
1:A:823:PHE:CD2	1:A:863:HIS:HB3	2.45	0.52
1:B:843:TRP:O	1:B:846:THR:OG1	2.26	0.52
1:B:938:ASN:OD1	1:B:938:ASN:N	2.42	0.52
1:B:1055:ALA:HB2	1:B:1065:VAL:HG21	1.90	0.52
1:C:414:ALA:O	1:C:418:ARG:N	2.42	0.52
1:D:177:ARG:H	1:D:177:ARG:NE	2.08	0.52
1:D:941:SER:HB3	1:D:944:ILE:HG12	1.92	0.52
1:A:147:ALA:HA	1:A:150:ILE:HD12	1.91	0.52
1:D:568:TRP:O	1:D:572:GLU:N	2.36	0.52
1:D:823:PHE:CD2	1:D:863:HIS:HB3	2.45	0.52
1:A:35:LEU:HD11	1:A:65:SER:HA	1.90	0.52
1:A:1036:GLU:O	1:A:1040:ALA:N	2.40	0.52
1:B:28:ARG:HB2	1:B:78:VAL:HA	1.91	0.52
1:D:414:ALA:O	1:D:418:ARG:N	2.43	0.52
1:D:460:TYR:O	1:D:464:VAL:HG23	2.10	0.52
1:B:884:THR:O	1:B:888:LEU:HG	2.10	0.51
1:C:505:LEU:O	1:C:510:ARG:NH2	2.34	0.51
1:D:686:THR:HG21	1:D:1075:LEU:HD13	1.91	0.51
1:B:101:LEU:HD22	1:B:106:GLY:HA3	1.92	0.51
1:B:443:PRO:CG	1:B:446:ARG:HE	2.00	0.51
1:B:538:ARG:CZ	1:B:538:ARG:H	2.23	0.51
1:B:824:PHE:O	1:B:865:GLN:N	2.41	0.51
1:B:90:HIS:HA	1:B:93:TYR:CD2	2.45	0.51
1:A:392:TYR:CE1	1:A:433:ARG:HB2	2.45	0.51
1:B:70:VAL:HG11	1:B:100:LEU:HD23	1.92	0.51
1:B:581:THR:HB	1:B:837:ARG:HE	1.75	0.51
1:C:450:LEU:CD2	1:C:800:PHE:CE2	2.93	0.51
1:D:152:ASP:O	1:D:156:ARG:HB2	2.11	0.51
1:D:481:HIS:HB2	1:D:494:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:837:ARG:NH1	1:D:938:ASN:HD22	2.09	0.51
1:A:222:LYS:NZ	1:A:310:GLU:OE2	2.43	0.51
1:B:56:GLU:OE2	1:B:282:ARG:NH2	2.43	0.51
1:D:347:MET:O	1:D:351:ALA:N	2.43	0.51
1:B:222:LYS:HD2	1:B:223:SER:N	2.25	0.51
1:B:330:TYR:CE2	1:B:332:MET:HB3	2.45	0.51
1:B:827:GLY:O	1:B:886:GLN:NE2	2.43	0.51
1:C:119:ILE:HD12	1:C:124:ILE:HD11	1.91	0.51
1:D:215:THR:O	1:D:331:VAL:N	2.43	0.51
1:D:398:ARG:HH22	1:D:441:ILE:CG1	2.21	0.51
1:D:829:ASP:OD1	1:D:829:ASP:N	2.42	0.51
1:D:1024:GLU:OE2	1:D:1028:GLN:NE2	2.43	0.51
1:B:731:VAL:HB	1:B:773:SER:HA	1.92	0.51
1:C:796:LEU:HG	1:C:959:PHE:CE2	2.42	0.51
1:C:849:ASP:OD1	1:C:849:ASP:N	2.42	0.51
1:B:849:ASP:N	1:B:849:ASP:OD1	2.42	0.51
1:B:887:ALA:O	1:B:891:ILE:HG12	2.11	0.51
1:C:28:ARG:HB2	1:C:78:VAL:HA	1.93	0.51
1:C:621:LYS:O	1:C:675:SER:N	2.35	0.51
1:D:628:ASP:OD2	1:D:653:SER:OG	2.28	0.51
1:D:683:PRO:HB3	1:D:1075:LEU:HD11	1.92	0.51
1:D:714:ASP:OD1	1:D:714:ASP:N	2.42	0.51
1:D:1048:MET:SD	1:D:1048:MET:N	2.83	0.51
1:A:92:GLU:O	1:A:96:TYR:HB3	2.11	0.51
1:B:314:ILE:HD13	1:B:314:ILE:H	1.76	0.51
1:C:1049:LEU:HA	1:C:1052:LEU:HD23	1.92	0.51
1:A:556:LEU:HD23	1:A:556:LEU:H	1.76	0.51
1:B:889:ILE:O	1:B:893:ASP:N	2.31	0.51
1:D:703:PHE:CE2	1:D:719:ILE:HD11	2.45	0.51
1:D:799:GLY:O	1:D:802:TYR:HB2	2.10	0.51
1:A:521:GLN:O	1:A:524:SER:OG	2.25	0.50
1:B:170:ASP:N	1:B:170:ASP:OD1	2.41	0.50
1:B:400:ASN:HD22	1:B:1059:ASN:HD21	1.58	0.50
1:B:686:THR:HG21	1:B:1075:LEU:HD13	1.92	0.50
1:C:359:PHE:HB3	1:C:395:GLN:HB2	1.93	0.50
1:C:402:ASP:N	1:C:402:ASP:OD1	2.41	0.50
1:A:197:VAL:HG12	1:A:201:HIS:CE1	2.46	0.50
1:B:461:HIS:CE1	1:B:841:ARG:HH22	2.29	0.50
1:B:1048:MET:SD	1:B:1048:MET:N	2.84	0.50
1:C:31:THR:O	1:C:59:HIS:ND1	2.36	0.50
1:C:58:ILE:HG12	1:C:260:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ARG:O	1:C:467:GLN:HG2	2.11	0.50
1:D:969:LEU:HA	1:D:972:MET:HE2	1.93	0.50
1:A:792:LEU:O	1:A:796:LEU:HG	2.12	0.50
1:A:923:LEU:HD23	1:B:1005:PHE:HB2	1.93	0.50
1:B:215:THR:HG22	1:B:311:THR:HG21	1.92	0.50
1:C:461:HIS:CE1	1:C:841:ARG:HH22	2.30	0.50
1:D:578:PHE:CZ	1:D:848:ARG:HD2	2.47	0.50
1:B:829:ASP:OD1	1:B:829:ASP:N	2.44	0.50
1:C:788:PRO:HB3	1:C:832:TYR:CE1	2.46	0.50
1:C:793:ALA:O	1:C:796:LEU:HB2	2.11	0.50
1:C:1092:ASN:H	1:C:1092:ASN:HD22	1.60	0.50
1:D:601:GLU:OE1	1:D:651:GLY:N	2.45	0.50
1:A:446:ARG:HH11	1:A:446:ARG:CG	2.09	0.50
1:A:714:ASP:N	1:A:714:ASP:OD1	2.45	0.50
1:A:1024:GLU:HA	1:A:1027:LYS:HD2	1.94	0.50
1:B:508:VAL:O	1:B:512:LEU:HG	2.12	0.50
1:C:661:LYS:HG2	1:C:694:THR:HG23	1.94	0.50
1:C:797:ALA:HA	1:C:800:PHE:CD2	2.47	0.50
1:C:800:PHE:CZ	1:C:959:PHE:CZ	2.99	0.50
1:D:629:SER:HA	1:D:632:LEU:HB2	1.94	0.50
1:D:712:THR:O	1:D:716:GLU:N	2.41	0.50
1:A:81:ILE:HB	1:A:111:VAL:HA	1.93	0.50
1:A:213:GLY:O	1:A:329:LEU:N	2.37	0.50
1:A:441:ILE:HD12	1:A:750:GLU:HA	1.91	0.50
1:B:239:ASP:OD1	1:B:239:ASP:N	2.45	0.50
1:B:699:GLN:HE21	1:B:719:ILE:HG13	1.77	0.50
1:B:763:PHE:O	1:B:767:GLN:N	2.44	0.50
1:B:1001:GLY:O	1:B:1006:ARG:NH2	2.36	0.50
1:C:746:ILE:HA	1:C:1089:TYR:HB3	1.94	0.50
1:D:166:PRO:HG2	1:D:179:ALA:HB2	1.93	0.50
1:D:798:ASN:O	1:D:801:THR:CG2	2.44	0.50
1:D:863:HIS:NE2	1:D:899:HIS:HB2	2.27	0.50
1:A:314:ILE:HD13	1:A:314:ILE:H	1.77	0.50
1:A:609:ARG:O	1:A:613:LEU:HG	2.12	0.50
1:B:569:LEU:O	1:B:573:ASN:ND2	2.45	0.50
1:B:892:TYR:HA	1:B:937:PRO:HG2	1.93	0.50
1:C:415:LEU:HB3	1:C:420:MET:HB3	1.93	0.50
1:D:601:GLU:H	1:D:607:THR:HG23	1.77	0.50
1:D:823:PHE:HD2	1:D:863:HIS:HB3	1.75	0.50
1:C:622:ARG:HA	1:C:675:SER:HB2	1.93	0.50
1:D:334:PRO:HD3	1:D:357:ASN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:O	1:B:59:HIS:ND1	2.29	0.50
1:A:529:VAL:HA	1:A:538:ARG:HA	1.94	0.49
1:A:628:ASP:OD1	1:A:628:ASP:N	2.27	0.49
1:B:642:ASP:OD1	1:B:643:ILE:N	2.44	0.49
1:C:449:TYR:HH	1:C:801:THR:HG23	1.77	0.49
1:D:376:GLN:OE1	1:D:384:SER:OG	2.30	0.49
1:D:787:ASN:C	1:D:789:ILE:HD12	2.32	0.49
1:B:567:LYS:HZ3	1:B:567:LYS:HB3	1.77	0.49
1:D:576:GLY:HA3	1:D:586:ALA:HB2	1.93	0.49
1:A:446:ARG:NH1	1:A:446:ARG:CG	2.72	0.49
1:A:557:PRO:HB3	1:B:942:PHE:CE1	2.47	0.49
1:B:219:GLY:H	1:B:222:LYS:HE2	1.76	0.49
1:C:747:PHE:HB3	1:C:751:PHE:HE2	1.76	0.49
1:D:210:PRO:HG2	1:D:306:LEU:HA	1.92	0.49
1:D:332:MET:HG3	1:D:356:ILE:HA	1.94	0.49
1:B:826:ASN:N	1:B:865:GLN:O	2.37	0.49
1:B:834:VAL:O	1:B:838:VAL:HG23	2.12	0.49
1:C:484:LEU:HG	1:C:489:HIS:HB2	1.94	0.49
1:C:784:ALA:HB1	1:C:981:ILE:HD11	1.94	0.49
1:C:815:ASP:N	1:C:815:ASP:OD1	2.44	0.49
1:C:1006:ARG:NH1	1:C:1007:ASN:OD1	2.44	0.49
1:D:603:ASP:OD1	1:D:606:ARG:HB3	2.12	0.49
1:A:242:SER:HB3	1:A:304:PHE:HD1	1.77	0.49
1:A:376:GLN:NE2	1:A:381:GLN:O	2.45	0.49
1:B:655:ALA:HB1	1:B:1034:LEU:HD13	1.94	0.49
1:D:801:THR:O	1:D:804:GLU:N	2.45	0.49
1:A:60:LEU:HD22	1:A:264:ILE:HA	1.94	0.49
1:A:181:ALA:HA	1:A:277:ARG:NH1	2.27	0.49
1:A:354:VAL:HB	1:A:391:VAL:HG22	1.93	0.49
1:A:474:ARG:HH11	1:A:474:ARG:HB3	1.77	0.49
1:A:571:ARG:HA	1:A:571:ARG:HH11	1.78	0.49
1:A:599:ALA:HB1	1:A:610:ARG:HD3	1.95	0.49
1:B:1051:ARG:HG3	1:B:1065:VAL:HG13	1.95	0.49
1:C:35:LEU:HA	1:C:63:ASN:HA	1.95	0.49
1:C:178:ARG:O	1:C:182:GLN:HG2	2.13	0.49
1:C:793:ALA:O	1:C:796:LEU:CB	2.61	0.49
1:C:863:HIS:NE2	1:C:899:HIS:HB2	2.27	0.49
1:C:1024:GLU:OE2	1:C:1028:GLN:NE2	2.45	0.49
1:D:603:ASP:OD2	1:D:605:PHE:N	2.44	0.49
1:A:345:ILE:O	1:D:252:ARG:NH2	2.45	0.49
1:A:864:ILE:HD12	1:A:895:CYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TYR:O	1:B:453:LEU:HG	2.13	0.49
1:B:1038:HIS:O	1:B:1042:GLN:N	2.46	0.49
1:C:76:GLU:OE1	1:C:277:ARG:HA	2.13	0.49
1:C:219:GLY:HA2	1:C:265:ARG:HH12	1.77	0.49
1:D:56:GLU:N	1:D:56:GLU:OE1	2.46	0.49
1:D:657:LEU:HD11	1:D:694:THR:OG1	2.12	0.49
1:D:1063:PHE:HA	1:D:1066:LEU:HB2	1.94	0.49
1:A:193:ASP:O	1:A:197:VAL:HG23	2.13	0.49
1:A:334:PRO:HD3	1:A:357:ASN:O	2.12	0.49
1:B:169:LEU:HD11	1:B:196:LEU:HD11	1.95	0.49
1:B:222:LYS:HA	1:B:225:LEU:HD12	1.95	0.49
1:D:466:ALA:O	1:D:470:LEU:HG	2.12	0.49
1:D:668:ASP:OD1	1:D:670:THR:OG1	2.31	0.49
1:D:698:GLN:HG2	1:D:702:ARG:HH21	1.78	0.49
1:B:218:GLY:HA2	1:B:222:LYS:HZ1	1.77	0.49
1:B:628:ASP:N	1:B:651:GLY:HA3	2.27	0.49
1:B:679:THR:HG22	1:B:732:GLN:HG3	1.94	0.49
1:D:505:LEU:HD22	1:D:510:ARG:HB2	1.95	0.49
1:A:824:PHE:O	1:A:865:GLN:N	2.45	0.49
1:B:792:LEU:O	1:B:796:LEU:HG	2.13	0.49
1:C:74:LEU:HD13	1:C:178:ARG:NH2	2.28	0.49
1:D:219:GLY:H	1:D:222:LYS:HE2	1.77	0.49
1:D:545:THR:HG23	1:D:547:SER:H	1.78	0.49
1:A:28:ARG:HH22	1:A:185:THR:HG22	1.77	0.48
1:A:44:ASN:O	1:A:48:ARG:HG3	2.13	0.48
1:A:679:THR:HA	1:A:732:GLN:HB2	1.95	0.48
1:B:58:ILE:HG12	1:B:260:LEU:HB2	1.95	0.48
1:B:507:ALA:HA	1:B:510:ARG:NH1	2.28	0.48
1:B:813:ILE:HG21	1:B:851:TYR:HB3	1.94	0.48
1:D:398:ARG:CZ	1:D:440:VAL:HA	2.42	0.48
1:D:402:ASP:O	1:D:405:THR:OG1	2.27	0.48
1:D:452:GLU:O	1:D:456:THR:OG1	2.30	0.48
1:D:703:PHE:HE2	1:D:719:ILE:HD11	1.77	0.48
1:D:854:ASN:OD1	1:D:857:SER:N	2.41	0.48
1:B:550:LYS:HB2	1:B:550:LYS:HE2	1.61	0.48
1:D:879:ASN:O	1:D:883:THR:OG1	2.30	0.48
1:B:827:GLY:HA2	1:B:867:SER:HB2	1.95	0.48
1:B:865:GLN:HG3	1:B:866:THR:O	2.13	0.48
1:C:53:GLN:NE2	1:C:55:CYS:SG	2.86	0.48
1:A:484:LEU:HD23	1:A:494:LEU:HD11	1.95	0.48
1:D:629:SER:O	1:D:633:TYR:CD2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ARG:CZ	1:A:538:ARG:H	2.26	0.48
1:B:36:PHE:CZ	1:B:635:GLU:HG3	2.49	0.48
1:C:739:ASP:O	1:C:743:ASN:ND2	2.45	0.48
1:C:824:PHE:HB2	1:C:864:ILE:HG12	1.95	0.48
1:D:855:ASP:OD1	1:D:855:ASP:N	2.43	0.48
1:A:74:LEU:HD21	1:A:101:LEU:HD22	1.95	0.48
1:A:466:ALA:O	1:A:470:LEU:HG	2.14	0.48
1:B:482:ASP:O	1:B:486:GLY:N	2.42	0.48
1:D:807:LEU:HD21	1:D:813:ILE:HB	1.96	0.48
1:A:891:ILE:HG13	1:A:925:ILE:HG21	1.95	0.48
1:B:599:ALA:HB1	1:B:610:ARG:HD2	1.94	0.48
1:B:939:GLN:HE21	1:B:939:GLN:HB3	1.48	0.48
1:B:1051:ARG:CZ	1:B:1065:VAL:HG22	2.44	0.48
1:C:863:HIS:HD2	1:C:864:ILE:H	1.62	0.48
1:C:986:LEU:O	1:C:989:GLU:HG2	2.14	0.48
1:D:1035:THR:O	1:D:1039:GLY:N	2.38	0.48
1:C:826:ASN:HD22	1:C:832:TYR:HB3	1.78	0.48
1:C:854:ASN:O	1:C:858:GLN:HG3	2.14	0.48
1:D:376:GLN:NE2	1:D:381:GLN:O	2.47	0.48
1:D:795:THR:HA	1:D:798:ASN:ND2	2.29	0.48
1:A:34:SER:HG	1:A:93:TYR:HE2	1.61	0.48
1:A:377:ARG:HG2	1:D:48:ARG:CZ	2.44	0.48
1:A:776:ILE:O	1:A:823:PHE:N	2.46	0.48
1:A:834:VAL:O	1:A:838:VAL:HG23	2.14	0.48
1:A:924:ILE:HG12	1:B:1000:ILE:HG13	1.95	0.48
1:B:330:TYR:HD2	1:B:354:VAL:HG13	1.78	0.48
1:B:878:PHE:O	1:B:882:ARG:HG3	2.14	0.48
1:D:800:PHE:CE1	1:D:843:TRP:HZ3	2.27	0.48
1:A:222:LYS:HD2	1:A:223:SER:N	2.29	0.47
1:A:1034:LEU:HG	1:A:1038:HIS:CE1	2.48	0.47
1:B:120:VAL:HB	1:B:123:GLU:HG3	1.95	0.47
1:B:402:ASP:OD1	1:B:402:ASP:N	2.47	0.47
1:B:609:ARG:O	1:B:613:LEU:HG	2.14	0.47
1:B:823:PHE:CD2	1:B:863:HIS:HB3	2.49	0.47
1:B:1068:ASP:OD1	1:B:1068:ASP:N	2.45	0.47
1:C:798:ASN:N	1:C:798:ASN:ND2	2.59	0.47
1:C:809:ARG:HB2	1:C:811:MET:HG2	1.95	0.47
1:D:843:TRP:O	1:D:847:MET:HG2	2.14	0.47
1:A:74:LEU:HD13	1:A:178:ARG:HH21	1.79	0.47
1:A:770:ASN:O	1:A:770:ASN:ND2	2.37	0.47
1:B:864:ILE:O	1:B:899:HIS:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ILE:HD11	1:C:295:VAL:HG13	1.95	0.47
1:C:639:GLU:OE2	1:C:640:ARG:NH1	2.47	0.47
1:C:953:GLU:O	1:C:957:GLN:HG2	2.15	0.47
1:D:800:PHE:CE1	1:D:843:TRP:CE3	2.96	0.47
1:A:843:TRP:O	1:A:847:MET:HG2	2.14	0.47
1:B:590:GLU:OE1	1:B:591:GLY:N	2.46	0.47
1:B:600:GLY:HA2	1:B:607:THR:HG22	1.95	0.47
1:D:184:ILE:HD11	1:D:295:VAL:HG13	1.96	0.47
1:A:657:LEU:HD13	1:A:690:MET:HB3	1.96	0.47
1:A:970:GLY:O	1:A:974:THR:OG1	2.26	0.47
1:A:1038:HIS:O	1:A:1042:GLN:N	2.47	0.47
1:C:252:ARG:HB3	1:C:255:SER:HB3	1.97	0.47
1:D:165:ALA:HA	1:D:182:GLN:HB3	1.96	0.47
1:D:461:HIS:CE1	1:D:841:ARG:HH12	2.32	0.47
1:D:866:THR:OG1	1:D:867:SER:N	2.47	0.47
1:A:1082:LEU:O	1:A:1085:VAL:HG12	2.13	0.47
1:C:1036:GLU:O	1:C:1040:ALA:N	2.44	0.47
1:D:248:ILE:HG22	1:D:312:SER:HB3	1.95	0.47
1:A:40:ASP:OD1	1:A:40:ASP:N	2.48	0.47
1:A:458:ARG:NH1	1:A:462:ARG:HH11	2.11	0.47
1:B:481:HIS:HA	1:B:494:LEU:HD13	1.97	0.47
1:C:712:THR:OG1	1:C:713:ALA:N	2.47	0.47
1:C:970:GLY:O	1:C:974:THR:OG1	2.28	0.47
1:D:32:ALA:HA	1:D:59:HIS:CE1	2.49	0.47
1:D:543:SER:O	1:D:551:ILE:N	2.23	0.47
1:D:557:PRO:HB3	1:D:559:PHE:CZ	2.50	0.47
1:A:647:VAL:HG11	1:A:1027:LYS:HB3	1.95	0.47
1:A:712:THR:OG1	1:A:713:ALA:N	2.48	0.47
1:A:723:VAL:O	1:A:727:VAL:N	2.48	0.47
1:B:328:SER:O	1:B:353:PHE:N	2.48	0.47
1:C:746:ILE:O	1:C:1089:TYR:N	2.45	0.47
1:D:785:GLY:O	1:D:869:ARG:NH1	2.46	0.47
1:D:787:ASN:CB	1:D:789:ILE:HD12	2.42	0.47
1:D:913:GLU:HB3	1:D:917:ARG:CZ	2.45	0.47
1:A:79:GLN:O	1:A:110:GLN:N	2.48	0.47
1:A:169:LEU:HD11	1:A:196:LEU:HD11	1.97	0.47
1:A:359:PHE:N	1:A:394:THR:O	2.47	0.47
1:A:647:VAL:HB	1:A:1027:LYS:HD3	1.97	0.47
1:B:1089:TYR:HE2	1:B:1091:ARG:HH11	1.63	0.47
1:C:656:THR:OG1	1:C:657:LEU:N	2.48	0.47
1:C:997:LEU:HD12	1:C:998:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:GLY:HA3	1:D:606:ARG:HD3	1.97	0.47
1:D:629:SER:HB2	1:D:633:TYR:CD2	2.50	0.47
1:A:704:ARG:O	1:A:708:GLY:N	2.48	0.47
1:A:887:ALA:O	1:A:891:ILE:HG12	2.14	0.47
1:A:923:LEU:HD11	1:A:927:ARG:HE	1.80	0.47
1:B:64:ARG:HA	1:B:64:ARG:HH11	1.80	0.47
1:B:999:ILE:O	1:B:1004:THR:N	2.48	0.47
1:D:794:PHE:CZ	1:D:958:GLU:OE2	2.68	0.47
1:D:1051:ARG:CZ	1:D:1065:VAL:HG22	2.45	0.47
1:A:75:GLN:HB3	1:A:275:PHE:HE1	1.80	0.47
1:C:597:MET:O	1:C:624:SER:N	2.44	0.47
1:D:887:ALA:O	1:D:891:ILE:HG12	2.14	0.47
1:B:271:HIS:HD2	1:B:274:ILE:HG13	1.80	0.46
1:B:788:PRO:HG2	1:B:831:GLU:OE1	2.16	0.46
1:B:817:ALA:HA	1:B:820:LEU:HG	1.95	0.46
1:C:152:ASP:O	1:C:156:ARG:HB2	2.16	0.46
1:C:181:ALA:HA	1:C:277:ARG:NH1	2.30	0.46
1:C:843:TRP:O	1:C:846:THR:OG1	2.28	0.46
1:D:177:ARG:HA	1:D:180:LEU:HB2	1.96	0.46
1:D:398:ARG:NH2	1:D:441:ILE:HG12	2.26	0.46
1:D:720:ARG:HH22	1:D:724:LEU:HD11	1.79	0.46
1:D:792:LEU:CD2	1:D:835:LEU:CD1	2.91	0.46
1:A:58:ILE:HG12	1:A:260:LEU:HD12	1.97	0.46
1:A:237:GLN:O	1:A:237:GLN:NE2	2.47	0.46
1:A:330:TYR:CE2	1:A:332:MET:HB3	2.50	0.46
1:A:712:THR:HG22	1:A:715:GLU:HG3	1.97	0.46
1:B:746:ILE:HD12	1:B:1089:TYR:H	1.80	0.46
1:B:989:GLU:HA	1:B:992:LYS:HE2	1.98	0.46
1:B:1055:ALA:HB1	1:B:1062:VAL:HG13	1.95	0.46
1:C:244:ALA:O	1:C:308:ILE:N	2.36	0.46
1:C:1053:ARG:O	1:C:1057:ILE:HG22	2.15	0.46
1:D:253:ARG:NH1	1:D:283:GLU:O	2.47	0.46
1:D:1069:ALA:O	1:D:1073:CYS:N	2.48	0.46
1:A:218:GLY:O	1:D:341:GLN:NE2	2.48	0.46
1:A:515:MET:O	1:A:519:MET:HG2	2.16	0.46
1:B:81:ILE:O	1:B:112:PHE:N	2.36	0.46
1:B:222:LYS:NZ	1:B:310:GLU:OE2	2.48	0.46
1:B:965:ARG:HH22	1:C:365:GLN:HB3	1.81	0.46
1:B:986:LEU:O	1:B:989:GLU:HG2	2.16	0.46
1:C:801:THR:HG23	1:C:968:VAL:HG21	1.92	0.46
1:D:442:VAL:HG21	1:D:804:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:NH1	1:A:467:GLN:HG3	2.30	0.46
1:A:818:PRO:HG3	1:A:857:SER:HA	1.97	0.46
1:A:986:LEU:O	1:A:989:GLU:HG2	2.15	0.46
1:D:581:THR:HG22	1:D:841:ARG:HG3	1.98	0.46
1:A:238:ASP:OD1	1:A:238:ASP:N	2.49	0.46
1:C:120:VAL:O	1:C:124:ILE:N	2.43	0.46
1:A:120:VAL:HG12	1:A:122:ASP:H	1.79	0.46
1:A:246:ILE:HG13	1:A:309:VAL:HG13	1.98	0.46
1:B:485:GLN:HE22	1:B:491:SER:H	1.63	0.46
1:B:630:VAL:HG13	1:B:635:GLU:HB2	1.97	0.46
1:B:720:ARG:HH22	1:B:724:LEU:HD21	1.81	0.46
1:D:398:ARG:HH22	1:D:441:ILE:CD1	2.28	0.46
1:D:403:GLY:HA2	1:D:406:MET:SD	2.55	0.46
1:D:518:GLN:HE21	1:D:518:GLN:HB3	1.50	0.46
1:A:246:ILE:HD11	1:A:309:VAL:HG22	1.98	0.46
1:A:554:VAL:HG23	1:A:935:GLU:HB2	1.98	0.46
1:C:696:ILE:HG23	1:C:719:ILE:HG21	1.97	0.46
1:A:445:ALA:C	1:D:448:ARG:NH1	2.69	0.46
1:A:605:PHE:HE1	1:A:662:VAL:HG11	1.80	0.46
1:A:628:ASP:O	1:A:631:THR:OG1	2.34	0.46
1:A:730:THR:HA	1:A:772:TYR:O	2.16	0.46
1:B:44:ASN:OD1	1:B:48:ARG:NE	2.49	0.46
1:B:433:ARG:HE	1:B:433:ARG:N	2.13	0.46
1:D:189:ASN:OD1	1:D:191:LYS:NZ	2.46	0.46
1:D:727:VAL:O	1:D:770:ASN:HB3	2.16	0.46
1:A:467:GLN:HE22	1:A:506:GLY:H	1.63	0.46
1:A:559:PHE:HB2	1:A:565:ILE:HD11	1.98	0.46
1:A:627:PHE:HD1	1:A:627:PHE:HA	1.66	0.46
1:A:1034:LEU:HD11	1:A:1074:SER:HB2	1.98	0.46
1:B:181:ALA:HA	1:B:277:ARG:NH1	2.31	0.46
1:C:796:LEU:CG	1:C:800:PHE:CZ	2.98	0.46
1:D:409:GLN:NE2	1:D:429:ASN:OD1	2.49	0.46
1:D:463:ARG:NH2	1:D:464:VAL:HG22	2.31	0.46
1:A:29:PHE:HB2	1:A:57:VAL:HG22	1.98	0.46
1:A:518:GLN:H	1:A:518:GLN:HG2	1.55	0.46
1:B:545:THR:HG23	1:B:547:SER:H	1.80	0.46
1:A:387:GLU:CD	1:A:387:GLU:H	2.18	0.45
1:B:847:MET:N	1:B:847:MET:SD	2.89	0.45
1:C:628:ASP:N	1:C:651:GLY:HA3	2.31	0.45
1:A:91:VAL:O	1:A:95:LYS:HE2	2.15	0.45
1:A:550:LYS:HE2	1:A:550:LYS:HB2	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:ARG:O	1:B:708:GLY:N	2.47	0.45
1:B:1034:LEU:HG	1:B:1038:HIS:CE1	2.50	0.45
1:D:253:ARG:HH22	1:D:281:THR:HG21	1.80	0.45
1:D:401:ASP:OD2	1:D:404:VAL:N	2.48	0.45
1:D:628:ASP:HB3	1:D:649:ASN:O	2.15	0.45
1:D:669:LEU:H	1:D:669:LEU:HG	1.41	0.45
1:D:779:TYR:HB2	1:D:823:PHE:CE1	2.51	0.45
1:A:501:ARG:O	1:A:505:LEU:N	2.47	0.45
1:A:964:GLU:O	1:D:362:LYS:NZ	2.46	0.45
1:B:56:GLU:N	1:B:56:GLU:OE1	2.49	0.45
1:B:848:ARG:HD3	1:B:849:ASP:OD1	2.16	0.45
1:C:1038:HIS:O	1:C:1042:GLN:N	2.49	0.45
1:D:458:ARG:NH1	1:D:462:ARG:HB2	2.31	0.45
1:D:511:LYS:O	1:D:515:MET:HG2	2.16	0.45
1:D:843:TRP:CD1	1:D:860:LEU:HB2	2.52	0.45
1:B:748:SER:OG	1:B:751:PHE:HB3	2.15	0.45
1:B:879:ASN:O	1:B:883:THR:OG1	2.35	0.45
1:C:409:GLN:NE2	1:C:429:ASN:OD1	2.49	0.45
1:C:763:PHE:HB3	1:C:768:VAL:HB	1.97	0.45
1:D:231:ARG:O	1:D:235:LEU:HG	2.17	0.45
1:D:531:LYS:HA	1:D:536:GLU:HA	1.97	0.45
1:D:580:TYR:CD1	1:D:584:VAL:HA	2.51	0.45
1:D:641:PRO:HA	1:D:644:TYR:CD2	2.52	0.45
1:D:670:THR:HB	1:D:726:ASN:ND2	2.31	0.45
1:D:788:PRO:HB3	1:D:832:TYR:CZ	2.51	0.45
1:A:555:VAL:HB	1:B:943:LEU:HD23	1.98	0.45
1:B:168:THR:OG1	1:B:169:LEU:N	2.49	0.45
1:A:759:ILE:HG12	1:A:763:PHE:CZ	2.52	0.45
1:B:392:TYR:CE1	1:B:433:ARG:HB2	2.52	0.45
1:B:443:PRO:HB2	1:B:446:ARG:HB2	1.99	0.45
1:C:47:ARG:HE	1:C:259:LEU:HD21	1.80	0.45
1:C:252:ARG:N	1:C:257:GLY:O	2.37	0.45
1:C:438:GLN:HG2	1:C:439:ASN:H	1.82	0.45
1:A:338:ALA:O	1:A:341:GLN:HG2	2.17	0.45
1:A:448:ARG:NH1	1:D:447:SER:OG	2.36	0.45
1:B:330:TYR:HE2	1:B:332:MET:HB3	1.82	0.45
1:C:214:ILE:HG23	1:C:329:LEU:HD12	1.99	0.45
1:C:883:THR:HA	1:C:886:GLN:HG2	1.98	0.45
1:C:907:ILE:O	1:C:1019:LEU:N	2.49	0.45
1:D:594:PRO:HB2	1:D:596:ARG:HE	1.81	0.45
1:D:843:TRP:CD2	1:D:860:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1068:ASP:OD1	1:D:1068:ASP:N	2.49	0.45
1:A:30:VAL:HG23	1:A:78:VAL:HG21	1.98	0.45
1:A:250:PRO:HD2	1:D:344:LYS:HZ1	1.81	0.45
1:A:725:GLN:HE21	1:A:725:GLN:HB3	1.62	0.45
1:B:578:PHE:CZ	1:B:848:ARG:HD2	2.52	0.45
1:C:787:ASN:ND2	1:C:790:SER:H	2.15	0.45
1:D:443:PRO:HG2	1:D:443:PRO:O	2.17	0.45
1:D:1080:HIS:HA	1:D:1083:PHE:CD2	2.51	0.45
1:A:119:ILE:HD12	1:A:124:ILE:HD11	1.99	0.45
1:B:29:PHE:HB2	1:B:57:VAL:HG22	1.98	0.45
1:C:239:ASP:N	1:C:239:ASP:OD1	2.50	0.45
1:C:727:VAL:HG11	1:C:768:VAL:HG13	1.99	0.45
1:C:840:ARG:HH12	1:C:893:ASP:HB3	1.82	0.45
1:A:165:ALA:HA	1:A:182:GLN:HB3	1.98	0.45
1:A:472:ARG:HH21	1:B:561:ASP:HA	1.82	0.45
1:A:785:GLY:HA2	1:A:869:ARG:HD3	1.98	0.45
1:B:44:ASN:O	1:B:48:ARG:HG3	2.17	0.45
1:C:64:ARG:HA	1:C:64:ARG:NH1	2.32	0.45
1:C:580:TYR:CD2	1:C:584:VAL:HA	2.52	0.45
1:C:865:GLN:HG3	1:C:866:THR:O	2.17	0.45
1:D:892:TYR:CD1	1:D:937:PRO:HG2	2.52	0.45
1:D:1052:LEU:HD13	1:D:1081:ALA:HB1	1.99	0.45
1:A:354:VAL:HB	1:A:391:VAL:HG13	2.00	0.44
1:A:448:ARG:HE	1:D:448:ARG:HH21	1.64	0.44
1:A:507:ALA:HA	1:A:510:ARG:NH1	2.31	0.44
1:A:879:ASN:HA	1:A:882:ARG:NE	2.31	0.44
1:A:943:LEU:HD22	1:B:555:VAL:HB	1.99	0.44
1:B:601:GLU:OE1	1:B:651:GLY:N	2.50	0.44
1:B:977:GLN:HE22	1:B:978:ARG:HG3	1.82	0.44
1:B:1063:PHE:HA	1:B:1066:LEU:HB2	1.99	0.44
1:D:136:TYR:CE1	1:D:149:MET:HG3	2.53	0.44
1:D:229:LEU:HD22	1:D:408:TYR:HD2	1.81	0.44
1:D:375:VAL:HA	1:D:378:ASN:ND2	2.32	0.44
1:D:514:ALA:O	1:D:517:PRO:HD2	2.16	0.44
1:D:628:ASP:N	1:D:651:GLY:HA3	2.33	0.44
1:D:643:ILE:O	1:D:647:VAL:HG23	2.16	0.44
1:D:878:PHE:O	1:D:882:ARG:HG3	2.17	0.44
1:B:901:ASN:OD1	1:B:901:ASN:N	2.50	0.44
1:B:929:TRP:HA	1:B:929:TRP:CE3	2.51	0.44
1:B:945:GLU:H	1:B:945:GLU:HG2	1.51	0.44
1:B:1029:SER:O	1:B:1033:ARG:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LEU:HD11	1:C:497:LEU:HB3	1.99	0.44
1:C:699:GLN:HG2	1:C:702:ARG:HH21	1.82	0.44
1:A:849:ASP:OD1	1:A:849:ASP:N	2.50	0.44
1:A:953:GLU:O	1:A:957:GLN:HG2	2.18	0.44
1:B:248:ILE:HD11	1:B:292:LEU:HD13	2.00	0.44
1:B:288:ILE:HG21	1:B:321:ILE:HD11	1.99	0.44
1:B:415:LEU:HB3	1:B:420:MET:HB3	1.99	0.44
1:C:707:ASN:HB3	1:C:709:ARG:NH1	2.32	0.44
1:D:193:ASP:H	1:D:196:LEU:HD23	1.82	0.44
1:D:432:GLY:HA2	1:D:433:ARG:HH21	1.82	0.44
1:A:509:GLU:H	1:A:509:GLU:CD	2.19	0.44
1:A:989:GLU:HA	1:A:992:LYS:HE2	1.98	0.44
1:C:177:ARG:HG2	1:C:275:PHE:CG	2.52	0.44
1:D:48:ARG:HG3	1:D:51:GLN:HE21	1.81	0.44
1:D:75:GLN:NE2	1:D:276:MET:O	2.50	0.44
1:D:209:VAL:HG22	1:D:300:LYS:HG2	1.99	0.44
1:D:938:ASN:OD1	1:D:938:ASN:N	2.51	0.44
1:A:267:ASN:HB2	1:A:1088:GLN:HE22	1.83	0.44
1:A:359:PHE:HB2	1:A:394:THR:C	2.38	0.44
1:A:627:PHE:HB3	1:A:632:LEU:HG	2.00	0.44
1:B:237:GLN:O	1:B:237:GLN:NE2	2.50	0.44
1:B:269:ILE:H	1:B:269:ILE:HG13	1.61	0.44
1:C:824:PHE:O	1:C:865:GLN:N	2.50	0.44
1:B:633:TYR:OH	1:B:744:THR:O	2.23	0.44
1:B:969:LEU:HD12	1:B:969:LEU:H	1.82	0.44
1:C:41:ALA:O	1:C:45:ILE:HG12	2.18	0.44
1:A:843:TRP:NE1	1:A:858:GLN:O	2.51	0.44
1:A:1005:PHE:HB2	1:B:923:LEU:HD23	1.99	0.44
1:A:1051:ARG:CZ	1:A:1065:VAL:HG22	2.47	0.44
1:B:965:ARG:NH2	1:C:365:GLN:HB3	2.32	0.44
1:C:581:THR:HG22	1:C:841:ARG:HB2	2.00	0.44
1:C:599:ALA:HB1	1:C:610:ARG:HD2	1.99	0.44
1:C:785:GLY:HA2	1:C:869:ARG:HD3	1.99	0.44
1:D:609:ARG:O	1:D:613:LEU:HG	2.17	0.44
1:B:246:ILE:HG13	1:B:309:VAL:HG13	2.00	0.44
1:B:643:ILE:O	1:B:647:VAL:HG23	2.18	0.44
1:B:815:ASP:OD1	1:B:815:ASP:N	2.51	0.44
1:C:796:LEU:HA	1:C:796:LEU:HD13	1.62	0.44
1:D:369:ARG:NE	1:D:370:ASP:OD1	2.51	0.44
1:D:557:PRO:HB3	1:D:559:PHE:CE2	2.52	0.44
1:A:64:ARG:HH22	1:A:68:GLU:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:SER:HB3	1:A:823:PHE:HB3	1.99	0.44
1:B:573:ASN:ND2	1:B:578:PHE:O	2.51	0.44
1:B:1030:GLN:HE21	1:B:1030:GLN:HB3	1.57	0.44
1:B:1075:LEU:HA	1:B:1078:ILE:HD12	2.00	0.44
1:C:446:ARG:C	1:C:446:ARG:HH11	2.21	0.44
1:C:686:THR:HG23	1:C:1070:VAL:HG12	2.00	0.44
1:D:353:PHE:CE2	1:D:390:PRO:HB2	2.52	0.44
1:D:856:ARG:HA	1:D:859:LYS:HE3	1.99	0.44
1:A:34:SER:OG	1:A:35:LEU:N	2.51	0.43
1:A:518:GLN:O	1:A:522:ALA:N	2.33	0.43
1:A:629:SER:HA	1:A:632:LEU:HB2	2.00	0.43
1:A:828:MET:HA	1:A:886:GLN:OE1	2.18	0.43
1:B:168:THR:OG1	1:B:170:ASP:OD1	2.35	0.43
1:B:778:GLY:HA2	1:B:781:ILE:HD12	2.00	0.43
1:B:912:ALA:O	1:B:915:VAL:HG22	2.18	0.43
1:D:193:ASP:O	1:D:197:VAL:HG23	2.18	0.43
1:D:515:MET:O	1:D:519:MET:HG2	2.18	0.43
1:A:642:ASP:OD1	1:A:643:ILE:N	2.48	0.43
1:B:374:GLN:OE1	1:B:378:ASN:ND2	2.47	0.43
1:D:1050:ALA:HA	1:D:1053:ARG:NH1	2.33	0.43
1:A:219:GLY:HA2	1:A:265:ARG:HH22	1.83	0.43
1:A:354:VAL:O	1:A:391:VAL:HA	2.17	0.43
1:A:360:ASP:OD1	1:A:360:ASP:N	2.51	0.43
1:A:431:GLU:N	1:A:431:GLU:OE1	2.51	0.43
1:A:443:PRO:HG2	1:A:446:ARG:HD2	2.00	0.43
1:A:501:ARG:HA	1:A:504:SER:HB2	2.00	0.43
1:A:815:ASP:OD1	1:A:815:ASP:N	2.51	0.43
1:D:30:VAL:HG23	1:D:78:VAL:HG21	1.99	0.43
1:B:60:LEU:HD12	1:B:69:VAL:HG22	2.01	0.43
1:C:500:GLU:OE1	1:C:501:ARG:NH1	2.51	0.43
1:C:817:ALA:HB3	1:C:857:SER:HB3	1.99	0.43
1:C:829:ASP:OD1	1:C:829:ASP:N	2.51	0.43
1:C:836:GLY:O	1:C:840:ARG:HG3	2.18	0.43
1:D:449:TYR:HH	1:D:801:THR:HB	1.76	0.43
1:D:458:ARG:HH12	1:D:462:ARG:HH11	1.67	0.43
1:A:211:VAL:HG22	1:A:307:VAL:HB	1.99	0.43
1:A:349:ASP:HB2	1:D:252:ARG:NH2	2.33	0.43
1:A:516:TRP:CH2	1:A:520:GLN:HB2	2.53	0.43
1:A:976:TYR:O	1:A:980:LYS:HG2	2.18	0.43
1:B:823:PHE:HD2	1:B:863:HIS:HB3	1.83	0.43
1:C:570:MET:SD	1:C:570:MET:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:GLU:O	1:C:808:ALA:N	2.44	0.43
1:D:381:GLN:HB3	1:D:384:SER:OG	2.18	0.43
1:A:31:THR:HG22	1:A:82:ALA:HB3	2.00	0.43
1:A:882:ARG:O	1:A:886:GLN:HG2	2.19	0.43
1:C:834:VAL:O	1:C:838:VAL:HG23	2.18	0.43
1:C:862:TYR:O	1:C:896:ASN:ND2	2.49	0.43
1:D:747:PHE:HB3	1:D:751:PHE:CE1	2.48	0.43
1:D:1081:ALA:O	1:D:1084:GLU:HB3	2.18	0.43
1:A:78:VAL:O	1:A:109:ILE:HD12	2.19	0.43
1:A:83:ILE:HB	1:A:113:GLY:HA2	1.99	0.43
1:A:990:GLN:O	1:A:994:ASP:HB2	2.18	0.43
1:B:621:LYS:N	1:B:673:SER:O	2.48	0.43
1:C:241:LEU:HD21	1:C:306:LEU:HD23	2.00	0.43
1:C:628:ASP:N	1:C:628:ASP:OD1	2.52	0.43
1:C:822:PHE:CE2	1:C:860:LEU:HD11	2.53	0.43
1:D:474:ARG:NH2	1:D:475:GLN:HA	2.34	0.43
1:D:881:ILE:H	1:D:881:ILE:HG13	1.58	0.43
1:D:976:TYR:CZ	1:D:980:LYS:HD3	2.53	0.43
1:D:1022:SER:HB3	1:D:1027:LYS:NZ	2.34	0.43
1:A:244:ALA:N	1:A:306:LEU:O	2.42	0.43
1:A:411:LEU:O	1:A:415:LEU:HG	2.18	0.43
1:A:449:TYR:O	1:A:453:LEU:HG	2.19	0.43
1:B:177:ARG:HG2	1:B:275:PHE:CG	2.54	0.43
1:B:215:THR:O	1:B:331:VAL:N	2.37	0.43
1:C:385:ARG:HA	1:C:385:ARG:HD2	1.76	0.43
1:C:418:ARG:HD2	1:C:418:ARG:HA	1.80	0.43
1:D:35:LEU:HD11	1:D:65:SER:HA	2.01	0.43
1:D:241:LEU:HD12	1:D:305:ASP:HB2	2.01	0.43
1:D:464:VAL:HG21	1:D:571:ARG:HH12	1.84	0.43
1:D:609:ARG:HA	1:D:609:ARG:HH11	1.84	0.43
1:D:942:PHE:O	1:D:945:GLU:HG2	2.19	0.43
1:A:178:ARG:O	1:A:182:GLN:HG2	2.19	0.43
1:A:540:GLY:O	1:A:553:LYS:NZ	2.38	0.43
1:D:100:LEU:O	1:D:104:HIS:N	2.52	0.43
1:D:359:PHE:HD1	1:D:359:PHE:HA	1.73	0.43
1:A:282:ARG:HA	1:A:282:ARG:HD3	1.66	0.43
1:A:381:GLN:HB3	1:A:384:SER:OG	2.19	0.43
1:A:385:ARG:HA	1:A:385:ARG:HD2	1.81	0.43
1:A:468:SER:HA	1:A:566:LEU:HD22	2.01	0.43
1:B:48:ARG:O	1:B:51:GLN:NE2	2.52	0.43
1:B:555:VAL:H	1:B:936:ASN:ND2	2.12	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:ASN:ND2	1:B:832:TYR:HB3	2.33	0.43
1:C:605:PHE:O	1:C:609:ARG:HG2	2.19	0.43
1:C:636:ASP:HB2	1:C:1076:GLY:HA3	2.00	0.43
1:C:1059:ASN:N	1:C:1059:ASN:OD1	2.52	0.43
1:D:29:PHE:HB2	1:D:57:VAL:HG22	2.01	0.43
1:D:418:ARG:HD2	1:D:418:ARG:HA	1.66	0.43
1:A:44:ASN:OD1	1:A:48:ARG:NE	2.49	0.42
1:A:433:ARG:H	1:A:433:ARG:HE	1.65	0.42
1:A:476:GLN:NE2	1:B:479:ALA:HB3	2.34	0.42
1:A:777:SER:HA	1:A:823:PHE:O	2.19	0.42
1:D:59:HIS:CE1	1:D:61:GLY:H	2.37	0.42
1:D:75:GLN:HE22	1:D:276:MET:HB3	1.83	0.42
1:D:262:ASP:HA	1:D:265:ARG:HE	1.84	0.42
1:D:441:ILE:HD11	1:D:750:GLU:HB2	2.01	0.42
1:D:713:ALA:HA	1:D:716:GLU:HB3	2.00	0.42
1:D:728:ARG:HG2	1:D:770:ASN:ND2	2.34	0.42
1:D:843:TRP:NE1	1:D:858:GLN:O	2.43	0.42
1:A:239:ASP:OD1	1:A:239:ASP:N	2.52	0.42
1:C:368:TRP:CZ2	1:C:433:ARG:HG3	2.54	0.42
1:C:585:PHE:HD1	1:C:585:PHE:HA	1.72	0.42
1:C:823:PHE:CD2	1:C:863:HIS:HB3	2.53	0.42
1:C:969:LEU:HA	1:C:972:MET:HE2	2.02	0.42
1:D:47:ARG:HH11	1:D:59:HIS:HD2	1.67	0.42
1:D:127:LEU:HB3	1:D:132:VAL:HG11	2.01	0.42
1:D:368:TRP:CD1	1:D:368:TRP:C	2.93	0.42
1:D:400:ASN:OD1	1:D:400:ASN:N	2.53	0.42
1:D:657:LEU:HD13	1:D:690:MET:HB3	2.01	0.42
1:D:777:SER:HA	1:D:823:PHE:HB3	2.01	0.42
1:A:91:VAL:HG22	1:A:127:LEU:HD21	2.01	0.42
1:A:377:ARG:NH2	1:D:49:ILE:HG13	2.35	0.42
1:A:923:LEU:HD12	1:A:923:LEU:HA	1.92	0.42
1:A:1081:ALA:HA	1:A:1084:GLU:HB3	2.00	0.42
1:B:596:ARG:HA	1:B:596:ARG:HD3	1.80	0.42
1:D:369:ARG:HG2	1:D:370:ASP:N	2.34	0.42
1:D:848:ARG:O	1:D:852:GLY:N	2.44	0.42
1:D:882:ARG:O	1:D:886:GLN:HG2	2.18	0.42
1:D:1045:ALA:HA	1:D:1048:MET:HG2	2.01	0.42
1:A:1078:ILE:O	1:A:1082:LEU:HG	2.18	0.42
1:B:282:ARG:HD3	1:B:282:ARG:HA	1.78	0.42
1:B:379:ARG:HA	1:B:379:ARG:NH1	2.34	0.42
1:B:411:LEU:HD22	1:B:411:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TYR:CE2	1:B:804:GLU:OE1	2.72	0.42
1:B:1001:GLY:N	1:B:1004:THR:O	2.43	0.42
1:C:446:ARG:O	1:C:446:ARG:HD3	2.19	0.42
1:C:571:ARG:HA	1:C:571:ARG:HH11	1.85	0.42
1:D:385:ARG:HB3	1:D:387:GLU:OE1	2.19	0.42
1:D:927:ARG:NE	1:D:928:GLU:OE2	2.53	0.42
1:A:415:LEU:HB3	1:A:420:MET:HB3	2.01	0.42
1:A:774:VAL:HG21	1:A:820:LEU:HD23	2.01	0.42
1:C:677:SER:HA	1:C:730:THR:HB	2.02	0.42
1:D:787:ASN:O	1:D:790:SER:HB2	2.19	0.42
1:A:219:GLY:HA2	1:A:265:ARG:NH2	2.35	0.42
1:A:608:ASN:ND2	1:A:662:VAL:O	2.50	0.42
1:A:813:ILE:HG21	1:A:851:TYR:HB3	2.02	0.42
1:B:186:ALA:O	1:B:190:GLY:N	2.52	0.42
1:B:510:ARG:HA	1:B:513:LEU:HB3	2.01	0.42
1:C:976:TYR:O	1:C:980:LYS:HG2	2.20	0.42
1:D:238:ASP:N	1:D:238:ASP:OD1	2.49	0.42
1:D:336:PHE:HE2	1:D:339:ALA:HA	1.83	0.42
1:D:883:THR:HA	1:D:886:GLN:HG2	2.01	0.42
1:A:215:THR:HA	1:A:311:THR:OG1	2.19	0.42
1:A:441:ILE:HG13	1:A:750:GLU:HB3	1.96	0.42
1:A:836:GLY:O	1:A:840:ARG:HG3	2.19	0.42
1:B:360:ASP:OD1	1:B:360:ASP:N	2.51	0.42
1:C:231:ARG:O	1:C:235:LEU:HG	2.19	0.42
1:C:234:ARG:HH21	1:C:271:HIS:HB2	1.85	0.42
1:D:865:GLN:HB2	1:D:899:HIS:HB3	2.00	0.42
1:A:63:ASN:HD21	1:A:744:THR:HG22	1.85	0.42
1:A:395:GLN:OE1	1:A:397:SER:N	2.52	0.42
1:A:866:THR:OG1	1:A:867:SER:N	2.53	0.42
1:B:559:PHE:HB2	1:B:565:ILE:HD11	2.02	0.42
1:C:330:TYR:HE2	1:C:332:MET:HB3	1.84	0.42
1:C:842:ILE:O	1:C:846:THR:HG23	2.20	0.42
1:D:218:GLY:HA2	1:D:222:LYS:NZ	2.34	0.42
1:A:1048:MET:HB3	1:A:1073:CYS:SG	2.60	0.42
1:A:1053:ARG:O	1:A:1057:ILE:HG22	2.20	0.42
1:B:725:GLN:HE21	1:B:725:GLN:HB3	1.64	0.42
1:B:952:GLU:O	1:B:956:LEU:HG	2.20	0.42
1:B:1090:ARG:H	1:B:1090:ARG:HD3	1.84	0.42
1:B:1090:ARG:HG2	1:B:1092:ASN:HD22	1.85	0.42
1:C:481:HIS:HA	1:C:494:LEU:HD13	2.01	0.42
1:C:601:GLU:OE1	1:C:651:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:GLU:OE1	1:D:277:ARG:HA	2.20	0.42
1:D:112:PHE:HB3	1:D:136:TYR:HE2	1.85	0.42
1:D:245:VAL:HA	1:D:308:ILE:O	2.20	0.42
1:A:152:ASP:O	1:A:156:ARG:HB2	2.19	0.42
1:A:160:ASP:OD1	1:A:163:ARG:NE	2.36	0.42
1:A:313:GLY:O	1:D:316:GLN:NE2	2.48	0.42
1:A:377:ARG:HH21	1:D:49:ILE:HG13	1.85	0.42
1:A:457:VAL:HG13	1:A:461:HIS:CE1	2.55	0.42
1:A:561:ASP:HA	1:B:472:ARG:HH21	1.85	0.42
1:A:850:LYS:HB3	1:A:851:TYR:CD2	2.54	0.42
1:A:850:LYS:HD2	1:A:851:TYR:CE1	2.55	0.42
1:B:515:MET:HA	1:B:518:GLN:OE1	2.20	0.42
1:B:625:THR:HB	1:B:678:MET:HA	2.02	0.42
1:C:669:LEU:H	1:C:669:LEU:HG	1.59	0.42
1:D:234:ARG:NH1	1:D:239:ASP:OD2	2.53	0.42
1:D:571:ARG:HA	1:D:571:ARG:HH11	1.85	0.42
1:D:601:GLU:O	1:D:607:THR:HG23	2.20	0.42
1:D:638:HIS:CE1	1:D:640:ARG:HG2	2.54	0.42
1:D:840:ARG:NH1	1:D:893:ASP:O	2.38	0.42
1:A:298:ALA:O	1:A:302:ALA:N	2.53	0.41
1:A:474:ARG:HB3	1:A:474:ARG:NH1	2.35	0.41
1:A:476:GLN:HA	1:B:476:GLN:HE21	1.85	0.41
1:A:627:PHE:CE1	1:A:652:VAL:HG13	2.55	0.41
1:A:1029:SER:O	1:A:1033:ARG:HG3	2.19	0.41
1:B:359:PHE:HB2	1:B:394:THR:C	2.41	0.41
1:B:577:SER:O	1:B:580:TYR:N	2.41	0.41
1:B:824:PHE:N	1:B:863:HIS:O	2.46	0.41
1:C:854:ASN:OD1	1:C:857:SER:N	2.48	0.41
1:C:882:ARG:O	1:C:886:GLN:HG2	2.19	0.41
1:D:28:ARG:HB2	1:D:78:VAL:HA	2.02	0.41
1:D:792:LEU:HD22	1:D:835:LEU:CG	2.50	0.41
1:D:850:LYS:HB3	1:D:851:TYR:CE2	2.54	0.41
1:D:879:ASN:HA	1:D:882:ARG:NE	2.34	0.41
1:A:432:GLY:HA2	1:A:433:ARG:NH2	2.35	0.41
1:A:475:GLN:NE2	1:A:562:GLU:H	2.17	0.41
1:A:727:VAL:O	1:A:770:ASN:HB3	2.21	0.41
1:B:628:ASP:OD2	1:B:653:SER:OG	2.36	0.41
1:C:328:SER:H	1:C:352:ASP:HB3	1.84	0.41
1:C:630:VAL:HG13	1:C:635:GLU:HB2	2.01	0.41
1:C:850:LYS:HB3	1:C:851:TYR:CD2	2.55	0.41
1:D:222:LYS:HD2	1:D:223:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:NH1	1:A:64:ARG:HA	2.36	0.41
1:A:1005:PHE:CE2	1:B:920:ALA:HB2	2.54	0.41
1:B:211:VAL:HA	1:B:307:VAL:O	2.21	0.41
1:D:95:LYS:HG2	1:D:130:TYR:CZ	2.55	0.41
1:D:236:ASP:HB2	1:D:427:LEU:HD11	2.02	0.41
1:D:329:LEU:HD22	1:D:330:TYR:N	2.36	0.41
1:D:511:LYS:HB3	1:D:511:LYS:HE3	1.86	0.41
1:D:518:GLN:O	1:D:522:ALA:N	2.48	0.41
1:D:545:THR:HG22	1:D:549:THR:H	1.86	0.41
1:D:843:TRP:O	1:D:846:THR:OG1	2.36	0.41
1:D:924:ILE:HG23	1:D:928:GLU:HB2	2.02	0.41
1:D:991:LEU:HD13	1:D:997:LEU:HD13	2.02	0.41
1:A:449:TYR:OH	1:A:801:THR:OG1	2.39	0.41
1:C:110:GLN:CD	1:C:156:ARG:HH12	2.23	0.41
1:D:29:PHE:HD1	1:D:80:GLY:HA3	1.85	0.41
1:D:737:LYS:HA	1:D:740:GLN:HG2	2.02	0.41
1:D:885:LEU:O	1:D:889:ILE:HG23	2.21	0.41
1:D:953:GLU:O	1:D:957:GLN:HG2	2.20	0.41
1:A:517:PRO:HA	1:A:520:GLN:OE1	2.21	0.41
1:B:354:VAL:HB	1:B:391:VAL:HG22	2.02	0.41
1:B:696:ILE:HG23	1:B:719:ILE:HG21	2.03	0.41
1:C:458:ARG:HE	1:C:458:ARG:HB3	1.72	0.41
1:D:597:MET:HB2	1:D:623:LEU:HA	2.02	0.41
1:D:1045:ALA:O	1:D:1049:LEU:HG	2.21	0.41
1:A:76:GLU:OE1	1:A:277:ARG:HD2	2.21	0.41
1:A:646:LYS:HB3	1:A:646:LYS:HE2	1.87	0.41
1:D:700:ILE:HG23	1:D:711:PRO:HG2	2.02	0.41
1:D:788:PRO:N	1:D:789:ILE:HD12	2.36	0.41
1:D:986:LEU:O	1:D:989:GLU:HG2	2.21	0.41
1:A:245:VAL:O	1:A:276:MET:HA	2.21	0.41
1:A:756:MET:O	1:A:759:ILE:HG22	2.20	0.41
1:A:987:TYR:O	1:A:991:LEU:HG	2.21	0.41
1:B:313:GLY:O	1:C:316:GLN:NE2	2.53	0.41
1:B:368:TRP:CZ2	1:B:392:TYR:HA	2.56	0.41
1:B:418:ARG:HA	1:B:418:ARG:HD2	1.81	0.41
1:B:546:LEU:H	1:B:546:LEU:HD22	1.86	0.41
1:B:581:THR:HG22	1:B:841:ARG:HB2	2.03	0.41
1:D:234:ARG:HG2	1:D:239:ASP:HA	2.02	0.41
1:D:271:HIS:CD2	1:D:274:ILE:HG13	2.55	0.41
1:D:431:GLU:N	1:D:431:GLU:OE1	2.54	0.41
1:A:742:GLN:O	1:A:744:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:GLN:HE21	1:A:1030:GLN:HB3	1.57	0.41
1:B:669:LEU:H	1:B:669:LEU:HG	1.59	0.41
1:C:368:TRP:CD1	1:C:368:TRP:C	2.94	0.41
1:D:415:LEU:HB3	1:D:420:MET:HB3	2.02	0.41
1:A:181:ALA:HA	1:A:277:ARG:HH12	1.85	0.41
1:A:275:PHE:CE2	1:A:277:ARG:HB2	2.56	0.41
1:A:621:LYS:HB2	1:A:674:THR:HA	2.02	0.41
1:A:778:GLY:O	1:A:782:ALA:N	2.37	0.41
1:A:881:ILE:H	1:A:881:ILE:HG13	1.55	0.41
1:A:1000:ILE:HG12	1:B:928:GLU:HG2	2.02	0.41
1:A:1045:ALA:HA	1:A:1048:MET:HG2	2.03	0.41
1:B:98:ILE:HD12	1:B:130:TYR:HE2	1.86	0.41
1:B:879:ASN:HA	1:B:882:ARG:NE	2.35	0.41
1:B:913:GLU:HB3	1:B:917:ARG:CZ	2.51	0.41
1:C:33:ALA:HB2	1:C:43:ILE:HD13	2.02	0.41
1:C:86:TYR:HD1	1:C:86:TYR:HA	1.69	0.41
1:C:264:ILE:HD11	1:C:1091:ARG:HG2	2.02	0.41
1:C:433:ARG:H	1:C:433:ARG:HE	1.69	0.41
1:C:627:PHE:HB3	1:C:631:THR:OG1	2.21	0.41
1:C:965:ARG:HA	1:C:965:ARG:HD3	1.79	0.41
1:C:1029:SER:O	1:C:1033:ARG:HG3	2.21	0.41
1:D:234:ARG:O	1:D:238:ASP:N	2.54	0.41
1:D:306:LEU:HD21	1:D:308:ILE:HD11	2.01	0.41
1:D:576:GLY:HA2	1:D:584:VAL:O	2.20	0.41
1:D:796:LEU:N	1:D:796:LEU:CD1	2.81	0.41
1:A:817:ALA:HA	1:A:820:LEU:HG	2.03	0.41
1:A:843:TRP:O	1:A:846:THR:OG1	2.31	0.41
1:B:788:PRO:HD3	1:B:869:ARG:HH22	1.86	0.41
1:B:1062:VAL:O	1:B:1066:LEU:HG	2.21	0.41
1:C:91:VAL:HG12	1:C:95:LYS:HE2	2.03	0.41
1:C:262:ASP:HA	1:C:265:ARG:HE	1.86	0.41
1:C:594:PRO:HB2	1:C:596:ARG:HH21	1.86	0.41
1:C:843:TRP:O	1:C:847:MET:HG2	2.21	0.41
1:D:107:GLU:H	1:D:107:GLU:CD	2.24	0.41
1:D:248:ILE:HA	1:D:279:LEU:O	2.20	0.41
1:D:581:THR:O	1:D:837:ARG:HG3	2.21	0.41
1:D:589:ARG:HA	1:D:589:ARG:HD2	1.94	0.41
1:D:922:GLN:HA	1:D:925:ILE:HD12	2.02	0.41
1:A:792:LEU:O	1:A:795:THR:OG1	2.33	0.40
1:B:245:VAL:HA	1:B:308:ILE:O	2.21	0.40
1:C:368:TRP:CZ3	1:C:392:TYR:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ARG:HE	1:D:433:ARG:N	2.19	0.40
1:D:585:PHE:HD1	1:D:585:PHE:HA	1.79	0.40
1:D:739:ASP:O	1:D:743:ASN:ND2	2.52	0.40
1:D:789:ILE:CD1	1:D:789:ILE:H	2.13	0.40
1:A:971:ALA:O	1:A:975:GLY:N	2.44	0.40
1:A:1062:VAL:O	1:A:1066:LEU:HG	2.21	0.40
1:C:243:ILE:HB	1:C:274:ILE:HG12	2.02	0.40
1:D:610:ARG:O	1:D:614:VAL:HG23	2.21	0.40
1:D:1062:VAL:O	1:D:1066:LEU:HG	2.21	0.40
1:A:696:ILE:HG23	1:A:719:ILE:HG21	2.02	0.40
1:A:938:ASN:OD1	1:A:938:ASN:N	2.52	0.40
1:B:219:GLY:HA2	1:B:265:ARG:HH12	1.87	0.40
1:B:263:ARG:HD2	1:B:276:MET:HG3	2.02	0.40
1:B:640:ARG:HD3	1:B:640:ARG:HA	1.89	0.40
1:C:431:GLU:OE1	1:C:431:GLU:N	2.53	0.40
1:C:507:ALA:HA	1:C:510:ARG:NH1	2.36	0.40
1:C:661:LYS:O	1:C:665:ASP:N	2.53	0.40
1:D:450:LEU:HB2	1:D:963:ALA:HB2	2.03	0.40
1:D:460:TYR:HE2	1:D:841:ARG:NH2	2.19	0.40
1:A:342:LEU:HD11	1:A:371:VAL:HG22	2.02	0.40
1:A:629:SER:O	1:A:633:TYR:N	2.32	0.40
1:A:827:GLY:C	1:A:886:GLN:HE22	2.25	0.40
1:C:428:PRO:O	1:C:430:LEU:HD22	2.22	0.40
1:C:621:LYS:HB2	1:C:674:THR:HA	2.02	0.40
1:C:855:ASP:O	1:C:859:LYS:HG3	2.22	0.40
1:D:178:ARG:O	1:D:182:GLN:HG2	2.21	0.40
1:D:1090:ARG:HG2	1:D:1092:ASN:HD22	1.86	0.40
1:A:184:ILE:HB	1:A:277:ARG:HH12	1.86	0.40
1:A:441:ILE:HD13	1:A:441:ILE:HA	1.94	0.40
1:A:545:THR:HG23	1:A:547:SER:H	1.86	0.40
1:B:29:PHE:O	1:B:57:VAL:HA	2.21	0.40
1:B:377:ARG:HG2	1:C:48:ARG:NH1	2.36	0.40
1:B:746:ILE:HA	1:B:1089:TYR:HB3	2.04	0.40
1:B:761:GLU:OE1	1:B:1061:ASN:ND2	2.51	0.40
1:C:90:HIS:CE1	1:C:119:ILE:HG23	2.56	0.40
1:C:463:ARG:NH1	1:C:509:GLU:OE2	2.54	0.40
1:C:573:ASN:HB2	1:C:579:PRO:HD2	2.01	0.40
1:C:597:MET:O	1:C:623:LEU:HD23	2.22	0.40
1:D:689:ALA:HB2	1:D:1063:PHE:HE1	1.86	0.40
1:D:1002:VAL:O	1:D:1006:ARG:NE	2.51	0.40

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	1053/1113 (95%)	1018 (97%)	34 (3%)	1 (0%)	51	86
1	B	1053/1113 (95%)	1026 (97%)	25 (2%)	2 (0%)	47	81
1	C	1053/1113 (95%)	1033 (98%)	20 (2%)	0	100	100
1	D	1053/1113 (95%)	1028 (98%)	23 (2%)	2 (0%)	47	81
All	All	4212/4452 (95%)	4105 (98%)	102 (2%)	5 (0%)	54	86

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	SER
1	B	447	SER
1	B	448	ARG
1	D	446	ARG
1	D	445	ALA

5.3.2   Protein sidechains ⓘ

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	826/906 (91%)	724 (88%)	102 (12%)	4	19
1	B	826/906 (91%)	729 (88%)	97 (12%)	5	20
1	C	826/906 (91%)	749 (91%)	77 (9%)	9	28
1	D	824/906 (91%)	724 (88%)	100 (12%)	5	20
All	All	3302/3624 (91%)	2926 (89%)	376 (11%)	9	21

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	44	ASN
1	A	53	GLN
1	A	62	HIS
1	A	86	TYR
1	A	96	TYR
1	A	104	HIS
1	A	110	GLN
1	A	119	ILE
1	A	149	MET
1	A	160	ASP
1	A	177	ARG
1	A	222	LYS
1	A	227	ASP
1	A	232	ARG
1	A	233	PHE
1	A	237	GLN
1	A	238	ASP
1	A	254	LYS
1	A	267	ASN
1	A	269	ILE
1	A	281	THR
1	A	283	GLU
1	A	287	GLU
1	A	294	ASP
1	A	314	ILE
1	A	318	ASP
1	A	329	LEU
1	A	333	THR
1	A	352	ASP
1	A	358	LYS
1	A	359	PHE
1	A	366	ASP
1	A	374	GLN
1	A	381	GLN
1	A	394	THR
1	A	402	ASP
1	A	422	LEU
1	A	433	ARG
1	A	446	ARG
1	A	474	ARG
1	A	475	GLN

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Mol	Chain	Res	Type
1	A	497	LEU
1	A	518	GLN
1	A	538	ARG
1	A	561	ASP
1	A	567	LYS
1	A	570	MET
1	A	585	PHE
1	A	607	THR
1	A	623	LEU
1	A	627	PHE
1	A	628	ASP
1	A	633	TYR
1	A	640	ARG
1	A	652	VAL
1	A	665	ASP
1	A	669	LEU
1	A	704	ARG
1	A	709	ARG
1	A	710	ASP
1	A	714	ASP
1	A	716	GLU
1	A	722	TRP
1	A	725	GLN
1	A	737	LYS
1	A	743	ASN
1	A	751	PHE
1	A	752	SER
1	A	753	LEU
1	A	761	GLU
1	A	762	TYR
1	A	770	ASN
1	A	787	ASN
1	A	822	PHE
1	A	855	ASP
1	A	856	ARG
1	A	860	LEU
1	A	865	GLN
1	A	875	GLU
1	A	881	ILE
1	A	883	THR
1	A	894	ASN
1	A	934	CYS

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Mol	Chain	Res	Type
1	A	938	ASN
1	A	942	PHE
1	A	943	LEU
1	A	974	THR
1	A	977	GLN
1	A	981	ILE
1	A	992	LYS
1	A	993	HIS
1	A	1004	THR
1	A	1030	GLN
1	A	1044	ASP
1	A	1052	LEU
1	A	1059	ASN
1	A	1068	ASP
1	A	1077	GLN
1	A	1080	HIS
1	A	1090	ARG
1	A	1091	ARG
1	B	43	ILE
1	B	44	ASN
1	B	53	GLN
1	B	62	HIS
1	B	86	TYR
1	B	110	GLN
1	B	119	ILE
1	B	149	MET
1	B	160	ASP
1	B	170	ASP
1	B	177	ARG
1	B	222	LYS
1	B	233	PHE
1	B	237	GLN
1	B	239	ASP
1	B	267	ASN
1	B	283	GLU
1	B	287	GLU
1	B	314	ILE
1	B	318	ASP
1	B	333	THR
1	B	347	MET
1	B	353	PHE
1	B	358	LYS

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Mol	Chain	Res	Type
1	B	387	GLU
1	B	402	ASP
1	B	409	GLN
1	B	411	LEU
1	B	422	LEU
1	B	433	ARG
1	B	455	ASP
1	B	456	THR
1	B	458	ARG
1	B	474	ARG
1	B	475	GLN
1	B	485	GLN
1	B	491	SER
1	B	518	GLN
1	B	538	ARG
1	B	542	ILE
1	B	543	SER
1	B	550	LYS
1	B	561	ASP
1	B	567	LYS
1	B	570	MET
1	B	585	PHE
1	B	607	THR
1	B	623	LEU
1	B	633	TYR
1	B	644	TYR
1	B	669	LEU
1	B	698	GLN
1	B	701	ASP
1	B	704	ARG
1	B	709	ARG
1	B	722	TRP
1	B	725	GLN
1	B	737	LYS
1	B	743	ASN
1	B	751	PHE
1	B	752	SER
1	B	754	LYS
1	B	761	GLU
1	B	762	TYR
1	B	765	HIS
1	B	770	ASN

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Mol	Chain	Res	Type
1	B	787	ASN
1	B	814	ASP
1	B	826	ASN
1	B	829	ASP
1	B	849	ASP
1	B	855	ASP
1	B	856	ARG
1	B	860	LEU
1	B	866	THR
1	B	875	GLU
1	B	881	ILE
1	B	883	THR
1	B	894	ASN
1	B	915	VAL
1	B	934	CYS
1	B	936	ASN
1	B	938	ASN
1	B	939	GLN
1	B	942	PHE
1	B	945	GLU
1	B	977	GLN
1	B	992	LYS
1	B	993	HIS
1	B	1004	THR
1	B	1030	GLN
1	B	1044	ASP
1	B	1052	LEU
1	B	1068	ASP
1	B	1080	HIS
1	B	1090	ARG
1	B	1091	ARG
1	C	48	ARG
1	C	53	GLN
1	C	62	HIS
1	C	86	TYR
1	C	110	GLN
1	C	119	ILE
1	C	122	ASP
1	C	128	GLN
1	C	160	ASP
1	C	177	ARG
1	C	222	LYS

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Mol	Chain	Res	Type
1	C	227	ASP
1	C	233	PHE
1	C	234	ARG
1	C	237	GLN
1	C	238	ASP
1	C	239	ASP
1	C	265	ARG
1	C	287	GLU
1	C	314	ILE
1	C	316	GLN
1	C	333	THR
1	C	352	ASP
1	C	358	LYS
1	C	360	ASP
1	C	374	GLN
1	C	381	GLN
1	C	385	ARG
1	C	387	GLU
1	C	394	THR
1	C	402	ASP
1	C	404	VAL
1	C	411	LEU
1	C	433	ARG
1	C	446	ARG
1	C	474	ARG
1	C	505	LEU
1	C	518	GLN
1	C	521	GLN
1	C	538	ARG
1	C	561	ASP
1	C	570	MET
1	C	585	PHE
1	C	607	THR
1	C	623	LEU
1	C	633	TYR
1	C	669	LEU
1	C	725	GLN
1	C	737	LYS
1	C	751	PHE
1	C	753	LEU
1	C	754	LYS
1	C	761	GLU

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Mol	Chain	Res	Type
1	C	762	TYR
1	C	770	ASN
1	C	772	TYR
1	C	796	LEU
1	C	798	ASN
1	C	809	ARG
1	C	815	ASP
1	C	849	ASP
1	C	855	ASP
1	C	856	ARG
1	C	860	LEU
1	C	977	GLN
1	C	981	ILE
1	C	1030	GLN
1	C	1044	ASP
1	C	1052	LEU
1	C	1053	ARG
1	C	1057	ILE
1	C	1059	ASN
1	C	1068	ASP
1	C	1085	VAL
1	C	1090	ARG
1	C	1091	ARG
1	C	1092	ASN
1	D	40	ASP
1	D	47	ARG
1	D	53	GLN
1	D	62	HIS
1	D	86	TYR
1	D	110	GLN
1	D	119	ILE
1	D	128	GLN
1	D	149	MET
1	D	177	ARG
1	D	196	LEU
1	D	222	LYS
1	D	227	ASP
1	D	233	PHE
1	D	234	ARG
1	D	237	GLN
1	D	238	ASP
1	D	239	ASP

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Mol	Chain	Res	Type
1	D	246	ILE
1	D	254	LYS
1	D	265	ARG
1	D	283	GLU
1	D	287	GLU
1	D	305	ASP
1	D	314	ILE
1	D	316	GLN
1	D	318	ASP
1	D	347	MET
1	D	352	ASP
1	D	358	LYS
1	D	359	PHE
1	D	366	ASP
1	D	369	ARG
1	D	374	GLN
1	D	381	GLN
1	D	387	GLU
1	D	394	THR
1	D	400	ASN
1	D	402	ASP
1	D	411	LEU
1	D	433	ARG
1	D	446	ARG
1	D	455	ASP
1	D	456	THR
1	D	458	ARG
1	D	474	ARG
1	D	505	LEU
1	D	518	GLN
1	D	520	GLN
1	D	538	ARG
1	D	556	LEU
1	D	561	ASP
1	D	570	MET
1	D	585	PHE
1	D	607	THR
1	D	628	ASP
1	D	640	ARG
1	D	665	ASP
1	D	669	LEU
1	D	681	ASN

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Mol	Chain	Res	Type
1	D	704	ARG
1	D	710	ASP
1	D	714	ASP
1	D	722	TRP
1	D	725	GLN
1	D	737	LYS
1	D	743	ASN
1	D	751	PHE
1	D	753	LEU
1	D	754	LYS
1	D	770	ASN
1	D	789	ILE
1	D	796	LEU
1	D	829	ASP
1	D	849	ASP
1	D	855	ASP
1	D	856	ARG
1	D	865	GLN
1	D	866	THR
1	D	875	GLU
1	D	881	ILE
1	D	883	THR
1	D	915	VAL
1	D	938	ASN
1	D	945	GLU
1	D	959	PHE
1	D	977	GLN
1	D	981	ILE
1	D	993	HIS
1	D	1004	THR
1	D	1030	GLN
1	D	1041	HIS
1	D	1044	ASP
1	D	1052	LEU
1	D	1068	ASP
1	D	1074	SER
1	D	1080	HIS
1	D	1085	VAL
1	D	1090	ARG
1	D	1091	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	203	GLN
1	A	237	GLN
1	A	273	ASN
1	A	381	GLN
1	A	409	GLN
1	A	467	GLN
1	A	476	GLN
1	A	573	ASN
1	A	671	ASN
1	A	699	GLN
1	A	725	GLN
1	A	726	ASN
1	A	765	HIS
1	A	767	GLN
1	A	770	ASN
1	A	780	HIS
1	A	858	GLN
1	A	863	HIS
1	A	865	GLN
1	A	939	GLN
1	A	957	GLN
1	A	1003	ASN
1	A	1041	HIS
1	A	1077	GLN
1	A	1092	ASN
1	B	53	GLN
1	B	75	GLN
1	B	237	GLN
1	B	267	ASN
1	B	271	HIS
1	B	273	ASN
1	B	376	GLN
1	B	381	GLN
1	B	400	ASN
1	B	409	GLN
1	B	467	GLN
1	B	476	GLN
1	B	573	ASN
1	B	671	ASN
1	B	681	ASN
1	B	699	GLN
1	B	725	GLN

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Mol	Chain	Res	Type
1	B	732	GLN
1	B	766	HIS
1	B	767	GLN
1	B	791	GLN
1	B	858	GLN
1	B	886	GLN
1	B	922	GLN
1	B	939	GLN
1	B	1092	ASN
1	C	51	GLN
1	C	53	GLN
1	C	75	GLN
1	C	90	HIS
1	C	203	GLN
1	C	267	ASN
1	C	273	ASN
1	C	316	GLN
1	C	341	GLN
1	C	381	GLN
1	C	409	GLN
1	C	429	ASN
1	C	573	ASN
1	C	671	ASN
1	C	699	GLN
1	C	725	GLN
1	C	732	GLN
1	C	767	GLN
1	C	787	ASN
1	C	798	ASN
1	C	858	GLN
1	C	865	GLN
1	C	886	GLN
1	C	922	GLN
1	C	938	ASN
1	C	977	GLN
1	C	1030	GLN
1	C	1038	HIS
1	C	1092	ASN
1	D	53	GLN
1	D	75	GLN
1	D	203	GLN
1	D	273	ASN

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Mol	Chain	Res	Type
1	D	376	GLN
1	D	381	GLN
1	D	409	GLN
1	D	467	GLN
1	D	518	GLN
1	D	573	ASN
1	D	671	ASN
1	D	693	ASN
1	D	699	GLN
1	D	725	GLN
1	D	740	GLN
1	D	765	HIS
1	D	767	GLN
1	D	826	ASN
1	D	858	GLN
1	D	865	GLN
1	D	886	GLN
1	D	896	ASN
1	D	922	GLN
1	D	977	GLN
1	D	1003	ASN
1	D	1030	GLN
1	D	1077	GLN
1	D	1092	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-40758. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
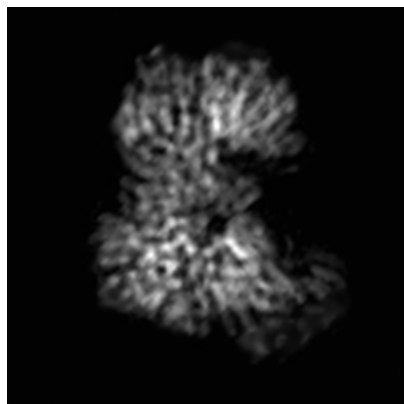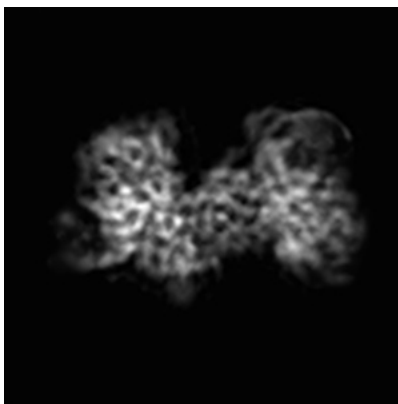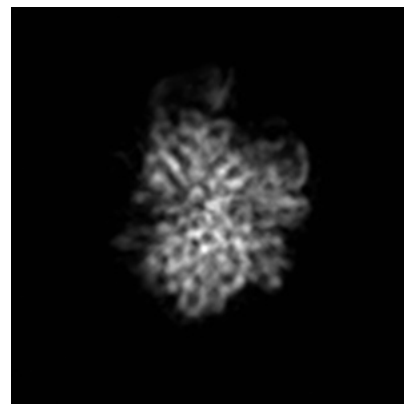
6.1.1 Primary map

X	Y	Z

6.1.2 Raw map

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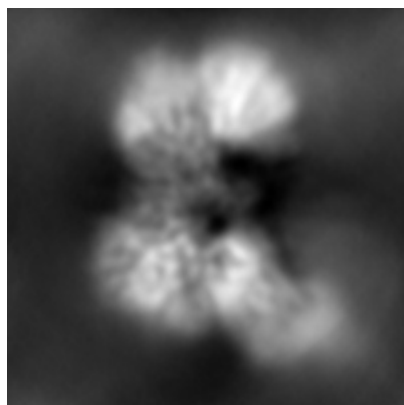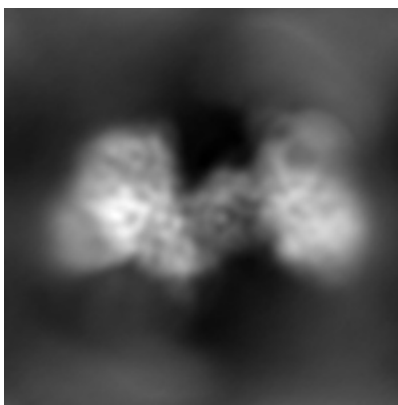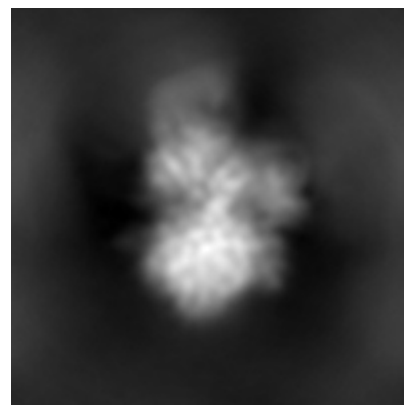
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
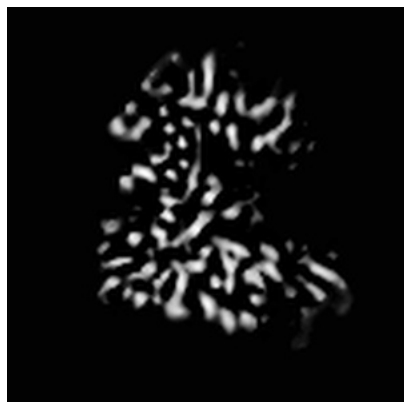
6.2.1 Primary map
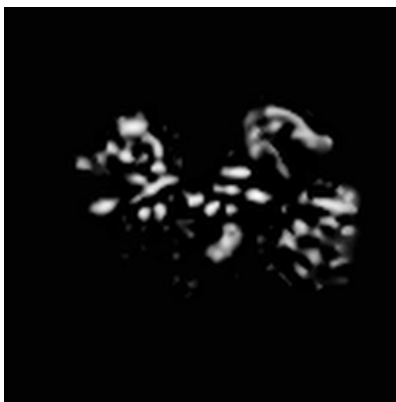
| X Index: 64 | Y Index: 64 | Z Index: 64 |

6.2.2 Raw map
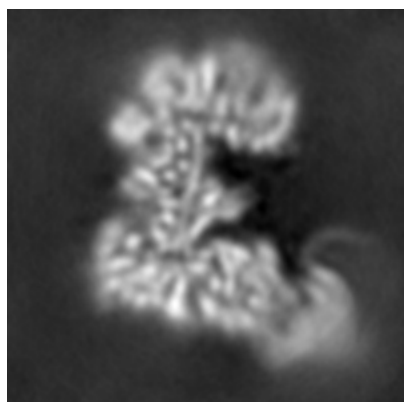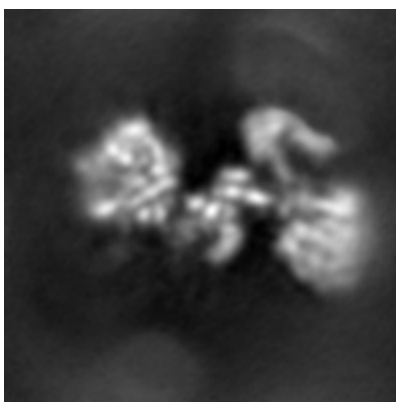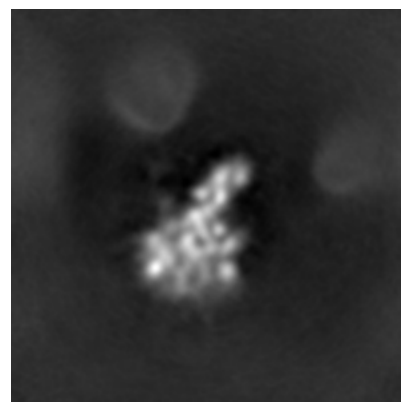
| X Index: 64 | Y Index: 64 | Z Index: 64 |

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

6.3 Largest variance slices ⓘ
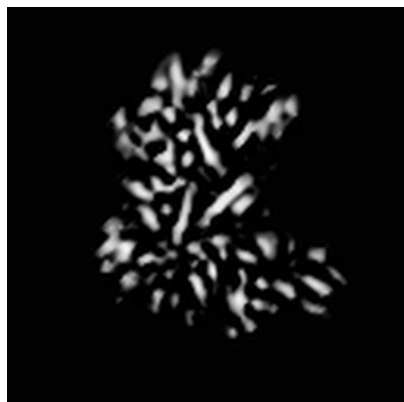
6.3.1 Primary map
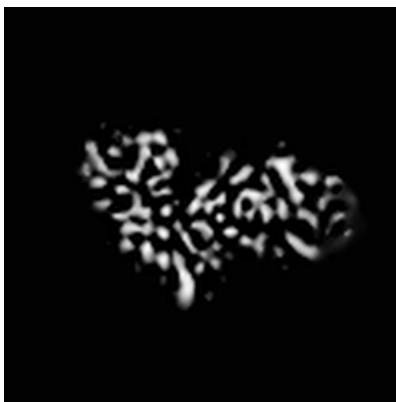
| X Index: 67 | Y Index: 51 | Z Index: 50 |

6.3.2 Raw map
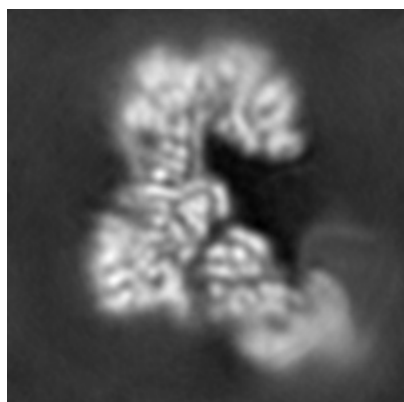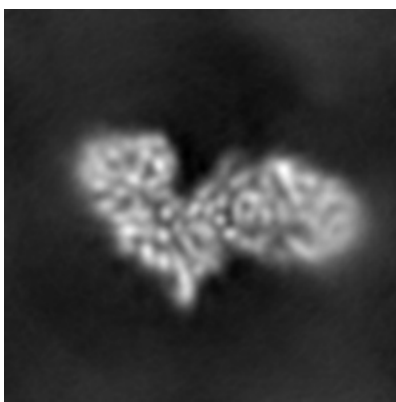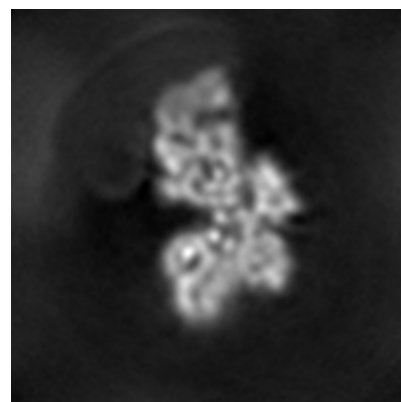
| X Index: 60 | Y Index: 51 | Z Index: 38 |

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
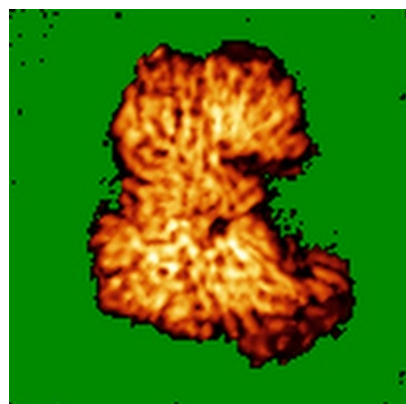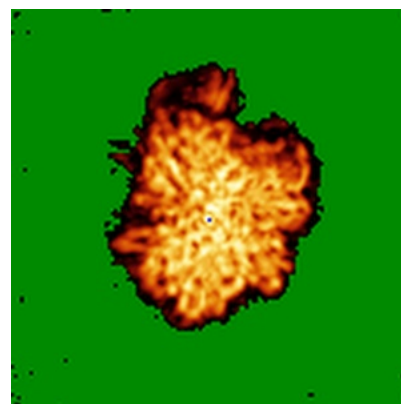
| X | Y | Z |

6.4.2 Raw map

| X | Y | Z |
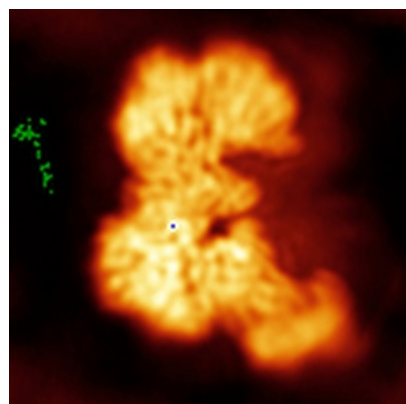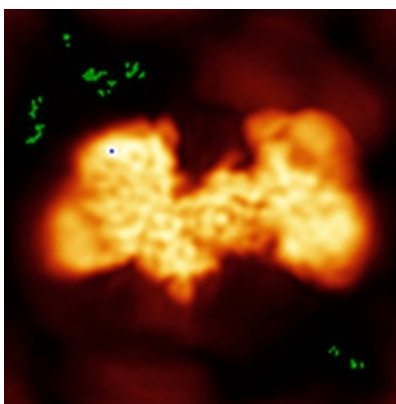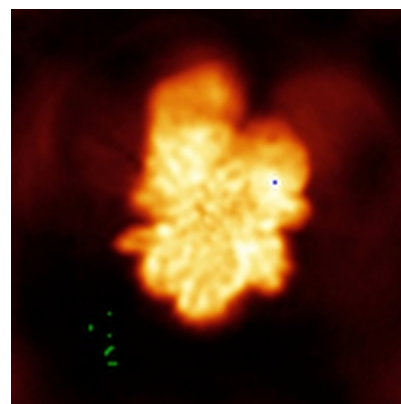
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
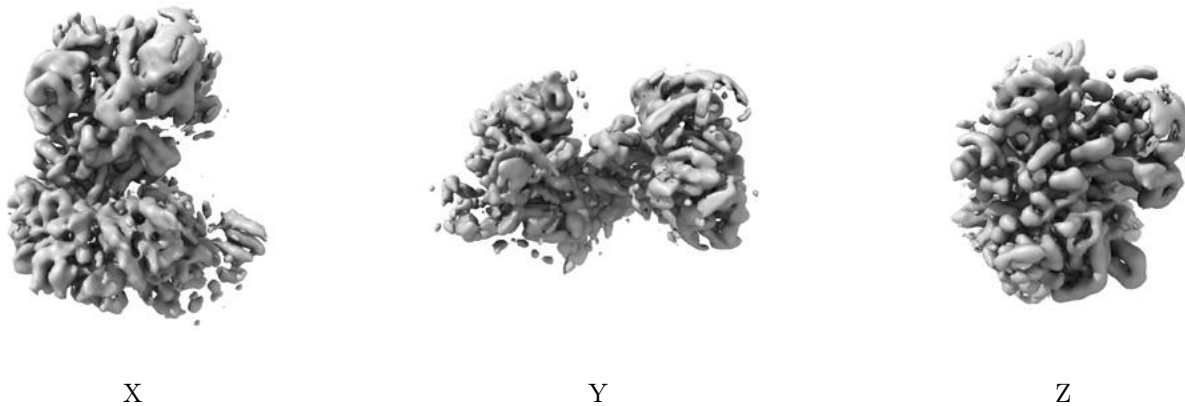
The images above show the 3D surface view of the map at the recommended contour level 2.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X   Y   Z
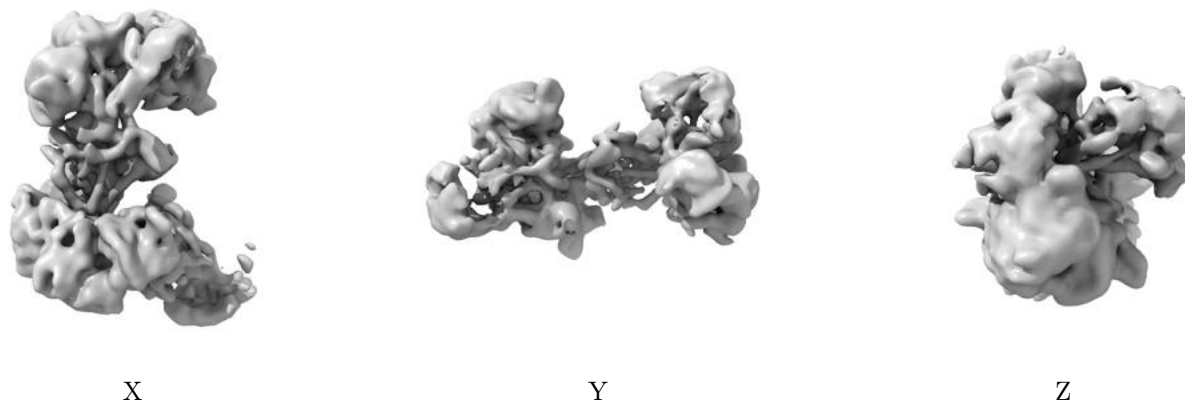
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 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 ⓘ
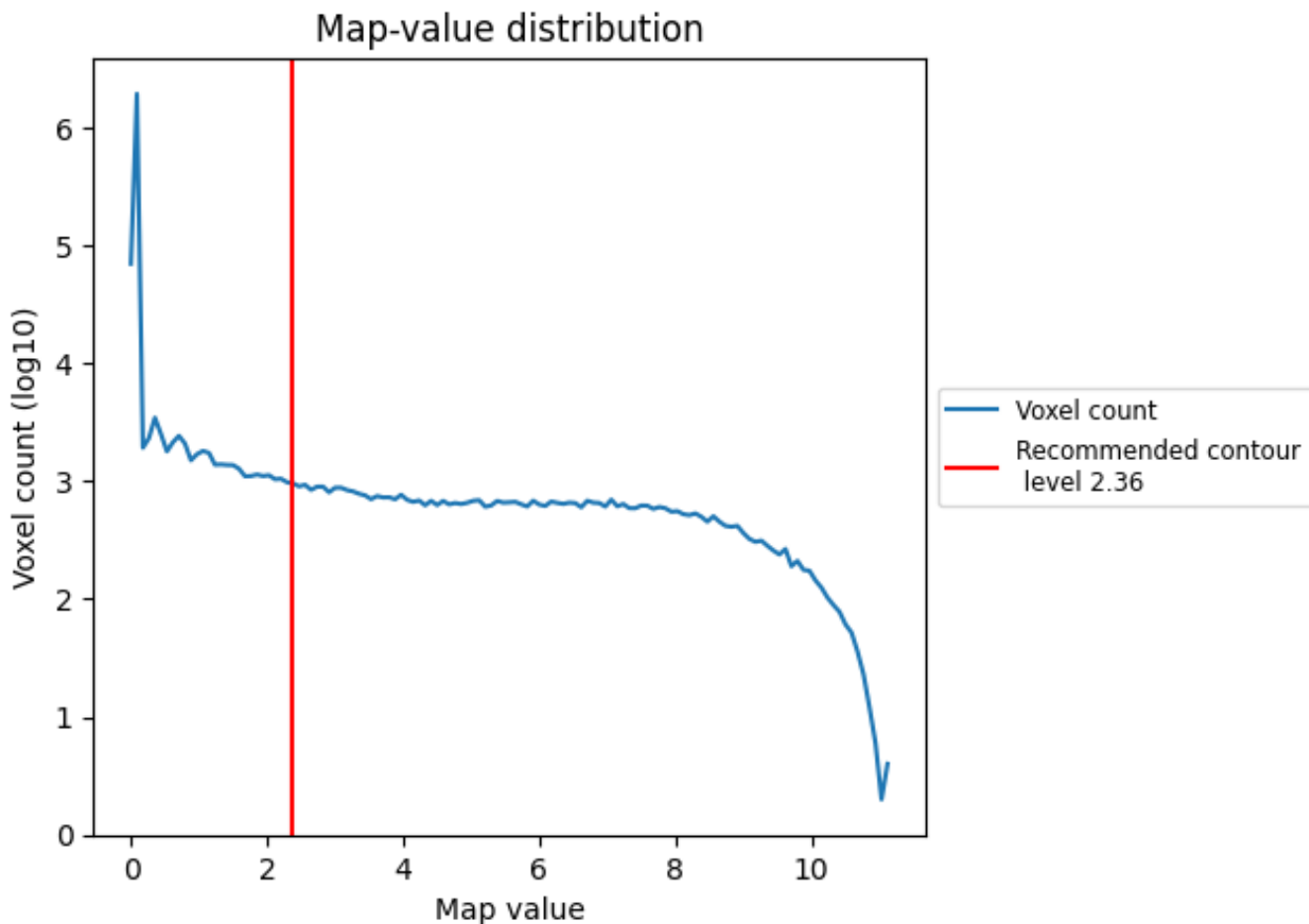
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
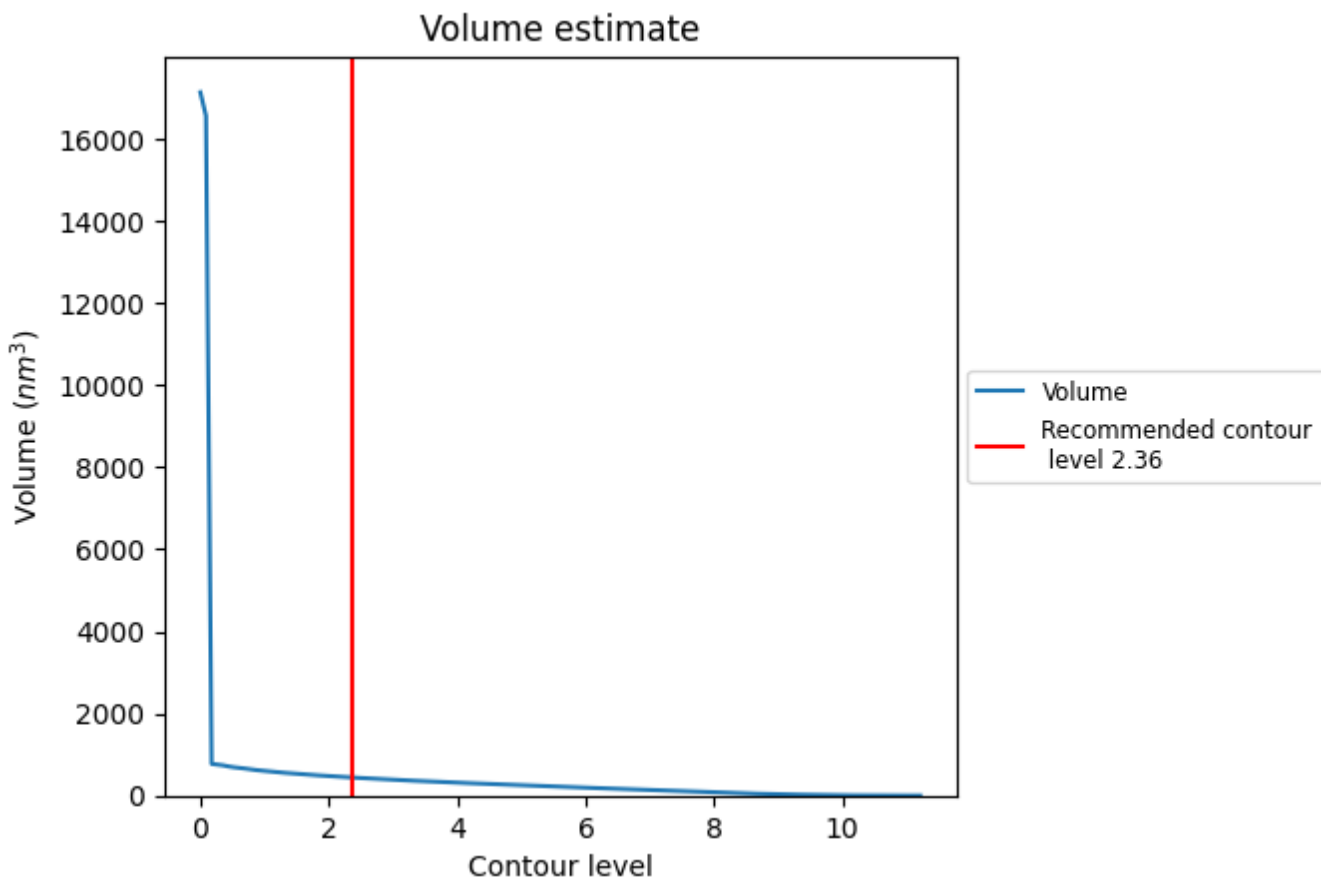
The volume at the recommended contour level is 440 nm^3; this corresponds to an approximate mass of 398 kDa.

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)
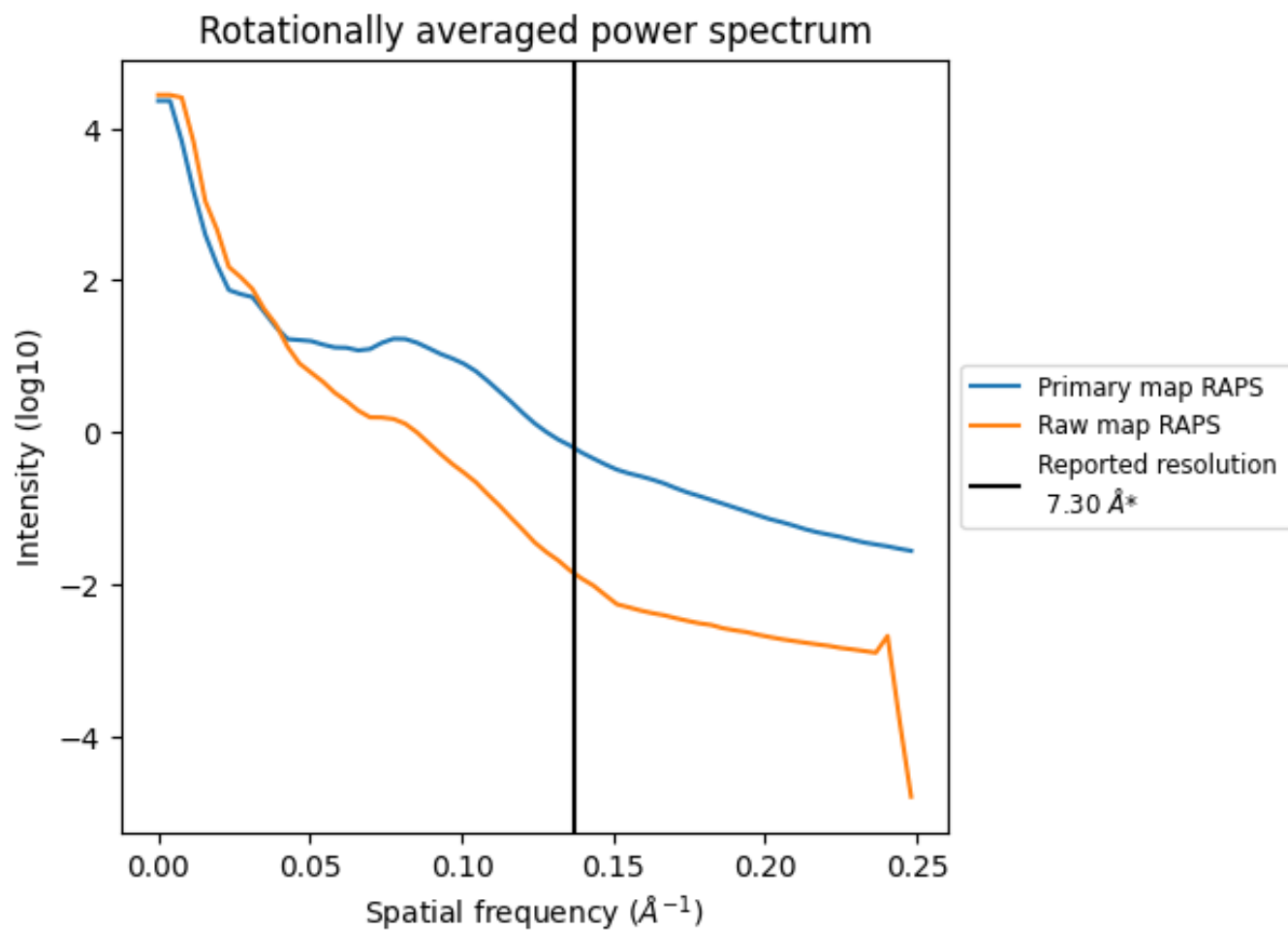
*Reported resolution corresponds to spatial frequency of 0.137 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ
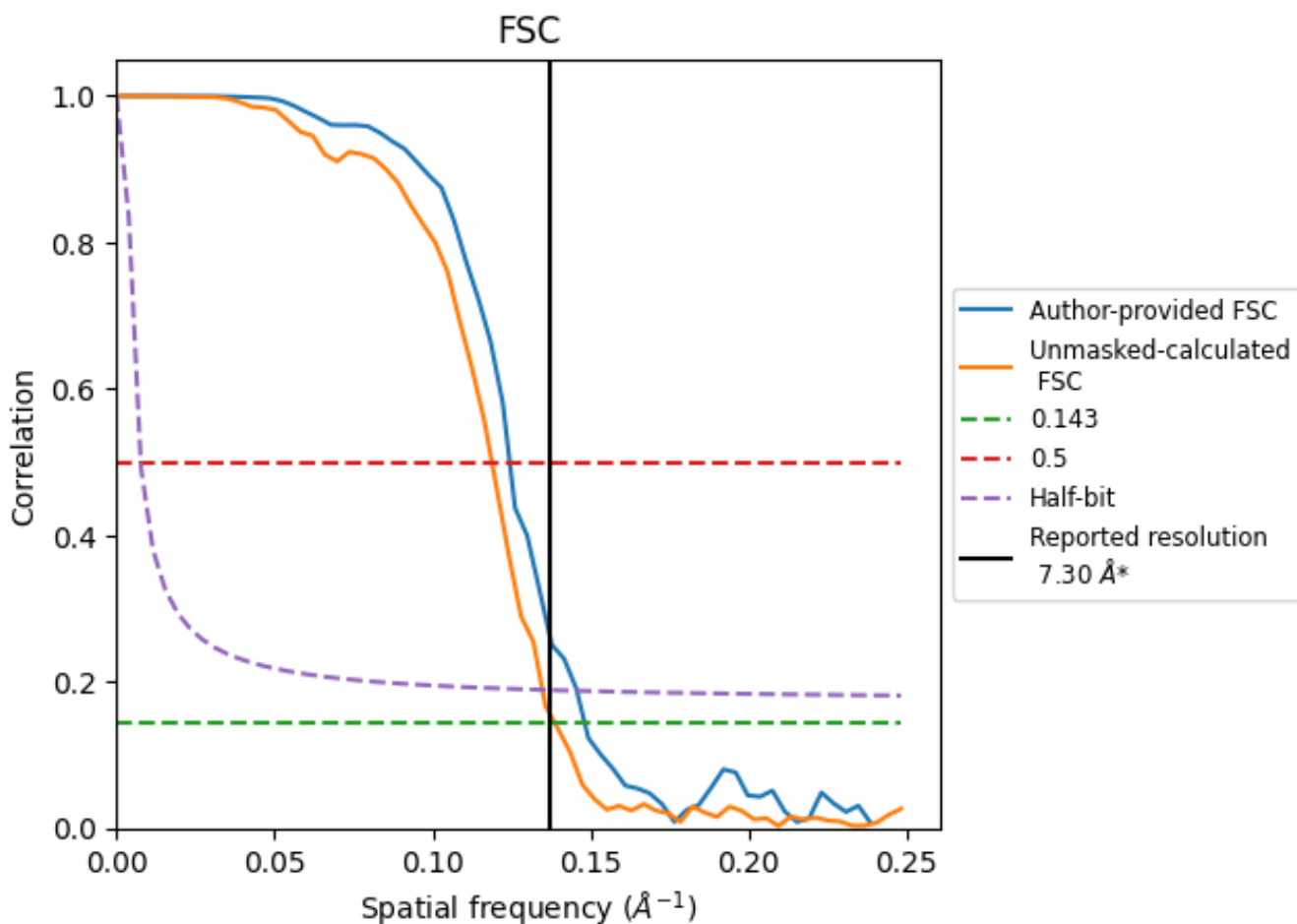
*Reported resolution corresponds to spatial frequency of 0.137 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	6.75	8.04	6.86
Unmasked-calculated*	7.21	8.42	7.42

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

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40758 and PDB model 8STA. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)

X	Y	Z
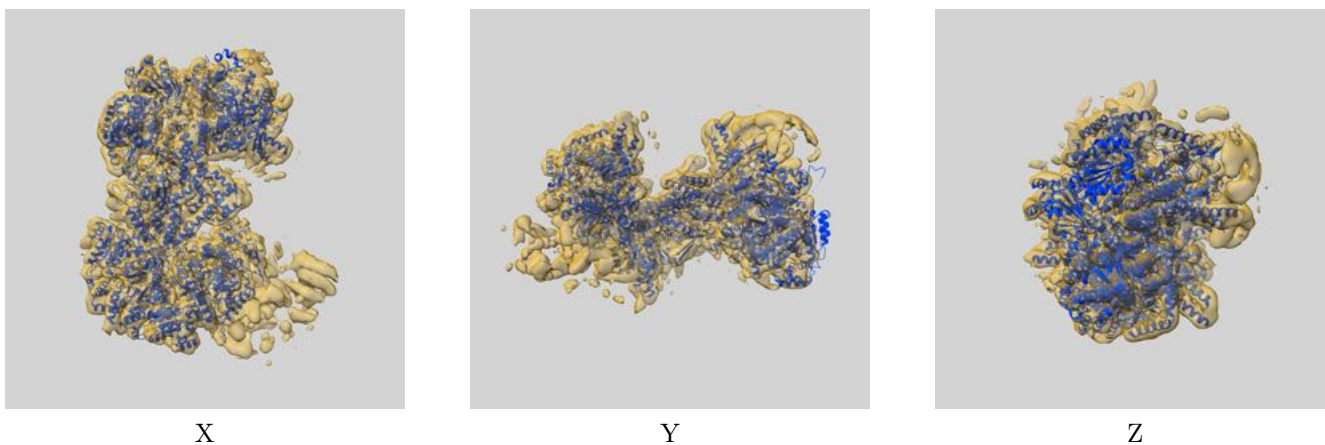
The images above show the 3D surface view of the map at the recommended contour level 2.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X   Y   Z
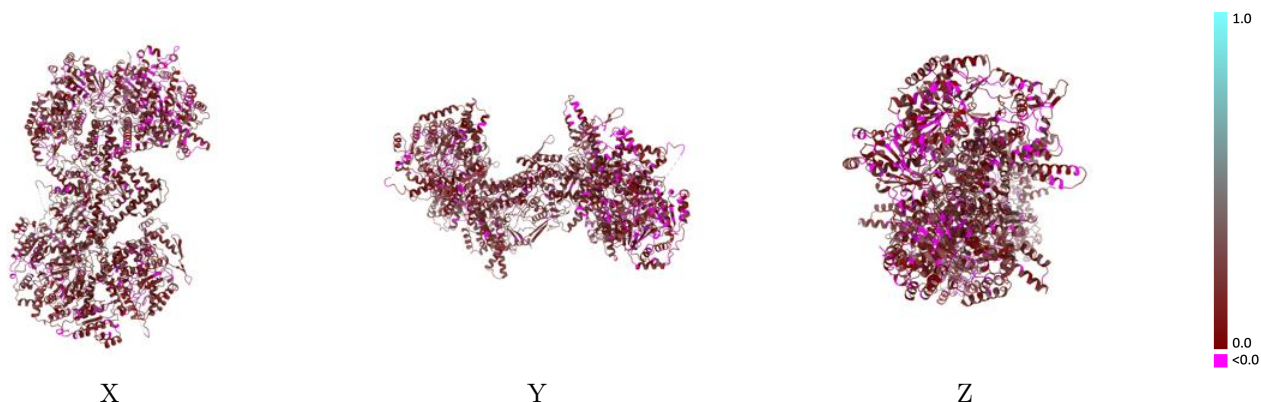
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ

X   Y   Z
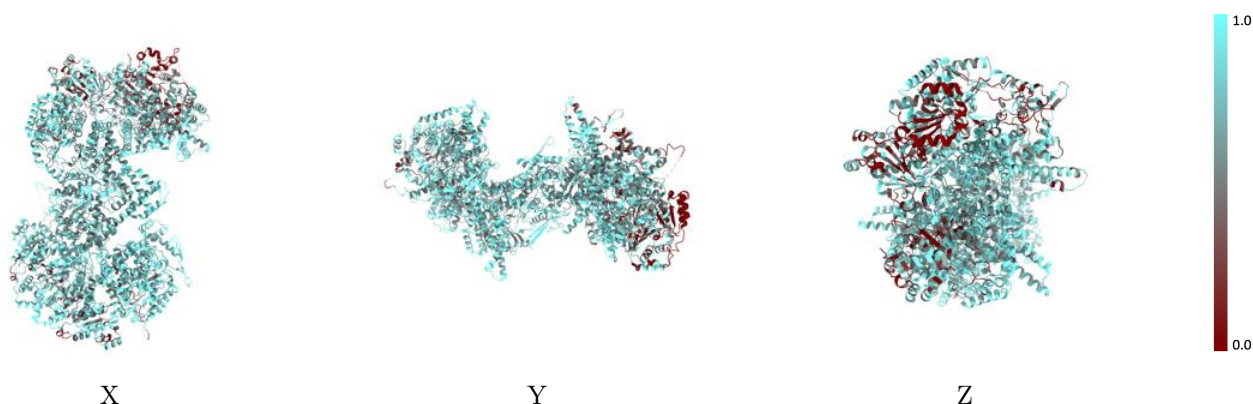
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.36).

9.4   Atom inclusion   ⓘ
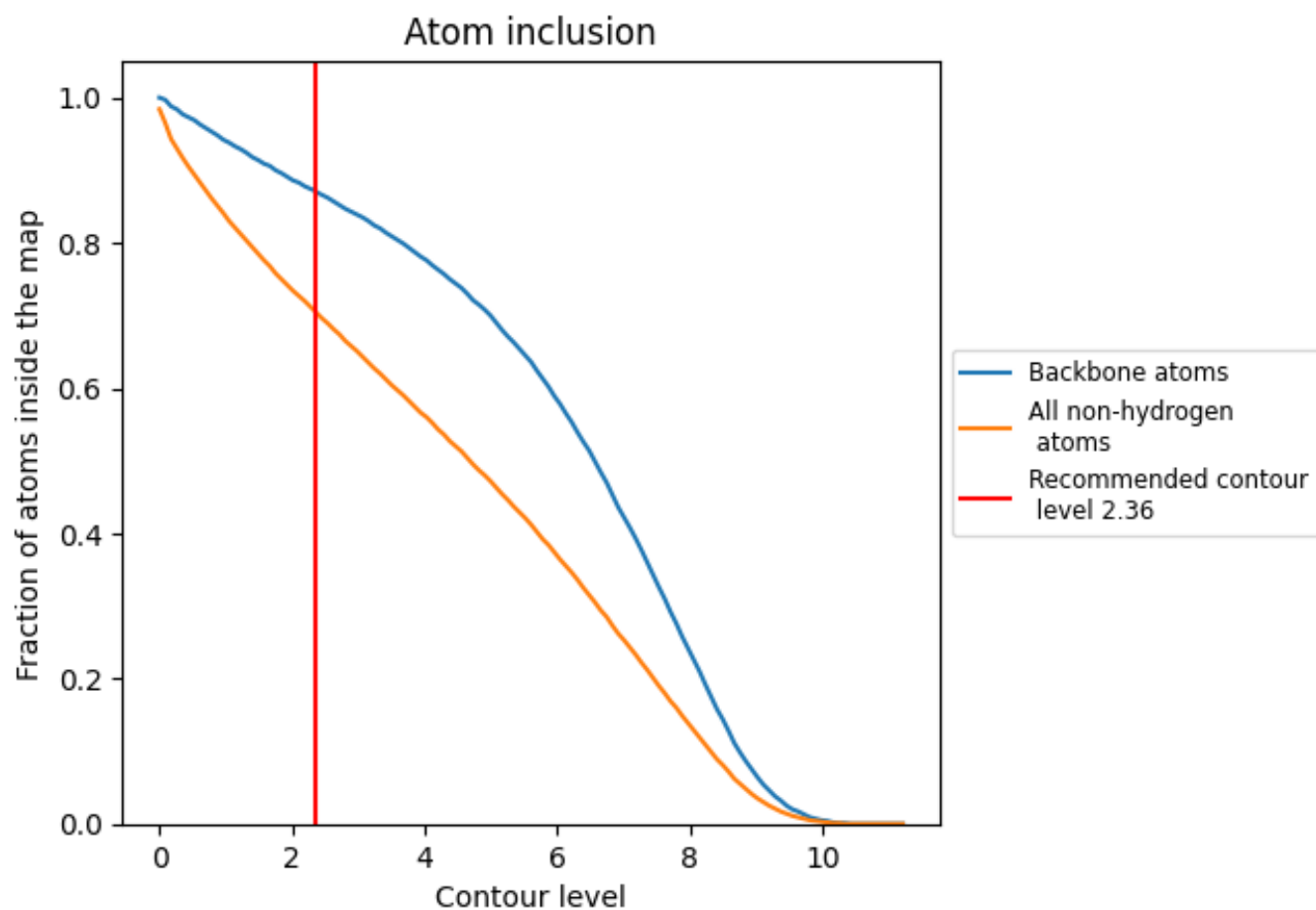
At the recommended contour level, 87% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.1490
A	0.7720	0.1720
B	0.7030	0.1500
C	0.5940	0.1150
D	0.7480	0.1600

1.0

0.0
<0.0