Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:47 PM UTC

PDB ID	:	8VLE / pdb_00008vle
EMDB ID	:	EMD-43337
Title	:	Composite structure of human FASN with NADPH in State 1
Authors	:	Schultz, K.; Marmorstein, R.
Deposited on	:	2024-01-11
Resolution	:	3.30 Å(reported)
Based on initial models	:	., 3HHD

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

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

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

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

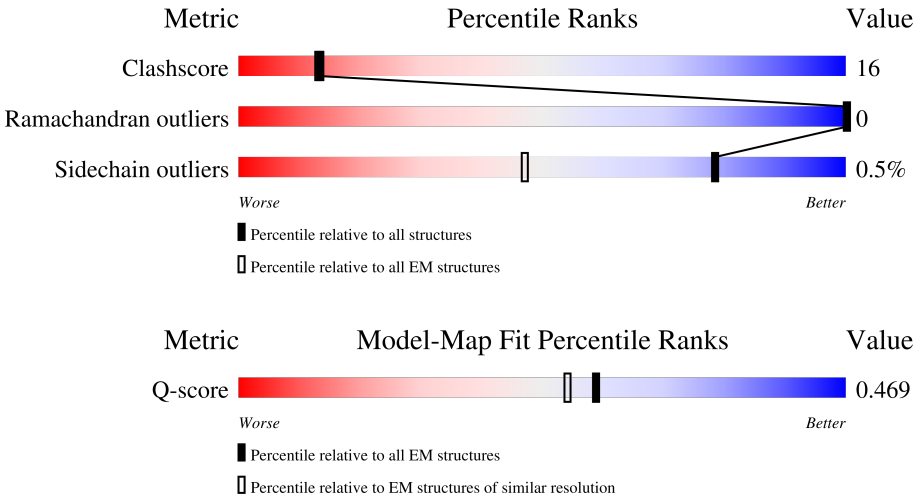
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	2553	59% 22% 19%
1	B	2553	59% 22% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 50715 atoms, of which 18833 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2068	Total	C	H	N	O	S	0	0
			25182	10041	9349	2785	2934	73		
1	B	2071	Total	C	H	N	O	S	0	0
			25237	10054	9380	2789	2941	73		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	expression tag	UNP P49327
A	-30	SER	-	expression tag	UNP P49327
A	-29	TYR	-	expression tag	UNP P49327
A	-28	TYR	-	expression tag	UNP P49327
A	-27	ASP	-	expression tag	UNP P49327
A	-26	TYR	-	expression tag	UNP P49327
A	-25	LYS	-	expression tag	UNP P49327
A	-24	ASP	-	expression tag	UNP P49327
A	-23	ASP	-	expression tag	UNP P49327
A	-22	ASP	-	expression tag	UNP P49327
A	-21	ASP	-	expression tag	UNP P49327
A	-20	LYS	-	expression tag	UNP P49327
A	-19	ASP	-	expression tag	UNP P49327
A	-18	TYR	-	expression tag	UNP P49327
A	-17	ASP	-	expression tag	UNP P49327
A	-16	ILE	-	expression tag	UNP P49327
A	-15	PRO	-	expression tag	UNP P49327
A	-14	THR	-	expression tag	UNP P49327
A	-13	THR	-	expression tag	UNP P49327
A	-12	GLU	-	expression tag	UNP P49327
A	-11	ASN	-	expression tag	UNP P49327
A	-10	LEU	-	expression tag	UNP P49327
A	-9	TYR	-	expression tag	UNP P49327
A	-8	PHE	-	expression tag	UNP P49327
A	-7	GLN	-	expression tag	UNP P49327
A	-6	GLY	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
A	1151	THR	LYS	conflict	UNP P49327
A	2512	LEU	-	expression tag	UNP P49327
A	2513	GLU	-	expression tag	UNP P49327
A	2514	HIS	-	expression tag	UNP P49327
A	2515	HIS	-	expression tag	UNP P49327
A	2516	HIS	-	expression tag	UNP P49327
A	2517	HIS	-	expression tag	UNP P49327
A	2518	HIS	-	expression tag	UNP P49327
A	2519	HIS	-	expression tag	UNP P49327
A	2520	HIS	-	expression tag	UNP P49327
A	2521	HIS	-	expression tag	UNP P49327
B	-31	MET	-	expression tag	UNP P49327
B	-30	SER	-	expression tag	UNP P49327
B	-29	TYR	-	expression tag	UNP P49327
B	-28	TYR	-	expression tag	UNP P49327
B	-27	ASP	-	expression tag	UNP P49327
B	-26	TYR	-	expression tag	UNP P49327
B	-25	LYS	-	expression tag	UNP P49327
B	-24	ASP	-	expression tag	UNP P49327
B	-23	ASP	-	expression tag	UNP P49327
B	-22	ASP	-	expression tag	UNP P49327
B	-21	ASP	-	expression tag	UNP P49327
B	-20	LYS	-	expression tag	UNP P49327
B	-19	ASP	-	expression tag	UNP P49327
B	-18	TYR	-	expression tag	UNP P49327
B	-17	ASP	-	expression tag	UNP P49327
B	-16	ILE	-	expression tag	UNP P49327
B	-15	PRO	-	expression tag	UNP P49327
B	-14	THR	-	expression tag	UNP P49327
B	-13	THR	-	expression tag	UNP P49327
B	-12	GLU	-	expression tag	UNP P49327
B	-11	ASN	-	expression tag	UNP P49327
B	-10	LEU	-	expression tag	UNP P49327
B	-9	TYR	-	expression tag	UNP P49327
B	-8	PHE	-	expression tag	UNP P49327

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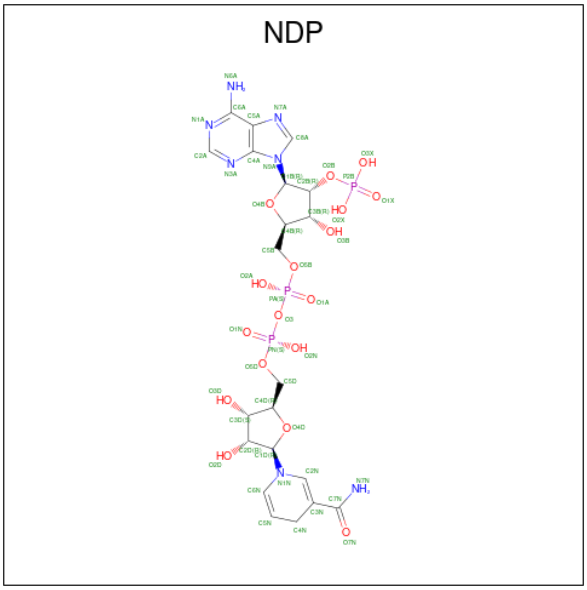
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLN	-	expression tag	UNP P49327
B	-6	GLY	-	expression tag	UNP P49327
B	-5	ALA	-	expression tag	UNP P49327
B	-4	MET	-	expression tag	UNP P49327
B	-3	GLY	-	expression tag	UNP P49327
B	-2	SER	-	expression tag	UNP P49327
B	-1	GLY	-	expression tag	UNP P49327
B	0	ILE	-	expression tag	UNP P49327
B	1	PRO	-	expression tag	UNP P49327
B	1151	THR	LYS	conflict	UNP P49327
B	2512	LEU	-	expression tag	UNP P49327
B	2513	GLU	-	expression tag	UNP P49327
B	2514	HIS	-	expression tag	UNP P49327
B	2515	HIS	-	expression tag	UNP P49327
B	2516	HIS	-	expression tag	UNP P49327
B	2517	HIS	-	expression tag	UNP P49327
B	2518	HIS	-	expression tag	UNP P49327
B	2519	HIS	-	expression tag	UNP P49327
B	2520	HIS	-	expression tag	UNP P49327
B	2521	HIS	-	expression tag	UNP P49327

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



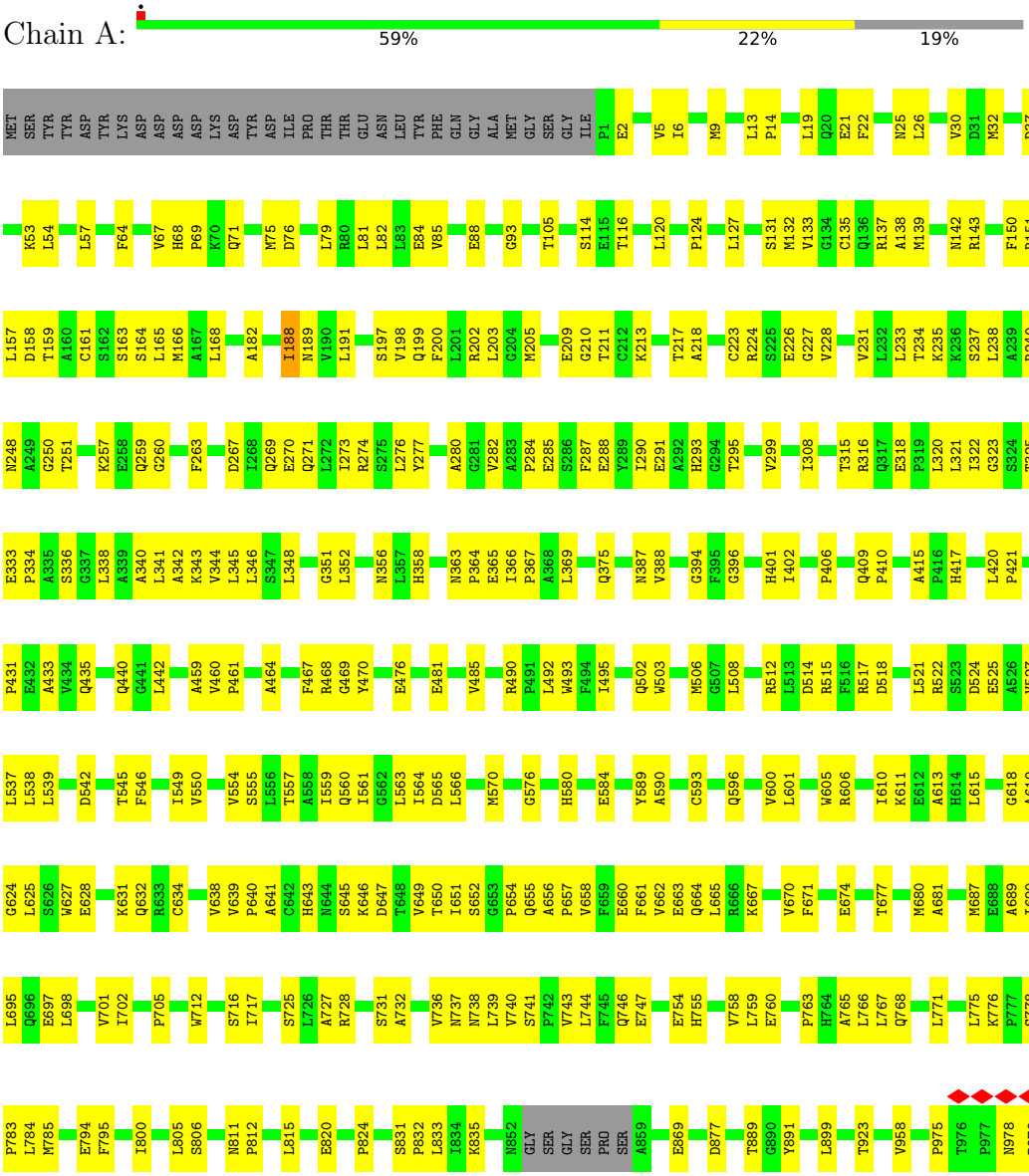
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

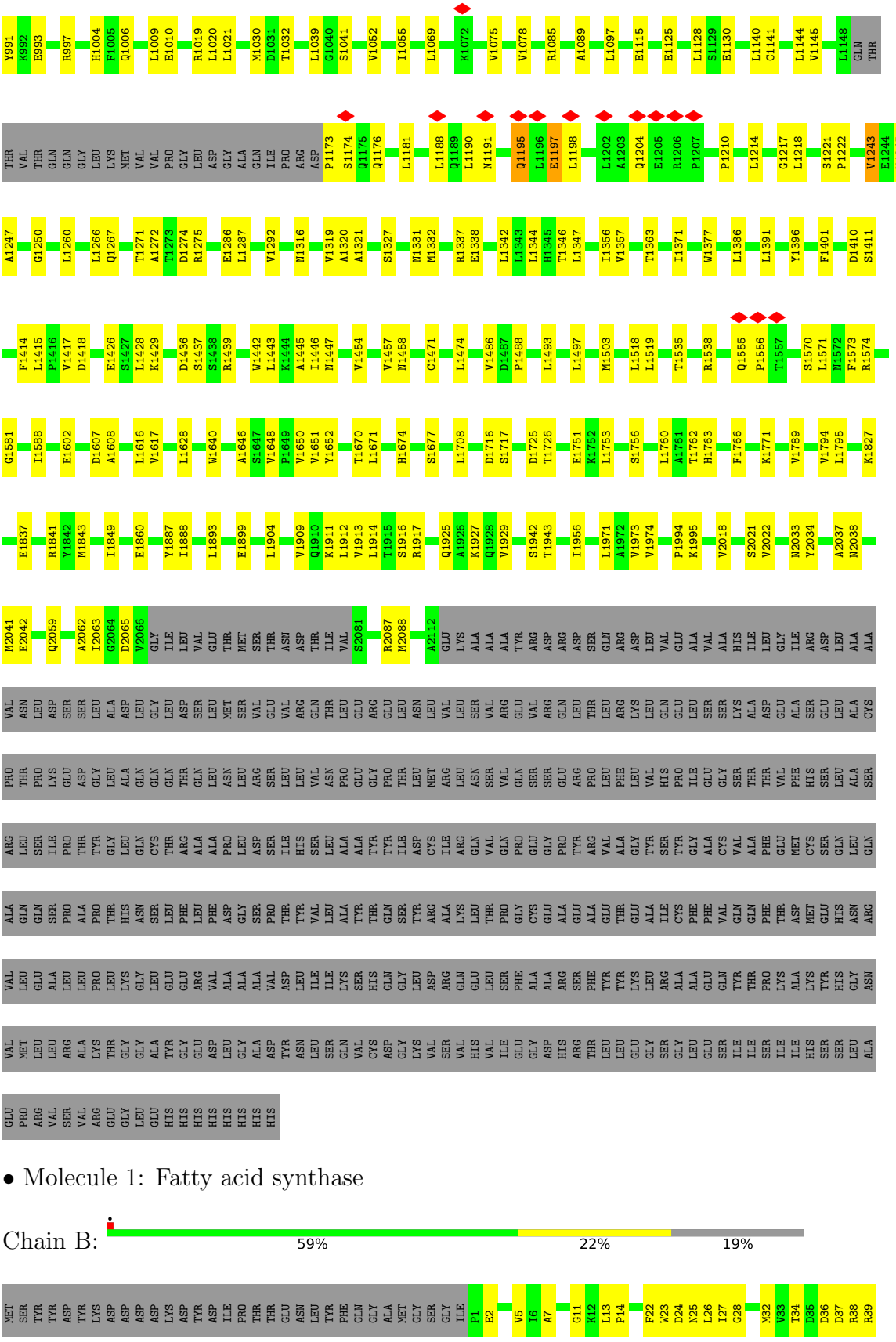
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fatty acid synthase

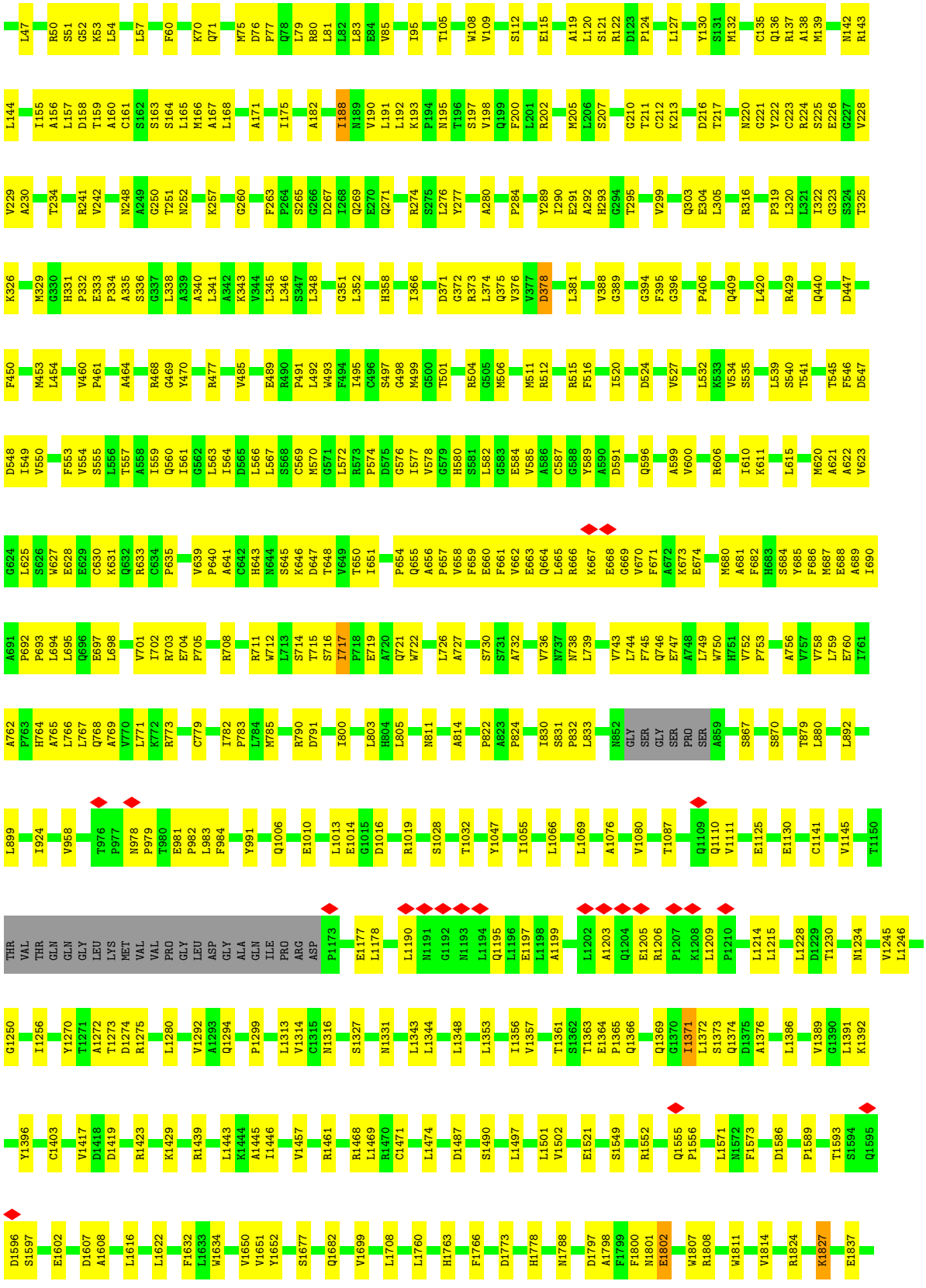
Chain A:

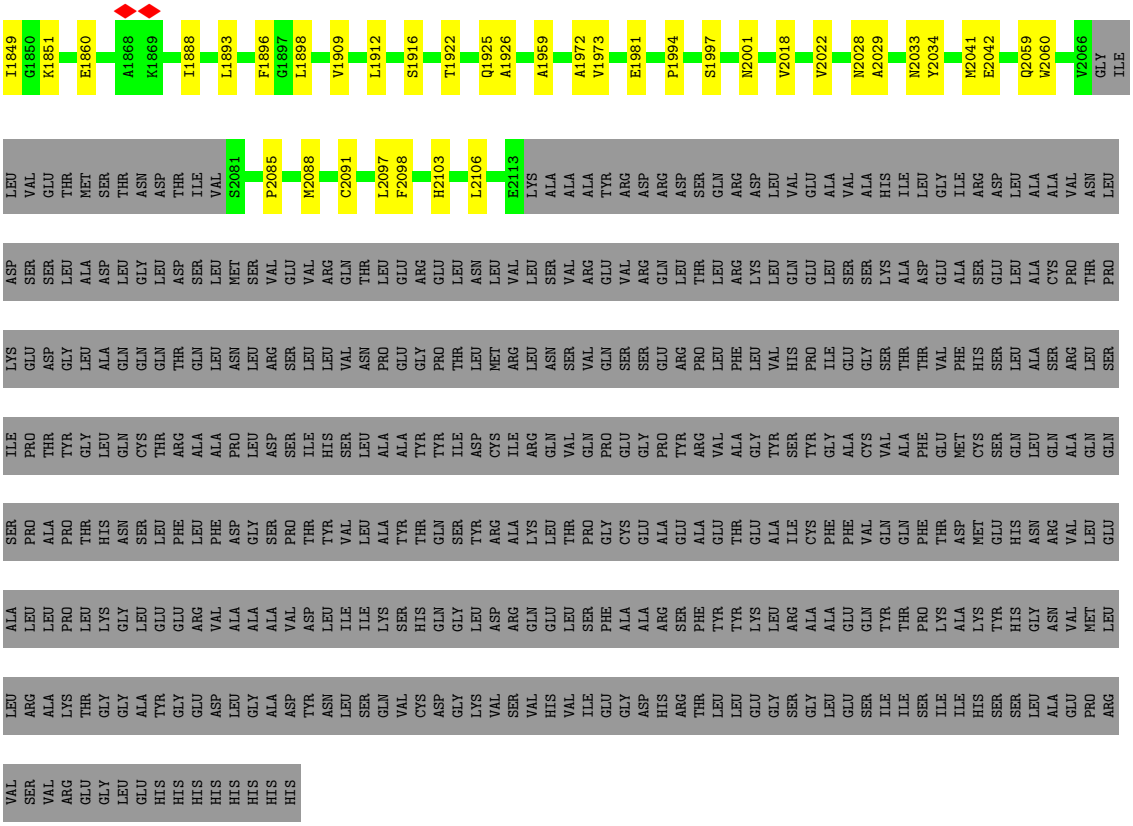




• Molecule 1: Fatty acid synthase

Chain B:


L47 R50 S51 G52 K53 L54 L57 F60 K70 Q71 M75 D76 P77 Q78 L79 R80 L81 L82 L83 E84 V85 I95 T105 W108 V109 S112 E115 A119 L120 S121 R122 D123 P124 L127 Y130 S131 M132 C135 Q136 R137 A138 M139 N142 R143
L144 I155 A156 L157 D158 T159 A160 C161 S162 S163 S164 L165 M166 A167 L168 A171 I175 A182 I188 N189 V190 L191 L192 K193 P194 N195 T196 S197 V198 Q199 F200 L201 R202 M205 L206 S207 G210 T211 C212 K213 D216 T217 N220 G221 Y222 C223 R224 S225 E226 G227 V228
V229 A230 T234 R241 V242 N248 A249 G250 T251 N252 K257 G260 F263 P264 S265 G266 D267 I268 Q269 E270 Q271 R274 S275 L276 Y277 A280 P284 Y289 I290 E291 A292 H293 G294 T295 V299 Q303 E304 L305 R316 P319 L320 L321 I322 G323 S324 T325
K326 M329 G330 H331 P332 E333 P334 A335 S336 G337 L338 A339 A340 L341 A342 K343 V344 L345 L346 S347 L348 G351 L352 H358 I366 D371 G372 R373 L374 Q375 V376 V377 D378 L381 V388 G389 G394 F395 G396 P406 Q409 L420 R429 Q440 D447
F450 M453 L454 V460 P461 A464 R468 G469 Y470 R477 V485 E489 R490 P491 L492 W493 F494 I495 C496 S497 G498 M499 G500 T501 R504 G505 M506 M511 R512 R515 F516 I520 D524 V527 L532 K533 V534 S535 L539 S540 T541 T545 F546 D547
D548 I549 V550 F553 V554 S555 L556 T557 A558 I559 Q560 I561 G562 L563 I564 D565 L566 L567 S568 C569 M570 G571 L572 R573 P574 D575 G576 I577 V578 G579 H580 S581 L582 G583 E584 V585 A586 C587 G588 Y589 A590 D591 Q596 A599 V600 R606 I610 K611 L615 M620 A621 A622 V623
G624 L625 S626 W627 E628 E629 C630 K631 Q632 R633 C634 P635 V639 P640 A641 C642 H643 N644 S645 K646 D647 T648 V649 T650 I651 P654 Q655 A656 P657 V658 F659 E660 F661 V662 E663 Q664 L665 R666 K667 E668 G669 V670 F671 A672 K673 E674 M680 A681 F682 H683 S684 Y685 F686 M687 E688 A689 I690
A691 P692 P693 L694 L695 Q696 E697 L698 V701 I702 R703 E704 P705 R708 R711 W712 L713 S714 T715 S716 I717 P718 E719 A720 Q721 W722 L726 A727 S730 S731 A732 V736 N737 N738 L739 V743 L744 F745 Q746 E747 A748 L749 W750 H751 V752 P753 A756 V757 V758 L759 E760 I761
A762 P763 H764 A765 L766 L767 Q768 A769 V770 L771 K772 R773 C779 I782 P783 L784 M785 R790 D791 I800 L803 H804 L805 N811 A814 P822 A823 P824 I830 S831 P832 L833 N852 GLY SER GLY SER PRO SER A859 S867 S870 T879 L880 L892
L899 I924 V958 T976 P977 N978 P979 T980 E981 P982 L983 F984 Y991 Q1006 E1010 L1013 E1014 G1015 D1016 R1019 S1028 T1032 Y1047 I1055 L1066 L1069 A1076 V1080 T1087 Q1109 Q1110 V1111 E1125 E1130 C1141 V1145 T1150
THR VAL THR GLN GLN GLY LEU LYS MET VAL VAL PRO GLY LEU ASP GLY ALA GLN ILE PRO ARG ASP P1173 E1177 L1178 L1190 N1191 G1192 N1193 L1194 Q1195 L1196 E1197 L1198 A1199 L1202 A1203 Q1204 E1205 R1206 P1207 K1208 L1209 P1210 L1214 L1215 L1228 D1229 T1230 N1234 V1245 L1246
G1250 I1256 Y1270 T1271 A1272 T1273 D1274 R1275 L1280 V1292 A1293 Q1294 P1299 L1313 V1314 C1315 N1316 S1327 N1331 L1343 L1344 L1348 L1353 I1356 V1357 T1361 S1362 T1363 E1364 P1365 Q1366 Q1369 G1370 I1371 L1372 S1373 Q1374 D1375 A1376 L1386 V1389 G1390 L1391 K1392
Y1396 C1403 V1417 D1418 D1419 R1423 K1429 R1439 L1443 K1444 A1445 I1446 V1457 R1461 R1468 L1469 R1470 C1471 L1474 D1487 S1490 L1497 L1501 V1502 E1521 S1549 R1552 Q1555 P1556 L1571 N1572 F1573 D1586 P1589 T1593 S1594 Q1595
D1596 S1597 E1602 D1607 A1608 L1616 L1622 F1632 L1633 W1634 V1650 V1651 Y1652 S1677 Q1682 V1699 L1708 L1760 H1763 F1766 D1773 H1778 N1788 D1797 A1798 F1799 F1800 N1801 E1802 W1807 R1808 W1811 V1814 R1824 K1827 E1837


I1849 G1850 K1851 E1860 A1868 K1869 I1888 L1893 F1896 G1897 L1898 V1909 L1912 S1916 T1922 Q1925 A1926 A1959 A1972 V1973 E1981 P1994 S1997 N2001 V2018 V2022 N2028 A2029 N2033 Y2034 M2041 E2042 Q2059 W2060 V2066 GLY ILE
LEU VAL GLU THR MET SER THR ASN ASP THR ILE VAL S2081 P2085 M2088 C2091 L2097 F2098 H2103 L2106 E2113 LYS ALA ALA ALA TYR ARG ASP ARG ASP SER GLN ARG ASP LEU VAL GLU ALA VAL ALA HIS ILE LEU GLY ILE ARG ASP LEU ALA ALA VAL ASN LEU
ASP SER SER LEU ALA ASP LEU GLY LEU ASP SER LEU MET SER VAL GLU VAL ARG GLN THR LEU GLU GLU LEU ASN LEU VAL LEU SER VAL ARG GLU VAL ARG GLN LEU THR LEU ARG LYS LEU GLN LEU SER GLU ALA ALA SER GLU LEU ALA CYS PRO THR PRO
LYS GLU ASP GLY LEU ALA GLN GLN GLN THR GLN LEU ASN LEU ARG SER LEU LEU VAL ASN PRO GLU GLY PRO THR LEU MET ARG LEU ASN SER VAL GLN SER SER GLU ARG PRO LEU PHE LEU VAL HIS PRO ILE GLU GLY SER THR THR VAL PHE HIS SER LEU ALA SER ARG LEU SER
ILE PRO THR TYR GLY LEU GLN CYS THR ARG ALA ALA PRO LEU ASP SER ILE HIS SER LEU ALA ALA TYR THR TYR ILE ASP CYS ILE ARG GLN VAL GLN PRO GLU GLY PRO TYR ARG VAL ALA GLY TYR SER TYR GLY ALA CYS VAL ALA PHE GLU MET CYS SER GLN LEU GLN GLN
SER PRO ALA PRO THR HIS ASN SER LEU PHE LEU PHE ASP GLY SER PRO THR TYR VAL LEU ALA TYR THR GLN SER TYR ARG ALA LYS LEU THR PRO GLY CYS GLU ALA GLU ALA GLU THR GLU GLU ALA ILE CYS PHE PHE VAL GLN GLN PHE THR ASP MET GLU HIS ASN ARG VAL LEU GLU
ALA LEU LEU PRO LEU LYS GLY LEU GLU GLU ARG VAL ALA ALA ALA VAL ASP LEU ILE ILE LYS SER HIS GLN GLY LEU ASP ARG GLN GLU LEU SER PHE ALA ALA ARG SER PHE TYR TYR LYS LEU ARG ALA ALA GLU GLN TYR THR PRO LYS ALA LYS TYR HIS GLY ASN VAL MET LEU
LEU ARG ALA LYS THR GLY GLY GLU ALA TYR GLY GLU ASP LEU GLY ALA ASP TYR ASN LEU SER GLN VAL CYS ASP GLY LYS VAL SER VAL HIS VAL ILE GLU GLY ASP HIS ARG THR LEU LEU GLU GLY SER GLY LEU GLU SER ILE ILE SER ILE ILE HIS SER SER LEU ALA GLU PRO ARG
VAL SER VAL ARG GLU GLY LEU GLU HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.750	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.171	Depositor
Map size (Å)	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/16198	0.32	6/22023 (0.0%)
1	B	0.19	0/16222	0.34	1/22055 (0.0%)
All	All	0.17	0/32420	0.33	7/44078 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1195	GLN	N-CA-C	-9.62	100.87	111.36
1	A	1197	GLU	N-CA-C	6.86	118.75	111.28
1	A	979	PRO	N-CA-C	-6.29	104.79	113.53
1	A	237	SER	N-CA-C	6.08	117.57	111.07
1	B	1814	VAL	N-CA-C	-5.75	104.73	111.00
1	A	975	PRO	N-CA-C	-5.71	105.59	113.53
1	A	39	ARG	N-CA-C	5.62	118.26	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15833	9349	15809	532	0
1	B	15857	9380	15826	510	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	96	52	52	23	0
2	B	96	52	52	11	0
All	All	31882	18833	31739	1027	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 16.

All (1027) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:PHE:CE2	1:B:665:LEU:HD11	1.80	1.15
1:A:1140:LEU:HD13	1:A:1174:SER:OG	1.50	1.11
1:A:1973:VAL:HB	2:A:2602:NDP:H3D	1.36	1.07
1:A:628:GLU:HA	1:A:631:LYS:HE2	1.33	1.05
1:A:619:ALA:HA	1:A:677:THR:HG21	1.36	1.03
1:B:716:SER:HB2	1:B:738:ASN:HD22	1.28	0.98
1:B:468:ARG:HD2	1:B:485:VAL:HG21	1.43	0.98
1:A:316:ARG:NH1	1:A:320:LEU:HD13	1.79	0.97
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.47	0.96
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.47	0.94
1:B:620:MET:HE1	1:B:682:PHE:HB2	1.49	0.94
1:A:2021:SER:HB2	2:A:2602:NDP:H6N	1.49	0.94
1:A:127:LEU:HD11	1:B:198:VAL:HG12	1.50	0.93
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.49	0.93
1:A:468:ARG:HD2	1:A:485:VAL:HG21	1.50	0.92
1:A:323:GLY:HA2	1:A:356:ASN:HD21	1.34	0.92
1:B:549:ILE:HD11	1:B:611:LYS:HG3	1.51	0.92
1:B:623:VAL:HG21	1:B:665:LEU:HD13	1.51	0.92
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.50	0.91
1:B:440:GLN:HG3	1:B:833:LEU:HD22	1.52	0.90
1:A:420:LEU:HD11	1:A:512:ARG:HB3	1.53	0.90
1:B:305:LEU:HD22	1:B:366:ILE:HD13	1.52	0.90
1:A:687:MET:HE2	1:A:739:LEU:HD11	1.53	0.88
1:A:646:LYS:HG3	1:A:647:ASP:OD1	1.72	0.88
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.56	0.88
1:B:1573:PHE:HD2	2:B:2601:NDP:O1A	1.58	0.86
1:B:164:SER:HB3	1:B:338:LEU:HG	1.56	0.86
1:A:1973:VAL:HG12	2:A:2602:NDP:O5B	1.76	0.84
1:B:290:ILE:HG23	1:B:322:ILE:HD12	1.58	0.84
1:A:640:PRO:HA	1:A:651:ILE:HG22	1.59	0.83
1:A:570:MET:HE2	1:A:815:LEU:HD11	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.43	0.83
1:B:661:PHE:CD2	1:B:665:LEU:HD11	2.14	0.82
1:A:768:GLN:HG3	1:A:781:ILE:HG21	1.61	0.82
1:A:1085:ARG:NH2	1:A:1097:LEU:O	2.13	0.81
1:B:1429:LYS:NZ	1:B:1981:GLU:O	2.14	0.81
1:A:139:MET:HE2	1:A:139:MET:HA	1.63	0.81
1:A:615:LEU:HB2	1:A:680:MET:HE1	1.62	0.81
1:A:2021:SER:OG	2:A:2602:NDP:H5N	1.79	0.81
1:B:322:ILE:HG21	1:B:374:LEU:HD21	1.63	0.80
1:A:623:VAL:HG12	1:A:625:LEU:H	1.45	0.80
1:B:293:HIS:N	1:B:304:GLU:OE2	2.13	0.79
1:A:549:ILE:HD11	1:A:611:LYS:HG3	1.64	0.79
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.64	0.79
1:B:633:ARG:NH2	1:B:668:GLU:OE2	2.15	0.78
1:B:250:GLY:HA3	1:B:276:LEU:HD21	1.65	0.78
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.64	0.78
1:A:1973:VAL:O	2:A:2602:NDP:H52A	1.83	0.78
1:A:189:ASN:HD22	1:A:334:PRO:HD2	1.49	0.78
1:B:429:ARG:NH1	1:B:464:ALA:O	2.16	0.78
1:B:1773:ASP:OD1	1:B:1778:HIS:ND1	2.17	0.77
1:B:305:LEU:HD23	1:B:366:ILE:HG21	1.67	0.77
1:A:274:ARG:HA	1:A:277:TYR:CE2	2.19	0.77
1:B:274:ARG:HA	1:B:277:TYR:CE2	2.19	0.77
1:B:1994:PRO:HB3	2:B:2602:NDP:H61A	1.50	0.77
1:A:213:LYS:HG2	1:A:358:HIS:HB3	1.65	0.77
1:A:1337:ARG:NH1	1:A:1338:GLU:O	2.18	0.77
1:B:1552:ARG:O	1:B:1555:GLN:NE2	2.18	0.76
1:A:316:ARG:HH12	1:A:320:LEU:HD13	1.49	0.76
1:A:1140:LEU:CD1	1:A:1174:SER:OG	2.31	0.76
1:B:1837:GLU:N	1:B:1837:GLU:OE1	2.19	0.76
1:B:705:PRO:HB3	1:B:730:SER:O	1.85	0.75
1:A:209:GLU:OE1	1:A:209:GLU:N	2.19	0.75
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.19	0.75
1:A:429:ARG:NH1	1:A:464:ALA:O	2.19	0.75
1:B:1327:SER:O	1:B:1331:ASN:ND2	2.19	0.75
1:B:596:GLN:O	1:B:600:VAL:HG23	1.86	0.75
1:B:1973:VAL:HG11	2:B:2602:NDP:H3D	1.68	0.75
1:A:692:PRO:O	1:A:695:LEU:HG	1.86	0.74
1:B:25:ASN:HB2	1:B:32:MET:HE2	1.70	0.74
1:B:216:ASP:OD1	1:B:217:THR:N	2.20	0.74
1:A:661:PHE:O	1:A:665:LEU:HG	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLU:OE1	1:A:628:GLU:N	2.20	0.74
1:A:21:GLU:O	1:A:25:ASN:ND2	2.20	0.74
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.69	0.74
1:A:620:MET:HB3	1:A:652:SER:HB2	1.70	0.73
1:A:625:LEU:HD21	1:A:670:VAL:HG11	1.70	0.73
1:A:784:LEU:O	1:A:785:MET:HG3	1.89	0.73
1:B:460:VAL:HG23	1:B:461:PRO:HD2	1.71	0.73
1:B:662:VAL:O	1:B:666:ARG:HG2	1.89	0.73
1:A:1995:LYS:HB3	1:A:2041:MET:SD	2.29	0.73
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.71	0.72
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.21	0.72
1:B:325:THR:HB	1:B:343:LYS:HD3	1.70	0.72
1:B:622:ALA:HA	1:B:650:THR:HA	1.71	0.72
1:A:1716:ASP:OD1	1:A:1717:SER:N	2.23	0.72
1:B:159:THR:CG2	1:B:163:SER:HA	2.19	0.72
1:B:1549:SER:O	1:B:1552:ARG:NH1	2.23	0.71
1:A:325:THR:HB	1:A:343:LYS:CD	2.20	0.71
1:B:623:VAL:HG11	1:B:665:LEU:HD22	1.71	0.71
1:A:716:SER:HB3	1:A:738:ASN:HD22	1.55	0.71
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.23	0.71
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.20	0.70
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.73	0.70
1:B:491:PRO:HG2	1:B:756:ALA:HA	1.73	0.70
1:B:765:ALA:HB1	1:B:768:GLN:HE21	1.55	0.70
1:A:737:ASN:OD1	1:A:741:SER:OG	2.09	0.70
1:B:71:GLN:HA	1:B:130:TYR:CE1	2.26	0.70
1:A:584:GLU:HG3	1:A:712:TRP:HZ2	1.56	0.70
1:A:596:GLN:O	1:A:600:VAL:HG23	1.91	0.70
1:B:322:ILE:CG2	1:B:374:LEU:HD21	2.21	0.70
1:A:522:ARG:NH1	1:A:596:GLN:OE1	2.24	0.70
1:B:1973:VAL:HG11	2:B:2602:NDP:C3D	2.21	0.70
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.74	0.70
1:B:651:ILE:O	1:B:651:ILE:HD12	1.91	0.70
1:B:124:PRO:HA	1:B:127:LEU:HD23	1.74	0.69
1:A:114:SER:OG	1:A:137:ARG:NH1	2.25	0.69
1:B:504:ARG:HH21	1:B:541:THR:HB	1.56	0.69
1:A:1973:VAL:O	2:A:2602:NDP:C5B	2.40	0.69
1:A:54:LEU:HD12	1:A:57:LEU:HD21	1.74	0.69
1:A:2021:SER:HB2	2:A:2602:NDP:C6N	2.20	0.69
1:A:325:THR:HB	1:A:343:LYS:HD2	1.74	0.69
1:A:1010:GLU:OE2	1:A:1019:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ASP:OD2	1:B:712:TRP:HB2	1.93	0.69
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.75	0.69
1:B:1205:GLU:O	1:B:1209:LEU:N	2.25	0.69
1:A:732:ALA:O	1:A:736:VAL:HG23	1.93	0.68
1:B:623:VAL:HG21	1:B:665:LEU:CD1	2.23	0.68
1:A:624:GLY:N	1:A:671:PHE:O	2.22	0.68
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.08	0.68
1:A:165:LEU:HD11	1:A:402:ILE:HD12	1.75	0.68
1:B:623:VAL:HG13	1:B:671:PHE:O	1.93	0.68
1:A:420:LEU:HD21	1:A:512:ARG:HE	1.58	0.68
1:B:166:MET:HE1	1:B:251:THR:HG21	1.75	0.68
1:B:163:SER:OG	1:B:334:PRO:HB3	1.93	0.67
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.75	0.67
1:A:820:GLU:OE1	1:A:820:GLU:N	2.26	0.67
1:A:132:MET:HE2	1:B:200:PHE:CZ	2.29	0.67
1:A:624:GLY:HA3	1:A:671:PHE:HB3	1.76	0.67
1:A:627:TRP:HA	1:A:649:VAL:HG21	1.75	0.67
1:B:1973:VAL:CG1	2:B:2602:NDP:H3D	2.23	0.67
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.28	0.67
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.24	0.66
1:A:620:MET:HB3	1:A:652:SER:CB	2.23	0.66
1:A:1538:ARG:NH2	1:A:1581:GLY:O	2.29	0.66
1:A:539:LEU:HD23	1:A:539:LEU:O	1.95	0.66
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.78	0.66
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.78	0.66
1:A:631:LYS:HG3	1:A:632:GLN:OE1	1.95	0.66
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.28	0.66
1:A:639:VAL:HB	1:A:640:PRO:HD2	1.77	0.66
1:B:371:ASP:OD1	1:B:372:GLY:N	2.25	0.66
1:B:625:LEU:HD21	1:B:670:VAL:HG11	1.77	0.66
1:A:9:MET:HG2	1:A:19:LEU:HD11	1.77	0.66
1:A:767:LEU:O	1:A:771:LEU:HD13	1.96	0.66
1:A:124:PRO:HG3	1:B:195:ASN:OD1	1.96	0.65
1:A:365:GLU:O	1:A:367:PRO:HD3	1.96	0.65
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.26	0.65
1:A:1573:PHE:HE1	2:A:2601:NDP:N7A	1.93	0.65
1:B:1246:LEU:HD11	1:B:1299:PRO:HG3	1.76	0.65
1:B:182:ALA:CB	1:B:234:THR:HG22	2.25	0.65
1:A:14:PRO:O	1:A:32:MET:HE2	1.97	0.65
1:A:138:ALA:HB1	1:B:160:ALA:HB2	1.78	0.65
1:B:639:VAL:HG13	1:B:640:PRO:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.78	0.65
1:B:277:TYR:CE1	1:B:284:PRO:HG3	2.31	0.65
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.78	0.65
1:A:570:MET:HE2	1:A:815:LEU:HD21	1.78	0.65
1:B:38:ARG:NH1	1:B:54:LEU:O	2.30	0.65
1:A:277:TYR:CE1	1:A:284:PRO:HG3	2.31	0.65
1:B:166:MET:HE1	1:B:251:THR:CG2	2.26	0.65
1:A:725:SER:HA	1:A:728:ARG:NH1	2.12	0.65
1:A:161:CYS:HA	1:A:333:GLU:O	1.97	0.64
1:A:1570:SER:OG	1:A:1646:ALA:O	2.15	0.64
1:B:627:TRP:NE1	1:B:631:LYS:HE2	2.12	0.64
1:A:211:THR:HG22	1:A:213:LYS:HG3	1.79	0.64
1:A:621:ALA:CB	1:A:674:GLU:HA	2.27	0.64
1:B:2033:ASN:OD1	1:B:2034:TYR:N	2.31	0.64
1:A:623:VAL:HG13	1:A:665:LEU:HD13	1.79	0.64
1:A:693:PRO:O	1:A:697:GLU:HG2	1.97	0.64
1:A:318:GLU:OE1	1:A:318:GLU:N	2.23	0.64
1:A:580:HIS:HD2	1:A:743:VAL:HG11	1.61	0.64
1:A:1327:SER:O	1:A:1331:ASN:ND2	2.31	0.64
1:B:697:GLU:O	1:B:701:VAL:HG23	1.98	0.64
1:B:769:ALA:O	1:B:773:ARG:HG2	1.98	0.64
1:A:1795:LEU:HA	2:A:2601:NDP:H72N	1.61	0.64
1:B:535:SER:O	1:B:539:LEU:HG	1.98	0.64
1:B:627:TRP:HE1	1:B:631:LYS:HE2	1.61	0.63
1:A:139:MET:HE1	1:B:396:GLY:HA3	1.78	0.63
1:A:705:PRO:HB3	1:A:731:SER:HB3	1.79	0.63
1:B:658:VAL:O	1:B:662:VAL:HG23	1.97	0.63
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.80	0.63
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.32	0.63
1:A:217:THR:HG22	1:A:364:PRO:HD3	1.80	0.63
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.62	0.63
1:A:831:SER:OG	1:A:832:PRO:HD3	1.98	0.63
1:A:182:ALA:CB	1:A:234:THR:HG22	2.29	0.63
1:A:877:ASP:OD2	1:A:1004:HIS:ND1	2.31	0.63
1:A:1573:PHE:CE1	2:A:2601:NDP:N7A	2.67	0.63
1:A:189:ASN:ND2	1:A:333:GLU:OE1	2.31	0.62
1:A:2:GLU:HG2	1:A:235:LYS:HB2	1.80	0.62
1:A:550:VAL:HG23	1:A:611:LYS:HD3	1.81	0.62
1:B:1652:TYR:OH	1:B:1824:ARG:O	2.11	0.62
1:B:1896:PHE:CE1	1:B:2088:MET:HE1	2.34	0.62
1:A:1141:CYS:O	1:A:1145:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:GLN:NE2	1:B:783:PRO:HB3	2.14	0.62
1:B:1439:ARG:O	1:B:1468:ARG:NH1	2.32	0.62
1:B:576:GLY:C	1:B:577:ILE:HD12	2.24	0.62
1:A:363:ASN:HB3	1:A:366:ILE:HD13	1.81	0.62
1:B:549:ILE:CD1	1:B:611:LYS:HG3	2.27	0.62
1:A:658:VAL:O	1:A:662:VAL:HG23	2.00	0.62
1:A:625:LEU:CD2	1:A:670:VAL:HG11	2.30	0.62
1:A:776:LYS:H	1:A:776:LYS:HD2	1.65	0.62
1:B:625:LEU:CD2	1:B:670:VAL:HG11	2.28	0.62
1:A:1221:SER:HB2	1:A:1222:PRO:HD2	1.82	0.61
1:A:978:ASN:HB3	1:A:980:THR:CG2	2.30	0.61
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.33	0.61
1:B:257:LYS:HE3	1:B:263:PHE:O	1.99	0.61
1:B:695:LEU:HD12	1:B:732:ALA:HB1	1.82	0.61
1:A:570:MET:CE	1:A:815:LEU:HD11	2.29	0.61
1:B:289:TYR:OH	1:B:323:GLY:HA3	2.00	0.61
1:B:1195:GLN:O	1:B:1199:ALA:N	2.33	0.61
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.34	0.61
1:A:133:VAL:O	1:A:139:MET:HG3	2.00	0.61
1:A:1973:VAL:CG1	2:A:2602:NDP:O5B	2.47	0.61
1:A:657:PRO:O	1:A:660:GLU:HG2	1.99	0.61
1:A:1893:LEU:HD12	1:A:1916:SER:OG	1.99	0.61
1:B:319:PRO:HB3	1:B:372:GLY:O	2.01	0.61
1:B:524:ASP:OD1	1:B:534:VAL:HB	2.00	0.61
1:A:276:LEU:HD12	1:A:401:HIS:HB3	1.81	0.61
1:B:492:LEU:HD11	1:B:759:LEU:HD12	1.81	0.61
1:B:978:ASN:O	1:B:981:GLU:HG3	2.00	0.61
1:B:732:ALA:O	1:B:736:VAL:HG23	2.00	0.61
1:B:574:PRO:CG	1:B:577:ILE:HD11	2.31	0.60
1:B:290:ILE:HG23	1:B:322:ILE:CD1	2.30	0.60
1:B:305:LEU:HD22	1:B:366:ILE:CD1	2.28	0.60
1:B:1391:LEU:HD23	1:B:1392:LYS:N	2.15	0.60
1:A:425:ARG:HH22	1:A:459:ALA:HB2	1.67	0.60
1:A:517:ARG:O	1:A:521:LEU:HG	2.00	0.60
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.83	0.60
1:A:203:LEU:HD13	1:A:205:MET:HE3	1.82	0.60
1:B:1272:ALA:O	1:B:1294:GLN:NE2	2.34	0.60
1:B:1602:GLU:OE2	1:B:1851:LYS:NZ	2.35	0.60
1:A:158:ASP:O	1:B:138:ALA:HB2	2.02	0.60
1:A:420:LEU:CD2	1:A:512:ARG:HE	2.14	0.60
1:A:431:PRO:HG3	1:A:467:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ASN:HD22	1:B:280:ALA:HB2	1.67	0.60
1:B:662:VAL:HA	1:B:665:LEU:HD12	1.84	0.60
1:A:580:HIS:CD2	1:A:743:VAL:HG11	2.37	0.60
1:B:182:ALA:HB1	1:B:234:THR:HG22	1.84	0.60
1:B:501:THR:OG1	1:B:764:HIS:HB3	2.01	0.60
1:A:199:GLN:OE1	1:B:121:SER:HB3	2.01	0.60
1:A:506:MET:HE3	1:A:559:ILE:HD12	1.82	0.60
1:A:605:TRP:CD1	1:A:701:VAL:HG21	2.37	0.59
1:B:23:TRP:O	1:B:27:ILE:HG13	2.02	0.59
1:B:305:LEU:CD2	1:B:366:ILE:HD13	2.30	0.59
1:A:68:HIS:HB3	1:A:71:GLN:OE1	2.01	0.59
1:B:71:GLN:O	1:B:71:GLN:NE2	2.35	0.59
1:B:1677:SER:O	1:B:1682:GLN:NE2	2.33	0.59
1:A:248:ASN:HB2	1:A:280:ALA:HB2	1.84	0.59
1:A:663:GLU:O	1:A:667:LYS:HG2	2.02	0.59
1:B:674:GLU:N	1:B:674:GLU:OE1	2.35	0.59
1:B:79:LEU:O	1:B:83:LEU:HD13	2.01	0.59
1:A:127:LEU:HD12	1:A:127:LEU:O	2.03	0.59
1:B:1028:SER:O	1:B:1032:THR:HG23	2.03	0.59
1:A:645:SER:HA	1:A:746:GLN:HE21	1.67	0.59
1:B:574:PRO:HG2	1:B:577:ILE:HD11	1.84	0.59
1:B:704:GLU:HG2	1:B:704:GLU:O	2.03	0.59
1:B:1019:ARG:HH12	1:B:1069:LEU:HD13	1.67	0.59
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.38	0.59
1:A:166:MET:HE1	1:A:251:THR:OG1	2.03	0.59
1:B:325:THR:HB	1:B:343:LYS:CD	2.32	0.59
1:A:527:VAL:HG11	1:A:600:VAL:HG12	1.84	0.59
1:B:105:THR:HG23	1:B:182:ALA:O	2.03	0.58
1:B:1445:ALA:O	1:B:1446:ILE:HD13	2.03	0.58
1:B:491:PRO:HG2	1:B:756:ALA:CA	2.33	0.58
1:A:5:VAL:HB	1:A:242:VAL:HG13	1.85	0.58
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.86	0.58
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.33	0.58
1:B:2022:VAL:HG13	1:B:2060:TRP:O	2.03	0.58
1:A:687:MET:HB2	1:A:740:VAL:HG12	1.85	0.58
1:A:1973:VAL:CG1	2:A:2602:NDP:PA	2.92	0.58
1:A:2033:ASN:OD1	1:A:2034:TYR:N	2.36	0.58
1:B:25:ASN:CB	1:B:32:MET:HE2	2.33	0.58
1:B:625:LEU:HB2	1:B:630:CYS:SG	2.44	0.58
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.35	0.58
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:HB2	1:A:234:THR:HG22	1.84	0.58
1:A:1640:TRP:CZ3	1:A:1648:VAL:HG21	2.39	0.58
1:B:274:ARG:HA	1:B:277:TYR:CD2	2.39	0.58
1:B:550:VAL:O	1:B:554:VAL:HG23	2.02	0.58
1:B:645:SER:HA	1:B:746:GLN:HE21	1.67	0.58
1:B:1487:ASP:N	1:B:1490:SER:OG	2.36	0.58
1:B:305:LEU:CD2	1:B:366:ILE:HG21	2.32	0.58
1:B:717:ILE:HD12	1:B:717:ILE:O	2.04	0.58
1:B:584:GLU:HG3	1:B:738:ASN:ND2	2.19	0.58
1:B:2028:ASN:OD1	1:B:2029:ALA:N	2.36	0.58
1:A:213:LYS:HE2	1:A:218:ALA:O	2.03	0.57
1:B:51:SER:O	1:B:53:LYS:NZ	2.37	0.57
1:B:205:MET:O	1:B:221:GLY:HA3	2.04	0.57
1:B:570:MET:HE1	1:B:800:ILE:HD11	1.86	0.57
1:A:1357:VAL:HG23	1:A:1371:ILE:HD13	1.86	0.57
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.04	0.57
1:A:987:GLN:NE2	1:A:1006:GLN:O	2.37	0.57
1:A:1128:LEU:HD21	1:A:1217:GLY:C	2.30	0.57
1:B:570:MET:HE1	1:B:800:ILE:CD1	2.34	0.57
1:B:694:LEU:O	1:B:698:LEU:HG	2.05	0.57
1:A:267:ASP:O	1:A:271:GLN:HG3	2.04	0.57
1:B:222:TYR:HB3	1:B:295:THR:CG2	2.34	0.57
1:A:615:LEU:CB	1:A:680:MET:HE1	2.33	0.57
1:A:783:PRO:HB2	1:A:795:PHE:HE2	1.69	0.57
1:A:1218:LEU:O	1:A:1221:SER:OG	2.19	0.57
1:B:1199:ALA:O	1:B:1203:ALA:N	2.34	0.57
1:A:492:LEU:HD11	1:A:759:LEU:CD1	2.35	0.57
1:A:518:ASP:O	1:A:522:ARG:HG3	2.04	0.57
1:A:534:VAL:O	1:A:538:LEU:HG	2.05	0.57
1:B:248:ASN:HB2	1:B:280:ALA:HB2	1.86	0.57
1:B:491:PRO:HG2	1:B:756:ALA:CB	2.35	0.57
1:B:1014:GLU:N	1:B:1014:GLU:OE1	2.35	0.57
1:A:891:TYR:OH	1:A:923:THR:HG22	2.05	0.57
1:A:550:VAL:O	1:A:554:VAL:HG23	2.05	0.57
1:B:39:ARG:NH2	1:B:226:GLU:OE1	2.35	0.57
1:B:628:GLU:OE1	1:B:628:GLU:N	2.30	0.57
1:A:198:VAL:O	1:A:202:ARG:HG2	2.05	0.57
1:A:332:PRO:O	1:A:336:SER:HB3	2.05	0.57
1:B:198:VAL:O	1:B:202:ARG:HG2	2.04	0.57
1:B:497:SER:OG	1:B:501:THR:HG21	2.04	0.57
1:A:76:ASP:HA	1:A:116:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLY:CA	1:A:356:ASN:HD21	2.14	0.56
1:B:983:LEU:HD13	1:B:1922:THR:O	2.04	0.56
1:A:139:MET:HE2	1:A:142:ASN:HB2	1.87	0.56
1:A:287:PHE:O	1:A:316:ARG:NH2	2.38	0.56
1:A:657:PRO:HA	1:A:660:GLU:HG2	1.87	0.56
1:B:191:LEU:C	1:B:192:LEU:HD12	2.31	0.56
1:B:585:VAL:HG12	1:B:599:ALA:HB1	1.85	0.56
1:A:321:LEU:HD23	1:A:375:GLN:HB3	1.86	0.56
1:B:621:ALA:HB3	1:B:651:ILE:CD1	2.35	0.56
1:B:628:GLU:O	1:B:631:LYS:HB2	2.06	0.56
1:B:645:SER:HA	1:B:746:GLN:NE2	2.21	0.56
1:B:1366:GLN:O	1:B:1369:GLN:N	2.38	0.56
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.37	0.56
1:B:506:MET:HE2	1:B:546:PHE:CZ	2.40	0.56
1:B:553:PHE:CD1	1:B:582:LEU:HD22	2.41	0.56
1:A:869:GLU:N	1:A:869:GLU:OE1	2.36	0.56
1:A:1214:LEU:O	1:A:1396:TYR:OH	2.07	0.56
1:A:1446:ILE:HD12	1:A:1447:ASN:N	2.21	0.56
1:B:468:ARG:CD	1:B:485:VAL:HG21	2.27	0.56
1:B:1125:GLU:N	1:B:1125:GLU:OE1	2.39	0.56
1:B:1197:GLU:OE1	1:B:1197:GLU:N	2.35	0.55
1:A:508:LEU:HD11	1:A:538:LEU:O	2.06	0.55
1:A:570:MET:CE	1:A:815:LEU:HD21	2.35	0.55
1:A:25:ASN:HA	1:A:30:VAL:HG12	1.87	0.55
1:A:780:THR:C	1:A:781:ILE:HD12	2.31	0.55
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.35	0.55
1:A:570:MET:HE2	1:A:815:LEU:CD1	2.33	0.55
1:A:1245:VAL:C	1:A:1246:LEU:HD12	2.30	0.55
1:B:120:LEU:HD12	1:B:135:CYS:SG	2.47	0.55
1:A:628:GLU:CA	1:A:631:LYS:HE2	2.22	0.55
1:A:1342:LEU:HD23	1:A:1386:LEU:HD21	1.89	0.55
1:B:547:ASP:OD1	1:B:548:ASP:N	2.39	0.55
1:B:983:LEU:HD12	1:B:1926:ALA:HB2	1.88	0.55
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.07	0.55
1:A:325:THR:HB	1:A:343:LYS:HD3	1.87	0.55
1:B:656:ALA:O	1:B:660:GLU:HG3	2.06	0.55
1:A:274:ARG:HA	1:A:277:TYR:CD2	2.42	0.55
1:B:495:ILE:CD1	1:B:578:VAL:HB	2.37	0.55
1:B:527:VAL:HG12	1:B:527:VAL:O	2.06	0.55
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.88	0.55
1:A:1535:THR:HG23	1:A:1535:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:GLN:O	1:B:668:GLU:HG3	2.07	0.55
1:A:620:MET:HG2	1:A:677:THR:HB	1.89	0.55
1:A:1418:ASP:OD2	1:A:1446:ILE:N	2.39	0.55
1:B:171:ALA:O	1:B:175:ILE:HG13	2.07	0.55
1:B:293:HIS:HB3	1:B:304:GLU:OE1	2.07	0.55
1:B:485:VAL:HG22	1:B:805:LEU:O	2.07	0.55
1:B:867:SER:O	1:B:870:SER:OG	2.24	0.55
1:A:618:GLY:HA3	1:A:681:ALA:HB2	1.89	0.55
1:A:2034:TYR:OH	2:A:2602:NDP:C6N	2.55	0.54
1:B:81:LEU:O	1:B:85:VAL:HG23	2.07	0.54
1:B:76:ASP:OD1	1:B:77:PRO:HD2	2.07	0.54
1:B:563:LEU:O	1:B:567:LEU:HD13	2.07	0.54
1:B:628:GLU:H	1:B:628:GLU:CD	2.13	0.54
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.06	0.54
1:A:420:LEU:HD21	1:A:512:ARG:NE	2.22	0.54
1:B:322:ILE:HG22	1:B:375:GLN:O	2.07	0.54
1:B:721:GLN:OE1	1:B:721:GLN:N	2.39	0.54
1:B:532:LEU:HD12	1:B:532:LEU:O	2.08	0.54
1:B:1616:LEU:HD21	1:B:1800:PHE:CE1	2.43	0.54
1:A:1342:LEU:HD23	1:A:1386:LEU:CD2	2.37	0.54
1:A:276:LEU:CD1	1:A:401:HIS:HB3	2.37	0.54
1:A:776:LYS:HD2	1:A:776:LYS:N	2.23	0.54
1:B:511:MET:CE	1:B:520:ILE:HG21	2.38	0.54
1:A:120:LEU:HD12	1:A:135:CYS:SG	2.48	0.54
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.90	0.54
1:A:197:SER:OG	1:A:224:ARG:NH1	2.39	0.54
1:A:235:LYS:CG	1:A:238:LEU:HD13	2.36	0.54
1:B:257:LYS:HE2	1:B:260:GLY:O	2.08	0.54
1:B:615:LEU:HD12	1:B:615:LEU:O	2.06	0.54
1:A:502:GLN:OE1	1:A:502:GLN:N	2.41	0.54
1:A:628:GLU:HA	1:A:631:LYS:CE	2.22	0.54
1:A:1973:VAL:CG1	2:A:2602:NDP:O3	2.55	0.54
1:A:1144:LEU:HD11	1:A:1173:PRO:HD3	1.90	0.53
1:B:322:ILE:CB	1:B:374:LEU:HD21	2.38	0.53
1:B:469:GLY:HA2	1:B:805:LEU:HD21	1.90	0.53
1:B:1909:VAL:HG11	1:B:1912:LEU:HD13	1.89	0.53
1:A:84:GLU:O	1:A:88:GLU:HG3	2.08	0.53
1:A:1418:ASP:OD1	1:A:1445:ALA:HB1	2.08	0.53
1:A:1616:LEU:HD13	1:A:1650:VAL:HG22	1.90	0.53
1:B:54:LEU:HD12	1:B:57:LEU:HD21	1.90	0.53
1:B:322:ILE:CG2	1:B:376:VAL:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:THR:C	1:B:880:LEU:HD12	2.33	0.53
1:B:1206:ARG:CZ	1:B:1209:LEU:HD13	2.38	0.53
1:A:716:SER:HB3	1:A:738:ASN:ND2	2.23	0.53
1:A:768:GLN:HG3	1:A:781:ILE:CG2	2.35	0.53
1:B:378:ASP:OD1	1:B:378:ASP:N	2.33	0.53
1:A:514:ASP:OD1	1:A:515:ARG:N	2.42	0.53
1:A:1760:LEU:HD11	1:A:1766:PHE:HB2	1.89	0.53
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	1.91	0.53
1:A:689:ALA:O	1:A:692:PRO:HD2	2.08	0.53
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.89	0.53
1:B:492:LEU:HD11	1:B:759:LEU:CD1	2.38	0.53
1:B:766:LEU:HD23	1:B:766:LEU:O	2.09	0.53
1:A:702:ILE:N	1:A:702:ILE:HD12	2.24	0.53
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.33	0.53
1:A:542:ASP:O	1:A:545:THR:HG22	2.08	0.53
1:B:24:ASP:HA	1:B:27:ILE:HD11	1.89	0.53
1:B:57:LEU:HD23	1:B:81:LEU:HD11	1.91	0.53
1:B:659:PHE:O	1:B:663:GLU:HG3	2.09	0.53
1:A:610:ILE:HA	1:A:690:ILE:HD13	1.91	0.53
1:B:182:ALA:HB2	1:B:234:THR:HG22	1.90	0.53
1:A:1346:THR:HG21	1:A:1377:TRP:NE1	2.23	0.53
1:B:470:TYR:CD1	1:B:805:LEU:HD11	2.44	0.53
1:B:627:TRP:HB2	1:B:643:HIS:CD2	2.44	0.53
1:A:468:ARG:CD	1:A:485:VAL:HG21	2.32	0.53
1:A:1275:ARG:NH2	1:A:1321:ALA:O	2.42	0.53
1:B:119:ALA:O	1:B:122:ARG:NH1	2.42	0.53
1:B:242:VAL:HG23	1:B:822:PRO:HB3	1.91	0.53
1:A:259:GLN:OE1	1:A:259:GLN:N	2.35	0.52
1:A:889:THR:HB	1:A:1030:MET:HE3	1.92	0.52
1:A:1973:VAL:H	2:A:2602:NDP:H52A	1.74	0.52
1:B:440:GLN:HG3	1:B:833:LEU:CD2	2.32	0.52
1:B:477:ARG:HH22	1:B:790:ARG:CD	2.22	0.52
1:A:664:GLN:O	1:A:667:LYS:HB2	2.09	0.52
1:A:978:ASN:HB3	1:A:980:THR:HG23	1.90	0.52
1:B:409:GLN:HB3	1:B:824:PRO:HA	1.92	0.52
1:B:460:VAL:CG2	1:B:461:PRO:HD2	2.39	0.52
1:B:702:ILE:HD12	1:B:702:ILE:N	2.24	0.52
1:B:715:THR:O	1:B:744:LEU:HB2	2.10	0.52
1:B:1699:VAL:HG11	1:B:1708:LEU:HD12	1.90	0.52
1:A:269:GLN:O	1:A:273:ILE:HG13	2.10	0.52
1:A:580:HIS:ND1	1:A:767:LEU:HD11	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HD12	1:B:28:GLY:N	2.24	0.52
1:B:767:LEU:O	1:B:771:LEU:HD13	2.08	0.52
1:A:168:LEU:HD23	1:A:168:LEU:O	2.10	0.52
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.92	0.52
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.72	0.52
1:B:332:PRO:O	1:B:336:SER:HB3	2.08	0.52
1:B:610:ILE:HG12	1:B:687:MET:HE1	1.91	0.52
1:B:2018:VAL:HB	1:B:2041:MET:HE2	1.91	0.52
1:A:624:GLY:CA	1:A:671:PHE:HB3	2.39	0.52
1:B:981:GLU:N	1:B:982:PRO:HD3	2.25	0.52
1:A:81:LEU:O	1:A:85:VAL:HG23	2.09	0.52
1:A:527:VAL:CG1	1:A:600:VAL:HG12	2.40	0.52
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.44	0.52
1:A:188:ILE:HG22	1:A:228:VAL:HG22	1.92	0.52
1:A:1794:VAL:C	1:A:1795:LEU:HD23	2.35	0.52
1:A:533:LYS:O	1:A:537:LEU:HG	2.10	0.52
1:B:1214:LEU:HD12	1:B:1214:LEU:C	2.35	0.52
1:B:1973:VAL:CG1	2:B:2602:NDP:C3D	2.87	0.52
1:A:1115:GLU:HG2	1:A:1518:LEU:HD23	1.90	0.52
1:B:168:LEU:O	1:B:168:LEU:HD23	2.10	0.52
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.45	0.52
1:B:570:MET:HG2	1:B:811:ASN:O	2.10	0.52
1:B:1363:THR:OG1	1:B:1366:GLN:OE1	2.27	0.52
1:A:433:ALA:HB2	1:A:835:LYS:HB2	1.92	0.51
1:A:442:LEU:HD23	1:A:442:LEU:C	2.35	0.51
1:A:199:GLN:HG2	1:B:127:LEU:HD13	1.92	0.51
1:B:623:VAL:CG2	1:B:665:LEU:HD13	2.30	0.51
1:B:1994:PRO:HB3	2:B:2602:NDP:N6A	2.22	0.51
1:B:1080:VAL:HG22	1:B:1087:THR:HG23	1.93	0.51
1:B:1807:TRP:CD1	1:B:1808:ARG:HH11	2.28	0.51
1:A:139:MET:HE1	1:B:396:GLY:CA	2.41	0.51
1:A:323:GLY:HA2	1:A:356:ASN:ND2	2.17	0.51
1:A:725:SER:HA	1:A:728:ARG:HH12	1.75	0.51
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.44	0.51
1:B:1808:ARG:HH22	1:B:1811:TRP:CG	2.29	0.51
1:B:1972:ALA:HB1	2:B:2602:NDP:C5A	2.40	0.51
1:A:476:GLU:HG3	1:A:794:GLU:OE2	2.11	0.51
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.46	0.51
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.91	0.51
1:B:36:ASP:OD1	1:B:37:ASP:N	2.38	0.51
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HG2	1:A:53:LYS:HD2	1.93	0.51
1:A:1245:VAL:HG21	1:A:1332:MET:HE2	1.92	0.51
1:A:105:THR:HG23	1:A:182:ALA:C	2.36	0.51
1:A:1415:LEU:HD22	1:A:1443:LEU:CD2	2.41	0.51
1:A:623:VAL:HG12	1:A:625:LEU:N	2.22	0.51
1:A:783:PRO:HB2	1:A:795:PHE:CE2	2.46	0.51
1:B:160:ALA:O	1:B:394:GLY:HA3	2.10	0.51
1:B:222:TYR:HB3	1:B:295:THR:HG23	1.93	0.51
1:B:555:SER:O	1:B:559:ILE:HG13	2.10	0.51
1:B:325:THR:HG21	1:B:340:ALA:HA	1.93	0.51
1:B:511:MET:HE1	1:B:520:ILE:HG21	1.92	0.51
1:A:203:LEU:HD12	1:B:132:MET:CE	2.41	0.50
1:A:270:GLU:OE2	1:A:274:ARG:NH2	2.27	0.50
1:A:276:LEU:HD12	1:A:401:HIS:CD2	2.46	0.50
1:B:210:GLY:O	1:B:223:CYS:HB2	2.11	0.50
1:B:326:LYS:HE3	1:B:331:HIS:CD2	2.45	0.50
1:B:694:LEU:HD23	1:B:698:LEU:HG	1.93	0.50
1:A:210:GLY:O	1:A:223:CYS:SG	2.70	0.50
1:A:1195:GLN:HG2	1:A:1363:THR:HG22	1.94	0.50
1:B:499:MET:HE2	1:B:582:LEU:HB2	1.94	0.50
1:B:647:ASP:OD2	1:B:773:ARG:NH1	2.44	0.50
1:A:694:LEU:O	1:A:694:LEU:HD23	2.11	0.50
1:A:1442:TRP:CZ2	1:A:1497:LEU:HD23	2.46	0.50
1:A:257:LYS:HE3	1:A:263:PHE:O	2.12	0.50
1:A:1827:LYS:NZ	1:A:1849:ILE:O	2.41	0.50
1:B:689:ALA:O	1:B:692:PRO:HD2	2.12	0.50
1:A:6:ILE:HG12	1:A:233:LEU:HD21	1.94	0.50
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.93	0.50
1:A:564:ILE:CD1	1:A:590:ALA:HB2	2.33	0.50
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.42	0.50
1:B:124:PRO:HA	1:B:127:LEU:CD2	2.42	0.50
1:B:621:ALA:HB3	1:B:651:ILE:HD12	1.94	0.50
1:B:623:VAL:HG12	1:B:625:LEU:HG	1.94	0.50
1:B:657:PRO:HA	1:B:660:GLU:OE1	2.11	0.50
1:B:743:VAL:HG12	1:B:745:PHE:H	1.76	0.50
1:B:1573:PHE:CD2	2:B:2601:NDP:O1A	2.50	0.50
1:A:9:MET:SD	1:A:345:LEU:HD12	2.51	0.50
1:A:570:MET:HE1	1:A:800:ILE:HG13	1.94	0.50
1:A:613:ALA:HB1	1:A:615:LEU:HG	1.93	0.50
1:A:692:PRO:HD2	1:A:693:PRO:HD2	1.93	0.50
1:A:188:ILE:HG22	1:A:228:VAL:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ILE:HD12	1:A:771:LEU:HD21	1.93	0.49
1:A:627:TRP:CA	1:A:649:VAL:HG21	2.42	0.49
1:A:660:GLU:O	1:A:663:GLU:HG2	2.12	0.49
1:A:247:LEU:HD23	1:A:282:VAL:CG2	2.42	0.49
1:A:606:ARG:O	1:A:610:ILE:HG13	2.11	0.49
1:A:6:ILE:HG12	1:A:233:LEU:CD2	2.42	0.49
1:A:282:VAL:HG11	1:A:387:ASN:HD22	1.76	0.49
1:A:717:ILE:CD1	1:A:727:ALA:HB2	2.42	0.49
1:A:755:HIS:ND1	1:A:778:SER:HB2	2.28	0.49
1:A:425:ARG:HD3	1:A:812:PRO:HD3	1.93	0.49
1:A:549:ILE:HD12	1:A:550:VAL:N	2.27	0.49
1:A:550:VAL:HG21	1:A:611:LYS:HE2	1.95	0.49
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.43	0.49
1:A:1973:VAL:HG12	2:A:2602:NDP:PA	2.53	0.49
1:B:212:CYS:SG	1:B:222:TYR:HA	2.53	0.49
1:A:1426:GLU:OE1	1:A:1429:LYS:NZ	2.44	0.49
1:A:1571:LEU:O	1:A:1843:MET:HE1	2.12	0.49
1:B:512:ARG:NH2	1:B:791:ASP:OD1	2.35	0.49
1:B:1214:LEU:O	1:B:1396:TYR:OH	2.20	0.49
1:B:1245:VAL:HG13	1:B:1313:LEU:HD21	1.94	0.49
1:A:623:VAL:CG1	1:A:665:LEU:HD13	2.41	0.49
1:B:191:LEU:HD22	1:B:224:ARG:HH21	1.77	0.49
1:B:569:CYS:SG	1:B:814:ALA:HB1	2.53	0.49
1:B:681:ALA:O	1:B:684:SER:OG	2.20	0.49
1:A:217:THR:HG22	1:A:364:PRO:CD	2.43	0.49
1:A:1346:THR:HG21	1:A:1377:TRP:HE1	1.78	0.49
1:B:322:ILE:HD13	1:B:374:LEU:HD11	1.94	0.49
1:B:655:GLN:HA	1:B:658:VAL:HG12	1.94	0.49
1:B:701:VAL:HB	1:B:702:ILE:HD12	1.94	0.49
1:A:155:ILE:N	1:A:155:ILE:HD12	2.27	0.49
1:A:189:ASN:HD22	1:A:334:PRO:CD	2.23	0.49
1:A:694:LEU:HD23	1:A:698:LEU:HG	1.94	0.49
1:B:23:TRP:HB2	1:B:346:LEU:HD13	1.94	0.49
1:B:1763:HIS:N	1:B:1788:ASN:O	2.45	0.49
1:B:1898:LEU:HD11	1:B:1925:GLN:HG2	1.94	0.49
1:A:189:ASN:O	1:A:226:GLU:HB2	2.12	0.49
1:A:200:PHE:CD1	1:B:132:MET:HE1	2.48	0.49
1:A:1753:LEU:C	1:A:1753:LEU:HD23	2.38	0.49
1:B:112:SER:C	1:B:137:ARG:HH21	2.20	0.49
1:B:213:LYS:HG2	1:B:358:HIS:HB3	1.93	0.49
1:A:127:LEU:HD12	1:A:127:LEU:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.94	0.49
1:B:627:TRP:CE3	1:B:643:HIS:HB2	2.48	0.49
1:B:719:GLU:HA	1:B:722:TRP:CG	2.48	0.49
1:B:1130:GLU:OE1	1:B:1130:GLU:N	2.37	0.49
1:A:288:GLU:HG2	1:A:288:GLU:O	2.12	0.48
1:B:22:PHE:CD1	1:B:32:MET:HE1	2.48	0.48
1:B:515:ARG:HB2	1:B:566:LEU:CD2	2.42	0.48
1:A:660:GLU:HA	1:A:663:GLU:HG2	1.95	0.48
1:A:978:ASN:C	1:A:980:THR:HG23	2.37	0.48
1:A:25:ASN:HA	1:A:30:VAL:CG1	2.43	0.48
1:A:1428:LEU:HD13	1:A:1443:LEU:HD21	1.95	0.48
1:B:52:GLY:O	1:B:225:SER:HA	2.12	0.48
1:B:136:GLN:HB3	1:B:139:MET:HG2	1.95	0.48
1:B:606:ARG:O	1:B:610:ILE:HG13	2.12	0.48
1:B:615:LEU:HD11	1:B:680:MET:HE1	1.95	0.48
1:B:621:ALA:O	1:B:651:ILE:N	2.40	0.48
1:A:342:ALA:O	1:A:346:LEU:HG	2.13	0.48
1:A:515:ARG:HB2	1:A:566:LEU:CD2	2.43	0.48
1:A:677:THR:OG1	1:A:680:MET:O	2.31	0.48
1:A:2062:ALA:O	1:A:2063:ILE:HD13	2.14	0.48
1:A:1417:VAL:HG13	1:A:1445:ALA:HB2	1.95	0.48
1:B:191:LEU:N	1:B:226:GLU:OE2	2.23	0.48
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.96	0.48
1:A:1909:VAL:HG11	1:A:1912:LEU:HD13	1.95	0.48
1:B:717:ILE:HG12	1:B:727:ALA:HB2	1.94	0.48
1:A:549:ILE:HD11	1:A:611:LYS:CG	2.38	0.48
1:A:329:MET:HE2	1:A:332:PRO:HD3	1.95	0.48
1:A:502:GLN:HA	1:A:506:MET:SD	2.53	0.48
1:A:584:GLU:HG3	1:A:712:TRP:CZ2	2.44	0.48
1:A:641:ALA:HB3	1:A:650:THR:O	2.14	0.48
1:A:1973:VAL:HB	2:A:2602:NDP:C3D	2.26	0.48
1:A:476:GLU:N	1:A:794:GLU:OE2	2.36	0.48
1:A:1837:GLU:OE2	1:A:1841:ARG:NH2	2.47	0.48
1:A:247:LEU:HD23	1:A:282:VAL:HG21	1.95	0.48
1:A:506:MET:HG2	1:A:546:PHE:HE2	1.79	0.48
1:A:2021:SER:CB	2:A:2602:NDP:H5N	2.43	0.48
1:B:620:MET:CE	1:B:682:PHE:HB2	2.32	0.48
1:B:654:PRO:O	1:B:658:VAL:HG12	2.14	0.48
1:B:207:SER:HB2	1:B:220:ASN:HB2	1.95	0.47
1:B:524:ASP:OD2	1:B:535:SER:OG	2.18	0.47
1:A:163:SER:OG	1:A:334:PRO:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLN:OE1	1:A:410:PRO:HD2	2.14	0.47
1:A:1210:PRO:HB3	1:A:1319:VAL:HG11	1.95	0.47
1:B:615:LEU:HD11	1:B:680:MET:CE	2.44	0.47
1:A:431:PRO:O	1:A:435:GLN:HG3	2.14	0.47
1:A:1771:LYS:CE	1:A:1795:LEU:HD22	2.44	0.47
1:A:1942:SER:O	1:A:1943:THR:OG1	2.19	0.47
1:B:516:PHE:O	1:B:520:ILE:HG12	2.15	0.47
1:B:83:LEU:HD12	1:B:144:LEU:HD21	1.96	0.47
1:B:692:PRO:HB2	1:B:693:PRO:HD3	1.96	0.47
1:A:1181:LEU:HD13	1:A:1204:GLN:HG2	1.95	0.47
1:B:1361:THR:HG21	1:B:1369:GLN:HE21	1.79	0.47
1:A:758:VAL:HG21	1:A:775:LEU:HD21	1.97	0.47
1:A:1446:ILE:HG21	1:A:1486:VAL:CG2	2.44	0.47
1:A:1887:TYR:CD1	1:A:1909:VAL:HG13	2.50	0.47
1:B:447:ASP:OD2	1:B:450:PHE:HB2	2.15	0.47
1:B:1190:LEU:O	1:B:1195:GLN:NE2	2.43	0.47
1:A:315:THR:O	1:A:315:THR:HG23	2.13	0.47
1:A:460:VAL:HG13	1:A:461:PRO:HD2	1.97	0.47
1:A:493:TRP:CE3	1:A:576:GLY:HA3	2.49	0.47
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.50	0.47
1:B:491:PRO:HG2	1:B:756:ALA:HB2	1.96	0.47
1:B:984:PHE:CD2	1:B:1010:GLU:HB2	2.50	0.47
1:B:1047:TYR:OH	1:B:1586:ASP:OD2	2.15	0.47
1:A:1555:GLN:HG3	1:A:1556:PRO:HD3	1.97	0.47
1:B:665:LEU:O	1:B:669:GLY:N	2.46	0.47
1:A:93:GLY:O	1:A:240:ARG:HB2	2.15	0.47
1:A:1555:GLN:N	1:A:1556:PRO:HD2	2.30	0.47
1:B:193:LYS:HE2	1:B:195:ASN:HB2	1.97	0.47
1:B:1270:TYR:HB3	1:B:1292:VAL:HG12	1.95	0.47
1:B:1798:ALA:O	1:B:1802:GLU:N	2.48	0.47
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.43	0.47
1:B:164:SER:OG	1:B:335:ALA:HA	2.15	0.47
1:A:13:LEU:HB3	1:A:14:PRO:CD	2.45	0.46
1:A:425:ARG:HH21	1:A:811:ASN:HD22	1.63	0.46
1:A:781:ILE:HD12	1:A:781:ILE:N	2.30	0.46
1:A:1009:LEU:HD21	1:A:1021:LEU:HD21	1.96	0.46
1:B:766:LEU:HD23	1:B:766:LEU:C	2.40	0.46
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	2.15	0.46
1:A:431:PRO:HG3	1:A:467:PHE:CD2	2.50	0.46
1:A:615:LEU:HB2	1:A:680:MET:CE	2.41	0.46
1:A:1021:LEU:HD23	1:A:1075:VAL:HG12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:LEU:HD11	1:A:1075:VAL:HG11	1.97	0.46
1:A:1995:LYS:HE2	1:A:2037:ALA:CB	2.45	0.46
1:B:690:ILE:N	1:B:690:ILE:HD12	2.29	0.46
1:B:1245:VAL:HB	1:B:1246:LEU:HD12	1.98	0.46
1:B:1589:PRO:HG3	1:B:1797:ASP:HB2	1.96	0.46
1:B:1997:SER:O	1:B:2001:ASN:ND2	2.45	0.46
1:B:2097:LEU:O	1:B:2097:LEU:HD23	2.15	0.46
1:A:25:ASN:CG	1:A:32:MET:HE3	2.39	0.46
1:A:82:LEU:HD22	1:A:188:ILE:HD13	1.96	0.46
1:A:211:THR:CG2	1:A:213:LYS:HG3	2.45	0.46
1:B:265:SER:O	1:B:269:GLN:NE2	2.48	0.46
1:B:687:MET:HE2	1:B:739:LEU:HD11	1.97	0.46
1:B:2088:MET:HE3	1:B:2091:CYS:HB2	1.96	0.46
1:A:363:ASN:HB3	1:A:366:ILE:CD1	2.43	0.46
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.22	0.46
1:A:899:LEU:HD22	1:A:958:VAL:HG22	1.96	0.46
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.41	0.46
1:B:168:LEU:HD23	1:B:168:LEU:C	2.40	0.46
1:B:188:ILE:HG22	1:B:228:VAL:HG13	1.97	0.46
1:B:577:ILE:HG21	1:B:587:CYS:HB3	1.97	0.46
1:A:290:ILE:HG12	1:A:308:ILE:HD13	1.98	0.46
1:A:692:PRO:CD	1:A:693:PRO:HD2	2.45	0.46
1:B:190:VAL:HA	1:B:226:GLU:HG2	1.96	0.46
1:B:1228:LEU:HD21	1:B:1256:ILE:HD12	1.98	0.46
1:A:557:THR:O	1:A:561:ILE:HG13	2.16	0.46
1:A:760:GLU:CD	1:A:765:ALA:HA	2.40	0.46
1:A:1130:GLU:OE1	1:A:1130:GLU:N	2.46	0.46
1:B:95:ILE:HD12	1:B:95:ILE:N	2.30	0.46
1:B:319:PRO:HA	1:B:373:ARG:O	2.16	0.46
1:B:351:GLY:C	1:B:352:LEU:HD12	2.41	0.46
1:B:574:PRO:O	1:B:711:ARG:HD2	2.16	0.46
1:A:54:LEU:HD12	1:A:57:LEU:CD2	2.44	0.46
1:A:409:GLN:HB3	1:A:824:PRO:HA	1.98	0.46
1:A:425:ARG:HD3	1:A:812:PRO:CD	2.45	0.46
1:A:514:ASP:OD1	1:A:515:ARG:HG2	2.16	0.46
1:A:760:GLU:OE2	1:A:765:ALA:HA	2.15	0.46
1:A:1899:GLU:HB3	1:A:2088:MET:HE2	1.96	0.46
1:B:5:VAL:HB	1:B:242:VAL:HG13	1.97	0.46
1:B:322:ILE:HG22	1:B:376:VAL:HA	1.98	0.46
1:B:2097:LEU:HD23	1:B:2097:LEU:C	2.41	0.46
1:B:34:THR:O	1:B:50:ARG:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.51	0.46
1:B:627:TRP:CZ3	1:B:643:HIS:HB2	2.50	0.46
1:B:663:GLU:O	1:B:667:LYS:HG3	2.15	0.46
1:B:1178:LEU:CD1	1:B:1214:LEU:HD11	2.46	0.46
1:B:1206:ARG:NH1	1:B:1209:LEU:HD13	2.31	0.46
1:A:613:ALA:HB1	1:A:615:LEU:CD2	2.45	0.46
1:A:698:LEU:HB2	1:A:732:ALA:HB1	1.98	0.46
1:A:1078:VAL:HG23	1:A:1089:ALA:HB2	1.98	0.46
1:A:1971:LEU:N	1:A:1971:LEU:HD12	2.31	0.46
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.98	0.46
1:B:746:GLN:OE1	1:B:750:TRP:NE1	2.49	0.46
1:B:1371:ILE:O	1:B:1372:LEU:HD12	2.16	0.46
1:A:6:ILE:HG23	1:A:231:VAL:CG1	2.46	0.45
1:A:139:MET:HE2	1:A:139:MET:CA	2.42	0.45
1:A:627:TRP:NE1	1:A:631:LYS:HD3	2.31	0.45
1:B:495:ILE:HD13	1:B:578:VAL:HB	1.98	0.45
1:B:645:SER:CA	1:B:746:GLN:HE21	2.29	0.45
1:A:565:ASP:OD1	1:A:589:TYR:OH	2.31	0.45
1:B:85:VAL:HG12	1:B:230:ALA:HB3	1.99	0.45
1:B:158:ASP:O	1:B:163:SER:HB3	2.16	0.45
1:A:235:LYS:HD2	1:A:238:LEU:CD1	2.46	0.45
1:A:766:LEU:HD23	1:A:766:LEU:O	2.16	0.45
1:B:450:PHE:CE2	1:B:454:LEU:HD11	2.51	0.45
1:B:540:SER:OG	1:B:545:THR:HG21	2.16	0.45
1:A:627:TRP:CZ3	1:A:643:HIS:HB2	2.52	0.45
1:B:322:ILE:HB	1:B:374:LEU:HD21	1.98	0.45
1:B:621:ALA:HB3	1:B:651:ILE:HD11	1.98	0.45
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.51	0.45
1:B:1445:ALA:C	1:B:1446:ILE:HD13	2.42	0.45
1:A:990:VAL:HG13	1:A:1039:LEU:HD12	1.97	0.45
1:A:1457:VAL:HG11	1:A:1471:CYS:HB2	1.99	0.45
1:B:477:ARG:NH2	1:B:790:ARG:HG2	2.31	0.45
1:A:490:ARG:HD3	1:A:806:SER:O	2.17	0.45
1:A:1995:LYS:HE2	1:A:2037:ALA:HB1	1.97	0.45
1:B:292:ALA:HB2	1:B:322:ILE:HD11	1.97	0.45
1:B:978:ASN:N	1:B:979:PRO:CD	2.79	0.45
1:A:131:SER:O	1:A:135:CYS:HB2	2.16	0.45
1:A:1188:LEU:HD12	1:A:1197:GLU:HG3	1.99	0.45
1:A:1794:VAL:O	1:A:1795:LEU:HD23	2.17	0.45
1:A:1860:GLU:N	1:A:1860:GLU:OE1	2.49	0.45
1:B:655:GLN:HA	1:B:658:VAL:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1246:LEU:HD12	1:B:1246:LEU:N	2.32	0.45
1:B:1446:ILE:CG2	1:B:1474:LEU:HD12	2.35	0.45
1:A:560:GLN:O	1:A:564:ILE:HG13	2.17	0.45
1:B:164:SER:OG	1:B:334:PRO:O	2.27	0.45
1:B:1314:VAL:HG12	1:B:1343:LEU:HB3	1.99	0.45
1:B:127:LEU:C	1:B:127:LEU:HD12	2.42	0.45
1:B:47:LEU:HD22	1:B:197:SER:HB3	1.99	0.45
1:B:83:LEU:HD12	1:B:144:LEU:CD2	2.46	0.45
1:B:493:TRP:NE1	1:B:753:PRO:HD2	2.32	0.45
1:B:549:ILE:HD11	1:B:611:LYS:CG	2.35	0.45
1:A:64:PHE:CD1	1:A:429:ARG:HD3	2.52	0.44
1:A:717:ILE:HD13	1:A:727:ALA:HB2	2.00	0.44
1:A:754:GLU:O	1:A:755:HIS:HB2	2.18	0.44
1:B:112:SER:CB	1:B:334:PRO:HG3	2.48	0.44
1:B:744:LEU:HB3	1:B:747:GLU:OE1	2.17	0.44
1:A:425:ARG:HH21	1:A:811:ASN:ND2	2.15	0.44
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.52	0.44
1:A:1391:LEU:HD23	1:A:1391:LEU:C	2.42	0.44
1:B:671:PHE:HE1	1:B:673:LYS:HD3	1.83	0.44
1:B:760:GLU:HB3	1:B:783:PRO:HA	1.99	0.44
1:A:625:LEU:HD11	1:A:665:LEU:HD22	1.99	0.44
1:A:692:PRO:N	1:A:693:PRO:HD2	2.32	0.44
1:A:39:ARG:NH2	1:A:226:GLU:OE2	2.50	0.44
1:A:420:LEU:CD1	1:A:512:ARG:HB3	2.37	0.44
1:A:508:LEU:HD11	1:A:538:LEU:C	2.42	0.44
1:B:211:THR:HG21	1:B:358:HIS:CE1	2.52	0.44
1:B:630:CYS:HA	1:B:633:ARG:HB2	2.00	0.44
1:B:1246:LEU:N	1:B:1273:THR:O	2.51	0.44
1:B:1250:GLY:O	1:B:1316:ASN:ND2	2.50	0.44
1:A:524:ASP:OD1	1:A:533:LYS:HA	2.17	0.44
1:A:601:LEU:HB3	1:A:701:VAL:HG11	1.99	0.44
1:B:489:GLU:HA	1:B:489:GLU:OE1	2.18	0.44
1:B:512:ARG:HH22	1:B:791:ASP:CG	2.22	0.44
1:B:515:ARG:HB2	1:B:566:LEU:HD21	1.99	0.44
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.53	0.44
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.53	0.44
1:A:159:THR:O	1:A:163:SER:HB3	2.18	0.44
1:A:321:LEU:HA	1:A:375:GLN:O	2.17	0.44
1:A:593:CYS:HG	1:A:712:TRP:HZ3	1.66	0.44
1:A:1973:VAL:CB	2:A:2602:NDP:H3D	2.26	0.44
1:A:2065:ASP:OD1	1:A:2087:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLU:OE1	1:B:2:GLU:HA	2.17	0.44
1:B:115:GLU:OE1	1:B:193:LYS:N	2.51	0.44
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.99	0.44
1:B:671:PHE:CE1	1:B:673:LYS:HD3	2.53	0.44
1:A:105:THR:HG23	1:A:182:ALA:O	2.18	0.44
1:A:570:MET:HE2	1:A:815:LEU:CD2	2.47	0.44
1:A:997:ARG:NH2	1:A:1041:SER:O	2.47	0.44
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	2.00	0.44
1:B:190:VAL:HG23	1:B:192:LEU:HD13	2.00	0.44
1:B:299:VAL:O	1:B:303:GLN:HG2	2.18	0.44
1:B:717:ILE:HG12	1:B:727:ALA:CB	2.48	0.44
1:A:163:SER:OG	1:A:334:PRO:HB2	2.17	0.44
1:A:341:LEU:O	1:A:345:LEU:HG	2.17	0.44
1:A:628:GLU:O	1:A:631:LYS:HG2	2.18	0.44
1:A:2034:TYR:OH	2:A:2602:NDP:H6N	2.16	0.44
1:B:646:LYS:HD2	1:B:646:LYS:HA	1.81	0.44
1:B:692:PRO:HB2	1:B:693:PRO:CD	2.47	0.44
1:B:1593:THR:HG22	1:B:1593:THR:O	2.17	0.44
1:A:39:ARG:HD2	1:A:191:LEU:O	2.17	0.44
1:B:830:ILE:HG22	1:B:830:ILE:O	2.17	0.44
1:A:68:HIS:CG	1:A:69:PRO:HD2	2.53	0.43
1:A:495:ILE:HD12	1:A:758:VAL:HG11	2.00	0.43
1:B:584:GLU:HG3	1:B:738:ASN:CG	2.42	0.43
1:B:695:LEU:HD12	1:B:732:ALA:CB	2.47	0.43
1:B:1760:LEU:HD11	1:B:1766:PHE:HB2	2.00	0.43
1:B:1896:PHE:CB	2:B:2602:NDP:H52N	2.48	0.43
1:A:492:LEU:HD11	1:A:759:LEU:HD12	2.00	0.43
1:A:620:MET:HA	1:A:651:ILE:O	2.17	0.43
1:A:1246:LEU:HD22	1:A:1320:ALA:HB1	2.00	0.43
1:B:719:GLU:HA	1:B:722:TRP:CD2	2.53	0.43
1:B:1364:GLU:N	1:B:1365:PRO:HD2	2.34	0.43
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.17	0.43
1:A:38:ARG:HH21	1:A:53:LYS:HE2	1.83	0.43
1:A:151:ARG:O	1:B:252:ASN:HB2	2.17	0.43
1:A:433:ALA:CB	1:A:835:LYS:HB2	2.48	0.43
1:A:763:PRO:O	1:A:785:MET:HE2	2.18	0.43
1:A:1287:LEU:O	1:A:1292:VAL:HG22	2.18	0.43
1:A:1417:VAL:CG1	1:A:1445:ALA:HB2	2.48	0.43
1:B:506:MET:HG3	1:B:559:ILE:HD11	1.99	0.43
1:A:503:TRP:CH2	1:A:506:MET:HA	2.54	0.43
1:A:1344:LEU:O	1:A:1401:PHE:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1674:HIS:NE2	1:A:1756:SER:OG	2.48	0.43
1:B:420:LEU:HD11	1:B:512:ARG:HD2	2.00	0.43
1:B:527:VAL:HG21	1:B:600:VAL:HG12	2.00	0.43
1:A:601:LEU:CB	1:A:701:VAL:HG11	2.48	0.43
1:B:560:GLN:O	1:B:564:ILE:HG13	2.19	0.43
1:A:690:ILE:O	1:A:690:ILE:HG22	2.19	0.43
1:B:241:ARG:NH2	1:B:453:MET:HE1	2.34	0.43
1:B:491:PRO:HG3	1:B:753:PRO:HG2	2.00	0.43
1:B:501:THR:HG1	1:B:764:HIS:HB3	1.82	0.43
1:B:532:LEU:HD12	1:B:532:LEU:C	2.44	0.43
1:B:655:GLN:O	1:B:658:VAL:HG12	2.18	0.43
1:B:1066:LEU:HD23	1:B:1076:ALA:HB2	2.01	0.43
1:B:1827:LYS:NZ	1:B:1849:ILE:O	2.49	0.43
1:A:366:ILE:HG22	1:A:369:LEU:H	1.84	0.43
1:A:470:TYR:HD1	1:A:805:LEU:HD11	1.84	0.43
1:A:515:ARG:HB2	1:A:566:LEU:HD21	2.00	0.43
1:A:716:SER:HB2	1:A:738:ASN:HA	2.01	0.43
1:A:1925:GLN:O	1:A:1929:VAL:HG23	2.19	0.43
1:B:13:LEU:HD13	1:B:22:PHE:CE1	2.54	0.43
1:A:64:PHE:HD1	1:A:429:ARG:HD3	1.84	0.43
1:A:210:GLY:O	1:A:223:CYS:CB	2.67	0.43
1:A:415:ALA:HB3	1:A:417:HIS:CE1	2.54	0.43
1:A:2062:ALA:C	1:A:2063:ILE:HD13	2.44	0.43
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.77	0.43
1:B:1571:LEU:CD2	1:B:1622:LEU:HD11	2.49	0.43
1:B:1632:PHE:CD1	1:B:1807:TRP:NE1	2.87	0.43
1:A:545:THR:HG23	1:A:546:PHE:N	2.34	0.43
1:A:613:ALA:HB1	1:A:615:LEU:HD21	2.00	0.43
1:A:2034:TYR:OH	2:A:2602:NDP:O2D	2.26	0.43
1:B:1389:VAL:HG21	1:B:1501:LEU:HD21	2.00	0.43
1:B:2103:HIS:HB2	1:B:2106:LEU:HD21	2.00	0.43
1:A:460:VAL:CG1	1:A:461:PRO:HD2	2.49	0.43
1:A:698:LEU:CB	1:A:732:ALA:HB1	2.48	0.43
1:B:7:ALA:HA	1:B:241:ARG:O	2.19	0.43
1:B:108:TRP:NE1	1:B:155:ILE:HD12	2.34	0.43
1:B:139:MET:O	1:B:143:ARG:HG2	2.19	0.43
1:B:316:ARG:NH1	1:B:320:LEU:HD13	2.34	0.43
1:B:351:GLY:O	1:B:352:LEU:HD12	2.19	0.43
1:B:506:MET:HE2	1:B:546:PHE:CE1	2.54	0.43
1:A:291:GLU:CG	1:A:340:ALA:HB1	2.46	0.42
1:A:293:HIS:CD2	1:A:295:THR:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:VAL:HG12	1:B:389:GLY:N	2.34	0.42
1:B:749:LEU:HA	1:B:752:VAL:HG23	2.01	0.42
1:B:1607:ASP:CG	1:B:1608:ALA:N	2.77	0.42
1:A:257:LYS:HE2	1:A:260:GLY:O	2.19	0.42
1:A:291:GLU:OE2	1:A:325:THR:HG22	2.20	0.42
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.19	0.42
1:A:2034:TYR:OH	2:A:2602:NDP:C2D	2.66	0.42
1:A:155:ILE:HG22	1:A:156:ALA:N	2.34	0.42
1:A:157:LEU:HD23	1:A:166:MET:CG	2.49	0.42
1:A:634:CYS:HB3	1:A:638:VAL:O	2.19	0.42
1:B:75:MET:HG3	1:B:79:LEU:HD23	2.00	0.42
1:B:157:LEU:N	1:B:157:LEU:HD12	2.34	0.42
1:B:470:TYR:CE1	1:B:805:LEU:HD11	2.54	0.42
1:A:54:LEU:HD21	1:A:227:GLY:HA2	2.01	0.42
1:A:68:HIS:ND1	1:A:69:PRO:HD2	2.33	0.42
1:A:366:ILE:HG22	1:A:366:ILE:O	2.18	0.42
1:A:420:LEU:HD11	1:A:512:ARG:CB	2.36	0.42
1:A:1888:ILE:CD1	1:A:1956:ILE:HD13	2.49	0.42
1:B:1602:GLU:HB3	1:B:1650:VAL:HG23	2.01	0.42
1:A:1411:SER:OG	1:A:1439:ARG:NH2	2.52	0.42
1:A:1677:SER:HA	1:A:1708:LEU:HD11	2.01	0.42
1:A:1913:VAL:C	1:A:1914:LEU:HD12	2.45	0.42
1:A:1917:ARG:NE	2:A:2602:NDP:O3X	2.53	0.42
1:B:159:THR:HG21	1:B:163:SER:HA	1.96	0.42
1:B:591:ASP:OD1	1:B:711:ARG:NH1	2.52	0.42
1:A:182:ALA:HB1	1:A:234:THR:HG22	2.00	0.42
1:A:621:ALA:HB2	1:A:674:GLU:HA	1.98	0.42
1:A:744:LEU:HB3	1:A:747:GLU:HG3	2.01	0.42
1:A:758:VAL:HG21	1:A:775:LEU:CD2	2.50	0.42
1:A:1020:LEU:HD22	1:A:1032:THR:CG2	2.49	0.42
1:A:1247:ALA:CB	1:A:1272:ALA:HB1	2.49	0.42
1:A:1414:PHE:CE1	1:A:1493:LEU:HD21	2.55	0.42
1:B:553:PHE:HE2	1:B:610:ILE:HD12	1.85	0.42
1:B:1214:LEU:HD12	1:B:1215:LEU:N	2.34	0.42
1:B:1651:VAL:HG23	1:B:1652:TYR:N	2.35	0.42
1:A:470:TYR:CE1	1:A:481:GLU:HB2	2.54	0.42
1:A:613:ALA:CB	1:A:615:LEU:HG	2.50	0.42
1:A:1190:LEU:O	1:A:1191:ASN:ND2	2.52	0.42
1:B:60:PHE:CG	1:B:80:ARG:HD2	2.54	0.42
1:B:108:TRP:HB3	1:B:167:ALA:HB1	2.02	0.42
1:A:277:TYR:CZ	1:A:284:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:HB3	1:A:732:ALA:CB	2.50	0.42
1:A:1760:LEU:HD13	1:A:1789:VAL:HG13	2.01	0.42
1:B:5:VAL:HG22	1:B:234:THR:O	2.18	0.42
1:B:11:GLY:HA2	1:B:85:VAL:CG1	2.50	0.42
1:B:1973:VAL:O	2:B:2602:NDP:H8A	2.20	0.42
1:A:9:MET:HE3	1:A:19:LEU:HD13	2.01	0.42
1:A:1346:THR:HG22	1:A:1347:LEU:N	2.35	0.42
1:B:1348:LEU:HD22	1:B:1374:GLN:HB3	2.02	0.42
1:B:1443:LEU:HD11	1:B:1469:LEU:HD12	2.01	0.42
1:B:1596:ASP:O	1:B:1597:SER:OG	2.24	0.42
1:B:1607:ASP:OD1	1:B:1608:ALA:N	2.52	0.42
1:A:67:VAL:HG21	1:A:75:MET:HE1	2.02	0.42
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.55	0.42
1:B:32:MET:SD	1:B:329:MET:HB3	2.59	0.42
1:B:572:LEU:HD11	1:B:803:LEU:HD23	2.01	0.42
1:B:983:LEU:O	1:B:1013:LEU:HD13	2.20	0.42
1:B:1373:SER:O	1:B:1376:ALA:N	2.53	0.42
1:B:1386:LEU:HD22	1:B:1403:CYS:HB3	2.02	0.42
1:A:627:TRP:O	1:A:631:LYS:HG2	2.20	0.41
1:A:1607:ASP:OD1	1:A:1608:ALA:N	2.43	0.41
1:B:60:PHE:CB	1:B:80:ARG:HD2	2.50	0.41
1:B:495:ILE:HG12	1:B:758:VAL:HG13	2.02	0.41
1:B:511:MET:HE1	1:B:520:ILE:CG2	2.50	0.41
1:B:643:HIS:ND1	1:B:746:GLN:HB3	2.35	0.41
1:B:685:TYR:HA	1:B:688:GLU:HG3	2.02	0.41
1:B:924:ILE:HD12	1:B:924:ILE:N	2.34	0.41
1:B:1344:LEU:C	1:B:1344:LEU:HD23	2.44	0.41
1:B:1357:VAL:O	1:B:1361:THR:HG23	2.20	0.41
1:B:1555:GLN:N	1:B:1556:PRO:HD2	2.35	0.41
1:A:38:ARG:NH2	1:A:53:LYS:HB2	2.35	0.41
1:A:157:LEU:HD23	1:A:166:MET:HG3	2.02	0.41
1:A:420:LEU:HB3	1:A:421:PRO:HD2	2.01	0.41
1:A:1771:LYS:HE2	1:A:1795:LEU:HD22	2.02	0.41
1:B:166:MET:HE1	1:B:251:THR:HG23	2.01	0.41
1:B:477:ARG:HH22	1:B:790:ARG:HD2	1.84	0.41
1:B:1230:THR:O	1:B:1234:ASN:ND2	2.49	0.41
1:B:1419:ASP:OD2	1:B:1423:ARG:NH2	2.53	0.41
1:A:1454:VAL:O	1:A:1458:ASN:ND2	2.54	0.41
1:B:557:THR:O	1:B:561:ILE:HG13	2.20	0.41
1:A:325:THR:HG21	1:A:340:ALA:HA	2.03	0.41
1:A:344:VAL:HG11	1:A:388:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1762:THR:HG22	1:A:1763:HIS:CD2	2.55	0.41
1:B:109:VAL:O	1:B:156:ALA:HA	2.20	0.41
1:B:670:VAL:HG12	1:B:671:PHE:N	2.34	0.41
1:B:703:ARG:HB2	1:B:704:GLU:OE1	2.21	0.41
1:B:1280:LEU:HD13	1:B:1294:GLN:HG2	2.02	0.41
1:B:1888:ILE:HD11	1:B:1959:ALA:CB	2.51	0.41
1:A:22:PHE:CE2	1:A:26:LEU:HD11	2.55	0.41
1:A:1436:ASP:OD1	1:A:1437:SER:N	2.51	0.41
1:B:70:LYS:O	1:B:130:TYR:CE1	2.73	0.41
1:B:477:ARG:HH22	1:B:790:ARG:HG2	1.86	0.41
1:B:621:ALA:HA	1:B:674:GLU:HA	2.01	0.41
1:B:1860:GLU:OE1	1:B:1860:GLU:N	2.53	0.41
1:A:1446:ILE:HD12	1:A:1446:ILE:C	2.44	0.41
1:B:984:PHE:CE2	1:B:1010:GLU:HB2	2.55	0.41
1:B:1110:GLN:NE2	1:B:2085:PRO:O	2.54	0.41
1:B:1353:LEU:HD22	1:B:1396:TYR:CD2	2.56	0.41
1:B:1616:LEU:CD1	1:B:1650:VAL:HG22	2.51	0.41
1:B:2098:PHE:CD1	1:B:2106:LEU:HD13	2.56	0.41
1:A:248:ASN:CB	1:A:280:ALA:HB2	2.49	0.41
1:A:285:GLU:OE2	1:A:315:THR:HG23	2.21	0.41
1:A:593:CYS:SG	1:A:712:TRP:HZ3	2.43	0.41
1:A:1052:VAL:HG11	1:A:1055:ILE:HD11	2.02	0.41
1:A:1519:LEU:HD12	1:A:1519:LEU:C	2.45	0.41
1:B:267:ASP:O	1:B:271:GLN:HG3	2.21	0.41
1:B:645:SER:CB	1:B:648:THR:HG1	2.26	0.41
1:B:803:LEU:HD12	1:B:803:LEU:HA	1.87	0.41
1:A:351:GLY:C	1:A:352:LEU:HD12	2.46	0.41
1:A:613:ALA:HB1	1:A:615:LEU:CG	2.50	0.41
1:A:655:GLN:HG2	1:A:656:ALA:N	2.36	0.41
1:A:763:PRO:HA	1:A:785:MET:CE	2.50	0.41
1:B:158:ASP:C	1:B:159:THR:HG22	2.46	0.41
1:B:501:THR:HG23	1:B:501:THR:O	2.21	0.41
1:B:756:ALA:O	1:B:779:CYS:HA	2.21	0.41
1:A:154:SER:C	1:A:155:ILE:HD12	2.46	0.41
1:A:263:PHE:CE1	1:A:299:VAL:HG11	2.56	0.41
1:A:503:TRP:CD2	1:A:506:MET:HB3	2.56	0.41
1:A:506:MET:HG2	1:A:546:PHE:CE2	2.56	0.41
1:A:687:MET:CB	1:A:740:VAL:HG12	2.49	0.41
1:A:1243:VAL:HG12	1:A:1271:THR:CG2	2.51	0.41
1:A:1260:LEU:HD23	1:A:1266:LEU:HD21	2.02	0.41
1:A:1274:ASP:OD1	1:A:1275:ARG:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ALA:N	1:B:650:THR:O	2.52	0.41
1:B:768:GLN:HE22	1:B:783:PRO:HB3	1.83	0.41
1:B:790:ARG:HG3	1:B:791:ASP:N	2.35	0.41
1:B:899:LEU:HD22	1:B:958:VAL:HG22	2.02	0.41
1:B:1228:LEU:HD21	1:B:1256:ILE:CD1	2.51	0.41
1:A:68:HIS:CE1	1:A:69:PRO:HD2	2.56	0.41
1:A:105:THR:O	1:A:150:PHE:HB3	2.21	0.41
1:A:691:ALA:HB3	1:A:692:PRO:HD3	2.03	0.41
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.36	0.41
1:B:610:ILE:HD13	1:B:682:PHE:CE1	2.56	0.41
1:B:892:LEU:HD21	1:B:1055:ILE:CD1	2.51	0.41
1:A:469:GLY:CA	1:A:805:LEU:HD21	2.47	0.40
1:A:570:MET:HE2	1:A:815:LEU:CG	2.51	0.40
1:A:1486:VAL:O	1:A:1493:LEU:HD22	2.20	0.40
1:B:13:LEU:HD21	1:B:229:VAL:CG2	2.51	0.40
1:B:71:GLN:HA	1:B:130:TYR:CD1	2.55	0.40
1:B:139:MET:HA	1:B:142:ASN:HB2	2.03	0.40
1:B:191:LEU:HD22	1:B:224:ARG:NH2	2.36	0.40
1:B:499:MET:HG2	1:B:582:LEU:HB2	2.02	0.40
1:B:692:PRO:HD2	1:B:693:PRO:HD2	2.03	0.40
1:B:694:LEU:O	1:B:694:LEU:HD23	2.21	0.40
1:B:1016:ASP:O	1:B:1080:VAL:N	2.42	0.40
1:A:521:LEU:O	1:A:525:GLU:HG2	2.21	0.40
1:A:783:PRO:O	1:A:784:LEU:HB2	2.20	0.40
1:A:990:VAL:HG13	1:A:1039:LEU:CD1	2.51	0.40
1:A:1019:ARG:CD	1:A:1075:VAL:HG21	2.51	0.40
1:A:1574:ARG:HD2	1:A:1588:ILE:HD12	2.04	0.40
1:B:108:TRP:HE1	1:B:155:ILE:HD12	1.85	0.40
1:B:205:MET:HE1	1:B:395:PHE:CD2	2.56	0.40
1:B:639:VAL:CG1	1:B:640:PRO:HD2	2.46	0.40
1:B:161:CYS:O	1:B:161:CYS:SG	2.80	0.40
1:B:352:LEU:HA	1:B:381:LEU:O	2.20	0.40
1:B:498:GLY:HA2	1:B:580:HIS:O	2.21	0.40
1:B:655:GLN:CA	1:B:658:VAL:HG12	2.51	0.40
1:A:203:LEU:HD12	1:B:132:MET:HE2	2.02	0.40
1:A:654:PRO:O	1:A:658:VAL:HG23	2.21	0.40
1:A:993:GLU:OE2	1:A:1927:LYS:NZ	2.55	0.40
1:A:1457:VAL:HG23	1:A:1503:MET:HE1	2.03	0.40
1:B:497:SER:HB3	1:B:762:ALA:HB2	2.02	0.40
1:B:615:LEU:HD21	1:B:680:MET:HE3	2.04	0.40
1:B:1461:ARG:HD2	1:B:1502:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1497:LEU:C	1:B:1497:LEU:HD12	2.46	0.40
1:B:1634:TRP:CD1	1:B:1811:TRP:CZ2	3.10	0.40
1:B:1893:LEU:HD12	1:B:1916:SER:CB	2.51	0.40
1:A:37:ASP:OD1	1:A:42:ALA:HB2	2.22	0.40
1:A:157:LEU:CD2	1:A:166:MET:HG3	2.51	0.40
1:A:276:LEU:HD12	1:A:401:HIS:HD2	1.86	0.40
1:A:555:SER:O	1:A:559:ILE:HG13	2.21	0.40
1:A:1446:ILE:HG22	1:A:1474:LEU:CD1	2.52	0.40
1:B:11:GLY:HA2	1:B:85:VAL:HG11	2.03	0.40
1:B:341:LEU:O	1:B:345:LEU:HG	2.22	0.40
1:B:670:VAL:HG12	1:B:671:PHE:H	1.87	0.40
1:B:831:SER:HB3	1:B:832:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2060/2553 (81%)	2014 (98%)	46 (2%)	0	100	100
1	B	2063/2553 (81%)	2018 (98%)	45 (2%)	0	100	100
All	All	4123/5106 (81%)	4032 (98%)	91 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1705/2117 (80%)	1699 (100%)	6 (0%)	84 84
1	B	1708/2117 (81%)	1698 (99%)	10 (1%)	78 81
All	All	3413/4234 (81%)	3397 (100%)	16 (0%)	78 83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ILE
1	A	563	LEU
1	A	1198	LEU
1	A	1243	VAL
1	A	1751	GLU
1	A	2022	VAL
1	B	188	ILE
1	B	378	ASP
1	B	717	ILE
1	B	726	LEU
1	B	782	ILE
1	B	785	MET
1	B	1371	ILE
1	B	1801	ASN
1	B	1802	GLU
1	B	1827	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	173	GLN
1	A	252	ASN
1	A	306	ASN
1	A	328	ASN
1	A	356	ASN
1	A	358	HIS
1	A	379	GLN
1	A	387	ASN
1	A	399	ASN
1	A	446	GLN
1	A	738	ASN

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Mol	Chain	Res	Type
1	A	746	GLN
1	A	764	HIS
1	A	804	HIS
1	A	852	ASN
1	A	949	ASN
1	A	987	GLN
1	A	1139	GLN
1	A	1193	ASN
1	A	1290	HIS
1	A	1296	GLN
1	A	1504	ASN
1	A	1595	GLN
1	A	1730	GLN
1	A	1778	HIS
1	A	1815	GLN
1	A	1835	GLN
1	A	2028	ASN
1	A	2101	GLN
1	A	2103	HIS
1	B	142	ASN
1	B	170	ASN
1	B	173	GLN
1	B	199	GLN
1	B	293	HIS
1	B	306	ASN
1	B	350	HIS
1	B	356	ASN
1	B	375	GLN
1	B	446	GLN
1	B	551	HIS
1	B	580	HIS
1	B	643	HIS
1	B	683	HIS
1	B	738	ASN
1	B	746	GLN
1	B	768	GLN
1	B	978	ASN
1	B	1006	GLN
1	B	1056	HIS
1	B	1294	GLN
1	B	1331	ASN
1	B	1345	HIS

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Mol	Chain	Res	Type
1	B	1447	ASN
1	B	1595	GLN
1	B	1709	GLN
1	B	1722	ASN
1	B	1735	HIS
1	B	1835	GLN
1	B	1845	GLN
1	B	1855	GLN
1	B	2086	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	B	2601	-	51,52,52	0.52	0	71,80,80	0.69	1 (1%)
2	NDP	A	2601	-	51,52,52	0.54	0	71,80,80	0.65	1 (1%)
2	NDP	A	2602	-	51,52,52	0.50	0	71,80,80	0.77	2 (2%)
2	NDP	B	2602	-	51,52,52	0.49	0	71,80,80	0.77	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	B	2601	-	-	13/34/77/77	0/5/5/5
2	NDP	A	2601	-	-	10/34/77/77	0/5/5/5
2	NDP	A	2602	-	-	9/34/77/77	0/5/5/5
2	NDP	B	2602	-	-	10/34/77/77	0/5/5/5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2602	NDP	P2B-O2B-C2B	-4.14	112.38	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.93	112.94	123.43
2	B	2601	NDP	P2B-O2B-C2B	-3.63	113.75	123.43
2	B	2602	NDP	C3N-C2N-N1N	-2.71	119.23	123.20
2	A	2602	NDP	C3N-C2N-N1N	-2.14	120.06	123.20
2	A	2601	NDP	O4D-C1D-C2D	-2.08	102.17	106.62

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5D-O5D-PN-O3
2	A	2601	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C3B-C4B-C5B-O5B
2	A	2602	NDP	C5D-O5D-PN-O3
2	A	2602	NDP	C5D-O5D-PN-O1N
2	B	2601	NDP	O4B-C4B-C5B-O5B
2	B	2601	NDP	C5D-O5D-PN-O1N
2	B	2601	NDP	O4D-C1D-N1N-C2N
2	B	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	C5B-O5B-PA-O2A
2	B	2602	NDP	C5B-O5B-PA-O3
2	B	2602	NDP	C4B-C5B-O5B-PA
2	B	2602	NDP	C5D-O5D-PN-O1N
2	B	2602	NDP	O4D-C1D-N1N-C6N
2	A	2602	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	A	2602	NDP	O4B-C4B-C5B-O5B
2	A	2601	NDP	C1B-C2B-O2B-P2B
2	A	2601	NDP	C3B-C2B-O2B-P2B
2	B	2601	NDP	C3B-C4B-C5B-O5B
2	B	2601	NDP	PA-O3-PN-O1N
2	A	2602	NDP	C4B-C5B-O5B-PA
2	A	2601	NDP	C2B-O2B-P2B-O1X
2	A	2601	NDP	C2N-C3N-C7N-O7N
2	A	2601	NDP	C5D-O5D-PN-O2N
2	A	2602	NDP	C5D-O5D-PN-O2N
2	B	2601	NDP	C5D-O5D-PN-O3
2	B	2601	NDP	C5D-O5D-PN-O2N
2	B	2602	NDP	C5B-O5B-PA-O1A
2	B	2601	NDP	O4B-C1B-N9A-C8A
2	B	2601	NDP	O4B-C1B-N9A-C4A
2	B	2601	NDP	C2B-O2B-P2B-O2X
2	B	2601	NDP	PA-O3-PN-O2N
2	B	2602	NDP	C4D-C5D-O5D-PN
2	A	2602	NDP	O4D-C4D-C5D-O5D
2	A	2602	NDP	C2B-C1B-N9A-C8A
2	B	2602	NDP	PN-O3-PA-O2A
2	A	2601	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	O4B-C4B-C5B-O5B
2	B	2601	NDP	C2B-O2B-P2B-O1X
2	B	2602	NDP	C2N-C3N-C7N-O7N

There are no ring outliers.

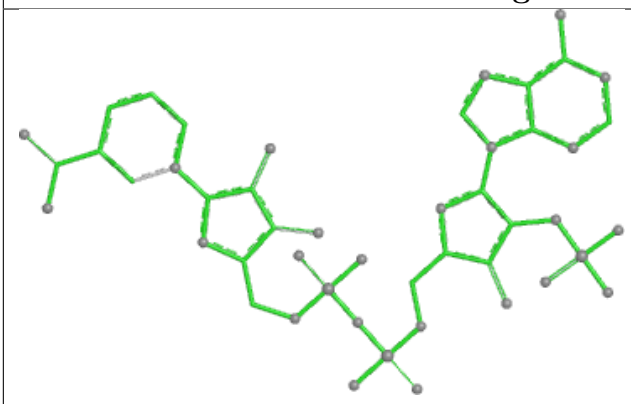
4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	NDP	2	0
2	A	2601	NDP	3	0
2	A	2602	NDP	20	0
2	B	2602	NDP	9	0

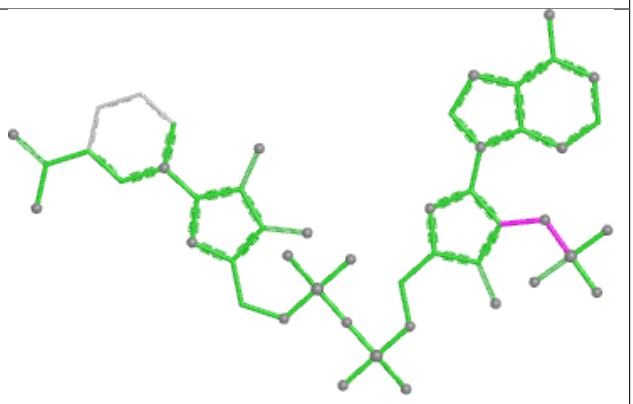
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

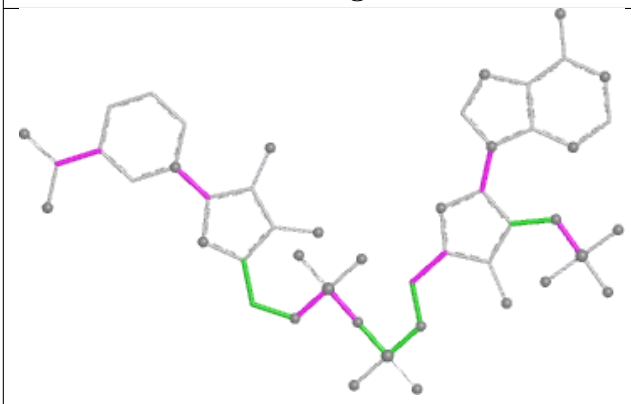
Ligand NDP B 2601



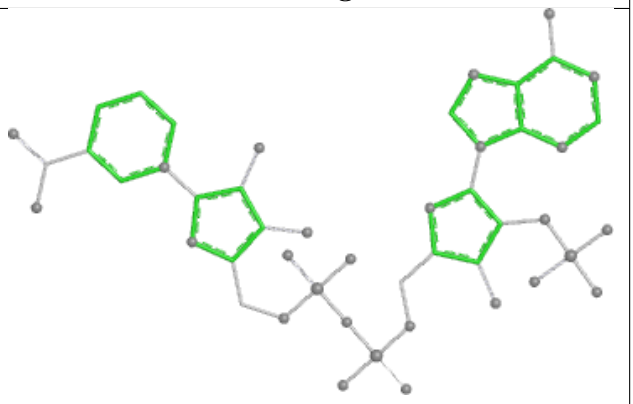
Bond lengths



Bond angles

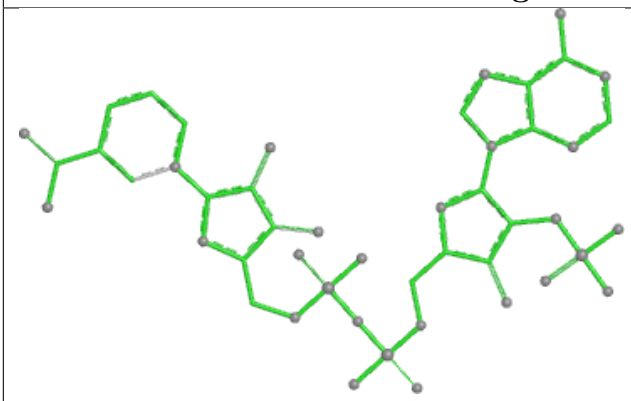


Torsions

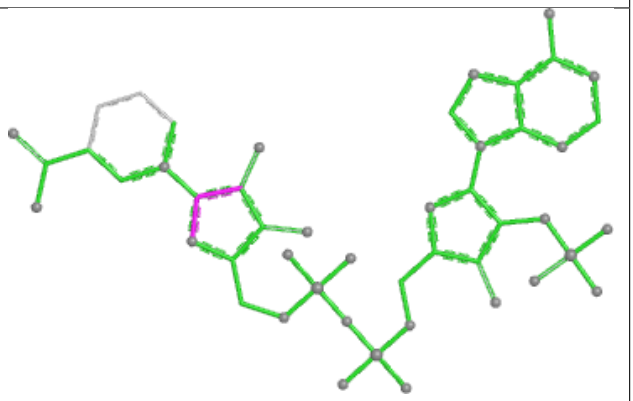


Rings

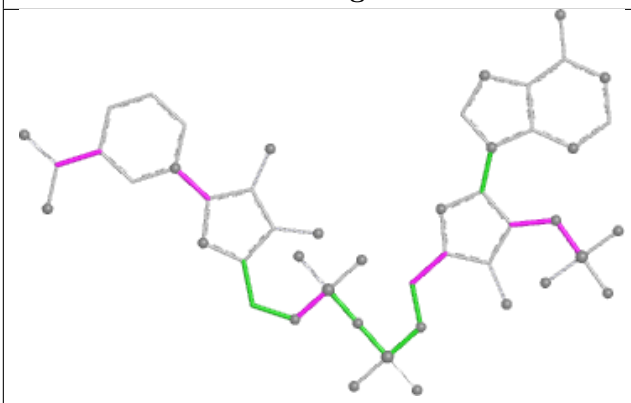
Ligand NDP A 2601



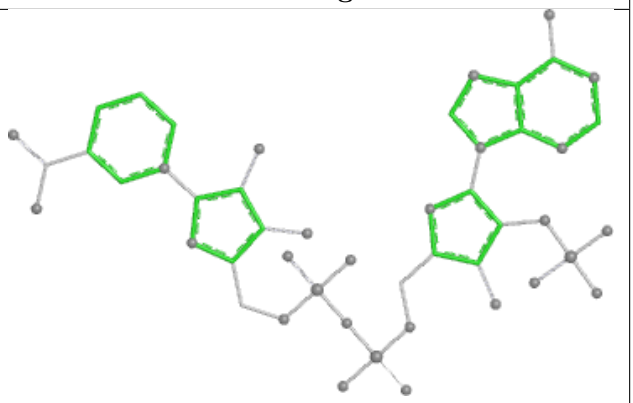
Bond lengths



Bond angles

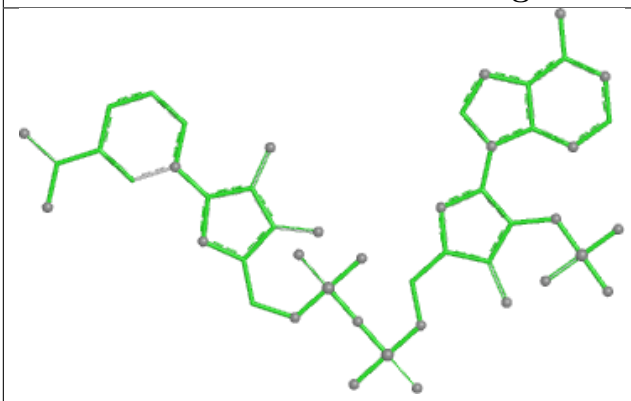


Torsions

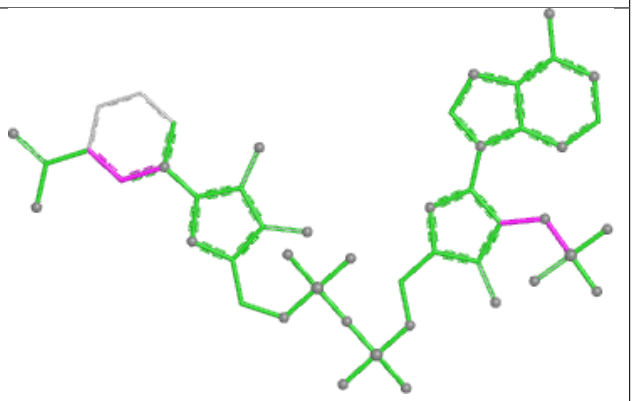


Rings

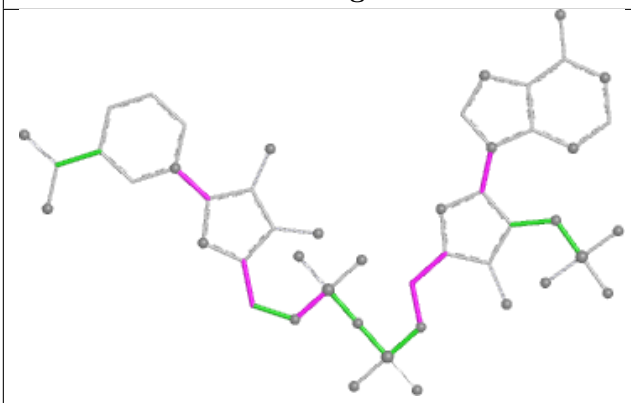
Ligand NDP A 2602



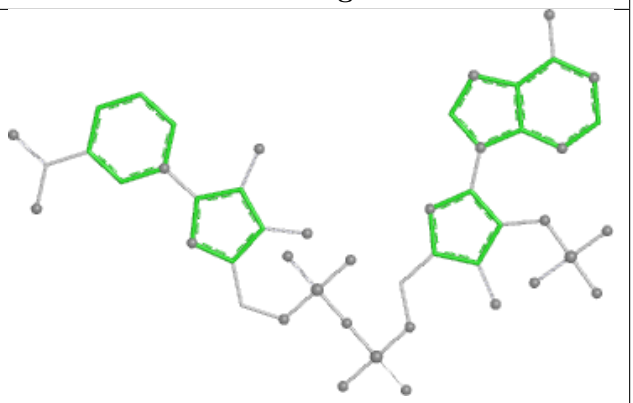
Bond lengths



Bond angles

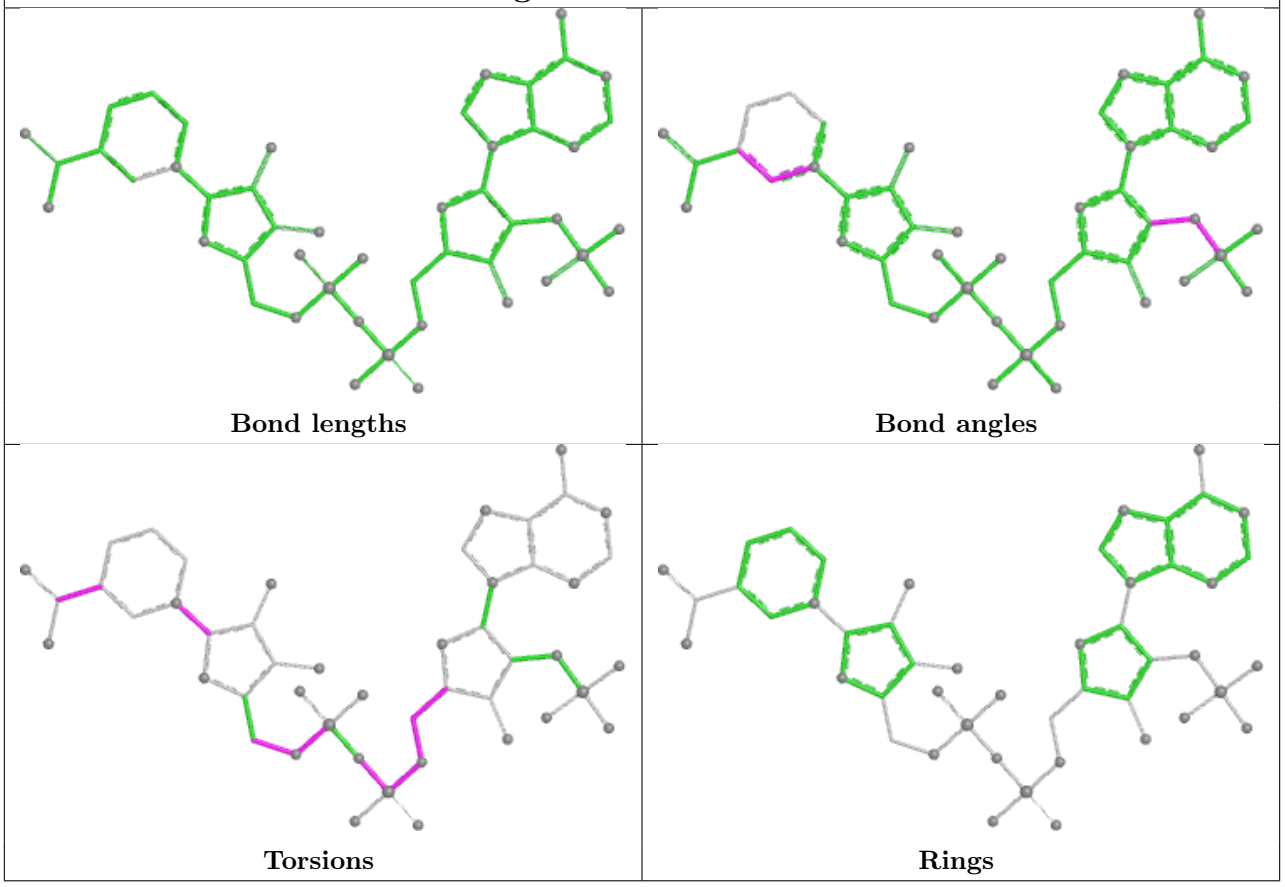


Torsions



Rings

Ligand NDP B 2602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

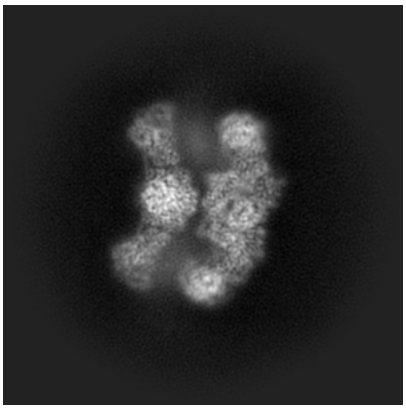
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43337. These allow visual inspection of the internal detail of the map and identification of artifacts.

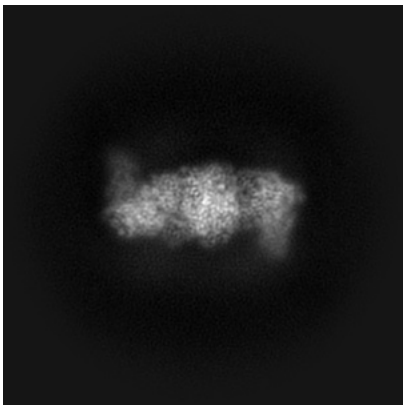
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

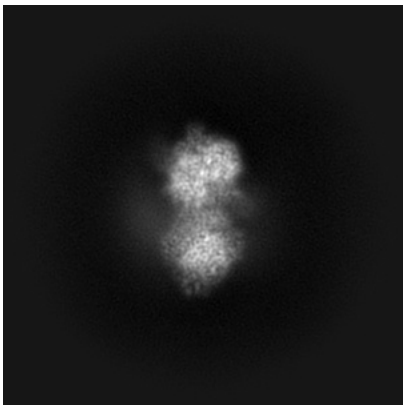
6.1.1 Primary map



X

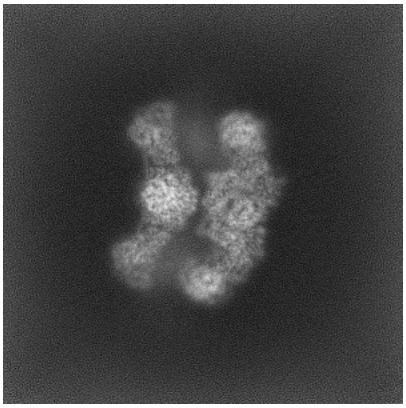


Y

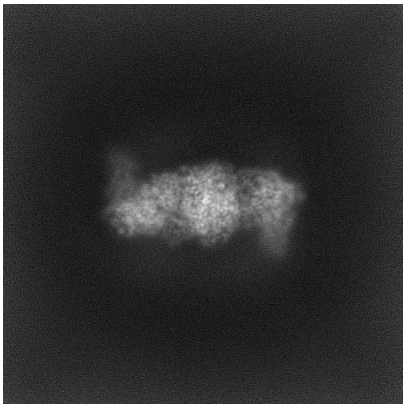


Z

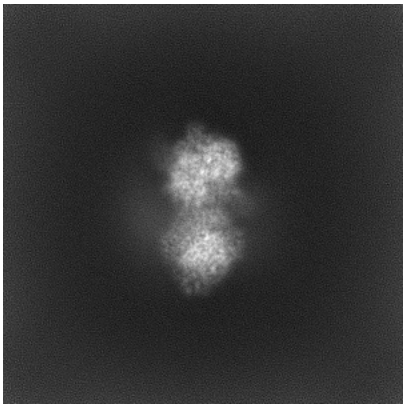
6.1.2 Raw map



X



Y

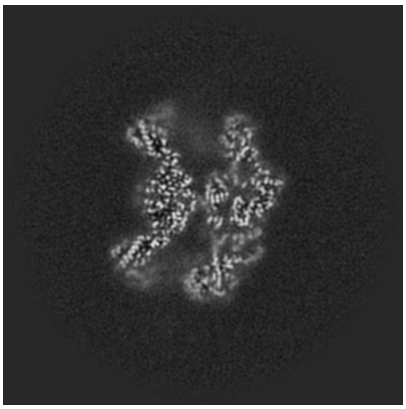


Z

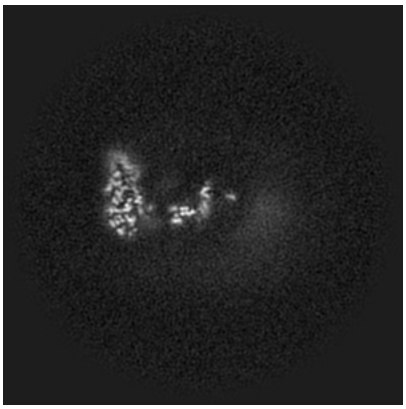
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

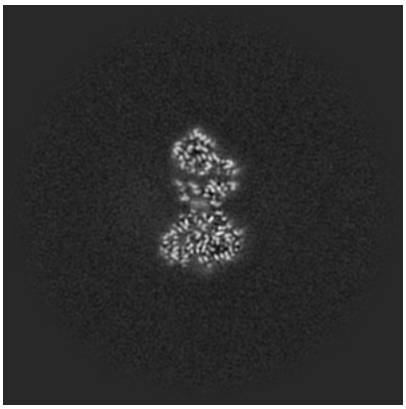
6.2.1 Primary map



X Index: 180

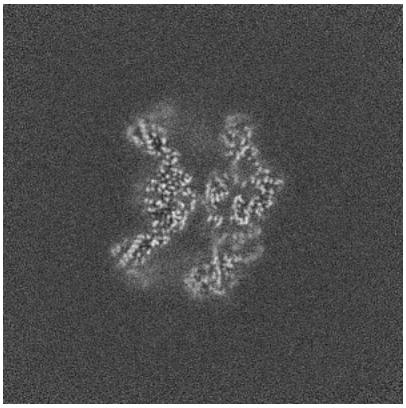


Y Index: 180

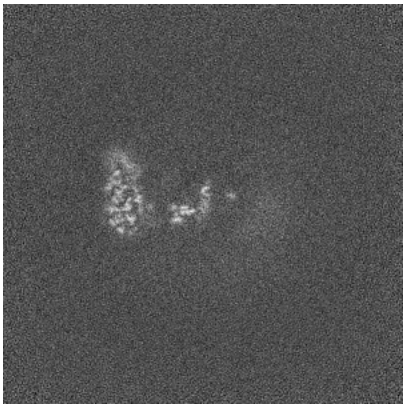


Z Index: 180

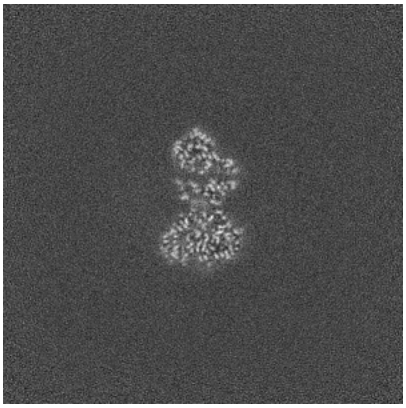
6.2.2 Raw map



X Index: 180



Y Index: 180

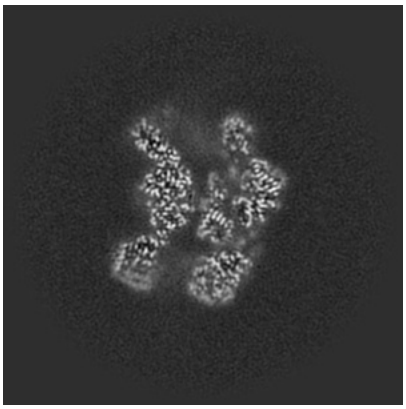


Z Index: 180

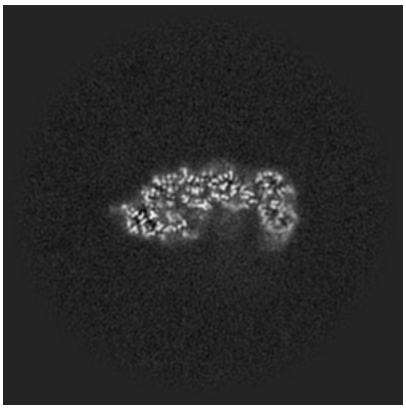
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

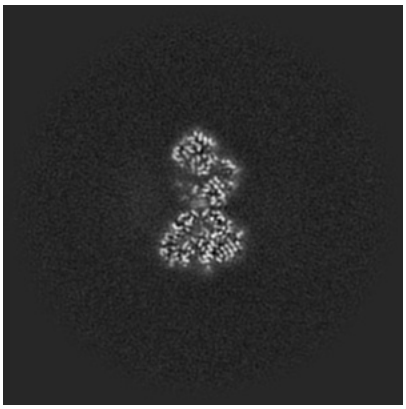
6.3.1 Primary map



X Index: 176

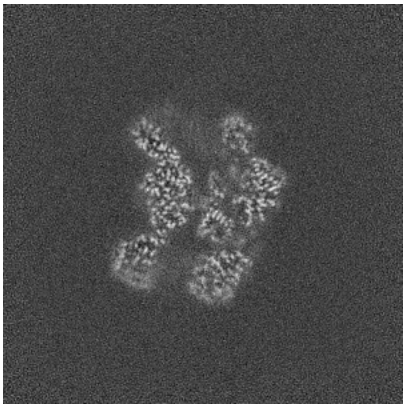


Y Index: 208

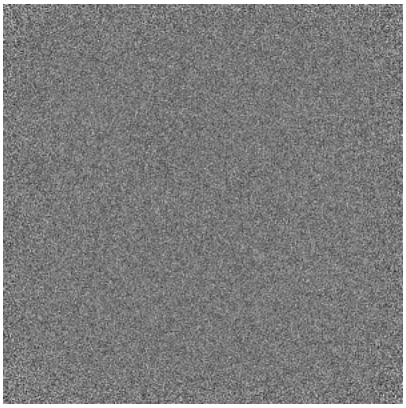


Z Index: 182

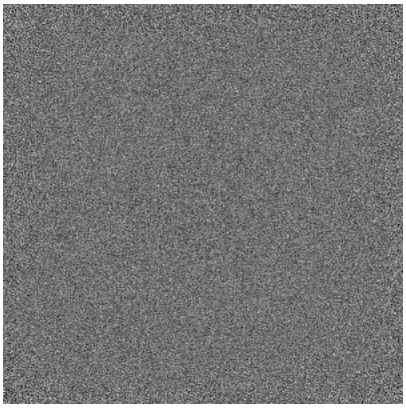
6.3.2 Raw map



X Index: 176



Y Index: 0

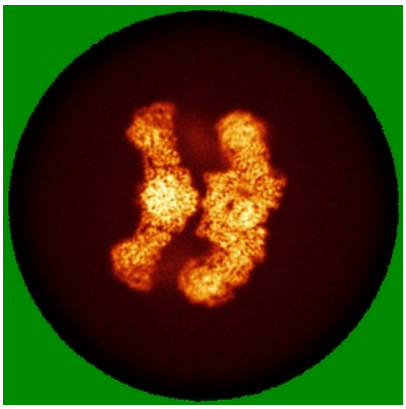


Z Index: 359

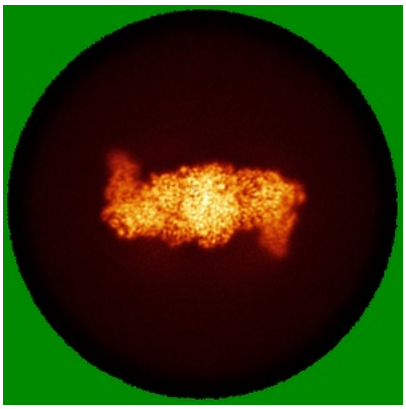
The images above show the largest variance slices of the map in three orthogonal directions.

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

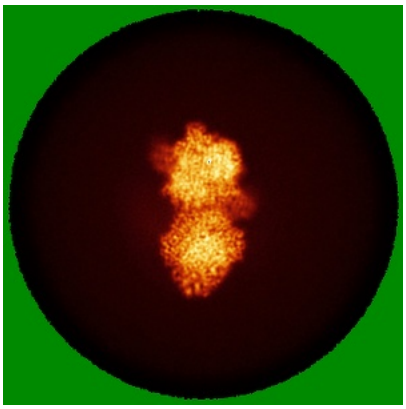
6.4.1 Primary map



X

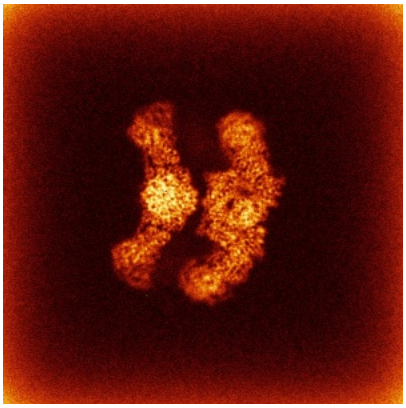


Y

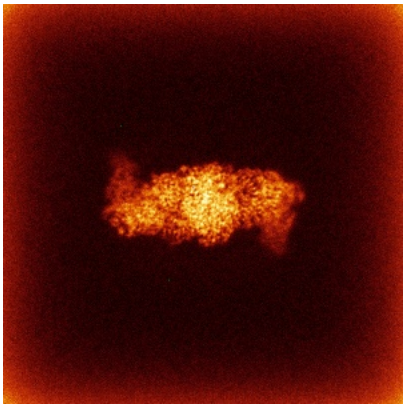


Z

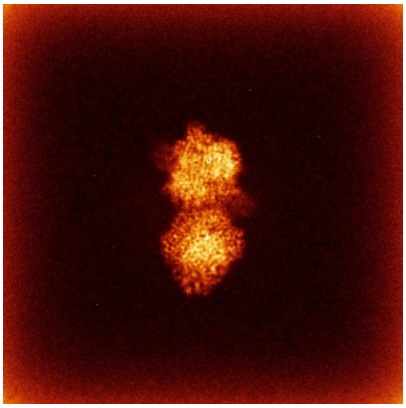
6.4.2 Raw map



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)

This section was not generated.

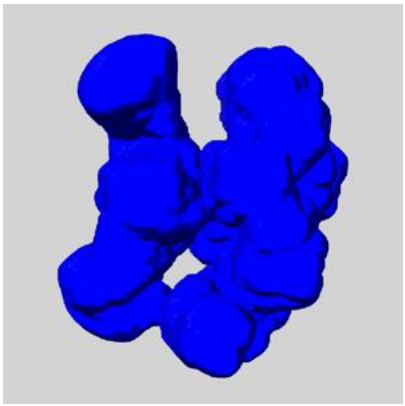
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

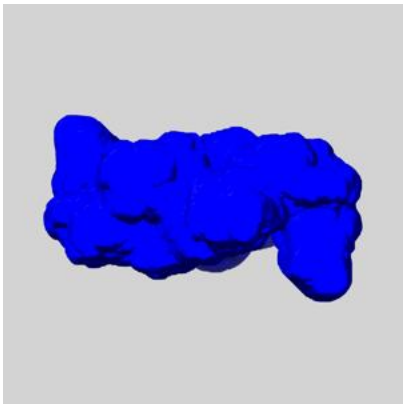
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

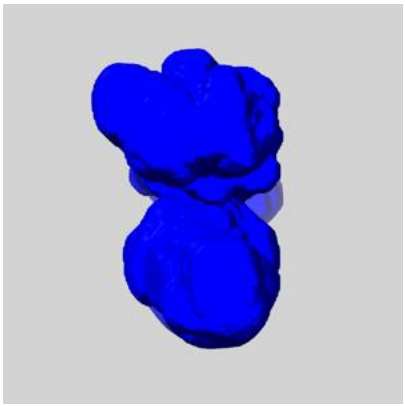
6.6.1 emd_43337_msk_1.map (i)



X



Y

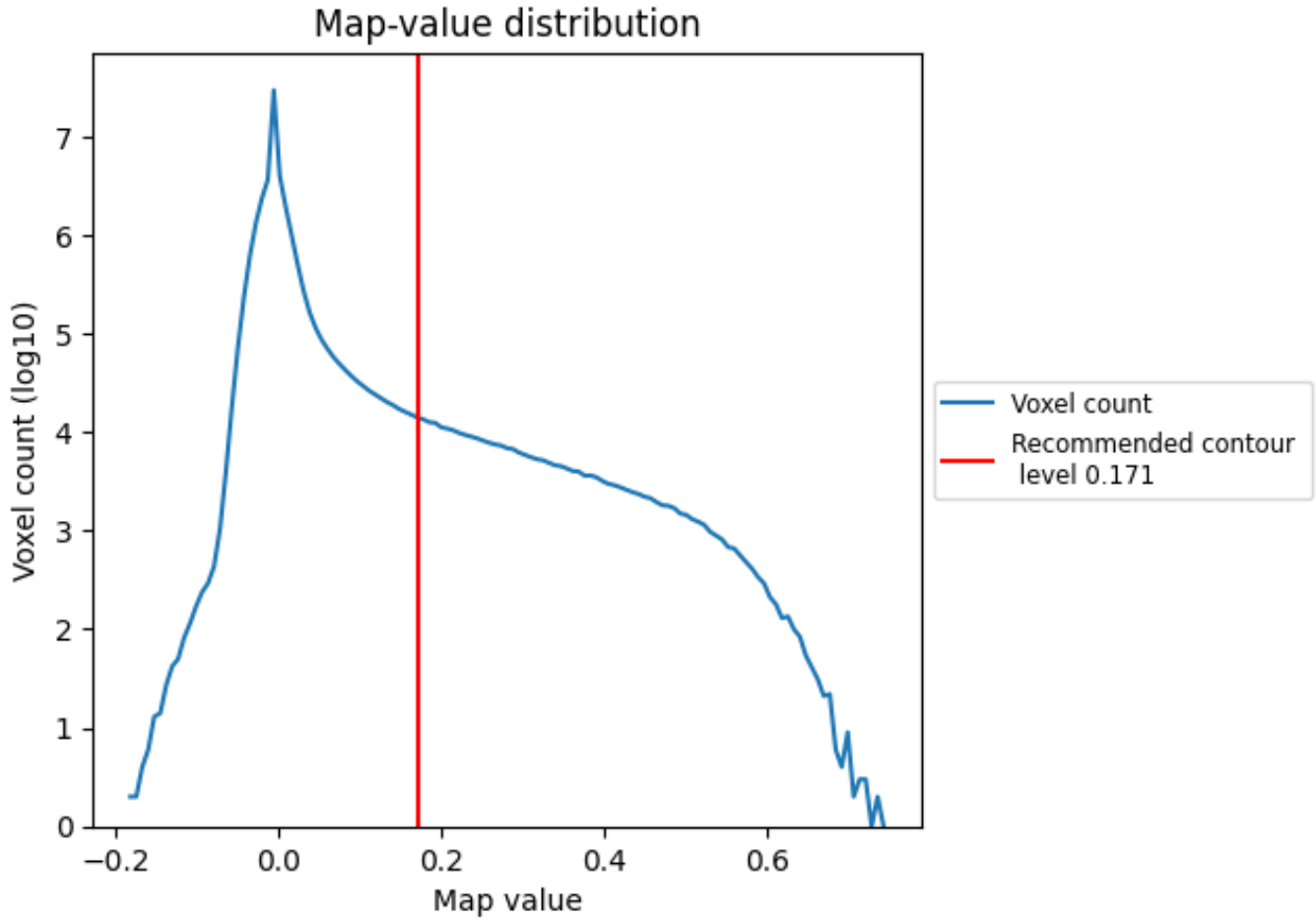


Z

7 Map analysis

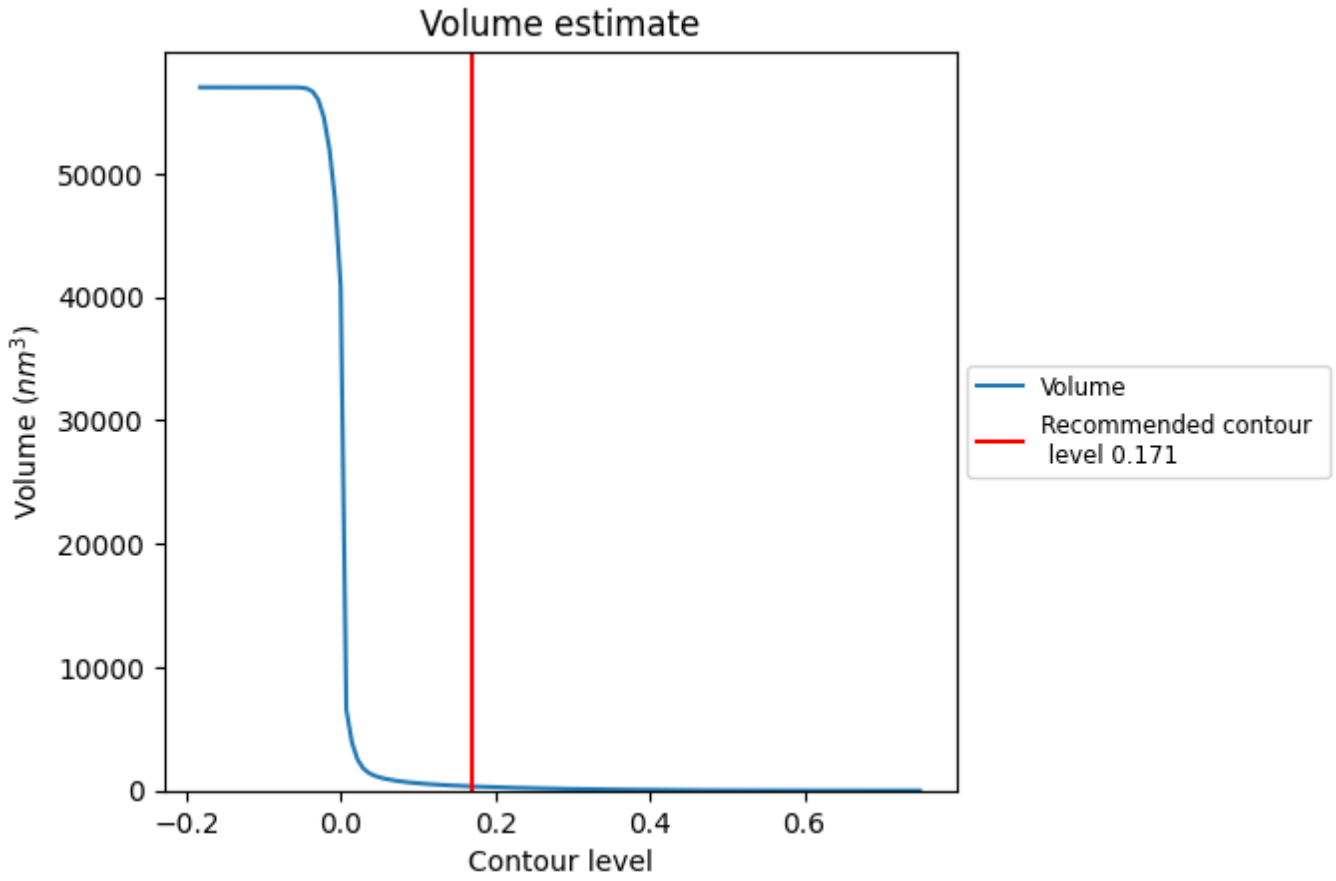
This section contains the results of statistical analysis of the map.

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.

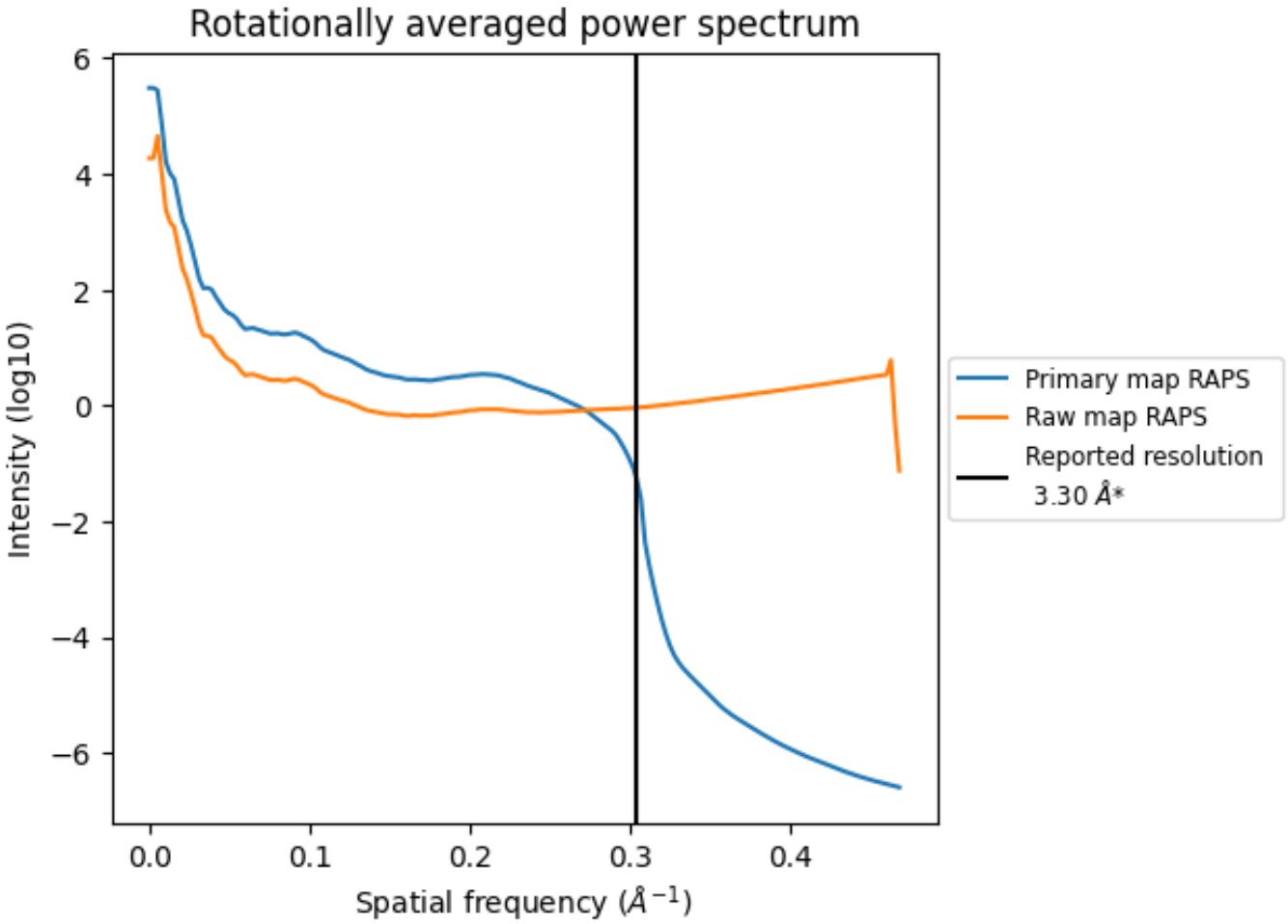
7.2 Volume estimate



The volume at the recommended contour level is 336 nm^3; this corresponds to an approximate mass of 304 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)

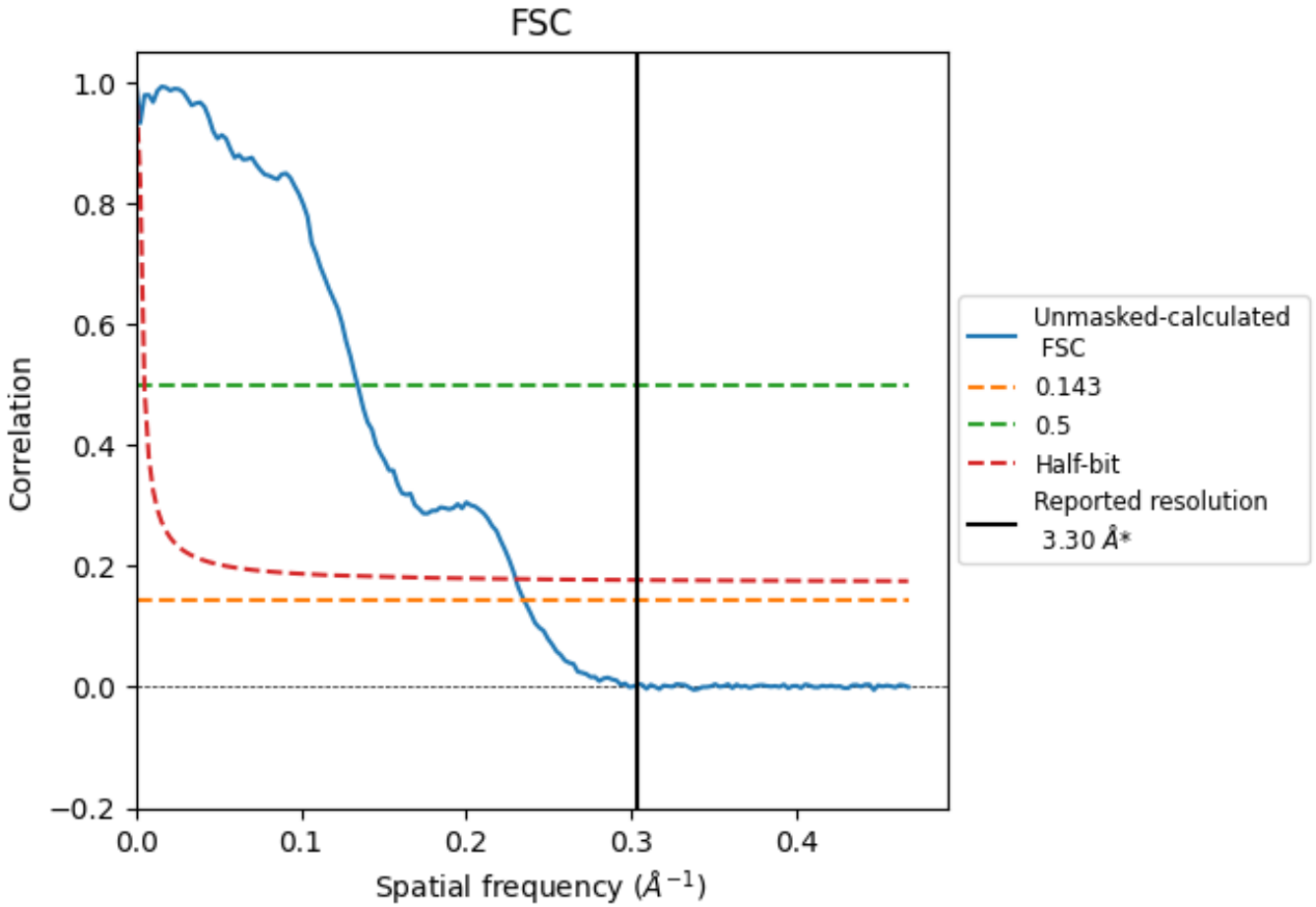


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

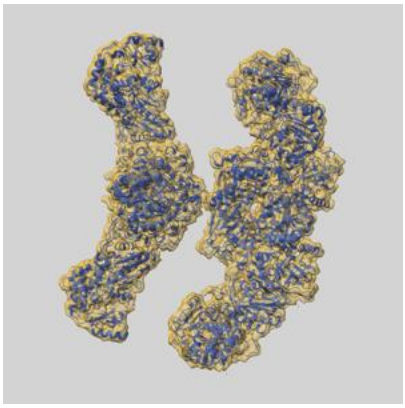
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.25	7.46	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.3 by more than 10 %

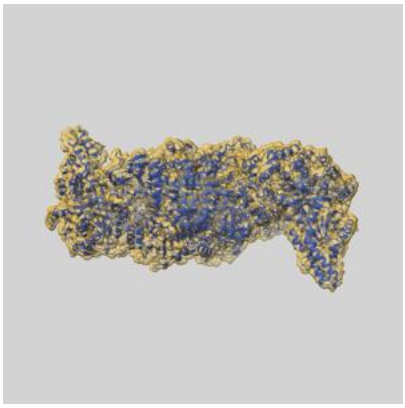
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43337 and PDB model 8VLE. Per-residue inclusion information can be found in section 3 on page 7.

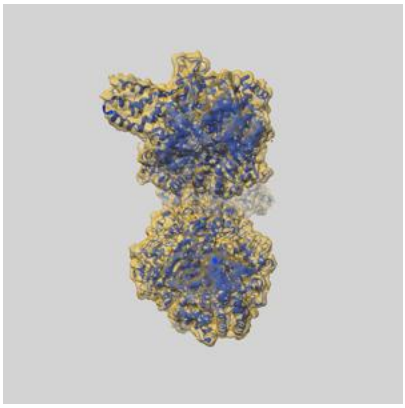
9.1 Map-model overlay



X



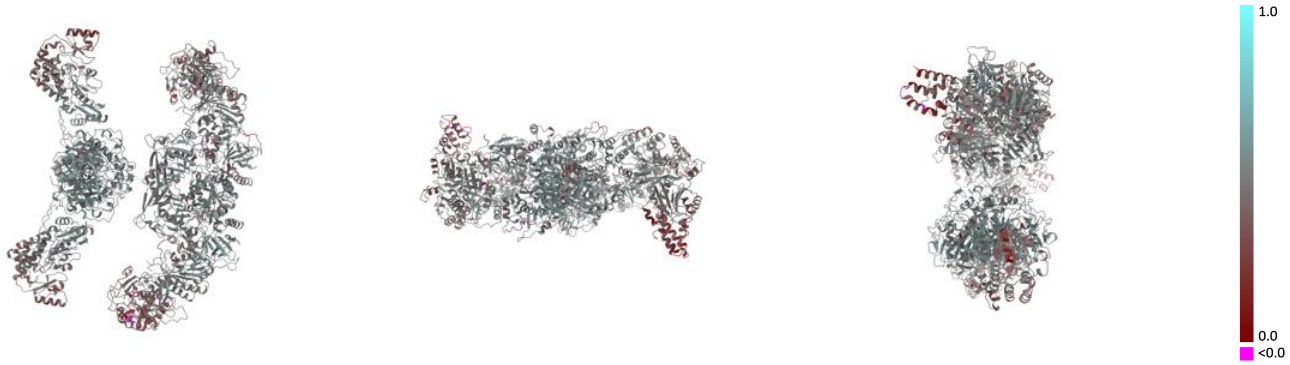
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



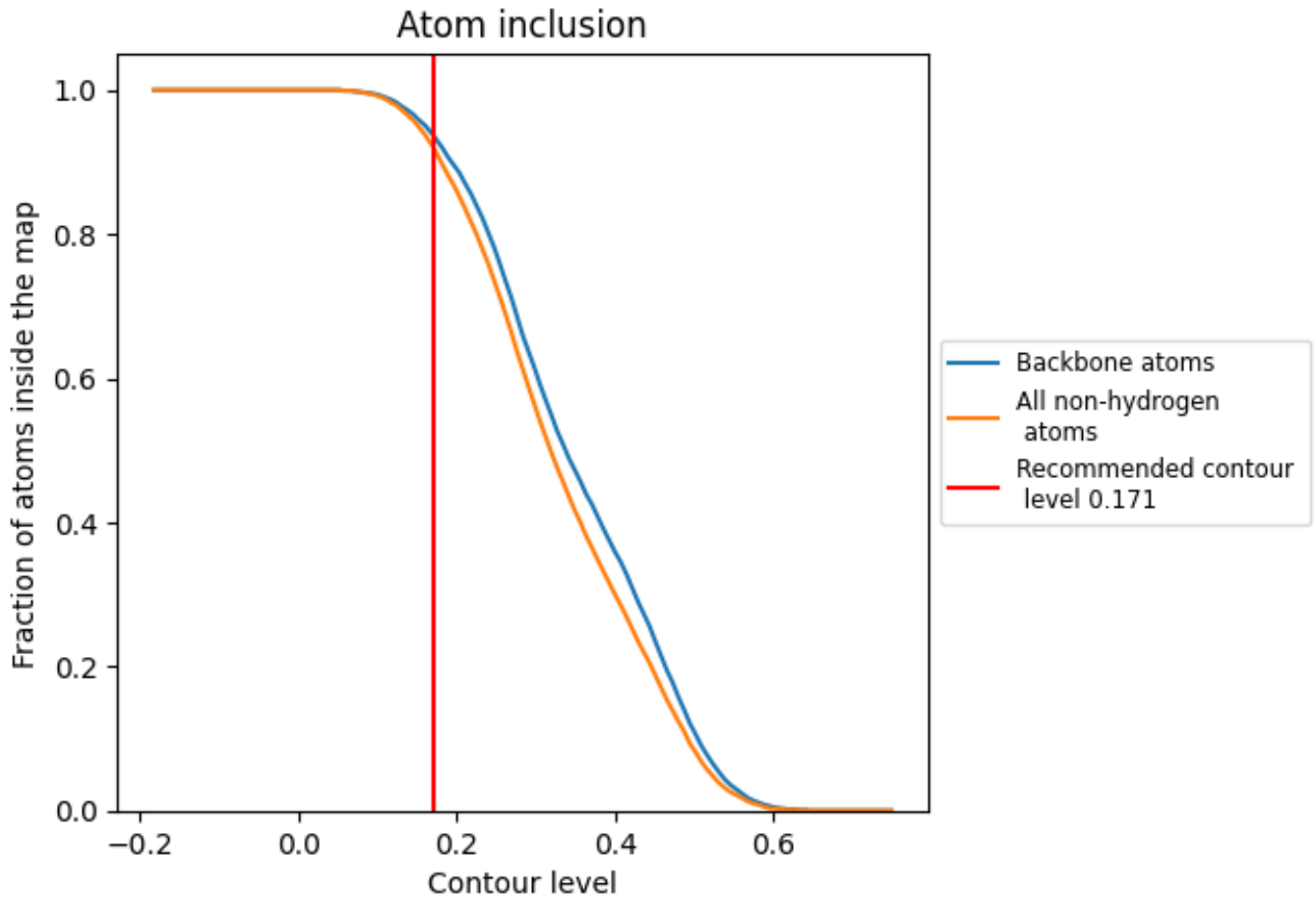
X Y Z

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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.171) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9200	0.4690
A	0.9220	0.4710
B	0.9160	0.4670